

## CURRICULUM VITAE

**Name** David Scott Wishart

**Position** Distinguished University Professor (University of Alberta)

**Address** Depts. of Computer Science and Biological Sciences  
Z-832 Biological Sciences Building  
University of Alberta  
Edmonton, Alberta  
Canada  
T6G 2E9

Phone: (780) 492-8574      FAX: (780) 492-1071

**Date of Birth** Dec. 7, 1961

**Marital Status** Married (to Debby), one daughter (Elizabeth), one son (Noah)

**Citizenship** Canadian

**Ethnic Identity** Metis (Cree and Assiniboine) - Metis ID#: 047448

**Education**

Ph.D. Molecular Biophysics & Biochemistry	Yale University, New Haven, U.S.A.	1991
M.Phil. Molecular Biophysics & Biochemistry	Yale University, New Haven, U.S.A.	1986

B.Sc. (Honours, First Class) Physics

University of Alberta,  
Edmonton, Canada

1983

### **Related Work Experience**

<b>Distinguished University Professor</b> Depts. of Computing Science and Biological Sciences, University of Alberta	2016- Present
<b>Chief Information Officer</b> Molecular You Corporation, Vancouver, BC	2016- Present
<b>Adjunct Professor</b> Department of Laboratory Medicine and Pathology, University of Alberta	2012- Present
<b>Program Coordinator for Metabolomic Sensors and Senior Research Office</b> NRC- National Institute of Nanotechnology (NINT)	2012-2016
<b>Director of Nanobiology and Senior Research Officer</b> NRC-National Institute of Nanotechnology (NINT)	2004-2012
<b>Professor</b> Department of Computing Science, University of Alberta	2003- Present
<b>Adjunct Professor</b> Faculty of Pharmacy, University of Alberta	2003- Present
<b>Cross-Appointed Member</b> NRC-National Institute of Nanotechnology (NINT)	2002-2004
<b>Associate Professor (Bristol-Myers Squibb Chair)</b> Faculty of Pharmacy, University of Alberta	2000-2003
<b>Assistant Professor (Bristol-Myers Squibb Chair)</b> Faculty of Pharmacy, University of Alberta	1995-2000
<b>Chief Scientific Officer and co-founder (Chenomx Inc. Edmonton, AB)</b>	2000-2005
<b>Chief Scientific Officer and co-founder (BioTools Inc. Edmonton, AB)</b>	1995-2005
<b>Postdoctoral Fellow</b> Department of Biochemistry, University of Alberta	1991-1995

Supervisor: Brian D. Sykes	
<b>Graduate Research Assistant</b> Department of Biochemistry, University of Alberta Supervisors: Brian D. Sykes and Frederic M. Richards	1988-1991
<b>Graduate Research Assistant</b> Department of Molecular Biophysics & Biochemistry, Yale University Supervisor: Frederic M. Richards	1985-1988

### Research Program

My laboratory is currently working in four areas of biotechnology and nanobiotechnology. In particular, we have active programs in: 1) metabolomics (quantitatively characterizing metabolites in biofluids), 2) bioinformatics, 3) structural biology, and 4) biosensors. Our work in metabolomics has focused on characterizing the human metabolome with a particular emphasis on developing technologies, resources and databases that can facilitate that process. We are using these techniques to improve our understanding of metabolism and help identify novel biomarkers of disease and/or nutritional imbalances. Our work in bioinformatics involves developing novel software and databases for protein function/structure prediction, MS and NMR spectral prediction, chemical structure/function prediction, metabolomics, natural products, microarray analysis, genome annotation, biomedical text mining, NMR spectral interpretation and biological simulation/visualization. Our work in structural biology focuses on using NMR to characterize a range of proteins involved in neurodegeneration including Abeta, alpha synuclein and the prion protein. We are actively developing both NMR and computational methods that can make the structural and dynamic analyses of these (and other large protein) systems better, faster and easier. Our work in biosensors is directed at developing compact or hand-held metabolomic sensing devices. These use enzyme-based or antibody-based colorimetric, impedance or electrochemical approaches to detect and quantify metabolites. These sensor systems are being used to develop systems for cancer testing in humans and veterinary applications for farm animals. Our expertise in machine learning and database development is also contributing to the biosensor development and optimization.

### Awards, Honours & Prizes

1) UofA Undergraduate Math Book Prize	Dept. of Mathematics, University of Alberta, Canada	1980
2) UofA Undergraduate Physics Book Prize	Dept. of Physics, University of Alberta, Canada	1981
3) UofA Summer Studentship	Dept. of Physics, University of Alberta, Canada	1981
4) M.J. Aamodt Prize in Classics	Dept. of Classics, University of Alberta, Canada	1982

5) UofA Summer Studentship	Dept. of Physics, University of Alberta, Canada	1982
6) Dean's Silver Medal in Science	University of Alberta, Canada	1983
7) N.S.E.R.C. Summer Studentship	Natural Sciences and Engineering Research Council, Canada	1983
8) UofA Summer Studentship	Dept. of Biochemistry, University of Alberta, Canada	1984
9) L. McKinney Undergraduate Scholarship (declined)	University of Alberta, Canada	1984
10) N.S.E.R.C. Postgraduate Scholarship	Natural Sciences and Engineering Research Council, Canada	1984-1988
11) Yale University Tuition Scholarship	Yale University	1985-1988
12) A.H.F.M.R. Postdoctoral Fellowship	Alberta Heritage Foundation for Medical Research, Canada	1991-1994
13) Eli Lilly Travel Award	Protein Society, USA	1994
14) Bristol-Myers Squibb Research Chair	PMAC-MRC and Bristol-Myers Squibb	1995-2000
15) New Investigator Award	American Assoc. Colleges of Pharmacy	1997
16) ASTech Prize in Innovation & Research	Awarded to BioTools Inc.	1999
17) Bristol-Myers Squibb Research Chair	CIHR-Rx&D and Bristol-Myers Squibb	2000-2005
18) Young Investigator Prize	Astra-Zeneca-CFPS	2001
19) Lifetime Honorary Fellow	International Metabolomics Society	2014
20) Top 100+ Most Influential Researchers (Biological Sciences)	Thomson Reuters	2014
21) Top 100+ Most Influential Researchers (Biological Sciences)	Thomson Reuters	2015
22) ANZMAG Lectureship	Australian-New Zealand Magnetic Resonance Society	2016

23) Top 100+ Most Influential Researchers (Biological Sciences)	Thomson Reuters/Clarivate Analytics	2016
24) Fellow of the Royal Society of Canada	Royal Society of Canada	2017
25) Top 100+ Most Influential Researchers (Biological Sciences)	Thomson Reuters/Clarivate Analytics	2017
26) Top 200 Most Influential Researchers (Biological Sciences)	Thomson Reuters/Clarivate Analytics	2018
27) University Alumni Award	University of Alberta	2018
28) Distinguished University Professor	University of Alberta	2018
29) Top 200 Most Influential Researchers (Biological Sciences)	Thomson Reuters/Clarivate Analytics	2019
30) Top 200 Most Influential Researchers (Biological Sciences/Biochemistry)	Thomson Reuters/Clarivate Analytics	2020
31) 2021 Innovation Award for Tricca Technologies Inc.	University of Alberta	2021
32) 2021 Innovation Award Molecular You Corporation	University of Alberta	2021
33) Top 200 Most Influential Researchers (Biological Sciences/Biochemistry)	Thomson Reuters/Clarivate Analytics	2021
34) 2022 Innovation Award MetabolomiX Inc	University of Alberta	2022
35) 2022 Innovation Award Q Boost Inc	University of Alberta	2022

**H-index = 124, Total number of citations > 105,500 (for 517 lifetime publications)**

### **Other Professional Activities**

- 1) Chief Scientific Officer of BioTools Inc. (1995-2001)
- 2) Member of the American Pharmaceutical Association (1995-1998)

- 3) Member of the American Association for the Advancement of Science (1995-2001)
- 4) Member of the Canadian Federation of Biological Scientists (1996-1998)
- 5) Chair and Organizer of Recent Advances in Biomacromolecular NMR Symposium (1996)
- 6) Member of Faculty of Pharmacy Student Appeals Committee (1997-1999)
- 7) Member, Organizing Committee for 12th International Symposium on HP Computing (1997)
- 8) Guest Editor: Biochemistry & Cell Biology (1998)
- 9) Member of the Canadian Society for Pharmaceutical Sciences (1998-2002)
- 10) Member of Agriculture/Forestry/Home Economics Faculty Council (1998-2001)
- 11) Member of the Alberta Proteomics Network Initiative Advisory Group (1999-2002)
- 12) Member of the NCI grant review panel in Virology and Structural Biology (1999-2000)
- 13) Chair of the PENCE Education and Training Committee (1999-2003)
- 14) Board Member and past Chair of BioTools Inc. (1999-2005)
- 15) Instructor and Co-Founder of the Canadian Bioinformatics Workshop Series (1999- present)
- 16) Chief Scientific Officer, Chenomx Inc. (2000-2003)
- 17) Scientific Consultant for Chenomx Inc. (2000-2005)
- 18) Board Member of Chenomx Inc. (2000-2006)
- 19) Chair of the Division of Pharmaceutical Sciences (2000-2002)
- 20) Member of the Prairie Genome Scientific Advisory Council (2000-2002)
- 21) Member of the AHFMR Studentship/fellowship Review Panel (2000-2002)
- 22) Member of the CIHR Multi-user Equipment Grant Review Panel (2001-2003)
- 23) Member of the NANUC advisory board (2001- present)
- 24) Member of the International Society for Computational Biology (2001- present)
- 25) Member of the UofA Nanotechnology Executive Council (2001-2004)

- 26) Chair of the Canadian Proteomics Initiative Conference (2001-2008)
- 27) Chair of the 10th ISCB Conference (2002) in Edmonton (2001-2002)
- 28) Member of the Metro Edmonton Health Industry Advisory (MEHIA) Board (2002-2006)
- 29) Chair and Co-organizer of the UofA Campus Nanotechnology Symposium (2002)
- 30) Member of the ANPI Advisory Board (2002-2003)
- 31) Director of the Genome Canada Bioinformatics Help Desk (2002-2011)
- 32) Director of the PENCE Bioinformatics Core Facility (2002-2006)
- 33) Faculty of Science Rep for the Faculty of Pharmacy Faculty Council (2003-2005)
- 34) Member of the 7th International ISSX Conference Organizing Committee (2003-2004)
- 35) Member of the BioMagResBank Scientific Advisory Board (2003-2008)
- 36) Member of the Learning Initiatives Committee- Biological Sciences (2004-2006)
- 37) Member of the Alberta Transplant Institute- Scientific & Management Council (2004-2007)
- 38) Member of the IBM Centre for Advanced Studies (CAS) Executive Committee (2005-2009)
- 39) Chair of the Alberta Metabolomics Symposium Conferences (2006-2008)
- 40) Co-Chair of the PSB Computational Aspects of Metabolomics Workshop (2006-2007)
- 41) Chair of the Toronto Prion Structure, Function & Dynamics Conference (2006)
- 42) Chair of the Calgary PrionNet Satellite Conference on Prion Structure & Dynamics (2006-2007)
- 43) Chair of the CFBS 5th Northern Lights Conference on Metabolomics (2006-2007)
- 44) Member of the Genome BC Microarray Platform Scientific Advisory Board (2006-2010)
- 45) Member of the International Metabolomics Society (2006-present)
- 46) Director of the Nano-Life Sciences Division for NINT (2006-2011)
- 47) Member of the Board, International Metabolomics Society (2007-2011)
- 48) Director of the Pan Alberta Metabolomics Platform- PANAMP (2008-2012)

- 49) Chair of the 5th Annual International Metabolomics Society Conference (2008-2009)
- 50) Organizing Committee for the 6th International Metabolomics Society Conference (2009-2010)
- 51) Member of the Metabolomics Australia Scientific Advisory Board (2009-present)
- 52) Member of the Prion2011 Conference Planning Committee (2010-2011)
- 53) Organizing Committee for the 7th International Metabolomics Society Conference (2010-2011)
- 54) Member, Scientific Advisory Board CoBRE, Montana State University, Bozeman (2010-2012)
- 55) Director of the PrioNet Prion Protein and Plasmid Production (PrP5) Facility (2010-2013)
- 56) Member, Scientific Advisory Board – Centre for Drug Research & Development (2011-2013)
- 57) Founder of Syntheteq Labs Inc. (2011)
- 58) Director of the Metabolomics Innovation Centre- TMIC (2011- present)
- 59) Program Leader for NRC-NINT- Metabolomic Sensors (2011-2014)
- 60) Board Member, EBI COSMOS Consortium on Metabolomics Data Standards (2012-2015)
- 61) Member of the wwPDB Validation Task Force on biomolecular NMR standards (2012-2017)
- 62) Chair & Organizer of Short Course on Metabolomic Profiling for 10th ISSX Symposium (2013)
- 63) Guest Editor for IEEE TBioCAS special issue on Biosensing (2013)
- 64) Member of the wwPDB NMR data exchange format committee (2013-2016)
- 65) Co-founder and board member of OMx Health Analytics Inc. (2015- present)
- 66) Co-founder, board member and CIO of Molecular You Inc. (2016- present)
- 67) Member, International Metabolomics Society 2016 Conference Organizing Committee (2015)
- 68) Member, International Metabolomics Society 2017 Conference Organizing Committee (2016)
- 69) Co-founder and board member of Tricca Inc. (2017- present)
- 70) Co-founder and board member of MetaSci Inc. (2017- present)
- 71) Organizer and Chair of “Metabolomics in Precision Medicine” Conference in Toronto (2017)



- 72) Member, International Metabolomics Society 2018 Conference Organizing Committee (2018)
- 73) Organizer and Chair of the “Metabolomics in Canada” Conference in Canmore (2018)
- 74) Organizer & Chair of the “2nd Annual Canadian Metabolomics Conference” in Canmore (2019)
- 75) Member of the TMIC All Nodes Leaders Committee (2019- present)
- 76) Co-founder and board member of Metabolomix Inc. (2019- present)
- 77) Chair of the NIH Common Fund Metabolomics Consortium Virtual Fall Meeting (2020)
- 78) Co-founder and board member of Q Boost Inc. (2021- present)
- 79) Co-founder and board member of Metabolomics Innovations Inc. (2021- present)
- 80) Member, Data and Safety Board for Dietary Biomarkers Development NIH (2022- present)
- 81) Member of the FoodPhyt steering Committee (2021-present)
- 82) Member, CIHR Bioinformatics & Health Data Sciences Planning Committee (2021-present)
- 83) Co-Chair, 4th Annual Metabolomics Association of North America Conference (2021-present)

### **University Committees**

- 1) Member of Faculty of Pharmacy Student Appeals Committee (1997-1999)
- 2) Member of Bachelor of Pharm. Sci. Curriculum Development Committee (1998)
- 3) External Member of the Agriculture/Forestry Faculty Council (1998-2001)
- 4) Member, Faculty of Science Bioinformatics Undergraduate Planning Committee (1999-2000)
- 5) Chair of Division of Pharmaceutical Sciences (Faculty of Pharmacy) (2000-2002)
- 6) Member of the NANUC advisory board (2001-2015)
- 7) Member of the UofA Nanotechnology Executive Council (2001-2006)
- 8) Faculty of Science Rep for the Faculty of Pharmacy Faculty Council (2003-2006)
- 9) Member of the Learning Initiatives Committee- Biological Sciences (2004-2006)

- 10) Member of the Alberta Transplant Institute- Scientific & Management Council (2004-2007)
- 11) Member of the IBM Centre for Advanced Studies (CAS) Executive Committee (2005-2009)
- 12) Director of the Nano-Life Sciences Division for NINT (2006-2011)
- 13) Faculty of Science Advisor for the Undergraduate Bioinformatics Program (2007-2017)
- 14) Member of Dept. of Computing Science Graduate Student Selection Committee (2008)
- 15) Program Leader for NRC-NINT – Metabolomics Sensors Program (2011-2016)
- 16) Member of the University Working Group on Precision Medicine (2016-present)
- 17) Member of the NRC-NINT Management and Group Leaders Committee (2012-2016)
- 18) Member of the Biological Metabolomics Faculty Position Search Committee (2016-2017)

### **Journal Reviewer**

- 1) Nature
- 2) Science
- 3) Journal of Molecular Biology
- 4) Nucleic Acids Research
- 5) Journal of Biomolecular NMR
- 6) BMC Bioinformatics
- 7) Magnetic Resonance in Chemistry
- 8) Biochemistry
- 9) Journal of the American Chemical Society
- 10) Protein Science
- 11) IEEE Nanotechnology
- 12) Bioinformatics
- 13) BMC Bioinformatics

- 14) PLoS One
- 15) In Silico Biology
- 16) Metabolomics
- 17) Metabolites
- 18) Journal of Magnetic Resonance
- 19) Analytical Chemistry
- 20) Journal of Proteome Research
- 21) Database
- 22) Biochimica Biophysica Acta
- 23) Acta Chimica

### **Editorships**

- 1) Guest Editor for Biochemistry and Cell Biology (special issue on NMR in Biochemistry) (1997)
- 2) Editorial board member for Biomolecular NMR Assignments (2005- present)
- 3) Editorial board member for Database (2011- present)
- 4) Guest Editor for IEEE TBioCAS special issue on Biosensing (2013)
- 5) Editorial board member for Current Metabolomics (2013-2018)
- 6) Editorial board member for Metabolites (2017- present)

### **Society Memberships and Society Board Memberships**

- 1) Member of the American Pharmaceutical Association (1995-1998)
- 2) Member of the Canadian Federation of Biological Scientists (1996-1998)
- 3) Member of the Canadian Society for Pharmaceutical Sciences (1998-2002)
- 4) Member of the American Association for the Advancement of Science (1995-2001)

- 5) Member of the International Society for Computational Biology (2001-present)
- 6) Member of the International Metabolomics Society (2006-present)
- 7) Board Member for the EBI-MetaboLights Initiative, Hinxton, UK (2011-present)
- 8) Member/Fellow of the Royal Society of Canada (2017-present)
- 9) Member of The American Chemical Society (2018-present)
- 10) Member of the Sigma Xi Society (2020-present)

### **National and International Conferences Chaired or Organized**

- 1) Chair and Organizer of Recent Advances in Biomacromolecular NMR Symposium (1996)
- 2) Member, Organizing Committee for 12th International Symposium on HP Computing (1997)
- 3) Chair of the 2001 Canadian Proteomics Initiative Conference (2001)
- 4) Chair of the 2002 Canadian Proteomics Initiative Conference (2002)
- 5) Chair of the 10th ISCB Conference (2002) in Edmonton (2001-2002)
- 6) Chair and Co-organizer of the UofA Campus Nanotechnology Symposium (2002)
- 7) Chair of the 2003 Canadian Proteomics Initiative Conference (2001-2008)
- 8) Chair of the 2004 Canadian Proteomics Initiative Conference (2001-2008)
- 9) Chair of the 2005 Canadian Proteomics Initiative Conference (2001-2008)
- 10) Chair of the 2006 Canadian Proteomics Initiative Conference (2001-2008)
- 11) Chair of the 2006 Alberta Metabolomics Symposium Conference (2006-2008)
- 12) Chair of the 2007 Canadian Proteomics Initiative Conference (2001-2008)
- 13) Chair of the 2007 Alberta Metabolomics Symposium Conference (2006-2008)
- 14) Co-Chair of the PSB Computational Aspects of Metabolomics Workshop (2006-2007)
- 15) Chair of the Toronto Prion Structure, Function & Dynamics Conference (2006)
- 16) Chair, Calgary PrionNet Conference on Prion Structure, Function & Dynamics (2006-2007)

- 17) Chair of the CFBS 5th Northern Lights Conference on Metabolomics (2006-2007)
- 18) Chair of the 2008 Alberta Metabolomics Symposium Conference (2006-2008)
- 19) Chair of the 5th Annual (2009) International Metabolomics Society Conference (2008-2009)
- 20) Organizing Committee for the 6th International Metabolomics Society Conference (2009-2010)
- 21) Member of the Prion2011 Conference Planning Committee (2010-2011)
- 22) Organizing Committee for the 7th International Metabolomics Society Conference (2010-2011)
- 23) Chair and Organizer of Short Course on Metabolomic Profiling for 10th ISSX Symposium (2013)
- 24) Member, International Metabolomics Society 2016 Conference Organizing Committee (2015)
- 25) Member, International Metabolomics Society 2017 Conference Organizing Committee (2016)
- 26) Chair and Organizer of “Metabolomics in Precision Medicine” Conference in Toronto (2017)
- 27) Member, International Metabolomics Society 2018 Conference Organizing Committee (2017-18)
- 28) Organizer and Chair of the “Metabolomics in Canada” Conference in Canmore (2018-2019)
- 29) Member, 4th Metabolomics Association of North America (MANA 2022) Conference Organizing Committee (2021- present)

### **Directorships of Research Service Centres and Service Cores**

- 1) Director of the Alberta Cancer Board Polyomx Bioinformatics Core (2002-2005)
- 2) Director of the Genome Canada Bioinformatics Help Desk (2002-2011)
- 3) Director of the PENCE Bioinformatics Core Facility (2002-2006)
- 4) Director of the Pan Alberta Metabolomics Platform – PANAMP (2008-2012)
- 5) Director of the PrioNet Prion Protein and Plasmid Production (PrP5) Facility (2010-2013)
- 6) Director of the Metabolomics Innovation Centre – TMIC (2011-2019)
- 7) Director of the Metabolomics Technology Demonstration Centre (2014-2018)
- 8) Co-director of the Metabolomics Innovation Centre – TMIC (2019- present)

**Peer Reviewed Grants Held**

\$75,000	Heritage Foundation for Medical Research Phase II Commercialization Grant	Operating (shared - 4)	1995
\$500,000	Medical Research Council University-Industry Chair (co-sponsored by Bristol-Myers Squibb)	Salary	1995-2000
\$215,000	Alberta Heritage Foundation for Medical Research Establishment Grant	Equipment & Operating	1995-1997
\$115,000	Protein Engineering Network of Centres of Excellence & AltaRex Inc.	Equipment & Operating (shared - 4)	1995-1996
\$10,000	Protein Engineering Network of Centres of Excellence (PENCE)	Operating	1995-1996
\$13,200	IRAP Technology Enhancement Grant (NRC)	Operating (shared - 4)	1995-1996
\$9000	Central Research Fund (University of Alberta)	Operating	1995-1996
\$119,500	Alberta Heritage Foundation for Medical Research	Equipment (shared - 5)	1996
\$63,500	Alberta Heritage Foundation for Medical Research	Equipment (shared - 4)	1996
\$31,500	Protein Engineering Network of Centres of Excellence (PENCE)	Operating	1996-1997

\$42,500	AltaRex Inc. & PENCE	Operating (shared - 3)	1996-1997
\$264,000	NSERC Strategic Grant	Operating (shared - 3)	1996-1999
\$496,000	Alberta Heritage Foundation for Medical Research Phase III Commercialization Grant	Operating (shared - 5)	1997-1998
\$165,000	MRC Group Equipment Grant (NMR support for 300 and 500 MHz machines)	Operating (shared - 6)	1997-2000
\$84,000	NSERC	Operating	1997-2000
\$11,200	PENCE	Operating	1997-1998
\$1,600,000	MRC and AHFMR (support for National NMR Centre)	Equipment (shared -10)	1997
\$2,552,000	ASRA and IIPP (support for Nat. NMR Centre)	Equipment (shared -10)	1997
\$17,000	American Association of Colleges of Pharmacy New Investigator Program	Operating	1997-1998
\$146,500	PENCE (NMR Technology Development)	Operating	1998-2001
\$28,000	PENCE (Antibacterial Peptide Design)	Operating	1998-1999

\$115,000	PENCE-BioTools Inc. (Bioinformatics)	Operating	1998-2001
\$5,718,000	CFI – Institute for Biomolecular Design	Equipment (shared -5)	1999
\$365,000	MRC Group Equipment Grant (NMR support for 300 and 500 MHz machines)	Operating (shared - 6)	2000-2005
\$169,000	NSERC	Operating	2000-2004
\$1,890,000	ACB Proteomics Initiative	Operating (shared - 8)	2000-2003
\$180,000	AHFMR Equipment Grant (MS spectrometer for ACB proteomics facility)	Equipment (shared - 4)	2000
\$390,000	MRC Group Equipment Grant (NMR support for 800 MHz NANUC facility)	Operating (shared - 5)	2000-2003
\$500,000	Rx&D CIHR University-Industry Chair (co-sponsored by Bristol-Myers Squibb)	Salary	2000-2005
\$117,500	PENCE (NMR Technology Development)	Operating	2001-2005
\$120,000	PENCE (Bioinformatics for Proteomics)	Operating	2001-2005
\$500,000	Alberta Heritage Foundation for Medical Research Phase III Commercialization Grant	Operating (Chenomx)	2001-2002



\$510,000	NSERC Strategic Grant (Engineering Protease Activity)	Operating (shared - 4)	2002-2004
\$150,000	PENCE (Bioinformatics Core Facility)	Operating	2002-2005
\$114,000	PENCE (Protein Fold Prediction)	Operating	2002-2005
\$117,000	PENCE (Proteomics of Pox Viruses)	Operating	2002-2005
\$410,000	Genome Canada (Bioinformatics Help Desk)	Operating	2002-2005
\$15,600,000	CFI/ASRIP (Project CyberCell, IBD)	Infrastructure (shared 6)	2004-2006
\$15,000,000	CFI/ASRIP (Integrated Nanosystems Facility)	Infrastructure (shared 8)	2004-2007
\$760,000	Genome Canada (4D Modeling of Genetic Disease)	Operating (shared - 5)	2005-2009
\$660,000	Genome Canada (Bioinformatics Help DeskII)	Operating	2005-2009
\$200,000	Genome Canada (Bioinformatics HelpDesk exp.)	Operating	2006-2008
\$290,000	Genome Canada (Microarrays in Organ Transplant)	Operating (shared - 3)	2005-2008

\$3,669,000	Genome Canada (Building Metabolomics Toolbox)	Operating (shared - 6)	2005-2008
\$235,000	NSERC (NMR without NOEs)	Operating	2004-2009
\$1,650,000	Alberta Prion Research Institute (Prion 3D struct)	Operating (shared - 5)	2006-2009
\$280,000	PrioNet (Prion dynamics)	Operating	2006-2009
\$440,000	National Research Council (Nanobot toolkit)	Operating	2006-2008
\$375,000	CIHR (Systems Biology Databases)	Operating	2007-2009
\$180,000	National Microbiology Lab (HIV infection)	Operating	2007-2008
\$400,000	PrioNet (Demiglobule hypothesis)	Operating (shared - 4)	2008-2010
\$75,000	ABIP-Ag-Canada (Cellulosic Biofuels)	Operating	2008-2011
\$50,000	Google Gift (Instant Wikipedia)	Operating (shared - 3)	2009
\$620,000	Genome Canada (Bioinformatics Help Desk)	Operating	2009-2011

\$700,000	Genome Canada (MS technology development)	Operating (shared - 2)	2008-2010
\$400,000	PrioNet (Metabolomic biomarkers for prions)	Operating (shared – 3 lead)	2008-2011
\$608,000	AAET/Genome Alberta (PANAMP)	Operating (shared – 4 lead)	2008-2009
\$600,000	AAET/Genome Alberta (PANAMP II)	Operating (shared – 4 lead)	2009-2010
\$1,200,000	CIHR (Bacteriophage therapy)	Operating (shared - 3)	2008-2012
\$1,600,000	APRI (Structure of Prions –core facility)	Operating (shared – 5 lead)	2008-2011
\$810,000	National Research Council (Nanobot toolkit)	Operating	2008-2011
\$390,000	CIHR (New Resources for Chemical Genomics)	Operating	2008-2011
\$200,000	NSERC (Cracking the Chemical Shift Code)	Operating	2009-2014
\$600,000	AARI (The Bovine Metabolome)	Operating (shared – 2 lead)	2009-2012
\$600,000	ALMA (LPS in prion disease etiology)	Operating (shared - 2)	2010-2012

\$270,000	APRI (LPS in prion disease etiology)	Operating (shared - 2)	2010-2012
\$300,000	APRI/ALMA (Biomarkers for prion disease)	Operating (shared – 4 lead)	2010-2012
\$150,000	APRI (Design rules for stabilized prions)	Operating (shared - 2)	2010-2012
\$1,600,000	NSERC/NRC/BDC (Nanotoxicology)	Operating (shared - 16)	2010-2012
\$810,000	AIHS-ACF (Tubulin isotype inhibitors)	Operating (shared - 3)	2011-2014
\$115,000	ALMA-AFC (Metabolomics and feeding)	Operating (shared - 2)	2012-2013
\$70,000	PrioNet (Demiglobule Hypothesis)	Operating	2011-2012
\$810,000	National Research Council (Nanobiosensors)	Operating	2011-2014
\$67,000	PrioNet (Prion vaccines)	Operating	2011-2012
\$140,000	PrioNet (Prion drug development)	Operating	2011-2012
\$300,000	PrioNet (SOD1 in ALS pathogenesis)	Operating (shared - 4)	2011-2012

\$220,000	PrioNet (PrP5 prion production facility)	Operating	2011-2012
\$67,000	PrioNet (Knowledge mobilization)	Operating	2011-2012
\$1,350,000	Genome Canada (Metabolomics Innovation Centre)	Operating (shared – 3 lead)	2011-2013
\$700,000	CIHR (New Resources for Chemical Genomics)	Operating	2011-2016
\$595,000	CIHR/NSERC (Alzheimer’s biomarker discovery)	Operating (shared - 4)	2012-2015
\$1,010,000	CIHR (Monitoring of pediatric kidney allografts)	Operating (shared - 7)	2012-2017
\$650,000	CIHR (Discovery of anti-amyloid compounds)	Operating	2012-2017
\$350,000	AIBS (Dietary therapies for IBD)	Operating (shared - 4)	2012-2015
\$480,000	AIBS (Alberta food metabolome)	Operating (shared – 2 lead)	2012-2015
\$484,000	AIBS (Substantiating health claims for pulses)	Operating (shared - 8)	2012-2014
\$100,000	Gates Foundation Grand Challenge (Biosensors)	Operating (shared – 2 lead)	2012-2013

\$500,000	ALMA (Biomarkers for dairy cattle disease)	Operating (shared - 2)	2012-2015
\$425,000	APRI (Targeting oligomers for neural disease)	Operating (shared - 3)	2013-2016
\$445,000	APRI (Glycolipids for prion conversion)	Operating (shared – 2 lead)	2013-2016
\$1,750,000	Genome Canada (Metabolomics Innovation Centre)	Operating (shared – 4 lead)	2013-2015
\$5,000,000	AIHS-CRIO (Devices for Personalized Medicine)	Operating (shared – 14 lead)	2013-2018
\$200,000	AIHS-Pfizer (Kits for metabolomics)	Operating (shared – 2 lead)	2013-2014
\$180,000	AIHS-Pfizer (metabolomics for polyps)	Operating (shared - 4)	2013-2014
\$495,000	AIBS (Bacteriocins for food safety)	Operating (shared - 4)	2013-2016
\$23,000,000	CIHR (Network for Transplant Research)	Operating (shared - 50)	2013-2018
\$298,000	APRI - Developing a Vaccine for CWD Using Attenuated PrP oligomers	Operating (shared – 2 lead)	2013-2017
\$700,000	APRI - Targeting Prion-Like Propagated Misfolding of SOD1 for ALS Immunotherapy	Operating (shared - 4)	2013-2018

\$450,000	CIHR (Food Biomarkers Alliance)	Operating (shared - 20)	2014-2017
\$310,000	NSERC Discovery - Improved Methods to Rapidly Characterize Protein Structure & Dynamics	Operating	2014-2019
\$2,983,800	WED (Metabolomics Technology Demonstration Centre)	Operating	2015-2018
\$1,877,857	Genome Canada (Metabolomics Innovation Centre)	Operating (shared – 4 lead)	2015-2017
\$914,790	Genome Canada (Metabolomics Innovation Centre)	Operating (shared – 4 lead)	2015-2017
\$93,430	Department of Defense – Suffield Metagenomics	Contract	2015-2016
\$24,000	NSERC – Engage grant (with BioMark)	Operating	2015
\$162,000	ALMA- Genomics and Metabolomics Analyses of Sheep Residual Feed Intake and Carcass Quality: A Follow Up Study	Operating (shared – 4)	2016-2018
\$25,000	NSERC Engage - Detecting Contaminants of Emerging Concern in Raw Water and Within Treatment Systems along the North Saskatchewan River	Operating	2016
\$123,000	University Health Foundation – ALNET metabolomics and proteomics of lymphedema	Operating (shared – 2)	2016-2022
\$2,114,000	CIHR - New Resources for Chemical Genomics and Metabolomics in Biomedicine	Operating	2016-2023

\$5,600,000	Genome Canada - Resilient Forests: Climate, Pests and Policy	Operating (shared – 7)	2016-2020
\$11,500,000	Genome Canada - Systems Biology and Molecular Ecology of Chronic Wasting Disease	Operating (shared – 8 lead)	2016-2020
\$6,013,000	Canada Foundation for Innovation – TMIC, The Metabolomics Innovation Centre	Operating (shared – 5 lead)	2017-2023
\$9,176,000	Genome Canada – TMIC, The Metabolomics Innovation Centre	Operating (shared – 5 lead)	2017-2023
\$6715	NSERC Connect – Metabolomics in Precision Medicine: From Theory to Practice	Conference	2017
\$140,000	Distinguished University Professor	Operating	2018-2025
\$300,000	Omni Personal Health Analytics Inc.	Operating	2021-2023
\$2,095,000	NIH Point of care, real time urine metabolomics test to diagnose colorectal cancers and polyps	Operating (shared – 8)	2017-2023
\$500,000	Genome Canada BCB - Illuminating the dark matter of the metabolome with convolutional neural networks	Operating (shared – 2)	2018-2021
\$571,000	NIH Battelle/PNNL - Pacific Northwest Advanced Compound Identification Core	Operating (shared – 2)	2019-2022
\$125,000	CIHR Catalyst - New metabolomics technologies to characterize cannabis safety and potency	Operating (shared – 2)	2019-2020



\$433,024	NSERC Discovery - Novel Approaches to spectral prediction and spectral deconvolution for metabolomics	Operating	2018-2025
\$750,000	Alberta Innovates Strategic Research Projects Advanced Materials for Precision Health in Dialysis	Operating (shared – 4)	2018-2022
\$150,000	APRI PET Metabolomics	Operating	2019-2021
\$4,100,000	Western Economic Development APEX	Operating	2019-2021
\$50,000	ProMIS Neurosciences, Inc: Structurally faithful cyclic peptides recapitulating the spike protein RBD loops that bind to ACE-2	Operating	2020-2021
\$305,000	CIHR: Development and clinical assessment of novel biomarker drugs targeting SSAT1 for detection and therapeutic monitoring of glioblastoma.	Operating (shared – 3)	2019-2023
\$135,000	Alberta Lamb Producers Association: Improved accuracy in diagnosing pregnancy and predicting litter size at early ewe gestation	Operating	2019-2020
\$783,000	NIH: Natural Products NMR Open Data Exchange	Operating (shared – 4)	2020-2025
\$245,000	Alberta Innovates: Development of a novel universal QSAR platform to design anti-Alzheimer's drugs via joint theoretical and experimental studies	Operating (shared – 2)	2019-2021
\$510,000	Mitacs: Portable Colorectal Screening Colorimetric Metabolite Biosensor	Operating	2020-2024
\$200,000	NMIN: Nanoparticle-enhanced, impedance-based biosensor development for cancer diagnostics	Operating	2020-2022

\$150,000	CCS/CIHR: A novel rapid, liquid biopsy early stage lung cancer diagnostic test	Operating	2021-2023
\$481,000	Alberta Innovates: An Analytic App for Arm-Chair Ranching	Operating (shared – 2)	2021-2023
\$220,545	Alberta Innovates: Predicting and Managing COVID-19 Pandemic Dynamics Using Machine Learning	Operating (shared – 4)	2020-2021
\$304,200	Alberta Innovates: Development and Clinical Validation of a Rapid Antibody Detection Device for COVID-19	Operating (shared – 3)	2020-2021
\$82,000 US	NIH: Alzheimer's Gut Microbiome Project	Operating	2021-2023
\$34,000 US	NIH: Gut Liver Brain Biochemical Axis in Alzheimer's Disease	Operating	2022-2023
\$24,000 US	NIH Supplement: Rare and Uncommon Metabolite Exchange (RUME) database	Operating	2021
\$32,400 US	NIH Supplement: Label-free polar metabolite quantification for untargeted metabolomics	Operating	2021-2022
\$253,840	NSERC: Comprehensive pathway generation of drug action and drug metabolism for DrugBank	Operating	2021 -2023
\$153,840	Alberta Innovates /CASBE: Comprehensive pathway generation of drug action and drug metabolism for DrugBank	Operating	2021 -2023
\$497,000	Alberta Innovates /SAFDAC: Defining Soil Health in the Digital Age: Using machine learning to predict and assess the impact of agricultural practices on soil health across Alberta	Operating (shared – 2)	2022 - 2023

\$180,000	Mitacs: Smart handheld device for automatic blood analysis: Innovative prediction of livestock pregnancy and litter size	Operating	2021-2025
\$145,000	Alberta Innovates /SAFDAC: Smart handheld device for automatic blood analysis: Innovative prediction of sheep pregnancy and litter size	Operating	2021-2023
\$248,000	RDAR: Handheld device for automatic blood analysis: Innovative prediction of sheep pregnancy and litter size	Operating	2021-2023
\$150,000	RDAR: Increasing participation of beef producers in financial and performance benchmarking to deliver new decision support tools	Operating	2022-2023
\$53,300	PROMIS: Computational modeling of misfolding specific epitopes	Operating	2022-2023
\$31,066	MetaboSensor LLC: Personalized Health and Nutrition	Operating	2022-2023
\$8,400,000	Canada Foundation for Innovation – TMIC, The Metabolomics Innovation Centre	Operating	2022-2029

### **Graduate Students and Postdoctoral Research Fellows**

\$65,000/Yr	Mitacs Postdoc Fellowship	Scott MacKay	01/12/2019	31/12/2022
\$60,000/Yr	Mitacs Postdoc Fellowship	Mai Yamamoto	19/06/2020	18/06/2022
\$60,000/Yr	CIHR/AI Postdoctoral Fellowship	Ammar Hassanzadeh	01/08/2020	30/07/2023
\$8,890/term	GTA	Afia Anjum	01/09/2020	31/12/2020

\$8,400/term	GTA	Shiful Islam	01/09/2020	31/12/2020
\$4,000	SM Blair RA	Seyed Ali Goldansaz	01/11/2020	30/08/2021
\$8,400/term	GTA	Shiful Islam	01/01/2021	30/04/2022
\$8,400/term	GTA	Dorna Varshavi	01/01/2021	30/04/2022
\$33,000	Student Work Placement Program	Multiple Students	05/01/2021	12/31/2021
\$6,000	Mitacs Globalink Research Award	Sajjad Janfaza	11/01/2021	05/01/2022
\$6,000	NSERC USRA	Irene Chen	01/05/2021	30/08/2021
\$8,648/term	GTA	Dorsa Rayat	01/09/2021	30/04/2022
\$8,890/term	GTA	Karla Trejo-Oliver	01/09/2021	31/12/2022
\$25,197/Yr	GRA	Mahi Zakir	01/09/2021	30/08/2022

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## **Patents**

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- 2) Preliminary Patent Application (M.R. Suresh, D.S. Wishart, S.M. Okarvi, G. Van Domselaar) A Simple and Efficient Method to Prepare  $^{99m}\text{Tc}$ -Labelled Peptides (filed Dec. 1997)
  
- 3) Patent (D.S. Wishart + 5 others) Compound Identification and Quantitation in Liquid Mixtures – Method and Process Using an Automated Nuclear Magnetic Resonance Measurement System (filed Jan. 12, 2001, awarded June 2005) UK Patent issued GB2410559.
  
