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Education

Ph.D. in Chemistry, Brandeis University, Waltham, MA, USA 1999
M.S. in Chemistry, Dalian Institute of Chemical Physics, Dalian, Liaoning, China 1994
B.S. in Physical Chemistry (major) and Polymer Science (minor)
University of Sci. and Tech. of China, Hefei, Anhui, China 1991

Professional Experience

Associate Director, Purdue Interdepartmental NMR Facility, Purdue University 2005-present
Senior Chemist, Discovery Chemistry Research and Technology, Eli Lilly and Company 2001-2004
Research Associate, Department of Molecular Biology, The Scripps Research Institute 1999-2001

Professional Associations

American Chemical Society

Skills

Structural biology and drug discovery

Conducted protein structural determination for terpredoxin, ARD and doppel
Performed protein SAR by NMR for therapeutic proteins
Characterized ligand-protein binding modes with nuclear hormone receptors by 2D NMR
Developed novel approaches for screening, hit validation and quality evaluation in drug discovery
Conducted SBDD and proposed a novel mechanism in ligand-protein interaction

Organic chemistry, modeling and structural calculation

Have independently designed & synthesized selectively labeled quaternary ammonium salts
Built various small molecule models using Insight & Macromodel
Conducted protein structural calculations/refinements by Xplor (CNS) & Amber

Molecular biology and protein chemistry

Site-directed mutagenesis & sub-cloning
Protein over-expression, uniform & selective labeling; protein refolding
Various separation techniques including analytical and preparative HPLC, ion exchange, hydrophobic interaction, size-exclusion & affinity chromatography
Protein characterization by ITC, Mass, CD, SDS-PAGE & ultra-centrifugation

NMR and Quantitative analysis

Proposed solvent concentration reference and receiving efficiency as two novel methods for cost-effective, universal and accurate quantitative analysis
Designed strategy and directed applications for concentration determination in complex biological systems
Developed, modified and implemented various nD sequences on both Varian and Bruker spectrometers
Determined structures for various small molecules, peptides and proteins by NMR
Conducted extensive instrument component analysis, pulse sequence and spectral simulation
Daily working experience with Unix/Linux/Windows, system administration, c/c shell and perl

Publications

33. Mo H* et al. “Quantitative NMR: influence of RF inhomogeneity”, manuscript in preparation
32. Weng J-K, Mo H, Chapple C. “Unusual lignin and disruption of pollen wall formation”, submitted

