Flora Meilleur

Associate Professor, Molecular and Structural Biochemistry, North Carolina State University
Neutron Scattering Scientist (IMAGINE and MaNDi), Neutron Sciences Directorate, Oak Ridge National Laboratory

Professional experience:

2015-pres Associate Professor, Department of Molecular and Structural Biochemistry, North Carolina State University, Raleigh, NC, USA; Joint appointment with Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN, USA
2007-2015 Assistant Professor, Department of Molecular and Structural Biochemistry, North Carolina State University, Raleigh, NC, USA; Joint appointment with Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN, USA
2006-2007 Research fellow, Spallation Neutron Source & Center for Structural Molecular Biology, Oak Ridge National Laboratory, Oak Ridge, TN, USA
2005-2006 Visiting scientist, Spallation Neutron Source & Center for Structural Molecular Biology, Oak Ridge National Laboratory, Oak Ridge, TN, USA
2004-2006 Physicist, Institut Laue Langevin, Grenoble, France

Education:

*Institution, Major, **Degree**, Year*
University J. Fourier, Grenoble, France, Physic & Chemistry, **B. Sc.** (Licence), 1998
University J. Fourier, Grenoble, France, Structural Biology, **M. Sc.** (Maîtrise, DEA), 2000
European Molecular Biology Laboratory & University J. Fourier, Grenoble, France, Structural Biology, **Ph. D.**, 2004

M. Sc. Thesis Title (Maîtrise): Quantum chemistry analysis of H-atom addition to cytosine; *Advisor:* André Grand (Commissariat à l'Energie Atomique)
M. Sc. Thesis Title (DEA): Neutron crystallographic and quantum chemistry studies of myoglobin; *Advisors:* Dean Myles (EMBL), André Grand (Commissariat à l'Energie Atomique)
Ph. D. Thesis Title: X-ray and Neutron Crystallographic Analysis of cytochrome P450cam and D-xylose isomerase; *Advisors:* Dean Myles (EMBL), Eva Pebay-Peyroula (University J. Fourier)

Scholarly and professional honors:

2013 ORNL Significant Event Award (Team award; Role: Science lead)
2000-2004 EMBL Ph. D. Fellowship
2000-2003 French government Ph. D. Fellowship
1999-2000 French government MSc (DEA) Fellowship

Membership in professional organizations:

2009-pres Neutron Scattering Society of America (NSSA)

2007-pres SNS-HFIR User Group (SHUG)
2006-pres American Crystallographic Association (ACA)

Elected position
2019-pres Secretary, Neutron Scattering Society of America (NSSA)

Appointed position
2015-pres Co-Editor, Journal of Applied Crystallography

Professional service
2021 NSF MCB panel reviewer
2010-pres Reviewer, Science, PNAS, ACS Catalysis, Scientific Reports, Protein Science, Biochemistry, FEBS Journal, Physical Chemistry Chemical Physics, Carbohydrate Research, Australian Journal of Chemistry, IUCr Journals (IUCRj, Acta Cryst. D and F)
2007-2017 Chair, Instrument Advisory Team (IAT) for the construction of a quasi-Laue diffractometer at the High Flux Isotope Reactor at Oak Ridge National Laboratory
2016 Member, Selection Committees NSSA Science and the Sustained Research Prizes
2009-2012 Member-at-large, NSSA Executive Committee
2011 Reviewer, Department of Energy, Early Career Award
2008-2010 Reviewer, American Heart Association
2007-2010 Member, SNS-HFIR User Group Executive Committee
2009 Member, Selection committee for NSSA Fellows
2007-2009 Member, Neutron Sciences Directorate Education Committee

Professional service on NCSU campus
2020-pres Chair, Biochemistry Dept. Post-Tenure Review committee
2019-2020 Member, NCSU Biochemistry Faculty Search Committee
2018-2019 Member, NCSU Biochemistry Dept. Graduate Curriculum Committee
2018-pres Chair, METRIC X-ray User Committee
2017-2019 Member, NCSU Biochemistry Dept. Graduate Student Recruiting Committee
2017-pres Reviewer, NCSU Biochemistry Undergrad. Fellowship
2016 Member, NCSU Biochemistry Head Search Committee
2015-2018 Administrator, NCSU Biochemistry Dept. Webpage
2014 Reviewer, NCSU CALS Dean's Enrichment Grants Program
2014 Member, NCSU Biochemistry Dept. Graduate student recruiting committee
2010 Internal (NCSU) reviewer, NIH U19
2008-pres Member, NCSU graduate student committee

Professional Service (ORNL)
2021-pre Coordinator, Neutron Scattering Division “Biology Initiative”

2021-pre Member, ORNL Student Programs Review Committee
2020 Member, ORNL STS SANS Instrument Development Scientist Interview Committee
2020 Member, ORNL NSD Group Leader, Labs & Soft Matter interview Committee
2011-pres Mentor, Appalachian Region. Comm. (ARC)/ORNL Math-Science-Tech. Institute

Teaching
2019-pres BCH 701 (Protein structure function; Fall semester)
2011-2019 BCH 705 (Molecular Biology of the cell; Spring semester)

Workshop Organization
2020-2021 Director, Virtual HFIR/SNS Advanced Neutron Diffraction and Scattering (HANDS)
2019 Director, HFIR/SNS Advanced Neutron Diffraction and Scattering (HANDS)
2010-2018 Director, Neutrons in Structural Biology (NCSU BCH 590E, Summer I semester)

