McGill | Faculty of Medicine and Health Sciences | Faculté de médecine et des sciences de la santé

Committee for Oversight of Research Units

Annual Reporting for Faculty Supported Research Centres and Networks

---

All Centres (provisional Centres; McGill Centres), Research groups and Networks that receive funding from the Faculty of Medicine and Health Sciences (FMHS) are required to provide an annual report to the Committee for Oversight of Research Units (CORU)

The reporting period is May 1, 2021 – April 30, 2022.

Please submit your report to the Research Office, Faculty of Medicine and Health Sciences (**riac.med@mcgill.ca**) before the following deadline:

Monday, May 2, 2022

Continued support from the Faculty is contingent on:

1. the receipt of the reporting documents on time,
2. the evaluation of reported activities by the Faculty's Committee for Oversight of Research Units (CORU),
3. the availability of Faculty funds.

Your strong engagement in the Faculty's mission for continued research excellence and financial stewardship is truly appreciated.

Annual Report of Activities and Outcomes

Name of the Unit: **McGill University Centre for Structural Biology (CSB),**

which also operates as FRQS-funded **Centre de Recherche en Biologie Structurale (CRBS)**

Name of Unit leader & email address:

Director: Dr. Martin Schmeing
martin.schmeing@mcgill.ca
Phone: 514-398-2331

Coordinator: Dr. Annick Guyot
csb.med@mcgill.ca
514-398-2293

Associate Director: **Dr. Natalie Zeytuni**
natalie.zeytuni@mcgill.ca
Phone: 514-398-6348

Associate Director: **Dr. Chris Thibodeaux**
christopher.thibodeaux@mcgill.ca
Phone: 514-398-3637

If the Unit is **a Senate-approved** McGill Research Centre, indicate date of approval:

May 14th ,2014 (for CSB)

Mission statement of the Unit (~ 2 sentences):

The mission of the CSB and CRBS is to exploit the power of structural biology and biophysics to produce the next wave of scientific breakthroughs in (i) determining the molecular basis of disease and treatments, and (ii) leveraging biophysical, chemical and synthetic biology for health. At the same time, we will train a new generation of structural biologists and biophysicists with outstanding expertise in using cross-disciplinary approaches for biomedical research to make structural biology and its many strengths accessible to the broader biomedical research and health community.

Total number of Unit members: 41 regular members

Number of members affiliated with McGill's FMHS: 22 regular members

Unit's website:

Please note the website needs to feature:

- all sources of funding support (including the FMHS logo),
- the list of Members and their institutional affiliation with appropriate links,
- the activities supported by the Unit,
- all previous Annual Reports.

Website address (URL): **http://crbsmcgill.ca**

Please respect the page limits, where indicated.

(minimum font size of 11 pts, use lay language)

1. Explain the significance of the Unit's mission at McGill and beyond (1/2 page max.)

Understanding the molecules that underlie all life function, and how they are altered in disease states, is of fundamental importance to health care. Equally, understanding the molecular mechanisms of therapeutics and leveraging new nanotechnologies will be key for the development of next-generation treatments. Practically all medicines are molecules (be they small molecules or biologics) and thus must be understood and developed with molecular level information. Structural biology and biophysics are the suite of multidisciplinary tools that provide precise molecular level information on the form and activity of the molecules of life. Clear examples of the importance of structural biology and biophysics for health include the massive structural biology and structure-function relationship initiatives developed in-house by biotechs and big pharma, the literally millions of lives saved by treatments which structural biology played a key role in developing, the eight Nobel prizes in the last two decades awarded for the use and/or development of structural biology and biophysics techniques, and the key role structural biology is assuming in the development of gene editing techniques. A recent meta-study (Westbrook & Burley, Structure 2019) revealed that structural information has been informative or critical for the development for 185 of the 210 new therapeutics approved by the US Food and Drug Administration between 2010 and 2016. Moreover, the influence of structural biology in the health sector is accelerating as researchers using electron microscopy and/or X-ray crystallography are increasingly successful at obtaining structures of more complex, therapeutically relevant targets and medically relevant cellular machines. Furthermore, the multi-disciplinary interrogation of these complexes with both structure determination and complementary biophysical techniques provides an unprecedented level of understanding of the systems and enhanced ability to inhibit or manipulate them to improve medical treatment outcomes. Modern structural biology and biophysics are making a broader impact in health than ever before, because structural information can now be leveraged for target discovery, new modes of action, and lead-to-therapeutic development for small molecules, biologics and gene editing.

We are very appreciative of the Faculties guaranteed ongoing contribution of $50,000 per year during the FRQS funding period.

2. Alignment with the Faculty's Strategic Research Plan (1/2 page max.)

-The CRBS supports numerous research activities that are central to the Faculty's mission of health science research and provide multidisciplinary training to McGill students.
-The CRBS held its 3rd Annual Symposium virtually on Monday, November 8, 2021 with ~100 attendees and 2 internationally renowned speakers. The CRBS also supports a student-run seminar series and several outreach activities (bench to bedside, bench to business, bootcamps)
-The CRBS has one student stipend program that support the recruitment and retention of high-quality students at McGill.
-The CRBS has several initiatives to support research projects from CRBS members and infrastructure funding
-The CRBS also manages –or contributes to the management of– several equipment platforms in the Bellini, Strathcona (FEMR), McIntyre (Mass Spec) and Otto Maas (QANUC) buildings. These platforms have contributed to the success of faculty members and the large number of high impact publications from CRBS.
-EDI: The SRP emphasizes the major importance of equity, diversity and inclusion throughout all aspects of research, from initial conception through implementation and ultimately translation to healthcare. We are undertaking a full review of our EDI activities and in conjunction with FRQS wil have a fully developed EDI policy in the coming year. We have already implemented several important steps, including a requirement for all members who receive funding to participate in sessions offered by McGill's Organizational Development Department

3. **Major joint publications over the past 12 months** (including shared software, data repositories; with links) co-authored by at least two PI members of the Unit:

CRBS members have published 155 publicatsion in the past 12 months, including in high profile journals such as Cell, Science and Nature. Around 14% of all publications of CRBS members were collaboration with another CRBS PI. These papers are listed here:

1. Design, synthesis and in vitro evaluation of novel SARS-CoV-2 3CL^{pro} covalent inhibitors.
Stille JK, Tjutrins J, Wang G, Venegas FA, Hennecker C, Rueda AM, Sharon I, Blaine N, Miron CE, Pinus S, Labarre A, Plescia J, Burai Patrascu M, Zhang X, Wahba AS, Vlaho D, Huot MJ, **Schmeing TM**, **Mittermaier AK**, Moitessier N.
Eur J Med Chem. 2022 Feb 5;229:114046. doi: 10.1016/j.ejmech.2021.114046. Epub 2021 Dec 11.PMID: 34995923

2. Structures and function of a tailoring oxidase in complex with a nonribosomal peptide synthetase module.
Fortinez CM, Bloudoff K, Harrigan C, Sharon I, **Strauss M**, **Schmeing TM.**
Nat Commun. 2022 Jan 27;13(1):548. doi: 10.1038/s41467-022-28221-y.PMID: 35087027

3. The chaperone HSPB1 prepares protein aggregates for resolubilization by HSP70.
Gonçalves CC, Sharon I, **Schmeing TM**, Ramos CHI, **Young JC**.
Sci Rep. 2021 Aug 24;11(1):17139. doi: 10.1038/s41598-021-96518-x.PMID: 34429462

