

Louis-Philippe Morency

Computational Pharmacologist · Docking-engine author

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$$\Delta G = \Delta H - T\Delta S$$

Computational pharmacologist building **thermodynamically honest docking**. Main author of **FlexAIDΔS** — a genetic-algorithm docking engine that computes the full $\Delta G = \Delta H - T\Delta S$, entropy term included, where enthalpy-only scorers guess. **Open-source by construction** (Apache 2.0). Anti-prohibitionist. Montréal.

96.4%

ASTEX DIVERSE 85 · TOP POSE

85%

CROSS-DOCK · RMSD < 2Å

94%

SHANNON · COLLAPSE

<1μs

PER TOKEN · SHANNON

// OPEN-SOURCE SOFTWARE

FlexAIDΔS C++26 · Python · PyMOL

Entropy-driven molecular docking engine. GA conformational search, Voronoi contact function, torsional ENCoM entropy, dead-end-elimination pruning, GPU batch scoring. Apache 2.0.

Shannon C++20 · Python

Entropy-collapse detector for frontier LLM agents. Same $H = -\sum p_i \log_2 p_i$ kernel that powers FlexAIDΔS binding — zero-shot deception & evaluation-awareness monitoring.

ClusterFuck Swift · HealthKit · CareKit

Multi-platform Apple biofeedback. Real-time HRV entropy → Shannon Collapse Index across Watch, iPhone, TV, Vision Pro.

NRGsuite Python · PyMOL

PyMOL plugin packaging the NRGLab docking toolchain for interactive use.

PoseBust C++26

PoseBusters-compatible geometric pose validation — physical plausibility checks for docked ligands.

// RESEARCH EXPERIENCE

Doctoral researcher

Fall 2017 – present

Najmanovich Research Group (NRGLab) · UdeM

Main author of FlexAIDΔS, Shannon, ClusterFuck and NRGsuite. 96.4% correct binding-mode recovery on Astex Diverse 85 without crystal coordinates; full $\Delta G = \Delta H - T\Delta S$ scoring.

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.

Open-source maintainer

2023 – present

Le Bonhomme Pharma · github.com/LeBonhommePharma

// EDUCATION

Ph.D. — Pharmacology

Université de Montréal · Najmanovich Research Group
in progress

M.Sc. — Biochemistry

Université de Sherbrooke · NRGLab
conferred

B.Sc. — Structural Bioinformatics

Université Laval
conferred

// SKILLS

LANGUAGES

C++26

C++20

Python

Swift

CMake

DOMAINS

Molecular docking

Statistical mechanics

Free-energy scoring

Shannon entropy

HRV signal processing

TOOLS

PyMOL

OpenMP

CUDA/GPU

Git

HealthKit

// SELECTED PUBLICATIONS & AWARDS

Gaudreault F, Morency L-P, Najmanovich RJ. NRGsuite: a PyMOL plugin for docking with FlexAID. Bioinformatics 31, 3856–3858 (2015).

Morency L-P, Gaudreault F, Najmanovich RJ. Applications of the NRGsuite and FlexAID in computational drug discovery. Methods Mol. Biol. (2018).

Médaille du Lieutenant-Gouverneur du Québec (bronze) · Cabinet du Lieutenant-gouverneur du Québec.

FRQ-NT doctoral research fellowship · Fonds de recherche du Québec — Nature et technologies.

Founder of an open-science pharmacology lab shipping reproducible, Apache-2.0
docking and entropy tooling from Little Burgundy.

LE BONHOMME PHARMA · RADICAL OPEN-SOURCE PHARMACOLOGY

DRUG IS ALWAYS AN ANSWER