

## Flora Meilleur

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

### Education:

<i>Institution</i>	<i>Major</i>	<i>Degree</i>	<i>Year</i>
University J. Fourier, Grenoble, France	Physic & Chemistry	BSc (Licence)	1999
University J. Fourier, Grenoble, France	Structural Biology	MSc (Maîtrise, DEA)	2000
European Molecular Biology Laboratory & University J. Fourier, Grenoble, France	Structural Biology	Ph. D.	2004
University J. Fourier, Grenoble, France	Structural Biology	Ph. D.	2004

*MSc Thesis Title (Maîtrise):* Quantum chemistry analysis of H-atom addition to cytosine;  
*Advisor:* André Grand (Commissariat à l'Énergie Atomique)

*MSc Thesis Title (DEA):* Neutron crystallographic and quantum chemistry studies of myoglobin;  
*Advisors:* Dean Myles (EMBL), André Grand (Commissariat à l'Énergie 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)

### Professional experience:

2015-present	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

### Membership in professional organizations:

2009-present	Neutron Scattering Society of America (NSSA)
2007-present	SNS-HFIR User Group (SHUG)
2006-present	American Crystallography Association

### Scholarly and professional honors:

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

## Professional service

2019-2022	Secretary, Neutron Scattering Society of America
2017-present	Reviewer, Albert Einstein Fellowship
2017-present	Reviewer, Science, Scientific Reports, Emerging Topics in Life Sciences
2016	Session chair, 24 <sup>th</sup> Congress – International Union of Crystallography
2016	Member, selection committee for the NSSA Science Prize
2016	Member, selection committee for the NSSA Sustained Research Prize
2015-present	Co-Editor, Journal Of Applied Crystallography
2015-present	Reviewer, FEBS Journal, Physical Chemistry Chemical Physics
2015	Member, ORNL- Duke University Neutron Workshop Organizing Committee
2015	Member, International Symposium on Diffraction Structural Biology Organizing Committee
2015	Member, Second Target Station Workshop Program Advisory Committee
2014-present	Reviewer, Australian Journal of Chemistry
2011-present	Mentor, Appalachian Regional Commission (ARC)/ORNL Math-Science-Technology Summer Institute
2011	Reviewer, Department of Energy, Early Career Award
2010-present	Reviewer, IUCr Acta Crystallographica, section D and F
2009-2012	Executive Committee member-at-large, Neutron Scattering Society of America
2009	NSSA Fellows, selection committee member
2008-2010	Reviewer, American Heart Association
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
2007-2010	Executive Committee member, SNS-HFIR User Group
2007-2009	Member, Neutron Sciences Directorate Education Committee

## Professional service on NCSU campus

2018-present	Chair, METRIC X-ray User Committee
2017-present	Reviewer, CALS undergraduate fellowship
2016	NCSU Biochemistry Head - Search Committee member
2015-present	NCSU Biochemistry Dept. Webpage Administrator
2014	NCSU CALS reviewer, Dean's Enrichment Grants Program
2014	NCSU Biochemistry Dept. Graduate student recruiting committee member
2010	NCSU internal reviewer, NIH: Engineered Nanomaterials: Linking Physical and Chemical Properties to Biology (U19)
2008-present	NCSU graduate student committee member

## Outreach activities

2017	Mentor, ORNL STEM Café
2017	Mentor, Hour of Code, Oak Ridge Elementary School
2017	Volunteer, Knoxville STEAM festival

2011-present Mentor, Appalachian Regional Commission (ARC)/ORNL Math-Science-  
Technology Summer Institute  
2013-present Volunteer, ORNL Science Fairs

## Teaching

<i>Course</i>	<i>Semester</i>	<i>Number of students</i>
BCH 590E (Neutron Structural Biology)	Summer 2017	15
BCH 705 (Molecular Biology of the cell)	Spring 2017	4
BCH 590E (Neutron Structural Biology)	Summer 2016	18
BCH 705 (Molecular Biology of the cell)	Spring 2016	5
BCH 590E (Neutron Structural Biology)	Summer 2015	15
BCH 705 (Molecular Biology of the cell)	Spring 2015	12
BCH 590E (Neutron Structural Biology)	Summer 2014	17
BCH 705 (Molecular Biology of the cell)	Spring 2014	13
BCH 590E (Neutron Structural Biology)	Summer 2013	15
BCH 705 (Molecular Biology of the cell)	Spring 2013	19
Physics 7410/4410 (U. Missouri; IGERT)	Fall 2012	10
BCH 590E (Neutron Structural Biology)	Summer 2012	15
BCH 705 (Molecular Biology of the cell)	Spring 2012	12
BCH 590E (Neutron Structural Biology)	Summer 2011	15
BCH 705 (Molecular Biology of the cell)	Spring 2011	12
BCH 590E (Neutron Structural Biology)	Summer 2010	15