4. Structural basis for plazomicin antibiotic action and resistance.
Golkar T, Bassenden AV, Maiti K, Arya DP, **Schmeing TM**, **Berghuis AM**.
Commun Biol. 2021 Jun 11;4(1):729. doi: 10.1038/s42003-021-02261-4.PMID: 34117352

5. Structural Dynamics of Cytochrome P450 3A4 in the Presence of Substrates and Cytochrome P450 Reductase.
Ducharme J, Sevrioukova IF, **Thibodeaux CJ**, **Auclair K**.
Biochemistry. 2021 Jul 20;60(28):2259-2271. doi: 10.1021/acs.biochem.1c00178. Epub 2021 Jul 1.PMID: 34196520

6. Combining Small-Molecule Bioconjugation and Hydrogen-Deuterium Exchange Mass Spectrometry (HDX-MS) to Expose Allostery: the Case of Human Cytochrome P450 3A4.
Ducharme J, Polic V, **Thibodeaux CJ**, **Auclair K**.
ACS Chem Biol. 2021 May 21;16(5):882-890. doi: 10.1021/acschembio.1c00084. Epub 2021 Apr 29.PMID: 33913317

7. Crystal structure of human PACRG in complex with MEIG1 reveals roles in axoneme formation and tubulin binding.
Khan N, Pelletier D, McAlear TS, Croteau N, Veyron S, Bayne AN, Black C, Ichikawa M, Khalifa AAZ, Chaaban S, Kurinov I, **Brouhard G**, **Bechstedt S**, **Bui KH**, **Trempe JF**.
Structure. 2021 Jun 3;29(6):572-586.e6. doi: 10.1016/j.str.2021.01.001. Epub 2021 Feb 1.PMID: 33529594

8. A dissipative pathway for the structural evolution of DNA fibres.
Rizzuto FJ, Platnich CM, Luo X, Shen Y, Dore MD, Lachance-Brais C, **Guarné A**, **Cosa G**, **Sleiman HF**.
Nat Chem. 2021 Sep;13(9):843-849. doi: 10.1038/s41557-021-00751-w. Epub 2021 Aug 9.PMID: 34373598

9. Endocytic proteins with prion-like domains form viscoelastic condensates that enable membrane remodeling.
Bergeron-Sandoval LP, Kumar S, Heris HK, Chang CLA, Cornell CE, Keller SL, François P, **Hendricks AG**, **Ehrlicher AJ**, Pappu RV, Michnick SW.
Proc Natl Acad Sci U S A. 2021 Dec 14;118(50):e2113789118. doi: 10.1073/pnas.2113789118.PMID: 34887356

10. Selective localization of Mfn2 near PINK1 enables its preferential ubiquitination by Parkin on mitochondria.
Vranas M, Lu Y, Rasool S, Croteau N, Krett JD, Sauvé V, **Gehring K**, Fon EA, Durcan TM, **Trempe JF**
Open Biol. 2022 Jan;12(1):210255. doi: 10.1098/rsob.210255. Epub 2022 Jan 19.PMID: 35042405

11. Structural basis for DNA targeting by the Tn7 transposon.
Shen Y, Gomez-Blanco J, Petassi MT, Peters JE, **Ortega J**, **Guarné A.**
Nat Struct Mol Biol. 2022 Feb;29(2):143-151. doi: 10.1038/s41594-022-00724-8. Epub 2022 Feb 16.PMID: 35173349

12. Mechanism of PINK1 activation by autophosphorylation and insights into assembly on the TOM complex.
Rasool S, Veyron S, Soya N, Eldeeb MA, **Lukacs GL**, Fon EA, **Trempe JF**.
Mol Cell. 2022 Jan 6;82(1):44-59.e6. doi: 10.1016/j.molcel.2021.11.012. Epub 2021 Dec 6.PMID: 34875213

13. Corrigendum to "Mineral tessellation in bone and the stenciling principle for extracellular matrix mineralization" [J. Struct. Biol. 214(1) (2022) 107823].
McKee MD, Buss DJ, **Reznikov N**.
J Struct Biol. 2022 Apr 22;214(2):107858. doi: 10.1016/j.jsb.2022.107858. Online ahead of print.PMID: 35468540 No abstract available.

14. Mineral tessellation in bone and the stenciling principle for extracellular matrix mineralization.
McKee MD, Buss DJ, **Reznikov N**.
J Struct Biol. 2022 Mar;214(1):107823. doi: 10.1016/j.jsb.2021.107823. Epub 2021 Dec 13.PMID: 34915130 Review.

15. Hierarchical organization of bone in three dimensions: A twist of twists.
Buss DJ, Kröger R, **McKee MD**, **Reznikov N**. 4
J Struct Biol X. 2021 Dec 9;6:100057. doi: 10.1016/j.yjsbx.2021.100057. eCollection 2022.PMID: 35072054

16. Using transient equilibria (TREQ) to measure the thermodynamics of slowly assembling supramolecular systems.
Hennecker CD, Lachance-Brais C, **Sleiman H**, **Mittermaier A.**
Sci Adv. 2022 Apr 8;8(14):eabm8455. doi: 10.1126/sciadv.abm8455. Epub 2022 Apr 6.PMID: 35385301

17. Tuning DNA Supramolecular Polymers by the Addition of Small, Functionalized Nucleobase Mimics.
Lachance-Brais C, Hennecker CD, Alenaizan A, Luo X, Toader V, Taing M, Sherrill CD, **Mittermaier AK**, **Sleiman HF**.
J Am Chem Soc. 2021 Dec 1;143(47):19824-19833. doi: 10.1021/jacs.1c08972. Epub 2021 Nov 16.PMID: 34783562

18. The amyloid-β_{1-42}-oligomer interacting peptide D-AIP possesses favorable biostability, pharmacokinetics, and brain region distribution.
Shobo A, James N, Dai D, Röntgen A, Black C, Kwizera JR, Hancock MA, **Huy Bui K**, **Multhaup G.**
J Biol Chem. 2022 Jan;298(1):101483. doi: 10.1016/j.jbc.2021.101483. Epub 2021 Dec 9.PMID: 34896396

19. Functional mimicry revealed by the crystal structure of an eIF4A:RNA complex bound to the interfacial inhibitor, desmethyl pateamine A.
Naineni SK, Liang J, Hull K, Cencic R, Zhu M, Northcote P, Teesdale-Spittle P, Romo D, **Nagar B**, **Pelletier J**.
Cell Chem Biol. 2021 Jun 17;28(6):825-834.e6. doi: 10.1016/j.chembiol.2020.12.006. Epub 2021 Jan 6.PMID: 33412110

20. Assessing eukaryotic initiation factor 4F subunit essentiality by CRISPR-induced gene ablation in the mouse.
Sénéchal P, Robert F, Cencic R, Yanagiya A, Chu J, **Sonenberg N**, Paquet M, **Pelletier J.**

Cell Mol Life Sci. 2021 Oct;78(19-20):6709-6719. doi: 10.1007/s00018-021-03940-5. Epub 2021 Sep 24.PMID: 34559254

21. Nonspecific binding of common anti-CFTR antibodies in ciliated cells of human airway epithelium.
Sato Y, Mustafina KR, Luo Y, Martini C, **Thomas DY**, **Wiseman PW**, Hanrahan JW.
Sci Rep. 2021 Dec 1;11(1):23256. doi: 10.1038/s41598-021-02420-x.PMID: 34853321

4. Major joint research projects funded over the past 12 months (involving at least two PI members of the Unit:

Extramural Grants:

