THIBAUD SOUTHIRATN

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SUMMARY

MSc. and **MEng.** dual degree student in Computer Science and Engineering.

I studied Computer Science in France, then researched AI-driven drug discovery in Korea where my thesis work was published in ICML'25.

SKILLS

- **Deep Learning & Cheminformatics**
  PyTorch, RDKit, PyMOL, AutoDock Vina, Transformers.
- **Programming & Tools**
  Python (mainly), Java, LaTeX, HTML/CSS.
- **Software Engineering**
  Git, Shell, Docker, HPC (Distributed Computing).
- Adaptability, Problem-solving, Team-work.

WORK EXPERIENCES

Nov 2025 – Sept 2025 **Cheminformatics Intern** • INTERNSHIP, 3 MONTHS **NovAliX** • Strasbourg, France
- End-to-end development/deployment of a robust and maintainable ADME prediction tool.
- Accelerating the workflow of the Drug Discovery team in early-stage screening.
- Co-authored a peer-reviewed publication.
- *Technologies*: Python, Scikit-Learn, PyTorch.

Aug 2025 – Sept 2023 **AI Researcher** • RESEARCH, 2 YEARS **Bio & Health Informatics Lab** • Seoul, Korea
- Published a paper in a top-tier AI conference (ICML'25).

My work is currently being used to attempt identifying selective CDK7 kinase inhibitors in a CRO.
- Co-authored a paper presented at a domestic conference (KCC'24, Korea).
- Peer reviewer of 4 papers (2x ICML'25, NeurIPS'25, KDD'24).
- *Topics*: Generative Models and Algorithms for Biomedicine and Cheminformatics.

PUBLICATIONS

CombiMOTS: Combinatorial Multi-Objective Tree Search for Dual-Target Molecule Generation **ICML'25**
Thibaud Southiratn, Bonil Koo, Yijingxiu Lu, Sun Kim

Deep Learning vs Classical Methods in Potency & ADME Prediction: Insights from a Computational Blind Challenge **American Chemical Society (JCIM)**
Yaelle Fischer, **Thibaud Southiratn**, Dhoha Triki, Ruel Cedeno

Web-based Exploratory Data Mining System for Analyzing the Gene-level Relationship between Intratumoral Heterogeneity of Promoter DNA Methylation and Drug Response **2024 Korea Computer Congress**
Tae Hoon Kweon, Bonil Koo, Sungjoon Park, **Thibaud Southiratn**, Sun Kim

PROJECTS & AWARDS

Owkin Decoding Biology Hackathon **[1st/12 Teams]** • AGENTIC ORCHESTRATION/LLM POST-TRAINING
- 3-day competition on building LLM agentic workflows to reason through real biomedical pre-specified Q&A-based data.
- Domain-specific data curation and exploration of post-training strategies (LoRA & Expert Model Merging).

Selective CDK7 Inhibitor Generation • PARETO OPTIMIZATION/MONTE-CARLO TREE SEARCH/PROPERTY PREDICTION
- Adapted CombiMOTS to attempt unveiling molecules biochemically active to CDK7 & inactive to CDK1-2-5-9-12-13.
- Identified potent candidates with motifs/warheads (acrylamide, chloroacetamide) found in relevant literature.

Efficient Molecule Captioning • TRANSFORMERS/CHEMICAL LANGUAGE MODELS
- Fine-tuned a Chemical Language Model (Text+ChemT5) to **improve performance (up to +5.4%)** on the "mol2text" task.
- Adapted an implementation of Speculative Decoding to **infer captions faster (+36.5%)** without changing output distribution.

EDUCATION

Aug 2025 – Sept 2023 **MSc. in Computer Science and Engineering** **Seoul National University, Korea**
- Bio and Health Informatics Lab, advised by Prof. Sun Kim.
- *Coursework*: Artificial Intelligence, Bioinformatics, Generative AI.
- Teaching Assistant: Lecturing & Mentoring
  Spring 2025 — "Machine Learning in Bioinformatics" (~50 students).
  Fall 2024 — "Computer Convergence Application" (~50 students).
- *GPA*: 3.82/4

Dec 2025 – Sept 2021 **MEng. in Computer Science and Engineering** **(Grande École) Télécom SudParis, France**
- *Coursework*: Machine Learning, Computer Vision, Network & Software Engineering.
- *GPA*: 3.72/4

June 2021 – Sept 2018 **Preparatory Class for Engineering** **Lycée Lakanal, France**
- Nationwide competitive exams.
- *Coursework*: Mathematics, Physics, Chemistry.

LANGUAGES

- **French** • Native
- **English** • Fluent (TOEIC 990/990)
- **Spanish** • Intermediate
- **Korean** • Scholar

INTERESTS

- **Gaming** (Reached Top 1% Europe on *CS:GO* & *Valorant*)
- **Photography** (Adobe Lightroom/Photoshop)
- **Weightlifting**
- **Trying everything**