Multi-Agent Drug Discovery Orchestra

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About

- Senior consultant @ D ONE (Zurich, Switzerland)
- Lead researcher @ ITMO University (St. Petersburg, Russia)

- Short vita:
  - 2018 – systems biology team lead @ BIOCAD LLC
  - 2022 – doctor of sciences @ ETH Zurich
  - 2024 – data & software engineer @ Calico Life Sciences LLC
  - 2025 – 3 posters and the Top Reviewer award @ NeurIPS conference

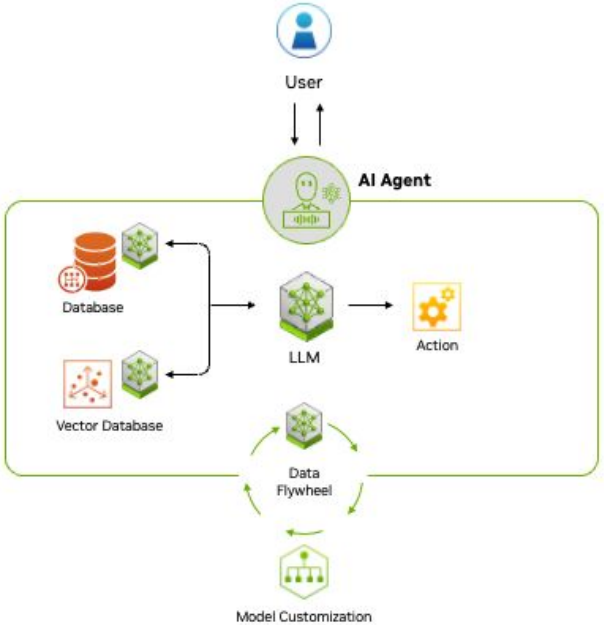
Center for AI in Chemistry @ ITMO University

- Since 2022
- Now >30 people
- A Master’s program (21 students)
- World-class research
- Academic and industrial collabs
- Core competences in:
  - Cheminformatics
  - Materials science
  - Bioinformatics
  - Artificial intelligence

Agentic AI is the new frontier

- Agent is:
  - a stateful LLM app designed to fulfil a particular role
  - equipped with tools and memory
  - free to reason, use tools, and perform actions in the real world

- Agent is, therefore, much like a human at work



Applications of agentic systems

nature › npj computational materials › articles › article

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Agent-based multimodal information extraction for nanomaterials

R. Odobesku, K. Romanova, S. Mirzaeva, O. Zagorulko, R. Sim, R. Khakimullin, J. Razlivina, A. Dmitrenko & V. Vinogradov

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Benchmarking Agentic Systems in Automated Scientific Information Extraction with ChemX

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MADD: Multi-Agent Drug Discovery Orchestra

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NEURAL INFORMATION PROCESSING SYSTEMS

EMNLP 2025 Suzhou, China 中国苏州

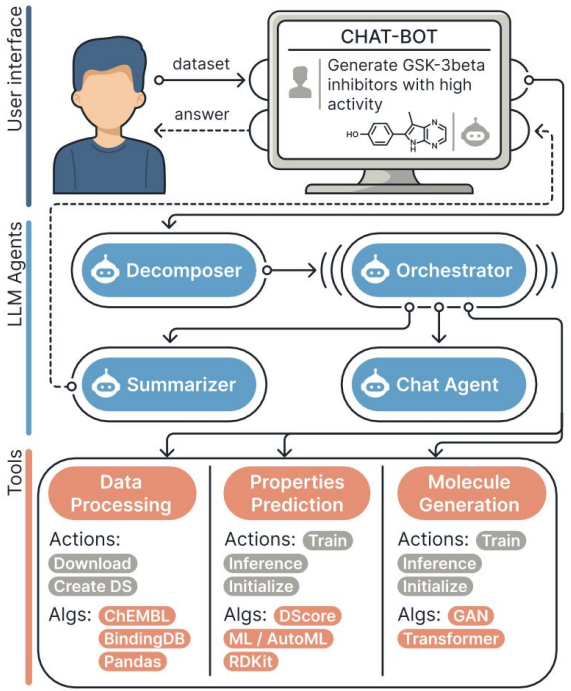
MADD

- A multi-agent system designed to address hit identification *in silico*
- Expects a user query in natural language as a default input

```
'input': 'Generate molecule of GSK-3beta
inhibitors with high docking score'
```