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- 5) Patent Application (B. McManus, D.S. Wishart + 10 others) Methods of Diagnosing Acute Cardiac Allograft Rejection (Appl. No. 61/071,057 - Filed April 2008).
  
- 6) Patent Application (B. McManus, D.S. Wishart + 10 others) Methods of Identifying Expression of Nucleic Acid and Proteomic Markers and Acute Allograft Status Thereof (PCT/CA2009/000516 – Filed April 2009).
  
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- 92) Tzur, D., Jeroncic, K., Jewell, K., Block, D., Knox, C., Eisner, R., Guo, A., Stothard, P., Forsythe, I, Shrivastava, S., Greiner, R., Wishart, D.S. "The Human Metabolome Database (HMDB)", poster presented at the Alberta Metabolomics Symposium: Understanding the Human Metabolome, Edmonton, AB, Oct. 25, 2005.
- 93) Wishart, D.S, Querengesser, L. "Metabolomics and the Human Metabolome Project", poster presented at the Alberta Metabolomics Symposium: Understanding the Human Metabolome, Edmonton, AB, Oct. 25, 2005.
- 94) Shrivastava, S., Knox, C., Stothard, P., Greiner, R., Wishart, D.S. "Data Mining Tools for Curation of the Human Metabolome Database", poster presented at the Alberta Metabolomics Symposium: Understanding the Human Metabolome, Edmonton, AB, Oct. 25, 2005.
- 95) Cruz, J., Tang, P., Arndt, D., Yang, R., Wishart, D.S. "SimCell: A Cellular Simulation System for Metabolic Modeling", poster presented at the Alberta Metabolomics Symposium: Understanding the Human Metabolome, Edmonton, AB, Oct. 25, 2005.
- 96) Pireddu, L., Poulin, B., Lu, P., Wishart, D.S. "Pathway Analyst: Automated Metabolic Pathway Prediction", poster presented at the Alberta Metabolomics Symposium: Understanding the Human Metabolome, Edmonton, AB, Oct. 25, 2005.
- 97) Pireddu, L., Poulin, B., Lu, P., Wishart, D.S. "Pathway Analyst: Automated Metabolic Pathway Prediction", poster presented at the 2005 IEEE Symposim on Computational Intelligence in Bioinformatics and Computational Biology, San Diego, CA, Nov. 12-14, 2005.
- 98) Andrew, L.C., Wishart, D.S. "Towards The NMR Solution Structure Of HAV 3c Proteinase", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.
- 99) Montgomerie, S., Sundararaj, S., Gallin, W.J., Wishart, D.S. "Secondary Structure Prediction at 88% Accuracy", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.

- 100) Cruz, J., Wishart, D.S., Meng, C., Soong, K., Yeh, E. "A Laboratory Information Management System for Transcriptomics", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.
- 101) Fung, C., Tang, P., Wishart, D.S. "Systems Biology using SimCell", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.
- 102) Gebremedhin, M., Nikolai, L., Amegbey, G., Li, L., Wishart, D.S. "Determination of Human Urine Metabolites by MS and NMR" poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.
- 103) Xia, J., Magor, K., Wishart, D.S. "EST Analysis Step-by-Step", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.
- 104) Semenchenko, V., Wishart, D.S. "How to Create a Monster. Part I: Birth of Prion", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.
- 105) Berjanskii, M.V., Wishart, D.S. "The Random Coil Index and Protein Flexibility", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.
- 106) Shrivastava, S., Guo, A.G., Forsythe, I., Wishart, D.S. "Data Mining Tools for DrugBank and The Human Metabolite Database", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.
- 107) Nikolai, L., Wishart, D.S., Li, L. "Identification and Quantification of Human Metabolites from Plasma Using HPLC, MS and NMR", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.
- 108) Materi, W., Wishart, D.S. "Genetically Engineering in vivo Adhesion in E. coli", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.
- 109) Coutouly, M., Maiti, R., Montgomerie, S., Langen, C., Wishart, D.S. "A Method to Determine Protein Structures with Minimal Information", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.

110) Zhang, N., Damaraju, S., Damarjau, V., Li, N., Mackey, J., Wishart, D.S., Li, L., Cass, C. "Influence of Tumor Suppressor Protein p53 on the Expression and Composition of Plasma Membrane Proteins in Breast Cancer Cell Lines MN1 and MDD2", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.

111) Cheng, D., Zhang, H., Young, N., Damaraju, S., Wishart, D.S. "PolySearch: A Web Based System Integrating PubMed, Human Genome Data and Primer Design Tools for Management of Pharmacogenomic Projects", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.

112) Ju, C., Liu, Y., Meng, C., Wishart, D.S., Gallin, W.J. "AffyPipe: A Web-based Customized Analysis Pipeline for Affymetrix GeneChip® Microarray", poster presented at the 6th International Conference of the Canadian Proteomics Initiative, Edmonton, AB, May 10-12, 2006.

113) Materi, W., Wishart, D.S. "Genetically Engineering in vivo Adhesion in E. coli", poster presented at the Synthetic Biology 2.0 Conference, Berkeley, CA May 20-22, 2006.

114) Nikolai, L., Wishart, D.S., Li, L. "Identification and Quantification of Human Metabolites from Plasma Using HPLC, MS and NMR", poster presented at the ASMS Conference on Mass Spectrometry, Seattle, WA, May 28-31, 2006.

115) Guo, N., Tzur, D., Young, N., Wishart, D.S., and Li, L. "Creation and Application of Human Metabolome MS/MS Database", poster presented at the ASMS Conference on Mass Spectrometry, Seattle, WA, May 28-31, 2006. 116) Gebremedhin, M., Nikolai, L., Amegbey, G., Wishart, D.S., and Li, L. "Metabolite Profiling in Human Urine by NMR and MS", poster presented at the ASMS Conference on Mass Spectrometry, Seattle, WA, May 28-31, 2006.

117) Wopereis, S., Van Ommen, B., Gibney, M., Gibney, S., German, B., Knox, C., Cheng, D., Wishart, D.S., Querengesser, L., "Development of the Public Wiki Nutritional Metabolomics Biology Database: NuGOwiki", poster presented at the 2nd Annual Metabolomics Society Meeting, Boston, MA, June 24-29, 2006.

118) Wishart, D.S., Li, L., Greiner, R., Marrie, T., Sykes, B.D., Bamforth, F., Vogel, H., Querengesser, L. "Metabolomics and the Human Metabolome Project", poster presented at the 2nd Annual Metabolomics Society Meeting, Boston, MA, June 24-29, 2006.

119) Young, N., Jewell, K., Block, D., Knox, C., Tang, P., Greiner, R., Wishart, D.S. "MetaboLIMS: A General Laboratory Information Management System For Metabolomics", poster presented at the 2nd Annual Metabolomics Society Meeting, Boston, MA, June 24-29, 2006.

120) Eisner, R., Greiner, R., Wishart, D.S., Knox, C. "Predicting Chemical Properties of Metabolites", poster presented at the 2006 ISMB (Intelligent Systems in Molecular Biology) Conference, Fortaleza, Brazil, Aug. 4-7, 2006.

121) Wishart, D.S., Sundararaj, S., Maiti, R., Coutouly, M.A., Berjanskii, M.V. "Single Spectrum Spectroscopy of Proteins" presented at the 4<sup>th</sup> Gordon Conference on Computational Aspects of Biomolecular NMR, Aussois, France, Sept. 23-26, 2006.

122) Hau, D.D., Xia, J., Wishart, D.S. "In Vitro Metabolic Mapping by NMR Spectroscopy: Part 1 of the Four-Dimensional Project", poster presented at the Second Annual Metabolomics Symposium: Exploring the Human Metabolome poster session, Timms Centre, University of Alberta, October 12, 2006.

123) Lewis, M.J., Nikolai, L.N., Jeroncic, K.G., Wishart, D.S. "Identification and Quantification of the Human CSF Metabolome", poster presented at the Second Annual Metabolomics Symposium: Exploring the Human Metabolome poster session, Timms Centre, University of Alberta, October 12, 2006.

124) Arndt, D., Fung, C., Cruz, J., Tang, P., Yang, R., Wishart, D.S. "SimCell: A Cellular Simulation System for Metabolic Modeling", poster presented at the Second Annual Metabolomics Symposium: Exploring the Human Metabolome poster session, Timms Centre, University of Alberta, October 12, 2006.

125) Young, N., Jewell, K., Block, D., Knox, C., Tang, P., Greiner, R., Wishart D.S. "MetaboLIMS: A General Laboratory Information Management System for Metabolomics", poster presented at the Second Annual Metabolomics Symposium: Exploring the Human Metabolome poster session, Timms Centre, University of Alberta, October 12, 2006.

126) Cheng, D., Zhang, H., Young, N., Knox, C., Stothard, P., Damaraju, S., Wishart, D.S. "PolySearch: A Web Based Text Mining System for Extracting Relationships between Diseases, Genes, Mutations, Drugs and Metabolites", poster presented at the Second Annual Metabolomics Symposium: Exploring the Human Metabolome poster session, Timms Centre, University of Alberta, October 12, 2006.

127) Ametaj, B.N., Emmanuel, D.G.V., Lewis, M.J., Jeroncic, K., Nikolai, L., Shanthipoosan, S., Wishart, D.S. "Bovine Metabolomics: Profiling of Rumen Fluid Metabolites in Dairy Cattle", poster presented at the Second Annual Metabolomics Symposium: Exploring the Human Metabolome poster session, Timms Centre, University of Alberta, October 12, 2006.

- 128) Wagner, J., Greiner, R., Baracos, V., Mourtzakis, M., Prado, C., Slupsky, C., Rankin, K., Chang, D., McGeer, A., Marrie, T., Nikolai, L., Lewis, M., Coutouly, M-A, Wishart, D.S. "Using Metabolomic Profiles to Diagnose Patients", poster presented at the Second Annual Metabolomics Symposium: Exploring the Human Metabolome poster session, Timms Centre, University of Alberta, October 12, 2006.
- 129) Eisner, R., Knox, C., Greiner, R., Wishart, D.S. "Predicting Chemical Properties of Small Molecules", poster presented at the Second Annual Metabolomics Symposium: Exploring the Human Metabolome poster session, Timms Centre, University of Alberta, October 12, 2006.
- 130) Cheng, D., Zhang, H., Young, N., Knox, C., Stothard, P., Damaraju, S., Wishart, D.S. "PolySearch: A Web Based Text Mining System for Extracting Relationships between Diseases, Genes, Mutations, Drugs and Metabolites", poster presented at the Alberta Cancer Board's Annual Research Meeting, Banff, AB. Nov. 7-9, 2006.
- 131) Zhou, J., Lin, G., Shi, Y., Wishart, D.S. "Structure Comparisons between a PrPsc Structure Model and All PDB Structures", poster presented at the PrP Canada 2007 Conference, Calgary, AB. Feb. 18-21, 2007.
- 132) Suriyamongkol, B., Duggan, D., Semenchenko, V., Wishart, D.S. "Expression and Purification of Recombinant Murine Wild Type and Mutant Prion Proteins", poster presented at the PrP Canada 2007 Conference, Calgary, AB. Feb. 18-21, 2007.
- 133) Eisner, R., Knox, C., Cheng, D., Greiner, R., Wishart, D.S. "Text Analysis in the Human Metabolome Project", poster presented at the 3<sup>rd</sup> Annual Meeting of the Metabolomics Society, Manchester UK, June 11-14, 2007.
- 134) Tzur, D., Tzur, D., Forsythe, I., Guo, A.C., Shrivastava, S., Tang, P., Wishart, D.S. "The Human Metabolome Library", poster presented at the 3<sup>rd</sup> Annual Meeting of the Metabolomics Society, Manchester UK, June 11-14, 2007.
- 135) Bhomkar, P., Materi, W., Semenchenko, V., Wishart, D.S. "E. coli as Intelligent Drug Delivery Machines: Possibilities and Perspectives", poster presented at the CPI 2007 Meeting, Ottawa ON, June 16-18, 2007.
- 136) Suriyamongkol, B., Semenchenko, V., Wishart, D.S. "Purification and Circular Dichroism Studies of Recombinant Syrian Hamster Wild Type and Mutant Prion Proteins", poster presented at the CPI 2007 Meeting, Ottawa ON, June 16-18, 2007.

- 137) Mongomerie, S., Cruz, J., Shrivastava, S., Arndt, D., Berjanskii, M., Wishart, D.S. “Proteus2: A Web Server for Comprehensive Protein Structure Prediction and Structure-Based Annotation”, poster presented at the CPI 2007 Meeting, Ottawa ON, June 16-18, 2007.
- 138) Tang, P., Arndt, D., Cruz, J., Yang, R., Fung, C., Wishart, D.S. “Dynamic Cellular Automata: An Alternative Approach to Cellular Simulation”, poster presented at the CPI 2007 Meeting, Ottawa ON, June 16-18, 2007.
- 139) Zhou, J., Shi, Y., Lin, G., Wishart, D.S. “A Contact Order Prediction Method”, poster presented at the CPI 2007 Meeting, Ottawa ON, June 16-18, 2007.
- 140) Liu, Y., Fyshe, A., Lu, P., Szafron, D., Greiner, R., Wishart, D.S., Percy, B., Poulin, B., Eisner, R., Ngo, D., Lamb, N. “Proteome Analyst: Machine Learning for Protein Annotation”, poster presented at the CPI 2007 Meeting, Ottawa ON, June 16-18, 2007.
- 141) Zhou, G.P., Suriyamongkol, B., Duggan, D., Semenchenko, V., Wishart, D.S. “NMR Characterization of the Reduced Form of the Syrian Hamster Prion”, poster presented at the CPI 2007 Meeting, Ottawa ON, June 16-18, 2007.
- 142) Sissons, P., Kawas, E., Senger, M., Wilkinson, M.D., Wishart, D.S, “BioMoby Extensions to the Taverna Workflow Management and Enactment Software”, poster presented at the CPI 2007 Meeting, Ottawa ON, June 16-18, 2007.
- 143) Bhomkar, P., Materi, W., Semenchenko, V., Wishart, D.S. “E. coli as Intelligent Drug Delivery Machines: Possibilities and Perspectives”, poster presented at the 5<sup>th</sup> Annual Northern Lights Summer Conference on Nanomedicine: Nanostructures and Their Biomedical Applications, Waterloo ON, June 20-22, 2007.
- 144) Eisner, R., Knox, C., Cheng, D., Greiner, R., Wishart, D.S. “Text Analysis in the Human Metabolome Project”, poster presented at the 5<sup>th</sup> Annual Northern Lights Summer Conference on Metabolomics, Technologies & Applications, Waterloo ON, June 20-22, 2007.
- 145) Wishart, D.S., Li, L., Greiner, R., Sykes, B., Bamforth, F., Clive, D., Forsythe, I., Vogel, H. “Metabolomics and the Human Metabolome Project”, poster presented at the 5<sup>th</sup> Annual Northern Lights Summer Conference on Metabolomics, Technologies & Applications, Waterloo ON, June 20-22, 2007.



- 146) Lewis, M.J., Morrissey, J., Jeroncic, K.G., Wishart, D.S. "Identification and Quantification of the Human CSF Metabolome", poster presented at the 5<sup>th</sup> Annual Northern Lights Summer Conference on Metabolomics, Technologies & Applications, Waterloo ON, June 20-22, 2007.
- 147) Tzur, D., Forsythe, I., Guo, A.C., Shrivastava, S., Tang, P., Wishart, D.S. "The Human Metabolome Library", poster presented at the 5<sup>th</sup> Annual Northern Lights Summer Conference on Metabolomics, Technologies & Applications, Waterloo ON, June 20-22, 2007.
- 148) Xia, J., Lewis, M.J., Wishart, D.S., "Automatics Metabolite Identification in Biofluids Using 2D TOCSY Spectroscopy", poster presented at the 5<sup>th</sup> Annual Northern Lights Summer Conference on Metabolomics, Technologies & Applications, Waterloo ON, June 20-22, 2007.
- 149) Peng, J., Hau, D.D., Xia, J., Lewis, M.J., Wishart, D.S. "Human Serum Metabolomics Studied by 1H NMR", poster presented at the 5<sup>th</sup> Annual Northern Lights Summer Conference on Metabolomics, Technologies & Applications, Waterloo ON, June 20-22, 2007.
- 150) Young, N., Jewell, K., Block, D., Knox, C., Tang, P., Greiner, R., Wishart, D.S. "MetaboLIMS: A General Laboratory Information Management System for Metabolomics", poster presented at the 5<sup>th</sup> Annual Northern Lights Summer Conference on Metabolomics, Technologies & Applications, Waterloo ON, June 20-22, 2007.
- 151) Reiz, B., Bujold, A., Wishart, D.S., Li, L. "Microwave-assisted Acid and Base Hydrolysis Combined with MALDI-MS for the Study of Prions", poster/abstract presented at PrP Canada 2008, Toronto, ON, Feb. 3-5, 2008.
- 152) Blinov, N., Dorosh, L., Wishart, D.S., Kovalenko, A. "Molecular Theory of Solvation: New Insights into Molecular Mechanisms of Misfolding and Aggregation of Prion Proteins", poster presented at PrP Canada 2008, Toronto, ON, Feb. 3-5, 2008.
- 153) Wishart, D.S., Arndt, D., Berjanskii, M., Tang, P., Shi, Y., Zhou, J. "CS23D, a Web Server for Rapid Generation of 3D Protein Structures from Chemical Shifts", poster presented at PrP Canada 2008, Toronto, ON, Feb. 3-5, 2008.
- 154) Zhou, G.P., Suryamongkol, B., Semenchenko, B., Wishart, D.S. "NMR Characterization of the Prion Beta Oligomer Form", poster presented at PrP Canada 2008, Toronto, ON, Feb. 3-5, 2008.

155) Peng, J., Psychogios, N, Wishart, D.S. “Human Blood Serum Metabolomics Studied by GC-MS”, poster presented at the Canadian Proteome Society Regional Meeting – Omics & Systems Biology, Edmonton, AB, Feb. 21-22, 2008.

156) Jia, L., Wishart, D.S. “NMR-Star Converter and Chemical Shift Editor”, poster presented at the Canadian Proteome Society Regional Meeting – Omics & Systems Biology, Edmonton, AB, Feb. 21-22, 2008.

157) Forsythe, I., Wishart, D.S., Li, L., Greiner, R., Sykes, B.D., Bamforth, F., Clive, D., Vogel, H. “Metabolomics – Revolutionizing Healthcare, Agriculture, Nutrition and Food Production in the 21<sup>st</sup> Century”, poster presented at the Canadian Proteome Society Regional Meeting – Omics & Systems Biology, Edmonton, AB, Feb. 21-22, 2008.

158) Eisner, R., Greiner, R., Wishart, D.S. “Chemical Class Prediction in the Human Metabolome”, poster presented at the Canadian Proteome Society Regional Meeting – Omics & Systems Biology, Edmonton, AB, Feb. 21-22, 2008.

159) Reiz, B., Bujold, A.R., Wishart, D.S., Li, L. “Microwave-Assisted Acid and Base Hydrolysis Combined with MALDI-MS for the Study of Prion Structures”, poster presented at the Canadian Proteome Society Regional Meeting – Omics & Systems Biology, Edmonton, AB, Feb. 21-22, 2008.

160) Tsang, J., Bujold, A.R., Wishart, D.S., Li, L. “A Novel Approach to Characterizing Prion Protein Structures Using Chemical Labeling, Microwave-Assisted Acid Hydrolysis and MALDI-MS”, poster presented at the Canadian Proteome Society Regional Meeting – Omics & Systems Biology, Edmonton, AB, Feb. 21-22, 2008.

161) Peng, J., Psychogios, N., Wishart, D.S. “Human Blood Serum Metabolomics Studied by GC-MS”, poster presented at the 8<sup>th</sup> Annual Canadian Proteomics Initiative Conference, Burnaby, BC, May 4-5, 2008.

162) Cheng, D., Knox, C., Young, N., Stothard, P., Damaraju, S., Wishart, D.S. “PolySearch: A Web Based Text Mining System for Extracting Relationships Between Human Diseases, Genes, Mutations, Drugs and Metabolites”, poster presented at the 8<sup>th</sup> Annual Canadian Proteomics Initiative Conference, Burnaby, BC, May 4-5, 2008.

163) Zhou, G.P., Liu, X-H., Semenchenko V., Wishart, D.S. “Some Insights into the Prion Conversion Process of PrP<sup>C</sup> to PrP<sup>Sc</sup>”, poster presented at the 8<sup>th</sup> Annual Canadian Proteomics Initiative Conference, Burnaby, BC, May 4-5, 2008.

164) Cruz, J., Montgomerie, S., Shrivastava, S., Arndt, D., Berjanskii, M., Wishart, D.S. "Proteus2: Protein Structure Prediction and Structure-Based Annotation", poster presented at the 8<sup>th</sup> Annual Canadian Proteomics Initiative Conference, Burnaby, BC, May 4-5, 2008.

165) Eisner, R., Xia, J., Hau, D., Stretch, C., Greiner, R., Baracos V., Wishart, D.S., "Machine Learning Analysis of Cancer Cachexia", poster presented at the 8<sup>th</sup> Annual Canadian Proteomics Initiative Conference, Burnaby, BC, May 4-5, 2008.

166) Liu, Y., Fyshe, A., Lu, P., Szafron, D., Greiner, R., Wishart, D.S., Percy, B., Poulin, B., Eisner, R., Ngo, D., Lamb, N. "Proteome Analyst: Machine Learning for Protein Annotation", poster presented at the 8<sup>th</sup> Annual Canadian Proteomics Initiative Conference, Burnaby, BC, May 4-5, 2008.

167) Blinov, N., Dorosh, L., Wishart, D.S., Kovalenko, A., "Thermodynamics of amyloid fibril formation: molecular theory of solvation perspective," poster presented at the 91st Canadian Chemical Society Conference and Exhibition (CSC 2008) Edmonton, AB, May 24-28, 2008.

168) Dorosh, L., Blinov, N., Wishart, D.S., Kovalenko, A. "Role of Molecular Solvation in Nano Assembly of Prion Proteins," poster presented at Nanoforum Canada 2008, Edmonton, AB, May 28-30, 2008.

169) Reiz, B., Wishart, D.S., Bujold, A., Li, L. "Microwave-Assisted Acid and Base Hydrolysis Combined with MALDI-MS for Structural Studies of the Prion Protein", poster presented at the 91st Canadian Chemical Society Conference and Exhibition (CSC 2008), Edmonton, AB, May 24-28, 2008.

170) Reiz, B., Wishart, D.S., Bujold, A., Li, L. "Microwave-Assisted Acid and Base Hydrolysis Combined with MALDI-MS for Structural Studies of the Prion Protein", poster presented at the 56<sup>th</sup> ASMS Conference on Mass Spectrometry, Denver, CO, June 1-5, 2008.

171) Wishart, D.S., Arndt, D., Berjanskii, M., Tang, P., Zhou, J., Lin, G. "CS23D: A Web Server for Rapid Protein Structure Generation Using NMR Chemical Shifts and Sequence Data", poster presented at the 16<sup>th</sup> ISMB Meeting, Toronto ON, July 19-23, 2008.

172) Cruz, J.A., Arndt, D., Berjanskii, M., Tang, P., Zhou, J., Lin, G., Wishart, D.S. "CS23D: A Web Server for Rapid Protein Structure Generation Using NMR Chemical Shifts and Sequence Data", poster presented at the 23<sup>rd</sup> Annual ICMRBS Meeting, San Diego, CA, Aug. 24-29, 2008.

- 173) Xia, J., Hau, D.D., Eisner, R., Stretch, C., Baracos, V., Greiner, R., Wishart, D.S. "Targeted Profiling and Analysis of the Urine Metabolome to Identify Potential Biomarkers Associated with Cancer Cachexia", poster presented at the 4<sup>th</sup> Annual Metabolomics Society Meeting, Boston, MA, Sept. 2-6, 2008.
- 174) Hau, D.D., Peng, J., Xia, J., Gautam, B., Tzur, D., Wishart, D.S. "The Human Serum Metabolome", poster presented at the 4<sup>th</sup> Annual Metabolomics Society Meeting, Boston, MA, Sept. 2-6, 2008.
- 175) Cruz, J., Larsen, I., Eisner, R., Knox, C., Wishart, D.S., West, L. "Web-based data collection tools and effective means to collect multi-centre information" poster presented at the Annual Research Day, Edmonton, AB, Nov. 15, 2008.
- 176) Wishart, D.S., Knox, C., Cruz, J., Guo, A., Gautam, B., Eisner, R., Young N. "New Resources for Disease Bioinformatics", poster presented at the 11th Annual Pacific Symposium in Biocomputing (PSB), Hawaii, Jan. 3-7, 2009.
- 177) Acharya, S., Saleem, F., Bjorndahl, T.C., Semenchenko, V., Wishart, D.S. "Characterizing Intermediate States in Prion Protein Conversion to the b-rich Isoform Under Mildly Denaturing Conditions Using Urea and Salt or SDS" poster presented at PrP Canada 2009, Edmonton, AB, March 1-3, 2009.
- 178) Blinov, N., Dorosh, L., Wishart, D.S., Kovalenko, A., "Thermodynamic stability and solvation properties of prion amyloid fibrils and small  $\beta$ -sheet oligomers" poster presented at PrP Canada 2009, Edmonton, AB, March 1-3, 2009.
- 179) Blinov, N., Berjanskii, M., Wishart, D.S., Stepanova, M. "Structural domains and main-chain flexibility in prion proteins" poster presented at PrP Canada 2009, Edmonton, AB, March 1-3, 2009.
- 180) Dorosh, L., Blinov, N., Berjanskii, M., Wishart, D.S., Kovalenko, A. "Thermodynamics of Prion Protein Unfolding" poster presented at PrP Canada 2009, Edmonton, AB, March 1-3, 2009.
- 181) Lo, A., Acharya, S., Wishart, D.S., Li, L., "Chemical Crosslinking and Mass Spectrometry for Prion Structure Determination," poster presented at PrP Canada 2009, Edmonton, AB, Mar. 1-3, 2009.
- 182) Reiz, B., Wishart, D.S. Li, L., "Microwave-assisted acid/base hydrolysis and mass spectrometry for prion structure characterization", poster presentation at PrP Canada 2009 in Edmonton, AB, Mar. 1-3, 2009.

- 183) Wang N., Wishart, D.S., Li. L., "Development and Application of Acid Hydrolysis Combined with LC-MS/MS for Prion Structure Characterization", poster presented at PrP Canada 2009, Edmonton, AB, Mar. 1-3, 2009.
- 184) Zhou, G.P., Liu, X.H., Bjorndhal, T.C., Semenchenko, V., Saleem, F., Acharya, S., Sobsey, C. Wishart, D.S. "Detailed Biophysical Characterization of the Syrian Hamster PrP<sup>C</sup> to PrP<sup>Sc</sup> Conversion Process" poster presented at PrP Canada 2009, Edmonton, AB, March 1-3, 2009.
- 185) Chatterjee, S., Julian, O., Acharya, S., Wishart, D.S., Sykes, B.D. "1H NMR Studies of the Urea Unfolding of the Boivne and Syrian Hamster Prion Proteins" poster presented at the 52<sup>nd</sup> Annual Meeting of the CSBMCB, Niagara-on-the-Lake, ON, June 2-5, 2009.
- 186) Blinov, N., Dorosh, L., Wishart, D., Kovalenko, A. "Bridging the Gap Between Implicit and Explicit Solvation Statistical-mechanical Molecular Theory of Solvation Perspective on Amyloidogenesis" poster presented at the 52<sup>nd</sup> Annual Meeting of the CSBMCB, Niagara-on-the-Lake, ON, June 2-5, 2009.
- 187) Eisner, R., Greiner, R., Knox, C., Cruz, J., Wishart, D.S. "Annotating Drugs and Metabolites with their Chemical Class" poster presented at the 17<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB), Stockholm, Sweden, June 27-July 2, 2009.
- 188) Xia, J., Young, N., Wishart, D.S. "MetaboAnalyst" poster presented at the First Annual Australasian Metabolomics Conference, Auckland, New Zealand, July 3-5, 2009.
- 189) Bouatra, S., Xia, J., Hau, D., Peng, J., Eisner, R., Mandal, R., Psychogios, N., Sinelnikov, I., Stretch, C., Baracos, V., Wishart, D.S. "The Human Urine Metabolome" poster presented at Metabolomics Society's 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.
- 190) Lim, E., Frolkis, A., Gautam, B., Liu, P., Guo, A.C., Knox, C., Jewison, T., Shrivastava, S., Law, V., Xia, J.G., Wishart, D.S., Ly, S. "Small Molecule Pathway Database: illustrating human metabolism at subcellular and organ level" poster presented at Metabolomics Society's 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.
- 191) Pon, A., Lim, E., Djoumbou, Y., Knox, C., Shrivastava, S., Guo, A.C., Wishart, D.S. "T3DB: The Toxin and Toxin Target Database" poster presented at Metabolomics Society's 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.

192) Sinelnikov, I., Dong, E., Huang, P., Young, N., Knox, C., Eisner, R., Guo, A.C., Bouatra, S., Xia J., Psychogios, N., Greiner, R., Wishart, D.S. “HMDB (version 2.5): Human Metabolome Database” poster presented at Metabolomics Society’s 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.

193) Young, N., Xia, J., Psychogios, N., Wishart, D.S. “MetaboAnalyst-A Web Service For Metabolomic Data Analysis” poster presented at Metabolomics Society’s 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.

194) Eisner, R., Xia, J., Stretch, C., Eastman, T., Greiner, R., Baracos, V., Wishart, D.S., Hau, D. “Diagnostic markers of cancer-associated skeletal muscle wasting using 1H-NMR profiling of urinary metabolites and machine learning approaches” poster presented at Metabolomics Society’s 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.

195) Neveu, V., Vos, F., Perez, J., Cruz, J., Eisner, R., Knox, C., Wishart, D.S., Scalbert, A. “Phenol-Explorer: a comprehensive database on the content of dietary polyphenols in foods” poster presented at Metabolomics Society’s 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.

196) Robson, P., Baracos, V., Mackey, J., Cass, C., Greiner, R., Yasui, Y., Wishart, D.S., Damaraju, S. “Establishing population based cohorts with urinary metabolome profiles, diet and lifestyle variables for comprehensive analysis to define health and disease status” poster presented at Metabolomics Society’s 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.

197) Saleem, F., Psychogios, N., Gautam, B., Eisner, R., Knox, C., Cruz, J., Bouatra, S., Sinelnikov, I., Zebeli, Q., Ametaj, B., Wishart, D.S. “Determination of the bovine metabolome” poster presented at Metabolomics Society’s 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.

198) Mandal, R., Bouatra, S., Sinelnikov, I., Psychogios, N., Krishnamurthy, R., Wishart, D.S. “Lipidomics: A Quantitative Approach for Analysis of Lipids in Biological and Plant Samples” poster presented at Metabolomics Society’s 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.

199) Mandal, R., Sinelnikov, I., Psychogios, N., Bouatra, S., Wishart, D.S., Bogumil, R., Dammeier, S. “Human Cerebrospinal Fluid Targeted Metabolomics Analysis using the BIOCRAATES AbsoluteIDQ Kit” poster presented at Metabolomics Society’s 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.

- 200) Psychogios, N., Hau, D., Peng, J., McManus, J., Pedersen, T., Bamforth, F., Greiner, R., McManus, B., Newman, J., Wishart, D.S. “The Human Serum Metabolome” poster presented at Metabolomics Society’s 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.
- 201) Psychogios, N., Saleem, F., Gautam, B., Bouatra, S., Mandal, R., Sinelnikov, I., Zebeli, Q., Ametaj, B., Wishart, D.S. “Metabolomic profiling of rumen fluid in dairy cows fed high concentrate/low forage diets” poster presented at Metabolomics Society’s 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.
- 202) Guo, A.C., Shrivastava, S., Knox, C., Mandal, R., Gautam, B., Wishart, D.S. “The E. coli Metabolome” poster presented at Metabolomics Society’s 5<sup>th</sup> Annual International Conference, Edmonton, Canada, Aug 30 – Sept 2, 2009.
- 203) Frolkis, A., Ziegler, K., Wishart, D.S. “Protein Interaction Databases: How Accurate Are They?” poster presented at the 12th Annual Pacific Symposium in Biocomputing (PSB), Hawaii, Jan. 4-8, 2010.
- 204) Zhou, J., Sobsey, C., Berjanskii, M., Liang, J., Lin, G., Wishart, D.S. “New Methods for the Assessment of Protein Structure Quality” poster presented at the 12th Annual Pacific Symposium in Biocomputing (PSB), Hawaii, Jan. 4-8, 2010.
- 205) Sinelnikov, I., Bouatra, S., Psychogios, N., Dong, E., Huang, P., Saleem, F., Krishna Murthy, R., Mandal, R., Wishart, D.S., Bogumil, R., Roehring, C., Kania A. “Targeted Metabolomics Analysis of Human Urine Using a Combined Flow Injection LC-MS/MS Assay” poster presented at the Metabolomics and More Symposium, Munich, Germany, March 10-12, 2010.
- 206) Bjorndahl, T.C., Perez-Pineiro, R., Lui, X., Acharya, S., Saleem, F., Semenchenko, V., Zhou, G.P., Wishart, D.S. “pH Induced Structural Changes and Fibrillar Formation of the Syrian Hamster Prion Protein (shPrP)” abstract presented at the PrP2010 Conference, Ottawa, Ontario, March 8-10, 2010.
- 207) Lo, A., Graham, C., Wishart, D.S., Li, L. “Biomarker Discovery in CWD-infected Elk by Mass Spectrometry” poster presented at the PrP2010 Conference, Ottawa, Ontario, March 8-10, 2010.
- 208) Bjorndahl, T.C., Liu, X., Zhou, G.P., Semenchenko, V., Saleem, F., Acharya, S., Bujold, A., Sobsey, C., Wishart, D.S. “Conversion of the Syrian Hamsters Prion Protein to Beta Oligomer and Fibril Forms Under Physiological pH Conditions” poster presented at the PrP2010 Conference, Ottawa, Ontario, March 8-10, 2010.

