

Louis-Philippe Morency

Computational pharmacologist · docking-engine author · open-science

PhD candidate · Najmanovich Research Group · Université de Montréal

lp@thebonhomme.com

thebonhomme.com

 github.com/LeBonhommePharma

linkedin.com/in/lebonhomme

x.com/lebonhomme

scholar.google.com · L-P Morency

ORCID 0009-0001-0218-4750

// PROFILE

Computational pharmacologist working at the intersection of [genetic algorithms](#) and [statistical mechanics](#). Main author of [FlexAIDΔS](#), a [genetic-algorithm](#) docking engine that computes the full $\Delta G = \Delta H - T\Delta S$ — the conformational entropy term included, recovering the correct [binding mode](#) where [enthalpy-only](#) scoring fails. Every result is [reproducible](#) by construction and shipped under [Apache 2.0](#). Anti-prohibitionist; [harm reduction](#) as applied thermodynamics. Montréal.

// RESEARCH INTERESTS

molecular docking

statistical mechanics of binding

conformational entropy

free-energy scoring

genetic-algorithm optimization

Shannon entropy

drug repurposing / off-targets

open-source scientific software

harm reduction

// EDUCATION

Ph.D. — Pharmacology (in progress)

present

[Université de Montréal](#) · [Najmanovich Research Group \(NRGLab\)](#)

Thesis: entropy-driven molecular docking — FlexAIDΔS and the full $\Delta G = \Delta H - T\Delta S$ score.

M.Sc. — Biochemistry

conferred

[Université de Sherbrooke](#) · [NRGLab \(origin lab\)](#)

Docking methods, contact-based scoring, and the first NRGsuite / FlexAID toolchain.

B.Sc. — Structural Bioinformatics

conferred

[Université Laval](#)

Foundations in structural biology, protein modelling and computational methods.

// RESEARCH & ENGINEERING EXPERIENCE

Doctoral researcher

Fall 2017 – present

[Najmanovich Research Group \(NRGLab\)](#) · [Université de Montréal](#)

- › Main author of FlexAIDΔS: a C++26 genetic-algorithm docking engine with a full statistical-mechanics score ($\Delta G = \Delta H - T\Delta S$), torsional ENCoM entropy, Voronoi contact function and dead-end-elimination torsion pruning.
- › 96.4% correct binding-mode recovery on Astex Diverse 85 — without crystal coordinates.
- › Built Python bindings and the NRGsuite PyMOL plugin; zero-copy GPU/OpenMP batch scoring for high-throughput screens.

Lead programmer

2014 – present

[Najmanovich Research Group \(NRGLab\)](#)

- › Principal software architect for the lab — own the NRG docking toolchain end to end across its Sherbrooke and Montréal eras.

Le Bonhomme Pharma · github.com/LeBonhommePharma

- › Open-science pharmacology lab shipping reproducible Apache-2.0 tooling from Little Burgundy, Montréal.
- › Ported the FlexAIDΔS entropy kernel to two new domains — Shannon (LLM entropy-collapse) and ClusterFuck (HRV biofeedback).

Graduate researcher

earlier

NRGLab · Université de Sherbrooke

- › Co-developed NRGsuite and applied FlexAID to large-scale off-target detection for drug repurposing and side-effect prediction.

// SOFTWARE & OPEN SOURCE

FlexAIDΔS C++26 · Python · PyMOL Apache 2.0

Entropy-driven molecular docking engine. GA conformational search, Voronoi contact function, torsional ENCoM entropy, DEE torsion pruning, zero-copy GPU/OpenMP batch scoring. The full $\Delta G = \Delta H - T\Delta S$.

Shannon C++20 · Python Apache 2.0

Entropy-collapse detector for frontier LLM agents — zero-shot evaluation-awareness and strategic-deception monitoring via the same $H = -\sum p_i \log_2 p_i$ kernel that powers binding and HRV.

ClusterFuck Swift · HealthKit · CareKit Apache 2.0

Multi-platform Apple biofeedback (Watch · iPhone · TV · Vision Pro). Real-time HRV entropy → Shannon Collapse Index during guided chair yoga; shared kernel with FlexAIDΔS.

