
BIOGRAPHICAL SKETCH

NAME: Ann McDermott

eRA COMMONS USER NAME (credential, e.g., agency login): MCDERMOTT

POSITION TITLE: Esther Breslow Professor of Biological Chemistry

EDUCATION/TRAINING

INSTITUTION AND LOCATION	DEGREE (if applicable)	Completion Date MM/YYYY	FIELD OF STUDY
Harvey Mudd College.	Bachelor	1981	Chemistry
University of California, Berkeley	PHD	1987	Physical Chemistry

A. Personal Statement

Ann McDermott is the Esther Breslow Professor of Biological Chemistry at Columbia University. She holds a B.Sc. in Chemistry from Harvey Mudd College, and a Ph.D. in Chemistry from U.C. Berkeley, where she worked with Kenneth Sauer and Melvin Klein; subsequently she had postgraduate training at MIT with Dr. Robert Griffin.

Her research concerns the remarkable ability of naturally occurring proteins to catalyze chemical reactions, focusing specifically on the inherent flexibility of enzymes and the coordination of chemistry to conformational exchange, using magnetic resonance methods. Her group carries out assignment and analysis of high-resolution MAS-based NMR spectra of proteins, including intrinsic membrane proteins in native lipid bilayers, microcrystalline proteins, large native assemblies like viral coats, and fibrillar or amyloid proteins.

She is the recipient of the Pure Award in Chemistry (1996) and the Eastern Analytic Symposium Award for Achievement in Magnetic Resonance (2005), and she is an elected member of both the American Academy of Arts and Sciences, and the National Academy of Sciences. At Columbia University she recently served as Associate Vice President for Academic Advising and Science Initiatives in the Arts and Sciences.

Ongoing and recently completed projects:

NSF 2020
Standard DMR *[Acquisition of a Dynamic Nuclear Polarization \(DNP\) Nuclear Magnetic Resonance \(NMR\) System](#)*
Marbella, Lauren; McDermott, Ann / Columbia University

NIH 2020
R01 GM *[Structural and Functional Studies of Potassium Channels by Solid State NMR](#)*
McDermott, Ann E. / Columbia University (N.Y.)

NSF 2019
Standard MCB *[Structural Characterization of Protein and Protein Assemblies by Solid State NMR](#)*
McDermott, Ann / Columbia University

NIH 2019
R01 GM *[Structural and Functional Studies of Potassium Channels by Solid State NMR](#)*
McDermott, Ann E. / Columbia University (N.Y.)

NIH 2018
R01 GM

Structural and Functional Studies of Potassium Channels by Solid State NMR
McDermott, Ann E. / Columbia University (N.Y.)

NIH 2017
R01 GM

Structural and Functional Studies of Potassium Channels by Solid State NMR
McDermott, Ann E. / Columbia University (N.Y.)

NIH 2016
R01 GM

Structural and Functional Studies of Potassium Channels by Solid State NMR
McDermott, Ann E. / Columbia University (N.Y.)

NIH 2015
R01 GM

Structural and Functional Studies of Potassium Channels by Solid State NMR
McDermott, Ann E. / Columbia University (N.Y.)

NSF 2014
Standard MCB

Structural Characterization of Proteins and Assemblies by Solid State NMR
McDermott, Ann / Columbia University

NIH 2014
R01 GM

Structural and Functional Studies of Potassium Channels by Solid State NMR
McDermott, Ann E. / Columbia University (N.Y.)

Publications:

1. [Fritzscheing, Keith. J.](#) , [Yang, Yizhuo.](#) , Pogue, Emily. M. , Rayman, Joseph. B. , Kandel, E.. and [McDermott, Ann. E.](#) # "Micellar TIA1 with folded RNA binding domains as a model for reversible stress granule formation" 2020. **Proc. Natl. Acad. Sci.** : [link info](#)
2. Zhang, Allison. , Howarth, Gary. , Parkin, Lia. A. and [McDermott, Ann. E.](#) # "NMR studies of lipid regulation of the K⁺ channel KcsA" 2020. **Biochimica et Biophysica Acta - Biomembranes** :183491 [link info](#)
3. [Fritzscheing, Keith. J.](#) , [Keeler, Eric. G.](#) , [He, Chengming.](#) and [McDermott, Ann. E.](#) # "Scaled Recoupling of Chemical Shift Anisotropies at High Magnetic Fields under MAS with Interspersed C-elements" 2020. **Journal of Chemical Physics** 153 :104201 [link info](#)
4. [Sun, Zhiyu.](#) , [Xu, Yunyao.](#) , Zhang, Allison. and [McDermott, Ann. E.](#) # "Probing allosteric coupling in a constitutively open mutant of the ion channel KcsA using solid-state NMR" 2020. **Proceedings of the National Academy of Sciences** 117 :7171-7175 [link info](#)
5. Zhang, Allison. , Itin, B.. and [McDermott, Ann. E.](#) # "TmDOTP: An NMR-based thermometer for magic angle spinning NMR experiments" 2019. **Journal of Magnetic Resonance** 308 :106574 [link info](#)
6. [Xu, Yunyao.](#) and [McDermott, Ann. E.](#) # "Inactivation in the potassium channel KcsA" 2019. **Journal of Structural Biology: X** 3 :100009 [link info](#)
7. [McCoy, Kelsey. M.](#) , Rogawski, Rivkah. , Stovicek, Olivia. and [McDermott, Ann. E.](#) # "Stability of nitroxide biradical TOTAPOL in biological samples" 2019. **Journal of Magnetic Resonance** 303 :115-120 [link info](#)
8. [Xu, Yunyao.](#) , Zhang, Allison. , Rogawski, Rivkah. , Nimigean, C.. and [McDermott, Ann. E.](#) # "Identifying coupled clusters of allostery participants through chemical shift perturbations" 2019. **Proceedings of the National Academy of Sciences of the United States of America** : [link info](#)
9. [Keeler, Eric. G.](#) , [Fritzscheing, Keith. J.](#) and [McDermott, Ann. E.](#) # "Refocusing CSA during magic angle spinning rotating-frame relaxation experiments" 2018. **Journal of Magnetic Resonance** : [link info](#)
10. Mompeán, Miguel. , Li, Wenbo. , Li, Jixi. , Laage, Ségolène. , Siemer, Ansgar. B. , Bozkurt, Gunes. , Wu, Hao.. # and [McDermott, Ann. E.](#) # "The Structure of the Necrosome RIPK1-RIPK3 core, a human hetero-amyloid signaling complex" 2018. **Cell** :in press [link info](#)
11. [Fritzscheing, Keith. J.](#) , Itin, B.. and [McDermott, Ann. E.](#) # "N,N-Diethylmethylamine as lineshape standard for NMR above 130 K" 2018. **Journal of Magnetic Resonance** 287 :110-112 [link info](#)