CRBS PIs: Albert Berghuis, Youla Tsantrizos
CIHR Project Grant
Validation of the human geranylgeranyl pyrophosphate synthase (hGGPPS) as a therapeutic target for cancer chemotherapy and design of pre-clinical candidates for the treatment of multiple myeloma, Grant
2018/10 - 2023/9
Total Funding - 883,194 (Canadian dollar)

CRBS PIs: Albert Berghuis, Youla Tsantrizos
FQRNT Team research project program grant
Surexpression de la géranylgéranyl pyrophosphate humaine (hGGPPS) et leur rôle dans la progression de la maladie d' Alzheimer's, Grant
Clinical Research Project?: No
2018/4 - 2022/3
Total Funding - 162,000 (Canadian dollar)

CRBS PIs: Allen Ehrlicher, Khanh Bui, Paul Wiseman
CIHR Project Grant
The role of lamin A/C in nuclear mechanotransduction and breast cancer metastasis
2022/4 - 2027/4 (Under review)
Total Funding - 660,000 (Canadian dollar)

CRBS PIs: Allen Ehrlicher, Gonzalo Cosa
CFI10
Dynamic Organization of the Building Blocks of Life (DOBBL)
2020/8 - 2025/4
Total Funding - 6,700,000 (Canadian dollar)

CRBS PIs: Alvin Shrier, Gergely Lukacs, Jason Young
CIHR Project Grant
Quality control and pharmacological rescue of heteromeric long QT mutants
2020/4 - 2025/3
Total Funding - 768,825 (Canadian dollar)

CRBS PIs: Hanadi Sleiman, Gonzalo Cosa, Masad Damha; Maureen McKeague
NSERC CREATE
Programmed Molecules for Therapeutics, Sensing and Diagnostics (PROMOTE)
2019/4 - 2025/3
Total Funding - 1,650,000 (Canadian dollar)
Portion of Funding Received - 165,000 (Canadian dollar)

CRBS PIs: Gonzalo Cosa, Hanadi Sleiman
NFRF

Toward automated synthesis of DNA nanomaterials
2021/4 - 2023/3
Total Funding - 200,000 (Canadian dollar)

CRBS PIs: JF Trempe, Kalle Gehring, Gergely Lukacs
CFI John R. Evans Leaders Fund
Conformational dynamics of complex proteins in health and diseases,
2020/4 - 2025/4
Total Funding - 1,481,590 (Canadian dollar)

CRBS PIs: JF Trempe, Joaquin Ortega
Michael J. Fox Foundation Target Optimization Award
Structure of human PINK1-TOM complex by Single-particle Cryo-EM.
2020/08 – 2022/07
Total Funding - 231,000 (US dollar)

CRBS PIs: Joaquin Ortega, Christopher Thibodeaux Natalie Zeytuni
FRQNT - Projet de recherche en équipe
Structural biology approaches to investigate the biosynthetic fidelity mechanisms in lanthipeptide synthetases.
2021/2 - 2022/1
Total Funding - 200,000 (Canadian dollar)

CRBS PIs: Marc McKee, Natalie Reznikov
Cryo-liftout system for preparing in situ lamellae in cryo-FIBSEM
NSERC RTI
2021/4 - 2022/3 Natural Sciences and Engineering Research Council of Canada
Research Tools and Instruments
Total Funding - 142,827 (Canadian dollar)

CRBS PIs: Marc McKee, Natalie Reznikov
Procter & Gamble Company Contract
Preserving dental biomechanical longevity: Bridging the gap when human life expectancy outpaces the evolutionary adaptation of dental tissues, Contract
2021/1 - 2021/12
Total Funding - 125,000 (Canadian dollar)

CRBS PIs: Nahum Sonenberg, Jerry Pelletier
CIHR Rapid Research Funding Opportunity
INTERCEPTORs: engINeered ThERapeutiC dEfensive Particles TO SARS-CoV-2, Grant,
2020/6 - 2022/5
Total Funding - 745,000 (Canadian dollar)

CRBS PIs: Tony Mittermaier, Maureen McKeague
Genome Quebec Genomics Integration Program
A rational design and in vitro screening pipeline to discover new classes of antibiotics targeting RNA
2021/6 - 2023/5
Total Funding - 400,000 (Canadian dollar)

CRBS PIs: Mike Straus, Adam Hendricks, Susanne Bechstedt, Huy Bui
NSERC RTI
Cryo-3D-super-resolution light microscope for correlative microscopy
04/2022 – 03/2023
Total Funding - 150,000 (Canadian dollar)

CRBS PIs: Martin Schmeing, Natalie Zeytuni, all CRBS PIs; application as a Centre in collaboration with MUHC-RI, Lady Davis and Douglas Hospital research centre
FRQS Tremplin Step 1
Tremplin program for trainees of McGill research centres funded by FRQS
11/2021 – 04/2022

Intramural funding provided in past 12 months

Blue sky funding competition: held in January 2022: 6 applications received, 4 funded for a total of $100,000. 1 funded application involves 2 CRBS members (**S. Bechstedt** and **M. Strauss**) ***Development of correlative cryo-SIM***

Infrastructure competition: held in December 2021. 3 applications received, 1 awarded for a total of $27,000. Involves 2 CRBS members (**J. Ortega** and **A. Guarné**). ***Cryo-EM grid storage system***

RTI competition: held in October 2021. 2 applications received, 1 funded for a total of $15,000. Involves 4 CRBS members (**M. Strauss, A. Hendricks, S. Bechstedt** and **H. Bui).** NSERC RTI Supplement. ***Cryo-3D-super-resolution light microscope for correlative microscopy***

5. Major outreach activities (e.g., seminar series, general public events):

-3rd CRBS Annual Symposium virtually held on Monday, November 8, 2021 with ~100 attendees and 2 internationally renowned speakers. See program in **Appendix 1.**

-CRBS Seminar Series: flagship event hosted by the CRBS student council that features trainee research. ~30 minutes presentations from trainees in CRBS labs. Open to CRBS community and adjacent departments. Held virtually 2/month from Sept-April, with 2 trainees presenting at each session. Talks are judged by faculty members and cash prizes are presented to the best presenters at the annual symposium. ~50 attendees per session. See schedule in **Appendix 2.**

-CRBS Methods Seminar Series: series hosted by the student council that introduces the CRBS audience to the wide variety of techniques and methods employed by different research groups at the CRBS. The goal is to make these techniques more accessible to CRBS trainees. Also to foster scientific collaboration within the CRBS by highlighting the infrastructure and the expertise available at the center. Held virtually 1/month with a 60-minute presentation by a trainee or staff member with expertise in a particular technique, covering basic theory and application of the technique and also showing how the technique has been employed at the CRBS in the past to answer important research questions. ~30 attendees per session. See schedule in **Appendix 3.**

-CRBS Invited Speakers Seminars: The CRBS student council invited two speakers (Assistant Professor Lorena Saelices of UT Southwestern, and Professor Tarun Kapoor of The Rockefeller University) to present on their research over an online seminar format. There was one seminar for each semester, with attendance of ~25 and ~60, respectively. These seminars were designed to stimulate discussion on research that is related to CRBS themes, but not found at McGill. Additionally, it provided an opportunity for trainees to interact with professors from outside of Canada. See announcements in **Appendix 4.**

-CRBS Research Showcase: The CRBS student council held the innagural online research showcase event for McGill undergraduate students in March 2022. The event was focused on introducing undergraduate students to research being done by CRBS trainees, showcasing common research themes within the CRBS. The event was held online, where CRBS trainees each had 3-5 minute lightning round sessions to highlight their research to undergraduate students at McGill. After the lightning round sessions, undergraduate students had an opportunity to gain more insight into CRBS research, and graduate research, at McGill. The graduate trainee to undergraduate ratio was 2:1. Overall turnout was ~10 people. See annoucement in **Appendix 5.**

-CRBS Professional Workshops: The CRBS Student Council has organized a series of professional workshops, which will be given online by Dr. Chris Corkery, the Technology Transfer Manager at McGill University. Topics for these workshops are manuscript preparation, poster presentation, and scientific presentations, and they will be held once a month for most of Winter/Summer semester. These professional workshops are designed to help trainees improve skills outside of the lab. See schedule in **Appendix 6.**

-CRBS Social Events: Three inperson social events were scheduled once a month from October to December of 2021. The first event was a scientific networking/mixer, while the other two events were meet and greets between CRBS members. These events were a great opportunity for trainees to network and interact with each other, in both formal and informal settings. For these events, the average inperson attendance was ~15 people. An additional social event occurred online in Winter semester, where the CRBS student council held a games night. Attendance for this event was 5 people. See announcements in **Appendix 7**.