- Provides a list of generated molecules as a target output


```
{'Smiles': {'0': 'OC12C3C=C(Br)C4=
    NCC5(CN6CC65)C4N1CC2CC3',
          '1': 'COC1(OC)C2C3C4CCN(
              C#N)C3C41c1nncn12'},
 'Brenk': {...}, 'QED': {...}, '
    Synthetic Accessibility':
    {...},
 'LogP': {...}, 'Polar Surface Area
    ': {...}, 'H-bond Donors':
    {...},
 'H-bond Acceptors': {...}, '
    Rotatable Bonds': {...},
 'Aromatic Rings': {...}, 'Glaxo':
    {...}, 'SureChEMBL': {...},
 'PAINS': {...}, 'Validity': {...},
     'Duplicates': {...},
 'docking_score': {...}, 'IC50':
    {...}}
```

MADD approach

- Case-driven:
  - Alzheimer’s
  - Parkinson’s
  - Multiple sclerosis
  - Lung cancer
  - Dislipidemia
  - Drug resistance

  \+ *Thrombocytopenia*

- Systematic:
  - Producing two benchmarking assets: the dataset of validated user queries and 3M of scored molecules

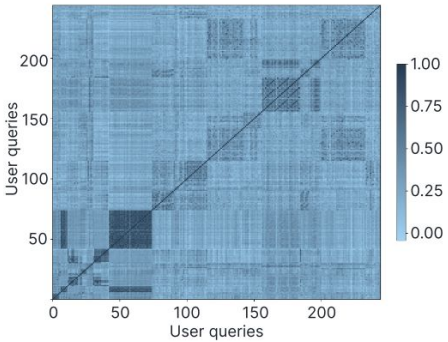
- Innovative:
  - Pioneering the application of AI-first drug design to five targets: STAT3, ABL, COMT, ACL, and PCSK9

Proposed benchmark

Queries — Dataset of >300 queries for 6 diseases

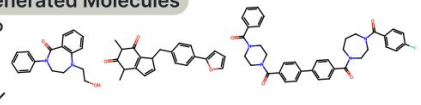
Example for Alzheimer:
Generate GSK-3beta inhibitors with high docking score and low brain-blood barrier permeability

Example for Dislipidemia:
Can you suggest molecules that inhibit Proprotein Convertase Subtilisin/Kexin Type 9 with enhanced bioavailability and the ability to cross the BBB?



Generated SMILES — >5000 molecules for 6 diseases

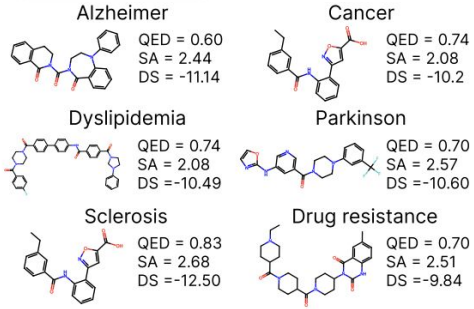
Generated Molecules



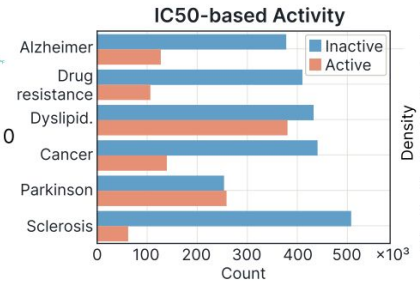
Filters

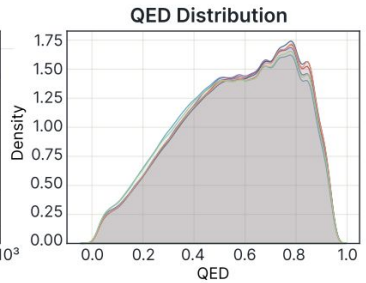
- DS <= -7
- IC50 = 1
- SA Score <= 3
- Brenk = 0
- SureChEMBL = 0
- Glaxo = 0
- PAINS = 0
- QED > 0.6