## Mentoring activities

### *Graduate students*

<i>Name</i>	<i>Period</i>	<i>Institution</i>
Gabriela Schroder	2015 - present	NCSU/ORNL
Wm Brad O'Dell	2012 - 2017	NCSU/ORNL
Annette Bodenheimer	2011 - 2016	NCSU/ORNL
Jason Bolsen	Summer 2009 (Rotation)	NCSU/ORNL

### *Graduate students hosted at ORNL:*

Leiah Carey, NCSU-Chemistry; January 2016-October 2016

Stephen Keable, Montana State University; March 2015-May 2015

### *Post-Doctoral Research Associate*

<i>Name</i>	<i>Period</i>	<i>Current institution and position</i>
Partha P. Munshi	Dec 10 – Dec 12	Shiv Nadir University, Assistant professor
Lilin He	May 08 – Mar 10	ORNL, GP-SANS beam line scientist
Yiming Mo	Sep 08 – Dec 09	Assurant Inc, Insurance Operations Data Analyst

### *Undergraduate students*

<i>Name</i>	<i>Period</i>	<i>Institution</i>	<i>Undergrad. Year</i>
Melissa Fee	2015	NCSU	Sophomore
Oksana Samarski	2009-2012	NCSU	Junior
Tabitha Donald	Summer 2010	Lane College	Senior

Sun-Lin Chung	Summer 2010	Yale	Freshman
Jillian Reich	Summer 2009	St Lawrence	Sophomore
Richard Goslen	2008-2009	NCSU	Senior
Lisa Gilligan	Summer 2007	NCSU	Senior
Hung Dang	Summer 2007	NCSU	Sophomore
Jia Kim	Summer 2007	NCSU	Sophomore

#### *High School Students*

Name	Period	High school
Keiara Holley	July 11	Newbern's Sunshine, AL
Chelsea King	July 11	Burkesville, KY
Kimberly Wilson	July 11	Loyall High School, KY

#### *Research Assistant*

Name	Period	Current institution and position
Lezlee Dice	Aug 07 – Jun 09	UTK, Research assistant

### **Graduate committee memberships**

#### *Current graduate committee*

1. Gabriela Schroder (NCSU; role: chair)
2. Robert Grinshpon (NCSU; role: graduate committee departmental member)
3. Sophia Juang (NCSU; role: graduate committee departmental member)
4. Walter Sandoval Espinola (NCSU; role: Graduate School Representative)
5. Paul Enriquez (NCSU; role: graduate committee departmental member)
6. Eric Waddell (NCSU; role: graduate committee departmental member)
7. Maddison Davidson (NCSU; role: graduate committee external member and Graduate School Representative)

#### *Past graduate (Ph. D.) committee*

1. Wm Brad O'Dell (NCSU/ORNL; role: chair)
2. Melvin Thomas (NCSU; role: graduate committee departmental member)
3. Annette Bodenheimer (NCSU; role: chair)
4. Sue Fetics (NCSU; role: graduate committee departmental member)
5. Craig Helstowski (UTK; role: graduate committee external member)

#### *Other Ph. D. Dissertation Committee*

2016 - Ryan Knithila, Northeastern University (role: external committee member)

## Publications

### Peer-reviewed articles

#### Published

1. Meilleur F., Coates L., Cuneo M. J., Myles D.A.A. (2018) The Neutron Macromolecular Crystallography Instruments at Oak Ridge National Laboratory: Advances, Challenges and Opportunities. *Crystals*. In press.
2. 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
3. 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
4. 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
5. G. C. Schroder, W. B. O'Dell, D. A. A. Myles, A. Kovalevsky, F. Meilleur. (2018) IMAGINE: neutrons reveal enzyme chemistry. In press, *Acta Cryst. Section D*
  - a. Supervised graduate students co-first author paper
6. A. M. Bodenheimer, W. B. O'Dell, C. B. Stanley, R. C. Oliver, S. Qian, F. Meilleur. (2018) Structural investigation of Cellobiose Dehydrogenase IIA: Insights from Small Angle Scattering into Intra- and Intermolecular Electron Transfer Mechanisms. *Biochem Biophys Acta*. **1862**:1031-1039
  - b. Supervised graduate students first and second author paper
7. 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
8. Hiromoto T., Meilleur F., Shimizu R., Shibasaki 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
9. 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
  - c. Supervised graduate students co-first author paper
10. 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.* **F73**:70-78
  - d. Supervised graduate student first author paper
11. Golden E., Duff A.P., Karton A., Blakeley M.P., Meilleur F., Vrieling 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
12. 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
  - e. Supervised graduate student first author paper
  - f. Front cover
13. 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