-Bench to Bedside events: 2 events held via Zoom **Appendix 8.**

April 22 2021: Ion channels and personalized medicine

April 19 2022: Focus on infectious diseases

-Bench to Business event: 1 event held via Zoom **Appendix 9.**

October 25 2021: From Laboratory Discovery to Big Pharma and back

-Virtual discovery day: held on Zoom on December 1 2021 **Appendix 10.**

-Radio interview: JF Trempe was interviewed and asked to comment on Alphafold on the Radio-Canada science show "Les Années Lumière".

Rattrapage du 1 août : Une possible révolution en biologie structurale, et la science dans l'assiette des athlètes (radio-canada.ca)

-Media interviews: Many members have been interviewed about structural biology research, for example:

https://www.manilatimes.net/2022/04/10/business/sunday-business-it/scientists-work-to-unlock-biological-machines/1839482

https://www.mcgill.ca/medhealthsci/channels/news/how-bacteria-create-piggy-bank-lean-times-334147

https://www.lightsource.ca/public/news/2021-22-q4-jan-march/creating-an-arsenal-of-covid-19-therapeutics.php

-Collaborations with other units: coordinate and co-hosts a virtual information seminar with QLS (November 23, 2021)

-Communications: @crbsmcgill (twitter)

http://crbsmcgill.ca

www.mcgill.ca/lifesciencescomplex/facilities/nmr

https://www.facebook.com/csbscmcgill/?ref=py_c&__xts__

6. **Major training activities** (e.g., summer schools, co-supervision of trainees, practical workshops):

-Summer bootcamps: 3 events held vis Zoom **Appendix 11.**

July 27 2021: Using Native Mass Spectrometry to Investigate Protein Tertiary and Quaternary Structure

August 3 2021: Investigating protein-ligand interactions using NMR

August 10 2021: Introduction to biological computations with Python

-CRBS Studentship award competition 2021-2022: held in the Spring, awards for the period Sept. 1, 2021 – Aug. 31, 2022. 31 applications received, 15 awards given, $10,000 each, for 1 year (5 M.Sc. students, 10 Ph.D. students including 1 co-supervised). The first annual Maximilian Eivaskhani In Memoriam Graduate Scholarship was awarded to Nuwani Weerasinghe, PhD candidate in the McGill Department of Chemistry, for the 2021-2022 academic year.

-DFW 2021: 3 awarded through GPS

TREMPLIN program (FRQS training grant for FRQS research centres): We have proposed a new program to address the career and professional development (CPD) needs of graduate students at our FRQS-funded McGill-affiliated centres (the Research Institute of the MUHC, the Douglas Research Centre, the Lady Davis Institute for Medical and the Centre de recherche en biologie structurale). Together the consortium brings together over 1700 research trainees, affiliated with the McGill University RUISSS, over more than five sites

in the city of Montréal. Student needs will be assessed through various consultations: 1) gathering already available data and literature on graduate CPD needs and 2) collecting quantitative and qualitative data from graduate students at our centres. Analysis and reflection on the acquired data by consortium members will determine how to integrate our four centres in the new program design, starting from currently available infrastructure for CPD at the Desjardins Centre for Advanced Training (DCAT).

So far, we were able to secure the first round of funding from the FRQS ($40,000) to conduct our needs assessment survey among graduate students and postdocs conducted by an external consultant. Following the analysis of available information, the needs assessment and two-day workshops, we will submit the full application (second round) in June 2022.

7. If applicable, **list new members** who joined the Unit in the past 12 months
(indicate: Name, title, full/associate member, affiliation):

-**Mehran Datsmalchi**, Assistant Professor, Full member, Plant Science, Faculty of Agricultural and Environmental Sciences

-**Marc McKee**, Professor, Full member, FMHS, Anatomy and Cell Biology & Faculty of Dental Medicine and Oral Health Sciences

-**Jérôme Waldispühl**, Associate Professor, Full member, School of Computer Science

8. If applicable, **list members who have left the Unit** in the past 12 months
(indicate: Name, title, full/associate member, affiliation):

-**Armando Jardim**, Associate Professor, Full member, Institute of Parasitology, Faculty of Agricultural and Environmental Sciences, has left McGill University

-**Jason Young**, Associate Professor, Full member, FMHS, Biochemistry, sadly passed away in February 2022

10. Explain why continued support from the FMHS is crucial to Unit (½ page max):

-The FMHS support allowed us to leverage funding from FRQS ($500K per year for 5 years, renewable) which leads to numerous CRBS activities but FMHS funding is still crucial for all CRBS activities.
-The letters of support and funding from McGill, with FMHS the biggest supporting body, were mentioned specifically in the review process and were clearly vital for securing this funding. FMHS generously pledged to continue to fund at the $50K level for the duration of the awarded FRQS Centre Grant.
-Specific initiatives that rely on FMHS funding include the Annual CRBS Symposium, intensive bootcamp training programs for students, community outreach and networking events, and essential equipment upgrades and maintenance.
-CRBS and its members will continue to win additional grants and apply for program funding and the FMHS funding is required to support additional activities that make us competitive when applying for other sources of funding.
-CRBS holds competitive opportunities for fellowships, seed funding and infrastructure. We are always unbiased and equal-opportunity or all our members, but as our mandate is structural biology and biophysics for health, FMHS members have been recipients of the majority of this funding.
-We have hired a full time Research Center officer, Kim Munro, who manages CRBS equipment and facilitates biophysical experiments for CRBS members, FMHS scientist and McGill colleagues. We require full funding from FRQS and FMHS to support this.
-Please note that there are exceptionally funds remaining in our Faculty of Medicine Fund at the end of 2021/22 which we rolled over to 2022/23. This is in large part because some of our activities (Bootcamp, CRBS symposium, CRBS seminar series) were held virtually this year at reduced costs, and others (biophysics for all mini-grants for use of infrastructure and consumables) were impractical with the density restrictions at McGill. These roll-over funds will be spent in 2022/23 for compensatory activities fundamental to the CRBS.

-The full funding of $50K as pledged .by FMHS at the time of FRQS grant application is required to continue our operations and research facilitation.

11. Provide suggestions about how the Faculty could do better to support the Unit and research efforts in general (**no page limit but please be specific and unleash your creativity!**)

The CRBS is very grateful for the support of the FMHS.

Any simplification of administration procedures is always welcome.

One of our main goals is to strengthen ties with the medical community. Support to coordinate efforts with other units/groups (both for students and PIs) within the Faculty would be welcome.

We are excited for the Infinity booking platform to be implemented. Thank you for allowing us to participate in that.