- 209) Subhrangsu, C., Julien, O., Sweeting, B., Acharya, S., Semenchenko, V., Pai, E.F., Chakrabarty, A., Wishart, D.S., Sykes, B.D. "Urea Unfolding Studies of Bovine, Syrian Hamster and Rabbit Prion Proteins" poster presented at the PrP2010 Conference, Ottawa, Ontario, March 8-10, 2010.
- 210) Dorosh, L., Blinov, N., Berjanskii, M., Wishart, D.S., Kovalenko, A. "Temperature Driven Unfolding of Human Prion Protein: Thermodynamics and Microscopic Solvation" poster presented at the PrP2010 Conference, Ottawa, Ontario, March 8-10, 2010.
- 211) Perez-Pineiro, R., Bjorndahl, T.C., Dong, Y.W., Wishart, D.S. "Does the Prion Protein Fixate, Transport or Utilize Thiamine?" poster presented at the PrP2010 Conference, Ottawa, Ontario, March 8-10, 2010.
- 212) Acharya, S., Saleem, F., Bjorndahl, T.C., Semenchenko, V., Wishart, D.S. "Characterizing the Intermediate States of Prion Protein Conversion to the Beta-rich Isoform Under Mildly Denaturing Conditions Using Urea and Salt" poster presented at the PrP2010 Conference, Ottawa, Ontario, March 8-10, 2010.
- 213) Psychogios, N., Mandal, R., Sinelnikov, I., Sobsey, C., Yang, J., Westaway, D., Guo, K., Peng, J., Li, L., Graham, C., Wishart, D.S. "Biomarkers of Disease State in Alzheimer's Disease Model Mice: A Tool for Understanding Neurodegenerative Amyloidoses" poster presented at the PrP2010 Conference, Ottawa, Ontario, March 8-10, 2010.
- 214) Mandal, R., Psychogios, N., Dong, Y.W., Bouatra, S., Saleem, F., Sinelnikov, I., Cosbsey, C., Daude, N., Westaway, D., Lo, A., Li, L., Graham, C., Wishart, D.S. "Using Metabolomics Approaches to Identify Novel Biomarkers for Preclinical Diagnosis and Monitoring of Prion Diseases in Elk" poster presented at the PrP2010 Conference, Ottawa, Ontario, March 8-10, 2010.
- 215) Zhou, J., Liang, Y., Berjanskii, M., Sobsey, C., Lin, G., Wishart, D.S. "New Methods for the Assessment of Protein Structure Quality: Applications to Prion Structures Deposited in the PDB" poster presented at the PrP2010 Conference, Ottawa, Ontario, March 8-10, 2010.
- 216) Frolkis, A., Brons, C., Mandal, R., Psychogios, N., Bouatra, S., Sinelnikov, I., Knox, C., Guo, A., Gautam, B., Eisner, R., Dong, Y.W., Huang, X.P., Krishnamurthy, R., Wishart, D.S. "Comprehensive quantitative characterization of the human CSF, serum, and urine metabolome" poster presented at the Metabolomics Society's 6<sup>th</sup> Annual International Conference, Amsterdam, Holland, June 27-July 1, 2010.
- 217) Xia, J., Wishart, D.S. "MSEA: A web-based tool to identify biologically meaningful patterns in quantitative metabolomics data" poster presented at the Metabolomics Society's 6<sup>th</sup> Annual International Conference, Amsterdam, Holland, June 27-July 1, 2010.



218) Issack B.B, Berjanskii, M., Wishart D.S., Stepanova M. “Probing the conformational dynamics of sheep prion dimers” presented at the 17<sup>th</sup> Canadian Symposium on Theoretical Chemistry, Edmonton, AB, July 25-30, 2010.

219) Santos, K.P., Berjanskii, M., Wishart D.S., Stepanova M. “Collective Dynamics in Prion Proteins: a Comparative Analysis of Disease-Prone and Disease-Resistant Species” presented at the 17<sup>th</sup> Canadian Symposium on Theoretical Chemistry, Edmonton, AB, July 25-30, 2010.

220) Ametaj, B.N., Saleem, F., Semenchenko, V., Sobsey, C., Wishart, D.S. “Lipopolysaccharide Interacts with Prion Protein and Catalytically Converts it into a Protease Resistant Beta-sheet Rich Isoform”, presented at the Prion 2010 conference, Salzburg, Austria, Sept. 8-11, 2010.

221) Perez-Pineiro, R., Bjorndahl, T.C., Dong, Y.W., Berjanskii, M.V., Li, L., Huang, A., Lee, R., Gibbs, E., Cashman, N., Wishart, D.S. “Probing prion interactions with small molecule human metabolites”, presented at the Prion 2010 conference, Salzburg, Austria, Sept. 8-11, 2010.

222) Semenchenko, V.V., Bjorndahl, T.C., Liu, X., Zhou, G.P., Saleem, F., Acharya, S., Bujold, A., Sobsey, C., Wishart, D.S. “Conversion of Syrian hamster prion protein to beta oligomer and fibril forms under physiological pH conditions”, presented at the Prion 2010 conference, Salzburg, Austria, Sept. 8-11, 2010.

223) Issack B.B, Berjanskii, M., Wishart D.S., Stepanova M. “Probing the conformational dynamics of sheep prion dimers” presented at the PrioNet/APRI Annual Scientific Meeting, Vancouver, BC, Oct. 24-26, 2010.

224) Santos, K.P., Berjanskii, M., Wishart D.S., Stepanova M. “Collective Dynamics in Prion Proteins: a Comparative Analysis of Disease-Prone and Disease-Resistant Species” presented at the PrioNet/APRI Annual Scientific Meeting, Vancouver BC, Oct. 24-26, 2010.

225) Guest, W.C., Gibbs, E., Grad, L.I., Semenchenko, V., Wishart, D.S. Plotkin, S.S., Cashman, N.R. “Misfolding of Wild-Type Superoxide Dismutase 1 Induced by Contact with Aggregated Mutant Superoxide Dismutase 1 in a Defined in vitro System: Generalization of the Prion “Protein-Only” Hypothesis to Amyotrophic Lateral Sclerosis” presented at the Prion 2011, Montreal QC, May 16-19, 2011.

226) Ametaj, B.N., Dunn, S.M., Bjorndahl, T.C., Saleem, F., Perez-Peneiro, R., Ladner, C., Sobsey, C., Wishart, D.S. “Is the Prion Protein an Innate Immune Response Protein?” presented at the Prion 2011, Montreal QC, May 16-19, 2011.

- 227) Blinov, N., Dorosh, L., Wishart, D.S., Kovalenko, A. “Thermodynamics of Formation and Inhibition of Amyloid Fibrils Studied with the Three-Dimensional Molecular Theory of Solvation” presented at the Prion 2011, Montreal QC, May 16-19, 2011.
- 228) Isaack, B.B., Santo, K.P., Frito, T., Berjanskii, M., Wishart, D.S., Stepanova, M. “Exploring the Conformational Dynamics of Prion Proteins to Understand the Mechanism of Susceptibility/Resistance to Pathological Conversion” presented at the Prion 2011, Montreal QC, May 16-19, 2011.
- 229) Ladner, C.L., Acharya, S., Bjorndahl, T.C., Suriyamongkol, B.P., Wishart, D.S. “A Novel, High-Resolution Native Gel Electrophoresis Technique for Characterizing PrP<sup>Sc</sup> Oligomers” presented at the Prion 2011, Montreal QC, May 16-19, 2011.
- 230) Pagadala, N.S., Blinov, N., Wishart, D.S., Kovalenko, A. “Computational Binding Studies of Thiamine and Receptor Based Discovery of New Antiprion Compounds Against Prion Protein via Docking and Pharmacophore Modeling” presented at the Prion 2011, Montreal QC, May 16-19, 2011.
- 231) Saleem, F., Bjorndahl, T.C., Semenchenko, V., Ametaj, B.N., Wishart, D.S. “Lipotechoic Acid (LTA) Interacts with the Prion Protein and Converts it into a Self-Propagating Proteinase Resistant Beta Rich Isoform” presented at the Prion 2011, Montreal QC, May 16-19, 2011.
- 232) Suriyamongkol, B.P., Abera, A. Semenchenko, V., Sobsey, C., Wishart, D.S. “The Prionet Prion Protein and Plasmid Production Platform Facility” presented at the Prion 2011, Montreal QC, May 16-19, 2011.
- 233) Chatterjee, S., Sykes, B.D., Julien, O., Bjorndahl, T.C., Wishart, D.S., Semenchenko, V., Sweeting, B., Acharya, S., Chakrabarty, A., Pai, E.P., Cashman, N. “Species Specific Urea Unfolding of Prion Proteins” presented at the Prion 2011, Montreal QC, May 16-19, 2011.
- 234) Ametaj, B.N., Hosseini, A., Lam, T., Farooq, U., Dunn, S.M., Wishart, D.S. “Lipopolysaccharide Affects Permeation of Prion Protein Through Gastrointestinal Tract of Rodents” presented at the Prion 2011, Montreal QC, May 16-19, 2011.
- 235) Saleem, F., Bjorndahl, T.C., Perez-Pineiro, R., Ladner, C., Semenchenko, V., Ametaj, B.N., Wishart, D.S. “Bacterial Lipopolysaccharide, a Trigger of Prion Fibrillar Disease?” presented at the Prion 2011, Montreal QC, May 16-19, 2011.
- 236) Berjanskii, M., Wishart, D.S. “ResProx – A new method to calculate protein coordinate quality” presented at the 5<sup>th</sup> Gordon Research Conference on Computational Aspects of Biomolecular NMR, Il Ciocco, Italy, May 22-27, 2011.

- 237) Han, B., Wishart D.S. “Accurate calculation of protein chemical shifts” presented at the 5<sup>th</sup> Gordon Research Conference on Computational Aspects of Biomolecular NMR, Il Ciocco, Italy, May 22-27, 2011.
- 238) Petrotchenko, E.V., Serpa, J.J., Wishart, D.S., Borchers, C.H. “Proteinase K Non-Specific Digestion for the Comprehensive Identification of Interpeptide Crosslinks: Application to Prion Proteins” presented at the ASMS 2011 Conference, Denver, CO, June 5-11, 2011
- 239) Peng, J., Guo, K., Xia, J., Zhou, J., Yang, J., Westaway, D., Wishart, D.S., Li, L. “A quantitative metabolomic study on transgenic mice urine samples of Alzheimer’s disease by dansylation labeling and LC-FTICR-MS” presented at the ASMS 2011 Conference, Denver, CO, June 5-11, 2011.
- 240) Petrochenko, E.V., Patterson, A., Cabecinha, A. Han, J., Serpa, J.J., Wishart, D.S., Borchers, C.H. “Structural Proteomics Characterization of Prion Protein Aggregation” presented at the ASMS 2011 Conference, Denver, CO, June 5-11, 2011.
- 241) Blydt-Hansen, T., Mandal, R., Wishart, D.S. “Urine metabolite profiles distinguish acute rejection from acute allograft injury and normal functioning allografts in pediatric renal transplant recipients” presented at the 6<sup>th</sup> IPTA Congress, Montreal QC, June 25-28, 2011.
- 242) Mandal, R., Sobsey, C., Krishnamurthy, R., Bouatra, S., Sinelnikov, I., Chaudhary, K., Dong, Y.W., Huang, X.P., Aziat, F., Liu, P., Xia, J., Li, L., Borchers, C., Wishart, D.S. “An Update on Canada’s National Metabolomics Platform – TMIC” presented at the 7<sup>th</sup> Annual Metabolomics Society Meeting, Cairns, Australia, June 27-30, 2011.
- 243) Mandal, R., Sobsey, C.A., Dong, Y., Iqbal, S., Dunn, S.M., Ametaj, B.N., Wishart, D.S. “Identification of Biomarkers Associated with the Onset and Progression of Major Metabolic and Infectious Diseases of Transition Dairy Cows” presented at the 7<sup>th</sup> Annual Metabolomics Society Meeting, Cairns, Australia, June 27-30, 2011.
- 244) Mandal, R., Farooq, U., Saleem, F., Krishnamurthy, R., Dong, Y., Sobsey, C.A., Guo, A., Dunn, S.M., Ametaj, B.N., Wishart, D.S. “The Bovine Milk Metabolome” presented at the 7<sup>th</sup> Annual Metabolomics Society Meeting, Cairns, Australia, June 27-30, 2011.
- 245) Neveu, V., Liu, Y., Guo, A.C., Guo, C, Djoumbou, Y., Scalberta, A., Wishart, D.S. “The FooDB: A Comprehensive Database on Food Constituents and their Health Promoting Effects” presented at the 5<sup>th</sup> International Conference on Polyphenols and Health, Barcelona, Spain, Oct. 17-20, 2011.

- 246) Wishart, D.S., Berjanskii, M., Zhou, J., Liang, Y., Lin, G. “Resolution by Proxy: A Simple Measure for Assessing and Comparing the Overall Quality of NMR Protein Structures” presented at the 14th Annual Pacific Symposium in Biocomputing Conference (PSB2012), Hawaii, USA, Jan. 4-8, 2012.
- 247) Blydt-Hansen, T., Mandal, R., Xia, J., Sarwal, M., Wishart, D.S. “Validation of urine metabolites (NMR) for detection of cell-mediated acute rejection in pediatric renal transplant recipients” presented at the 3<sup>rd</sup> International Conference on Transplantomics and Biomarkers in Organ Transplantation, La Jolla, CA, March 8-10, 2012.
- 248) Blydt-Hansen, T., Mandal, R., Xia, J., Wishart, D.S. “Urine metabolites (MS) distinguish cell-mediated rejection from acute allograft injury and normal functioning allografts in pediatric renal transplant recipients” presented at the 3<sup>rd</sup> International Conference on Transplantomics and Biomarkers in Organ Transplantation, La Jolla, CA, March 8-10, 2012.
- 249) Pan, J., Zhang, S., Petrotchenko, E., Han, J., Wishart, D.S., Borchers, C.H. “Deciphering Prion Conformational Changes during Monomer to Oligomer Conversion by Top-Down HDX with Electron Capture Dissociation” presented at the 60<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Vancouver, BC, May 20-24, 2012.
- 250) Peng, J., Guo, K., Xia, J., Zhou, J., Yang, J., Westaway, D., Wishart, D.S., Li, L. “A quantitative metabolomic study on transgenic mice urine samples of Alzheimer’s disease by dansylation labeling and LC-FTICR-MS” presented at the 60<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Vancouver, BC, May 20-24, 2012.
- 251) Petrochenko, E., Patterson, A., Cabecinha, A., Han, J., Serpa, J., Wishart, D.S., Borchers, C.H. “Structural Proteomics Characterization of Prion Protein Aggregation” presented at the 60<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Vancouver, BC, May 20-24, 2012.
- 252) Ladner, C.L., Perez-Pineiro, R., Li, L., Gibbs, E., Bjorndahl, T., Cashman, N., Wishart, D.S. “Native electrophoresis techniques for the identification of oligomerization-interfering small compounds” presented at the Joint PrP-Canada and Protein Folding and Disease Conference, Toronto ON, June 25-27, 2012.
- 253) Saleem, F., Bjorndahl, T.C., Perez-Pineiro, R., Semenchenko, V., Ametaj, B.N., Wishart, D.S. “Lipopolysaccharide Induced Catalytic Self-Propagation of Recombinant Prion Misfolding” presented at the Joint PrP-Canada and Protein Folding and Disease Conference, Toronto ON, June 25-27, 2012.

254) Stepanova, M., Issack, B.B., Santo, K.P., Berjanskii, M., Wishart, D.S. “Structure and essential dynamics of prion proteins: comparative analysis for evolutionarily diverse vertebrate species, polymorphic variants and mutants” presented at the Joint PrP-Canada and Protein Folding and Disease Conference, Toronto ON, June 25-27, 2012.

255) Hosseini, A., Lam, T., Farooq, U., Dunn, S.M., Wishart, D.S., Ametaj, B.N. “Lipopolysaccharide affects permeation of prion protein through gastrointestinal tract of rodents” presented at the Joint PrP-Canada and Protein Folding and Disease Conference, Toronto ON, June 25-27, 2012.

256) Ametaj, B.N. and Wishart, D.S. “A new understanding of the functions of prion protein” presented at the Joint PrP-Canada and Protein Folding and Disease Conference, Toronto ON, June 25-27, 2012.

257) Sobsey, C.A., Mandal, R., Krishnamurthy, R., Bouatra, S., Sinenikov, I., Guo, A.C., Liu, P., Chaudhary, K.K., Dong, E., Azit, F., Yallou, F.S., Wishart, D.S. “Characterizing diseases using multi-platform metabolomics techniques” presented at the 8<sup>th</sup> Annual Metabolomics Society Meeting, Washington, DC, June 25-28, 2012.

258) Bouatra, S., Aziat, F., Guo, A.C., Mandal, R., Sinenikov, I., Liu, P., Chaudhary K.K., Dong, E., Yallou, F.S., Bogumil, R., Wishart, D.S. “The Human Urine Metabolome” presented at the 8<sup>th</sup> Annual Metabolomics Society Meeting, Washington, DC, June 25-28, 2012.

259) Rush, D., Mandal, R., Wishart, D.S., Wiebe, C., Ho, J., Storsley, L., Karpinski, M., Gibson, I., Nickerson, P. “Non-invasive Diagnosis of Renal Allograft Inflammation using Quantitative Urine Metabolomics” presented at the 24<sup>th</sup> International Congress of the Transplantation Society, Berlin, Germany, July 15-19, 2012.

260) Bahado-Singh, R., Akolekar, R., Mandal, R., Chelliah, A., Dong, E., Xiz, J., Kruger, M., Wishart, D.S., Nicolaides, K. “Metabolic prediction of trisomy 18 first trimester pregnancies” presented at the 33<sup>rd</sup> Annual Meeting of the Society for Maternal-Fetal Medicine: The Pregnancy Meeting, San Francisco, CA, Feb. 11-16, 2013.

261) Kenny, L.C., Broadhurst, D.I., Hong, W., Stanley, J., Andersson, I., Rueda-Clausen, C., Mandal, R., Wishart, D., Baker, P.N. “NMR Profiling in Early Pregnancy Reveals a Metabolomic Signature that Predicts the Subsequent Development of Preeclampsia” Presented at the 60<sup>th</sup> Society for Gynecologic Investigation Meeting, Orlando, Florida, USA, Mar. 20-23, 2013.

262) Baker, P.N., Hong, W., Stanley, J.L., Andersson, I.J., Sibley, C., Davidge, S., Kenny, L.C., Mandal, R., Wishart, D., Broadhurst, D. “Sildenafil Therapy Alters the Aberrant Metabolomic Profile

in a Mouse Model of Preeclampsia/Fetal Growth Restriction” Presented at the 60<sup>th</sup> Society for Gynecologic Investigation Meeting, Orlando, Florida, USA, Mar. 20-23, 2013.

263) Perez-Pineiro, R., Bjorndahl, T.C., Berjanskii, M., Ladner, C., Pagadala, N.S., Wishart, D.S. “Interaction of a diazirine modified curcumin analog with the beta-oligomeric form of the Syrian hamster prion protein” presented at the Prion 2013 Conference, Banff, AB, May 26-29, 2013.

264) Glaves, J.P.J., Daude, N., Wishart, D.S., Westaway, D., Sykes, B.D. “Metabolite profiles allow pre-symptomatic diagnosis of mouse prion infections” presented at the Prion 2013 Conference, Banff, AB, May 26-29, 2013.

265) Kovalenko, A., Blinov, N., Wishart, D.S. “A new computational platform for predictive description of pathological conversion of prion proteins” presented at the Prion 2013 Conference, Banff, AB, May 26-29, 2013.

266) Ladner, C.L., Wishart, D.S. “Shaking alone converts PrP<sup>C</sup> to beta-sheet rich fibrils” presented at the Prion 2013 Conference, Banff, AB, May 26-29, 2013.

267) Blinov, N., Huang, W., Wishart, D.S., Kovalenko, A. “Thermodynamic stability of amyloid fibrils and beta-sheet oligomers: perspective of molecular theory of solvation” presented at the Prion 2013 Conference, Banff, AB, May 26-29, 2013.

268) Hailamariam, D., Goldansaz, S.A., Saleem, F., Daude, N., Wishart, D.S., Westaway, D., Ametaj, B.N. “Chronic subcutaneous lipopolysaccharide aggravated transmissible spongiform encephalopathy in mice teated subcutaneously with RML and mouse recombinant PrP<sup>B</sup>” presented at the Prion 2013 Conference, Banff, AB, May 26-29, 2013.

269) Goldansaz, S.A., Hailamariam, D., Saleem, F., Daude, N., Wishart, D.S., Westaway, D., Ametaj, B.N. “Brain histology changes detected at 11 weeks post-infection in RML and PrP<sup>B</sup> subcutaneously infected mice” presented at the Prion 2013 Conference, Banff, AB, May 26-29, 2013.

270) Goldansaz, S.A., Hailamariam, D., Saleem, F., Daude, N., Wishart, D.S., Westaway, D., Ametaj, B.N. “Subcutaneous injection of lipopolysaccharide-converted mouse PrP beta modulated gene expression in the brain of FVB/N mice” presented at the Prion 2013 Conference, Banff, AB, May 26-29, 2013.

271) Pagdala, N.S., Perez-Pineiro, R., Bjorndahl, T., Saini, R., Ladner, C., Berjanskii, M., Gibbs, E., Cahsman, N., Wishart, D.S. “In silico PrP<sup>Sc</sup> inhibitor screening of 60,000 commercially available compounds” presented at the Prion 2013 Conference, Banff, AB, May 26-29, 2013.

- 272) Bjorndahl, T., Perez-Pineiro, R., Saini, R., Ladner, C., Pagdala, N.S., Berjanskii, M., Li, L., Gibbs, E., Cahsman, N., Wishart, D.S. “Binding of epigallocatechin gallate to monomeric, oligomeric and fibril forms of the Syrian hamster prion protein” presented at the Prion 2013 Conference, Banff, AB, May 26-29, 2013.
- 273) Serpa, J., Petrotchenko, E., Wishart, D.S., Borchers, C. “Using Isotopically-Coded Hydrogen Peroxide as a Surface Modification Reagent for the Structural Characterization of Prion-Protein Aggregates” presented at the 61<sup>st</sup> American Society for Mass Spectrometry (ASMS) Conference, Minneapolis, MN, June 9-13, 2013.
- 274) Serpa, J., Petrotchenko, E., Wishart, D.S., Borchers, C. “Inter-subunit contacts in prion oligomers studied by crosslinking of 15N-metabolically labeled prion proteins” presented at the 61<sup>st</sup> American Society for Mass Spectrometry (ASMS) Conference, Minneapolis, MN, June 9-13, 2013.
- 275) Mandal, R., Lim, T., Li, L., Harynuk, J., Borchers, C., Wishart, D.S. “Targeted and Non-targeted Quantitative Metabolomics Using A Multi-Platform Approach” Presented at the University of Alberta OMICS Symposium, Edmonton, AB, June 17, 2013.
- 276) Mandal, R., Lim, T., Krishnamurthy, R., Bjorndahl, T.C., Aziat, F., Dame, Z., Dong, E., Bouatra, S., Liu, P.B., Guo, A.C., Han, B., Wilson, M., Yallou, F., Li, L., Harynuk, J., Borchers, C., Wishart, D.S. “Targeted and Non-targeted Quantitative Metabolomics Using A Multi-Platform Approach” Presented at the 9<sup>th</sup> Annual Conference of the Metabolomics Society, Glasgow, Scotland, July 1-4, 2013.
- 277) Mandal, R. Bahado-Singh, R.O., Akolekar, R., Nicolaidis, K., Broadhurst, D.I., Kenny, L.C., Murray, D.M., Wishart, D.S. “Application of Quantitative Metabolomics in Human Maternal, Prenatal and Neonatal Disease Biomarker Studies” Presented at the 9<sup>th</sup> Annual Conference of the Metabolomics Society, Glasgow, Scotland, July 1-4, 2013.
- 278) Ravanbakhsh, S., Liu, P.B., Bjorndahl, T.C., Wilson, M., Mandal, R., Eisner, R., Sinelnikov, I., Dong, E., Wishart, D.S. “Fully Automated NMR Spectral Profiling for Metabolomics – BAYESIL” Presented at the 9<sup>th</sup> Annual Conference of the Metabolomics Society, Glasgow, Scotland, July 1-4, 2013.
- 279) Scalbert, A., Neveu, V., Knox, C., Wishart, D.S. “The Phenol-Explorer Database on The Polyphenol Metabolome as an Aid to Identify Novel Biomarkers of Dietary Exposure for Nutritional Epidemiology” Presented at the 9<sup>th</sup> Annual Conference of the Metabolomics Society, Glasgow, Scotland, July 1-4, 2013.

- 280) Sulek, K., Baker, P.N., Wishart, D.S., Kenny, L. “Mouse Model of Fetal Growth Restriction Shows an Altered Serum Metabolic Profile Which is Reversible Following Treatment with Sildenafil Citrate” Presented at the 9<sup>th</sup> Annual Conference of the Metabolomics Society, Glasgow, Scotland, July 1-4, 2013.
- 281) Blydt-Hansen, T., Mandal, R., Gibson, I., Wishart, D. “Urine Metabolites for Diagnosis of Clinical and Subclinical Rejection in Pediatric Kidney Transplants”, Presented at the 7<sup>th</sup> Congress on Pediatric Transplantation, Warsaw, Poland, July 13-16, 2013.
- 282) Blinov, N., Huang, W., Nikolic, D., Wishart, D.S., Kovalenko, A. “Biomolecular Recognition Based on 3D Molecular Theory of Solvation”, Presented at the 58<sup>th</sup> Annual Meeting of the Biophysical Society, San Francisco, Feb. 15-19, 2014.
- 283) Sulek, K., Han, T.L., Villas-Boas, S.G., Kwek, K., Chong, Y.S., Wishart, D.S., Kenny, L.C., Baker, P.N. “Metabolic Profiling Identifies Biomarkers of FGR in Maternal Hair”, Presented at the 61<sup>st</sup> Annual Meeting of the Society for Gynecologic Investigation, Florence, Italy, March 26-29, 2014.
- 284) Hsin, M.K., Zamel, R., Cypel, M., Hashimoto, K., Chen, M., Machuca, T., Wishart, D., Han, B., Waddell, T.K., Liu, M., Keshavjee, S. “Metabolic Profiling of Perfusate from Clinical Ex Vivo Lung Perfusion Yields Potential Biomarkers of Early Lung Transplant Outcomes” Presented at the 34<sup>th</sup> Annual International Society for Heart and Lung Transplantation (ISHLT) Meeting, San Diego, CA, April 10-13, 2014.
- 285) Moehn, S., Mandal, R., Bjorndahl, T., Yallou, F., Wishart, D., Pencharz, P., Ball, R., Plastow, G. “Effects of pregnancy status, individual animal and age of pigs on plasma metabolome” Presented at the Experimental Biology 2014 Conference, San Diego, CA, April 26-30, 2014.
- 286) Moehn, S., Han, B., Krishnamurthy, R., Liu, P., Bouatra, S., Wishart, D., Pencharz, P., Ball, R., Plastow, G. “Effects of amino acid intake level in pregnant pigs on plasma metabolome” Presented at the Experimental Biology 2014 Conference, San Diego, CA, April 26-30, 2014.
- 287) Keshteli, A.H., van den Brand, F.F., Wishart, D., Mandal, R., Bjorndahl, T.C., Han, B., Baarda, J., Kroeker, K.I., Valcheva, R., Fedorak, R.N., Madsen, K., Dieleman, L.A. “Dietary Fat Intake, Fecal Calprotectin and Metabolomic Profiles Predict Relapse of Ulcerative Colitis” Presented at the Digestive Disease Week (DDW) 2014 Conference, Chicago, USA, May 3-6, 2014.



- 288) Goldansaz, S.A., Hailemariam, D., Westaway, D., Mandal, R., Wishart, D., Ametaj, B.N. “Metabolomics approach reveals lipid and carbohydrate alterations in the urine of FVB/N female mice subcutaneously infected with RML and RML plus lipopolysaccharide” Presented at the Prion 2014 Conference, Trieste, Italy, May 27-30.
- 289) Goldansaz, S.A., Hailemariam, D., Daude, N., Westaway, D., Wishart, D., Ametaj, B.N. “In vitro generated mouse prion protein causes brain neurodegeneration in FVB/N female mice” Presented at the Prion 2014 Conference, Trieste, Italy, May 27-30.
- 290) Deng, L., Mandal, R., Wishart, D.S. “Adductomics Analysis of Human Serum Albumin by Mass Spectrometry” Presented at the American Society for Mass Spectrometry (ASMS) Conference, Baltimore, MD, June 15-19, 2014.
- 291) Deng, L., Mandal, R., Wishart, D.S. “Adductomics Analysis of Human Serum Albumin by Mass Spectrometry” Presented at the 10<sup>th</sup> International Metabolomics Society Conference, Tsuruoka, Japan, June 23-26, 2014.
- 292) Ravanbakhsh S., Liu, P.B., Bjorndahl, T.C., Wilson, M., Mandal, R., Grant, J., Wisner, T., Han, B., Krishnamurthy, R., Aziat, F., Dong, E., Greiner, R., Wishart, D.S. “Automated NMR, GC-MS-based Kits for Quantitative Metabolomics” Presented at the 10<sup>th</sup> International Metabolomics Society Conference, Tsuruoka, Japan, June 23-26, 2014.
- 293) Dame, Z.T., Aziat, F., Mandal, R., Lim, T., Krishnamurthy, R., Bouatra, S., Borzouie, S., Guo, A.C., Liu, P.B., Saleem F., Dong, E., Wishart, D.S. “The Human Saliva Metabolome” Presented at the 10<sup>th</sup> International Metabolomics Society Conference, Tsuruoka, Japan, June 23-26, 2014.
- 294) Mandal, R., Reid, J., Bjorndahl, T.C., Krishnamurthy, R., Aziat, F., Dame, Z., Deng, L., Han, B., Dong, E., Liu, P.B., Guo, A.C., Wilson, M., Pon, A., Lim, T., Reid, C., Harynuck, J., Li, L., Borchers, C., Wishart, D.S. “Application of Targeted and Non-targeted Quantitative Metabolomics in Human Disease Biomarker Studies” Presented at the 10<sup>th</sup> International Metabolomics Society Conference, Tsuruoka, Japan, June 23-26, 2014.
- 295) Wishart, D.S., Jewison, T., Pon, A., Wilson, M., Knox, C., Disfany, F.M., Maciejewski, A., Su, Y. “PathWhiz: a Web Server for High Quality Pathway Generation and Visualization in Systems Biology” Presented at the 15<sup>th</sup> International Conference of on Systems Biology, Melbourne Australia, Sept. 14-18, 2014.
- 296) Pon, A., Jewison, T., Wilson, M., Knox, C., Su, Y., Disfany, F.M., Maciejewski, A., Wishart, D.S. “PathWhiz: a Web Server for High Quality Pathway Generation” Presented at the Pacific Symposium on Biocomputing 2015, Hawaii, Jan. 4-8, 2015.

- 297) Ravanbakhsh, S., Liu, P., Bjorndahl, T.C., Mandal, R., Grant, J.R., Wilson, M., Eisner, R., Sinelnikov, I., Hu, X., Luchinat, C., Greiner, R., Lim, T., Wishart, D.S. “Automated molecular phenotyping using Bayesil” Presented at the Pacific Symposium on Biocomputing 2015, Hawaii, Jan. 4-8, 2015.
- 298) Blydt-Hansen, T., Wishart, D., Mandal, R., Sharma, A., Gibson, I., Ho, J., Rush, D., Nickerson, P. “Urine metabolomics for identifying risk of late antibody-mediated rejection”. Presented at the International Pediatric Transplant Association 8<sup>th</sup> Congress on Pediatric Transplantation, San Francisco, USA, March 28-31, 2015.
- 299) Keshteli, A.H., van den Brand, F.F., Valcheva, R., Wishart, D.S., Mandal, R., Kroeker, K., Fedorak, R.N., Madsen, K., Dieleman, L.A. “Ulcerative Colitis Patients With and Without Subclinical Inflammation Can Be Differentiated From Healthy Controls Through Metabolomic Profiling”. Presented at Digestive Disease Week, Washington, DC, USA, May 16-19, 2015.
- 300) Dervishi, E., Zwierzchowski, G., Hailemariam, D., Lam, T.H., Dunn, S., Wishart, D., Ametaj, B. “Mouse recombinant prion protein alone or in combination with bacterial LPS modulated production of colon proteins involved in innate immune responses in Fvb/N mice” Presented at Prion 2015, Fort Collins, CO, USA May 26-29, 2015.
- 301) Hailemariam, D., Lam, T.H., Dervishi, E., Zwierzchowski, G., Dunn, S., Wishart, D., Ametaj, B. “Recombinant mouse prion protein alone or combined with detoxified lipopolysaccharide affects colon immune protein levels of Fvb/N mice”. Presented at Prion 2015, Fort Collins, CO, USA May 26-29, 2015.
- 302) Zwierzchowski, G., Daude, N., Dunn, S., Wishart, D., Ametaj, B. “Intracranial injection of LPS-converted mouse recombinant PrP alone or with LPS causes brain neurodegeneration in Fvb/N mice”. Presented at Prion 2015, Fort Collins, CO, USA May 26-29, 2015.
- 303) Zwierzchowski, G., Hailemariam, D., Dunn, S., Wishart, D., Ametaj, B. “Subcutaneously administered LPS-converted recombinant mouse prion protein alone or in combination with LPS modulates the content of prion-related proteins in the brain of Fvb/N mice”. Presented at Prion 2015, Fort Collins, CO, USA May 26-29, 2015.
- 304) Wishart, D.S., Berjanskii, M. “A Robust Method for Optimizing Protein Structures Using Chemical Shifts” Presented at the Gordon Research Conference Computational Aspects of Biomolecular NMR, Il Ciocco, Italy, June 7-12, 2015.