12. Rogawski, Rivkah. , Sergeyev, I. , Zhang, Yinglu. , Tran, T. , Yongjun, Li. , Tong, L. and [McDermott, Ann. E.](#) # "NMR Signal Quenching from Bound Biradical Affinity Reagents in DNP Samples" 2017. **J. Phys. Chem. B**, 121 :10770-10781 [link info](#)
13. Rogawski, Rivkah. , Sergeyev, I. , Li, Y. , Ottaviani, M. , Cornish, V. and [McDermott, Ann. E.](#) "Dynamic Nuclear Polarization Signal Enhancement with High-Affinity Biradical Tags" 2017. **Journal of Physical Chemistry B** 121 :1169-1175 [link info](#)
14. [Xu, Yunyao.](#) , Bhate, M. and [McDermott, Ann. E.](#) "Transmembrane allosteric energetics characterization for strong coupling between proton and potassium ion binding in the KcsA channel" 2017. **Proceedings of the National Academy of Sciences of the United States of America** 114 :8788-8793 [link info](#)
15. Sergeyev, I. , Itin, B. , Rogawski, Rivkah. , Day, L. and [McDermott, Ann. E.](#) "Efficient assignment and NMR analysis of an intact virus using sequential side-chain correlations and DNP sensitization" 2017. **Proceedings of the National Academy of Sciences of the United States of America** 114 :5171-5176 [link info](#)
16. Rogawski, Rivkah. and [McDermott, Ann. E.](#) "New NMR tools for protein structure and function: Spin tags for dynamic nuclear polarization solid state NMR" 2017. **Archives of Biochemistry and Biophysics** 628 :102-113 [link info](#)
17. Harris, M. , Struppe, J. , Wylie, B. , [McDermott, Ann. E.](#) and Thompson, L. "Multidimensional Solid-State Nuclear Magnetic Resonance of a Functional Multiprotein Chemoreceptor Array" 2016. **Biochemistry** 55 :3616-3624 [link info](#)
18. Wylie, B. , Dzikovski, B. , Pawsey, S. , Caporini, M. , Rosay, M. , Freed, J. and [McDermott, Ann. E.](#) "Dynamic nuclear polarization of membrane proteins: Covalently bound spin-labels at protein-protein interfaces" 2015. **Journal of Biomolecular NMR** 61 :361-367 [link info](#)
19. Laage, Ségolène. , Tao, Y. and [McDermott, Ann. E.](#) "Cardiolipin interaction with subunit c of ATP synthase: Solid-state NMR characterization" 2015. **Biochimica et Biophysica Acta - Biomembranes** 1848 :260-265 [link info](#)
20. Mompeán, M. , Hervás, R. , [Xu, Yunyao.](#) , Tran, T. , Guarnaccia, C. , Buratti, E. , Baralle, F. , Tong, L. , Carrión-Vázquez, M. , [McDermott, Ann. E.](#) and Laurents, D. "Structural Evidence of Amyloid Fibril Formation in the Putative Aggregation Domain of TDP-43" 2015. **Journal of Physical Chemistry Letters** 6 :2608-2615 [link info](#)
21. Wylie, B. , Bhate, M. and [McDermott, Ann. E.](#) "Transmembrane allosteric coupling of the gates in a potassium channel" 2014. **Proceedings of the National Academy of Sciences of the United States of America** 111 :185-190 [link info](#)
22. Sergeyev, I. , Bahri, S. , Day, L. and [McDermott, Ann. E.](#) "Pf1 bacteriophage hydration by magic angle spinning solid-state NMR" 2014. **Journal of Chemical Physics** 141 : [link info](#)
23. Catalano, J. , Sadre-Bazzaz, K. , Amodeo, G. , Tong, L. and [McDermott, Ann. E.](#) "Structural evidence: A single charged residue affects substrate binding in cytochrome P450 BM-3" 2013. **Biochemistry** 52 :6807-6815 [link info](#)
24. Bhate, M. , Wylie, B. , Thompson, A. , Tian, L. , Nimigeon, C. and [McDermott, Ann. E.](#) "Preparation of uniformly isotope labeled KcsA for solid state NMR: Expression, purification, reconstitution into liposomes and functional assay" 2013. **Protein Expression and Purification** 91 :119-124 [link info](#)
25. Raveendra, B. , Siemer, Ansgar. B. , Puthanveetil, S. , Hendrickson, W. , Kandel, E. and [McDermott, Ann. E.](#) "Characterization of prion-like conformational changes of the neuronal isoform of Aplysia CPEB" 2013. **Nature Structural and Molecular Biology** 20 :495-501 [link info](#)
26. Li, Wenbo. and [McDermott, Ann. E.](#) "Detection of slow dynamics by solid-state NMR: Application to L-phenylalanine hydrochloride" 2013. **Concepts in Magnetic Resonance Part A: Bridging Education and Research** 42 A :14-22 [link info](#)
27. Siemer, Ansgar. B. , Huang, K. and [McDermott, Ann. E.](#) "Protein Linewidth and Solvent Dynamics in Frozen Solution NMR" 2012. **PLoS ONE** 7 : [link info](#)
28. Li, J. , McQuade, T. , Siemer, Ansgar. B. , Napetschnig, J. , Moriwaki, K. , Hsiao, Y. , Damko, E. , Moquin, D. , Walz, T. , [McDermott, Ann. E.](#) , Chan, F. and Wu, Hao. "The RIP1/RIP3 necrosome forms a functional amyloid signaling complex required for programmed necrosis" 2012. **Cell** 150 :339-350 [link info](#)
29. Quinn, C. and [McDermott, Ann. E.](#) "Quantifying conformational dynamics using solid-state R1p experiments" 2012. **Journal of Magnetic Resonance** 222 :1-7 [link info](#)
30. Li, Wenbo. and [McDermott, Ann. E.](#) "Investigation of slow molecular dynamics using R-CODEX" 2012. **Journal of Magnetic Resonance** 222 :74-80 [link info](#)