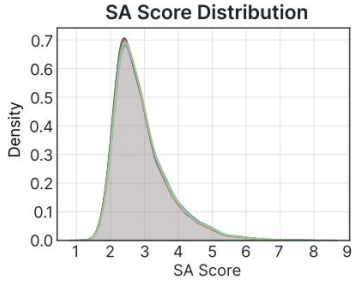
Selected Molecules

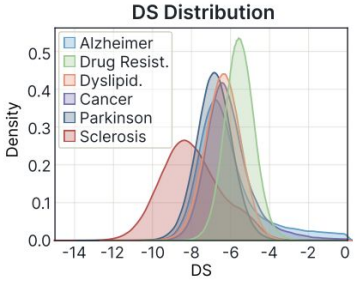


Molecule properties — Molecular properties dataset (DS, IC50, SA, QED) for >3M molecules









Agentic system design

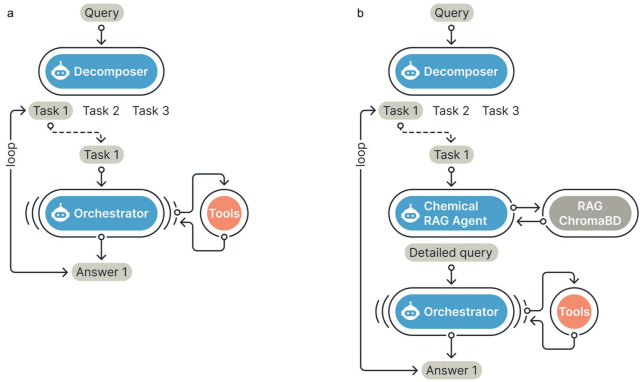


Figure 12: Visualisation of MADD-v2A and MADD-v3 systems.

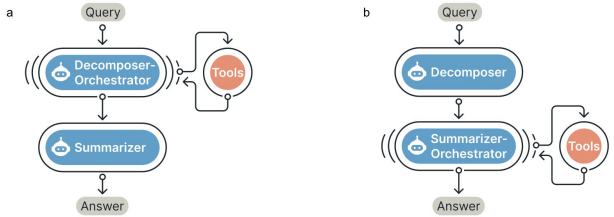
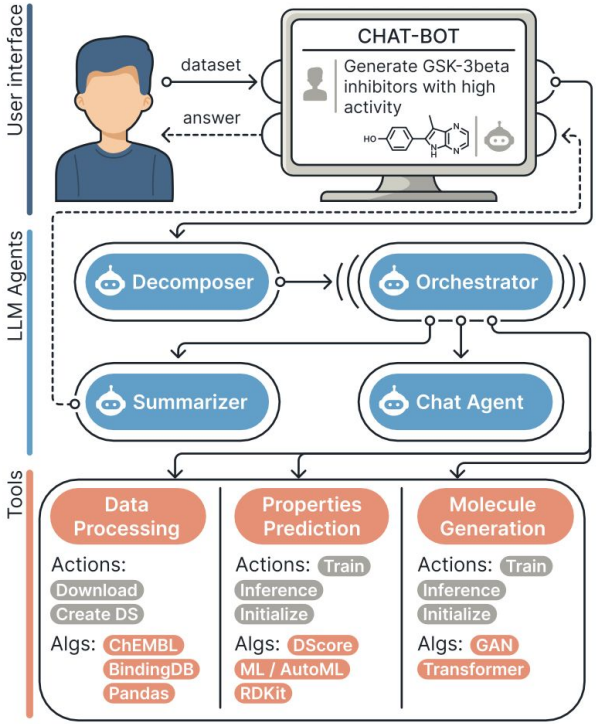


Figure 13: Visualisation of MADD-v2C and MADD-v2B systems.