- 305) Ahmed, R., Reid, J., Sitar, D., Maksymiuk, A., Mandal, R., Wishart, D.S. “Discovery of novel metabolite biomarkers for early diagnosis of lung cancer and monitoring chemotherapy treatment response” Presented at the 11<sup>th</sup> International Conference of the Metabolomics Society, Burlingame, CA, USA, June 29-July 2, 2015.
- 306) Mandal, R., Goldansaz, S., Saleem, F., Guo, A.C., Deng, L., Lin, H., Dong, E., Ametaj, B., Wishart D.S. “The Bovine Milk Metabolome” Presented at the 11<sup>th</sup> International Conference of the Metabolomics Society, Burlingame, CA, USA, June 29-July 2, 2015.
- 307) Borzouie, S., Sajed, T., Mandal, R., Krishnamurthy, R., Bouatra, S., Guo, A.C., Deng, L., Lin, H., Liu, P., Dong, E., Wishart, D.S. “Application of metabolomics to measure the Foodome” Presented at the 11<sup>th</sup> International Conference of the Metabolomics Society, Burlingame, CA, USA, June 29-July 2, 2015.
- 308) Gibbons, H., Carr, E., Wishart, D.S. Frost, G., Brennan, L. “Metabolomics based discovery of a panel of biomarkers for the assessment of red meat intake” Presented at the 11<sup>th</sup> International Conference of the Metabolomics Society, Burlingame, CA, USA, June 29-July 2, 2015.
- 309) Wishart, D.S., Pon, A., Jewison, T., Su, Y., Liang, Y., Knox, C., Maciejewski, A., Wilson, M. “PathWhiz: A Web-enabled Pathway Drawing Tool” Presented at the 11<sup>th</sup> International Conference of the Metabolomics Society, Burlingame, CA, USA, June 29-July 2, 2015.
- 310) Deng, L., Mandal, R., Bjorndahl, T., Liu, P., Ravanbakhsh, S., Han, B., Dong, E., Allen, F., Greiner, R., Li, L., Lin, G., Wishart, D.S. “Automated Software for Quantitative Metabolomics” Presented at the 11<sup>th</sup> International Conference of the Metabolomics Society, Burlingame, CA, USA, June 29-July 2, 2015.
- 311) Jayaseelan, K.V., Xia, J., Nainala, V., Haug, K., Mingo, P., Wishart, D.S., Steinbeck, C. “R-Cloud based analysis of metabolomics data with MetaboAnalyst in MetaboLights Labs” Presented at the 11<sup>th</sup> International Conference of the Metabolomics Society, Burlingame, CA, USA, June 29-July 2, 2015.
- 312) Xia, J., Wishart D.S. “Making Metabolomics More Meaningful – Introducing MetaboAnalyst 3.0 and MetabolomeNet” Presented at the 11<sup>th</sup> International Conference of the Metabolomics Society, Burlingame, CA, USA, June 29-July 2, 2015.
- 313) Zhang, G., Dervishi, E., Hailemariam, D., Deng, Q., Goldansaz, S., Dunn, S., Mandal, R., Han, B., Wishart, D., Ametaj, B. “Metabolomics identifies potential screening and diagnostic serum

biomarkers of laminitis in transition dairy cows” Presented at the 11<sup>th</sup> International Conference of the Metabolomics Society, Burlingame, CA, USA, June 29-July 2, 2015.

314) Zhang, G., Dervishi, E., Hailemariam, D., Deng, Q., Goldansaz, S., Dunn, S., Mandal, R., Han, B., Wishart, D., Ametaj, B. “Metabolomics reveals pathways and biomarkers perturbed before clinical appearance of milk fever in transition dairy cows” Presented at the 11<sup>th</sup> International Conference of the Metabolomics Society, Burlingame, CA, USA, June 29-July 2, 2015.

315) Wishart, D.S., Weinert, C., Pujos-Guillot, E., Ulaszewska, M., Giacomoni, F., Mattivi, F., Urpi-Sarda, M., Andres-Lacueva, C., Kulling, S.E., Dragsted, O., Manach, C. “FoodComEx, a new chemical library for food compounds and their metabolites” Presented at the 4<sup>th</sup> International Foodomics Conference, Cesena, Italy, Oct. 8, 2015.

316) Ametaj, B.N., Hailemarim, D., Zwierzchowski, G., Willing, B.P., Wishart, D.S., Dunn, S.M. “Subcutaneous Administration of Mouse Recombinant Prion Protein Resistant or RML Trigger Long-term Alterations in Composition of Intestinal Microbiota in FVB/N Female Mice” Presented at the Prion 2016 Conference, Tokyo, Japan, May 10-13, 2016

317) Dunn, S.M., Zwierzchowski, G., Hailemarim, D., Willing, B.P., Wishart, D.S., Ametaj, B.N. “Early Age Oral Administration of Mouse Recombinant Prion Protein Resistant or RML Trigger Lifelong Modifications in the Composition of Intestinal Microbiota in FVB/N Female Mice” Presented at the Prion 2016 Conference, Tokyo, Japan, May 10-13, 2016.

318) Blinov, N., Cashman, N.R., Wishart, D.S., Kovalenko, A. “From Misfolding to Aggregation: Sequence Effects on Conformational Properties of Amyloidogenic Peptides Implicated in Neurodegeneration”, Presented at the Prion 2016 Conference, Tokyo, Japan, May 10-13, 2016.

319) Kumari, M., Chow, A., Bridgman, S.L., Tun, M., Mandal, R., Wishart, D.S., Sears, M.R. Subbarao, P., Mandhane, P.J., Turney, S.E., Becker, A.B., Scott, J.A., Kozyrskyj, A.L. “Maternal depression during pregnancy and fecal short chain fatty acid levels in infants” Presented at the 8<sup>th</sup> Annual AllerGen Conference, Vancouver, BC, May 29-June 1, 2016.

320) Manach, C., Weinert, C., Dragsted, L.O., Durang, S., Giacomoni, F., Knox, C., Kulling, S.E., Llorach, R., Neveu, V., Pratico, G., Pujos-Guillot, E., Remus-Rosana, A., Rothwell, J.A., Sajed, T., Ulaszewska, M., Urpi-Sarda, M., Vasquez-Fresno, R., Vazquez-Manjarrez, N., Scalbert, A., Wishart, D.S. “New databases on food compounds and the food metabolome to support discovery of novel dietary biomarkers – A FoodBALL initiative” Presented at the 12<sup>th</sup> International Conference of the Metabolomics Society, Dublin, Ireland, June 27-30, 2016.

321) Vazquez-Fresno, R., Borzouie, S., Mandal, R., Wishart, D.S. “Application of Multi-platform Metabolomics to Characterize the Chemical Composition of Food” Presented at the 12<sup>th</sup> International Conference of the Metabolomics Society, Dublin, Ireland, June 27-30, 2016.

- 322) Mandal, R., Deng, L., Stanislaus, A., Vazquez-Fresno, R., Rezaei-Darestani, R., Zhang, Y., Han, B., Bjorndahl, T.C., Dong, E., Guo, A.C., Stanley, B., Chamot, D., Harynuk, J., Li, L., Borchers, D., Wishart, D.S. “Innovations and Applications of Quantitative Metabolomics in Human Health” Presented at the 12<sup>th</sup> International Conference of the Metabolomics Society, Dublin, Ireland, June 27-30, 2016.
- 323) Wishart, D.S., Djoumbou Feunang, Y., Knox, C., Sajed, T., Allen, Y., Liu, Y., Shi, Z., Budinski, Z., Greiner, R. “New Bioinformatics Tools for Metabolomics”, Presented at the 12<sup>th</sup> International Conference of the Metabolomics Society, Dublin, Ireland, June 27-30, 2016.
- 324) Chamot, D., Deng, L., Mandal, R., Bjorndahl, T., Ravanbakhsh, S., Grant, J., Wilson, M., Han, B., Serra-Cayuela, A., Dong, E., Greiner, R., Wishart, D.S. Automated kits and software for quantitative metabolomics”, Presented at the 12<sup>th</sup> International Conference of the Metabolomics Society, Dublin, Ireland, June 27-30, 2016.
- 325) Wishart, D.S., Marcu, A., Guo, A.C., Anwar, A., Johannessen, S., Knox, C., Wilson, M., Borchers, C.H., Cullis, P., Fraser, R. “Integration, Interpretation and Display of Multi-omic Data for Precision Medicine”, Presented at the 20<sup>th</sup> Pacific Symposium on Biocomputing, Kona, Hawaii, Jan. 4-8, 2017.
- 326) LeVatte, M., Ladner, Keay, C., Berjanskii, M., Bjorndahl, T., Wishart, D.S. “Purification and Characterization of a Highly Soluble Alzheimer’s Disease A $\beta$ 42 Peptide”, Presented at the Alberta Prion Research Institute Scientific Meeting, Edmonton, AB, Feb. 28-March 1, 2017
- 327) Keshteli, A.H., Madsen, K., Nickurak, C., Mandel, R., Kroeker, K., Wishart, D.S., van zanten, S., Halloran, B.P., Fedorak, R.N., Valcheva, R., Dieleman, L.A. “Adherence to an Anti-Inflammatory Diet Prevents Increases in Colonic Inflammation in Ulcerative Colitis Patients in Remission”, Poster abstract presented at Digestive Disease Week 2017, Chicago, USA, May 6-9, 2017.
- 328) Vozza, N., Wishart, D.S. “Development of Assays and Sensors for Metabolomics Screens”, Presented at the 2<sup>nd</sup> Personalized Medicine Summit, Vancouver, BC, June 11-13, 2017.
- 329) Marcu, A., Wishart, D.S., Guo, A.C., Anwar, A., Johannessen, S., Knox, C., Wilson, M., Borchers, C.H., Cullis, P., Fraser, R. “Integration, Interpretation and Display of Multi-omic Data for Personalized Medicine”, Presented at the 2<sup>nd</sup> Personalized Medicine Summit, Vancouver, BC, June 11-13, 2017.

- 330) Swardfager, W., Lanctôt, K.L., Mandal, R., Wishart, D.S., Levitt, A.J. “A Pilot Metabonomic Study of Major Depressive Disorder with Winter-type Seasonal Pattern” Poster presented at Society for Light Treatment and Biological Rhythms, 29th Annual Meeting, Berlin, Germany, June 23-25, 2017.
- 331) Wishart, D.S., Vazquez-Fresno, R., Serray Cayuela, A., Mandal, R., Bhattacharyya, D., Zhang, Y., Iynkkaran, I., Zhang, Z., Assempour, N., Berjanskii, M., Voza, N., Jafari, S. Mari, S. “Automated Kits and Devices of Quantitative Metabolomics”, Presented at the 13<sup>th</sup> Annual Conference of the International Metabolomics Society, Brisbane, Australia, June 25-29, 2017.
- 332) Karu, N., Sajed, T., Djoumbou, Y., Zayeeda, Z., Guo, A.C., Arndt, D., Wishart, D.S. “ContaminantDB: The Environmental Contaminant Database”, Presented at the 13<sup>th</sup> Annual Conference of the International Metabolomics Society, Brisbane, Australia, June 25-29, 2017.
- 333) Kwan, A., Schirra, H., Wishart, D.S. “Developing an Open Learning Environment Unit on Metabolomics”, Presented at the 13<sup>th</sup> Annual Conference of the International Metabolomics Society, Brisbane, Australia, June 25-29, 2017.
- 334) Somerset, A., Bayci, A., Hothem, Z., Turkoglu, O., Keidan, R., Mandal, R., Graham, S., Wishart, D., Bjorndahl, T., Bahado-Singh, R., Han, B. “Metabolomic Identification of Diagnostic Biomarkers for Malignant Melanoma”, Presented at the 13<sup>th</sup> Annual Conference of the International Metabolomics Society, Brisbane, Australia, June 25-29, 2017.
- 335) Reid, J., Mandal, R., Zhang, J., Zhang, Y., Vazquez-Fresno, R., Serray Cayuela, A., Karu, N., Dong, E., Daneshfar, R., Harynuk, J., Li, L., Britz-Mckibbin, P., Overduin, M., Borchers, C., Wishart, D.S. “Targeted and Non-targeted Quantitative Metabolomics Using a Multi-platform Approach”, Presented at the 13<sup>th</sup> Annual Conference of the International Metabolomics Society, Brisbane, Australia, June 25-29, 2017.
- 336) Mandal, R., Bahado-Singh, R., Blydt-Hansen, T., Zhang, G., Ametaj, B., Wishart, D.S. “Application of Quantitative Metabolomics in Disease Biomarker Studies”, Presented at the 13<sup>th</sup> Annual Conference of the International Metabolomics Society, Brisbane, Australia, June 25-29, 2017.
- 337) Mandal, R., Chamot, D., Wishart, D.S. “Application of Targeted Quantitative Metabolomics in Disease Biomarker Studies”, Presented at the MSACL 2018 Meeting, Palm Springs, CA, USA, Jan. 21-25, 2018.

- 338) Fuenang, Y.D., Wishart, D.S. “BioTransformer: A tool for metabolism prediction of small molecules”, Presented at the 255<sup>th</sup> American Chemical Society Meeting, New Orleans, LA, USA, March 18-22, 2018.
- 339) Feunang, Y.D., Wishart, D.S. “Cheminformatics tools for supporting environmental chemistry”, Presented at the 255<sup>th</sup> American Chemical Society Meeting, New Orleans, LA, USA, March 18-22, 2018.
- 340) St. John-Williams L., Pham, T.H., Wolf, B., Koal, T., Kalli, A., Huhmer, A.F.R., Bowden, J.A., Koeniger, S., Raynaud, F.I., Pal, A., Asad, Y., Winder, C.L., Southam, A., Viant, M., Dunn, W., O’Neill, D., Prehn, C., Adamski, J., Shen, T., Valdiviez, L., Fiehn, O., Byram, G., Chamot, D, Mandal, R., Zheng, J., Zhang, A, Wishart, D. Fernandez, F.M., Gaul, D.A., Vasilopoulou, C.G., Meier, F., Mann M., Naser, F.J, Patti, G.J., Dang, V.D., Borts, D.J., Lucas, J.E., Moseley, A., Thompson, J.W. ”Results of an International Ring Trial for the Biocrates AbsoluteIDQ p400HR Targeted Metabolomics Kit”, Presented at the 14<sup>th</sup> Annual International Metabolomics Society Meeting, Seattle, WA, USA, June 24-28, 2018.
- 341) Zheng, J., Mandal, R., Wishart, D.S. “A Sensitive, High-Throughput LC-MS/MS Method for Measuring Catecholamines in Low Volume Serum”, Presented at the 14<sup>th</sup> Annual International Metabolomics Society Meeting, Seattle, WA, USA, June 24-28, 2018.
- 342) Mandal, R., Zheng, J., Wishart, D.S. “Mass Spectrometry –based High-throughput Quantitative Assays and Applications to Metabolomics”, Presented at the 14<sup>th</sup> Annual International Metabolomics Society Meeting, Seattle, WA, USA, June 24-28, 2018.
- 343) Chamot, D., Lipfert, M., Rout, M, Berjanskii, M., Xia, Y., Dong, E., Chowdhury, D., Zheng, J., Mandal, R., Wishart, D.S. “Automated NMR and GC-MS Kits for Quantitative Metabolomics”, Presented at the 14<sup>th</sup> Annual International Metabolomics Society Meeting, Seattle, WA, USA, June 24-28, 2018.
- 344) Djoumbou Feunang, Y., Wishart, D.S. “Cheminformatics Tools For Enabling Metabolomics”, Presented at the 14<sup>th</sup> Annual International Metabolomics Society Meeting, Seattle, WA, USA, June 24-28, 2018.
- 345) Reid, J., Karu, N., Deng, L., Slae, M., Guo, A.C., Sajed, T., Huynh, H., Wine, E., Wishart, D.S. “The Human Fecal Metabolome Database”, Presented at the 14<sup>th</sup> Annual International Metabolomics Society Meeting, Seattle, WA, USA, June 24-28, 2018.
- 346) Zhang, G., Dervishi, E., Wishart, D.S., Ametaj, B. “Targeted metabolomics profiling for identification of novel serum biomarkers in early prediction of subclinical mastitis in transition dairy

cows”, Presented at the 2018 American Society of Animal Science (ASAS) Annual Meeting and Trade Show, Vancouver, BC, Jul. 8-12, 2018.

347) Hailemariam, D., Zhang, G., Wishart, D.S., Ametaj, B. “Identification of urine metabolite signatures for monitoring dairy cows for susceptibility to metritis by DI/LC-MS/MS-based metabolomics”, Presented at the 2018 American Society of Animal Science (ASAS) Annual Meeting and Trade Show, Vancouver, BC, Jul. 8-12, 2018.

348) Dervishi, E., Zhang, G., Wishart, D.S., Ametaj, B “Novel DI/LC-MS/MS-based urinary metabolite signatures for monitoring dairy cows for occurrence of retained placenta”, Presented at the 2018 American Society of Animal Science (ASAS) Annual Meeting and Trade Show, Vancouver, BC, Jul. 8-12, 2018.

349) Ametaj, B., Zhang, G., Dervishi, E., Wishart, D.S. “Milk metabotyping by DI/LC-MS/MS demonstrated major alterations in metabolites related to lipid and amino acid metabolism in dairy cows affected by subclinical mastitis”, Presented at the 2018 American Society of Animal Science (ASAS) Annual Meeting and Trade Show, Vancouver, BC, Jul. 8-12, 2018.

350) Ametaj, B., Zhang, G., Dervishi, E., Wishart, D.S. “Urinary metabotyping around parturition indicates consistent metabolite signatures that can be used for monitoring and diagnosing of subclinical mastitis in dairy cows”, Presented at the 2018 American Society of Animal Science (ASAS) Annual Meeting and Trade Show, Vancouver, BC, Jul. 8-12, 2018.

351) Zhang, G., Dervishi, E., Wishart, D.S., Ametaj, B. “ICP-MS based ionotyping reveals altered ionome in the serum, urine, and milk of pre-milk fever (MF), MF, and post-MF dairy cows”, Presented at the 2018 American Society of Animal Science (ASAS) Annual Meeting and Trade Show, Vancouver, BC, Jul. 8-12, 2018.

352) Feunang, Y.D., Wishart, D.S., Karu, N., Marcu, A., Lo, E., Guo, A.C. “ChemOnt: A semantic-based ontology for chemical and biological data integration”, Presented at the 256<sup>th</sup> ACS National Meeting & Exposition, Boston, MA, Aug. 19-23, 2018.

353) Deng, L., Ismond, K., Liu, Z. Zheng, J., Chang, D., Kingham, P. Alatisse, O., Wishart, D.S., Wang, H., Fedorak, R. “Urine Metabolomic Biomarker Panel for Colorectal Cancer” Presented at the American College of Gastroenterology 2018 Annual Scientific Meeting, Philadelphia, PA. Oct. 5-8, 2018.



- 354) Pirimoghadam, H. Bhumireddy, S. Mandal, R. Wishart, D.S. “Development of a LC-MS/MS Metabolomics Assay for Quantitation of Polyphenols and Flavonoids in Spruce and Pine Samples”, Presented at the 2<sup>nd</sup> Annual Canadian Metabolomics Conference, Canmore, AB, May 1-2, 2019.
- 355) Bhattacharyya, D., Magha, S., Voza, N., Khaniani, Y., Wishart, D.S. “A Novel Chemical Assay for the Detection of Kynurenine in Human Urine Samples”, Presented at the 2<sup>nd</sup> Annual Canadian Metabolomics Conference, Canmore, AB, May 1-2, 2019.
- 356) Zheng, J., Zhang, L., Mandal, R., Wishart, D.S. “Mass Spectrometry – Based High-Throughput Quantitative Platforms for Urine Analysis”, Presented at the 2<sup>nd</sup> Annual Canadian Metabolomics Conference, Canmore, AB, May 1-2, 2019.
- 357) Zhang, L., Zheng, J., Berjanskii, M., Dong, Y., Mandal, R., Wishart, D.S. “Identification of Biomarkers of Chronic Wasting Disease by a Mass Spectrometry – Based High-Throughput Quantitative Method”, Presented at the 2<sup>nd</sup> Annual Canadian Metabolomics Conference, Canmore, AB, May 1-2, 2019.
- 358) Gautam, M., Zheng, J., Mandal, R., Wishart, D.S. “Quantitative Metabolomics of Uremic Toxins in Human Serum”, Presented at the 2<sup>nd</sup> Annual Canadian Metabolomics Conference, Canmore, AB, May 1-2, 2019.
- 359) Mandal, R., Han, J., De la Mata, P., Shanmuganathan, M., Mercier, P., Zahedi, R., Overduin, M., Harynuk, J., Britz-McKibbin, P., Li, L., Borchers, C., Wishart, D.S. “Quantitative Analysis of Over 600 Metabolites in a NIST Human Plasma Reference Material (SRM 1950) Using Multiple Analytical Platforms”, Presented at the 2<sup>nd</sup> Annual Canadian Metabolomics Conference, Canmore, AB, May 1-2, 2019.
- 360) MacKay, S., Keen, C., Liu, Y., Chen, J., Wishart, D.S. “Design of an Inexpensive Colour-based Metabolomic Biosensor System”, Presented at the 2<sup>nd</sup> Annual Canadian Metabolomics Conference, Canmore, AB, May 1-2, 2019.
- 361) Khaniani, Y., Wishart, D.S. “Maple Syrup Urine Disease”, Presented at the 2<sup>nd</sup> Annual Canadian Metabolomics Conference, Canmore, AB, May 1-2, 2019.
- 362) Keshtili, A.H., Chibbar, R., Mandal, R., Wishart, D.S., Dieleman, L.A. “Ulcerative Colitis (UC) Patients with Primary Sclerosing Cholangitis (PSC) Have Distinctive Serum Metabolomic Fingerprints Versus UC Patients Without PSC”, Presented at the Digestive Disease Week Meeting, San Diego, CA, May 18-21, 2019.

- 363) Hinge, V.K., Blinov, N., Roy, D., Allison, W.T., Wishart, D.S., Kovalenko, A. “Design and optimization of nucleic acid derivatives for inhibition of prion-like propagation at W32 site of SOD1 enzyme in Amyotrophic Lateral Sclerosis”, Presented at the Prion 2019 Conference, Edmonton, AB, May 21-24, 2019.
- 364) Blinov, N., Wishart, D.S., Cashman, N.R., Kovalenko, A. “Structural characterization of amyloidogenic proteins implicated in neurodegeneration under conditions of intracellular crowding and in nonpolar environments”, Presented at the Prion 2019 Conference, Edmonton, AB, May 21-24, 2019.
- 365) Mandal, R., Zheng, J., Zhang, L., Berjanskii, M., Zahraei, S., Borchers, C.H., Britz-McKibbin, P., Overduin, M., Harynuk, J., Liang, L., Wishart, D.S. “Quantitative Analysis of Over 600 Metabolites in the NIST Human Plasma Reference Material (SRM 1950) Using Multiple Analytical Platforms”, Presented at the MANA Virtual Summer Symposium 2020, Oct. 4, 2020.
- 366) Wang, Y., Bhumireddy, S., Zheng, J., Wishart, D.S. “MS-Based Assays for the Absolute Quantification of Primary and Secondary Metabolites in Plant Samples”, Presented at the MANA Virtual Summer Symposium 2020, Oct. 4, 2020.
- 367) Zhang, L., Zheng, J., Gautam, M., Mandal, R., Wishart, D.S. “A Comprehensive Targeted Metabolomic Assay for Uremic Toxin Quantification”, Presented at the MANA Virtual Summer Symposium 2020, Oct. 4, 2020.
- 368) Cort, J., Wishart, D.S. The Natural Products Magnetic Resonance Database (NP-MRD). Presented at the MANA Virtual Summer Symposium 2020, Oct. 4, 2020.
- 369) Hiebert, M., Inchehborouni, G., Cao, X., Guo, A.C. LeVatte, M., Liigand, J., Wang, F., Bhumireddy, S., Wang, Y., Zheng, J., Mandal, R., Wishart, D.S. The Chemical Composition of Cannabis. Presented at the MANA Virtual Summer Symposium 2020, Oct. 4, 2020.
- 370) Tian, S., Cao, X., Guo, AnChi, Li, C., Geiner, R., Wishart, D.S. CyProduct: A software tool for accurately predicting the byproducts of human cytochrome P450 metabolism. Presented at the 16th Annual Conference of the Metabolomics Society (Virtual), Oct. 27, 2020.
- 371) Wang, F., Tian, S., Liggand, J., Greiner, R., Wishart, D.S. “Accurate MS/MS Spectral Prediction with CFM-ID 4.0”, Presented at the 16th Annual Conference of the Metabolomics Society (Virtual), Oct. 28, 2020.

- 372) Zheng, J., Johnson, M., Mandal, R., Wishart, D S. “A Comprehensive Targeted Metabolomics Assay for Crop Plant Sample Analysis”, Presented at Metabolomics 2021 Online, the second virtual conference, June 22-24, 2021.
- 373) Mandal, R., Zheng, J., Zhang, L., Fraser, D D., López-Hernández. Y., Wishart, D S. “Targeted Metabolomics Identifies High Performing Diagnostic and Prognostic Biomarkers for COVID-19”, Presented at Metabolomics 2021 Online, the second virtual conference, June 22-24, 2021.
- 374) Zhang, L., Zheng, J., Mandal, R., Wishart, D S. “A Comprehensive Targeted Metabolomic Assay for Uremic Toxin Quantification”, Presented at the Metabolomics 2021 Online, the second virtual conference, June 22-24, 2021.
- 375) Hiebert, M., Maayah, Z H., Inchehborouni, G., Cao, X., Guo, A C., LeVatte, M., Liigand, J., Wang, F., Bhumireddy, S., Wang, Y., Zheng, J., Mandal, R., Dyck, J., Wishart, D S. “The Cannabis Compound Database and Novel Cannabis Metabolite Assays”, Presented at Metabolomics 2021 Online, the second virtual conference, June 22-24, 2021.
- 376) Chan, Y C., LeBlanc, P., Khanini, Y., MacKay, S., Kovur, P., Wishart, D S. “Metabolomics on a Chip: Development of an Impedance-Based Metabolite Biosensor for Early Diagnosis of Colon Cancer”, Presented at Metabolomics 2021 Online, the second virtual conference, June 22-24, 2021.
- 377) Wishart, D.S., Bartok, B., Oler, E., Liang, K., Budinski, Z., Brejanskii, M., Guo, A., Cao, X., Wilson, M. “MarkerDB: A Web Database of Molecular Biomarkers”, Presented at Metabolomics 2021 Online, the second virtual conference, June 22-24, 2021.
- 378) Wishart, D.S., Sayeeda, Z., Budinski, Z., Lee, B., Rout, M., Peters, H., Dizon, R., Mah, R., Torres Calzada, C., Giesbrecht, M., Varshavi, D., Varshavi, D., Oler, E., Allen, D., Cao, X., Gautum, V., Maras, A., Poynton, E., Tavangar, P., Yang, V., Santen, J., Ghosh, R., Sarma, S., Knutson, E., Sullivan, V., Jystad, A., Renslow, R., Sumner, L., Linington, R., Cort. J. “NP-MRD: The World’s Largest NMR Database for Natural Products”, Presented at Metabolomics 2021 Online, the second virtual conference, June 22-24, 2021.
- 379) Chan, Y. C., LeBlanc, P., Khanini, Y., MacKay, S., Kovur, P., Wishart, D S. “Metabolomics on a Chip: Development of an Impedance-Based Metabolite Biosensor for Early Diagnosis of Colon Cancer”, the Nanomedicines Innovation Network (NMIN) Theme 3 Virtual Workshop, June 30, 2021.
- 380) Zheng, J., Johnson, M., Mandal, R., Wishart, D. S. “A Comprehensive Targeted Metabolomics Assay for Crop Plant Sample Analysis”, Presented at the 3rd Annual MANA Conference (Virtual) – Columbus, Ohio, Oct. 18-21, 2021.

381) Mandal, R., Zheng, J., Zhang, L., Fraser, D D., López-Hernández. Y., Wishart, D S. “Targeted Metabolomics Identifies High Performing Diagnostic and Prognostic Biomarkers for COVID-19”, Presented at the 3rd Annual MANA Conference (Virtual) – Columbus, Ohio, Oct. 18-21, 2021.

382) Zhang, L., Zheng, J., Mandal, R., Wishart, D S., A Comprehensive Targeted Metabolomic Assay for Uremic Toxin Quantification”, Presented at the 3rd Annual MANA Conference (Virtual) – Columbus, Ohio, Oct. 18-21, 2021.

383) Hiebert, M., Maayah, Z H., Inchehborouni, G., Cao, X., Guo, A C., LeVatte, M., Liigand, J., Wang, F., Bhumireddy, S., Wang, Y., Zheng, J., Mandal, R., Dyck, J., Wishart, D.S. “The Cannabis Compound Database and Novel Cannabis Metabolite Assays”, Presented at the 3rd Annual MANA Conference (Virtual) - Columbusm Ohio, Oct. 18-21, 2021.

384) Chan, Y.C., LeBlanc, P., Khanini, Y., MacKay, S., Kovur, P., Wishart, D S. “Metabolomics on a Chip: Development of an Impedance-Based Metabolite Biosensor for Early Diagnosis of Colon Cancer”, Presented at the 3rd Annual MANA Conference (Virtual) – Columbus, Ohio, Oct. 18-21, 2021.

385) Mandal, R., Zheng, J., Zhang, L., Fraser, D.D., Wishart, D.S. “Targeted Metabolomics Identifies High Performing Diagnostic and Prognostic Biomarkers for COVID-19”, Presented at the 69<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Philadelphia, PA Oct. 31 – Nov. 4, 2021.

386) Zhang, L., Zheng, J., Mandal, R. Karu, N., Wishart, D.S. “A Comprehensive Targeted Metabolomic Assay for Uremic Toxin Quantification”, Presented at the 69<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Philadelphia, PA Oct. 31 – Nov. 4, 2021.

387) Zheng, J., Johnson, M., Mandal, R., Wishart, D.S. “A Comprehensive Targeted Metabolomics Assay for Plant Sample Analysis”, Presented at the 69<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Philadelphia, PA Oct.31 – Nov. 4, 2021.

### **Invited Lectures**

1) Wishart, D.S., "Protein Structure Prediction", presented at the Third Annual Symposium of the Protein Society, Seattle, WA (August 1989).

2) Wishart, D.S., "Databases for Design, Construction & Prediction of Protein Structure", presented at Connaught Laboratories of Canada, Willowdale, ON (June 1992).

- 3) Wishart, D.S., "Unravelling the Protein Folding Problem", presented at the Ontario Cancer Institute, Toronto, ON (December 1992).
- 4) Wishart, D.S., "Understanding Protein Sequence Analysis", presented at the NCE Molecular Biology Software Workshop, Mississauga, ON (September 1993).
- 5) Wishart, D.S., "Protein Sequence Analysis using SEQSEE", presented at the NCE Molecular Biology Software Workshop, Mississauga, ON (September 1993).
- 6) Wishart, D.S., "The Design of a Water-Soluble  $\beta$ -sheet Model and its Utility as a Miniglobulin Template" Presented at the 3rd P.E.N.C.E. Annual General Meeting, Whistler, BC (June 1994).
- 7) Wishart, D.S., "NMR Without NOE's: Applications of Chemical Shifts and JHNH $\alpha$  Coupling Constants to Protein Structure Determination", presented at the 78th Canadian Society of Chemistry Conference and Exhibition, Guelph, ON (May 1995).
- 8) Wishart, D.S., "How to Interpret Chemical Shifts in Biomolecules", presented at the University of Calgary, Calgary, AB (February 1996).
- 9) Wishart, D.S., "Biotechnology - Its Impact on the Future of Pharmacy", presented at the Banff Seminar -- Western Branches, Canadian Society of Hospital Pharmacists, Banff, AB (March 1996).
- 10) Wishart, D.S., "NMR and Computer-Aided Drug Design", presented at the CERCA symposium on Perspectives in Pharmaceutical Design by Computers, Montreal, PQ (May 1996).
- 11) Wishart, D.S. "Bioinformatics and Computer-Aided Drug Design", presented at the PENCE Computer-Aided Drug Design Workshop, Montreal, PQ (May 1996).
- 12) Wishart, D.S. "Predicting Protein Folds -- A Short History", presented at the PENCE Protein Folding Symposium, Toronto, ON (May 1997).
- 13) Wishart, D.S. "Simple Methods to Extract Complex Structural Data from NMR Spectra", presented at the 40th Annual CFBS Meeting, Quebec City, PQ (June 1997).
- 14) Wishart, D.S. "Interaction of PENCE on the Development of BioTools", presented at the 1st Annual International Health Opportunities Business Conference, Calgary, AB (October 1997).

- 15) Wishart, D.S. "Building Better Tools for Drug Discovery and Drug Delivery" presented at the Bristol Myers Squibb Pharmaceutical Research Institute, Lawrenceville, NJ (October 1998).
- 16) Wishart, D.S. "NMR without NOEs -- How to Make the Most from Chemical Shifts" presented at the Gordon Research Conference in Computer Techniques in Biomolecular NMR, Barga, Italy (June 1999).
- 17) Wishart, D.S. "Bioinformatics and Computer Aided Drug Design" presented at the PENCE Annual General Meeting, Whistler, BC (June 1999).
- 18) Wishart, D.S. "From Desktop to Drug Shoppe" presented at the Campus Computing Symposium '99, Edmonton, AB (June 1999).
- 19) Wishart, D.S. "Bioinformatics and Drug Discovery" presented at the Second Annual Meeting of the Canadian Society for Pharmaceutical Sciences, Montreal, PQ (August 1999).
- 20) Wishart, D.S. "Structural Proteomics: The Next Frontier in Structural Biology" presented at the University of Southern Illinois, Carbondale, IL (October 1999).
- 21) Wishart, D.S. "Structural Proteomics: The Nexus of Computers and Biology" presented at the SGI-Oracle Workshop Series for New Technologies for Discovery Research, Palo Alto, CA (February 2000).
- 22) Wishart, D.S. "Structural Proteomics: The Nexus of Computers and Biology" presented at the SGI-Oracle Workshop Series for New Technologies for Discovery Research, San Diego, CA (February 2000).
- 23) Wishart, D.S. "Bioinformatics in the 21st Century" presented at the University of Southern Florida, Tampa, FL (February 2000).
- 24) Wishart, D.S. "Bioinformatics and Proteomics" presented at the Dept. of Pharmacology, University of Alberta, Edmonton, AB (March 2000).
- 25) Wishart, D.S. "Bioinformatics, Proteomics and Cancer" presented at the Cross Cancer Clinic Oncology Grand Rounds, University of Alberta, Edmonton, AB (March 2000).

- 26) Wishart, D.S. “Lessons from the Field: How to Start a University Spin-off Company” presented at the Westlink “Going Corporate Seminar Series”, Edmonton, AB (May 2000).
- 27) Wishart, D.S. “What’s Next for Bioinformatics” presented at the 1<sup>st</sup> Annual BioFuture 2000 Conference, Calgary, AB (September 2000).
- 28) Wishart, D.S. “New Technologies for the Post-Genomic Era” presented at the NRC Technical Training Symposium, Calgary, AB (September 2000).
- 29) Wishart, D.S. “Getting the Most From Your Bioinformatics Toolbox” presented at the Dept. of Experimental Oncology, University of Alberta, Edmonton, AB (September 2000).
- 30) Wishart, D.S. “BRONCO – The ACB Bioinformatics Resource for Oncology” presented at Cancer Research: Paradigms for a New Millennium, Banff, AB (November 2000).
- 31) Wishart, D.S. “Nanotechnology – Life Sciences Applications” presented at the National Research Council symposium on Nanotechnology Research, University of Alberta, Edmonton, AB (November 2000).
- 31) Wishart, D.S. “Project Cyber-Cell” presented at the BIND Database Symposium, Centre for Molecular Medicine and Therapeutics, Vancouver, BC (January 2001).
- 33) Wishart, D.S. “Bioinformatics and Drug Discovery” presented at the University of Toronto, Toronto, ON (February 2001).
- 34) Wishart, D.S. “The Next Step for Bioinformatics: Total Cellular Simulation” presented at the University of Toronto, Toronto, ON (February 2001).
- 35) Wishart, D.S. “Bioinformatics and Cancer: From Genotype to Phenotype” presented at the BC Cancer Research Centre, Vancouver, BC (February 2001).
- 36) Wishart, D.S. “Bioinformatics Tools for Genomic Data Storage and Retrieval” presented at the ASCPT 2001 Annual General Meeting, Orlando, FL (March 2001).
- 37) Wishart, D.S. “What’s Next for Bioinformatics: A Peek into the Future of Computational Biology” presented at the Dept. of Biological Sciences, University of Alberta, Edmonton, AB (May 2001)

- 38) Wishart, D.S. “Bioinformatics and Proteomics” presented at the CSBMCB/PENCE AGM conference, Alliston ON (June 2001).
- 39) Wishart, D.S. “Proteomics at the University of Alberta” presented at the CIHR Proteomics Workshops, Kingstson, ON (August 2001).
- 40) Wishart, D.S. “What’s Next for Bioinformatics” presented at the University of Alberta ITC Bioinformatics Forum (Telus Centre), Edmonton, AB (November 2001)
- 41) Wishart, D.S. “Proteomics: The Past, Present and Future of Nanotechnology” presented at the Applications of Microsystems and Nanotechnology in the Life Sciences Conference, Banff, AB (November 2001).
- 42) Wishart, D.S. “Life Sciences in the 21<sup>st</sup> Century – Looking into the Past to See the Future” public lecture presented at the Richmond Community Centre, Richmond, BC (December 2001).
- 43) Wishart, D.S. “PolyomX and BioinformatX” presented at the PolyomX bioinformatics retreat at the University of Alberta, Edmonton, AB (January 2002).
- 44) Wishart, D.S. “Bioinformatics, Genomics, Proteomics and Cancer” presented at the University of Calgary, Calgary, AB (February 2002).
- 45) Wishart, D.S. “Bioinformatics, Genomics and Cancer” presented at the University of British Columbia, Vancouver, BC (February 2002).
- 46) Wishart, D.S. “In the Beginning... There was Nanotech” presented at the University of Alberta ITC Nanotechnology Forum (ECERF), Edmonton, AB (March 2002).
- 47) Wishart, D.S. “Microbial Cell Simulation: Building a Virtual E. Coli Cell” presented at the UA-UC Conference on Infectious Diseases, Banff, AB (April 2002).
- 48) Wishart, D.S. “Protein Fold Prediction: New Approaches to an Old Problem” presented at the 10<sup>th</sup> PENCE Annual General Meeting, Edmonton, AB (May 2002).
- 49) Wishart, D.S. “How NMR is Changing Pharmaceutical Sciences” presented at the University of British Columbia, Vancouver BC (May 2002).