Appendix 1

3ème Colloque Annuel du CRBS – 8 novembre 2021
3rd Annual CRBS Symposium - November 8, 2021

CRBS Centre de Recherche en Biologie Structurale

Séance 1 / Session 1 – on Zoom

8h45 Mots d'Ouverture / Opening Words – Martin Schmeing, *CRBS Director, McGill University*

Sous la Présidence de / Session Chair: Susanne Bechstedt, *CRBS Executive member, McGill University*

9h00-9h50 Andrew Carter, *MRC-LMB, Cambridge, UK*
Dynein motors: from axons to axonemes

9h50-10h20 Mehran Dastmalchi, *McGill University*
Leveraging plant metabolic diversity to engineer biosynthetic pathways

10h20-10h35 Thomas McAlear, *McGill University* - Prix Annuel Excellence du FRQ-S 2020-2021
The mitotic spindle protein CKAP2 is a potent microtubule assembly factor

10h35-11h25: Ben Engel, *Helmholtz Zentrum München, Neuherberg, Germany*
Exploring molecular landscapes inside cells with *in situ* cryo-electron tomography

Pause / Break

Séance 2 / Session 2 – on Fourwaves

11h35-12h35 Poster session

Diner / Lunch

Séance 3 / Session 3 – on Zoom

Sous la Présidence de / Session Chair: Natalie Zeytuni, *CRBS co-Associate Director*, *McGill University*

13h05-13h55 Susan Lea, *NCI-CCR, Frederick, USA*
Using protons in the bacterial cytoplasmic membrane

13h55-14h25 Natalie Reznikov, *McGill University*
Multiscale 3D imaging of bone

14h25-14h40 Javier Rodriguez Gonzalez, *McGill University* - Prix Annuel Excellence du FRQ-S 2020-2021
Recruitment and activation of the DNA structure-specific endonuclease Rad1-Rad10

Séance 4/ Session 4 – on Zoom – Two parallel sessions at the same time

<u>Séance 4A/ Session 4A</u>

Sous la Présidence de / Session Chair: Jia Yin Xiao, *CRBS Student Consortium, McGill University*

14h40-14h55 Shannon Sim, *McGill University*
The role of γ-tubulin phosphorylation in the kinesin-5 dependent organization of spindle microtubules

14h55-15h10 Juan Carvajal, *McGill University*
A RNA-ligand docking study to improve the prediction of molecular fingerprints - RNAmigos study case

15h10-15h25 **Yeganeh Habibi, *McGill University***
Exploring the effects of substrate post-translational modification on the structural dynamics of a lanthipeptide synthetase

15h25-15h40 **Francis Noël, *Laval University***
The membrane interaction of the S100A16 protein studying with the Langmuir monolayer model and biomolecular modeling

Séance 4B/ Session 4B

Sous la Présidence de / Session Chair: Madeline Shred, *CRBS Student Consortium, McGill University*

14h40-14h55 **Mélanie Côté-Cyr, *Université du Québec à Montréal***
Guiding the self-assembly of the protein flagellin into immunostimulatory nanoring structures as antigen delivery system

14h55-15h10 **Armando Palacios, *McGill University***
Machine learning techniques allow direct visualization of complex maturation steps in the ribosome assembly process

15h10-15h25 **Corbin Black, *McGill University***
Structure of the ciliary outer junction

15h25-15h40 **Ismael Abu-Baker, *McGill University***
Highly organized arrays of gold nanorings assembled on tobacco mosaic virus coat protein

Pause / Break

Séance 5/ Session 5 – on Fourwaves

15h50-16h50 **Poster session**

Séance 6 / Session 6 – on Zoom

16h50-17h00 **Présentation des Prix & Remerciements / Présentation of Awards & Closing Words**
Khanh Huy Bui, *CRBS Executive member, McGill University*

Meet the exhibitors on Fourwaves: 11h35-12h35 and 15h50-16h50

Appendix 2

Centre de Recherche en Biologie Structurale
2021-2021 Seminar Series

2nd and 4th Friday of every month.
The seminars are held virtually (via ZOOM)
The meeting link will be provided on the day of presentation
12.30pm – 1.30pm

Date	Speaker	Lab
September 10	Jacklyn Vogel	Jacklyn Vogel
September 24	Yeganeh Habibi	Christopher Thibodeaux
	Sebastian Morales	Paul Wiseman
October 8	Sofia Cruz Tetlalmatzi	Gary Brouhard
	Rayan Fakih	Kalle Gehring
October 22	Armando Palacios	Joaquin Ortega
	Micaela Belleperche	Maureen McKeague
November 12	Daniel Buss	Natalie Reznikov
	Katherine Morelli	Jackie Vogel
November 26	Olivia Kovecses	Maureen McKeague
	Anshu Saran	Natalie Zeytuni
December 10	Lauralicia Sacre	Alba Guarné
	Jingyu Sun	Joaquin Ortega
January 14	Daniel Beaudet	Adam Hendricks
	Halle Barber	Masad Damha
January 28	Anna Clouvel	Allen Ehrlicher
	Shannon Sim	Jackie Vogel
February 11	Annie Shao	Chris Thibodeaux
	Ashkan Karimi	Nathan Luedtke
February 25	Claire Edrington	Gary Brouhard
	Angelos Pistofidis	Martin Schmeing
March 25	Harry McFarlane	Mike Strauss
April 8	Peter Yang	Alba Guarné
	Nuwani Weerasinghe	Chris Thibodeaux
April 22	Julia McCain	Gonzalo Cosa

Centre de Recherche en Biologie Structurale
2021-2022 Methods Seminar Series

Appendix 3

3rd Friday of every month.
The seminars are held virtually (via ZOOM)

Date	Speaker	Topic
March 11	Mohini Ramkaran	Atomic Force Microscopy
April 1	Andrew Bayne	Proteomics
May 27	Jorge Eduardo Ramos Sanchez	Single Molecule Fluorescence

CRBS

Appendix 4

Special Seminar Announcement

Deciphering the structures of amyloid fibrils to design therapeutic and diagnostic tools

Lorena Saelices, PhD.
Assistant Professor
Department of Biophysics
UT Southwestern

Amyloid diseases, such as transthyretin amyloidosis, are caused by the accumulation of fibrils in tissues leading to organ failure and death. These fibrils are made of proteins that self-associate forming beta-rich structures that are resilient to degradation and clearance. Possibly related to this feature, amyloid diseases are cureless. Moreover, current treatments show limited effects at the late stages of the disease, which is when patients are often diagnosed. In our laboratory, we study the structures of amyloid fibrils using cryogenic electron microscopy and crystallography and use this information to design therapeutic molecules for late disease stages and design diagnostic tools for early detection. We have developed peptides that block fibril polymerization of transthyretin in vitro, in flies, and patient samples. Our results indicate that our peptides can hinder amyloid seeding, which is the proposed mechanism that drives disease progression at late stages. Additionally, we are currently designing peptide probes for the detection of transthyretin fibrils in patient samples. Our peptide-based tools may represent novel avenues for the early diagnosis of transthyretin amyloidosis and its treatment at late stages.

