STEVEN R. LAPLANTE, PH.D.

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PROFILE

Senior biophysical medicinal chemist and professor with +25 years of drug discovery experience in the pharmaceutical industry and in academia. Proven track record of creating innovative solutions to chemical and biological challenges. A skilled team-leader in interdisciplinary strategic planning and research. Effective collaborator and communicator.

- NMR specialist with applications of X-ray crystallography and molecular modeling.
- Developed novel strategies that led to discoveries of many drug candidates (HIV, HCV).
- Key inventor of advanced drugs for treating hepatitis C infection (Deleobuvir, Faldaprevir and Ciluprevir).
- Developed novel strategies for fragment-, structure- and property-based drug discovery.
- Discovered the phenomenon of drug self-assemblies (nano-entities), and currently exploring its implications for nano-biotechnology.
- Budgeted and managed NMR facility and many research projects.
- Forward interests: Discovering drugs, exposing drug aggregates or nano-entities, and exploiting nano-properties for novel discovery strategies. Also, monitoring nano-particles with regards to toxicology, along with elucidating metabolites, promoting atropisomer chirality, and understanding effects of climate change.
- Citations of my publications 5078, h-index 32 (Google Scholar)

EMPLOYMENT AND EDUCATION

Employment:

- University of Québec, INRS (Board of Directors) 2017-2020
- Drug Discovery Network
  - Founder 2019-date
- University of Québec, INRS-IAF (Associate Professor) 2015-date
- Harvard University (Fragment Screening, Consultant and Collaborator) 2014-date
- Broad Institute (Visiting Scientist) 2014-date
- NMX Research and Solutions Inc.
  - Founder 2014-date
  - President (website: nmxresearch.com) 2014-2015
- Boehringer Ingelheim (Canada) Ltd., Top 15 Pharmaceutical Company. 1991–2013
  - Senior Research Scientist, NMR Spectroscopy, Structural Research, Drug Design.
- University René Descartes, France, Government-based National Center for Scientific Research (CNRS). Research Scientist (CR2), tenured position. 1990-1991

Education:

- Postdoctorate – CNRS and Ecole Polytechnique, France. 1988-1990
- Ph.D. Syracuse University, USA, Biophysics (Chemistry, Biology, Physics) 1983-1988
- B.A. - State University of New York, Potsdam, USA, Chemistry and Biology. 1979-1983

EXPERIENCE AND KEY EXPERTISE

Experienced in fragment-, structure- and property-based drug design:

- Designed many compounds that target viruses: HIV,HCV,HCMV,HRV,RSV.
- Discovered inhibitors of proteases, polymerases, helicases & protein-protein interactions
- Implicated in a variety of areas of drug discovery and development:
  - Fragment, substrate and high-throughput screening.

- Lead identification (hit validation, triaging for quality ligands).
- Lead optimization (potency, physicochemical properties, metabolite ID, tox predictions).
- Peptide-based drug design and macrocycles

Designed novel strategies that led to drugs:
- Created new NMR methods to detect ligand binding to targets.
- Screened substrate-based compounds for lead identification.
- Optimized potency via structure- and dynamics-based drug design.
- Identified new lead series via torsion angle rigidifications and scaffold hopping.
- Developed hit triaging methods for eliminating false-positives and promoting quality leads.
- Implemented rapid metabolite ID methods using ^{1}H and ^{19}F NMR techniques.
- Quantified drug entities (single molecules, aggregates, precipitates) and impurities by NMR.
- Implemented robust methods to distinguish N- vs. O-alkylations and synthetic regioisomers.
- Elucidated primary structures of compounds (complete and high-throughput).
- Predicted drug promiscuity and toxicity by NMR.
- Designed a cooling system for computer clusters for virtual screening.

Discovered and exploited unusual drug properties:
- Discovered drug self-aggregation properties that affect most levels of R&D.
- Correlated aggregation with off-target promiscuity and toxicity – used as a prediction tool.
- Identified avenues for detecting, avoiding and exploiting various aggregation properties.
- Uncovered atropisomer axial chirality properties of compounds.
- Implemented industry-wide classification schemes with the US FDA for dealing with atropisomerism at the discovery and development stages.
- Discovered new drug candidates via exploitation of atropisomeric properties.
- Deciphered various types of chemical and conformational exchange phenomena.