- 50) Wishart, D.S. "The CyberCell Database" presented at the EMC<sup>2</sup> meeting on E. coli Simulation, Chicago, Illinois (May 2002).
- 51) Wishart, D.S. "Metabonomics and Chemomx: Applications of Metabolic Profiling" presented at the Schering Plough Research Institute, Newark, NJ (June 2002).
- 52) Wishart, D.S. "NMR in Drug Discovery and Development" presented at the University of Toronto, Toronto, ON (June 2002).
- 53) Wishart, D.S. "Cyberinformatics: Bioinformatics and the CyberCell" presented at BIO2002, Toronto, ON (June 2002).
- 54) Wishart, D.S. "DrugBank: Bringing Bioinformatics, Proteomics and Drug Discovery Together" presented at the 10<sup>th</sup> Chemical Society of Canada Conference, Vancouver, BC (June 2002).
- 55) Wishart, D.S. "Bioinformatics Solutions for the Post Genomic Era" presented at the 10<sup>th</sup> ISMB conference, Edmonton AB (August 2002).
- 56) Wishart, D.S. "Do's Don't's and No NOEs in Biomolecular NMR" presented at the 20<sup>th</sup> ICMRBS conference, Toronto, ON (August 2002).
- 57) Wishart, D.S. "NMR in Drug Discovery and Design" presented at the University of Rhode Island, Kingston, RI (September 2002).
- 58) Wishart, D.S. "Nanotechnology for Nanodetection" Presented at 2002 conference of the Provincial Laboratory for Public Health (Microbiology) Technology and Research Symposium, Calgary, AB (October 2002).
- 59) Wishart, D.S. "Rapid Metabolite Identification by NMR – Applications and Innovations" presented at the 2002 CPSA (Chemical and Pharmaceutical Structural Analysis) conference, Princeton, NJ (October 2002).
- 60) Wishart, D.S. "Mixture Analysis with NMR" presented at the 37<sup>th</sup> MidWest Regional Conference of the American Chemical Society, Lawrence, Kansas (October 2002).

- 61) Wishart, D.S. “Using NMR to Understand Protein Structure and Folding” presented at the University of Kansas, Lawrence, Kansas (October 2002).
- 62) Wishart, D.S. “Metabolic Profiling: Seeing Living Systems Through the Eyes of A Chemist” presented at the Edmonton Council for Advanced Technology (ECAT) Spring Meeting, University of Alberta, Edmonton, AB (April 2003).
- 63) Wishart, D.S. “Protein Feature Identification” presented at the University of Calgary, Calgary, AB (February 2003).
- 64) Wishart, D.S. “Nanotechnology and Biotechnology” presented at the AIBA conference, University of Alberta, Edmonton, AB. (May 2003).
- 65) Wishart, D.S. “Grand Challenges in Bioinformatics” presented at the 6<sup>th</sup> CBW workshop in Bioinformatics, University of Ottawa, Ottawa, ON. (June 2003).
- 66) Wishart, D.S. “Programmable, Adaptable Nanomaterials” presented at the Silicon vs. Carbon – Thinking Small, Thinking Fast Symposium, Banff Centre, Banff, AB (August 2003).
- 67) Wishart, D.S. “LIMS for the Masses” presented at The Protein Engineering Network of Centres of Excellence (PENCE) Bioinformatics Theme Meeting, University of Alberta, Edmonton, AB (September 2003)
- 68) Wishart, D.S. “Protein Structure Assessment and Protein Interactions” presented at the NHGRI (National Human Genome Research Institute), Bethesda, MD (October 2003).
- 69) Wishart, D.S. “Metabolic Profiling and Functional Proteomics” presented at the 2<sup>nd</sup> Annual Human Proteome Organization (HUPO) Congress, Montreal, QC (October 2003).
- 70) Wishart, D.S. “Nanotechnology: What it Means and Where it’s Going” presented at the Edmonton Y’s Men meeting, Edmonton, AB (October 2003).
- 71) Wishart, D.S. “Project CyberCell: Computational Challenges to Cellular Modelling” presented at the 3<sup>rd</sup> Annual BioNorth Conference, Ottawa, ON (November 2003)

- 72) Wishart, D.S. “Bioinformatics and AI: Current Projects and Future Challenges” presented at the University of Alberta, Dept. of Computing Science Artificial Intelligence Seminar Series, Edmonton, AB (December 2003).
- 73) Wishart, D.S. “Single Spectrum Spectroscopy” presented at the 3<sup>rd</sup> Gordon Research Conference on Computational Aspects of Biomolecular NMR, Ventura, CA (January 2004).
- 74) Wishart, D.S. “Protein Feature Identification” presented at the University of Calgary, Calgary, AB (February 2004).
- 75) Wishart, D.S. “Structural Proteomics: What it is and where it’s going” presented at the 31<sup>st</sup> Annual Biology Symposium, York University, Toronto, ON (March 2004).
- 76) Wishart, D.S. “Mining Medical Mountains: How Bioinformatics Can Help Medical Science” presented at the Cross Cancer Oncology Grand Rounds, Edmonton, AB (March 2004).
- 77) Wishart, D.S. “Progress Report on the Structure and Production of HAV, HRV and SARS Viral Proteases” presented at the The Protein Engineering Network of Centres of Excellence (PENGE) Protease Theme Meeting, University of Alberta, Edmonton, AB (March 2004)
- 78) Wishart, D.S. “Seeing the Unseeable: The Science Behind Cellular Simulation” presented at the First Banff Summit on Simulation and Other Re-enactments: Modeling the Unseen, Banff, AB (April 2004).
- 79) Wishart, D.S. “Nanobiology and NINT” presented to the Dept. of Biological Sciences, University of Alberta, Edmonton, AB (May 2004).
- 80) Wishart, D.S. “Protein Structure Prediction: Seeing Some Light at the End of the Protein Folding Funnel” presented at the 14<sup>th</sup> Annual PENGE AGM, Montreal, QC (May 2004).
- 81) Wishart, D.S. “Cellular Simulation Using Cellular Automata” presented at the Dagstuhl Seminar 04281 Integrative Bioinformatics - Aspects of the Virtual Cell Biological Simulation Workshop, Schloss Dagstuhl Germany. (July 2004).
- 82) Wishart, D.S. “Bioinformatics in Drug Development and Discovery” presented at the 7th International Society for the Study of Xenobiotics (ISSX) conference, Vancouver, BC (August 2004).

- 83) Wishart, D.S. “Project CyberCell” presented at Computational Cell Biology, MITRE Inc. McLean, Virginia, USA (September 2004)
- 84) Wishart, D.S. “Nanorobotics: Can We Make Intelligent Bacteria” presented at the Alberta Ingenuity Centre for Machine Learning (AICML) Seminar Series, Edmonton, AB (October 2004).
- 85) Wishart, D.S. “Am I Able – Mobile Technologies: A Synopsis of New Technologies” presented at the Am-I-Able Mobile Technologies Summit, Banff Centre, Banff, AB (November 2004).
- 86) Wishart, D.S. “SimCell: A Novel Computational Approach to Cellular Simulation” presented at the University of Toronto, Toronto, ON (December 2004).
- 87) Wishart, D.S. “NMR & Metabolomics: The Possibilities and the Limitations” presented at the NRC-GHI workshop on Metabolomics, Ottawa, ON (December 2004).
- 88) Wishart, D.S. “Computational Microbiology” presented as a guest lecture at Microbiology 606/607, University of Alberta, Edmonton, AB (January 2005).
- 89) Wishart, D.S. “Mass Spectrometric Peptide Identification using MASCOT” presented at the ABRF 2005 workshop on Computational Proteomics, Savannah, Georgia (February 2005).
- 90) Wishart, D.S. “Protein Structure Analysis and Protein-Protein Interactions” presented at the NHGRI (National Human Genome Research Institute), Bethesda, MD (February 2005).
- 91) Wishart, D.S. “Protein Feature Identification” presented at the University of Calgary, Calgary AB (March 2005).
- 92) Wishart, D.S. “Genomics and Drug Discovery” presented at the Canadian Bioinformatics Workshop on Genomics, Calgary AB (April 2005).
- 93) Wishart, D.S. “The Human Metabolome Project and its Impact on Human Disease” presented at the Garrod Association Annual Symposium, Ottawa, ON (May 2005).
- 94) Wishart, D.S. “The Human Metabolome Project” presented at the PolyomX Research Seminar Series, Edmonton, AB (June 2005).

- 95) Querengesser, L. and Wishart, D.S. "The Human Metabolome Project and its Impact on Human Disease" presented at the 1<sup>st</sup> Annual Meeting of the Metabolomics Society, Tsuruoka City, Japan (June 2005)
- 96) Wishart, D.S. "Between Biological and Digital Memory" presented at the Bodies in Motion: Memory, Personalization, Mobility and Design Summit, Banff, AB (June 2005).
- 97) Wishart, D.S. "Metabolomics: The Basics" presented at the 8<sup>th</sup> International Banff Symposium on Organ Transplantation, Edmonton, AB (July 2005)
- 98) Wishart, D.S. "The Human Genome Project and What it Means to be Human" Public lecture presented at the Cape Cod Synagogue, Hyannis, MA (August 2005).
- 99) Wishart, D.S. "The Human Metabolome Project: Its Application to Disease Diagnosis and Monitoring" presented at the 3<sup>rd</sup> Annual GHI (Genomics and Health Initiative) Conference, Ottawa, ON (September 2005).
- 100) Wishart, D.S. "Systems Biology in Bioscience and Medicine" presented at the DGKL (German Society of Clinical Laboratory Medicine) Annual Conference, Jena, Germany (October 2005).
- 101) Wishart DS. "The Bioinformatics of Small Molecules" presented at the Vancouver Bioinformatics User Group (VanBUG) Monthly Meeting, Vancouver, BC (October 2005).
- 102) Wishart DS. "The Human Metabolome Project" presented at the Alberta Metabolomics Symposium: Understanding the Human Metabolome, Edmonton, AB (October 2005).
- 103) Wishart, D.S. "Functional Genomics and Bioinformatics" presented at the Karolinska Institute, Stockholm Sweden (February 2006).
- 104) Wishart DS. "Integrative Bioinformatics and Cheminformatics" presented at the Stockholm Bioinformatics Centre, Stockholm, Sweden (February 2006).
- 105) Wishart, D.S. "Protein Feature Identification" presented at the University of Calgary, Calgary, AB (March 2006).

- 106) Wishart DS. "The Human Metabolome Project" presented at the LMC Genome Canada Nutrigenomics Workshop, Roskilde, Denmark (March 2006).
- 107) Wishart, D.S. "NMR, Structural Genomics and Metabolomics – What's the Connection" presented at the 6<sup>th</sup> Annual Protein Structure Initiative Bottlenecks Workshop, Bethesda, MD, (April 2006).
- 108) Wishart, D.S. "A New Strategy for Disease Diagnosis" presented at the University of Alberta Alumni Association Meeting, Edmonton, AB (April 2006).
- 109) Wishart, D.S. "New Approaches for Monitoring Prion Dynamics and Prion Assembly" presented at the Misfolding Diseases: Prion Dynamics and Roles of Chaperones -- CPI06 Satellite Workshop, Edmonton, AB (May 2006).
- 110) Wishart, D.S. "Programmable Adaptable Nanomaterials" presented at the University of Alberta Nanomedicine Workshop, Edmonton, AB (June 2006).
- 111) Wishart, D.S. "The Human Metabolome Project" presented at the 2nd Annual Metabolomics Society Meeting, Boston, MA (June 2006).
- 112) Wishart, D.S. "MetaboLIMS: A general Laboratory Information Management System for Metabolomics" presented at the 2nd Annual Metabolomics Society Meeting, Boston, MA (June 2006).
- 113) Wishart, D.S. "Metabolomics in Canada" presented at the Genome Canada Proteomics Workshop, Montreal, QC (July 2006).
- 114) Wishart, D.S. "Proteomics and Informatics: The Fundamentals" presented at the APIII 2006 (Advancing Practice through Instruction, Innovation and Informatics) Conference, Vancouver, BC. (August 17, 2006).
- 115) Wishart, D.S. "Metabolomics: The Other Side of Proteomics" presented at the APIII 2006 (Advancing Practice through Instruction, Innovation and Informatics) Conference, Vancouver, BC. (August 17, 2006).
- 116) Wishart, D.S. and Berjanskii M.V. "Using Chemical Shifts to Improve Accuracy and Precision in NMR Structures" presented at the 4<sup>th</sup> Gordon Conference on Computational Aspects of Biomolecular NMR, Aussois, France (September 25, 2006).

- 117) Wishart, D.S. “Nutrigenomics Research in Alberta” presented at the Canadian Nutrigenomics Workshop, Montreal, Quebec (October 3, 2006).
- 118) Wishart, D.S. “The Human Metabolome Project: An Update” presented at the 2<sup>nd</sup> Annual Conference on Understanding the Human Metabolome. Edmonton, AB (October 12, 2006).
- 119) Wishart, D.S. “Protein Structure Analysis and Protein-Protein Interactions II” presented at the at the NHGRI (National Human Genome Research Institute), Bethesda, MD (October 15, 2006).
- 120) Wishart, D.S. “Nanotechnology – A New Direction for Alberta” presented at the Edmonton ProBus (Professional Business) meeting, Edmonton, AB (October 24, 2006).
- 121) Wishart, D.S. “Novel Bioinformatics Systems” presented at the IBM Centre for Advanced Studies (CAS) board meeting, Edmonton, AB (November 29, 2006).
- 122) Wishart, D.S. “Metabolomics: The Next Frontier for Bioinformatics?” presented at the Rocky 06 Conference, Snowmass CO, (December 2, 2006).
- 123) Wishart, D.S. “Computational Approaches to Metabolomics: A Tutorial” presented at the 2007 Pacific Symposium on Biocomputing, Maui, Hawaii (January 4, 2007).
- 124) Wishart, D.S. “Introduction to Computational Aspects of Metabolomics” presented at the 2007 Pacific Symposium on Biocomputing, Maui, Hawaii (January 4, 2007).
- 125) Wishart, D.S. “A Novel Approach to Characterize Prion Aggregates and the Prion Propagation Complex” presented at the PrP Canada 2007 Conference, Calgary AB (February 20, 2007).
- 126) Wishart, D.S. “What does PrPc Tell Us About PrPsc?” presented at the PrP Canada 2007 Satellite Workshop, Calgary AB (February 21, 2007).
- 127) Wishart, D.S. “Bioinformatics and the Human Metabolome Project” presented at the first annual Who We Are and What We Eat Conference, Charlotte NC (April 17, 2007).
- 128) Wishart, D.S. “Metabolomics and Structural Proteomics” presented at the University of Toronto and the Structural Genomics Consortium, Toronto ON (April 25, 2007).

- 129) Wishart, D.S. “The Human Metabolome Project: Past, Present and Future” presented at Agilent Technologies, Santa Clara CA (May 11, 2007).
- 130) Wishart, D.S. “Protein Feature Identification” presented at the University of Calgary, Calgary AB (May 17, 2007).
- 131) Wishart, D.S. “The Human Metabolome Project: An Update for 2007” presented at the 3<sup>rd</sup> Annual Conference of the Metabolomics Society, Manchester UK (June 12, 2007).
- 132) Wishart, D.S. “Looking Ahead: What’s Next for the Protein Sciences” presented at the CPI07 Conference, Ottawa ON (June 17, 2007).
- 133) Wishart, D.S. “The Metabolomics ToolBox: Applications to Organ Transplant Monitoring” presented at the ATAGC Conference – Using Omics Technologies to Phenotype Diseases, Edmonton AB (June 18, 2007).
- 134) Wishart, D.S. “The Human Metabolome Project” presented at the 5<sup>th</sup> Northern Lights Summer Conference on Metabolomics: Technologies & Applications, Waterloo ON (June 21, 2007).
- 135) Wishart, D.S. “The Human Metabolome Project” What it Means for Pharmaceutical Research” presented at the Faculty of Pharmacy, State University of Washington, Pullman WA (July 27, 2007).
- 136) Wishart, D.S. “How Bioinformatics Helped Reveal the Human Metabolome” presented at InCOB 2007, Hong Kong (August 28, 2007).
- 137) Wishart, D.S. “NMR and the Human Metabolome Project” presented at the Dept. of Chemistry, SUNY Buffalo, Amherst NY (September 14, 2007).
- 138) Wishart, D.S. “Metabolite Identification” presented at the NuGO International Workshop on Tools and Methods for MS Metabolomics in Nutrition, Clermont-Ferrand, France (December 14, 2007).
- 139) Wishart, D.S. “DrugBank2” presented at the EBI Druggability Portal Workshop, Cambridge, England (February 4, 2008).
- 140) Wishart, D.S. “Studies of Prion Structure and Dynamics by NMR and MS Methods” presented at the Northern Lights Seminar Series, Dept. of Biochemistry, University of Alberta, Edmonton, AB (February 8, 2008).



- 141) Wishart, D.S. “Applications of Metabolomics in Nutritional Science” presented at the University of North Carolina (Chapel Hill), Chapel Hill, NC (February 13, 2008).
- 142) Wishart, D.S. “Metabolomics: The Capstone to Systems Biology” presented at the Omics & Systems Biology CPS-Regional Meeting, Edmonton, AB (February 21, 2008).
- 143) Wishart, D.S. “Protein Structure Analysis and Protein-Protein Interactions” presented at the NHGRI Bioinformatics Workshops, Bethesda, MD (April 14, 2008).
- 143) Wishart, D.S. “Applications of Metabolomics in Nutritional Science” presented at the Dow Agrosiences Institute, Indianapolis, Indiana (April 28, 2008).
- 144) Wishart, D.S. “Towards Quantitative Metabolomics” presented at the Bio-IT World Conference, Boston, MA (April 30, 2008).
- 145) Wishart, D.S. “New Tools for Structural Proteomics” presented at the CPI08 Conference, Burnaby BC (May 5, 2008).
- 146) Wishart, D.S. “Automated Metabolite Identification and Quantification by NMR” presented at the 5<sup>th</sup> Gordon Research Conference on Computational Aspects of Biomolecular NMR, Il Ciocco, Italy (May 20, 2008).
- 147) Wishart, D.S. “Calculation of Protein Structure and Dynamics from NMR Chemical Shifts” presented at the Dept. of Computing Science, Ludwig Maximilians University, Munich, Germany (June 25, 2008).
- 148) Wishart, D.S. “New Approaches to Studying Prion (and Protein) Structures” presented at the Hospital for Sick Children, Toronto, Ontario (July 21, 2008).
- 149) Wishart, D.S. “Canadian Bioinformatics Platform – HelpDesk Update” presented at the Genome Canada Bioinformatics Platform Annual General Meeting, Banff, AB (September 10, 2008).
- 150) Wishart, D.S. “Using Metabolomics and Proteomics to Identify Biomarkers for Prion Diseases” presented at the PrionNet Networking Meeting, Toronto, ON (September 19, 2008).

- 151) Wishart, D.S. “Clinical Biomarkers from Biofluid Metabolomics” presented at the CHI Biomarkers Summit – 9<sup>th</sup> Biomarkers Conferences, Philadelphia, PA (September 30, 2008).
- 152) Wishart, D.S. “Metabolomics in Food Science and Nutrition” presented at the Institute for Human Nutrition, University of Alberta, Edmonton, AB (October 21, 2008).
- 153) Wishart, D.S. “DrugBank: An Update” presented at the 2<sup>nd</sup> Druggability Portal Workshop, European Bioinformatics Institute (EBI), Hinxton, England (November 7, 2008).
- 154) Wishart, D.S. “Omics” in Alberta: Building on Excellence”, presented at the Genome Alberta Board Retreat, Cochrane, AB (November 10, 2008).
- 155) Wishart, D.S. “The 4D Project: Metabolomics of Mice, Rats and Humans – An Update” presented at the Genome Canada 4D Modeling of Genomics Annual General Meeting, Banff, AB (November 14, 2008).
- 156) Wishart, D.S. “The Human Metabolome Project” presented at the NIH Glue Grant Metabolomics Workshop, Bethesda MD (December 17, 2008).
- 157) Wishart, D.S. “Informatics and Metabolomics” presented at the ELIXIR/EBI International Metabolomics Workshop, Hinxton, UK (January 27, 2009).
- 158) Wishart, D.S. “The Human Biofluid Metabolome(s): Different Answers from Different Technologies”, presented at the NuGO & SysDiet Metabolomics Workshop, Copenhagen, DK (February 23, 2009).
- 159) Wishart, D.S. “Prion Bioinformatics Workshop”, presented at the PrP Canada 2009 Meeting, Edmonton, AB (March 2, 2009).
- 160) Wishart, D.S. “Studies of Prion Conversion by Integrated Biophysical Methods”, presented at the PrP Canada 2009 Satellite Workshop on Prion Structure & Dynamics, Edmonton, AB (March 4, 2009).
- 161) Wishart, D.S. “Metabolomics for Monitoring and Optimizing Microbial Xylose Fermentation” presented at the First Annual CBioNet Meeting, Montreal, Quebec (March 27, 2009).

162) Wishart, D.S. “How the Prion Converts in Disease”, presented at the From Baden to Banff 2009 TSE Conference, Banff, AB (April 25, 2009).

163) Wishart, D.S. “The Human Metabolome Project: Potential Applications to Structural and Functional Genomics”, presented at Columbia University, NY (April 27, 2009).

164) Wishart, D.S. “Proteomics and Metabolomics for Prion Biomarker Discovery”, presented at the Workshop on Live Animal Testing and the Clinical and Biological Perspective of Atypical BSE, Edmonton, AB (May 6, 2009).

165) Wishart, D.S. “Using Proteomics to Enable Metabolomics and Vice Versa”, presented at the 4<sup>th</sup> International Experimental Technologies in Proteomics (ETP) Symposium, Vancouver, BC (May 14, 2009).

166) Wishart, D.S. “Metabolomics for Monitoring Kidney Transplants”, presented at the World Congress of Nephrology (WCN) 2009, Milan Italy (May 25, 2009).

167) Wishart, D.S. “A Molecular Picture of the Prion Conversion Process” presented at the 52nd Meeting of the CSBMCB, Niagara-on-the-Lake (June 1-5, 2009).

168) Wishart, D.S. “Cord Blood Banking and Informatics” presented at the Alberta Cord Blood Bank Symposium, Edmonton, AB (June 17, 2009).

169) Wishart, D.S. & Psychogios, N. “The Human Metabolome Database: A General Metabolomics Resource” presented at the 11<sup>th</sup> International Congress of Inborn Errors of Metabolism, San Diego, USA (Aug. 30, 2009).

170) Wishart, D.S. “Pathways and Statistics in Metabolomics” workshop/tutorial presented at the 5<sup>th</sup> International Metabolomics Society Meeting, Edmonton, AB (Aug. 30, 2009).

171) Wishart, D.S. “Tools, Issues and Opinions on Structure Validation” presented at the wwPDB NMR Structure Validation Task Force Workshop, Paris, France (Sept. 21, 2009).

172) Wishart, D.S. “Using Proteomics and Metabolomics to ID Biomarkers for Prion Diseases” presented at the 3<sup>rd</sup> Annual PrioNet Networking Meeting, Vancouver, BC (Oct. 21, 2009).

173) Wishart, D.S. “Metaboomics For Cancer Diagnosis, Prognosis and Prediction” presented at the Alberta Cancer Research Institute (ACRI) Research Meeting 2009, Banff, AB (Nov. 26, 2009).

174) Wishart, D.S. “Food, Nutrition and the Human Metabolome” presented at The 4th International Conference on Polyphenols & Health (ICPH 2009), Harrogate, UK (Dec. 11, 2009).

175) Wishart, D.S. “Personal Genomics: The Answer Isn’t Always in the Genes” presented at the Pacific Symposium in Biocomputing (PSB) 2010. Kohala Coast, Hawaii (Jan. 5, 2010).

176) Wishart, D.S. “Metabolomics and Nanotechnology” presented at the NRC-NINT seminar series, NINT, Edmonton (Jan. 21, 2010).

177) Wishart, D.S. “Applications of Metabolomics to the Pharmaceutical Sciences” presented at the Faculty of Pharmacy, University of Alberta, Edmonton, AB (Feb. 3, 2010).

178) Wishart, D.S. “Metabolomics in Biological fluids” presented at the Transplantomics and Biomarkers in Organ Transplantation Conference, San Francisco, CA (Feb. 26, 2010).

179) Wishart, D.S. “An Update on the Human Metabolome Project” presented at the Therapeutic Applications of Computational Biology and Chemistry (TACBAC) Conference, Hinxton, UK (March 2, 2010).

180) Wishart, D.S. “Metabolite Identification and Quantification: New Approaches to an Old Problem” presented at the Metabolomics and More Symposium, Munich, Germany (March 11, 2010).

181) Wishart, D.S. “Trends in Quantitative Metabolomics” presented at the ABRF (Association of Biomolecular Resource Facilities) Meeting, Sacramento CA (March 22, 2010).

182) Wishart, D.S. “Cracking the Chemical Shift Code: How to Use Chemical Shifts in “Omics” Research” presented at Harvard Medical School, Boston, MA (March 29, 2010).

183) Wishart, D.S. “Metabolomics and Neuronomics” presented at the Neuronomics CFRI Workshop, Vancouver, BC (April 9, 2010).

184) Wishart, D.S. “Nanotoxicology: Effects on Human Health and the Environment” presented at the Association of Professional Engineers, Geologists and Geophysicists of Alberta (APEGGA) Annual Conference, Edmonton, AB (April 16, 2010).

185) Wishart, D.S. “Metabolomics: Future Trends in Laboratory Diagnostics” presented at the Canadian College of Microbiologists Workshop on Future Trends in Laboratory Diagnostics, Edmonton, AB (May 5, 2010).

186) Wishart, D.S. “Metabolomics: The Capstone to Systems Biology” presented at the Systems Biology 2010 Conference – From Gene to Metabolite Networks, Melbourne, Australia (May 17, 2010).

187) Wishart, D.S. “Applications of Metabolomics to Drug Research and Development” presented at the Centre for Drug Research and Development, Vancouver, BC (June 10, 2010).

188) Wishart, D.S. “FooDB and the Construction of an International Consortium” presented at the 3<sup>rd</sup> NUGO Workshop on Nutritional Metabolomics, Vlaardingen, The Netherlands (July 1-2, 2010).

189) Wishart, D.S. “The Future of Prion Disease Diagnosis” presented at the CJD 2010 and CJD Foundation Family Conference, Washington DC (July 17, 2010).

190) Wishart, D.S. “The Human Metabolome: Applications to Clinical Chemistry” presented at the AACC Annual Meeting 2010, Anaheim CA (July 26-28, 2010).

191) Wishart, D.S. “Using Chemical Shifts to Build and Assess Protein Structures”, presented at the XXIV ICMRBS Meeting, Cairns, Australia (Aug. 25, 2010).

192) Wishart, D.S. “PANAMP- The Pan-Alberta Metabolomics Platform” presented at the Centre for Drug Research and Discovery, Vancouver, BC (Oct. 8, 2010).

193) Wishart, D.S. “Metabolomics as a Capstone to Systems Biology” presented at the Centre for Analysis of Cellular Mechanisms and Systems Biology Workshop on Metabolomics, Bozeman, Montana (Oct. 12, 2010).

194) Wishart, D.S. “An Integrated Approach to Characterize the Structure and Dynamics of Prions”, presented at the PrionNet/APRI Joint Scientific Meeting, Vancouver, BC (Oct. 25, 2010).

- 195) Wishart, D.S. “Novel Inhibitor Development for Prion Conversion” presented at the PrioNet/APRI Joint Scientific Meeting, Vancouver, BC (Oct. 25, 2010).
- 196) Wishart, D.S. “Quantitative Metabolomics: How Far Can We Go?” presented at Pacificchem2010, Honolulu, Hawaii (Dec. 18, 2010).
- 197) Wishart, D.S. “Tools, Issues and Suggestions on Structure Validation” presented at the wwPDB NMR Structure Validation Task Force Workshop, Rutgers, NJ (Jan. 15, 2011).
- 198) Wishart, D.S. “Metabolomics, Past, Present and Future” presented at the Pathology Grand Rounds for the Vancouver Women’s and Children’s Hospital, Vancouver, BC (March 1, 2011).
- 199) Wishart, D.S. “What the Heck is That? The Challenge of Metabolite Identification in Metabolomics” ACS-CSC Young Investigator Award Symposium, PittCon 2011, Atlanta Georgia (March 16, 2011).
- 200) Wishart, D.S. “NINT and Metabolomics” presented at the NRC-National Institute for Nanotechnology Visioning Workshops, Edmonton, AB (April 20, 2011).
- 201) Wishart, D.S. “Structure Determination by Mass Spectrometry” presented at the Canadian National Proteomics Network (CNPN/ETP) Joint Symposium, Banff, AB (May 8, 2011).
- 202) Wishart, D.S. “Predicting Chemical Shifts from Structure and Structure from Chemical Shifts” presented at the Gordon Research Conference on Computational Aspects of Biomolecular NMR, Il Ciocco, Italy (May 23, 2011).
- 203) Wishart, D.S. “The Bioinformatics of Small Molecules” presented at the Canadian Society for Pharmaceutical Sciences (CSPS) Symposium, Montreal, QC (May 25, 2011).
- 204) Ametaj, B.N. and Wishart, D.S. “Applications of Metabolomics Technology in Dairy Cattle Research” presented at the 7<sup>th</sup> Annual Metabolomics Society Meeting, Cairns, Australia (June 28, 2011).
- 205) Xia, J., Sinelnikov, I.V., and Wishart, D.S. “METTAT – A Web-based Metabolomic Tool for Analyzing Two-Factor and Time-Series Data” presented at the 7<sup>th</sup> Annual Metabolomics Society Meeting, Cairns, Australia (June 29, 2011).

206) Wishart, D.S. “Biostatistics for Metabolomics” presented at the 7<sup>th</sup> Annual Metabolomics Society Meeting, Cairns, Australia (June 27, 2011).

207) Wishart, D.S. “MarkerDB – The Biomarker Database” presented at the 7<sup>th</sup> Annual Metabolomics Society Meeting, Cairns, Australia (June 28, 2011).

208) Wishart, D.S. “The Future of Prion Disease Diagnostics” presented at the CJD 2011 & CJD Foundation Family Conference, Washington DC (July 9, 2011).

209) Wishart, D.S. “Metabolomics Resources, Initiatives and Core Facilities in Canada” presented at the NIH-CF Metabolomics Initiative Meeting, Bethesda MD (Sept. 15, 2011).

210) Wishart, D.S. “Databases in Metabolomics” presented at the Max Rubner Conference on Food Metabolomics, Karlsruhe, Germany (Oct. 9-11, 2011).

211) Wishart, D.S. “Bioinformatic Tools and Databases in Nutrition Research” presented at the 5<sup>th</sup> International Conference on Polyphenols and Health, Barcelona, Spain (Oct. 17-20, 2011).

212) Wishart, D.S. “Metabolomics Databases – What Can We Learn from Past “Omics” Efforts” presented at the NMR Standards & Biobanks Workshop, Florence, Italy (Nov. 18, 2011).

213) Wishart, D.S. “Metabolomics in Orphan Disease Research” Presented at the Orphan Diseases Workshop, Ottawa ON (Nov. 29, 2011).

214) Wishart, D.S. “Metabolomics and Personalized Medicine” Presented at the University of Toronto, Toronto, ON (Dec. 2, 2011).

215) Wishart, D.S. “Metabolomics and Personalized Medicine” Presented at McMaster University, Hamilton, ON (Dec. 2, 2011).

216) Wishart, D.S. “Metabolomics and Personalized Medicine” Presented at the University of Alberta, Edmonton, AB (Dec. 8, 2011).

217) Wishart, D.S. “Metabolomics and Personalized Medicine” Presented at McGill University, Montreal, Quebec (Jan. 13, 2012).

- 218) Wishart, D.S. “The PrioNet Prion Protein Production Platform: PrP<sup>5</sup>” Presented at the PrioNet-APRI Network and Collaboration Meeting, Vancouver BC (Jan. 18, 2012).
- 219) Wishart, D.S. “Detection of Pre-clinical Prion Disease Biomarkers by Metabolomics” Presented at the PrioNet-APRI Network and Collaboration Meeting, Vancouver BC (Jan. 18, 2012).
- 220) Wishart, D.S. “Vaccination of Mice Against Prion Disease Using Attenuated PrP Oligomers” Presented at the PrioNet-APRI Network and Collaboration Meeting, Vancouver BC (Jan. 18, 2012).
- 221) Wishart, D.S. “Identification, Characterization and Development of Novel Inhibitors of Prion Conversion” Presented at the PrioNet-APRI Network and Collaboration Meeting, Vancouver BC (Jan. 18, 2012).
- 222) Wishart, D.S. “An Integrated Approach to Characterize the Structure and Dynamics of Prions – Phase II” Presented at the PrioNet-APRI Network and Collaboration Meeting, Vancouver BC (Jan. 18, 2012).
- 223) Wishart, D.S. “Using Chemical Shifts to Understand Structured and Unstructured Proteins” Presented at the Structural & Unstructural Biology of Viral Proteins Workshop, CERM, Florence, Italy (Jan. 24-26, 2012).
- 224) Wishart, D.S. “The Metabolomics Innovation Centre” Presented at the Annual Genome Canada Science Technology and Innovation Centre Meeting, Vancouver, BC (Feb. 9, 2012).
- 225) Wishart, D.S. “Bioinformatics: Solving the Big Problems in Life Science” Presented at the University of Alberta, Edmonton, AB (Feb. 12, 2012).
- 226) Wishart, D.S. “Metabolomics and Personalized Medicine” Presented at the University of Manitoba, Winnipeg, MB (Feb. 24, 2012).
- 227) Wishart, D.S. “Starting, Propagating and Stopping Prion Conversion – Some Structural Insights” Prion Science Brazil-Canada Meeting, Sao Paulo, Brazil (March 7, 2012).
- 228) Wishart, D.S. “Plasma Metabolomics in Transplantation” Presented at the 3<sup>rd</sup> Transplantomics and Biomarkers in Organ Transplantation Conference, San Diego, CA (March 10, 2012).