Thursday, Dec. 9th, 2021
3:30 pm EST, via ZOOM

Link: https://bit.ly/30bAkJO
Meeting ID: 831 6940 7865
Passcode: CRBS2021

CRBS

Special Seminar Announcement

Chemical biology of drug resistance

Tarun Kapoor, PhD.
The Pels Family Professor
The Rockefeller University

I will discuss how the analysis of resistance, which is generally considered to be a limitation of molecularly targeted therapeutics, can be leveraged to address major challenges in chemical biology. First, characterizing chemotype-specific resistance can help deconvolve a chemical inhibitor's mechanism of action in human cells and achieve 'gold standard' validation of its direct target, i.e. when a silent mutation in the target suppresses drug activity in cell-based and biochemical assays. Second, examining resistance can help with the use of chemical inhibitors as probes of cellular mechanisms. In particular, phenotypes due to target inhibition can be identified as those observed in wildtype cells, across a range of inhibitor concentrations, but not in matched cells with a silent resistant-conferring mutation in the target. Finally, I will highlight our recent efforts to design new chemical inhibitors for AAA+ (ATPases associated with diverse cellular activities) proteins. Our approach, named RADD (Resistance Analysis During Design), involves testing selected chemical scaffolds against constructs with engineered silent mutations. Identifying mutations that confer resistance lead to robust inhibitor-target binding models that guide improvements in inhibitor potency and selectivity. These data can also help develop chemical strategies to overcome or delay the emergence of resistance.

Wednesday, Feb. 2nd, 2022
12:30 pm EST, via ZOOM

Zoom Link:
https://mcgill.zoom.us/j/81472776630?pwd=bFJVeGVoWjU0VXpPWTFUeHRFcW15Zz09

Meeting ID: 814 7277 6630
Passcode: CRBS2022

Appendix 5

CRBS Centre de recherche en biologie structurale

Undergraduate Introduction to Research in Structural Biology

March 1st, 2022 @ 12:30pm

Join graduate students on Zoom for a lightning round style event discussing their research in the **CRBS** (Center for Structural Biology Research), and a chance to connect with structural biology researchers at McGill! Research performed by CRBS members is centered around applications in health and disease.

Undergraduate students can register at:

https://docs.google.com/forms/d/e/1FAIpQLSf2dsrJQdcW5-UA1UMs89jW6cpoWcWCAecJUkOYHHEyB7nH_A/viewform

McGill

Fonds de recherche Santé Québec

Centre de Recherche en Biologie Structurale
2021-2022 Professional Workshops

Appendix 6

Date	Speaker	Topic
January 21	Dr. Chris Corkery	Manuscript Preparation
April 29	Dr. Chris Corkery	Poster Presentations
May 20	Dr. Chris Corkery	Scientific Presentations

CRBS Centre de Recherche en Biologie Structurale

PROFESSIONAL DEVELOPMENT WORKSHOP

Manuscript Preparation

Chris Corkery, PhD

Chris is a Technology Transfer manager in the Office of Innovation and Partnerships. He earned a certificate in graduate education from Western University in 2011 and has taught at McGill since 2012. His courses focus on research project management and technical writing for graduate students. He runs workshops or seminars on research communication (poster and oral presentations, manuscript or grant writing) and anything related to patents and intellectual property management.

Friday, Jan 21st, 2022.
12:00 - 1:00 pm, Via ZOOM

Meeting Link: bit.ly/3qbDszN
Meeting ID: 891 8733 8478
Passcode: CRBS2022

CRBS Centre de Recherche en Biologie Structurale

Professional Development Workshop

Poster Presentations

Dr. Chris Corkery

Technology Transfer Manager

Office of Innovation and Partnerships

In many fields, the poster presentation is a key form of scholarly communication. Well-conceived posters present research findings effectively and launch conversations with fellow scholars and future collaborators. Attend this seminar to help you optimize your poster presentations for scholarly conferences and be prepared for the conversations your posters will invoke.

Friday, April 29th, 2022, 12 -1 pm

mcgill.zoom.us/j/87221394725?pwd=ODdiR2wwUoxzcnUxUGxXdGovN3FRQT09

Meeting ID: 872 2139 4725
Passcode: CRBS2021

CRBS Centre de Recherche en Biologie Structurale

Appendix 7

NETWORKING EVENT ANNOUCEMENT

CRBS Graduate Students Scientific Networking Event

Pizza will be available.
Bring your own drinks, blanket and jacket.

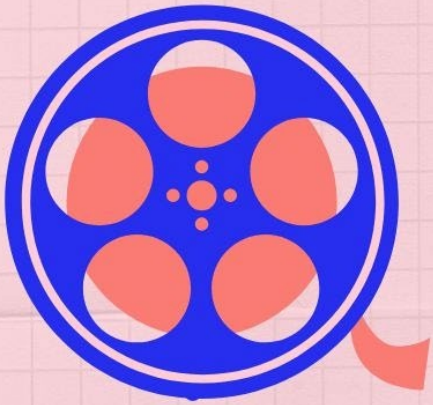
Friday, Oct 1st, 2021.
5:00 - 7:30 pm, Jeanne-Mance Parc.
Meetup at Monument a Sir George-Etienne Cartier and proceed to seating in Jeanne-Mance Parc.

Subject: CRBS Social Announcement Friday Nov 5th 6PM @ Thomson House
Date: Monday, October 25, 2021 at 6:45:36 PM Eastern Daylight Time
From: Hedi Zhou

Dear all,
Congratulations on finishing the first two months of back on campus. Some of CRBS student council members will come together to have some food and drinks on Friday Nov 5th, 6PM, in Thomson House. Feel free to drop by or bring friends to Thomson house.

Please note this is more of a casual event, and not a formal networking event. VaxiCode, piece of ID and McGill student card is required by Thomson house.

Best,
CRBS Student Council



CRBS
STUDENT
COUNCIL
PRESENTS

MOVIE NIGHT

Dec 3rd, 2021
5:00-8:30PM
Room 230 Bellini Life
Sciences Complex

Appendix 8

CRBS Bench-to-Bedside online workshop
April 22nd 2021, 10:00am-noon
Ion channels and personalized medicine.

Dear colleagues,

The *Centre de Recherche en Biologie Structurale* (CRBS) is proud to announce the second event of the CRBS Bench-to-Bedside workshop series. This initiative seeks to bring awareness of the power of structural biology to the greater biomedical community, as well as to foster collaborations between clinicians and basic scientists.

The event, titled "**Ion channels and personalized medicine**", will take place online via Zoom on **April 22nd 2021 from 10:00 to noon**. First, **Dr. Derek Bowie** *(McGill University, Canada)* will give an introduction of ion channel families and how they give insight into understanding complex diseases. Then **Dr. David Bennett** *(University of Oxford, UK)* will focus on the diagnosis and clinical outcomes of mutations in Nav channels with therapeutic avenues. Finally, **Dr. Steve Traynelis** *(Emory University School of Medicine, USA)* will discuss the translational potential of studying point mutations in NMDA-type ionotropic glutamate receptors towards personalized medicine. The presentations will be followed by a panel discussion with the speakers and CRBS members Jean-François Trempe and Gergely Lukacs.

Program:

10:00 – 10:15	Introduction – Dr. Derek Bowie Title: Introduction to ion channel structure and function
10:15 – 10:30	Guest speaker, Dr. David Bennett Title: Human Pain Channelopathies
10:30 – 11:00	Guest speaker, Dr. Steve Traynelis Title: Insight into the glutamate receptor function provided by genetic variation
11:00 – 11:30	Panel Discussion with Dr. Jean-François Trempe and Dr. Gergely Lukacs
11:30 – 11:35	Conclusion

Registration: https://forms.gle/PACfWHq4sYBUuhGMA

Zoom link:
https://mcgill.zoom.us/j/5150839283?pwd=OHd3M0hMQlVyblE2ZGZNaXc5SGJCUT09
Meeting ID: 515 083 9283
Passcode: CRBS2021

Finally, we would like to ask all of you to **distribute this invitation** to whoever you think could be or **SHOULD be involved** in this initiative, or just wants to listen in. If you know a clinician scientist whose work could benefit from structural biology, or conversely if you know a structural biologist who seeks greater interactions with clinicians, please invite them!