Conference Organization
2022 Member, International Conference on Neutron Scattering International Program, Committee, Buenos Aires, Argentina
2021 Session chair, PACIFICHEM2020 (New Era of Quantum Beam in Biology), Honolulu, HI
2021 Session chair, 71st ACA meeting (Redox enzymes), Virtual conference
2021 Session chair, 25th Congress of International Union of Crystallography (Macromolecular neutron diffraction) Prague, Czech Republic (Hybrid meeting)
2020 NSSA Secretary, American Conference on Neutron Scattering (ACNS) 2020, Boulder, Co (virtual)
2019 Member, International Symposium on Diffraction Structural Biology International Advisory Committee, Osaka, Japan
2017 Session organizer, 24th Congress of International Union of Crystallography (Advanced neutron sources in biological and materials sciences) Hyderabad, India
2015 Member, ORNL- Duke University Neutron Workshop Organizing Committee, Durham, NC
2015 Member, Int. Symposium Diffraction Structural Biology Organizing Committee, Knoxville, TN
2015 Member, Second Target Station Workshop Program Advisory Committee, Oak Ridge, TN
2013 Session chair, SNS/HFIR User meeting (Biological Sample Environment/Sample Preparation; Structural Biology) Oak Ridge, TN, USA
2009 Session chair, International Conference on Neutron Scattering (Protein Structures) Knoxville, TN

Mentoring activities

Graduate students

Gabriela Schroder, 2015-present, NCSU/ORNL
Wm Brad O'Dell, 2012-2017, NCSU/ORNL
Annette Bodenheimer, 2011-2016, NCSU-ORNL

Graduate students hosted at ORNL:

Tobias Tandrup, February 2019, August 2019 - December 2019, University of Copenhagen
Leiah Carey, January 2016-October 2016, NCSU (Chemistry)
Stephen Keable, March 2015-May 2015, Montana State University

Post-doctoral research associate (Current position)

Partha P. Munshi, 2010-2012 (Associate professor and department chair, Shiv Nadir University)
Lilin He, 2008-2010 (Neutron scattering scientist, ORNL)
Yiming Mo, 2008-2009 (Insurance Operations Data Analyst, Assurant Inc)

Undergraduate students

Melissa Fee, 2015, NCSU, Sophomore
Oksana Samarski, 2009-2012, NCSU, Sophomore-senior
Tabitha Donald, 2010, Lane College, Senior
Sun-Lin Chung, 2010, Yale, Freshman
Jillian Reich, 2009, St Lawrence, Sophomore
Richard Goslen, 2008-2009, NCSU, Junior-Senior
Lisa Gilligan, 2007, Senior
Hung Dang, 2007, Sophomore
Jia Kim, 2007, Sophomore

High school students

Keiara Holley, 2011, Newbern's Sunshine High School, AL
Kimberly Wilson, 2011, Loyall High School, KY
Chelsea King, 2011, Burkesville High School, KY

Research assistant (current position)

Lezlee Dice, 2007-2009 (Research assistant, UTK)

Graduate committee memberships

Current graduate committee

1. Gabriela Schroder (NCSU/Biochemistry; role: chair)
2. Olivia Manley (NCSU/Biochemistry; role: graduate committee departmental member)
3. Suman Das (NCSU/Biochemistry; role: graduate committee departmental member)

4. Madison Moore (NCSU/Plant and Microbial Biology; role: graduate committee external member & Graduate School Representative)

Past graduate (Ph. D.) committee

13. Yue Yuan (NCSU/TECHS; role: graduate committee external member)
12. Donna Liebert (NCSU/Biochemistry; role: graduate committee departmental member**)**
11. Maddison Davidson (NCSU/Chemistry; role: graduate committee external member and Graduate School Representative)
10. Sophia Yang (NCSU/Biochemistry; role: graduate committee departmental member)
9. Paul Enriquez (NCSU/Biochemistry; role: graduate committee departmental member)
8. Eric Waddell (NCSU/Biochemistry; role: graduate committee departmental member)
7. Robert Grinshpon (NCSU; role: graduate committee departmental member**)**
6. Wm Brad O'Dell (NCSU/ORNL; role: chair)
5. Melvin Thomas (NCSU; role: graduate committee departmental member)
4. Walter Sandoval Espinola (NCSU; role: Graduate School Representative)
3. Annette Bodenheimer (NCSU; role: chair)
2. Sue Fetics (NCSU; role: graduate committee departmental member)
1. Craig Helstowski (UTK; role: graduate committee external member)

Other Ph. D. Dissertation Committee

1. Ryan Knithila, Northeastern University (role: external committee member)

Publications

Peer-reviewed articles

55. Schröder G.C., O'Dell W.B., Swartz P.D., **Meilleur F.** (2021)Preliminary results of neutron and X-ray diffraction data collection on a lytic polysaccharide monooxygenase under reduced and acidic conditions. *Acta Cryst. F* **77**:128-133.
a. Supervised graduate student first author paper
54. Schröder G. C., **Meilleur F.** (2020) Neutron Crystallography Data Collection and Processing for Modelling Hydrogen Atoms in Protein Structures *J. Vis. Exp.* doi: 10.3791/61903.
a. Supervised graduate student first author paper
53. Pierce J., Crow L., Cuneo M., Edwards M., Herwig K.W., Jennings A., Jones A., Li L., **Meilleur F.**, Myles D.A.A., Robertson L., Standaert R., Wonder A. Zhao J.K. (2019) A prototype system for dynamically polarized neutron protein crystallography. *Nucl Instrum Methods Phys Res A. https://doi.org/10.1016/j.nima.2019.06.023*
52. Lu X., Selvaraj B., Ghimire-Rijal S., Orf G.S., **Meilleur F.**, Blankenship R.E., Cuneo M.J., Myles D.A.A. (2019) Neutron and X-ray analysis of the Fenna-Matthews-Olson photosynthetic antenna complex from *Prosthecochloris aestuarii*. *Acta Cryst. F* **75**:171-175