- 229) Wishart, D.S. “The Food Metabolome Database and Markers of Dietary Intake”, NutriTech Launch Meeting, Amsterdam, the Netherlands (March 12, 2012).
- 230) Wishart, D.S. “Bioinformatics for Metabolomics” Presented at the ISCB 2012 Latin America Workshop on Insights on Metabolomics and its Applications. Santiago, Chile (March 25, 2012).
- 231) Wishart, D.S. “MS23D: From Mass Spectra to 3D Protein Structures”, Presented at the Canadian National Proteomics Network (CNP) Conference, Toronto, ON (April 24, 2012).
- 232) Wishart, D.S. “NINT, Nanotechnology and Metabolomics Sensors” Presented at the Joint NRC-AIST Workshop on Nanotechnology, Tsukuba, Japan (April 27, 2012).
- 233) Wishart, D.S. “Metabolomics and Personalized Medicine” Presented at the Alberta Health Industry Association, Edmonton, AB (May 4, 2012).
- 234) Wishart, D.S. “The Alberta Food Metabolome Project: What’s in Your Food?” Presented at the AI-Bio Impact Innovation 2012 Seminar Series, Edmonton, AB, May 16, 2012.
- 235) Wishart, D.S. “The Alberta Food Metabolome Project: What’s in Your Food?” Presented at the AI-Bio Impact Innovation 2012 Seminar Series, Calgary, AB, May 17, 2012.
- 236) Wishart, D.S. “The Human Metabolome Database and Its Associated Software Resources” Presented at the EMBL-EBI Industry Programme and MetaboLights Project Workshop, Hinxton, UK, May 23, 2012.
- 237) Wishart, D.S. “The Tricorder Project: Using Nanotechnology to Assess Food Safety and Quality” Presented at the ACAMP – Agriculture and Forestry Seminar Series, Edmonton, AB, June 5, 2012.
- 238) Wishart, D.S. “The Human Plasma Metabolome” Presented at the 72<sup>nd</sup> Annual American Diabetes Association Meeting, Philadelphia, PA, June 11, 2012.
- 239) Wishart, D.S. “Metabolomics and Personal Medicine: Research, New Oportunities and Commercialization” Presented to the NRC-IRAP National Life Sciences Representatives, Edmonton, AB, June 13, 2012.

- 240) Wishart, D.S. “Small Molecules Inhibitors of Protein Misfolding” Presented at the Joint PrP-Canada and Protein Folding and Disease Conference, Toronto, ON, June 26, 2012.
- 241) Wishart, D.S., Kaddurah-Daouk, R., Fiehn, O., Steinbeck, C., Hankemier, T., Higachi, R, Raftery, D. “Bottlenecks in Metabolomics” Presented at the 8<sup>th</sup> International Conference of the Metabolomics Society, Washington, DC, June 26, 2012.
- 242) Wishart, D.S. and Mandal, R. “Canadian Initiatives and Innovations in Metabolomics” Presented at the 8<sup>th</sup> International Conference of the Metabolomics Society, Washington, DC, June 28, 2012.
- 243) Wishart, D.S. “Chemical Shift Calculation and Protein Structure Refinement” Presented at the 25<sup>th</sup> ICMRBS Meeting, Lyon, France, Aug. 20, 2012.
- 244) Wishart, D.S. “Curation of Biological Data – Perspectives for the 21<sup>st</sup> Century” Presented at the International Agency for Cancer Research (IARC), Lyon, France, Aug. 21, 2012.
- 245) Wishart, D.S. “Comprehensive Characterization of the Human Biofluid Metabolomes” Presented at the 4<sup>th</sup> Annual Australasian Metabolomics Meeting, Shah Alam, Malaysia, Sept. 4, 2012.
- 246) Wishart, D.S. “Metabolomics and Personalized Medicine” Presented at the NSFC-CIHR Canada-China Joint Health Research Initiative, Montreal, Quebec, Sept. 12, 2012.
- 247) Wishart, D.S. “The Toxin, Toxin-Target Database – T3DB” Presented at the EMBL-EBI Industry Programme Workshop Systems Toxicology: Systems Biology for Tox Pathways, Hinxton, England, Sept. 25, 2012.
- 248) Wishart, D.S. & Mandal, R. “Early Diagnostics – Metabolomics in Osteoarthritis” Presented at the OA (Osteoarthritis) Alberta Annual Team Meeting, Edmonton, AB, Oct. 16, 2012.
- 249) Wishart, D.S. “Metabolomics and Personalized Phenotyping” Presented at the UBC/CIHR Workshop on Personalized Medicine, Vancouver, BC, Nov. 12, 2012.
- 250) Wishart, D.S. “A Primer in Bioinformatics” Presented at Computing Science 495, University of Alberta, Edmonton, AB, Nov. 18, 2012.

- 251) Wishart, D.S. “The Human Metabolome Project in 2012” Presented at 2012 Omics Australasia Symposium, Freemantle, Australia, Nov. 26, 2012.
- 252) Wishart, D.S. “Using Metabolomics to Discover Novel Biomarkers for Common Diseases” Presented at the University of Alabama Birmingham Symposium: Metabolomics, The Underlying Basis of Disease, Birmingham, AL, Dec. 12, 2012.
- 253) Wishart, D.S. “Metabolomics, Biomarkers, Nutrition and Metabolism” Presented at AFNS 501 (Advanced Human Metabolism), University of Alberta, Edmonton, AB, Feb. 25, 2013.
- 254) Wishart, D.S. “Metabolomics, Genomics and Human Disease” Presented at the CIFAR Genetic Networks Program Meeting, Banff, AB, April 6, 2013.
- 255) Wishart, D.S. “T3DB – The Toxin, Toxin-Target Database” Presented at the Communities of Practice – US EPA National Center for Computational Toxicology Monthly Seminar/Webinar, Edmonton, AB/Washington, DC, April 25, 2013.
- 256) Wishart, D.S. “Metabolomics: Its Role In Nutrition, Disease & the Gut Microbiome” Presented at the Western Canada Pediatric GI Meeting, Edmonton, AB, April 26, 2013.
- 257) Wishart, D.S. “Clearing the Biomarker Barrier, Moving from the Bench to the Bedside” Presented at the 7<sup>th</sup> Annual ETP (Experimental Technologies for Proteomics) Symposium, Toronto, ON, May 1, 2013.
- 258) Wishart, D.S. “Disruptive Technologies for Molecular Detection” Presented at the Genome Canada Disruptive Technologies Workshop, Toronto, ON, May 10, 2013.
- 259) Wishart, D.S. “The Future of NMR in Metabolomics Research” Presented at the Gordon-Merck Research Seminar - Computational Aspects of Biomolecular NMR, Mount Snow Resort, Vermont, June 1, 2013.
- 260) Wishart, D.S. “Analyzing Metabolomic and Metabolism Data” Presented at the Gordon Research Conference - Computational Aspects of Biomolecular NMR, Mount Snow Resort, Vermont, June 5, 2013.
- 261) Wishart, D.S. “Metabolomics and Medicine” Presented at the University of Alberta OMICS Symposium, Edmonton, AB, June 17, 2013.

262) Wishart, D.S. “Metabolomics in Alberta: Past, Present and Future” Presented at the Genome Alberta Board Meeting, Calgary, AB, June 25, 2013.

263) Wishart, D.S. “NMR and Metabolomics: Bringing Medicine and NMR Closer Together” Presented at the University of Toronto, Toronto, AB, Aug. 8, 2013.

264) Wishart, D.S. “Metabolomics and Metagenomics – Meta-omics” Presented at the Microbial Multi-Omics Workshop, Montreal, QC, Sept. 23, 2013.

265) Wishart, D.S. “Metabolomics and Xenobiotics” Presented at the 10<sup>th</sup> International ISSX Conference Short Course on Metabolomic Profiling, Toronto, ON, Sept. 29, 2013.

266) Wishart, D.S. “NMR and Metabolomics: Pushing the Limits of Speed, Sensitivity and Coverage” Presented at the NJACS NMR Topical Group Symposium, Rutgers University, New Brunswick, New Jersey, Oct. 2, 2013.

267) Wishart, D.S. “New and Improved Resources for Metabolomics Research” Presented at Bristol-Myers-Squibb, Princeton, New Jersey, Oct. 3, 2013.

268) Wishart, D.S. “The Metabolomics Innovation Centre” Presented to Servier Pharmaceuticals Inc., Edmonton, AB, Oct. 8, 2013.

269) Wishart, D.S. “Validation of Protein Structure Models Against Chemical Shift Data”, Presented at the wwPDB Protein Structure VTF Workshop, Duxford, UK, Nov. 17, 2013.

270) Wishart, D.S. “Handling NMR Data in CS23D, GeNMR and PROSESS”, Presented at the wwPDB Workshop on Unified Restraints Formats, Duxford, UK Nov. 18, 2013.

271) Wishart, D.S. “Quantitative Metabolomics and Medical Biomarkers”, Presented at the Liggins Institute, University of Auckland, Auckland, NZ, Dec. 4, 2013.

272) Wishart, D.S. “Metabolomics and Medicine: From Biomarkers to Treatment”, Presented at the AB Heart STEADI-HF Seminar, University of Alberta, Edmonton, AB, Dec. 12, 2013.

273) Wishart, D.S. “The Metabolomics Innovation Centre”, Presented at the Genome Canada Science and Technology Innovation Centres Platform Meeting, Ottawa, ON, Dec. 17, 2013.

- 274) Wishart, D.S. “Disease Biomarkers and Metabolomics”, Presented at the University of Alberta Pathology Grand Rounds, Edmonton, AB, Dec. 19, 2013.
- 275) Wishart, D.S. “Genomics, Metabolomics and Agriculture”, Presented at the Faculty of Agriculture, University of Alberta, Edmonton, AB, Feb. 8, 2014.
- 276) Wishart, D.S. “Metabolomics and Veterinary Medicine”, Presented to the University of Calgary Veterinary Medicine School via Video Conference, Feb. 26, 2014.
- 277) Wishart, D.S. “Genomics, Metabolomics and AgriFood Research”, Presented at the University of Saskatchewan, Saskatoon, SK, March 19, 2014.
- 278) Wishart, D.S. “Metabolomic Databases in Canada”, Presented at the COSMOS Consortium Meeting, Hinxton, UK, Apr. 2, 2014.
- 279) Wishart, D.S. “Genomics, Metabolomics and AgriFood Research”, Presented at the University of Calgary (Faculty of Science), Calgary, AB., Apr. 17, 2014.
- 280) Wishart, D.S. “Using Metabolomics to Detect Biomarkers of Food Consumption”, Presented at the American Society for Nutrition Meeting, San Diego, CA. Apr. 30, 2014.
- 281) Wishart, D.S. “Metabolomics – How to Make Metabolism Interesting for Students”, Presented at the Edmonton Biology and Chemistry Regionals Annual Conference, Edmonton, AB, May 2, 2014.
- 282) Wishart, D.S. “Using Metabolomics to Shed New Light on Genetic Diseases”, Presented at the CIHR Meeting on Statistical Genetics and Human Disease, Victoria BC, May 5, 2014.
- 283) Wishart, D.S. “Genomics, Metabolomics and AgriFood Research”, Presented at the UBC-Okanagan Campus, Kelowna, BC, May 6, 2014.
- 284) Wishart, D.S. “Metabolomics in AgriFood Research”, Presented at the University of Guelph, Guelph, ON, May 14, 2014.
- 285) Wishart, D.S. “Metabolomics, Biomarkers and Human Health – The Next Frontier”, University of Toronto, Dept. of Gastroenterology, Toronto, ON, May 15, 2014.

286) Wishart, D.S. “Quantitative Metabolomics and Medical Biomarkers: Challenges and Opportunities” Presented at the GTC-Metabolomics Symposium: Advances and Applications in Human Disease, Cambridge, MA, May 22, 2014.

287) Wishart, D.S. “Mining Metabolites for Medically Meaningful Biomarkers”, Presented at the International Agency for Research on Cancer (IARC), Lyon, France, May 27, 2014.

288) Wishart, D.S. “Getting the Most from Your Protein Chemical Shift Data”, Presented at the EMBO/Chianti Workshop, Grosseto, Italy, June 5, 2014.

289) Wishart, D.S. “Chemical Shift Refinement”, Presented at the EMBO/Chianti Workshop, Grosseto, Italy, June 5, 2014.

290) Wishart, D.S. “Making Metabolomics Matter”, Presented at the 10<sup>th</sup> International Conference of the Metabolomics Society, Tsuruoka, Japan, June 25, 2014.

291) Wishart, D.S. “Making Metabolomics Matter”, Presented at the Metabolomics Data Standards and Data Processing Workshop, Edmonton, AB, July 14-15, 2014.

292) Wishart, D.S. “Translational Biomarker Discovery in Clinical Metabolomics”, Presented at the World Transplant Congress, San Francisco, CA, July 29, 2014.

293) Wishart, D.S. “Making Metabolomics Matter”, Presented at MIT, Cambridge, Mass. Aug. 20, 2014.

294) Wishart, D.S. “Making Metabolomics Matter”, Presented at the University of Melbourne, Melbourne, Australia. Sept. 18, 2014.

295) Wishart, D.S. “Metabolomics and Lymphedema”, Presented at the Alberta Lymphedema Workshop, Edmonton, AB, Sept. 29, 2014.

296) Wishart, D.S. “Metabolomics, Epigenetics, Environment and Health”, Presented at the CEERHC Workshop, Vancouver, BC, Oct. 10, 2014.

297) Wishart, D.S. “Data Mining and Question Answering for the Life Sciences”, Presented at the Dept. of Computing Science, University of Alberta, Edmonton, AB, Oct. 29, 2014.

- 298) Wishart, D.S. “Clinical Metabolomics: Moving from the Bench to the Bedside”, Presented as CSMU, Taichung, Taiwan, Nov. 6, 2014.
- 299) Wishart, D.S. “Clinical Metabolomics: Moving from the Bench to the Bedside”, Presented as Chang Gung University, Taiwan, Nov. 6, 2014.
- 300) Wishart, D.S. “Neonicotinoids and Bees”, Presented at St. Paul’s United Church, Edmonton, AB, Nov. 13, 2014.
- 301) Wishart, D.S. “Inducers and Inhibitors of Prion Formation and Propagation”, Presented at the Advances in the Science of Prion and Prion-Like Misfolding Diseases, Ubatuba, Brazil, Nov. 17-18, 2014.
- 302) Wishart, D.S. “Metabolomics in Drug Research and Development”, Presented at McGill University, Montreal, QC, Nov. 28, 2014.
- 303) Wishart, D.S. “The Metabolome, The Exposome & Pregnancy-Related Diseases”, Presented at the 2<sup>nd</sup> International Pregnancy Research Alliance Symposium, Chongqing, China, Dec. 4, 2014.
- 304) Wishart, D.S. “Metabolomics for Environmental Health Decisions”, Presented at the NRC ESEH Committee Meeting, Washington DC, Dec. 12, 2014.
- 305) Wishart, D.S. “Validation of Protein Structure Models Against Chemical Shift Data”, Presented at the VTF (Validation Task Force) Workshop 3.0, Rutgers University, New Jersey, Jan. 9, 2015.
- 306) Wishart, D.S. “Prion Conversions and Prion Vaccines”, Presented at the APRI Scientific Meeting, Edmonton, AB, Jan. 26, 2015.
- 307) Wishart, D.S. “A Diet to Defy Cancer”, Presented at the Edmonton Jewish Drop-in Centre, Edmonton, AB, Feb. 3, 2015.
- 308) Wishart, D.S. “An Introduction to Metabolomics and its Applications”, Presented at the 20<sup>th</sup> Annual Biochemistry and Microbiology Graduate Student Symposium, Victoria BC, Feb. 12, 2015.
- 309) Wishart, D.S. “Moving Metabolomics from the Benchtop to the Bedside”, Presented at the University of Florida, Gainesville, FL, Feb. 15, 2015.

- 310) Wishart, D.S. “Updates and Upgrades to the Alberta NMR Software Suite”, Presented at the University of Leicester, Leicester, UK, Feb. 23, 2015.
- 311) Wishart, D.S. “Updates and Upgrades to the Alberta NMR Software Suite”, Presented at the European Bioinformatics Institute, Hinxton, UK, Feb. 24, 2015.
- 312) Wishart, D.S. “Metabolomics for Diagnosis and Monitoring of GI and Liver Disease”, Presented at the Canadian Association for Gastroenterology Meeting, Banff, AB, Feb. 28, 2015.
- 313) Wishart, D.S. “Metabolomics in Drug Research and Development”, Presented to Tech Edmonton, Edmonton, AB, March 25, 2015.
- 314) Wishart, D.S. “Metabolism, Metabolomics and Cancer”, Presented at the ASBMB Meeting, Metabolism: Warburg at 90, Boston, MA, March 31, 2015.
- 315) Wishart, D.S. “Making NMR the Method of Choice in Metabolomics”, Presented at the 56<sup>th</sup> Experimental NMR Conference, Pacific Grove, CA, USA, Apr. 21, 2015.
- 316) Wishart, D.S. “Translational Lipidomics: Linking Lipidomics to Laboratory Medicine”, Presented at the LipidMaps Meeting, Lipidomics: Impact on Cancer, Metabolic and Inflammatory Diseases, La Jolla, CA, May 12, 2015.
- 317) Wishart, D.S. “Using Metabolomics to Characterize Exposure”, Presented at the National Academy of Science Workshop on Metabolomics as a Tool for Characterizing the Exposome, Washington DC, May 28, 2015.
- 318) Wishart, D.S. “Understanding Exposure and Disease Etiology, Case Study: Eosinophilic Esophagitis”, Presented at the National Academy of Science Workshop on Metabolomics as a Tool for Characterizing the Exposome, Washington DC, May 28, 2015.
- 319) Wishart, D.S. “Metabolomics, TMIC and Personalized Medicine”, Presented at the University of British Columbia, Vancouver, BC, June 2, 2015.
- 320) Wishart, D.S. “Automating NMR-Based Metabolomics”, Presented at the GRC-Computational Aspects of Biomolecular NMR, Il Ciocco, Italy, June 9, 2015.



- 321) Wishart, D.S. “The Future of Metabolomics”, Presented at the University of Alabama Birmingham, Birmingham, AL, June 18, 2015.
- 322) Wishart, D.S. “Metabolism, Metabolomics and Cancer”, Presented at the University of Alabama Birmingham, Birmingham, AL, June 19, 2015.
- 323) Wishart, D.S. “Moving Metabolomics from the Benchtop to the Bedside”, Presented at the 1<sup>st</sup> International Symposium on Metabolomics in Mexico, Guadalajara, MX, June 25, 2015.
- 324) Wishart, D.S. “The Metabolomics Innovation Centre”, presented at the Genome Canada Genomics Innovation Network Meeting, Toronto, ON, July 15, 2015.
- 325) Wishart, D.S. “New Databases and Software Tools for the Non-targeted Identification of Xenobiotics”, US-EPA Non-targeted Analysis Workshop, Research Triangle Park, NC, USA, Aug. 18, 2015.
- 326) Wishart, D.S. “Computational Challenges in Metabolomics”, presented at the Dagstuhl Seminar on Computational Mass Spectrometry, Schloss Dagstuhl, Germany, Aug. 24, 2015.
- 327) Wishart, D.S. “FoodBall Research Activities”, presented at the FoodBall-NuGO week Joint Meeting, Barcelona, Spain, Sept. 9, 2015.
- 328) Wishart, D.S. and Reid, J. “Metabolomics, The Metabolomics Innovation Centre and Plant Biotechnology”, presented at the 11<sup>th</sup> ISBAB Symposium, Banff, AB, Sept. 14, 2015.
- 329) Wishart, D.S. “Metabolomic Devices for Companion Diagnostics and Personalized Medicine” presented at the First Annual Tricorder AIHS-CRIO AGM, Sept. 24, 2015.
- 330) Wishart, D.S. “How Metabolomics is Changing Our Understanding of Human Disease” presented at HUPO 2015, Vancouver, BC, Sept. 29, 2015.
- 331) Wishart, D.S. “Chemical Ontologies – How To’s and Use Cases” presented at the OntoChem Workshop, Basel, Switzerland, Oct. 2, 2015.
- 332) Wishart, D.S. “FooDB: A Database of Food Constituents & Their Health Effects” presented at the 4<sup>th</sup> International Foodomics Conference, Cesena, Italy, Oct. 8, 2015.

- 333) Wishart, D.S. “Metabolomics and Food Databases” presented at the 12<sup>th</sup> European Nutrition Conference, Berlin, Germany, Oct. 21, 2015.
- 334) Wishart, D.S. “Moving Metabolomics from the Benchtop to the Bedside” presented at the Biocrates Workshop on Targeted Metabolomics, Munich Germany, Oct. 22, 2015.
- 335) Wishart, D.S. “Introduction to the TMIC Symposium on Metabolomics and NMR”, presented at the first TMIC Symposium, Edmonton, AB, Nov. 5, 2015.
- 336) Wishart, D.S. “Identifying the Dark Matter of Metabolism”, presented at the NIH Beyond the Known Metabolome Workshop, Bethesda, MD, Nov. 17, 2015.
- 337) Wishart, D.S. “Metabolomics in Drug Research and Development”, presented at the University of Alberta Annual Industry Day Presentations, Edmonton, AB, Nov. 23, 2015.
- 338) Wishart, D.S. “Data Exchange and Public Reference Data”, presented at the Dagstuhl Computational Metabolomics Workshop, Schloss Dagstuhl, Germany, Nov. 30, 2015.
- 339) Wishart, D.S. “Searching in Molecular Structure Databases”, presented at the Dagstuhl Computational Metabolomics Workshop, Schloss Dagstuhl, Germany, Dec. 1, 2015.
- 340) Wishart, D.S. “A Prion Research Update”, presented at the 2016 Alberta Prion Research Institute (APRI) Annual Meeting, Calgary, AB, Feb. 3, 2016.
- 341) Wishart, D.S. “Metabolomics Software Resources”, presented at the EMBO Practical Course on Metabolomics Bioinformatics for Life Sciences”, Hinxton, UK, Feb. 15, 2016.
- 342) Wishart, D.S. “Translational Metabolomics: Moving Metabolomic Discoveries from the Bench to the Bedside”, presented at the University of Calgary, Calgary, AB, Feb. 19, 2016.
- 343) Wishart, D.S. “Metabolomics and its Applications to Human Disease”, presented at the Yunnan Cancer Hospital, Kunming, China, March 9, 2016.
- 344) Wishart, D.S. “Classifying Chemistry: Current Efforts in Canada”, presented at the 251<sup>st</sup> ACS Chemistry Meeting, San Diego CA, March 15, 2016.

- 345) Wishart, D.S. “Metabolomics, Epigenetics and Precision Medicine – What’s the Connection?” presented at the Alberta Epigenetics Network Summit, Banff, Alberta, March 22, 2016.
- 346) Wishart, D.S. “How Metabolomics is Changing our Understanding of Human Disease”, presented at the ANZMET 2016 meeting, Melbourne, Australia, March 31, 2016.
- 347) Wishart, D.S. “Bioinformatics and Statistical Methods for Metabolomics”, presented at the MSB (Microscale Separations & Bioanalysis) 2016 Conference, Niagara-on-the-Lake, ON, Apr. 3, 2016.
- 348) Wishart, D.S. “New Resources for Enabling Food & Nutritional Metabolomics”, presented at the MSB (Microscale Separations & Bioanalysis) 2016 Conference, Niagara-on-the-Lake, ON, Apr. 7, 2016.
- 349) Wishart, D.S. “Deciphering the Dark Matter of Metabolism”, presented at the CFABS 2016 Toronto Spring MS Group Meeting, Toronto, ON, May 18, 2016.
- 350) Wishart, D.S. “Identifying the Dark Matter of the Chemical Exposome”, presented at the Non-Target 2016 Conference, Ascona, Switzerland, May 31, 2016.
- 351) Wishart, D.S. “Biotransformation Prediction with BioTransformer”, presented at the Non-Target 2016 Conference, Ascona, Switzerland, June 2, 2016.
- 352) Wishart, D.S. “Reading the Hidden Meaning of Chemical Shifts: Applications to Structural Biology and Metabolomics”, presented at CIC bioGUNE, Bilbao, Spain, June 6, 2016.
- 353) Wishart, D.S. “Standardizing NMR-Based Metabolomics”, presented at the University of Wisconsin, Madison, Wisconsin, June 10, 2016.
- 354) Wishart, D.S. “Introduction to Metabolomics”, presented at the Universidad Autonoma del Estado de Morelos, Curenavaca, Mexico, June 17-18, 2016.
- 355) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at the EUROMAR 2016 conference, Aarhus, Denmark, July 6, 2016.
- 356) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at the University of Sydney, Sydney, Australia, July 25, 2016.

357) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at the University of New South Wales, Sydney, Australia, July 26, 2016.

358) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at the Australia National University, Canberra, Australia, July 27, 2016.

359) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at La Trobe University, Melbourne, Australia, July 28, 2016.

360) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at the University of Melbourne, Melbourne, Australia, July 29, 2016.

361) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at the University of Queensland, Brisbane, Australia, Aug. 1, 2016.

362) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at Griffith University, Gold Coast, Australia, Aug. 2, 2016.

363) Wishart, D.S. ANZMAG Lectureship (14 Lectures over 3 days on NMR in metabolomics), presented at the University of Queensland, Brisbane, Australia, Aug. 3-5, 2016.

364) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at Murdoch University, Perth, Australia, Aug. 8, 2016.

365) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at the University of Auckland, Auckland, New Zealand, Aug. 9, 2016.

366) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at the University of Otago, Dunedin, New Zealand, Aug. 10, 2016.

367) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at Victoria University, Wellington, New Zealand, Aug. 11, 2016.

368) Wishart, D.S. “Why NMR Matters in Metabolomics”, presented at the Queensland University of Technology, Brisbane, Australia, Aug. 12, 2016.

369) Wishart, D.S. “New Software Tools and Resources for MS-based Metabolomics”, presented at the University of Copenhagen, Copenhagen, Denmark, Sept. 9, 2016.

370) Wishart, D.S. “Is Cancer a Genetic Disease or a Metabolic Disease”, presented at the How to Bridge Metabolomics & Genomics Conference, Pula, Sardinia, Italy, Sept. 12, 2016.

371) Wishart, D.S. “What you Need to Know in Metabolomics”, presented at the How to Bridge Metabolomics & Genomics Conference, Pula, Sardinia, Italy, Sept. 13, 2016.

372) Wishart, D.S. “Pharmacometabolomics: Applications in Drug Safety and Efficacy”, presented at the JSPS/SPS/CSPT Meeting, Vancouver, BC, Sept. 20, 2016.

373) Wishart, D.S. “Metabolomics and Clinical Applications: Why Urine is Golden”, presented at the International Society of Nephrology – Forefronts Symposium, San Diego, CA, Sept. 24, 2016.

374) Wishart, D.S. “Applications of Quantitative Metabolomics to Food Analysis”, presented at the 2016 Max Rubner Conference on Food Metabolomics, Karlsruhe, Germany, Oct. 10, 2016.

375) Wishart, D.S. “Metabolomic Devices for Companion Diagnostics & Personalized Medicine”, presented at the AIHS-CRIO AGM, Edmonton, AB, Oct. 19, 2016.

376) Wishart, D.S. “New Approaches for Plant Natural Product Identification”, presented at the XVth Fall Workshop: Frontiers in Biotechnology, Merida, Mexico, Oct. 24, 2016.

377) Wishart, D.S. “The Future of NMR in Metabolomics”, presented at the 55<sup>th</sup> Annual Meeting of the NMR Society of Japan, Hiroshim, Japan, Nov. 17, 2016.

378) Wishart, D.S. “Metabolomics and Metabolic Syndrome”, presented at the Montreal Diabetes Research Centre, Montreal, QC, Dec. 14, 2016.

379) Wishart, D.S. “Metabolomics, TMIC and Precision Medicine”, presented at the Metabolic Grand Rounds, University of Alberta, Edmonton, AB, Dec. 16, 2016.

380) Wishart, D.S. “Metabolomics, the Microbiome & Precision Health”, presented at the AMED Alberta Workshop for Medical Innovation, Calgary, AB, Feb. 25, 2017.

- 381) Wishart, D.S. “Prion Project Research Update”, presented at the Alberta Prion Research Institute 2017 Scientific Meeting, Edmonton, AB, March 1, 2017.
- 382) Wishart, D.S. “Precision Medicine in Alberta: Bringing 21<sup>st</sup> Century Science to 19<sup>th</sup> Century Medical Practices”, presented at the Alberta Health Industry Association Breakfast Meeting, Edmonton, AB, March 1, 2017.
- 383) Wishart, D.S. “Precision Medicine and Metabolomics”, presented at McMaster University, Hamilton, ON, March 16, 2017.
- 384) Wishart, D.S. “New Technologies for Large Scale Analysis of Small Molecules”, presented at the 2017 HUPO Meeting, San Diego, CA, March 21, 2017.
- 385) Wishart, D.S. “Metabolomics, TMIC and Agri-Tech”, presented at the UK-Alberta Agritech Meeting, Edmonton, AB, March 24, 2017.
- 386) Wishart, D.S. “Metabolomics, TMIC and Endless Possibilities”, presented at the University of Alberta, Edmonton, AB, March 29, 2017.
- 387) Wishart, D.S. “Time Series Data Analysis Using MetaboAnalyst”, presented at the FoodBALL Webinar Series, Edmonton, AB, March 30, 2017.
- 388) Wishart, D.S. “Metabolomics, Biomarkers and Human Health – The Next Frontier”, presented at the University of Toronto, Dept. of Gastroenterology, April. 3, 2017.
- 389) Wishart, D.S. “Metabolomics Networking Meeting”, presented a McGill University, Montreal, Quebec, May 10, 2017.
- 390) Wishart, D.S. “Metabolomics: Making an Impact in Alberta”, presented at the Western Economic Diversification Forum, Edmonton, AB, May 17, 2017.
- 391) Wishart, D.S. “New Databases and Software Tools for Metabolomics, Exposomics and Toxicological Assessment”, presented at the Pacific Northwest National Lab, Richland, WA, May 31, 2017.

- 392) Wishart, D.S. “Metabolomics, Precision Medicine and the Future of Health”, presented at the Conference on Metabolomics in Precision Medicine: From Theory to Practice, Mt. Sinai Hospital, Toronto, ON, June 8, 2017.
- 393) Wishart, D.S. “Molecular Analysis for Personalized, Precision Health: Metabolomics”, presented at the 2<sup>nd</sup> Personalized Medicine Summit, Vancouver, BC, June 11, 2017.
- 394) Wishart, D.S. “Omic Databases and Their Role in Clinical Decision Making”, presented at the 2<sup>nd</sup> Personalized Medicine Summit, Vancouver, BC, June 12, 2017.
- 395) Wishart, D.S. “TMIC: The Metabolomics Innovation Centre”, presented at the Genome Canada GTP Webinar, Edmonton, AB, June 19, 2017.
- 396) Wishart, D.S. “In Silico Metabolomics: New Tools and Techniques to Measure the Dark Matter of the Metabolome”, presented at the 13<sup>th</sup> International Conference of the Metabolomic Society, Brisbane, Australia, June 28, 2017.
- 397) Wishart, D.S. “Metabolomics for Food Composition and Food Biomarker Analysis”, presented at the 2017 ILSI North American FNSP Mid-Year Meeting, Arlington, Virginia, USA, July 18, 2017.
- 398) Wishart, D.S. “The Metabolomics Innovation Centre”, presented at the University of Alberta for Boehringer Ingelheim, Edmonton, AB, Aug. 18, 2017.
- 399) Wishart, D.S. “Metabolomics Applications in Precision Medicine and Wellness”, presented at the 2017 Swedish Metabolomics Conference, Gothenburg, Sweden, Aug. 24, 2017.
- 400) Wishart, D.S. “Development of an Assay for Dietary and Exposome Measurements for Precision Medicine”, presented at NUGO Week, Varna, Bulgaria, Aug. 29, 2017
- 401) Wishart, D.S. “Methodological Strategies for the Discovery of Novel Biomarkers of Food Intake”, presented at the 2017 FoodBALL meeting, Varna, Bulgaria, Aug. 31, 2017
- 402) Wishart, D.S. “Update on FoodDB, FoodBALL wiki and Biotransformer”, presented at the 2017 FoodBALL meeting, Varna, Bulgaria, Aug. 31, 2017

- 403) Wishart, D.S. “Metabolomics for Cancer Prevention and Screening”, presented at the European Cancer Summit, Rome, Italy, Sept. 4, 2017
- 404) Wishart, D.S. “Metabolomics for Precision Cancer Prevention and Screening”, presented at the MSACL 2017 EU Conference, Salzburg, Austria, Sept. 13, 2017.
- 405) Wishart, D.S. “The Future of Metabolomics”, presented at Biocrates LLC, Innsbruck, Austria, Sept. 18, 2017.
- 406) Wishart, D.S. “Metabolomics Resources”, webinar presented for HST and the European Bioinformatics Institute, Sept. 29, 2017.
- 407) Wishart, D.S. “Bioinformatic Tools for Polyphenol Analysis”, presented at the International Conference on Polyphenols and Health 2017, Quebec City, Quebec, Oct. 4, 2017.
- 408) Wishart, D.S. “What’s Next for Medical Metabolomics?”, presented at the Mayo Clinic Metabolomics Symposium, Rochester, MN, USA, Oct. 13, 2017.
- 409) Wishart, D.S. “Environmental Metabolomics: New Tools & Techniques to Measure the Exposome”, presented at the International Workshop on Environmental Omics – Integration and Modeling, Barcelona, Spain, Oct 19, 2017
- 410) Wishart, D.S. “Tools and Kits for Food Biomarker Discovery and Analysis”, presented at the University of Barcelona, Barcelona, Spain, Oct. 20, 2017.
- 411) Wishart, D.S. “Metabolomics for Biomarker and Drug Discovery”, presented at Denali Therapeutics Inc. San Francisco, CA, Oct. 27, 2017.
- 412) Wishart, D.S./Mandal, R. “Metabolomics in AgriFood Research”, presented at TEAGASC, Cork, Ireland, Nov. 12, 2017.
- 413) Wishart, D.S. “Cancer as a Metabolic Disease”, presented at the Canadian Cancer Research Conference, Vancouver BC, Nov. 6, 2017.
- 414) Wishart, D.S. “Metabolomics for Precision Medicine”, presented at the University of Missouri, Columbia, Missouri, Nov. 10, 2017.



- 415) Wishart, D.S. “Computational Challenges in Environmental Metabolomics & Exposomics”, presented at the Dagstuhl Seminar on Computational Mass Spectrometry, Schloss Dagstuhl, Germany, Dec. 4, 2017.
- 416) Wishart, D.S. “Untargeted Metabolomics and Novel Data Analysis Strategies to Identify Biomarkers of Diet and Type 2 Diabetes”, presented at the Swedish University of Agricultural Sciences, Uppsala, Sweden, Dec. 11, 2017.
- 417) Wishart, D.S. “Grand Challenges in Metabolomic Data Processing”, Metabolomics Society Webinar, presented at the University of Alberta, Edmonton, AB, Dec. 20, 2017.
- 418) Wishart, D.S. “The Metabolomics Innovation Centre”, International Scientific Advisory Committee Meeting for TMIC, presented at the University of Alberta, Edmonton, AB, Jan. 9, 2018.
- 419) Wishart, D.S. “Methodological strategies for the discovery of novel biomarkers of food intake”, presented at the 2018 FoodBALL Meeting, Bern, Switzerland, Jan. 25, 2018.
- 420) Wishart, D.S. “Update on FooDB, the FoodBall Wiki, the FoodBall Website & BioTransformer”, presented at the 2018 FoodBALL Meeting, Bern, Switzerland, Jan. 25, 2018.
- 421) Wishart, D.S. “Medical Metabolomics”, presented at the Edmonton-NIH-Nigeria Meeting, Edmonton, AB, Feb. 16, 2018.
- 422) Wishart, D.S. “Standardizing NMR and MS-Based Metabolomics”, presented at the Pittcon 2018 Conference, Orlando, FL, USA, Mar. 1, 2018.
- 423) Wishart, D.S. “The Metabolomics Innovation Centre – An Update”, presented at the University of Alberta for Boehringer Ingelheim, Edmonton, AB, Mar. 5, 2018.
- 424) Wishart, D.S. “Medical Metabolomics”, presented at the Beijing Academy of Science, Beijing, China, Mar. 17, 2018.
- 425) Wishart, D.S./Feunang, Y.D. “BioTransformer: An accurate, freely available tool for predicting small molecule metabolism-applications in drug discovery”, presented at the 255<sup>th</sup> American Chemical Society National Meeting, New Orleans, LA, USA, Mar. 20, 2018.