We are looking forward to seeing you at the event and hope many participate!

The CRBS Outreach committee:
Jean-François Trempe (CRBS Outreach committee)
Susanne Bechstedt (CRBS Outreach committee)
Annick Guyot (CRBS coordinator)

CRBS Bench-to-bedside workshop

***Focus on Infectious Diseases* – April 19th 2022, 14:00-16:00**

Please register and submit your questions/ideas before April 15th:

https://forms.gle/eHYPLtDhqCtc2Dor5

Zoom link:
https://mcgill.zoom.us/j/81555995697 (password CRBS2022)

Guest speakers:

Dr Dao Nguyen
Dept of Microbiology and Immunology
Research Institute of the McGill University Health Centre

Dr Bastien Castagner
Dept of Pharmacology & Therapeutics
McGill University

Dr Fernando Lopes
Institute of Parasitology
McDonald Campus, McGill University

Program:

14:00 – 14:05	Opening words - Jean-François Trempe
14:05 – 14:30	Dao Nguyen, RI-MUHC, Microbiology & Immunology Title: *Tacking difficult respiratory infections: from bacteria to patients*
14:35 – 15:00	Bastien Castagner, McGill Pharmacology & Therapeutics Title: *Disarming Clostridioides difficile: the therapeutic potential of inositol phosphate analogues*
15:05 – 15:30	Fernando Lopes, McGill Institute of Parasitology Title: *Tolerogenic Properties of Helminth-Derived Metabolites*
15:35 – 16:00	Panel Discussion, chaired by Jean-François Trempe With Drs Nguyen, Castagner, Lopes

CRBS Bench-to-Bedside online workshop
Focus on infectious diseases
April 19th 2022, 14:00-16:00

Dear colleagues,

The *Centre de Recherche en Biologie Structurale* (CRBS) is proud to announce our next CRBS Bench-to-Bedside workshop titled "**Focus on infectious diseases**". It will take place online via Zoom on **April 19th 2022 from 14:00 to 16:00**. The COVID-19 pandemic brought to the forefront the importance of investigating infectious diseases. Yet, while COVID has received much attention in the last two years, other infectious diseases remain prevalent and disproportionally affect vulnerable populations. Here, we will have presentations by researchers that are at the crossroad of basic and clinical research in infectious diseases. **Dr Dao Nguyen** will tell us about bacteria responsible for airway infections, from a clinical point of view. Then **Dr Bastien Castagner** will show how protein structure and chemistry can inform design of novel therapeutics avenues for treating *C. difficile* infections. Finally, **Dr Fernando Lopes** will explain how worm infections affect the immune system of their hosts. The presentations will be followed by a panel discussion with the speakers and CRBS members.

Program:

14:00 – 14:05	Opening words - Jean-François Trempe
14:05 – 14:30	Dao Nguyen, RI-MUHC, Microbiology & Immunology Title: *Tacking difficult respiratory infections: from bacteria to patients*
14:35 – 15:00	Bastien Castagner, McGill Pharmacology & Therapeutics Title: *Disarming Clostridioides difficile: the therapeutic potential of inositol phosphate analogues*
15:05 – 15:30	Fernando Lopes, McGill Institute of Parasitology Title: *Tolerogenic Properties of Helminth-Derived Metabolites*
15:35 – 16:00	Panel Discussion, chaired by Jean-François Trempe With Dr Nguyen, Castagner, Lopes

Registration: https://forms.gle/eHYPLtDhqCtc2Dor5

Zoom link:
https://mcgill.zoom.us/j/81555995697
Meeting ID: 815 5599 5697
Passcode: CRBS2022

This initiative seeks to bring awareness of the power of structural biology to the greater biomedical community, as well as to foster collaborations between clinicians and basic scientists. Thus, **please distribute this invitation** to anyone you think could be interested or should be involved in this initiative. If you know a clinician scientist whose work could benefit from structural biology, or conversely if you know a structural biologist who seeks greater interactions with clinicians, please invite them! Also, when you register, please submit questions for our panellists (see examples below).

We are looking forward to seeing you at the event and hope many participate!

The CRBS Outreach committee:
Jean-François Trempe (CRBS member, Event chair)
Susanne Bechstedt (CRBS Outreach committee)
Annick Guyot (CRBS coordinator)

Panel discussion questions - examples

1- How can structural biology and biophysics guide our understanding of host-pathogen interactions?

2- Can we use protein structures to fight emergence of drug resistance in bacteria?

Appendix 9

CRBS Bench-to-Business online workshop
October 25th 2021, 11:00am-1:00pm
From Laboratory Discovery to Big Pharma and back

Dear colleagues,

The *Centre de Recherche en Biologie Structurale* (CRBS) is proud to announce the inaugural event of the CRBS Bench-to-Business workshop series. This initiative seeks to bring awareness of the power of structural biology to the greater biomedical community, as well as to foster collaborations between scientists, clinicians and industry.

The event, titled "**From Laboratory Discovery to Big Pharma and back**", will take place online via Zoom on **October 25th 2021 from 11:00am to 1:00pm**. First, **Dr. Youla Tsantrizos** *(Professor, Chemistry Department, McGill University, Canada)* will give a talk on the role of structural research in drug discovery. Then **Dr. Uwe Schoenbeck** *(Senior Vice President, Chief Scientific Officer, Emerging Science and Innovation, Worldwide Research, Development, and Medical, Pfizer, USA)* will focus on recent developments from Pfizer. The presentations will be followed by discussion with the speakers.

Program:

11:00 – 11:05	Introduction: Dr. Susanne Bechstedt
11:05 – 11:50	**Dr. Youla Tsantrizos** Seminar Title: ***Discovery of Thienopyrimidine-Based Bisphosphonates with a Novel Mechanism of Action and Antimyeloma Activity in Vivo***
11:50 – 12:00	Questions & Discussion
12:00 – 12:45	**Dr. Uwe Schoenbeck** Seminar Title: ***Breakthrough Therapies enabled through Partnerships***
12:45 – 12:55	Questions & Discussion
12:55 – 13:00	Conclusion: Dr. Susanne Bechstedt

Registration: https://forms.gle/WBit7N1dtSS4vRm59

Zoom link:
https://mcgill.zoom.us/j/85248038900?pwd=elJvMW9mbi9Fem9kZ1ZxcnlweHN5UT09
Meeting ID: 852 4803 8900
Passcode: CRBS2021

Finally, we would like to ask all of you to **distribute this invitation** to whoever you think could be or **SHOULD be involved** in this initiative, or just wants to listen in.

We are looking forward to seeing you at the event and hope many participate!

The CRBS Outreach committee:
Susanne Bechstedt (CRBS Outreach committee)
Jean-François Trempe (CRBS Outreach committee)
Annick Guyot (CRBS coordinator)

Canadian Medical Hall of Fame
Discovery Days in HEALTH SCIENCES

Temple de la renommée médicale canadienne
Journées Découvertes en SCIENCES DE LA SANTÉ

Proudly presented by
Fièrement présenté par
MD Financial Management
Gestion financière MD

2021 Evaluation Report

McGill University and The Neuro – December 1, 2021

Appendix 10

Results indicate that Discovery Days prime youth for a career in the health sciences

A total of 149 students and teachers participated in this year's event. Of those who completed our evaluation survey, we learned that:

99% would **recommend** Discovery Day to another student or teacher
84% stated that Discovery Day **exceeded** or **fully met** their expectations
96% rated their interactive workshops **valuable**
96% felt that the career panel was **valuable**

When we compared students' beliefs and attitudes towards a career in the health sciences before and after Discovery Day, we learned that:

82% expressed an increase or the same level of **interest**
74% expressed an increase or the same level of **excitement**
88% expressed an increase or the same level of **knowledge**
81% were more or equally as certain about their **future plans**

Once again, Discovery Day received terrific feedback from the participants. Our favourite comments include:

'I loved learning everything and being able to interact with pros. It was very fun and I am happy I was able to participate."