51. Knihtila R., Volmar A. Y., **Meilleur F.**, Mattos C. (2019) Titration of ionizable groups in proteins using multiple neutron data sets from a single crystal: application to the small GTPase Ras. *Acta Cryst. F* **75**:111-115
50. Ashkar R. *et al.* (2018) Neutron scattering in the biological sciences: progress and prospects. *Acta Cryst.* D**74**:1129-1168
49. **Meilleur F.**, Coates L., Cuneo M. J., Kovalevsky A. Y., Myles D.A.A. (2018) The Neutron Macromolecular Crystallography Instruments at Oak Ridge National Laboratory: Advances, Challenges and Opportunities. *Crystals* **8**, 388
48. Coates L., Cao H. B., Chakoumakos B. C., Frontzek M. D., Hoffmann C., Kovalevsky A. Y., Liu Y., **Meilleur F.**, dos Santos A. M., Myles D. A. A., Wang X. P., Ye F. (2018) A suite-level review of the neutron single-crystal diffraction instruments at Oak Ridge National Laboratory. *Rev. Sci. Instr.* **89**, 092802
47. Haberl B., Dissanayake S., Wu Y., Myles D. A. A., dos Santos A. M., Loguillo M., Rucker G. M., Armitage D. P., Cochran M., Andrews K. M., Hoffmann C., Cao H., Matsuda M., **Meilleur F.**, Ye F., Molaison J. J., Boehler R. (2018) Next-generation diamond cell and applications to single-crystal neutron diffraction. *Rev. Sci. Instr.* **89**, 092902
46. Duff M. R., Borreguero J. M., Cuneo M., Ramanathan A., He J., Kamath G., Chennubhotla C. S., **Meilleur F.**, Howell E. E, Herwig K. W., Myles D. A. A., Agarwal P. K. (2018) Modulating enzyme activity by altering protein dynamics with solvent. *Biochemistry* **57**:4263-4275
45. Schroder G. C., O'Dell W. B. , Myles D. A. A., Kovalevsky A., **Meilleur F.** (2018) IMAGINE: neutrons reveal enzyme chemistry. *Acta Cryst.* D**74**:778-786
a. Supervised graduate students co-first author paper
44. Bodenheimer A.M., O'Dell W.B., Oliver R.C., Qian S., Stanley C.B., **Meilleur F.** (2018) Structural investigation of cellobiose dehydrogenase IIA: Insights from small angle scattering into intra- and intermolecular electron transfer mechanisms. *Biochim. Biophys. Acta.* **1862**:1031-1039
a. Supervised graduate student first author paper
43. Li L., Shukla S., **Meilleur F.**, Standaert R.F., Pierce J., Myles D.A., Cuneo M.J. (2017) Neutron crystallographic studies of T4 lysozyme at cryogenic temperature. *Protein Sci*. **26**:2098-2104
42. Hiromoto T., **Meilleur F.**, Shimizu R., Shibazaki C., Adachi M., Tamada T., Kuroki R. (2017) Neutron structure of the T26H mutant of T4 phage lysozyme provides insight into the catalytic activity of the mutant enzyme and how it differs from that of wild type. *Protein Sci.* **26**:1953-1963
41. Bodenheimer A.M., O'Dell W.B., Stanley C.B., **Meilleur F.** (2017) Structural studies of Neurospora crassa LPMO9D and redox partner CDHIIA using neutron crystallography and small-angle scattering. *Carbohydr. Res.* **448**:200-204
a. Supervised graduate students co-first author paper

40. O'Dell W.B., Swartz P., Weiss K., **Meilleur F.** (2017) Crystallization of a fungal lytic polysaccharide monooxygenase expressed from glycoengineered Pichia pastoris for X-ray and neutron diffraction *Acta Cryst.* F**73**:70-78
a. Supervised graduate student first author paper
39. Golden E., Yu L.G., **Meilleur F.**, Blakeley M.P., Duff A.P., Karton A., Vrielink A. (2017) An extended N-H bond driven by a conserved second order interaction orients the flavin N5 orbital in cholesterol oxidase. *Scientific Reports* **7**, Article Number 40517
38. O'Dell W. B., Aggarwal P., **Meilleur F.** (2017) Oxygen Activation at the Active Site of a Fungal Lytic Polysaccharide Monooxygenase. *Angew. Chem. Int. Ed.* **56**:767-770
a. Supervised graduate student first author paper
b. Front cover
37. Bodenheimer A. M., **Meilleur F.** (2016) Crystal structures of wild-type Trichoderma reesei Cel7A catalytic domain in open and closed states. *FEBS Letters* **590**:4429-4438
a. Supervised graduate student first author paper
36. O'Dell W.B., Bodenheimer A.M., **Meilleur F.** (2016) Neutron protein crystallography: insight into enzyme chemistry. *Arch Biochem. Biophys.* **602**:48-60
a. Supervised graduate students first and second author paper
35. Zhaoa JK, Pierce J., Myles D.A., Robertson J.L., Herwig K.W., Standaert R., Cuneo M., Li L., **Meilleur F.** (2016) Dynamically polarized samples for neutron protein crystallography at the Spallation Neutron Source. DOI: 10.1088/1742-6596/746/1/012008
34. Knihtila R., Holzapfel G., Weiss K.L., **Meilleur F.**, Mattos C. (2015) Neutron Crystal Structure of RAS GTPase puts in question the Protonation State of the GTP γ-Phosphate. *J. Biol. Chem.* **290**:31025-31036
33. Zhuravleva M., Lindsey A., Chakoumakos B.C., Custelcean R., **Meilleur F.**, Hughes R.W., Kriven W.M., Melcher C.L. (2015) Crystal structure and thermal expansion of a $CsCe_2Cl_7$ scintillator. J. Solid State Chem. **227**:142-149
32. Golden E., Attwood P.V., Duff A.P., **Meilleur F.**, Vrielink A. (2015) Production and characterization of recombinant perdeuterated cholesterol oxidase. Anal Biochem. ***485***:102-106
31. Bodenheimer A.M., Cuneo M., Schwarz P., O'Neill H., Myles D.A., Evans, B., **Meilleur F.** (2014) Crystallization and preliminary X-ray diffraction analysis of *Hypocrea jecorina* cel7a in two new crystal forms. *Acta Cryst.* F**70**:773-336
a. Supervised graduate student first author paper
30. Munshi P., Snell E.H, Van der Woerd M.J., Judge R.A., Myles D.A., Ren Z., **Meilleur F.** (2014) Hydrogen bonding interaction at the active site of cyclic glucose bound xylose isomerase E186Q mutant. *Acta Cryst.* D**70**:414-420
a. Supervised post-doctoral fellow first author paper
29. Gruene T., Hahn H.W., **Meilleur F.**, Sheldrick G.M. (2014) Refinement of macromolecular structures against neutron data with SHELXL-2013. *J. Appl. Cryst*. **47**:462-466