31. Bhate, M.. and [McDermott, Ann. E.](#) "Protonation state of E71 in KcsA and its role for channel collapse and inactivation" 2012. **Proceedings of the National Academy of Sciences of the United States of America** 109 :15265-15270 [link info](#)
32. Mao, L.. , Inoue, K.. , Tao, Y.. , Montelione, G.. , [McDermott, Ann. E.](#) and Inouye, M.. "Suppression of phospholipid biosynthesis by cerulenin in the condensed Single-Protein-Production (cSPP) system" 2011. **Journal of Biomolecular NMR** 49 :131-137 [link info](#)
33. Sergeyev, I.. , Day, L.. , Goldbourt, A.. and [McDermott, Ann. E.](#) "Chemical shifts for the unusual DNA structure in Pf1 bacteriophage from dynamic-nuclear-polarization-enhanced solid-state NMR spectroscopy" 2011. **Journal of the American Chemical Society** 133 :20208-20217 [link info](#)
34. Bauer, A.. , Gieschler, S.. , Lemberg, K.. , [McDermott, Ann. E.](#) and Stockwell, B.. "Functional model of metabolite gating by human voltage-dependent anion channel 2" 2011. **Biochemistry** 50 :3408-3410 [link info](#)
35. Huang, K.. , Amodeo, G.. , Tong, L.. and [McDermott, Ann. E.](#) "The structure of human ubiquitin in 2-methyl-2,4-pentanediol: A new conformational switch" 2011. **Protein Science** 20 :630-639 [link info](#)
36. Huang, K.. , Siemer, Ansgar. B. and [McDermott, Ann. E.](#) "Homonuclear mixing sequences for perdeuterated proteins" 2011. **Journal of Magnetic Resonance** 208 :122-127 [link info](#)
37. Xu, Yimin. , Lorieau, J.. and [McDermott, Ann. E.](#) "Triosephosphate Isomerase: 15N and 13C Chemical Shift Assignments and Conformational Change upon Ligand Binding by Magic-Angle Spinning Solid-State NMR Spectroscopy" 2010. **Journal of Molecular Biology** 397 :233-248 [link info](#)
38. Love, J.. , Mancina, F.. , Shapiro, L.. , Punta, M.. , Rost, B.. , Girvin, M.. , Wang, D.. , Zhou, M.. , Hunt, J.. , Szyperski, T.. , Gouaux, E.. , MacKinnon, R.. , [McDermott, Ann. E.](#) , Honig, B.. , Inouye, M.. , Montelione, G.. and Hendrickson, W.. "The New York Consortium on Membrane Protein Structure (NYCOMPS): A high-throughput platform for structural genomics of integral membrane proteins" 2010. **Journal of Structural and Functional Genomics** 11 :191-199 [link info](#)
39. Siemer, Ansgar. B. , Huang, K.. and [McDermott, Ann. E.](#) "Protein-ice interaction of an antifreeze protein observed with solid-state NMR" 2010. **Proceedings of the National Academy of Sciences of the United States of America** 107 :17580-17585 [link info](#)
40. Goldbourt, A.. , Day, L.. and [McDermott, Ann. E.](#) "Intersubunit hydrophobic interactions in Pf1 filamentous phage" 2010. **Journal of Biological Chemistry** 285 :37051-37059 [link info](#)
41. Bhate, M.. , Wylie, B.. , Tian, L.. and [McDermott, Ann. E.](#) "Conformational dynamics in the selectivity filter of KcsA in response to potassium ion concentration" 2010. **Journal of Molecular Biology** 401 :155-166 [link info](#)
42. Quinn, C.. and [McDermott, Ann. E.](#) "Monitoring conformational dynamics with solid-state R1ρ experiments" 2009. **Journal of Biomolecular NMR** 45 :5-8 [link info](#)
43. and [McDermott, Ann. E.](#) "Structure and dynamics of membrane proteins by magic angle spinning solid-state NMR" 2009. **Annual Review of Biophysics** 38 :385-403 [link info](#)
44. Li, Wenbo. and [McDermott, Ann. E.](#) "Characterization of slow conformational dynamics in solids: Dipolar CODEX" 2009. **Journal of Biomolecular NMR** 45 :227-232 [link info](#)
45. Huang, L.. and [McDermott, Ann. E.](#) "Partial site-specific assignment of a uniformly 13C, 15N enriched membrane protein, light-harvesting complex 1 (LH1), by solid state NMR" 2008. **Biochimica et Biophysica Acta - Bioenergetics** 1777 :1098-1108 [link info](#)
46. Siemer, Ansgar. B. and [McDermott, Ann. E.](#) "Solid-state NMR on a type III antifreeze protein in the presence of ice" 2008. **Journal of the American Chemical Society** 130 :17394-17399 [link info](#)
47. Lorieau, J.. , Day, L.. and [McDermott, Ann. E.](#) "Conformational dynamics of an intact virus: Order parameters for the coat protein of Pf1 bacteriophage" 2008. **Proceedings of the National Academy of Sciences of the United States of America** 105 :10366-10371 [link info](#)
48. Goldbourt, A.. , Gross, B.. , Day, L.. and [McDermott, Ann. E.](#) "Filamentous phage studied by magic-angle spinning NMR: Resonance assignment and secondary structure of the coat protein in Pf1" 2007. **Journal of the American Chemical Society** 129 :2338-2344 [link info](#)
49. Ravindranathan, K.. , Gallicchio, E.. , [McDermott, Ann. E.](#) and Levy, R.. "Conformational dynamics of substrate in the active site of cytochrome P450 BM-3/NPG complex: Insights from NMR order parameters" 2007. **Journal of the American Chemical Society** 129 :474-475 [link info](#)
50. Jovanovic, T.. , Harris, M.. and [McDermott, Ann. E.](#) "Cytochrome P450 BM-3 in complex with its substrate: Temperature-dependent spin state equilibria in the oxidized and reduced states" 2007. **Applied Magnetic Resonance** 31 :411-429 [info](#)
51. Gross, B.. and [McDermott, Ann. E.](#) "Locating hydrogen atoms in single crystal and uniaxially aligned amino acids by solid-state NMR" 2007. **Journal of Magnetic Resonance** 185 :12-18 [link info](#)