'I am glad I was given the opportunity to attend this event. I feel more knowledgeable and aware of what I want to do and how I will get there. I have learned from our speakers to deal with life obstacles and accept failure in order to continue along my path despite the ups and downs."

'Incredible group of speakers. Great timing for me to attend."

'I entered this event thinking it would be a very mild experience, little did I know all of my unconscious questions were being answered without even needing to ask for a rephrase. This experience overall was amazing, and I learned many things that will definitely stay with me for a lifetime. Thank you for this unforgettable experience!"

What participants told us about your workshop...

A09 - Biomedical Sciences: What Can Proteins at the nanoscale tell us about health and diseases?

Low				High		
1	**2**	**3**	**4**	**5**	**N/A**	**Total**
0	3	2	4	5	0	14
0.0%	21.4%	14.3%	28.6%	35.7%		

- Very informative and interesting
- Learned a lot and was very interesting.
- It was so interesting when he was showing the molecules in 3D.
- I liked the presentation and the models that they used to show the protein structures. I also liked the video of what happens during a lab and the different types of people like the professors and undergrads. It was also nice that they got to teach us a little bit and I felt like I learned more from them.
- Well set-up, just not a topic I would want to pursue. Also there was not enough interactive "stuff" and it made the presentation feel longer than it was.
- My connection was very bad, so I missed a bunch of it, but from what I saw it was pretty interesting. We are learning about this in my biology class at school.
- We talked about many different diseases and how they affect the human body which was very fascinating to me. This panel really helped me grasp the basics and confirmed my interest in biomedical science.

CRBS Centre de Recherche en Biologie Structurale

Appendix 11

The McGill *Centre de Recherche en Biologie Structurale* (CRBS) is pleased to announce another round of Structural Biology Boot Camps for the Summer of 2021.

These short (half-day), intensive courses are free of charge, and will familiarize attendees with the cutting-edge biophysical tools and computational approaches being conducted by researchers at the CRBS to investigate the frontiers of structural biology. Courses will be led by CRBS researchers, who will cover both theoretical and practical aspects of biophysical and computational approaches to problems in structural biology. The 2021 courses will all be held remotely as Zoom meetings (hopefully for the last time!), but future iterations of the CRBS Structural Biology Boot Camps will include practical components as well as live, hands-on demonstrations. The 2021 CRBS Structural Biology Boot Camps are:

Using Native Mass Spectrometry to Investigate Protein Tertiary and Quaternary Structure
Instructor: Christopher Thibodeaux
Date: Tuesday, July 27, 2021
Time: 1 – 4 PM

Investigating protein-ligand interactions using NMR
Instructors: Jean-Francois Trempe & Tara Sprules
Date: Tuesday, August 3, 2021
Time: 1 – 4PM

Introduction to Biological Computations with Python
Instructor: Juan Carvajal
Date: Tuesday, August 10, 2021
Time: 1 – 4 PM

Registration for the 2021 Boot Camps is ***free*** at the following link: https://forms.gle/CjTa3zSkrfjWrJ1u9
Prior to your course, you will be e-mailed a Zoom invitation to the course, as well as access to any materials you may need to get the most out of your Boot Camp.

We look forward to seeing you at the Boot Camps and please don't hesitate to contact us at csb.med@mcgill.ca if you have any questions.

Best Wishes,
Christopher Thibodeaux & Natalie Zeytuni
Co-chairs, CRBS Training and Awards Committee

CRBS Summer Bootcamp

Using Native Mass Spectrometry to Investigate Protein Tertiary and Quaternary Structure

Instructor: Christopher Thibodeaux
Date: Tuesday, July 27, 2021
Time: 1 – 4 PM

https://mcgill.zoom.us/j/87083468891

This bootcamp will cover the theoretical and practical aspects of conducting mass spectrometry experiments on natively folded proteins to investigate tertiary/quaternary structure and ligand binding interactions. The seminar will consist of four sections:

1. Native MS basics: What is native MS and what is the theoretical basis for maintaining proteins in a natively folded state in gas phase MS experiments? What are the experimental requirements for conducting native MS experiments? How do you know that your protein is natively folded in the gas phase?
2. Practical aspects for (cheaply!!!) preparing native MS experiments: How to make nanospray ESI emitters, how to prepare protein samples for native MS analysis, how to load protein samples into emitters and onto the MS.
3. Live (virtual) demo illustrating how to tune the MS instrument to maintain native structure in the gas phase. The demo will take place on a Waters Synapt G2-Si ion mobility mass spec (the most popular model for performing native MS experiments).
4. (Time permitting) Examples from the literature where native MS has been used to characterize ligand binding, protein conformational changes, determine binding equilibria, study allostery, and investigate quaternary structure.

The session will take about 2 hours, but it may overflow to 3 hours depending on how many questions we get. **Feel free to interrupt at any time during the seminar if you have questions!!**

A recording of the tutorial will be made freely available to those who registered for the Bootcamp.

Looking forward to seeing you on July 27!
Chris Thibodeaux

CRBS Summer Bootcamp

Investigating protein-ligand interactions using NMR

Instructors: Jean-François Trempe and Tara Sprules
Date: Tuesday, August 3, 2021
Time: 1 – 4 PM

Join Zoom Meeting
https://mcgill.zoom.us/j/82228892810?pwd=YWdIWkxkOC9RUzEyMkkyb0c5WWhhZz09
Meeting ID: 822 2889 2810
Passcode: 608266

In this boot camp seminar, we will introduce basic concepts of NMR spectroscopy that relate specifically to the study of protein-ligand interactions. The tutorial will concentrate on practical aspects, from sample preparation to data acquisition and interpretation. We will cover the following specific topics: 1) 1D NMR and chemical shifts, 2) Relaxation and linewidths, 3) saturation-transfer difference and WATER-LOGSY methods, 4) Kd determination, 5) 2D NMR and HSQC, and 6) ZZ-exchange method for interface mapping.

The session will take about 2 hours, but it may overflow to 3 hours depending on how many questions we get.

A recording of the tutorial will be made freely available to those who registered for the Bootcamp.

Looking forward to seeing you!

Jean-François & Tara

CRBS Summer Bootcamp

Introduction to biological computations with Python

Instructor: Juan Guillermo Carvajal Patiño
Date: Tuesday, August 10, 2021
Time: 1 – 4 PM

https://mcgill.zoom.us/j/88007897680?pwd=SFlmd3R0U0ZmUTBhTWk5c2NnQ1RoQT09
Meeting ID: 880 0789 7680
Passcode: CRBS2021

In this boot camp seminar, you will learn the basics of Python programming language and after it you will be able to perform some biological computations. The tutorial will focus on 1) the Python interpreter, 2) Python virtual environment, 3) control flow structures, 4) main data structures, 5) input and output, 6) Open Babel to the interconversion of chemical data from one format to another, and 7) Biopython to perform some for biological computation.

The session will take about 2 hours, but it may overflow to 3 hours depending on how many questions we get.

A recording of the tutorial will be made freely available to those who registered for the Bootcamp.

Looking forward to seeing you!

Juan Carvajal