28. **Meilleur F.**, Munshi P., Kovalevsky A., Koritsanszky T., Blessing R., Robertson L., Stoica A.D., Crow L., Myles D.A. (2013) IMAGINE: First Neutron Protein Structure and New capabilities for neutron macromolecular crystallography. *Acta Cryst.* D**69:**2157-2160

27. Ankner J., Heller W.T., Herwig K., **Meilleur F.**, Myles D.A. (2013) Neutron scattering techniques and application in structural biology. *Current Protoc. Prot. Sci.* Chapter 17:Unit17.16

26. Martin S.L., He L., **Meilleur F.**, Guenther R.H., Sit T.L., Lommel S.A., Heller W.T. (2013) New insight into the structure of RNA in red clover necrotic mosaic virus and the role of divalent cations revealed by small-angle neutron scattering. *Arch Virol.* **158**:1661-1669

15. Jayasundar J.J., Ju J.H., He L., Liu D., **Meilleur F.**, Zhao J., Callaway D.J., Bu Z. (2012) Open conformation of Erzin bound to PIP2 and to F-actin revealed by neutron scattering. *J. Biol. Chem.* **44**:37119-37133

24. Myles D.A., Dauvergne F., Blakeley M.P., **Meilleur F.** (2012) Neutron protein crystallography at ultra- low (<15K) temperatures. *J. Appl. Cryst.* **45**:686-692

23. He L., Piper A., **Meilleur F.**, Hernandez R., Heller W.T., Brown D.T. (2012) Conformational changes in Sindbis virus induced by decreased pH revealed by small-angle neutron scattering. *J. Virology*. **86**:1982-1987

a. Supervised post-doctoral fellow first author paper

22. Munshi P., Chung S.-L., Weiss K.L., Blakeley M.P., Myles D.A., **Meilleur F.** (2012) Rapid visualization of hydrogen positions in neutron crystallography structures. *Acta Cryst.* D**68**:35-41

a. Supervised post-doctoral fellow first author paper

b. Article highlighted in the International Union of Crystallography (IUCr) Newsletter (Volume 20, Number 1)

21. Borreguero J.M., He J., **Meilleur F.**, Weiss K.L., Brown C.M., Myles D.A., Herwig K.W., Agarwal P.K. (2011) Redox-Promoting Protein Motions in Rubredoxin. *J. Phys. Chem.* B. **115**:8925-8936

20. Li X., Shew C.-Y., He L., **Meilleur F.**, Myles D.A., Liu E., Zhang Y., Smith G., Herwig K., Pynn R., Chen W.-R. (2011) Scattering functions of Platonic solids *J. Appl. Cryst*. **44**: 545-557

19. Martin S.L., Guenther R.H., Sit T.L., Swartz P.D., Meilleur F., Lommel S.A., Rose R.B. Crystallization and preliminary X-ray diffraction analysis of red clover necrotic mosaic virus. *Acta Cryst.* F**66**:1458-1462

18. Gardberg A.S., Del Castillo A.R., Weiss K., **Meilleur F.**, Blakeley M.P., Myles D.A. (2010) Unambiguous determination of hydrogen atom positions: comparing results from neutron and high-resolution X-ray crystallography. *Acta Cryst*. D**66**:558-567

17. He L., Piper A., **Meilleur F.**, Myles D.A., Hernandez R., Brown D.T., Heller W.T. (2010) The structure of Sindbis virus produced from vertebrate and invertebrate hosts determined by small-angle neutron scattering. *J. Virol.* **84**:5270-5276

a. Supervised post-doctoral fellow first author paper

16. Wilkinson C., Lehmann M.S., **Meilleur F.**, Blakeley M.P., Myles D.A., Vogelmeier S., Thoms M., Walsh M., McIntyre G.J. (2009) Characterization of image plates for neutron diffraction *J. Appl. Cryst.* **42**:1-9