31. Mo H*, Balko K, Colby DA* “A Practical No-D NMR Method for the Rapid Determination of 1-Octanol/Water Partition Coefficients of Pharmaceutical Agents”, Bioorg Med Chem Lett. accepted
30. Mo H*, Harwood JS, Raftery D, “A quick diagnostic test for NMR receiver gain compression”, in press
29. Ye T, Zhang S, Mo H, Tayyari F, Nagana Gowda GA, Raftery D, Anal. Chem, 2010, 82: 2303–9.
28. Mo H*, Harwood JS, Raftery D “Receiver gain function: the actual NMR receiver gain” Magn. Res. Chem., 2010, 48: 235-38
27. Mo H*, Harwood J, Zhang S, Xue Y, Santini R, Raftery D ”R: A quantitative measure of NMR signal receiving efficiency", J. Magn. Reson, 2009, 200: 239-44
26. Ye T, Mo H, Shanaiah N, Gowda N, Zhang S, Raftery D "A chemoselective ^{15}N tag for sensitive and high resolution NMR profiling of the carboxyl-containing metabolome" Anal. Chem., 2009, 81: 4882-88
25. Mo H*, Raftery D “Solvent signal as an NMR concentration reference” Anal. Chem, 2008; 80: 9835–39
24. Bai G, Mo H, Shapiro M “NMR evaluation of adipocyte fatty acid binding protein (aP2) with R and S ibuprofen” Bioorg Med Chem 2008; 16: 4323-30
23. Mo H*, Raftery D. “Improved residual water suppression: WET180” J Biomol NMR 2008; 41: 105-111
22. Mo H*, Raftery D. “PreSAT180: a simple and effective method for residual water suppression” J Magn Reson 2008; 190: 1-6
21. Zartler ER, Mo H "Practical Aspects of NMR-based Fragment Discovery", Curr. Top. Med. Chem. 2007, 7:1592-99
20. Hsiung HM, Hertel J, Zhang XY, Smith DP, Smiley DL, Heiman ML, Yang DD, Husain S, Mayer JP, Zhang L, Mo H, Yan LZ “A novel and selective beta-melanocyte-stimulating hormone-derived peptide agonist for melanocortin 4 receptor potently decreased food intake and body weight gain in diet-induced obese rats” Endocrinology 2005, 46: 5257-66
19. Flora D, Mo H, Mayer JP, Khan MA, Yan LZ “Detection and control of aspartimide formation in the synthesis of cyclic peptides” Bioorg Med Chem Lett 2005, 15: 1065-68
18. Yan J, Kline AD, Mo H, Shapiro MJ, Zartler ER “The absolute sign of J coupling constants determined using the order matrix calculation” Magn Reson Chem 2004; 42: 962-67
17. Yan J, Delaglio F, Kaerner A, Kline AD, Mo H, Shapiro MJ, Smitka TA, Stephenson GA, Zartler ER “Complete relative stereochemistry of multiple stereocenters using only residual dipolar couplings” J Am Chem Soc 2004; 126: 5008-17
16. Zartler ER, Hanson J, Jones BE, Kline AD, Martin G, Mo H, Shapiro MJ, Wang R, Wu H, Yan J “RAMPED-UP NMR: multiplexed NMR-based screening for drug discovery” J Am Chem Soc 2003,125:10941-46
15. Yan J, Kline AD, Mo H, Shapiro MJ, Zartler ER “The effect of relaxation on the epitope mapping by saturation transfer difference NMR” J. Magn. Reson 2003, 163:270-76
14. Kroon GJA, Mo H, Martinez-Yamont MA, Dyson HJ, Wright PE “Changes in structure and dynamics of the Fv fragment of a catalytic antibody upon binding of inhibitor” Prot. Sci. 2003, 12:1386-94
13. Yan J, Kline AD, Mo H, Shapiro MJ, Zartler ER “A novel method for the determination of stereochemistry in six-membered chair-like rings using residual dipolar couplings” J Org Chem 2003, 68:1786-95
12. Zartler ER, Yan J, Mo H, Kline AD, Shapiro MJ “ID NMR Methods in ligand-receptor interactions” Curr Top Med Chem. 2003, 3:25-37
11. Pochapsky TC, Pochapsky SS, Ju T, Mo H, Al-Mjeni F, Maroney MJ “Modeling and experiment yields the structure of acireductone dioxygenase from Klebsiella pneumoniae” Nat Struct Biol, 2002, 9:966-72.
10. Yan J, Kline AD, Mo H, Zartler ER, Shapiro MJ “Epitope mapping of ligand-receptor interactions by diffusion NMR” J Am Chem Soc 2002, 124: 9984-85
9. Kostic M, Pochapsky SS, Obenauer J, Mo H, Pagani GM, Pejchal R, Pochapsky TC “Comparison of functional domains in vertebrate-type ferredoxins” Biochem., 2002, 41:5978-89
8. Nicholson EM, Mo H, Prusiner SB, Cohen FE, Marqusee S “Differences between the prion protein and its homolog Doppel: a partially structured state with implications for scrapie formation” J Mol Biol. 2002, 316: 807-15
7. Mo H, Moore RC, Cohen FE, Westway D, Prusiner SB, Wright PE, Dyson HJ “Two different neurodegenerative diseases caused by proteins with similar structures” PNAS USA 2001, 98:2352-57
6. Mo H, Dai Y, Pochapsky SS, Pochapsky TC “1H, 13C and 15N NMR assignments for a carbon monoxide generating metalloenzyme from Klebsiella pneumoniae” J Biomol NMR 1999, 14:287–88

5. Mo H, Pochapsky SS, Pochapsky TC “A model for the solution structure of oxidized terpredoxin, a Fe2S2 ferredoxin from pseudomonas” Bioch., 1999, 38: 5666-75
4. Mo H, Wang A, Wilkinson PS, Pochapsky TC Closed-shell ion pairs: cation and aggregate dynamics of tetraalkylammonium salts in an ion-pairing solvent. J Am Chem Soc 1997; 119: 11666-73
3. Mo H, Pochapsky TC, "Intermolecular Interactions Characterized by Nuclear Overhauser Effects" Prog. NMR Spec. 1997, 30: 1-38
2. Mo H, Pochapsky TC “Self-Diffusion Coefficients of Paired Ions” J Phys Chem B 1997; 101: 4485-86.
1. Pochapsky SS, Mo H, Pochapsky TC "Closed-Shell Ion Pair Aggregation in Non-Polar Solvents Characterized By NMR Diffusion Measurements", J. Chem. Soc., Chem. Comm. (1995), 2513-14

Presentations

Mo H (invited talk) “Quantitative NMR: if it can be observed, then it can be quantified”, Pittcon, Orlando, FL 2010
Mo H “Universal Quantitations by NMR”, Chicago Area NMR Discussion Group, Chicago, IL 2009
Mo H at al. “A universal NMR quantification method”, Experimental NMR Conference, Pacific Grove, CA 2008
Mo H et al. “NMR solution structure of DOPPEL”, Experimental NMR conference, Orlando, FL 2001
Mo H et al. “Contact ion pairs”, Experimental NMR conference, Orlando, FL 1997