52. Rozovsky, S.. and [McDermott, Ann. E.](#) "Substrate product equilibrium on a reversible enzyme, triosephosphate isomerase" 2007. **Proceedings of the National Academy of Sciences of the United States of America** 104 :2080-2085 [link info](#)
53. Varga, K.. , Tian, L.. and [McDermott, Ann. E.](#) "Solid-state NMR study and assignments of the KcsA potassium ion channel of *S. lividans*" 2007. **Biochimica et Biophysica Acta - Proteins and Proteomics** 1774 :1604-1613 [link info](#)
54. Goldbourt, A.. , Day, L.. and [McDermott, Ann. E.](#) "Assignment of congested NMR spectra: Carbonyl backbone enrichment via the Entner-Doudoroff pathway" 2007. **Journal of Magnetic Resonance** 189 :157-165 [link info](#)
55. [McDermott, Ann. E.](#) and Polenova, T.. "Solid state NMR: new tools for insight into enzyme function" 2007. **Current Opinion in Structural Biology** 17 :617-622 [link info](#)
56. Lorieau, J.. and [McDermott, Ann. E.](#) "Conformational flexibility of a microcrystalline globular protein: Order parameters by solid-state NMR spectroscopy" 2006. **Journal of the American Chemical Society** 128 :11506-11512 [link info](#)
57. Ravindranathan, K.. , Gallicchio, E.. , Friesner, R.. , [McDermott, Ann. E.](#) and Levy, R.. "Conformational equilibrium of cytochrome P450 BM-3 complexed with N-palmitoylglycine: A replica exchange molecular dynamics study" 2006. **Journal of the American Chemical Society** 128 :5786-5791 [link info](#)
58. Lorieau, J.. and [McDermott, Ann. E.](#) "Order parameters based on $^{13}\text{C}1\text{H}$, $^{13}\text{C}1\text{H}_2$ and $^{13}\text{C}1\text{H}_3$ heteronuclear dipolar powder patterns: A comparison of MAS-based solid-state NMR sequences" 2006. **Magnetic Resonance in Chemistry** 44 :334-347 [link info](#)
59. Jovanovic, T.. , Farid, R.. , Friesner, R.. and [McDermott, Ann. E.](#) "Thermal equilibrium of high- and low-spin forms of cytochrome P450 BM-3: Repositioning of the substrate?" 2005. **Journal of the American Chemical Society** 127 :13548-13552 [link info](#)
60. Gross, B.. , Tanski, J.. and [McDermott, Ann. E.](#) "Structure determination of aligned systems by solid-state NMR magic angle spinning methods" 2005. **Journal of Magnetic Resonance** 176 :223-233 [link info](#)
61. Igumenova, T.. and [McDermott, Ann. E.](#) "Homo-nuclear ^{13}C J-decoupling in uniformly ^{13}C - enriched solid proteins" 2005. **Journal of Magnetic Resonance** 175 :11-20 [link info](#)
62. Zech, S.. , Wand, A.. and [McDermott, Ann. E.](#) "Protein structure determination by high-resolution solid-state NMR spectroscopy: Application to microcrystalline ubiquitin" 2005. **Journal of the American Chemical Society** 127 :8618-8626 [link info](#)
63. [McDermott, Ann. E.](#) , Gustafsson, M.. , Elsam, T.. , Hui, C.. , Emerson Jr., C.. and Borycki, A.. "Gli2 and Gli3 have redundant and context-dependent function in skeletal muscle formation" 2005. **Development** 132 :345-357 [link info](#)
64. Jovanovic, T.. and [McDermott, Ann. E.](#) "Observation of ligand binding to cytochrome P450 BM-3 by means of solid-state NMR spectroscopy" 2005. **Journal of the American Chemical Society** 127 :13816-13821 [link info](#)
65. Marulanda, D.. , Tasayco, M.. , [McDermott, Ann. E.](#) , Cataldi, M.. , Arriaran, V.. and Polenova, T.. "Magic angle spinning solid-state NMR spectroscopy for structural studies of protein interfaces. Resonance assignments of differentially enriched *Escherichia coli* thioredoxin reassembled by fragment complementation" 2004. **Journal of the American Chemical Society** 126 :16608-16620 [link info](#)
66. Zech, S.. , Olejniczak, E.. , Hajduk, P.. , Mack, J.. and [McDermott, Ann. E.](#) "Characterization of protein-ligand interactions by high-resolution solid-state NMR spectroscopy" 2004. **Journal of the American Chemical Society** 126 :13948-13953 [link info](#)
67. and [McDermott, Ann. E.](#) "Structural and dynamic studies of proteins by solid-state NMR spectroscopy: Rapid movement forward" 2004. **Current Opinion in Structural Biology** 14 :554-561 [link info](#)
68. Igumenova, T.. , [McDermott, Ann. E.](#) , Zilm, K.. , Martin, R.. , Paulson, E.. and Wand, A.. "Assignments of carbon NMR resonances for microcrystalline ubiquitin" 2004. **Journal of the American Chemical Society** 126 :6720-6727 [link info](#)
69. Igumenova, T.. , Wand, A.. and [McDermott, Ann. E.](#) "Assignment of the Backbone Resonances for Microcrystalline Ubiquitin" 2004. **Journal of the American Chemical Society** 126 :5323-5331 [link info](#)
70. Guallar, V.. , Jacobson, M.. , [McDermott, Ann. E.](#) and Friesner, R.. "Computational Modeling of the Catalytic Reaction in Triosephosphate Isomerase" 2004. **Journal of Molecular Biology** 337 :227-239 [link info](#)
71. Desamero, R.. , Rozovsky, S.. , Zhadin, N.. , [McDermott, Ann. E.](#) and Callender, R.. "Active site loop motion in triosephosphate isomerase: T-jump relaxation spectroscopy of thermal activation" 2003. **Biochemistry** 42 :2941-2951 [link info](#)