15. Weiss K.L., **Meilleur F.**, Blakeley M.P., Myles D.A. (2008) Preliminary neutron crystallographic analysis of selectively CH3-protonated, deuterated rubredoxin from Pyrococcus furiosus. *Acta Cryst.* F**64**:537-540.
14. Teixeira S. C. et al. (2008) New sources and instrumentation from neutron in biology. *Chem. Phys.* **345:**133-151
13. Blakeley M.P., Ruiz F., Cachau R., Hazemann I., **Meilleur F.**, Mitschler A., Ginell S., Afonine P., Ventura O. N., Cousido-Siah A, Haertlein M., Joachimiak A., Myles D. A., Podjarny A. (2008) Quantum model of catalysis based on a mobile proton revealed by subatomic x-ray and neutron diffraction studies of h-aldose reductase. *Proc. Natl. Acad. Sci.* **105**:1844-1846
12. Di Constanzo L., Moulin M., Haertlein M., **Meilleur F.**, Christianson D.W. (2007) Expression, purification, assay, and crystal structure of perdeuterated human arginase I. *Arch. Biochem. Biophys.* **465**:82-89
11. Snell E.H., van der Woerd M.J, Damon M., Judge R.A., Myles D.A., **Meilleur F.** (2006) Optimizing crystal volume for neutron diffraction: D-Xylose Isomerase. *Eur. Biophys. J.* **35:**621-632 --
10. **Meilleur F.**, Myles D.A., Blakeley M.P. (2006) Neutron Laue macromolecular crystallography. *Eur. Biophys. J.* **35**:611-620
9. **Meilleur F.**, Snell E.H., van der Woerd M.J., Judge R.A., Myles D.A. (2006) A Quasi-Laue Neutron Crystallographic Study of D-Xylose Isomerase. *Eur. Biophys. J.* **35:**601-609
8. Blakeley M.P., Mitschler A., Hazemann I., **Meilleur F.**, Myles D.A., Podjarny A. (2006) Comparison of hydrogen determination with X-ray and neutron crystallography in a human aldose reductase-inhibitor complex. *Eur. Biophys. J.* **35:**577-583
7. Budayova-Spano M., Bonnete F., Ferte N., El Hajji M., **Meilleur F.**, Blakeley M.P., Castro B. (2006) A preliminary neutron diffraction study of rasburicase, a recombinant urate oxidase enzyme, complexed with 8-azaxanthin. *Acta Cryst.* F**62**:306-309
6. Buffet J.C., Clergeau J.F., Cooper R.G., Darpentigny J., De Laulany A., Fermon C., Fetal S., Fraga F., Guérard B., Kampmann R., Kastenmueller A., Mc Intyre G.J., Manzin G., **Meilleur F.**, Millier F., Rhodes N., Rosta L., Schooneveld E., Smith G.C., Takahashi H., Van Esch P., Van Vuure T.L. and Zeitelhack K. (2005) Advances in detectors for single crystal neutron diffraction. *Nuclear Instruments and Methods in Physics Research* A**554**:392-405
5. Hazemann I., Dauvergne M.T., Blakeley M.P., **Meilleur F.**, Haertlein M., Van Dorsselaer A., Mitschler A., Myles D.A.A & Podjarny A.D. (2005) High-resolution neutron protein crystallography with radically small crystal volumes; application of perdeuteration to human Aldose Reductase. *Acta Cryst*. D**61**:1413-1417
4. Bennett B.C., **Meilleur F.**, Myles D.A., Howell E.E., Dealwis C.G. (2005) Preliminary neutron diffraction studies of Escherichia coli dihydrofolate reductase bound to the anticancer drug methotrexate. *Acta Cryst.* D**61**:574-579
3. **Meilleur F.**, Dauvergne M.T., Schlichting I., Myles D.A.A. (2005) X-Ray crystallographic analysis of fully deuterated cytochrome P450cam. *Acta Cryst.* D**61:**539-544

2. **Meilleur F.**, Contzen J., Myles D.A.A., Jung C. (2004) Structural stability and dynamics of hydrogenated and perdeuterated cytochrome P450cam (CYP101). *Biochemistry* **43**:8744-8753
1. Adamo C., Heitzman M., **Meilleur F.**, Grand A., Cadet J. & Barone V. (2001) Interplay of intrinsic and environmental effects on the magnetic properties of free radicals issuing from H-atom addition to cytosine. *J. Am. Chem. Soc.* **123**:7113-7117

Book chapters
5. Pierce J., Cuneo M.J., Jennings A., Li L., **Meilleur F.**, Zhao J.K., Myles D.A.A. (2020) Dynamic nuclear polarization enhanced neutron crystallography: Amplifying hydrogen in biological crystals. *Methods In Enzymology. https://doi.org/10.1016/bs.mie.2019.11.018*
4. **Meilleur F.**, Kovalevsky A.Y., Myles D.A. (2020) IMAGINE: The Neutron Protein Crystallography Beamline at the High Flux Isotope Reactor. *Methods In Enzymology*. *https://doi.org/10.1016/bs.mie.2019.11.016*
3. **Meilleur F.**, Weiss K.L., Myles D.A. (2009) Deuterium Labeling for Neutron Structure-Function-Dynamics Analysis. *Methods in Mol. Bio.* **544**:281-292
2. **Meilleur F**., Blakeley M.P & Myles D.A.A. (2005). Hydrogen and hydration-sensitive structural biology. Editors Niimura N., Mizuno H., Helliwell J.R., Westhof E., pages 75-85. Neutron Laue analysis of hydrogen and hydration in protein structure.
1. Blakeley M.P., Hazemann I., Mitschler A., **Meilleur F.**, Dauvergne M.T., El Kabbani O., Cousido A., Joachimiak A., Petrova T., Myles D.A.A., Podjarny A. (2005) Hydrogen and hydration-sensitive structural biology. Editors Niimura N., Mizuno H., Helliwell J.R., Westhof E, pages 87-102. Combined high resolution X-ray and neutron crystallography to observe protonation states in human aldose reductase

Non-peer reviewed article
1. **Meilleur F.** (2020) Beginner's guide to neutron macromolecular crystallography. *The Biochemist*. https://doi.org/10.1042/BIO20200078 (invited contribution)

Educational workshop reports
7. **Meilleur F.** (2020) ORNL hosts first virtual HANDS workshop. *Neutron News*. *Neutron News* **31**(2-4)
6. **Meilleur F.** (2020) HANDS 2019 - A decade of neutron scattering education in structural biology at Oak Ridge National Laboratory. *Neutron News* **31**(2-4)
5. **Meilleur F.** (2014) The Neutrons in Structural Biology Workshop celebrates its 5th Edition. *Neutron News* **25**(4):11
4. **Meilleur F.** (2014) ORNL welcomed IMAGINE first external users and the participants of the fourth workshop on Neutron Scattering Applications in Structural Biology. *Neutron News* **25**:12
3. **Meilleur F.** (2013) Third school on the applications of Neutron Scattering Applications in Structural Biology, Oak Ridge, TN. *Neutron News* **24**:4

2. **Meilleur F.** (2011) ORNL hosted second graduate course on neutron scattering applications in structural biology. *Neutron News* **22**:4-5
1. **Meilleur F.** (2010) First graduate course on neutron scattering applications in structural biology at Oak Ridge. *Neutron News* **21:**30-31

Letter Of Intent
1. IMAGINE: a single crystal neutron diffractometer at the High Flux Isotope Reactor (2007)