- g. Supervised graduate student first author paper
14. O'Dell W.B., Bodenheimer A.M., Meilleur F. (2016) Neutron protein crystallography: insight into enzyme chemistry. *Arch Biochem. Biophys.* **602**:48-60
- h. Supervised graduate students first and second author paper
15. Zhao J.K., 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
16. Knihtila R., Holzappel G., Weiss K.L., Meilleur F., Mattos C. (2015) Neutron Crystal Structure of RAS GTPase puts in question the Protonation State of the GTP  $\gamma$ -Phosphate. *J. Biol. Chem.* **290**:31025-31036
17. 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<sub>2</sub>Cl<sub>7</sub> scintillator. *J. Solid State Chem.* **227**:142-149
18. 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
19. 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. F70*: 773-336
- i. Supervised graduate student first author paper
20. 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. D70*:414-420
- j. Supervised post-doctoral fellow first author paper
21. 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
22. 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. D69*:2157-2160
23. 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
24. 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
25. Jayasundar J.J., Ju J.H., He L., Liu D., Meilleur F., Zhao J., Callaway D.J., Bu Z. (2012) Open conformation of Erzinc bound to PIP2 and to F-actin revealed by neutron scattering. *J. Biol. Chem.* **44**:37119-37133
26. 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
27. 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
- k. Supervised post-doctoral fellow first author paper
28. 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. D68*:35-41
- l. Supervised post-doctoral fellow first author paper
- m. Article highlighted in the International Union of Crystallography (IUCr) Newsletter (Volume 20, Number 1)
29. Borreguero J.M., He J., Meilleur F, Weiss K.L., Brown C.M., Myles D.A., Herwig K.W., Argarwal P.K. (2011) Redox-Promoting Protein Motions in Rubredoxin. *J. Phys. Chem. B.* 115(28):8925-8936

30. 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
31. 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.* **F66**:1458-1462
32. 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.* **D66**:558-567
33. 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  
n. Supervised post-doctoral fellow first author paper
34. 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
35. Weiss K.L., Meilleur F., Blakeley M.P., Myles D.A. (2008) Preliminary neutron crystallographic analysis of selectively CH<sub>3</sub>-protonated, deuterated rubredoxin from *Pyrococcus furiosus*. *Acta Cryst.* **F64**:537-540.
36. Teixeira S. C. et al. (2008) New sources and instrumentation from neutron in biology. *Chem. Phys.* **345**:133-151
37. 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
38. 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
39. 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
40. Meilleur F., Myles D.A., Blakeley M.P. (2006) Neutron Laue macromolecular crystallography. *Eur. Biophys. J.* **35**:611-620
41. 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
42. 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
43. 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.* **F62**:306-309
44. 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
45. 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.* **D61**:1413-1417
46. 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

47. 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
48. 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
49. 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*

1. 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.
3. 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

#### *Meeting reports*

1. Meilleur F. (2014) The Neutrons in Structural Biology Workshop celebrates its 5<sup>th</sup> Edition. *Neutron News* **25**(4):11
2. 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
4. Meilleur F. (2011) ORNL hosted second graduate course on neutron scattering applications in structural biology. *Neutron News* **22**:4-5
5. 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*

1. 'On your mark, get set' Neutrons run enzyme's reactivity for better biofuel production (2017)  
<https://www.ornl.gov/news/your-mark-get-set>
2. Imagine finalizes cryogenic sample environment (2016)  
<https://neutrons.ornl.gov/content/imagine-finalizes-cryogenic-sample-environment>
3. 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>
4. 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>
6. IMAGINE beam line at HFIR welcomes first external user (2013)  
<https://www.ornl.gov/news/imagine-beam-line-hfir-welcomes-first-external-user>
7. Neutrons Go Viral (2011)  
<https://www.ornl.gov/news/neutrons-go-viral-ornl>
8. New graduate course utilizes neutron scattering techniques to study structural biology (2010)  
<http://www.ornl.gov/university-partnerships/>
9. Successful Neutron-Scattering Proposal (2009)  
<http://news-from-mtsu.blogspot.com/2009/09/075-mtsu-chemistry-researcher.html>