72. Igumenova, T.. and [McDermott, Ann. E.](#) "Improvement of resolution in solid state NMR spectra with J-decoupling: An analysis of lineshape contributions in uniformly ^{13}C -enriched amino acids and proteins" 2003. **Journal of Magnetic Resonance** 164 :270-285 [link info](#)
73. Jogl, G.. , Rozovsky, S.. , [McDermott, Ann. E.](#) and Tong, L.. "Optimal alignment for enzymatic proton transfer: Structure of the Michaelis complex of triosephosphate isomerase at 1.2-Å resolution" 2003. **Proceedings of the National Academy of Sciences of the United States of America** 100 :50-55 [link info](#)
74. Sauve, A.. , Cahill, S.. , Zech, S.. , Basso, L.. , Lewandowicz, A.. , Santos, D.. , Grubmeyer, C.. , Evans, G.. , Furneaux, R.. , Tyler, P.. , [McDermott, Ann. E.](#) , Girvin, M.. and Schramm, V.. "Ionic states of substrates and transition state analogues at the catalytic sites of N-ribosyltransferases" 2003. **Biochemistry** 42 :5694-5705 [link info](#)
75. Kisko, J.. , Torzilli, M.. , Liu, K.. , [McDermott, Ann. E.](#) and Beer, R.. "An iron(III)trichloride adduct of N-isopropylsalicylaldehyde: Preparation, x-ray structure and NMR spectroscopic characterization" 2002. **Inorganic Chemistry Communications** 5 :283-287 [link info](#)
76. Wei, Y.. , Lee, D.. , [McDermott, Ann. E.](#) and Ramamoorthy, A.. "A 2D MAS solid-state NMR method to recover the amplified heteronuclear dipolar and chemical shift anisotropic interactions" 2002. **Journal of Magnetic Resonance** 158 :23-35 [link info](#)
77. [McDermott, Ann. E.](#) , Polenova, T.. , Bockmann, A.. , Zilm, K.. , Paulson, E.. , Martin, R.. and Montelione, G.. "Erratum: Partial NMR assignments for uniformly (^{13}C , ^{15}N)-enriched BPTI in the solid state (Journal of Biomolecular NMR (2000) vol. 16 (209-219))" 2001. **Journal of Biomolecular NMR** 19 :389 [info](#)
78. Rozovsky, S.. , Jogl, G.. , Tong, L.. and [McDermott, Ann. E.](#) "Solution-state NMR investigations of triosephosphate isomerase active site loop motion: Ligand release in relation to active site loop dynamics" 2001. **Journal of Molecular Biology** 310 :271-280 [link info](#)
79. Rozovsky, S.. and [McDermott, Ann. E.](#) "The time scale of the catalytic loop motion in triosephosphate isomerase" 2001. **Journal of Molecular Biology** 310 :259-270 [link info](#)
80. Gilchrist Jr., M.. , Monde, K.. , Tomita, Y.. , Iwashita, T.. , Nakanishi, K.. and [McDermott, Ann. E.](#) "Measurement of interfluorine distances in solids" 2001. **Journal of Magnetic Resonance** 152 :1-6 [link info](#)
81. Song, X.. , Rienstra, Chad. and [McDermott, Ann. E.](#) "N-H bond stretching in histidine complexes: A solid-state NMR study" 2001. **Magnetic Resonance in Chemistry** 39 :S30-S36 [info](#)
82. Song, X.. and [McDermott, Ann. E.](#) "Proton transfer dynamics and N-H bond lengthening in N-H...N model systems: A solid-state NMR study" 2001. **Magnetic Resonance in Chemistry** 39 :S37-S43 [info](#)
83. Turro, N.. , Lei, X.. , Li, Wenbo. , Liu, Z.. , [McDermott, Ann. E.](#) , Ottaviani, M.. and Abrams, L.. "Photochemical and magnetic resonance investigations of the supramolecular structure and dynamics of molecules and reactive radicals on the external and internal surface of MFI zeolites" 2000. **Journal of the American Chemical Society** 122 :11649-11659 [link info](#)
84. Monde, K.. , Tomita, Y.. , Gilchrist Jr., M.. , [McDermott, Ann. E.](#) and Nakanishi, K.. "Design and preparation of polyphenyl distance markers for solid-state ^{19}F NMR" 2000. **Israel Journal of Chemistry** 40 :301-306 [info](#)
85. Peshkovsky, A.. and [McDermott, Ann. E.](#) "Dipolar Interactions in Molecules Aligned by Strong AC Electric Fields" 2000. **Journal of Magnetic Resonance** 147 :104-109 [info](#)
86. Li, Wenbo. , Lei, X.. , Lem, G.. , [McDermott, Ann. E.](#) , Turro, N.. , Bottke, N.. and Adam, W.. "Oxygen and structural effects on silicalite ^{29}Si spin-lattice relaxation studied by high-resolution ^{29}Si solid-state NMR" 2000. **Chemistry of Materials** 12 :731-737 [link info](#)
87. [McDermott, Ann. E.](#) , Polenova, T.. , Bockmann, A.. , Zilm, K.. , Paulsen, E.. , Martin, R.. and Montelione, G.. "Partial NMR assignments for uniformly (^{13}C , ^{15}N)-enriched BPTI in the solid state" 2000. **Journal of Biomolecular NMR** 16 :209-219 [link info](#)
88. Dekker, L.. , Leitges, M.. , Altschuler, G.. , Mistry, N.. , [McDermott, Ann. E.](#) , Roes, J.. and Segal, A.. "Protein kinase C- β contributes to NADPH oxidase activation in neutrophils" 2000. **Biochemical Journal** 347 :285-289 [link info](#)
89. Polenova, T.. and [McDermott, Ann. E.](#) "A coherent mixing mechanism explains the photoinduced nuclear polarization in photosynthetic reaction centers" 1999. **Journal of Physical Chemistry B** 103 :535-548 [info](#)
90. Wei, Y.. and [McDermott, Ann. E.](#) "Effects of hydrogen bonding on ^1H chemical shifts" 1999. **ACS Symposium Series** 732 :177-193 [info](#)
91. Peshkovsky, A.. and [McDermott, Ann. E.](#) "NMR spectroscopy in the presence of strong AC electric fields: Degree of alignment of polar molecules" 1999. **Journal of Physical Chemistry A** 103 :8604-8611 [info](#)