Press release
12. Chasing Better Biofuels: Biochemistry's Flora Meilleur (2019) *https://cals.ncsu.edu/molecular-and-structural-biochemistry/news/chasing-better-biofuels-biochemistrys-flora-meilleur/*
11. Doctoral student creating "scrubber" textiles discovers neutron analysis techniques at ORNL (2019) *https://neutrons.ornl.gov/content/doctoral-student-creating-%E2%80%9Cscrubber%E2%80%9D-textiles-discovers-neutron-analysis-techniques-ornl*
10. Spinach Used in Neutron Studies Could Unearth Secret to Stronger Plant Growth (2018) *https://neutrons.ornl.gov/content/spinach-used-neutron-studies-could-unearth-secret-stronger-plant-growth*
9. 'On your mark, get set' Neutrons run enzyme's reactivity for better biofuel production (2017) *https://www.ornl.gov/news/your-mark-get-set*
8. Imagine finalizes cryogenic sample environment (2016) *https://neutrons.ornl.gov/content/imagine-finalizes-cryogenic-sample-environment*
7. ORNL hosts Seventh Annual Neutron Scattering School on Structural Biology (2016) *https://neutrons.ornl.gov/content/ornl-hosts-seventh-annual-neutron-scattering-school-structural-biology*
6. High school teacher mentoring: Summer Science *https://www.ornl.gov/news/summer-science* (2016)
5. Joint NCSU-ORNL faculty position: Best of Both Worlds (2015) *https://www.ornl.gov/news/best-both-worlds*
4. IMAGINE beam line at HFIR welcomes first external user (2013) *https://www.ornl.gov/news/imagine-beam-line-hfir-welcomes-first-external-user*
3. Neutrons Go Viral (2011) *https://www.ornl.gov/news/neutrons-go-viral-ornl*
2. New graduate course utilizes neutron scattering techniques to study structural biology (2010) *http://www.orau.org/university-partnerships/*
1. Successful Neutron-Scattering Proposal (2009) *http://news-from-mtsu.blogspot.com/2009/09/075-mtsu-chemistry-researcher.html*

Graduate student spotlight

3.https://cals.ncsu.edu/molecular-and-structural-biochemistry/news/like-taking-apart-a-tiny-machine-biochemistrys-gabriela-schroder/
2. https://cals.ncsu.edu/news/student-spotlight-i-enjoy-the-challenge-of-solving-problems/
1. https://cals.ncsu.edu/news/outstanding-december-graduate-william-brad-odell/

Web pages
9. *https://conference.sns.gov/event/291/* (HANDS2021 - virtual)
8. *https://conference.sns.gov/event/217/* (HANDS2020 - virtual)
7. *https://conference.sns.gov/event/125/* (HANDS2019)
6. *http://biochem.ncsu.edu/faculty/meilleur/*
5. *http://neutrons.ornl.gov/imagine/*
4. *https://neutrons.ornl.gov/mandi*
3. *https://conference.sns.gov/event/99/* ((9th Workshop on Neutron Scattering Applications in Structural Biology; 2018)
2. *https://conference.sns.gov/event/66/* (8th Workshop on Neutron Scattering Applications in Structural Biology; 2017)
1. *https://conference.sns.gov/event/15/* (7th Workshop on Neutron Scattering Applications in Structural Biology; 2016)

Oral presentations
(* Invited presentations at conferences; >20)
(** Invited presentations at university seminar series or colloquiums)
(^International presentations)

54. **2021 University of California San Francisco (Virtual)
Neutron Protein Crystallography: Practical Considerations
53. *^2021 CCP4 study week-end (virtual)
Neutron diffraction and scattering to study metalloenzyme chemistry and redox complexes
52. *^2020 X National Congress of The Mexican Society of Crystallography (virtual)
The mechanism of lytic polysaccharide monooxygenases: what can we learn from neutron diffraction?
51. 2020 American Conference on Neutron Scattering (Virtual)
Characterization of biomass-degrading enzymes using neutron diffraction and scattering
50. *2020 22th National School on Neutron X-ray Scattering, Oak Ridge, TN
Science and Capabilities on IMAGINE at the HFIR
49. *^2019 Chemical Society for Canada meeting, Quebec, Canada
Cellulose-degrading oxidative enzymes: structural insights from neutron diffraction and scattering
48. **2019 Louisiana State University, Baton Rouge, LA
Cellulose-degrading oxidative enzymes: structural insights from neutron diffraction and scattering

47. **2019 CCNY, New York, NY
Cellulose-degrading oxidative enzymes: structural insights from neutron diffraction and scattering
46. *^2018 31th European Crystallographic Meeting, Oviedo, Spain
Neutron macromolecular crystallography to elucidate the mechanisms of industrial and biomedical enzymes
45. *2018 20th National School on Neutron X-ray Scattering, Oak Ridge, TN
Science and Capabilities on IMAGINE at the HFIR
44. ^*2018 "Quantum Beam Science in Biology and Soft Material Sciences" international conference, Mito, Japan
Neutron diffraction and scattering of metallo-enzymes involved in the oxidative deconstruction of cellulose
43. **2018 University of Missouri, Columbia, MO
Oxidative enzymatic deconstruction of cellulose: structural insights from neutron diffraction and scattering
42. **2017 Massachusetts Institute of Technology, Cambridge, MA
Structural and functional studies of cellulolytic enzymes using neutron protein crystallography (NPC) and small angle neutron scattering (SANS)
41. *2017 8th Workshop on Applications of Neutron Scattering in Struct. Biology, Oak Ridge, TN
Radiation damage free structural studies of cellulolytic redox enzymes using neutron scattering and diffraction
40. ^**2017 Uppsala Biomedical Center, Uppsala, Sweden
Structural enzymology using neutron crystallography and small angle scattering
39. ^*2017 Swedish Neutron Scattering Society Annual Meeting Uppsala, Sweden
Structural studies of cellulolytic enzymes using neutron scattering and diffraction
38. ^*2016 1st Symposium on Lytic Polysaccharide Monooxygenases, Copenhagen, Denmark
Structural studies of cellulolytic redox enzymes using neutron scattering and diffraction
37. *2016 12th International Conference on Synchrotron Radiation, Palo Alto, CA
Radiation damage free structural studies of cellulolytic redox enzymes using neutron scattering and diffraction
36. *2016 Southeastern Regional Meeting of the American Chemistry Society
Structural studies of cellulolytic redox enzymes using neutron scattering and diffraction
35. *2016 12th International Conference on Synchrotron Radiation
Radiation damage free structural investigation of cellulose oxidative enzymes
34. 2016 5th International Symposium on Diffraction in Structural Biology
IMAGINE: new capability and sciences opportunities at the HFIR
33. ^*2016 16th International Conference on Crystallization of Macromolecules, Prague, Czech Republic
Crystallization of a fungal polysaccharide monooxygenase for neutron crystallography
32. *2015 NCSU Stewards of the Future – Water for a Growing World, Raleigh, NC