- 426) Wishart, D.S. “Exposomics and Epigenetics: Building Linkages”, presented at the Alberta Epigenetics Network Summit, Edmonton, AB, Mar. 26, 2018.
- 427) Wishart, D.S. “Metabolomic Devices for Companion Diagnostics & Personalized Medicine”, presented at the 3<sup>rd</sup> Annual CRIO Meeting, Edmonton, AB, Mar. 27, 2018.
- 428) Wishart, D.S. “Metabolomics and the Microbiome”, presented at the Alberta Microbiome Day Symposium, Edmonton, AB, Mar. 28, 2018.
- 429) Wishart, D.S. “Nanobiology, Nanosensing and Nanomedicine”, presented at the 5<sup>th</sup> Annual Alberta Nano Research Symposium, Red Deer, AB, May 3, 2018.
- 430) Wishart, D.S. “Expanding the Commercial Impact of The Metabolomics Innovation Centre”, presented to Alberta Ingenuity, Edmonton, AB, May 17, 2018.
- 431) Wishart, D.S. “Metabolomics in the Post-Modern Era”, presented at the 101<sup>st</sup> Canadian Chemical Society Conference, Edmonton, AB, May 30, 2018.
- 432) Wishart, D.S. “Looking Back at 30 Years of Science with the Sykes Lab”, presented at the Brian Sykes Career Celebration Symposium, Edmonton, AB, Jun. 14, 2018.
- 433) Wishart, D.S. “The Metabolomics Innovation Centre”, presented at the Metabolomics in Canada Meeting, Canmore, AB, Jun. 21, 2018.
- 434) Wishart, D.S. “The Metabolomics Innovation Centre – Activities in the Wishart Node”, presented at the Metabolomics in Canada Meeting, Canmore, AB, Jun. 21, 2018.
- 435) Wishart, D.S. “The Human Metabolome Database: A Major Update for 2018”, presented at the 14<sup>th</sup> International Conference of the Metabolomic Society, Seattle, WA, Jun. 25, 2018.
- 436) Wishart, D.S. “Precision Medicine & Metabolomics: A Commercial Perspective”, presented at the 14<sup>th</sup> International Conference of the Metabolomics Society – Workshop on Metabolomics & Precision Medicine, Seattle, WA, Jun. 25, 2018.

- 437) Wishart, D.S./Xia, J. “Introduction to Data Workflows – MetaboAnalyst 4.0”, presented at the 14<sup>th</sup> International Conference of the Metabolomics Society – Workshop on MetaboAnalyst 4.0, Seattle, WA, Jun. 25, 2018.
- 438) Wishart, D.S. “TMIC: A Technology Update”, presented at the Bruker Booth for the 14<sup>th</sup> International Conference of the Metabolomics Society, Seattle, WA, Jun. 25, 2018.
- 439) Wishart, D.S. “Cancer as a Metabolic Disease”, presented at the Yunnan International Cancer Conference, Kunming, China, Jul. 7, 2018.
- 440) Wishart, D.S. “The Metabolomics Innovation Centre”, presented at the University of Alberta for ReliantID, Edmonton, AB, Jul. 17, 2018.
- 441) Wishart, D.S. “Characterizing the Dark Matter of the Metabolome”, presented at the Frontiers in Metabolomics Conference, Telluride, CO, Jul. 30, 2018.
- 442) Wishart, D.S. “New Resources for Metabo-Informatics”, presented at the European Bioinformatics Institute, Hinxton, UK, Aug. 17, 2018.
- 443) Wishart, D.S. “NMR in Metabolomics: The Future is Bright”, presented at the 28<sup>th</sup> Annual ICMRBS Conference, Dublin, Ireland, Aug. 21, 2018.
- 444) Wishart, D.S. “Making Metabolomics More Affordable”, presented at the ANZMET 2018 Conference, Auckland, NZ, Aug. 30, 2018.
- 445) Wishart, D.S. “New Technologies to Make Precision Medicine More Accessible & Affordable”, presented at the 2018 International Conference on Pharmaceutical Innovation & Development, Yantai, China, Sept. 7, 2018.
- 446) Wishart, D.S. “Metabolomics and Medical Genetics: Fro Newborn Screening to Precision Medicine”, presented at the Medical Genetics Seminar Series, Edmonton, AB, Sept. 19, 2018.
- 447) Wishart, D.S. “What’s in our Food?”, presented at the NIH Workshop on Biomarkers of Dietary Intake and Exposure: Exploration with Omic Approaches, Bethesda, MD, Sept. 27, 2018.

- 448) Wishart, D.S. “Metabolomics and the Dream of Precision Nutrition”, presented at the NutriMet - Summer School in Nutritional Metabolomics, Pula, Sardinia, Italy Oct. 1, 2018.
- 449) Wishart, D.S. “In Silico Metabolomics & Novel Compound ID in Nutrition Studies”, presented at the NutriMet - Summer School in Nutritional Metabolomics, Pula, Sardinia, Italy Oct. 4, 2018.
- 450) Wishart, D.S. “Metabolomics and The Future of Precision Medicine”, presented at the Beaumont Metabolomics Symposium, Royal Oak, Michigan, Oct. 10, 2018.
- 451) Wishart, D.S. “Bioinformatic Tools for Clinical Metabolomics”, presented at Clinical Metabolomics Copenhagen 2018, Copenhagen, DK, Oct. 25, 2018.
- 452) Wishart, D.S. “Computational Tools for the Identification of Unknowns”, 3rd International Electronic Conference on Metabolomics, Edmonton, AB, Nov. 15, 2018.
- 453) Wishart, D.S. “Metabolomics and Precision Medicine”, presented at Boston University, Boston MA, Nov. 19, 2018.
- 454) Wishart, D.S. “Metabolomics and the Dream of Precision Nutrition”, presented at the University of Alberta, Edmonton, AB, Nov. 23, 2018.
- 455) Wishart, D.S. “Metabolomic Databases & Compound Identification”, presented at the ASMS 2018 Fall Meeting, San Francisco, CA Nov. 28, 2018.
- 456) Wishart, D.S. “Moving Metabolomic Discoveries into the Clinic: Lessons from the Front Lines”, presented at the 2019 Gordon Research Conference on Metabolomics & Human Health, Ventura CA, Feb. 3, 2019.
- 457) Wishart, D.S. “Computational Tools for the Identification of the Unknowns of the Exposome”, presented at PittCon 2019, Philadelphia, PA, March 18, 2019.
- 458) Wishart, D.S. “PNACIC – Kickoff Meeting”, presented at the Pacific Northwest National Laboratory, Richland, WA, March 28, 2019.
- 459) Wishart, D.S. “Metabolomics and Precision Medicine: A Look Ahead”, presented at the 2019 Korean Metabolomics Society Meeting, Seoul, South Korea, Apr. 4, 2019.

- 460) Wishart, D.S. “New Tools and Technologies for Metabolomics”, presented at the 2019 X-omics Festival, Nijmegen, Holland, Apr. 16, 2019.
- 461) Wishart, D.S. “The Human Metabolome Database – Present & Future”, presented at the HMDB Meets Felix Symposium, Nijmegen, Holland, Apr. 17, 2019.
- 462) Wishart, D.S. “What’s Next for NMR-based Metabolomics?”, presented at the UGA-NMR Conference on Building on Strength for a New Tomorrow, University of Georgia, Athens, GA, May 18, 2019.
- 463) Wishart, D.S. “Moving Metabolomic Discoveries into the Clinic: A Practical Perspective”, presented at the University of Eastern Finland, Kuopio, Finland, May 21, 2019.
- 464) Wishart, D.S. “Miniaturizing Metabolomics”, presented at the Canadian Chemistry Conference and Exhibition (CCCE) 2019 – Subgroup: Metabolomics: Applications & Techniques, Quebec City, Quebec, June 7, 2019.
- 465) Wishart, D.S. “Moving Metabolomics Discoveries into the Clinic: Lessons from the Front Lines”, presented at the Metabolomics Enabling Tools for Large Studies and Biobank Initiatives: A Precision Medicine Approach at the 2019 International Metabolomics Society Meeting, The Hague, The Netherlands, June 23, 2019.
- 466) Wishart, D.S. “Metabolomics and Precision Medicine: A Look Ahead”, presented at the 2019 International Metabolomics Society Meeting, The Hague, The Netherlands, June 25, 2019.
- 467) Wishart, D.S. “From Microbes to Metabolites: Tools to Help Integrate Metabolomics with Microbiomics”, presented at the 2019 Multi-Omics for Microbiomes Conference, The Department of Energy’s Pacific Northwest National Laboratory (PNNL), Richland, Washington, July 26, 2019.
- 468) Wishart, D.S. “Databases and Software Tools for Data Integration in Metabolomics” presented at the University of Missouri Metabolomics Workshop, Lloyd Sumner meeting in Columbia, August 9, 2019.
- 469) Wishart, D.S. “Tools and Databases for In Silico Compound Identification”, presented at the 2019 American Chemical Society, San Diego, CA, August 26, 2019.

- 470) Wishart, D.S. “Cancer as a Metabolic Disease – what metabolomics tells us”, presented at the Metabolomics and Cancer Biomarkers and Therapy Summer School, Pula, Sardinia, Italy, September 10, 2019.
- 471) Wishart, D.S. “Moving Metabolomics into the Clinic: Case Studies with Cancer”, presented at the Metabolomics and Cancer Biomarkers and Therapy Summer School, Pula, Sardinia, Italy, September 12, 2019.
- 472) Wishart, D.S. “Is Cancer a Genetic Disease, a Metabolic Disease or an Environmental Disease?”, presented at the International Agency for Research on Cancer (IARC), Lyon, France, September 17, 2019.
- 473) Wishart, D.S. "What's Next for Metabolomics", presented at the EMBO Practical Course on Metabolomics & Bioinformatics in Human Health in Lyon, France, September 19, 2019.
- 474) Wishart, D.S. & Allen Zhang “New Resources for Metabo-Informatics”, presented at BioNet University of Lethbridge in Lethbridge, AB, September 20, 2019.
- 475) Wishart, D.S. “From Microbes to Metabolites” (Keynote) presented at the 6th Munich Metabolomics Symposium, Munich, Germany, September 26, 2019.
- 476) Wishart, D.S. “Metabolomics and the Future of Precision Medicine”, presented at the 6th Munich Metabolomics Symposium, Munich, Germany, September 27, 2019.
- 477) Wishart, D.S. "Tools for Data Integration in Metabolomics", presented at the Murdoch University, Perth, Australia, October 3, 2019.
- 478) Wishart, D.S. “Metabolomics and Precision Medicine: Looking Back and Looking Ahead”, presented at the 8th Symposium of the Mexican Proteomics Society, Acapulco, Mexico, October 20, 2019.
- 479) Wishart, D.S. “Metabolomics and Multi-Omic Data Integration”, presented at the ResFor Annual Team Meeting, Edmonton, AB, November 6, 2019.
- 480) Wishart, D.S. “MS-based Metabolite Identification and Annotation Using the Web”, presented at the SINP School and Symposium on Advances in Biomedical Mass Spectrometry (SSABMS 2019), Saha Institute of Nuclear Physics (SINP), Kolkata, India, November 11, 2019.

- 481) Wishart, D.S. “In Silico Metabolomics: New Tools and Techniques to Measure the “Dark Matter” of the Metabolome”, presented at the SINP School and Symposium on Advances in Biomedical Mass Spectrometry (SSABMS 2019), Saha Institute of Nuclear Physics (SINP), Kolkata, India, November 13, 2019.
- 482) Wishart, D.S. & Hamed Pirimoghadam “Making Metabolomics Faster and Cheaper”, presented at the GIDRM-Advances in NMR and MS-Based Metabolomics, Lucca, Italy, November 20-22, 2019.
- 483) Wishart, D.S. “Metabolomics: Pathways and Pathway Interpretation”, presented at the UNI-BIOLAC, Mexico, July 7, 2019.
- 484) Wishart, D.S. “MetaboAnalyst for Metabolomic Data Analysis”, presented at the UNI-BIOLAC, Mexico, July 7, 2019.
- 485) Wishart, D.S. “Public Databases for Metabolite Identification”, presented at the UNI-BIOLAC, Mexico, July 7, 2019.
- 486) Wishart, D.S. “In Silico Metabolomics: New Tools and Techniques to Measure the “Dark Matter” of the Metabolome”, presented at the Schloss Dagstuhl workshop on Computational Mass spectrometry, Schloss Dagstuhl, Germany, January 27, 2020.
- 487) Wishart, D.S. “In Silico Metabolomics: New Tools and Techniques to Measure the “Dark Matter” of the Food Metabolome”, presented at the FoodPhyt Kick-off Meeting, Paris, France, February 3, 2020.
- 488) Wishart, D.S. “NMR Metabolomics: A Look Ahead”, presented at the 61st ENC (Experimental Nuclear Magnetic Resonance Conference), Baltimore, Maryland, March 10, 2020.
- 489) Wishart, D.S. “In Silico Metabolomics: New Tools and Techniques to Measure the “Dark Matter” of the Metabolome”, presented at the CIDC (Compound Identification Cores) Team Meeting, (virtual meeting hosted by the NIH and PNNL), April 13, 2020.
- 490) Wishart, D.S. “Machine Learning in Genomics: What We Can Learn from Big Data”, presented at the University of Alberta, April 28, 2020.
- 491) Wishart, D.S. “Mass Spectral Libraries and Databases”, presented at the ABSciex Virtual Podium 2020, May 8, 2020.

492) Wishart, D.S. “Metabolomics, Natural Resources and The Environment”, presented at the TMIC/Genome Canada Virtual Symposium, University of Alberta, June 6, 2020.

493) Wishart, D.S. “In Silico Metabolomics: Tools to Illuminate the “Dark Matter” of the Metabolome”, presented at the Intelligent Systems for Molecular Biology (ISMB) 2020 Virtual Conference, Montreal, QC, July 16, 2020.

494) Wishart, D.S. “Metabolomics and Immunology”, presented at the Virtual Immunet Seminar, University of Alberta, July 21, 2020.

495) Wishart, D.S. “In Silico Metabolomics: Using Machine Learning to Identify the “Dark Matter” of the Metabolome”, presented at the Telluride Science Research Center Virtual Conference on Frontiers in Metabolomics, Telluride Science Research Center, July 29, 2020.

496) Wishart, D.S. “Uncovering the Unknown: Libraries and Databases for Fecal Metabolomics”, presented at the Advancing Metabolomics of the Gut Microbiome (AMGM) Virtual Workshop, University of Alberta, August 6, 2020.

497) Wishart, D.S. “Moving Metabolomics into the Clinic”, American Chemical Society Conference Fall 2020 Virtual Meeting & Expo, August 17, 2020.

498) Wishart, D.S. “In Silico Tools for the Generation and Identification of Novel Metabolites” presented at the American Chemical Society Fall 2020 Virtual Meeting & Expo – Agrochemicals, August 17, 2020.

499) Wishart, D.S. “Software and Databases to Enable Omics-based Regulatory Science” presented at the Virtual Global Summit on Regulatory Science (GSRS20-Virtual), US Food and Drug Administration, September 28, 2020.

500) Wishart, D.S. “Moving Metabolomics into The Clinic”, presented at the Virtual Summer Symposium 2020, West Coast Metabolomics Centre, MANA, October 4, 2020.

501) Wishart, D.S. "What's Next for Metabolomics? Challenges and Opportunities for Metabolomics over the Coming Decade", presented at Swiss-Metabolomic Society Annual Meeting (Virtual), October 6, 2020.



- 502) Wishart, D.S. “Systemizing and Centralizing Data for Biomodeling”, presented at the 2020 Computational Modeling in Biology Network (COMBINE) Virtual Conference, October 8, 2020.
- 503) Wishart, D.S. “Food Metabolomics Kits, Databases and Software Resources”, presented at the Artificial Intelligence Institute of Next Generation Food Systems Virtual Workshop, Artificial Intelligence Institute of Next Generation Food Systems, October 8, 2020.
- 504) Wishart, D.S. “Moving Metabolomics into the Clinic”, presented at the Symposium on Metabolomics and Disease, Chongqing Medical University (Virtual), October 9, 2020.
- 505) Wishart, D.S. “The ClassyFire algorithm”, presented at the Chalmers University MetId Workshop (Virtual), October 19, 2020.
- 506) Wishart, D.S. “Web Tools for in Silico Metabolite Identification”, presented at the MetID Online Workshop (Virtual Version), Chalmers University of Technology, October 23, 2020.
- 507) Wishart, D.S. “The ClassyFire algorithm”, presented at the MetId Online Workshop (Virtual Version), Chalmers University of Technology, October 23, 2020.
- 508) Heibert, M., & Wishart, D.S. “A GC-MS Based Assay for the Identification and Quantification of Terpenes in Cannabis sativa L.”, presented at the 16th Annual Conference Metabolomics Society, October 27, 2020.
- 509) Wang, F., & Wishart, D.S. “Accurate MS/MS Spectral Prediction with CFM-ID 4.0 Technologies for Fecal Metabolomics”, presented at presented at the 16th Annual Conference Metabolomics Society, October 27, 2020.
- 510) Wishart, D.S. “Moving Biomarkers to Applications”, presented at the Dietary BioMarkers – Where to Next? Virtual Conference, University College, Dublin, Ireland, October 27, 2020.
- 511) Wishart, D.S. “Technologies for Fecal Metabolomics”, presented at the NIH U19 Annual Meeting and Workshop (Virtual), NIH, October 27, 2020.
- 512) Zheng, J., & Wishart, D.S., “Metabolomics Assays for Absolute Quantification of Primary and Secondary Metabolites in Plant Samples”, presented at the 16th Annual Conference Metabolomics Society (Virtual), October 28, 2020.

- 513) Berjanskii, M., & Wishart, D.S. “Automated metabolomic profiling of 1D 1H NMR spectra with MagMet”, presented at the 16th Annual Conference Metabolomics Society (Virtual), October 28, 2020.
- 514) Zhang, L., & Wishart, D.S. “A Comprehensive Targeted Metabolomic Assay for Urine Analysis”, presented at the 16th Annual Conference Metabolomics Society (Virtual), October 28, 2020.
- 515) Tian, S., & Wishart, D.S. “CyProduct: A software tool for accurately predicting the byproducts of human cytochrome P450 metabolism.”, presented at the 16th Annual Conference Metabolomics Society (Virtual), October 28, 2020.
- 516) Wishart, D.S. “New Metabolomics Technologies to Characterize Cannabis Safety and Potency”, presented at the Cannabis CRUPA-CIHR Virtual Conference on Cannabis, November 9, 2020.
- 517) Wishart, D.S. "New Data Resources for Microbial Metabolomics", presented at the New York Academy of Sciences Conference (Virtual), November 10, 2020.
- 518) Wishart, D.S. " Metabolomics and the Discovery of Novel Biomarkers of Food Intake", presented at the Canadian Nutrition Society Mini Conference, University of Alberta, November 20, 2020.
- 519) Wishart, D.S. “COVID-19: What is it? Where did it come from? How to avoid it” presented at the educational meeting, Ngemba Cultural And Development Association Alberta, Edmonton, AB, January 19, 2021.
- 520) Wishart, D.S. "Machine Learning, Multi-Omics Measurements and Precision Health - Where are we Now?", presented at the Precision Health 2021, an event hosted by the Integrative Pharmacogenomics Institute, Universiti Teknologi MARA (Virtual), Malaysia, February 24, 2021.
- 521) Wishart, D.S. "Metabolomics and Precision Nutrition: Key Outcomes from the JPL Food Biomarker Alliance (FoodBall) Project", presented at the Virtual Lectureship Presentation to CIHR-INMD Institute Advisory Board, February 26, 2021.
- 522) Wishart, D.S. "Using Machine Learning to Optimize the COVID Pandemic Response", presented at the Symposium - Artificial Intelligence in Medicine Student Society (AIMSS), Edmonton, March 13, 2021.

523) Wishart, D.S. "Innovation and Bioinformatics", presented at the Operation Medical School Conference, Operation Medical School Calgary, March 26, 2021.

524) Wishart, D.S. "Metabolomics and Life Sciences", presented at TMIC Precision Medicine Webinar Series, TMIC, Edmonton, AB, May 4, 2021.

525) Wishart, D.S. "Metabolomics and Precision Medicine", presented at the TMIC Precision Medicine Webinar Series, TMIC, Edmonton, AB, May 12, 2021.

526) Wishart, D.S. "Integrating Machine Learning and Omics Analyses to Understand Neurodegeneration", presented at the 2021 Promoting Healthy Brain Aging and Preventing Dementia International Symposium, Campus Alberta Neuroscience, Edmonton, AB, May 19, 2021.

527) Wishart, D.S. "Analyzing and Interpreting Big Metabolomics Data with MetaboAnalyst", presented at the UNL CIBC Workshop (Virtual), May 19, 2021.

528) Wishart, D.S. "Metabolomics and Agri-Food", presented at TMIC Precision Medicine Webinar Series, TMIC, Edmonton, AB, May 19, 2021.

529) Wishart, D.S. "Metabolomics and The Environment: Find Out How Metabolomics Can Be Used for Environmental Research & Monitoring", presented at TMIC Precision Medicine Webinar Series, TMIC and BioAlberta, Edmonton, AB, May 27, 2021.

530) Wishart, D.S. "Food Informatics" presented at the Metabolomics project event "Know FOOD-COMPOSITION (Part 2): Better food composition data. Better diets. Better health.", KnowFOOD live, Canada, May 27 (Virtual), 2021.

531) Wishart, D.S. "Metabolomics and drug discovery and development", presented at the The Canadian Center for Bioinnovation (Virtual), May 27, 2021.

532) Wishart, D.S. "FoodDB: new resource on food constituents and chemistry", presented at the Food Science Webinar 2021 (Virtual), June 4, 2021.

533) Wishart, D.S. "Metabolomics for Investigating Physiological and Pathophysiological Processes in the Public Health Context", presented at the 2021 Nutrition 2021 Conference (Virtual), June 7, 2021.

- 534) Wishart, D.S. "Expanding Metabolite Coverage via In Silico Metabolomics", presented at the Metabolomics 2021 Conference (Virtual), June 23, 2021.
- 535) Wishart, D.S. "Metabolomics on a Chip: Impedance-Based Metabolite Biosensor for Early Diagnosis of Colon Cancer", presented at the Metabolomics 2021 Conference (Virtual), June 23, 2021.
- 536) Wishart, D.S. "Expanding Metabolite Coverage via In Silico Metabolomics", presented at the 1st Chinese American Society for Mass Spectrometry Virtual Conference, August 9, 2021.
- 537) Wishart, D.S. "Using machine learning to improve the accuracy MS-based compound identification", presented at the Analytical Division, ACS Annual Meeting (Virtual), August 22, 2021.
- 538) Wishart, D.S. "Biotransformer 3.0: An improved in silico metabolism prediction tool", presented at the ACS Annual Meeting (Virtual), August 23, 2021.
- 539) Wishart, D.S. "Chemistry, big data, and machine learning", presented at the University of British Columbia, Vancouver, BC, September 21, 2021.
- 540) Wishart, D.S. "Chemistry, big data, and machine learning", presented at Simon Fraser University, Burnaby, BC, September 22, 2021.
- 541) Wishart, D.S. "Databases- what's needed?", presented at the Alzheimer Gut Microbiome Project (U19) Workshop 1: Precision Nutrition, Gut Microbiome and Brain Health (Virtual), September 27, 2021.
- 542) Wishart, D.S. "Foodomics & Dietary Biomarkers Databases: What's Needed?", presented at the NIH Common Fund Metabolomics Consortium Virtual Fall Meeting, September 28, 2021.
- 543) Wishart, D.S. "Uremic Toxin Assay", presented at the NIH Common Fund Metabolomics Consortium Virtual Fall Meeting, September 28, 2021.
- 544) Wishart, D.S. "Automated Analysis of Wine and Beer by NMR Spectroscopy", presented at the ABC-2021 Analytical and Bioanalytical Methods Conference, Boston Online, October 18, 2021.
- 545) Wishart, D.S. "Wine Tasting by NMR Workshop", presented at the Metabolomics Association of North America (MANA)-2021 Conference (Virtual), October 18, 2021.

546) Wishart, D.S. " Machine learning and Metabolomics", presented at the Metabolomics Association of North America (MANA)-2021 Conference (Virtual), October 19, 2021.

547) Wishart, D.S. " Liquid Biopsy in Cancer Screening: The Contribution of Metabolomics", presented at the III ISLB Annual Congress (Virtual), October 22, 2021.

548) Wishart, D.S. "Deciphering Dementia with Metabolomics", presented at the University of Calgary – Dementia Academic Rounds (Virtual), Calgary, AB, November 12, 2021.

549) Wishart, D.S. "Metabolomics for the Discovery of Disease Biomarkers", presented at the 2<sup>nd</sup> Symposium on Metabolism and Diseases (Virtual), Chongqing Medical University, China, November 18, 2021.

550) Wishart, D.S. "MiMeDB: The Microbiome Metabolome Database", presented at the Reshaping the Microbiome Through Nutrition Conference (Session IV) – Virtual, UCSD, San Diego, USA, November 18, 2021.

551) Wishart, D.S. "New Tools in Metabolomics for Multi-Omics Integration", presented at the Virtual Poidum Asia Pacific (VPAP) Conference, Singapore, November 29, 2021.

552) Wishart, D.S. "Automating NMR Spectral Interpretation: What the Future Holds", presented at the Pacificchem 2021 Virtual Conference, Honolulu, Hawaii, USA, December 17, 2021.

553) Wishart, D.S. "The Do's and Don'ts of Metabolomics", presented at the Exercise Metabolomics Mini-Meeting (Virtual), Liverpool John Moores University, Liverpool, UK, January 20, 2022.

554) Wishart, D.S. Livestock Gentec Interactions with the Wishart Lab", presented at the Livestock Gentec Virtual Board Meeting, Edmonton, AB, January 28, 2022

555) Wishart, D.S. "Using Artificial Intelligence to Predict the Next Designer Drugs", presented at the Ohio Narcotics Intelligence Center Drug Summit, Columbus, Ohio, USA, March 2, 2022.

556) Wishart, D.S. "Understanding the Human Metabolome", presented at the University of Toronto, Dept. of Molecular Genetics Winter Colloquium (Virtual), Toronto, ON, March 7, 2022.

557) Wishart, D.S. “Connecting the Microbiome and the Metabolome through Diet”, presented at the Frncombe Family Digestive Health Research Institute Seminar (Virtual), McMaster University, Hamilton, ON, March 9, 2022.

558) Wishart, D.S. “Databases in Metabolomics Research”, presented at the JPI FoodPhyt PI’s webinar for ECS, University of Clermont-Auvergne. France, May 12, 2022.

559) Wishart, D.S. “The future of NMR-based metabolomics”, presented at the 2022 ANZMAG Virtual Seminar Series. Australia, June 14, 2022.

560) Wishart, D.S. "Metabolomics in Environmental Science: Identifying Dark Matter", presented at the Environmental Sciences: Water Gordon Research Conference, USA, June 20, 2022.

561) Wishart, D.S. “Illuminating the dark matter of the metabolome with convolutional neural networks”, presented at the Genome BC Close-Out Meeting, BC, Canada, June 16, 2022.

562) Wishart, D.S. "Comprehensive Targeted Metabolomics Platforms for Various Biological Samples", presented at the Metabolomics Society Conference, Spain, June 20, 2022.

563) Wishart, D.S. "A Comprehensive Targeted Metabolomic Assay for Uremix Toxin Quantification", presented at the Metabolomics Society Conference, Spain, June 20, 2022.

564) Wishart, D.S. "Comprehensive Targeted Metabolomics Platforms for Serum Samples", presented at the Metabolomics Society Conference, Spain, June 20, 2022.

565) Wishart, D.S. “What is Metabolomics?”, presented at the ILSI Annual Meeting, Belgium, June 27, 2022.

566) Wishart, D.S. “Metabolomics to Analyze Food Components & Current Database Development”, presented at the ILSI Annual Meeting, Belgium, June 29, 2022.

567) Wishart, D.S. “The coming revolution of the Omics sciences: Metabolomics and Foodomics for increased understanding of food nutrients, quality, traceability and health impacts”, presented at the ILSI Annual Meeting, Belgium, June 28, 2022.

568) Wishart, D.S., “Machine Learning and Predictive Metabolomics”, presented at the Telluride Science Research Centre Workshop Frontiers in Metabolomics, USA, July 26, 2022.

569) Wishart, D.S., “ClassyFire - automated chemical classification in application contexts”, presented at the virtual NFDI for Chem Ontology Workshop, September 8, 2022.

570) Wishart, D.S., “Omics on call for prevention of diabetic neuropathy”, presented at the Technological workshop, Steno Diabetes Center Copenhagen, August 7, 2022.

571) Wishart, D.S., "Recent Developments in BioTransformer for Predicting Biotransformations", presented at the virtual Scientific Advancement Seminar, Boehringer Ingelheim, September 21, 2022.

572) Wishart, D.S., “Fermentation product analysis via Metabolomics.”, presented at the virtual seminar Saskatchewan Food Industry Development Centre Inc, September 21, 2022.

573) Wishart, D.S. “Wine and beer tasting with Metabolomics”, presented at the MANA-2022 conference Workshop, Edmonton, Canada, September 16, 2022.

#### **Web-based Databases (Developed and Maintained)**

- 1) BMDB <https://bovinedb.ca/>
- 2) MCDB <https://mcdb.ca/>
- 3) LMDB <https://lmdb.ca/>
- 4) ContaminantDB <https://contaminantdb.ca/>
- 5) CypComp <https://cypcomp.ca/>
- 6) DrugBank <https://www.drugbank.com/>
- 7) ECMDB <https://ecmdb.ca/>
- 8) FooDB <https://foodb.ca/>
- 9) AFCDB <https://www.afcdb.ca/>
- 10) HMDB <https://hmdb.ca/>

- 11) MarkerDB <https://markerdb.ca/>
- 12) NP-MRD <https://np-mrd.org/>
- 13) PathBank <https://pathbank.org/>
- 14) SMPDB <https://smpdb.ca/>
- 15) PathWiz <https://smpdb.ca/pathwhiz>
- 16) T3DB <http://www.t3db.ca/>
- 17) YMDB <http://www.ymdb.ca/>
- 18) Serum Metabolome <https://serummetabolome.ca/>
- 19) CSF Metabolome <https://csfmetabolome.ca/>

#### **Web-based Metabolomics Tools (Developed and Maintained)**

- 1) Bayesil <http://bayesil.ca/>
- 2) Biotransformer <https://biotransformer.ca/new>
- 3) CFMID 3.0 <https://cfmid.wishartlab.com/>
- 4) ClassyFire <http://classyfire.wishartlab.com/>
- 5) MolDB <https://moldb.wishartlab.com/>
- 6) NMRlib <http://nmrlib.wishartlab.com/>
- 7) GC-AutoFit <http://gc-autofit.wishartlab.com/>
- 8) MagMet <http://magmet.ca/users/login>

#### **Web-based Proteomics Tools (Developed and Maintained)**

- 1) CS23D <http://www.cs23d.ca/index.php>



- 2) CSI3.0 <http://csi.wishartlab.com/cgi-bin/index.py>
- 3) E-Thrifty <http://ethrifty.ca/>
- 4) GENMR <http://www.genmr.ca/index.php>
- 5) MovieMaker <http://wishart.biology.ualberta.ca/moviemaker/>
- 6) PANA V <http://panav.wishartlab.com/>
- 7) PepMake <http://pepmake.wishartlab.com/>
- 8) PPT-DB <http://www.pptdb.ca>
- 9) PREDITOR [http://wishart.biology.ualberta.ca/shiftor/cgi-bin/preditor\\_current.py](http://wishart.biology.ualberta.ca/shiftor/cgi-bin/preditor_current.py)
- 10) PROSESS <http://www.prosess.ca/>
- 11) PROTEUS <http://www.proteus2.ca/proteus/>
- 12) PROTEUS2 <http://www.proteus2.ca/proteus2/>
- 13) RCI-Main Chain [http://www.randomcoilindex.ca/cgi-bin/rci CGI\\_current.py](http://www.randomcoilindex.ca/cgi-bin/rci CGI_current.py)
- 14) RCI -Side Chain [http://www.randomcoilindex.ca/cgi-bin/rci CGI\\_current.py](http://www.randomcoilindex.ca/cgi-bin/rci CGI_current.py)
- 15) Ref-DB <http://refdb.wishartlab.com/>
- 16) RESPROX <http://www.resprox.ca/>
- 17) ShiftX <http://shiftx.wishartlab.com/>
- 18) SHIFTX2 <http://www.shiftx2.ca/>
- 19) ShiftASA <http://shiftasa.wishartlab.com/cgi-bin/index.py>
- 20) SuperPose <http://superpose.wishartlab.com/>
- 21) Vadar <http://vadar.wishartlab.com/>
- 22) GAMDY <http://www.gamdy.ca/>
- 23) Shiftcor <http://shiftcor.wishartlab.com/>
- 24) Metaboanalyst <https://www.metaboanalyst.ca/>

### **Web-based Genomics Tools (Developed and Maintained)**

- 1) BacMap <http://wishart.biology.ualberta.ca/BacMap/>
- 2) GWAS-ROCS <https://gwasrocs.ca/>
- 3) Metagenassist <http://www.metagenassist.ca/METAGENassist/faces/Home.jsp>
- 4) Plasmapper <http://wishart.biology.ualberta.ca/PlasMapper/>
- 5) PHASTER <https://phaster.ca/>

### **Other Web servers (Developed and Maintained)**

- 1) COVID Mapper <https://covidmapper.ca/>
- 2) HeatMapper <http://www.heatmapper.ca/>
- 3) PA3 <http://pa.wishartlab.com/pa/>
- 4) PolySearch2 <http://polysearch.ca/index>
- 5) Phenol Explorer <http://phenol-explorer.eu/>

### **Supervision – Undergraduate Students**

- 1) Yamini Ramamoorthy 1998
- 2) Scott Ellerbeck 1998-1999
- 3) Anuj Ranjan 1999-2001
- 4) Nelson Young 2001-2002
- 5) Sydney Young 2001-2002
- 6) Jennifer Tran 2001

7) Jennifer Woolsey	2001
8) Michael Madlansacay	2002
9) Ryan de los Angeles	2002
10) Phil Luk	2002
11) Murtaza Hassanali	2002-2005
12) Robert Yang	2003-2004
13) Brian O'Neill	2004
14) David Arndt	2004
15) Joseph Cruz	2004
16) Scott Montgomerie	2004
17) Craig Knox	2005
18) Joel Jackson	2005
19) Kevin Jeroncic	2005-2006
20) Moustafa Mourad	2006
21) Patrick Kong	2006
22) Byron Barth	2007

23) Asdrubal Burgos	2007
24) Brenna Brown	2007
25) Jill Pang	2007
26) Summit Sawahney	2007
27) You Zhou	2007-2008
28) Jack Liang	2007-2008
29) Shannon Deane	2008
30) Jessica D'Amico	2008
31) Phillip Liu	2008
32) Jon Hung	2008
33) Paul Huang	2008-2010
34) Paul Lam	2008
35) Emilia Lim	2008
36) Lydia Fang	2008
37) Allison Pon	2008
38) Alex Frolkis	2009

39) Alex Wolkow	2009
40) Kirby Ziegler	2009
41) Bowei Wang	2009
42) Tim Jewison	2010
43) Kyra Leimert	2010
44) Kruti Chaudhary	2010
45) Mike Wilson	2011
46) Jacqueline Lee	2011-2012
47) Patrick Lo	2012
48) Vivian Law	2010-2011
49) Faizath Yallou	2011-2013
50) Jessica Huynh	2012-2013
51) Jenna Poelzer	2012-2013
52) Alexandra Tang	2013
53) Geraldine Gabriel	2012-2013
54) Carol Ly	2013

55) Sakina Adamjee	2013
56) Marianna Nogueira Limas	2013
57) Adam Maciejewski	2013
58) Yilu Su	2013-2014
59) Danny Golec	2013-2014
60) Tanvir Sajed	2014
61) Sasha Babicki	2015
62) Ana Marcu	2015
63) Anthony Wu	2015
64) Joseph Landy	2015
65) Miguel Ramirez	2015
66) Noah Wishart	2016-2018
67) John Bacon	2016-2018
68) Tuvieri Onookome-Okome	2016
69) Zachary Budinski	2016
70) Eric Sun	2017

71) Ian Splinter	2017
72) Elvis Lo	2017
73) Daniel Johnson	2017
74) Carin Li	2017
75) Hasan Badran	2017
76) Elizabeth Wishart	2017
77) Graeme Splinter	2017
78) Vishrut Gulhati	2017
79) Chelsea Hong	2017-2019
80) Philip Kirwin	2018
81) Xuan Cao	2018-2019
82) Jonas Patron	2018-2019
83) Debra Lipton	2018-2019
84) Sarah Davis	2018-2020
85) Adam Cruse	2019
86) Yushan Liu	2019