#### *Web pages*

1. <http://biochem.ncsu.edu/faculty/meilleur/>
2. <http://neutrons.ornl.gov/imagine/>
3. <https://conference.sns.gov/event/66/> (8th Workshop on Neutron Scattering Applications in Structural Biology; 2016)
4. <https://conference.sns.gov/event/15/> (7<sup>th</sup> Workshop on Neutron Scattering Applications in Structural Biology; 2016)
5. <https://public.ornl.gov/neutrons/conf/gcnb2015/> (6<sup>th</sup> Workshop on Neutron Scattering Applications in Structural Biology; 2015)

#### **Oral presentations**

(\* Invited presentations at conferences)

(\*\* Invited presentations at university seminar series or colloquiums)

#### *Scheduled*

\*2018 20<sup>th</sup> National School on Neutron X-ray Scattering, Oak Ridge, TN

\*2018 31<sup>th</sup> European Crystallographic Meeting, Oviedo, Spain

#### *Given*

\*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*

\*\*2018 University of Missouri, Columbia, MO

*Oxidative enzymatic deconstruction of cellulose: structural insights from neutron diffraction and scattering*

\*\*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)*

\*2017 8<sup>th</sup> Neutron Scattering Applications in Structural Biology

*Radiation damage free structural studies of cellulolytic redox enzymes using neutron scattering and diffraction*

\*\*2017 Uppsala Biomedical Center, Uppsala, Sweden

*Structural enzymology using neutron crystallography and small angle scattering*

\*2017 Swedish Neutron Scattering Society Annual Meeting Uppsala, Sweden

*Structural studies of cellulolytic enzymes using neutron scattering and diffraction*

\*2016 1<sup>st</sup> Symposium on Lytic Polysaccharide Monooxygenases, Copenhagen, Denmark

- Structural studies of cellulolytic redox enzymes using neutron scattering and diffraction*
- \*2016 12th International Conference on Synchrotron Radiation, Palo Alto, CA  
*Radiation damage free structural studies of cellulolytic redox enzymes using neutron scattering and diffraction*
  - \*2016 Southeastern Regional Meeting of the American Chemistry Society, Columbia, MO  
*Structural studies of cellulolytic redox enzymes using neutron scattering and diffraction*
  - 2016 5<sup>th</sup> International Symposium on Diffraction in Structural Biology, Knoxville, TN  
*IMAGINE: new capability and sciences opportunities at the HFIR*
  - \*2016 16<sup>th</sup> International Conference on Crystallization of Macromolecules, Prague, Czech Republic  
*Crystallization of a fungal polysaccharide monooxygenase for neutron crystallography*
  - \*2015 NCSU Stewards of the Future – Water for a Growing World, Raleigh, NC  
*Protein Crystallography for Sustainability*
  - 2015 American Crystallography Association meeting, Philadelphia, PA  
*Locating Hydrogen Atoms in Enzymes Using Neutron Protein Crystallography*
  - \*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*
  - \*2014 Gordon Research Conference on Diffraction methods (July 27-August 1, 2014)  
*IMAGINE: new capability for neutron diffraction in the U.S.*
  - 2014 American Conference on Neutron Scattering, Knoxville, TN  
*IMAGINE, A Quasi-Laue Single Crystal Neutron Diffractometer at the HFIR*
  - 2014 American Crystallography Association meeting, Albuquerque, NM  
*Recent results from the new neutron diffractometer IMAGINE*
  - 2013 Oak Ridge National Laboratory, Oak Ridge, TN  
*The IMAGINE instrument at HFIR*
  - \*\*2013 North Eastern University, Boston, MA  
*Neutron Protein crystallography: application to Xylose Isomerase*
  - \*2013 Pittsburg Diffraction Society Meeting, Buffalo, NY  
*Locating Hydrogen Atoms in Enzymes Using Neutron Protein Crystallography*
  - \*\*2013 Molecular and Structural Biochemistry Department, Raleigh, NC  
*Protonation in protein structure and function*
  - 2013 Mid-Atlantic Macromolecular Crystallography Conference, Durham, NC  
*Locating hydrogen atoms in enzymes using neutron protein crystallography*
  - 2012 American Crystallography Association Meeting, Boston, MA  
*Locating hydrogen atoms in Xylose Isomerase using neutron protein crystallography*
  - \*\*2012 University of Tennessee Science Forum, Knoxville, TN  
*Neutrons for Biology and Bioenergy*
  - 2010 Neutron Scattering Sciences Division, ORNL, Oak Ridge, TN  
*Rapid visualization of deuterium atoms in Rubredoxin*
  - 2009 North Carolina State University, Molecular and Structural Biochemistry Dpt, Raleigh, NC, USA  
*Structural Biology with Neutrons*
  - \*2008 International Union of Crystallography meeting, Osaka, Japan  
*Neutron crystallographic analysis of deuterated and selectively CH<sub>3</sub>-protonated deuterated rubredoxin*
  - 2008 American Conference on Neutron Scattering, Santa Fe, NM, USA  
*IMAGINE: Supra- and Macro-molecule Quasi-Laue Neutron Diffractometer at HFIR*
  - 2007 Neutrons in Biology, Didcot, United Kingdom  
*Rubredoxin: H-D labeling for neutron direct methods*