Protein Crystallography for Sustainability
31. 2015 American Crystallographic Association meeting, Philadelphia, PA
Locating Hydrogen Atoms in Enzymes Using Neutron Protein Crystallography
29/30. ^*2014 RACIRI Summer School, 2014 "Imaging with X-rays and Neutrons in Life and Material Sciences"(August 24-31, Stockholm area, Sweden)
Lecture 1: Neutron Macromolecular Diffraction
Lecture 2: Structural biology with neutrons
28. *2014 Gordon Research Conference on Diffraction methods
IMAGINE: new -capability for neutron diffraction in the U.S.
27. 2014 American Conference on Neutron Scattering, Knoxville, TN
IMAGINE, A Quasi-Laue Single Crystal Neutron Diffractometer at the HFIR
26. 2014 American Crystallographic Association meeting, Albuquerque, NM
Recent results from the new neutron diffractometer IMAGINE
25. 2013 Oak Ridge National Laboratory, Oak Ridge, TN
The IMAGINE instrument at HFIR
24. **2013 NorthEastern University, Boston, MA
Neutron Protein crystallography: application to Xylose Isomerase
23. *2013 Pittsburgh Diffraction Society Meeting, Buffalo, NY
Locating Hydrogen Atoms in Enzymes Using Neutron Protein Crystallography
22. **2013 Molecular and Structural Biochemistry Department, Raleigh, NC
Protonation in protein structure and function
21. 2013 Mid-Atlantic Macromolecular Crystallography Conference, Durham, NC
Locating hydrogen atoms in enzymes using neutron protein crystallography
20. 2012 American Crystallographic Association Meeting, Boston, MA
Locating hydrogen atoms in Xylose Isomerase using neutron protein crystallography
19. **2012 University of Tennessee Science Forum, Knoxville, TN
Neutrons for Biology and Bioenergy
18. 2010 Neutron Scattering Sciences Division, ORNL, Oak Ridge, TN
Rapid visualization of deuterium atoms in Rubredoxin
17. 2009 North Carolina State University, Molecular and Structural Biochemistry Dpt, Raleigh, NC,
Structural Biology with Neutrons
16. ^*2008 International Union of Crystallography meeting, Osaka, Japan
Neutron crystallographic analysis of deuterated and selectively CH3-protonated deuterated rubredoxin
15. 2008 American Conference on Neutron Scattering, Santa Fe, NM, USA
IMAGINE: Supra- and Macro-molecule Quasi-Laue Neutron Diffractometer at HFIR
14. ^2007 Neutrons in Biology, Didcot, United Kingdom
Rubredoxin: H-D labeling for neutron direct methods
13. 2007 American Crystallographic Association meeting, Salt Lake City, UT, USA

The Enzymatic Mechanism of D-Xylose Isomerase Revealed by Neutron Protein Crystallography
12. ^*2007 International Workshop on Laue Diffraction in Frontier Science, Grenoble, France
Neutron Macromolecular Crystallography: Current Capabilities, Future Horizons
11. ^*2006 CNRS school "Water in biological environment", Roscoff, France
Visualisation des molécules d'eau dans une structure cristallographique aux neutrons
10. *2006 Hauptman-Woodward Institute, Buffalo, NY, USA
Neutron Macromolecular Crystallography: Application to D-xylose isomerase
9. 2006 Tennessee Structural Biology Meeting, Knoxville, TN, USA
Neutron Macromolecular Crystallography: Current Capabilities, Future Horizons
8. 2006 American Crystallographic Association meeting, Honolulu, HI, USA
Neutron cryo-crystallography
7. 2006 Spallation Neutron Source, Oak Ridge, TN, USA
Neutron macromolecular crystallography: New Horizons
6. ^2006 International Meeting for Construction and Utilization of iBIX, Hitachi, Japan
Neutron quasi-Laue crystallography at a steady state reactor
5. ^2005 International Conference on Neutron Scattering, Sydney, Australia
Neutron macromolecular crystallography with LADI
4. *2005 Neutrons in Biology, Grenoble, France
Neutron protein crystallography with LADI
3. ^*2004 European Molecular Biology Laboratory, Hamburg, Germany
Neutron macromolecular crystallography
2. **2004 Institut de Biologie Structurale, Grenoble, France
Neutron Crystallographic studies of D-xylose isomerase and cytochrome P450cam
1. *2003 Partnership for Structural Biology (PSB) Science day, Sassenage, France
Neutron macromolecular crystallography: visualizing protons in proteins

Poster presentations
2020 GRC Metal in Biology (Flora Meilleur: presenter)
Structural Insights into the Mechanism Of Lytic Polysaccharide Monooxygenases
2019 International Conference on Cytochrome P450 (Gabriela Schroder: presenter; Flora Meilleur: PI)
Investigating the catalytic cycle and redox partner protein dependent dynamics of cytochrome P450 (CYP450) by neutron scattering
2019 Pittsburgh Diffraction Conference (Gabriela Schroder: presenter; Flora Meilleur: PI)
Toward Elucidating the Mechanism of Lytic Polysaccharide Monooxygenases: Chemical Insights from X-ray and Neutron Crystallography
2019 SNS/HFIR User Meeting (Gabriela Schroder: presenter; Flora Meileulr: PI)
Toward Elucidating the Mechanism of Lytic Polysaccharide Monooxygenases: Chemical Insights from X-ray and Neutron Crystallography
2017 SNS HFIR User meeting (Flora Meilleur: presenter)