Budgeted, implemented and managed NMR facility and research projects:
- INRS: NSERC Discovery and CFI grants awarded.
- Established and managed NMR analytical and computational facility: 700, 600 and two 400 MHz spectrometers, Linux computer clusters, microTOF-Q II MS, SPE, and LC.
- Managed production, isolation and MS-NMR characterization of drug metabolites.
- Analyzed primary structures of numerous organic molecules and metabolites.
- Collaborated with ACD to develop semi-automated structure determinations.
- Implemented high-throughput structure verifications of compound libraries.
- Coordinated research projects and collaborations.
  - Corporate BI projects: Canada, USA and Europe.
  - External projects: Univ. Montreal, NRC-BRI, ACD, Bruker, Harvard Univ., McGill Univ.
- Extensive experience in budgeting and securing funding for new equipment and operating costs (>$4 million in new equipment and >$300,000 in yearly operating funding).

LANGUAGES AND CITIZENSHIPS

- **Languages:** English and French. **Citizenships:** USA and CANADA.

RESEARCH PAPERS, REVIEWS & PATENTS

1. Protocol for probing the free-state solution behavior of drugs and their tendencies to self-associate into nano-entities, **LaPlante, S.R.**; Roux, V.; Shahout, F.; Laplante, G.; Woo, S.; Ayotte, Y.; Denk, M.; Larda, S.T., Nature Protocols, **2021 (in press)**
2. Sodium Tetraphenylborate Displays Selective Bactericidal Activity against Neisseria meningitidis and N. gonorrhoeae and Is Effective at Reducing Bacterial Infection Load. Bernet E, Lebughe M, Vincent AT, Haghdoost MM, Golbaghi G, **LaPlante S**, Castonguay A, Veyrier FJ.
   Antimicrob Agents Chemother. **2021** Jan 20;65(2)

3. Development of LM98, a Small-Molecule TEAD Inhibitor Derived from Flufenamic Acid. Mélin L, Abdullayev S, Fnaiche A, Vu V, González Suárez N, Zeng H, Szewczyk MM, Li F, Senisterra G, Allali-Hassani A, Chau I, Dong A, Woo S, Annabi B, Halabelian L, **LaPlante SR**, Vedadi M, Barsyte-Lovejoy D, Santhakumar V, Gagnon A.
   ChemMedChem. **2021** Jun 23. doi: 10.1002/cmdc.202100432.
4. Searching for potential drugs against SARS-CoV-2 through virtual screening on several molecular targets. Almeida JSFD, Botelho FD, de Souza FR, Dos Santos MC, Goncalves ADS, Rodrigues RLB, Cardozo M, Kitagawa DAS, Vieira LA, Silva RSF, Cavalcante SFA, Bastos LDC, Nogueira MOT, de Santana PIR, Brum JOC, Nepovimova E, Kuca K, **LaPlante SR**, Galante EBF, Franca TCC.
   J Biomol Struct Dyn. **2021** Jan 8:1-14.
5. Docking and molecular dynamics studies of potential new leads against DBL3x derived from chondroitin sulfate A (CSA): a new approach for the treatment of malaria. Spadeto JPM, Cormanich RA, Franca TCC, **LaPlante SR**, Goncalves AS.
   J Biomol Struct Dyn. 2021 Apr 16:1-10. doi: 10.1080/07391102.2021.1911859.
6. Identification of novel potential ricin inhibitors by virtual screening, molecular docking, molecular dynamics and MM-PBSA calculations: a drug repurposing approach.
   Botelho FD, Santos MC, Gonçalves AS, França TCC, **LaPlante SR**, de Almeida JSFD.
   J Biomol Struct Dyn. **2021** Jan 7:1-11.
7. Fatty acid mimetic PBI-4547 restores metabolic homeostasis via GPR84 in mice with non-alcoholic fatty liver disease, Jean-Christophe Simard, J.C.; Thibodeau, J.F.; Leduc, M.; Tremblay, M.; Laverdure, A.; Sarra-Bournet, F.; Gagnon, W.; Ouboudinar, J.; Gervais, L.; Felton, A.; Letourneau, S.; Geerts, L.; Cloutier, M.P.; Hince, K.; Corpuz, R.; Blais, A.; Marques Quintela, V.; Duceppe, J.-S.; Abbott, S.D.; Blais, A.; Zacharie, B.; Laurin, P.; **LaPlante, S.R**.; Kennedy, C.; Hebert, R.; Leblond, F.A.; Grouix, B. Gagnon, L.
   Scientific Reports, **2020**, 10, 12778. 1-16.
8. Synthesis and biological activity of hydrazones and derivatives: A review, Brum,J.O.C.; França, T.C.C; **LaPlante, S.R**.; Villara,J.D.F.
   Mini Reviews in Medicinal Chemistry, **2020**, 20, 342-368.
9. Reactivation of VX-inhibited human acetylcholinesterase by deprotonated pralidoxime. A complementary quantum mechanical study, Valle da Silva, J.A,; Pereira, A.F.; **LaPlante, S.R.;** Kuca, K.; Ramalho, T.C.; Franca, T.C.C., Biomolecules, **2020**, 10, 192-200.
10. Structure-Thermodynamics-Relationships of Hepatitis C Viral NS3 Protease Inhibitors, Wypych, R.M.; **LaPlante, S.R**.; White, P.W.; Martin, S.F.,
    European Journal of Medicinal Chemistry, **2020**, 192, 112195, 1-9.
11. NMR-based Approaches to the Study of GPCRs and GPCR-ligand Interactions
    Pandey, A.; Larda, S.T.; **LaPlante, S.R.**; Prosser, R.S.
    GPCRs Structure, Function, and Drug Discovery **2020,** 65-80**.**
12. Ligand-Based Virtual Screening, Molecular Docking, Molecular Dynamics, and MM-PBSA Calculations towards the Identification of Potential Novel Ricin Inhibitors. Botelho, F. D., dos Santos, M. C., Goncalves, A. D., Kuca, K., Valis, M., **LaPlante, S. R**., Franca, T. C. C., & de Almeida, J.
    Toxins, **2020**, 12(e746), 1-14.
13. Synthesis and Biological Activity of Hydrazones and Derivatives: A Review. Brum, J. D. C., Franca, T. C. C., **LaPlante, S**., & Villar, J. D. F.
    Mini-Reviews in Medicinal Chemistry, **2020**, 20(5), 342-368.
14. Exposing Small-molecule Nano-entities By An NMR Relaxation Assay
    Ayotte,Y.; Marando,V.M.; Vaillancourt,L.; Bouchard,P.; Heffron,G.; Coote,P.W.; Larda,S.T.; **LaPlante,S.R**.