92. Wei, Y., De Dios, A. and [McDermott, Ann. E.](#) "Solid-state ^{15}N NMR chemical shift anisotropy of histidines: Experimental and theoretical studies of hydrogen bonding" 1999. **Journal of the American Chemical Society** 121 :10389-10394 [link info](#)
93. Lee, H., Ortiz De Montellano, P. and [McDermott, Ann. E.](#) "Deuterium magic angle spinning studies of substrates bound to cytochrome P450" 1999. **Biochemistry** 38 :10808-10813 [link info](#)
94. Lee, H., Polenova, T., Beer, R. and [McDermott, Ann. E.](#) "Lineshape fitting of deuterium magic angle spinning spectra of paramagnetic compounds in slow and fast limit motion regimes" 1999. **Journal of the American Chemical Society** 121 :6884-6894 [link info](#)
95. Gu, Z., Drueckhammer, D., Kurz, L., Liu, K., Martin, D. and [McDermott, Ann. E.](#) "Solid state NMR studies of hydrogen bonding in a citrate synthase inhibitor complex" 1999. **Biochemistry** 38 :8022-8031 [link info](#)
96. Standley, D., Eyrich, V., Felts, A., Friesner, R. and [McDermott, Ann. E.](#) "A branch and bound algorithm for protein structure refinement from sparse NMR data sets" 1999. **Journal of Molecular Biology** 285 :1691-1710 [link info](#)
97. Turro, N., [McDermott, Ann. E.](#), Lei, X., Li, Wenbo., Abrams, L., Ottaviani, M., Beard, H., Houk, K., Beno, B. and Lee, P. "Photochemistry of ketones adsorbed on size/shape selective zeolites. A supramolecular approach to persistent carbon centered radicals" 1998. **Chemical Communications** :697-698 [info](#)
98. Standley, D., Gunn, J., Friesner, R. and [McDermott, Ann. E.](#) "Tertiary structure prediction of mixed α/β proteins via energy minimization" 1998. **Proteins: Structure, Function and Genetics** 33 :240-252 [link info](#)
99. Liu, K., Williams, J., Lee, H., Fitzgerald, M., Jensen, G., Goodin, D. and [McDermott, Ann. E.](#) "Solid-state deuterium nmr of imidazole ligands in cytochrome C peroxidase" 1998. **Journal of the American Chemical Society** 120 :10199-10202 [link info](#)
100. Williams, J. and [McDermott, Ann. E.](#) "Variable NMR spin-lattice relaxation times in secondary amides: Effect of ramachandran angles on librational dynamics" 1998. **Journal of Physical Chemistry B** 102 :6248-6259 [info](#)
101. Rompel, A., Cinco, R., Latimer, M., [McDermott, Ann. E.](#), Guiles, R., Quintanilha, A., Krauss, R., Sauer, K., Yachandra, V. and Klein, M. "Sulfur K-edge x-ray absorption spectroscopy: A spectroscopic tool to examine the redox state of S-containing metabolites in vivo" 1998. **Proceedings of the National Academy of Sciences of the United States of America** 95 :6122-6127 [link info](#)
102. [McDermott, Ann. E.](#), Zysmilich, M. and Polenova, T. "Solid state NMR studies of photoinduced polarization in photosynthetic reaction centers: Mechanism and simulations" 1998. **Solid State Nuclear Magnetic Resonance** 11 :21-47 [info](#)
103. Turro, N., Lei, X., Li, Wenbo., [McDermott, Ann. E.](#), Abrams, L., Oftavianai, M. and Beard, H. "Photochemistry and magnetic resonance spectroscopy as probes of supramolecular structures and migration pathways of organic molecules and radicals adsorbed on zeolites" 1998. **Chemical Communications** :695-696 [info](#)
104. Polenova, T., Iwashita, T., Palmer III, A. and [McDermott, Ann. E.](#) "Conformation of the trypanocidal pharmaceutical suramin in its free and bound forms: Transferred nuclear overhauser studies" 1997. **Biochemistry** 36 :14202-14217 [link info](#)
105. Zysmilich, M. and [McDermott, Ann. E.](#) "Natural abundance solid-state carbon NMR studies of photosynthetic reaction centers with photoinduced polarization" 1996. **Proceedings of the National Academy of Sciences of the United States of America** 93 :6857-6860 [link info](#)
106. Gu, Z., Ebisawa, K. and [McDermott, Ann. E.](#) "Hydrogen bonding effects on amine rotation rates in crystalline amino acids" 1996. **Solid State Nuclear Magnetic Resonance** 7 :161-172 [link info](#)
107. Palmer III, A., Williams, J. and [McDermott, Ann. E.](#) "Nuclear magnetic resonance studies of biopolymer dynamics" 1996. **Journal of Physical Chemistry** 100 :13293-13310 [info](#)
108. Zysmilich, M. and [McDermott, Ann. E.](#) "Photochemically induced nuclear spin polarization in bacterial photosynthetic reaction centers: Assignments of the ^{15}N SSNMR spectra" 1996. **Journal of the American Chemical Society** 118 :5867-5873 [link info](#)
109. Gu, Z., Ridenour, C., Bronnimann, C., Iwashita, T. and [McDermott, Ann. E.](#) "Hydrogen bonding and distance studies of amino acids and peptides using solid state 2D ^1H - ^{13}C heteronuclear correlation spectra" 1996. **Journal of the American Chemical Society** 118 :822-828 [info](#)
110. Becerra, L., Gerfen, G., Bellew, B., Bryant, J., Hall, D., Inati, S., Weber, R., Un, S., Prisner, T., [McDermott, Ann. E.](#), Fishbein, K., Kreischer, K., Temkin, R., Singel, D. and Griffin, R. "A Spectrometer for Dynamic Nuclear Polarization and Electron Paramagnetic Resonance at High Frequencies" 1995. **Journal of Magnetic Resonance, Series A** 117 :28-40 [link info](#)

111. Williams, J.. and [McDermott, Ann. E.](#) "Dynamics of the Flexible Loop of Triosephosphate Isomerase: The Loop Motion Is Not Ligand Gated" 1995. **Biochemistry** 34 :8309-8319 [link info](#)
112. Liu, K.. , Ryan, D.. , Nakanishi, K.. and [McDermott, Ann. E.](#) "Solid State NMR Studies of Paramagnetic Coordination Complexes: A Comparison of Protons and Deuterons in Detection and Decoupling" 1995. **Journal of the American Chemical Society** 117 :6897-6906 [link info](#)
113. Gu, Z.. , Zambrano, R.. and [McDermott, Ann. E.](#) "Hydrogen Bonding of Carboxyl Groups in Solid-State Amino Acids and Peptides: Comparison of Carbon Chemical Shielding, Infrared Frequencies, and Structures" 1994. **Journal of the American Chemical Society** 116 :6368-6372 [link info](#)
114. [McDermott, Ann. E.](#) , Creuzet, F.. , Griffin, R.. , Gebhard, R.. , van der Hoef, K.. , Lugtenburg, J.. , Levitt, M.. and Herzfeld, J.. "Determination of Internuclear Distances and the Orientation of Functional Groups by Solid-State NMR: Rotational Resonance Study of the Conformation of Retinal in Bacteriorhodopsin" 1994. **Biochemistry** 33 :6129-6136 [link info](#)
115. O'Connor, E.. , Tomita, Y.. and [McDermott, Ann. E.](#) "Synthesis of (1, 2-¹³C₂) 2-phosphoglycolic acid" 1994. **Journal of Labelled Compounds and Radiopharmaceuticals** 34 :735-740 [link info](#)
116. Copié, V.. , [McDermott, Ann. E.](#) , Beshah, K.. , Griffin, R.. , Williams, J.. , Spijker-Assink, M.. , Gebhard, R.. , Lugtenburg, J.. and Herzfeld, J.. "Deuterium Solid-State Nuclear Magnetic Resonance Studies of Methyl Group Dynamics in Bacteriorhodopsin and Retinal Model Compounds: Evidence for a 6-s-Trans Chromophore in the Protein" 1994. **Biochemistry** 33 :3280-3286 [link info](#)
117. Zysmilich, M.. and [McDermott, Ann. E.](#) "Photochemically Induced Dynamic Nuclear Polarization in the Solid-State ¹⁵N Spectra of Reaction Centers from Photosynthetic Bacteria Rhodobacter spbaeroides R-26" 1994. **Journal of the American Chemical Society** 116 :8362-8363 [link info](#)
118. Tomita, Y.. , O'Connor, E.. and [McDermott, Ann. E.](#) "A Method for Dihedral Angle Measurement in Solids: Rotational Resonance NMR of a Transition-State Inhibitor of Triose Phosphate Isomerase" 1994. **Journal of the American Chemical Society** 116 :8766-8771 [link info](#)
119. Auger, M.. , [McDermott, Ann. E.](#) , Robinson, V.. , Castelhana, A.. , Billedeau, R.. , Pliura, D.. , Krantz, A.. and Griffin, R.. "Solid-State ¹³C NMR Study of a Transglutaminase-Inhibitor Adduct" 1993. **Biochemistry** 32 :3930-3934 [link info](#)
120. Gu, Z.. and [McDermott, Ann. E.](#) "Chemical Shielding Anisotropy of Protonated and Deprotonated Carboxylates in Amino Acids" 1993. **Journal of the American Chemical Society** 115 :4282-4285 [link info](#)
121. Prisner, T.. , [McDermott, Ann. E.](#) , Un, S.. , Norris, J.. , Thurnauer, M.. and Griffin, R.. "Measurement of the g-tensor of the P700+ signal from deuterated cyanobacterial photosystem I particles" 1993. **Proceedings of the National Academy of Sciences of the United States of America** 90 :9485-9488 [info](#)
122. Williams, J.. and [McDermott, Ann. E.](#) "Cis-trans energetics in urea and acetamide studied by deuterium NMR" 1993. **Journal of Physical Chemistry** 97 :12393-12398 [info](#)
123. [McDermott, Ann. E.](#) , Creuzet, F.. , Kolbert, A.. and Griffin, R.. "High-resolution magic-angle-spinning NMR spectra of protons in deuterated solids" 1992. **Journal of Magnetic Resonance (1969)** 98 :408-413 [link info](#)
124. Un, S.. , Prisner, T.. , Weber, R.. , Seaman, M.. , Fishbein, K.. , [McDermott, Ann. E.](#) , Singel, D.. and Griffin, R.. "Pulsed dynamic nuclear polarization at 5 T" 1992. **Chemical Physics Letters** 189 :54-59 [link info](#)
125. Thompson, L.. , [McDermott, Ann. E.](#) , Raap, J.. , van der Wielen, C.. , Lugtenburg, J.. , Herzfeld, J.. and Griffin, R.. "Rotational Resonance NMR Study of the Active Site Structure in Bacteriorhodopsin: Conformation of the Schiff Base Linkage" 1992. **Biochemistry** 31 :7931-7938 [link info](#)
126. DeRose, V.. , Yachandra, V.. , [McDermott, Ann. E.](#) , Britt, R.. , Sauer, K.. and Klein, M.. "Nitrogen Ligation to Manganese in the Photosynthetic Oxygen-Evolving Complex: Continuous-Wave and Pulsed EPR Studies of Photosystem II Particles Containing ¹⁴N or ¹⁵N" 1991. **Biochemistry** 30 :1335-1341 [link info](#)
127. Spencer, R.. , Auger, M.. , [McDermott, Ann. E.](#) , Griffin, R.. , Halverson, K.. , Griffin, R.. and Lansbury, Jr.. "An Unusual Peptide Conformation May Precipitate Amyloid Formation in Alzheimer's Disease: Application of Solid-State NMR to the Determination of Protein Secondary Structure" 1991. **Biochemistry** 30 :10382-10387 [link info](#)
128. [McDermott, Ann. E.](#) , Thompson, L.. , Winkel, C.. , Lugtenburg, J.. , Farrar, M.. , Pelletier, S.. , Herzfeld, J.. and Griffin, R.. "Mechanism of Proton Pumping in Bacteriorhodopsin by Solid-State NMR: The Protonation State of Tyrosine in the Light-Adapted and M States" 1991. **Biochemistry** 30 :8366-8371 [link info](#)