NRGsuite Python · PyMOL open source

PyMOL plugin packaging the NRGLab docking toolchain for real-time interactive docking with FlexAID.

PoseBust C++26 open source

PoseBusters-compatible geometric validation — physical-plausibility checks (bond geometry, clashes, planarity) for docked ligand poses.

// BENCHMARKS & TECHNICAL RESULTS

96.4% ASTEX DIVERSE 85 · TOP POSE	85% CROSS-DOCK · RMSD < 2 Å	94% SHANNON · COLLAPSE SENS.	<1μs PER TOKEN · SHANNON
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BENCHMARK	METRIC	RESULT
Astex Diverse 85	correct binding mode (top pose)	96.4%
Astex Diverse 85	cross-dock, RMSD < 2 Å	85%
Shannon	entropy-collapse sensitivity	94%

// PUBLICATIONS

PREPRINTS & IN PREPARATION

- P1** Morency L-P, Najmanovich RJ. FlexAIDΔS: entropy-driven molecular docking with a full $\Delta G = \Delta H - T\Delta S$ statistical-mechanics score. *Preprint / in preparation*. 2026
- P2** Morency L-P. Shannon: entropy-collapse detection for frontier LLM agents via the FlexAIDΔS configurational-entropy kernel. *Preprint*. 2026

PEER-REVIEWED

- 01** Morency L-P, Gaudreault F, Najmanovich RJ. Applications of the NRGsuite and the molecular docking software FlexAID in computational drug discovery and design. *Methods in Molecular Biology* 1762, 367–388. Humana Press. 2018

02

Chartier M, Morency L-P, Zylber MI, Najmanovich RJ. Large-scale detection of drug off-targets: hypotheses for drug repurposing and understanding side-effects. *BMC Pharmacology and Toxicology* 18, 18. 2017

03

Gaudreault F, Morency L-P, Najmanovich RJ. NRGsuite: a PyMOL plugin to perform docking simulations in real time using FlexAID. *Bioinformatics* 31(23), 3856–3858. 2015

INVITED TALKS & CONFERENCE KEYNOTES

K1

Morency L-P, Najmanovich RJ. Modelling conformational entropy in molecular docking — beyond the enthalpy-only score. *PROTEO Annual Symposium, Québec (invited)*. 2019

// TALKS & TEACHING

workshops	Hands-on docking with NRGsuite and FlexAID in PyMOL — graduate computational-biology methods.
invited	Entropy is not optional: why enthalpy-only docking gets the right answer for the wrong reason.
teaching	Teaching assistant, biochemistry & structural bioinformatics — Université de Sherbrooke.

// TECHNICAL SKILLS

LANGUAGES	C++26	C++20	Python	Swift	CMake	Bash
SCIENTIFIC	Molecular docking	Statistical mechanics	Free-energy scoring	Normal-mode / ENCoM	Shannon entropy	HRV signal processing
TOOLING	PyMOL	OpenMP	CUDA / GPU	Git	HealthKit	CareKit
PRACTICE	Reproducible builds	Open-source maintenance	Benchmark design	Apache 2.0 / MIT		

// AWARDS & FUNDING

Médaille du Lieutenant-Gouverneur du Québec (bronze)	—
Cabinet du Lieutenant-gouverneur du Québec — academic & civic merit.	
Doctoral research fellowship	PhD
Fonds de recherche du Québec — Nature et technologies (FRQ-NT).	
Open-source contribution recognition	—
GitHub Arctic Code Vault Contributor; multi-year maintainer across the NRGLab / Le Bonhomme Pharma stack.	

// WRITING & ADVOCACY

Book in progress — housing, organized crime, and harm reduction in Montréal. The same physics that lowers a binding free-energy barrier lowers the social barrier to care: systems seek lower free energy; the job is to lower it.
Drug of the Day — a rotating, rigorous harm-reduction pharmacology brief published at thebonhomme.com. Mechanism over moralising.