J. Med. Chem. **2019**, 62, 17, 7885-7896.

15. Revealing Drug Self-Associations Into Nano-entities
Dlim, W.M.; Shahout, F.S.; Khabir, M.K.; Labonté, P.P.**; LaPlante, S.R**.
ACS Omega **2019**, 4, 588919-58925.
16. Synthesis of NSC 106084 and NSC 14778 and evaluation of their DNMT inhibitory activity
Leroy, M; Mélina, l.; **LaPlante, S.R**.; Medina-Franco, J.L.; Gagnon, A.
Bioorganic and Medicinal Chemistry Letter, **2019**, 29, 826-831.
17. Fragment-Based Phenotypic Lead Discovery: Cell-Based Assay to Target Leishmaniasis.
Ayotte Y, Bilodeau F, Descoteaux A, **LaPlante SR.**
ChemMedChem (**2018**) 18;13(14):1377-1386.
18. Revealing dye and dye-drug aggregation into nano-entities using NMR
Murugesan, J.R.; Shahout, F.; Dlim, M.; Langella, M.; Cuadra-Foy, E.; Forgione, P.; **LaPlante, S.R.**
Dyes and Pigments (**2018**) 153, 300-306.
19. NMR strategies to support medicinal chemistry workflows for primary structure determination
Oguadinma, P.; Bilodeau, F.; **LaPlante, S.R.**
Bioorganic & Medicinal Chemistry Letters, (**2017**) 27, 242-247.
20. Resurgence of Phenotypic Screening for Discovering Drug Leads
Ayotte, Y & LaPlante, S.R., EC Microbiology 7.3, **2017**, 80-82.
21. The Rise of Academia-Pharma Partnerships for Discovering New Chemical Matter for Future Drugs, **LaPlante, S**; Bilodeau, F. EC Microbiology 4.5 (**2016**): 756-758.
22. Aligning Potency and Pharmacokinetic Properties for Pyridine-Based NCINIs.
Fader, LD; Bailey, M; Beaulieu, E; Bilodeau, F; Bonneau, P; Bousquet, Y; Carson, RJ; Chabot, C; Coulombe, R; Duan, J; Fenwick, C; Garneau, M; Halmos, T; Jakalian, A; James, C; Kawai, SH; Landry, S; **LaPlante, SR**; Mason, SW; Morin, S; Rioux, N; Simoneau, B; Surprenant, S; Thavonekham, B; Thibeault, C; Trinh, T; Tsantrizos, Y; Tsoung, J; Yoakim, C; Wernic, D
ACS Med Chem Lett. **(2016)** 7(8), 797-801.
23. Multi-parameter optimization of aza-follow-ups to BI 207524, a thumb pocket 1 HCV NS5B polymerase inhibitor. Part 2: Impact of lipophilicity on promiscuity and in vivo toxicity.
Beaulieu, PL; Bolger, G; Deon, D; Duplessis, M; Fazal, G; Gagnon, A; Garneau, M; **LaPlante, S**; Stammers, T; Kukolj, G; Duan, J
Bioorg Med Chem Lett. **(2015)** 25(5),1140-5.
24. Conformation-Based Restrictions and Scaffold Replacements in the Design of HCV Polymerase Inhibitors: Discovery of Deleobuvir (BI 207127)
LaPlante, Steven R.; Bos, Michael; Brochu, Christian; Chabot, Catherine; Coulombe, René; Gillard, James R.; Jakalian, Araz; Poirier, Martin; Rancourt, Jean; Stammers, Timothy; Thavonekham, Bounkham; Beaulieu, Pierre L.; Kukolj, George; Tsantrizos, Youla S.
J. Med. Chem., (**2014**) *57*, 1845-1854. Special HCV therapies issue.
25. Ligand Bioactive Conformation Plays a Critical Role in the Design of Drugs That Target the Hepatitis C Virus NS3 Protease
LaPlante, Steven R.; Nar, Herbert; Lemke, Christopher; Jakalian, Araz; Aubry, Norman; Kawai, Stephen,
J. Med. Chem., (**2014**) *57*, 1777-1789. Special HCV therapies issue.
26. Integrated Strategies for Identifying Leads that Target the NS3 Helicase of the Hepatitis C Virus
LaPlante, Steven R.; Padyana, Anil; Abeywardnae, Asitha; Bonneau, Pierre R; Cartier, Mireille; Colombe, Rene; Jakalian, Araz; Jones, Jessi; Li, Xiang; Liang, Shuang; McKercher,