87) Omar Mohamud	2019
88) Leon Tran	2019
89) Jordan Lamash	2019
90) Chris Chan	2019
91) Mailys Paccoud	2019
92) Eponine Oler	2019
93) Krissa Li	2019
94) Adam Cruse	2019-2020
95) Christiana Garros	2019-2020
96) William Wei	2019 – 2021
97) Aadhavya Sivakumaran	2020 – pres.
98) Yifan Yang	2020
99) Payton LeBlanc	2020-2021
100) Selena Sanford	2020-pres.
101) Nitya Khetarpal	2020-pres.
102) Karxena Harford	2020-2021



103) Kristen Yee	2020-2021
104) Rehab Al-Hajj	2020-2021
105) Jeanne Coleongco	2020-2021
106) Samuel Stuart	2020-pres.
107) Angela Chan	2021
108) Shahzaib Ahmed	2021
109) August Sieben	2021
110) Samuel Hudianto	2021
111) Robert Mah	2021
112) Raynard Dizon	2021
113) Varun Aggarwal	2021
114) Fleur Isaac	2021
115) Abby Kropielnicki	2021-pres.
116) Harrison Peters	2021-pres.
117) Irene Chen	2021-pres.
118) Rahil Doshi	2021

119) Boris Ignatev	2021-2022
120) Mateo Echeverry	2021-pres.
121) Ryan Bererton	2022-pres.
122) Hayden Gowing	2022-pres.
123) Albert Dinh	2022-pres.
124) Abhishek Solanki	2022-pres.
125) Suyenna Huang	2022-pres.
126) Robert Joseph	2022
127) Lisa Nig	2022
128) Sagan Girod	2022
129) Sukanta Saha	2022
130) Ralph Milford	2022
131) Scott Han	2022
132) Hieu Ngyuen	2022

**Supervision - Graduate Students**

1) Yunjun Wang	"Dissecting the Structure and Activity of a Prostate Cancer Antibody"	Ph.D. 1996 - 1999
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|--------------------------|---|-------------------|
| 2) Gary Van Domselaar    | "Design and Synthesis of Targetable Peptide Micelles"     | Ph.D. 1996 – 2003 |
| 3) Scott Watson          | "NMR Assignments of Hepatitis A protease"                 | M.Sc. 1996 - 2000 |
| 4) Alan Gibbs            | "Structure-Activity Relationships of Antibiotic Peptides" | Ph.D. 1997 – 2001 |
| 5) Haiyan Zhang          | "Development of Advanced Bioinformatics Databases"        | M.Sc. 1997 – 2002 |
| 6) Sudeepa Bhattacharyya | "Structural Proteomics of a Thermophile"                  | M.Sc. 1998 - 2001 |
| 7) Ping Li               | "Expression of Human Rhinovirus Protease "                | M.Sc. 1998 - 2000 |
| 8) Steve Neal            | "NMR chemical shift prediction"                           | M.Sc. 1999 – 2003 |
| 9) Trent Bjorndahl       | "SAR of Hepatitis A protease and HRV protease"            | Ph.D. 1999 – 2006 |
| 10) Lena Andrew          | "Solid phase Protein Synthesis"                           | Ph.D. 2000-2009X  |
| 11) Godwin Amegbey       | "Development and Testing of Protease Inhibitors"          | Ph.D. 2000 – 2006 |
| 12) Zhan Chang           | "Structural Proteomics of a Thermophile"                  | M.Sc. 2000 – 2003 |
| 13) Raj Maiti            | "Bioinformatics and Protein Folding"                      | M.Sc. 2002 – 2005 |
| 14) Shan Sundararaj      | "Bioinformatics Applications to Protein Structure"        | Ph.D. 2002 –2004X |
| 15) Savita Shrivistava   | "Whole Proteome Annotation"                               | M.Sc. 2003 –2004  |

16) Steve Neal	“Nanobiotechnology and Nanorobots”	Ph.D. 2004–2005X
17) Dean Cheng	“Text Mining in Bioinformatics”	M.Sc. 2005 – 2007
18) Jeff Xia	“Metabolomics Software Development”	Ph.D. 2006 – 2011
19) Fozia Saleem	“Prion Structure and Dynamics”	Ph.D. 2008 – 2013
20) Yifeng Liu	“Computational Question Answering”	Ph.D. 2009 – 2016
21) You Zhou	“Minimal Constraints for NMR Structures”	M.Sc. 2009-2012
22) Yannick Djoumbou	“Chemical Taxonomies”	Ph.D. 2010-2017
23) Susan M. Dunn	“Bovine Metabolomics”	Ph.D. 2010-2011X
24) Noor Hafsa	“Computational Structure Determination”	Ph.D. 2011-2016
25) Timothy Jewison	“Small Molecule Pathway Database”	M.Sc. 2011-2014
26) Shima Borzouie	“The Alberta Food Metabolome”	M.Sc. 2012-2016
27) Shahrzad Rafatnia	“Machine Learning for Metabolite Annotation”	M.Sc. 2013-2014X
28) Mordechaie Slae	“Metabolomics of Eosinophil Esophagitis”	M.Sc. 2013-2015X
29) Seyed Ali Goldansaz	“Metabolomics of Dairy and Beef Cattle”	PhD. 2015-2021
30) Massih Khorvash	“Simulating Amyloid Folding”	PhD. 2014-2020
31) Aidin Fouradin	“Metabolomics/Genomics of Bovine Fecundity”	PhD. 2015-2020

32) Tanvir Sajed	“NMR Chemical Shift Prediction”	M.Sc. 2016-2017X
33) Amel Hamza	“Bisphosphonate Detection in Serum	M.Sc. 2017-2019
34) Fei Wang	“Mass Spectral Spectrum Prediction”	Ph.D. 2017-pres.
35) Siyang Zhang	“Site of Reaction Prediction”	M.Sc. 2016-2019
36) Zinat Sayeeda	“NMR Spectral Analysis”	M.Sc. 2017-pres.
37) Nazanin Khameneh	“Machine Learning”	M.Sc. 2018-2019X
38) Shiful Islam	“Artificial gut microbiota and microbial diversity in different environments”	M.Sc 2019-pres
39) Dorna Varshavi	“Metabolic profiling of dried blood spots”	M.Sc. 2021-pres.
40) Dorsa Yahya Rayat	“Predicting the effect of precision nutrition on Autism using machine learning methods”	M.Sc. 2020-pres.
41) Afia Anjum	"Reliable identification of unknown and in-silico compounds through Gas Chromatography Retention Index and Electron Ionization Mass Spectrometry Predictions”	M.Sc. 2020-pres.
42) Karla Trejo-Oliver	“Metabolomic analysis of the Microbiota-Immune-Brain interaction”.	Ph.D. 2021-pres.
43) Ryan Nabozniak	“Application of machine learning to recognize spousal abuse”	M.Sc. 2021-pres.
44) Mahi Zakir 2022-pres.	“Optimizing metabolomics data for faster model predictions using machine learning”	M.Sc.

45) Gina Sykes	“Investigation by machine learning of the human blood transcriptome and metabolome for stroke biomarkers and improved understanding the molecular etiology of stroke”	Ph.D. 2021-pres
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### **Supervision - Postdoctoral Fellows**

1) Alex Nip	"Cracking the Chemical Shift Code"	1996-1999
2) Diane Jette	"Purification of a Prostate Cancer Single Chain Fv"	1996-1998
3) Kathy Wang	"Expression of a Prostate Cancer Antibody in P. pastoris"	1996
4) Hassan Monzavi	"SAR of Hepatitis A protease using NMR"	1997-2003
5) Dong Luo	"Improving PSA Detection through Protein Engineering"	1998-1999
6) Subir Okarvi	“Technicium peptide labeling”	2000
7) Bahram Habibi-Nazhad	“Computer-aided Drug Design”	2001-2003
8) AnChi Guo	“Bioinformatics for Project CyberCell	2002-2007
9) Gary Van Domselaar	“Bioinformatics and Proteome Annotation	2003-2009
10) Paul Stothard	“Canadian Bioinformatics Help Desk”	2003-2006

11) Mark Berjanskii	“NMR Structure from Chemical Shifts”	2004-2009
12) Wayne Materi	“Bacterial Nanobots”	2004-2006
13) Marie-Aude Coutouly	“NMR Structure from Chemical Shifts”	2005-2007
14) Godwin Amegbey	“Metabolomics”	2006
15) Trent Bjorndahl	“NMR of proteins and metabolites”	2006-2011
16) Nick Pyschogios	“Metabolomics”	2007-2011
17) Souhaila Bouatra	“Metabolomics”	2007-2012
18) Xuehui Liu	“Prion Structure and Dynamics”	2007-2009
19) Guoping Zhou	“Prion Structure and Dynamics”	2007-2010
20) Prasanna Bhomkar	“Bacterial Nanobots”	2007-2011
21) Sandipta Acharya	“Prion Structure and Dynamics”	2008-2010
22) Igor Sinelnikov	“MS-based Metabolomics”	2008-2011
23) BeomSoo Han	“Machine Learning and Bioinformatics”	2008-2011
24) Carol Ladner	“Prion proteins and amyloids”	2008-2012
25) Monika Kalla	“Enzymatic synthesis of metabolite derivatives”	2009-2010
26) Ram Krishnamurthy	“Metabolomics of Lipids”	2010-2014

27) Farid Aziat	“Metabolomic Method Development”	2010-2014
28) Jeff Xia	“Metabolomics Software Development”	2011-2012
29) Jianjun Zhou	“Protein structure prediction and clustering”	2011-2012
30) Zerihun Dame	“Metabolomics Technology Development”	2011-2015
31) Nataraj Pagadala	“Prion protein simulation and modeling”	2012-2013
32) Rabab Ahmed	“Phage Display for Metabolomic Devices”	2013-2014
33) Fozia Saleem	“Metabolomics for Biomarker Discovery”	2013-2014
34) Lu Deng	“Adductomics and Metabolomics”	2013-2016
35) Nicolas Vozza	“Single chain Antibodies”	2014-2018
36) Ithayavani Iynkkaran	“Clinical Metabolomics”	2014-2017
37) Rosa Vazquez-Fresno	“Food Metabolomics and Biomarkers”	2015-2017
38) Arnau Serra Cayuela	“Statistics of GWAS and Metabolomic Data”	2015-2017
39) Naama Karu	“Development of a Uremic Toxin Metabolomics Kit	2016-2017
40) Shiva Kalhor Monfared	“Chemical Synthesis of GNP-metabolite Conjugates	2016-2017
41) Yeganeh Khaniani	“Chemical Synthesis of GNP-metabolite Conjugate	2017-2020
42) Lun (Allen) Zhang	“Prion Metabolomics”	2017-2021



43) Yannick Djoumbou	“Cheminformatics”	2017-2018
44) Sandeep Singhal	“Metabolomics and Bioinformatics”	2017-2018
45) Matthias Lipfert	“NMR-based Metabolomics”	2017-2019
46) Sudarshana Bhumireddy	“Plant/Forestry Metabolomics”	2018-2021
47) Hamed Pirimoghadam	“Metabolomics Technology Development”	2018-2020
48) Maheswor Gautam	“Integrated Metabolomics”	2018-2019
49) Shiyang Zhao	“Applied statistics in biology”	2021-pres.
50) Sajjad Janfaza	“Plasma separation, molecularly imprinted polymer, functionalized magnetic nanoparticles, electrochemical biosensors”	2021-2022
51) Dorsa Varshavi	“Development of colorimetric assays for detection of Colorectal cancer biomarkers”	2021-2022
52) Ammar H. Keshteli	“Metabolomics and gastrointestinal diseases”	2020-pres.
53) Mai Yamamoto	“Bioinformatics and urinary metabolome analysis”	2020-2022.
54) Scott MacKay	“Biosensor design”	2017-pres.
55) Yanna Xiao	“Colorimetric assays for metabolite detection in biofluids”	2021-pres.
56) Jaanus Liigand	“Computational metabolomics”	2019-2020
57) Mickel Hiebert	“Metabolomics method development”	2019-2022

58) Claudia Torres	“Colorimetric assays for metabolite detection”	2021-pres.
59) Saira Ali	“Colorimetric assays for metabolite detection”	2020-2021

### **Research Associates**

1) Zoltan Gombos	“Bacterial Nanobots”	2005-2006
2) Wayne Materi	“Bacterial Nanobots”	2006-2010
3) AnChi Guo	“Bioinformatics for Project CyberCell”	2007-pres.
4) Trent Bjorndahl	“NMR for protein chemistry”	2007-2016
5) Graham Banting	“Bacterial Nanobots”	2008-2009
6) Ruparsi Mandal	“MS-based Metabolomics”	2008-pres.
7) Guoping Zhou	“Prions and NMR”	2010-2011
8) Mark Berjanskii	“NMR and structural bioinformatics”	2010-pres.
9) Rolando Perez-Pinero	“Prions and Tubulins”	2010-2013
10) Prasanna Bhomkar	“Nanobiosensors”	2011-2014
11) Carol Ladner	“Prion chemistry and amyloids”	2012-2017 2019
12) Beomsoo Han	“Metabolomics and Informatics”	2012-2019

13) Jason Grant	“Bioinformatics, Genomics, Metabolomics”	2014-2016
14) Marcia LeVatte	“Prion chemistry and amyloids”	2014-2018
15) Rambod Daneshfar	“Metabolomics”	2016-2017
16) Nicolas Vozza	“Metabolomic Devices”	2014-2018
17) Dipanjan Bhattacharrya	“Chemical Synthesis”	2018-pres.
18) Upasana Singh	“Metabolomic Devices”	2018-pres.
19) Brian Lee	“NMR, MS and Prion Diseases”	2019-pres.
20) Yeganeh Khaniani	“Chemical Synthesis”	2017-pres.
21) Sindhu Gopinathan Nair	“ISO Quality Assurance”	2019-pres.
22) Lun (Allen) Zhang	“Metabolomics”	2021-pres.
23) Vasuk Gautam	“Bioinformatics and software development”	2021-pres.

### **Supervision – Technicians/Programmers**

1) Gary Van Domselaar	"Peptide Synthesis and Purification"	1995 – 1996
2) Yi Zhang	"Cloning and Expression of Antibody Fragments"	1995 – 1996
3) Imke Gronwald	"HPLC purification and analysis"	1995 – 1997
4) Jane Nagel	"Peptide Synthesis of Antibody Reductants"	1996 – 1997 2017 – 2018

5) Wei Xia	"Expression of a Prostate Cancer Antibody in <i>P. pastoris</i> "	1997 – 1998
6) Ashenafi Abera	"Peptide Synthesis and Protein Expression"	1998 – 2000 2004 – 2013 2016 – 2017 2019 – 2021
7) Lena Andrew	"Peptide Synthesis and NMR"	2000 – 2000
8) Nelson Young	"Alberta Cancer Board Bioinformatics Core Facility"	2002-2011
9) Ian Forsythe	"Canadian Bioinformatics Help Desk"	2003-2010
10) Dan Tzur	"Protein Purification, metabolomics & NMR"	2003-2008
11) Xiaoli Dong	"Bioinformatics and Lab Information Management"	2003-2006
12) Val Semenchenko	"Protein Purification, Bacterial Nanobots, Prions"	2004-2013
13) Joseph Cruz	"Bioinformatics in Microarray Analysis"	2004-2012
14) Chunyan Meng	"PENCE Bioinformatics Core Facility"	2005-2007
15) Savita Shrivastava	"Canadian Bioinformatics Help Desk"	2004-2009
16) David Arndt	"Bioinformatics and Prion Structure"	2006-2008 2010-pres.
17) Criag Knox	"Bioinformatics for Metabolomics"	2006-pres.
18) Leslie Jia	"Bioinformatics for Metabolomics"	2006-2009

19) Peter Tang	“System Administration & SimCell”	2006-2011
20) David Hau	“NMR and Metabolomics”	2007-2010
21) Jun Peng	“GC-MS and Metabolomics”	2007-2010
22) Michael Lewis	“Metabolomics and HMDB”	2007-2008
23) Kevin Jeroncic	“Metabolomics and HMDB”	2007
24) Mitchel Flegel	“Metabolomics and HMDB”	2007
25) Joshua Morrissey	“Metabolomics and HMDB”	2007
26) Ryan Fradette	“Metabolomics”	2007
27) Bijaya Gautam	“Metabolomic Annotations”	2008-2010 2016
28) Jack Liang	“Bioinformatics and Prion Structure”	2008-2020
29) Roman Eisner	“Bioinformatics, Google Gift”	2008-2009
30) Edison Dong	“Metabolomics”	2008-pres.
31) Philip Liu	“Metabolomics”	2009-2014
32) Adina Bujold	“Prion protein purification”	2009
33) Bow Suryiamongkol	“Protein production and cloning”	2009-2012

34) Vanessa Neveu	“Food Metabolome”	2009-2011
35) Mike Wilson	“Bioinformatics”	2011-2015
36) Ritesh Saini	“Fluorescent proteins”	2012-2013
37) You Zhou	“Bioinformatics”	2012-2013
38) Fatemeh Miri Disfany	“SMPDB and Bioinformatics”	2013
39) Oxana Tarassova	“Protein production and cloning”	2013-2020
40) Allison Pon	“Bioinformatics”	2013-2015
41) Nazanin Assempour	“Chemistry and Metabolomics”	2014-2017
42) Adam Maciejewski	“DrugBank and Supercapacitors”	2014-2017
43) Bob Stanley	“Metabolomics”	2015-2016
44) Erin (Yiran) Zhang	“Metabolomics”	2015-2017
45) Yichen (Ashley) Xia	“Metabolomics”	2015-2019
46) Fatemeh Shahin	“Chemistry and Supercapacitors”	2016-2021
47) Jiamin (Tammy) Zheng	“Metabolomics”	2016-pres.
48) Ana Marcu	“Precision Medicine”	2016-2019
49) Upasana Singh	“Metabolomics”	2016-2018

50) Debjani Bhattacharyya	“Metabolomics”	2016-2018
51) Annie Wong	“Protein chemistry”	2016-2017
52) Carin Li	“Bioinformatics”	2017- 2020
53) Manoj Rout	“Bioinformatics and NMR”	2017-2021
54) Elvis Lo	“Cheminformatics”	2017-2018
55) Zachary Budinski	“Data Mining & Text Composition”	2017-2021
56) Hasan Badran	“Data Mining & Cheminformatics”	2017-2019
57) Rahmatollah Rajabza	“GC-MS Analysis”	2018-2020
58) Shirin Zahraei	“ICP-MS and the HML”	2018-pres.
59) Yongjie Liang	“Bioinformatics”	2008-2020
60) Gozal Inchehborouni	“GC-MS Analysis”	2019-2020
61) Lusine Tonoyan	“Machine Learning in Bioinformatics”	2019-2020
62) Ishu Jain	“Bioinformatics”	2020-2020
63) Xuan Cao	“Bioinformatics”	2019-2021
64) Yilin Wang	“Metabolomics”	2019-2021
65) Siyang Tian	“Bioinformatics”	2019-pres.

66) Eponine Oler	“Bioinformatics and databases”	2019-pres.
67) Vicki Lui	“Software development and databases commercialization”	2021-pres.
68) John Bacon	“Biosensors engineering”	2020-pres.
69) Dana Allen	“Databases, LIMS and TMIC website maintenance”	2020-pres.
70) Laura Bony	“Colorimetric detection of UTI metabolites”	2020-2021
71) Leif Wilm	“Machine learning, software development”	2020-pres.
72) Claudia Torres	“Colorimetric assays for metabolite detection”	2021
73) Nikolay Blinov	“Biophysical modelling and software development”	2021-pres.
74) Karla Trejo-Oliver	“Metabolomics”	2021
75) Arian Ramezani	“Bioinformatics”	2021
76) Robert Sullivan	“Metabolomics”	2021-pres.
77) Ashley Zubkowski	“Metabolomics”	2021-pres.
78) Juan Jovel	“Bioinformatics”	2021-pres.
79) Olawunmi Taiwo	“Metabolomics”	2021-2022
80) Mathew Johnson	“Metabolomics”	2018-pres.
81) Karxena Harford	“Bioinformatics”	2021-pres.



82) Kevin Liang	“Bioinformatics”	2020
83) Louisa Normington	“Bioinformatics”	2020-pres.
84) Rachel Kruger	“Bioinformatics”	2022-pres
85) Jennifer Bui	“Structural simulations of proteins”	2022-pres.
86) James Cook	“Biosensors engineering”	2020-pres.
87) Krishna Kovur	“Bioinformatics”	2021-pres.
88) Samuel Stuart	“Bioinformatics”	2020-pres.
89) Abigail Wipf	General Lab assistance	2021-pres.
90) Seyedehamideh Razavi	“Metabolomics”	2021
91) Alyaa Selim	“Metabolomics”	2021
92) Jenna Poelzer	“Bioinformatics”	2022
93) Ameneh Mohammadnezhad	“Metabolomics and biosensors”	2022

### **Assistants and Research Coordinators**

1) Lori Querengesser	Research Manager	2005-2007
2) Treena Neufeld	Faculty Assistant	2006-2007
3) Jill Walshaw	Faculty Assistant	2007-2008

4) Connie Sobsey	Research Coordinator	2007-2012
5) Ian Forsythe	Research Manager	2007-2008
6) Bobby-Jo Miller	Faculty Assistant	2008-2014 2017
7) Ann O'Neill	Research Coordinator	2008-2009
8) Jamie Kulchitsky	Faculty Assistant	2012-2020
9) Tamara Lim	Research Coordinator	2012-2015
10) Jennifer Reid	Business Developer	2012-pres.
11) Christopher Reid	Research Coordinator	2013-2015 2017-2019
12) Dana Chamot	Research Coordinator	2015-2019
13) Chris Kazala	Research Coordinator	2016-2017
14) Reza Jafari	Program Manager	2016-2017
15) Julie Peddle	Executive Assistant	2017-2018
16) Galina Durant	Executive Assistant	2018-pres.
17) Nicolas Vozza	Junior Research Coordinator	2018-2019
18) Danielle Girard	Executive Assistant	2019-2020

19) Manmeet Mamik	Business Developer	2019-2020
20) Prashanthi Kovur	Research Coordinator	2020-pres.
21) Oxana Tarassova	Administrative Assistant (HR)	2020-pres.
22) Jamie Kulchitsky	Digital Marketer	2021-pres.
23) Marcia LeVatte	Scientific articles and grant writing	2020-pres.

### **Visiting Professors**

1) Hassan Monzavi	“NMR analysis of Stoeffel Polymerase Peptides’	1996 – 1997
2) Bahram Habibi-Nazhad	“Computer-aided Drug Design”	2000 – 2001
3) Brent W Winston	“Metabolomics in Critical Care”	2020 – 2020
4) Cristina Andres-Lacueva	“Barcelona Brain Health Initiative, FOBI-ontology applications and further connections to HMDB database”	2021 – pres.

### **Visiting Researchers:**

Karen Machin	Canada	University of Alberta	2011-2012
Soenke Moehn	Canada	University of Alberta	2011-2013
Nicole Afacan	Canada	University of British Columbia	2012
Walter Swardfager	Canada	University of Toronto	2012
Fardin Ghobakhlou	Canada	Universite Laval	2013
Kasper Skov	Denmark	Technical University of Denmark	2013-2014

Margie Gruber	Canada	University of Saskatchewan	2013-2014
Vanessa Neveu	France	IARC	2013
Guanshi Zhang	Canada	University of Alberta	2013-2014
Adriana Buzatto	Brazil	UNICAMP	2014
Eoin Fahy	USA	University of California, San Diego	2014
Helena Gibbons	Ireland	University College Dublin	2014
Karolina Sulek	New Zealand	University of Auckland	2014
Mordechai Slae	Israel	University of Alberta	2014
Rosa Vazquez Fresno	Spain	University of Barcelona	2014
Petya Koleva	Canada	University of Alberta	2015-2016
David DeSouza	Australia	Metabolomics Australia	2015
Douglas Kiss	Canada	University of Lethbridge	2015
Ian Garber	Canada	University of British Columbia	2015
Paul Ryan	Ireland	Moorepark Food Research Centre	2015-2016
Saravanan Dayalan	Australia	Metabolomics Australia	2015
Aaron Abraham	Canada	University of Calgary	2016
Silvia Mari	Spain	Mestrelab	2016
Albert Tsiu	Canada	Royal Alexandra Hospital	2016
Mellisa Lorenzo	USA	Queens University	2016
Vi Dang	Canada	McMaster University	2017
Tom O'Callaghan	Ireland	Teagasc Food Research Centre	2017
Beata M. Mickiewicz	Canada	University of Calgary	2017
Katie Powell	Australia	Kolling Institute of Med. Research	2017
Amir Alizad	Iran	IPM	2017-2018
Mickel Hiebert Giesbrecht	Mexico	Unidad de biotecnologia CICY	2018

Jonathan Magnan	Ireland	TEAGACS	2018
Alberto Gil de la Fuente	Spain	CEU-San Pablo University	2018
Gabriele Rocchetti	Italy	Universita Catolica sel Sacro Cuore	2018
Claudia Valeria Saucedo	Mexico	Autonomous Univ. of Nuevo Leon	2018
Ralph Sclapbach	Switzerland	Functional Genomics Center Zurich	2018
Obrayan Gomez Gonzalez	Mexico	Instituto Tecnologico	2018
Hossein Ghahremani	Iran	Shahid Beheshti University of Medical Sciences	2018-2019
Ann Kwan	Australia	University of Sidney	2018-2019
Gustavo Bueno Duarte	Brazil	University of C�mpin�s	2019
Urja Verma	India	University of Baroda	2019
Sean Bennet	Canada	Queens University	2019
Zafer Ugu	USA	Beaumont Health	2019
Anas El-Aneed	Canada	University of Saskatchewan	2019
Carlos Fernando Mel	Brazil	University of Campinas	2019
Claudia Blakebrough-Hall	Australia	University of Sidney	2019
Denise Biagini	Italy	University of Pisa	2019
Deying Chen	China	Zhejiang University	2019
Gerardo Cebrian Torrejon	Guadeloupe	University of Valencia	2019
Izzah Shahid	Pakistan	University of Central Punjab	2019
Mengxuan Wang	China	Fudan University	2019
Paiboon Tunsagool	Thailand	Prince of Songkla University	2019
Ralph Sclapbach	Switzerland	University of Zurich	2019

Wei Huang	China	Second Institute of Oceanography, Hangzhou	2019
Xiaowei Shi	China	Zhejiang University, Hangzhou	2019
Yamile Lopez	Mexico	Universidad de San Luis Potosí	2019
Alyaa Hatem Ibrahim	Egypt	Sohag University	2021
Hannah Charnock	Canada	Brock University	2022
Marina Bellot	Spain	Chemical Institute of Sarrià	2022
Anna Damato	Italy	University of Padua	2022

### **University of Alberta Courses Taught**

FNS 501	Advanced Human Metabolism	2013
Biol 299	Research Opportunity Program	2007 – 2013
Biol 398	Research Project	2019 – pres.
Biol 490	Individual Study	2006
Biol 498	Research Project	2007 – 2010
Biol 499	Research Project	2005 – pres.
Biol 501	Applied Bioinformatics	2009 – pres.
Bioin 301	Bioinformatics I	2001 – pres.
Bioin 401	Bioinformatics II	2003 – pres.
Cell 398	Research Project	2009

Comput 495	Honors Seminar	2012 – 2014
Comput 499	Topics in Computing Science	2004 – pres.
Comput 603	Teaching and Research Methods	2003 – pres.
Comput 605	Topics in Computing Science	2010
Microb 343	Analysis of Microbial Macromolecules	2005 – 2007
Microb 607	Microbiology Seminar	2005
Pharm 321	Pharmacy Biotechnology and Immunology	2007 – pres.
Pharm 325	Introduction to Quantitative Pharmaceutical Analysis	1996 – 2006
Pharm 341	Quantitative Pharmaceutical Analysis	2006 – 2010
Pharm 360	Pharmaceutics	2001 – 2006
Pharm 361	Pharmaceutics 2	2007 – pres.
Pharm 493	Pharmaceutical Biotechnology	1997 – 2007
Pharm 498	Research and Directed Studies	1998
Pharm 570	Advanced Pharmaceutical Analysis - Spectroscopy	1995 – pres.
Pharm 580	Introduction to Computer-Aided Drug Design	1998 – pres.
Pharm 604	Applied Problems in Current Research	1997 – 1998
Pharm 610	Advanced Drug Delivery Systems	1998 – pres.
Pharm 624	Application of Nuclear Magnetic Resonance Spectroscopy to Medicinal and Pharmaceutical Chemistry	2010

Pharm 694	Directed Project	1998 – 2000
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### **External Courses Developed and Taught**

<b>Course</b>	<b>Location</b>	<b>Period</b>
Canadian Bioinformatics Workshops (CBW) - Bioinformatics	Across Canada	1999 – 2007
Canadian Bioinformatics Workshops (CBW) - Proteomics	Across Canada	2002 – 2007
Canadian Proteomics Initiative – Practical Bioinformatics	Across Canada	2002 – 2005
Genome Canada – Advanced Computational Genomics Course (Programming)	Across Canada	2003 – 2011
NIH Bioinformatics Workshop - Structural Biology	Bethesda, USA	2003 – 2008
BCIT and NRC-Vitesse – Bioinformatics for Proteomics	Vancouver, BC	2004 – 2006
BCIT and NRC-Vitesse – Bioinformatics for Microarrays	Vancouver, BC	2004 – 2006
BCIT and NRC-Vitesse – Tools for Drug Discovery	Vancouver, BC	2005 – 2006
Canadian Bioinformatics Workshops (CBW) – Informatics for Metabolomics	Across Canada	2010 – pres.



Bioinformatics and Statistical Methods in Metabolomics	Niagara Falls, ON	2016
Bioinformatics and Metabolomics	Curenavaca, MX	2016
NMR-based Metabolomics	Brisbane, AUS	2016
Canadian Bioinformatics Workshops (CBW) – Machine Learning for Bioinformatics	Across Canada	2020 – pres.

### **Examining Committees**

- 1) Ph.D. candidacy examining committee for Ryan McKay (Biochemistry) Oct. 1999
- 2) Ph.D. examining committee (final oral) for Iqbal Goralwalla (Comp. Sci.) March 16, 1998
- 3) Ph.D. candidacy examining committee for Christine Lutsiak (Pharmacy) June 2, 1998
- 4) M.Sc. examining committee (final oral) for Ulunma Imo (Pharmacy) Jan. 23, 1998
- 5) M.Sc. examining committee (final oral) for Fei Lui (Comp. Sci.) Jan. 18, 1999
- 6) Ph.D. examining committee (final oral) for Ryan McKay (Biochemistry) April 16, 1999
- 7) Ph.D. examining committee (final oral) for Brian Trippet (Biochemistry) July 15, 1999
- 8) Ph.D. candidacy examining committee for Chun Shung Liu (Chemistry) Nov. 19, 1999
- 9) Ph.D. candidacy examining committee for Jennifer Kaplan (Chemistry) Nov. 26, 1999
- 10) Ph.D. examining committee (candidacy) for Sean McKenna (Biochemistry) May 31, 2002
- 11) Ph.D. examining committee (final oral) Christine Lutsiak (Pharmacy) Sept. 20, 2002

- 12) Ph.D. examining committee (candidacy) for Karen Kawulka (Chemistry) Nov. 20, 2002
- 13) M.Sc. examining committee for Nathalie Guo, Jan. 24, 2006
- 14) Ph.D. examining committee for Danielle Kemmer, Feb. 23, 2006
- 15) Ph.D. examining committee for Theodore Laskowski, July 12, 2006
- 16) Ph.D. examining committee for Ben Zhou, Dec. 2009
- 17) Ph.D. examining committee for David Chang, Feb. 2009
- 18) M.Sc. examining committee for Bela Reiz, Jan. 2009
- 19) M.Sc. examining committee for Wei Wei, Jan. 2009
- 20) Ph.D. examining committee for Ci Song, May, 2009
- 21) M.Sc. examining committee for Siamak Ravanbakhsh, Sept. 2009
- 22) Ph.D. candidacy examining committee for Wael Soliman, Jan. 2010
- 23) Ph.D. candidacy examining committee for Cynthia Stretch, Jun. 2010
- 24) Ph.D. examining committee for Madhuri Newa, Apr. 2012
- 25) Ph.D. examining committee for Paul Weldman, Apr. 2013
- 26) Ph.D. examining committee for Hao Yu, Jun. 2013
- 27) M.Sc. examining committee for Zheng Shi, Dec. 2015
- 28) Ph.D. examining committee for Adriana Nori de Macedo, Mar. 2017
- 29) Ph.D. examining committee for Fabini Orata, Nov. 2017
- 30) Ph.D. examiner for Lin Shi, Dec. 2017

- 31) M.Sc. examining committee for Amel Hamza, Dec. 2018
- 32) M.Sc. examining committee for Siyang Tian, Apr. 2019
- 33) Ph.D. examiner for Ville Koistinen, May 2019
- 34) M.Sc. examiner for Fei Wang, Jan. 2020
- 35) Ph.D. examining committee for MD. Shaheen, Feb. 2020
- 36) Ph.D. examining committee for Aidin Foroutannaddafi, July, 2020
- 37) Ph.D. examining committee for Massih Khovash, Aug, 2020
- 38) M.Sc. examining committee for Louisa Normington, Sep 2020
- 39) M.Sc. examining committee for Klevis Haxhiaj, June 2021
- 40) Ph.D. examining committee for Ali Goldansaz, June 2021

### **Supervisory Committee Member**

- 1) Ph.D. supervisory committee for Bin Li (Biology), Jan. 1, 2001
- 2) Ph.D. supervisory committee for Karen Kawalka (Chemistry), Sept. 1, 2001
- 3) M.Sc. supervisory committee for Michael Pedersen, Sept. 1, 2002
- 4) M.Sc. supervisory committee for Rajesh Vij, Sept. 1, 2002
- 5) Ph.D. supervisory committee for Jake Stymiest, Sept. 1, 2003
- 6) M.Sc. supervisory committee for Eric Cheong, Jan. 1, 2003
- 7) Ph.D. supervisory committee for Douglas Burr, Jan. 1, 2003

- 8) M.Sc. supervisory committee for Theodore Tegos, April 1, 2004
- 9) Ph.D. supervisory committee for Xian Wang, Aug. 19, 2004
- 10) M.Sc. supervisory committee for Jeff Xia, May 19, 2005
- 11) Ph.D. supervisory/candidacy committee for Ryan Hoffman, Aug. 31, 2006
- 12) Ph.D. supervisory/candidacy committee for Gabriella Moise, Dec. 12, 2006
- 13) Ph.D. supervisory/candidacy committee for Jianjun Zhou, June 26, 2006
- 14) Ph.D. supervisory committee for Nirosha Bunasekara, Mar 2008
- 15) M.Sc. supervisory committee for Sheehan Khan, Feb. 2010
- 16) M.Sc. supervisory committee for Saman Vaisipour, Feb. 2010
- 17) Ph.D. supervisory committee for Siamak Ravanbakhsh, Sept. 2011
- 18) Ph.D. supervisory committee for Mohsen Hajiloo, Feb. 2012
- 19) Ph.D. supervisory committee for Michael Burns, April. 2012
- 20) Ph.D. supervisory committee for Felicity Allen, Aug. 2012
- 21) Ph.D. supervisory committee for Meduri Newa, Aug. 2012
- 22) Ph.D. supervisory committee for Massih, Khorvash, Sep. 2012
- 23) Ph.D. supervisory committee for Guanshi Zhang, Jun. 2013
- 24) Ph.D. supervisory committee for Fabini Orata, Jan. 2014
- 25) Ph.D. supervisory committee for Kirby Zeigler, Jan. 2014
- 26) Ph.D. supervisory committee for Ali, Goldansaz, Aug. 2015

- 27) M.Sc. supervisory committee for Louisa Normington, Sept. 2016
- 28) M.Sc. supervisory committee for Amel Hamza, Dec. 2017
- 29) M.Sc. supervisory committee for Siyang Tian, Apr. 2018
- 30) M.Sc. supervisory committee for Fei Wang, Feb. 2019
- 31) M.Sc. supervisory committee for Afia Anjum, March, 2020
- 32) M.Sc. supervisory committee for Shiful, Islam, June, 2020
- 33) M.Sc. supervisory committee for Zinat, Sayeeda, Sep. 2020
- 34) M.Sc. supervisory committee for Aidin, Foroutannaddafi, March, 2020