129. Creuzet, F., [McDermott, Ann. E.](#), Gebhard, R., van der Hoef, K., Spijker-Assink, M., Herzfeld, J., Lugtenburg, J., Levitt, M. and Griffin, R. "Determination of membrane protein structure by rotational resonance NMR: Bacteriorhodopsin" 1991. **Science** 251 :783-786 [info](#)
130. Guiles, R., Zimmermann, J., [McDermott, Ann. E.](#), Yachandra, V., Cole, J., Dexheimer, S., Britt, R., Wieghardt, K., Bossek, U., Sauer, K. and Klein, M. "The S3 State of Photosystem II: Differences between the Structure of the Manganese Complex in the S2 and S3 States Determined by X-ray Absorption Spectroscopy" 1990. **Biochemistry** 29 :471-485 [link info](#)
131. Herzfeld, J., Das Gupta, S., Farrar, M., Harbison, G., [McDermott, Ann. E.](#), Pelletier, S., Raleigh, D., Smith, S., Winkel, C., Lugtenburg, J. and Griffin, R. "Solid-State ¹³C NMR Study of Tyrosine Protonation in Dark-Adapted Bacteriorhodopsin" 1990. **Biochemistry** 29 :5567-5574 [link info](#)
132. Guiles, R., Yachandra, V., [McDermott, Ann. E.](#), Cole, J., Dexheimer, S., Britt, R., Sauer, K. and Klein, M. "The S0 State of Photosystem II Induced by Hydroxylamine: Differences between the Structure of the Manganese Complex in the S0 and S1 States Determined by X-ray Absorption Spectroscopy" 1990. **Biochemistry** 29 :486-496 [link info](#)
133. [McDermott, Ann. E.](#), Creuzet, F., Griffin, R., Zawadzke, L., Ye, Q. and Walsh, C. "Rotational resonance determination of the structure of an enzyme-inhibitor complex: Phosphorylation of an (aminoalkyl)phosphinate inhibitor of D-alanyl-D-alanine ligase by ATP" 1990. **Biochemistry** 29 :5767-5775 [link info](#)
134. [McDermott, Ann. E.](#), Yachandra, V., Guiles, R., Sauer, K., Klein, M., Parrett, K. and Golbeck, J. "EXAFS Structural Study of FX, the Low-Potential Fe-S Center in Photosystem I" 1989. **Biochemistry** 28 :8056-8059 [link info](#)
135. Yachandra, V., Guiles, R., [McDermott, Ann. E.](#), Cole, J., DeRose, V., Zimmermann, J., Sauer, K. and Klein, M. "X-ray absorption spectroscopy of Mn in the photosynthetic apparatus" 1989. **Physica B: Physics of Condensed Matter** 158 :78-80 [link info](#)
136. [McDermott, Ann. E.](#), Yachandra, V., Guiles, R., Cole, J., Dexheimer, S., Britt, R., Sauer, K. and Klein, M. "Characterization of the Manganese O2-Evolving Complex and the Iron-Quinone Acceptor Complex in Photosystem II from a Thermophilic Cyanobacterium by Electron Paramagnetic Resonance and X-ray Absorption Spectroscopy" 1988. **Biochemistry** 27 :4021-4031 [link info](#)
137. [McDermott, Ann. E.](#), Yachandra, V., Guiles, R., Britt, R., Dexheimer, S., Sauer, K. and Klein, M. "Low-Potential Iron-Sulfur Centers in Photosystem I: An X-ray Absorption Spectroscopy Study" 1988. **Biochemistry** 27 :4013-4020 [link info](#)
138. Cole, J., Yachandra, V., Guiles, R., [McDermott, Ann. E.](#), Britt, R., Dexheimer, S., Sauer, K. and Klein, M. "Assignment of the g = 4.1 ERP signal to manganese in the S2 state of the photosynthetic oxygen-evolving complex: An X-ray absorption edge spectroscopy study" 1987. **BBA - Bioenergetics** 890 :395-398 [link info](#)
139. Golbeck, J., [McDermott, Ann. E.](#), Jones, W. and Kurtz, D. "Evidence for the existence of [2Fe-2S] as well as [4Fe-4S] clusters among FA, FB and FX. Implications for the structure of the Photosystem I reaction center" 1987. **BBA - Bioenergetics** 891 :94-98 [link info](#)
140. Golbeck, J., Parrett, K. and [McDermott, Ann. E.](#) "Photosystem I charge separation in the absence of center A and B. III. Biochemical characterization of a reaction center particle containing P-700 and FX" 1987. **BBA - Bioenergetics** 893 :149-160 [link info](#)
141. Klein, M., Sauer, K., Britt, R., Yachandra, V., Guiles, R., [McDermott, Ann. E.](#), Cole, J. and Dexheimer, S. "Comparison of the Structure of the Manganese Complex in the S1 and S2 States of the Photosynthetic O2-Evolving Complex: An X-ray Absorption Spectroscopy Study" 1987. **Biochemistry** 26 :5974-5981 [link info](#)
142. Cole, J., Yachandra, V., Britt, R., [McDermott, Ann. E.](#), Guiles, R., Sauer, K., Klein, M. and Dexheimer, S. "Structure of the Manganese Complex of Photosystem II upon Removal of the 33-Kilodalton Extrinsic Protein: An X-ray Absorption Spectroscopy Study" 1987. **Biochemistry** 26 :5967-5973 [link info](#)
143. Yachandra, V., Guiles, R., [McDermott, Ann. E.](#), Britt, R., Dexheimer, S., Sauer, K. and Klein, M. "The state of manganese in the photosynthetic apparatus. 4. Structure of the manganese complex in Photosystem II studied using EXAFS spectroscopy. The S1 state of the O2-evolving Photosystem II complex from spinach" 1986. **BBA - Bioenergetics** 850 :324-332 [link info](#)