Ginette; White, Peter W; Zhang, Qiang; Taylor, Steven J., *J. Med. Chem*., (**2014**) *57*, 2074-2090. Special HCV therapies issue.

27. Enantiomeric Atropisomers Inhibit HCV Polymerase and/or HIV Matrix: Characterizing Hindered Bond Rotations and Target Selectivity
LaPlante, Steven R.; Forgione, Pat; Boucher, Colette; Coulombe, René; Gillard, James; Hucke, Oliver; Jakalian, Araz; Joly, Marc-André; Kukolj, George; Lemke, Christopher; McCollum, Robert; Titolo, Steve; Beaulieu, Pierre L.; Stammers, Timothy,
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28. Discovery of BI 224436, a Non-Catalytic Site Integrase Inhibitor (NCINI) of HIV-1.
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29. Preclinical Profile of BI 224436, a Novel HIV-1 Non-Catalytic-Site Integrase Inhibitor
Fenwick, Craig; Amad, Ma'an; Bailey, Murray D.; Bethell, Richard; Bös, Michael, Bonneau, Pierre; Cordingley, Michael; Coulombe, René; Duan, Jianmin; Edwards, Paul; Fader, Lee D.; Faucher, Anne-Marie; Garneau, Michel; Jakalian, Araz; Kawai, Stephen; Lamorte, Louie; **LaPlante, Steven**; Luo, Laibin; Mason, Steve; Poupart, Marc-André; Rioux, Nathalie; Schroeder, Patricia; Simoneau, Bruno; Tremblay, Sonia; Tsantrizos, Youla, Witvrouw, Myriam; Yoakim, Christiane
Antimicrobial Agents and Chemotherapy, (**2014**), *56*, 17, 7073–7083.
30. Minimizing the Contribution of Enterohepatic Recirculation to Clearance in Rat for the NCINI Class of Inhibitors of HIV
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ACS Med. Chem. Lett., (**2014**), *5*, 711–716.
31. Monitoring Drug Self-Aggregation and Potential for Promiscuity in Off-Target In Vitro Pharmacology Screens by a Practical NMR Strategy
LaPlante, Steven R.; Aubry, Norman; Bolger, Gordon; Bonneau, Pierre; Carson, Rebekah; Coulombe, René; Sturino, Claudio; Beaulieu Pierre L.,
J. Med. Chem., (**2013**), *56*, 17, 7073–7083.
32. Compound Aggregation in Drug Discovery: Implementing a Practical NMR Assay for Medicinal Chemists
LaPlante, Steven R.; Carson, Rebekah; Gillard, James; Aubry, Norman; Coulombe, René; Bordeleau, Sylvain; Bonneau, Pierre; Little, Michael; O'Meara, Jeff; Beaulieu, Pierre L.,
J. Med. Chem., (**2013**), *56*, 12, 5142–5150.
33. N- versus O-alkylation: Utilizing NMR Methods to Establish Reliable Primary Structure Determinations for Drug Discovery
LaPlante, Steven R.; Bilodeau, François; Aubry, Norman; Gillard, James R.; O'Meara, Jeff; Coulombe, René,
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34. Anthranilic Acid-based Thumb Pocket 2 HCV NS5B polymerase Inhibitors with Sub-micromolar Potency in the Cell-based Replicon Assay
Stammers, Timothy A.; Coulombe, René; Duplessis, Martin; Fazal, Gulrez; Gagnon, Alexandre; Garneau, Michel; Goulet, Sylvie; Jakalian, Araz; **LaPlante, Steven**; Rancourt, Jean; Thavonekham, Bounkham; Wernic, Dominik; Kukolj, George; Beaulieu, Pierre L.,