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

#### *Conference Session Chair*

- 2017 24<sup>th</sup> Congress, International Union of Crystallography  
 Session: Advanced neutron sources in biological and materials sciences
- 2013 SNS/HFIR User meeting, Oak Ridge, TN, USA  
 Session: Biological Sample Environment/Sample Preparation  
 Session: Structural Biology
- 2009 International Conference on Neutron Scattering, Knoxville, TN, USA  
 Session: Protein Structures

#### *Poster presentations*

- 2017 SNS HFIR User meeting (Flora Meilleur: presenter)  
*IMAGINE: Image Plate Diffractometer at the HFIR*
- 2016 5<sup>th</sup> Symposium on Diffraction in Structural Biology (Annette Bodenheimer: presenter; Flora Meilleur: PI)  
*The close state of Cel7a*
- 2016 American Conference on Neutron Scattering (Brad ODell: 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 Crystallography 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 (W. (Brad) 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 Crystallography 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 Crystallography Association Meeting, Boston, MA (Annette Bodenheimer, presenter; Flora Meilleur: PI)  
*Structural analysis of Cel7a*
- 2011 American Crystallography 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 Crystallography Association meeting, Chicago, USA (Flora Meilleur, presenter & PI)  
*IMAGINE, a quasi-Laue single crystal neutron diffractometer at the HFIR*
- 2010 American Crystallography 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 Crystallography Association meeting, Knoxville, TN, USA (Flora Meilleur, presenter & PI)  
*IMAGINE, a quasi-Laue single crystal neutron diffractometer at the HFIR*
- 2008 American Crystallography Association meeting, Knoxville, TN, USA (Flora Meilleur, presenter & PI)  
*The enzymatic mechanism of xylose isomerase revealed by neutron protein crystallography*
- 2006 American Crystallography 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 Cytochrome 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*

## Sponsored grant

### Current funding

<i>Title</i>	<i>Role</i>	<i>Funding Agency</i>	<i>Award</i>	<i>Period</i>
1) GO! Graduate Opportunity at ORNL	PI	ORNL/UT-Battelle	\$194,190	FY15 – present
2) IGERT: Neutron Scattering for the Science and Engineering of the 21st Century	Co-PI	NSF (Missouri U)	\$3,000,000 (NCSU subcontract: \$237,720)	FY12 – FY18
3) Joint appointment NCSU-ORNL	Faculty	ORNL/UT-Battelle	\$ 745,210	FY07 – present

### Past funding

<i>Title</i>	<i>Role</i>	<i>Funding Agency</i>	<i>Award</i>	<i>Period</i>
1) MRI: Acquisition of a neutron single crystal diffractometer	Co-PI	NSF	\$1,831,600	FY10 – FY13
2) Neutron Structural Virology	PI	DOE - ORNL	\$646,000	FY07 – FY10
3) Mapping the Protein Structure-Function-Dynamics Landscape	Co-PI	DOE - ORNL	\$306,000	FY07 – FY10

### Education grants

<i>Title</i>	<i>Role</i>	<i>Funding Source</i>	<i>Award</i>	<i>Period</i>
BCH590E	PI	ORNL/NSSD	\$140,000	FY10 – FY14
BCH590E	PI	TN DOE EPSCoR	\$21,600	FY10 – FY15
BCH590E	PI	ORAU	\$17,900	FY10 – FY14
BCH590E	PI	UT/ORNL JINS	\$36,000	FY10 – FY14

### Letter of Intent

<i>Title</i>	<i>Role</i>	<i>Year</i>	<i>Outcome</i>
IMAGINE: a single crystal diffractometer at HFIR	PI	2007	CG4-D beamline position at HFIR awarded to the project