IMAGINE: Image Plate Diffractometer at the HFIR
2016 5th Symposium on Diffraction in Structural Biology (Annette Bodenheimer: presenter; Flora Meilleur: PI)
The close state of Cel7a
2016 American Conference on Neutron Scattering (William B. O'Dell: presenter; Flora Meilleur: PI)
Pichia pastoris as a source of biomolecules for neutron scattering
2015 Second target Station Workshop, Oak Ridge, TN (Flora Meilleur, presenter)
IMAGINE: New Science Capabilities at HFIR
2015 SNS HFIR User Meeting, Oak Ridge, TN (Annette Bodenheimer, presenter; Flora Meilleur: PI)
Structural Biology of Cellulotic Enzymes
2015 American Crystallographic Association Meeting, Philadelphia, PA (Annette Bodenheimer: presenter; For a Meilleur: PI)
Effect of Cations and pH on N. Crassa CDHIIA Dimensions Investigated by Small Angle Scattering
2015 Mid-Atlantic Crystallography Meeting, Baltimore, MD (William B. O'Dell, presenter; Flora Meilleur: PI)
Structural Biology of Cellulotic Enzymes
2014 Mid-Atlantic Crystallography Meeting/SER-CAT Symposium, Rockville, MD (Annette Bodenheimer, presenter; Flora Meilleur: PI)
Crystallization and preliminary X-ray analysis of Cel7a
2012 American Crystallographic Association Meeting, Boston, MA (Parthapratim Munshi, presenter; Flora Meilleur: PI)
Neutron Crystallographic Studies of Ligand-Free, Substrate-Bound and Inhibitor-Bound D-Xylose Isomerase GLU186GLN Mutant
2012 American Crystallographic Association Meeting, Boston, MA (Annette Bodenheimer, presenter; Flora Meilleur: PI)
Structural analysis of Cel7a
2011 American Crystallographic Association meeting, New Orleans, USA (Parthapratim Munshi, presenter; Flora Meilleur: PI)
IMAGINE, a quasi-Laue neutron diffractometer for protein crystallography at the HFIR
2010 SER-CAT symposium, Knoxville, TN, USA (Flora Meilleur, presenter and PI)
IMAGINE, a quasi-Laue neutron diffractometer for protein crystallography at the HFIR
2010 SER-CAT symposium, Knoxville, TN, USA *(Tabitha Donald, presenter; Flora Meilleur: PI)*
Optimizing Growth of Beta Lactoglobulin Crystal for Neutron Crystallography
2010 American Crystallographic Association meeting, Chicago, USA (Flora Meilleur, presenter & PI)
IMAGINE, a quasi-Laue single crystal neutron diffractometer at the HFIR

2010 American Crystallographic Association meeting, Chicago, USA (William Heller, presenter; Flora Meilleur: PI)
Small-angle neutron scattering study of Sindbis virus produced from vertebrate and invertebrate hosts
2009 International Conference on Neutron Scattering, Knoxville, TN, USA (Flora Meilleur: presenter and PI)
IMAGINE, a supra- and macromolecular quasi-Laue neutron Diffractometer for materials research and discovery at HFIR
2009 International Conference on Neutron Scattering, Knoxville, TN, USA (Lilin He, presenter; Flora Meilleur: PI)
Solution Structure of Sindbis Virus: A Small Angle Neutron Scattering (SANS) Study
2009 International Conference on Neutron Scattering, Knoxville, TN, USA (Yiming Mo, presenter; Flora Meilleur: PI)
SANS Investigations on E1 protein from Sindbis virus
2008 American Crystallographic Association meeting, Knoxville, TN, USA (Flora Meilleur, presenter & PI)
IMAGINE, a quasi-Laue single crystal neutron diffractometer at the HFIR
2008 American Crystallographic Association meeting, Knoxville, TN, USA (Flora Meilleur, presenter & PI)
The enzymatic mechanism of xylose isomerase revealed by neutron protein crystallography
2006 American Crystallographic Association meeting, Honolulu, HI, USA (Flora Meilleur, presenter & PI)
Neutron Macromolecular Crystallography: Future Horizons
2005 Conference on New Frontiers in Neutron Macromolecular Crystallography, Oak Ridge, TN, USA (Flora Meilleur, presenter & PI)
Neutron Crystallography with LADI
2005 International Biophysics Meeting, Montpellier, France (Flora Meilleur, presenter & PI)
Neutron Crystallography of perdeuterated protein on LADI
2005 American Crystallographic Association meeting, Orlando, TN, USA (Flora Meilleur, presenter & PI)
The enzymatic mechanism of xylose isomerase revealed by neutron protein crystallography
2005 High resolution crystallography and drug design meeting, Strasbourg, France (Flora Meilleur, presenter & PI)
Neutron crystallographic studies of Cyctochrome P450cam
2004 European Crystallographic Meeting, Budapest, Hungary (Flora Meilleur, presenter & PI)
Neutron macromolecular crystallography with LADI
2003 International Conference on Cytochrome P450, Prague, Czech Republic (Flora Meilleur, presenter; Dean Myles: PI)
Neutron crystallographic studies of P450cam

2002 European Spallation Source Conference, Bonn, Germany (Flora Meilleur, presenter; Dean Myles: PI)
Neutron crystallographic studies of P450cam
2001 European Crystallographic Meeting, Krakow, Poland (Flora Meilleur, presenter; Dean Myles: PI)
Neutron crystallographic studies of P450cam
2001 Protons in Protein, Grenoble, France (Flora Meilleur, presenter; Dean Myles: PI)
Neutron crystallographic studies of P450cam
2000 HERCULES, Grenoble, France (Flora Meilleur, presenter; Dean Myles: PI)
Neutron crystallographic studies of P450cam