

Luciano Mueller

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EDUCATION

February 1979 – June 1980: Postdoctoral Research Fellow, University of California, Berkeley, California 94720. Research with Prof. Alexander Pines in magic angle spinning and multiple quantum NMR in solids.

May, 1978 - February, 1979: Postdoctoral Research Fellow, Varian Associates, Inc., Palo Alto, California 94303. Research with Dr. Robert Codrington in two-dimensional NMR and software development.

February, 1973 - February, 1978: Ph.D., ETH Zurich, Switzerland. Thesis in “two-dimensional NMR and high-resolution carbon-13 NMR in solids” under the supervision of Nobel prize Laureate Prof. Richard Ernst.

October, 1968 - November, 1972: Undergraduate study in chemistry, ETH Zurich, Switzerland.

PROFESSIONAL EXPERIENCE

December, 1989 - 2022: Scientific Senior Director since January 2021
Bristol-Myers Squibb, Department of Discovery Chemistry Platforms
P.O. Box 4000, Princeton, New Jersey 08543-4000,

June, 1983 - December, 1989: Fellow
Smith Kline & French Laboratories, Department of Physical and Structural Chemistry,
Mail code: L940, P. O. Box 1539, King of Prussia, Pennsylvania 19406-0939

June, 1980 - June, 1983: Manager (Spectroscopist until May, 1982)
Southern California Regional NMR Facility, California Institute of Technology,
Department of Chemistry, Pasadena, California, 91125

AWARDS
Bristol-Myers Chemistry Leadership Award, 2011
AAA Fellow. award, 2018
BMS ARC Lifetime achievement award 2022
ACS Fellowship award, 2023

SCHOLARSHIPS/ MEMBERSHIPS

Swiss National Science Foundation Scholarship, 1979.
Member of the American Chemical Society.
Member of American Association for the Advancement of Science.
Member of Editorial Advisory Board of Biochemistry from 1992-2000. Member of NRMFAM scientific advisory board, 2002-2005

LEADERSHIP ROLES

IN PROFESSIONAL ORGANIZATIONS

NJACS NMR Topical Group chair, 2013
 NJACS NMR Topical Group Scientific advisor, 2014 - present
 NJACS chair-elect, 2015, NJACS chair 2016
 Maurice Rohrbach Fund for Swiss American Cultural Exchange president, 2014 – present
 Swiss Benevolent Society, Philadelphia chapter, board member, 2013 – present

Skills

Extensive expertise in NMR
 NMR methods development
 NMR experiment customization
 Bruker pulse programming, au-programming
 Spectrometer trouble-shooting
 NMR resonance assignments
 3d-structure calculations using NMR derived restraints
 Experience in structure-based drug design,
 Knowledge in:
 nmrPipe, Sparky, ACD-Labs software, nmrView, NMR2, CYANA, AMIX, Maestro,
 Glide, Macromodel, Pymol, Gaussian, Sigmaplot.
 Familiarity in: C, C-shell, AWK Perl scripting
 Experience in project management, NMR facility- and team management

PUBLICATIONS; Representative sub-set

1. J. Caceres-Cortes, B. Falk, **L. Mueller**, T. G. Murali Dhar, "Perspectives on NMR in Drug Discovery", (2024) J. Med. Chem. 67 (3), 1701-1733.
2. A. N. Jain, Alexander Brueckner, C. Jorge, A. E. Cleves, P. Khandelwal, J. Caceres-Cortes, **L. Mueller**, "Complex Peptide Optimization combining NMR-restraints with Conformational Analysis to Guide Structure-based Ligand Optimization, (2023) J. Comput.-Aided Mol. Des. 37, 519-535
3. M. J. Smith, H. Tang, P. Morin, H. Malone, **L. Mueller** "Methods and Composition for Deuterated Biologics", US patent application (2019) 12979-US-NP.
4. Mary Harner, **Luciano Mueller**, Kevin Robbins and Michael Reily "NMR in Drug Design", (2017) Archives of Biochem. and Biophys. 628, 132-147.
5. .P. Glunz, **L. Mueller** , D. L. Cheney, V. Ladziata, Y. Zou, N. R. Wurtz, A. Wei, W. C. Wong, R. Wexler, E. S. Priestley, "Atropisomer Control in Macrocyclic Factor VIIa Inhibitors", (2016) J. Med. Chem.59, 4007-4018.
6. Rie Nygaard, Yaozhong Zou, Ron O. Dror, Thomas J. Mildorf, Daniel H. Arlow, Aashish Manglik, Albert C. Pan, Corey W. Liu, Juan Jose Fung, Michael P. Bokoch, Foon Sun Thian, Tong Sun Kobilka, David E. Shaw, **Luciano Mueller**, R. Scott Prosser, and Brian K. Kobilka,* "The Dynamic Process of b2-Adrenergic Receptor Activation" (2013) Cell 152, 532-542.
7. M. P. Bokoch, Y. Zou, S. G. F. Rasmussen, C. W. Liu, R. Nygaard, D. M. Rosenbaum, J. J. Fung, H. J. Choi, F. S. Thian, T. S. Kobilka, J. D. Puglisi, W. L. Weis, L. Pardo, R. S. Prosser, **L. Mueller** & B. K. Kobilka "Ligand-specific regulation of the extra-cellular surface of G-protein-coupled receptor" (2010) Nature 463(7), 108-112.
8. L. Mueller "An Alternate SOFAST-experiment for recording 1H,15N-Correlation Spectra at a High Through-Put", (2008) J. Biomol. NMR 42, 129-137.
9. K. L. Constantine, M. E. Davis, W. J. Metzler, **L. Mueller** & B. Claus "Protein-Ligand NOE Matching: A High-Throughput Method for Binding Pose Evaluation that does not Require Protein NMR Resonance Assignments", (2006) J. Amer. Chem. Soc. 128, 7252-7263.
10. M. R. Hansen, **L. Mueller** and A. Pardi "Tunable Alignment of Macromolecules by Filamentous Phage Yields Dipolar Coupling Interactions", (1998) Nature Structural Biology 5, 1065-1074.
11. W. J., Metzler, J. Bajorath, W. Fenderson, S.-Y. Shaw, K. L. Constantine, J. Naemura, G. Leytze,