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35. Identification of Benzofurano[3,2-d]pyrimidin-2-ones, a New Series of HIV-1 Nucleotide-competing Reverse Transcriptase Inhibitors
Tremblay, Martin; Bethell, Richard C.; Cordingley, Michael G.; DeRoy, Patrick; Duan, Jianmin; Duplessis, Martin; Edwards, Paul J.; Faucher, Anne-Marie; Halmos, Ted; James, Clint A.; Kuhn, Cyrille; Lacoste, Jean-Éric; Lamorte, Louie; **LaPlante, Steven R.**; Malenfant, Éric; Minville, Joannie; Morency, Louis; Morin, Sébastien; Rajotte, Daniel; et al
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36. Discovery of the First Thumb Pocket 1 NS5B Polymerase Inhibitor (BILB 1941) with Demonstrated Antiviral Activity in Patients Chronically Infected with Genotype 1 Hepatitis C Virus (HCV)
Beaulieu, Pierre L.; Bos, Michael; Cordingley, Michael G.; Chabot, Catherine; Fazal, Gulrez; Garneau, Michel; Gillard, James R.; Jolicoeur, Eric; **LaPlante, Steven**; McKercher, Ginette;..
Journal of Medicinal Chemistry (**2012**), *55*, 17, 7650-7666.
37. Revealing Atropisomer Axial Chirality in Drug Discovery
LaPlante, Steven R.; Edwards, Paul J.; Fader, Lee D.; Jakalian, Araz; Hucke, Oliver
ChemMedChem (**2011**), *6*, 3, 505-513.
38. Peptides as Leads for Drug Discovery
Edwards, Paul J.; **LaPlante, Steven R.** - Edited by Castanho, Miguel; Santos, Nuno C ,
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39. Assessing Atropisomer Axial Chirality in Drug Discovery and Development
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40. Importance of Ligand Bioactive Conformation in the Discovery of Potent Indole-Diamide Inhibitors of the Hepatitis C Virus NS5B
LaPlante, Steven R.; Gillard, James R.; Jakalian, Araz; Aubry, Norman; Coulombe, Rene; Brochu, Christian; Tsantrizos, Youla S.; Poirier, Martin; Kukolj, George; Beaulieu, Pierre L.
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41. The Effect of the P1 Side Chain on the Binding of Optimized Carboxylate and Activated Carbonyl Inhibitors of the Hepatitis C Virus NS3 Protease
Kawai, Stephen H.; **LaPlante, Steven R**.; Llinas-Brunet, Montse; Hucke, Oliver
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Yoakim, Christiane; Bailey, Murray D.; Bilodeau, Francois; Carson, Rebekah J.; Fader, Lee; Kawai, Stephen; **LaPlante, Steven**; Simoneau, Bruno; Surprenant, Simon; *et al.*
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45. Preparation of 2-(quinolin-2-yl)acetic Acid Derivatives as Inhibitors of Human Immunodeficiency Virus Replication
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47. The Use of Chemical Double-mutant Cycles in Biomolecular Recognition Studies: Application to HCV NS3 Protease Inhibitors
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Coulombe, Rene; Beaulieu, Pierre Louis; Jolicoeur, Eric; Kukolj, George; **LaPlante, Steven**; Poupart, Marc-Andre
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