B. Positions, Scientific Appointments, and Honors

Positions and Scientific Appointments

1991– Present Professor, Department of Chemistry, Columbia University, NY

Honors

the DuPont Young Investigator Award (1992)

the Cottrell Scholars Award (1994)

the [Alfred P. Sloan](#) Research Fellowship (1995)

The Pure Award in Chemistry (1996)

the Eastern Analytic Symposium Award for Achievement in Magnetic Resonance (2005)

the Royal Society of Chemistry's [Bourke Award](#) (2014)

Fellow of American Academy of Arts and Sciences (2000)

Member of the National Academy of Sciences (2006)

BIOGRAPHICAL SKETCH

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POSITION TITLE: Postdoctoral

EDUCATION/TRAINING

INSTITUTION AND LOCATION	DEGREE (if applicable)	Completion Date MM/YYYY	FIELD OF STUDY
Hunan University	Bachelor	06/2011	Chemistry
Columbia University	PHD	06/2018	Chemistry
Columbia University	Postdoctoral	08/2018-	Chemistry

A. Personal Statement

My research is focused on connecting structural and functional states of KcsA, a model bacterial potassium channel, as it undergoes activation, potassium conduction, and subsequent inactivation. I am particularly interested in the C-type inactivation process, in which the channel slowly inactivates spontaneously after activation. By combining solid-state NMR with other biophysical methods, including electrophysiology and site-directed mutagenesis, my work elucidates the strong allosteric coupling between the activation gate and the potassium selectivity filter and connects this allostery to the functional role of the channel in controlling potassium ion permeation.

I am also working on a project combining SSNMR and CryoEM to study the three-dimensional structure of fibrils formed by TDP-43, which caused lethal neurodegenerative diseases.

Publications:

Z. Sun, **Y. Xu**, D. Zhang, A. E McDermott, Probing Allosteric Coupling of a Constitutively Open Mutant of the Ion Channel KcsA using Solid State NMR, Proceedings of the National Academy of Science, 2020, 117 (13) 7171-7175

Y. Xu, D. Zhang, R. Rogwaski, C. Nimigean, A. McDermott, Coupled Clusters of Allostery Participants: Identification by Chemical Shift, *Proceedings of the National Academy of Science*, 2019,116 (6), 2078-2085

Y. Xu, A. McDermott, Inactivation in KcsA, *Journal of Structural Biology*,: X, 100009

Y. Xu, M. Bhate, A. McDermott, Transmembrane allosteric energetics characterization for strong coupling between proton and potassium ion binding in the KcsA channel, *Proceedings of the National Academy of Science*, 2017, 114 (33) 8788-8793;

M. Mompeán, R. Hervás, Y. Xu, et al. Structural Evidence of Amyloid Fibril Formation in the Putative Aggregation Domain of TDP-43. *The journal of physical chemistry letters*. 2015 6(13):2608-2615.

Y. Xu, L. Deng, H. Wang, J. Li, and R. Yang, Metal-induced aggregation of mononucleotides-stabilized gold nanoparticles: an efficient approach for simple and rapid colorimetric detection of Hg(II), *Chem. Commun.*, **2011**, 47, 6039-6041.

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POSITION TITLE: Junior Principal Investigator (since 2019)			
EDUCATION/TRAINING			
INSTITUTION AND LOCATION	DEGREE (if applicable)	Completion Date MM/YYYY	FIELD OF STUDY
IQFR-CSIC	PHD	2015	Biophysics

Personal Statement

Miguel Mompeán holds two BSc degrees (Chemistry, 2010, and Biochemistry, 2015), and a European MSc in Theoretical Chemistry and Computational Modelling, an initiative from > 30 participating institutions from different countries (2013). In 2011, MM joined the IQFR-CSIC, obtaining his international PhD in Biophysics in 2015. During this period, he was trained in protein NMR and biophysical techniques, and merged this expertise with his interests in computational approaches to tackle the complex biological question of protein aggregation in health and disease. After four years trained as a postdoc in advanced NMR and computational methods, including theoretical aspects and hardware implementation, solid-state NMR and hyperpolarization techniques, MM obtained a Junior Leader fellowship from la Caixa Foundation, and re-joined the IQFR-CSIC as a Junior Principal Investigator. This allowed MM to initiate a new research line to study homo- and hetero-amyloids and other protein aggregate forms, using a unique, powerful combination of NMR techniques in solution and in the solid-state, combined with hyperpolarization strategies and a myriad of computational approaches that range from quantum mechanical calculations to molecular or spin dynamics simulations to match theory and experiment in the quest

for relevant biological answers and new methods.

Funding

La Caixa Banking Foundation – Junior Leader Programme

Publication:

Google Scholar: <https://scholar.google.com/citations?user=qXcUZdAAAAAJ&hl=es&authuser=1>