- R. J. Peach, T. B. Lavoie, **L. Mueller** and P. S. Linsley "Solution Structure of Human CTLA-4 and Delineation of a CD80/86 Binding Site Conserved in CD28", (1997) *Nat., Struct. Biol.* 4, 527 - 531.
12. M. Wittekind, C. Mapelli, B. T. Farmer II, V. Goldfarb, J. Tsao, T. Lavoie, C. A. Meyers and **L. Mueller** "Solution Structure of the Grb2 N-terminal SH3 Domain Complexed with a Ten-Residue Peptide Derived from SOS: Direct Refinement Against NOEs, J-couplings and ¹H and ¹³C Chemical Shifts", (1997) *J. Molecular Biology* 267, 933 - 952.
 13. **L. Mueller**, P. Legault and A. Pardi, "Improved RNA Structure Determination by Detection of NOE Contacts to Exchange-Broadened Amino Protons", *J. Amer. Chem. Soc.* 117, 11043 (1995).
 14. Wittekind, C. Mapelli, B. T. Farmer II, K.-L. Suen, V. Goldfarb, J. Tsao, T. Lavoie, M. B. T. Farmer II and **L. Mueller**, "Simultaneous Acquisition of [¹³C, ¹⁵N]- and [¹⁵N, ¹⁵N]-Separated 4D Gradient Enhanced NOESY Spectra in Proteins," *J. Biomol. NMR* 4, 673-687 (1994).
 15. W. J. Metzler, K. L. Constantine, M. S. Friedrichs, A. J. Bell, E. G. Ernst, T. B. Lavoie and L. M. Wittekind and **L. Mueller**, "HNCACB: A High Sensitivity 3D NMR Experiment to Correlate Amide Proton and Nitrogen Resonances with the Alpha and Beta Carbon Resonances in Proteins," *J. Magn. Reson.* B101, 201 (1993).
 16. K. L. Constantine, M. S. Friedrichs, V. Goldfarb, P. D. Jeffrey, S. Sheriff and L. Mueller, E. Kay, M. Wittekind, M. A. McCoy, M. S. Friedrichs and **L. Mueller**, "4D NMR Triple-Resonance Experiments for Assignment of Protein Backbone Nuclei Using Shared Constant-Time Evolution Periods," *J. Magn. Reson.* 98, 443 (1992).
 17. B. T. Farmer II, R. Venters, L. Spicer, M. G. Wittekind and **L. Mueller**, "A Refocused and Optimized HNCA: Increased Sensitivity and Resolution in large Macromolecules," *J. Biomol. NMR* 2, 195 (1992).
 18. T. P. Kline, F. K. Brown, S. C. Brown, P. W. Jeffs, K. D. Kopple and **L. Mueller**, "Solution Structures of Human Transforming Growth Factor alpha derived from ¹H NMR data," *Biochemistry*, 29, 7805 (1990).
 19. S. C. Brown, P. L. Weber and **L. Mueller**, "Towards complete ¹H NMR spectra in proteins," *J. Magn. Reson.* 77, 166 (1988).
 20. **L. Mueller**, S. L. Heald and P. W. Jeffs, "The Binding of the Ardicin Aglycon to Bacterial Cell Wall Precursors," *J. Amer. Chem. Soc.* 111, 496 (1989).
 21. **L. Mueller**, "Excitation of Deuterium Double Quantum Transitions in Liquids," *Chem. Phys. Letters* 91, 303 (1982).
 22. **L. Mueller**, "Sensitivity Enhanced Detection of Weak Nuclei using Heteronuclear Multiple Quantum Coherence," *J. Amer. Chem. Soc.* 101, 4481 (1979).
 23. **L. Mueller** and R. R. Ernst, "Coherence Transfer in the Rotating Frame, Application to Heteronuclear Cross-Correlation Spectroscopy," *Molecular Physics* 38, 963 (1979).
 24. **L. Mueller**, A. Kumar and R. R. Ernst, "Two-Dimensional Carbon-13 NMR Spectroscopy," *J. Chem. Phys.* 63, 5490 (1975).