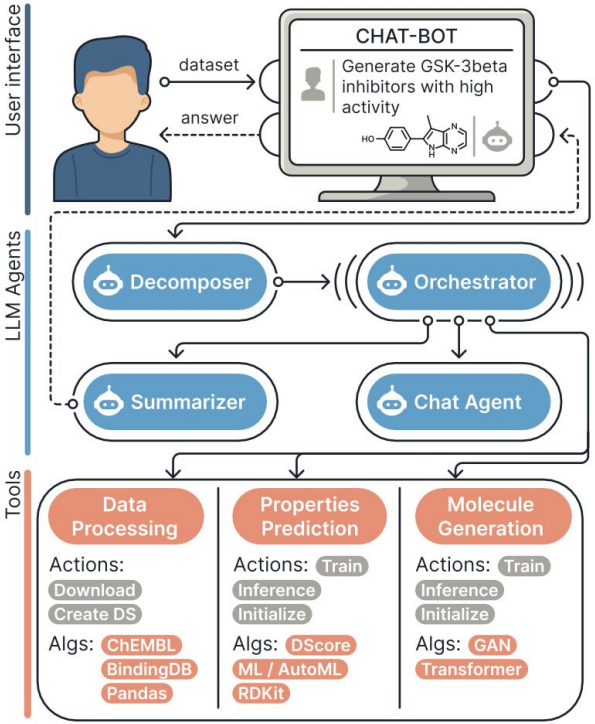


Agentic system design

Table 1: Comparison of MADD with other candidate architectures for multi-agent systems by TS, SSA, and FA metrics.

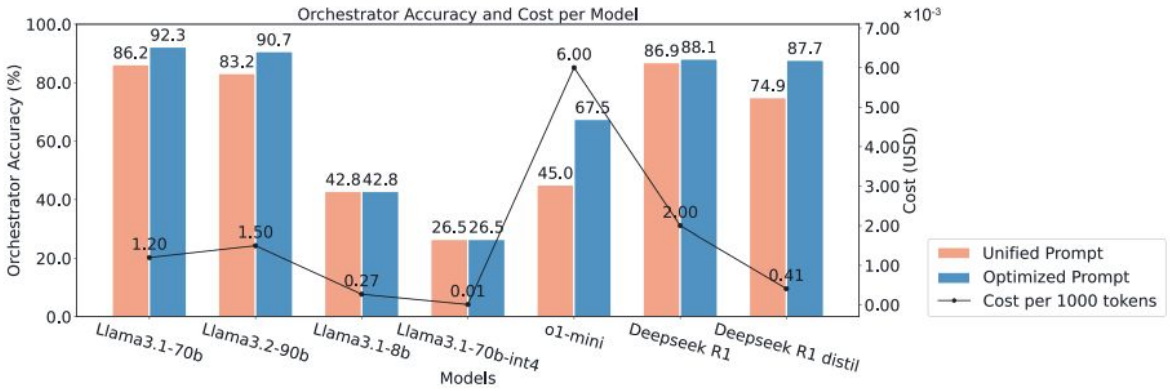
Metric	TS	SSA	FA
MADD	**83.7**	**95.3**	**79.8**
MADD-v1	42.5	70.0	29.8
MADD-v2A	35.0	65.1	22.8
MADD-v2B	76.7	95.3	73.0
MADD-v2C	81.4	53.7	43.7
MADD-v3	46.5	75.6	35.2

- TS – Tool Selection
- SSA – System Summarization Accuracy
- FA – Final Accuracy



Agentic system design

- Orchestration is all you need



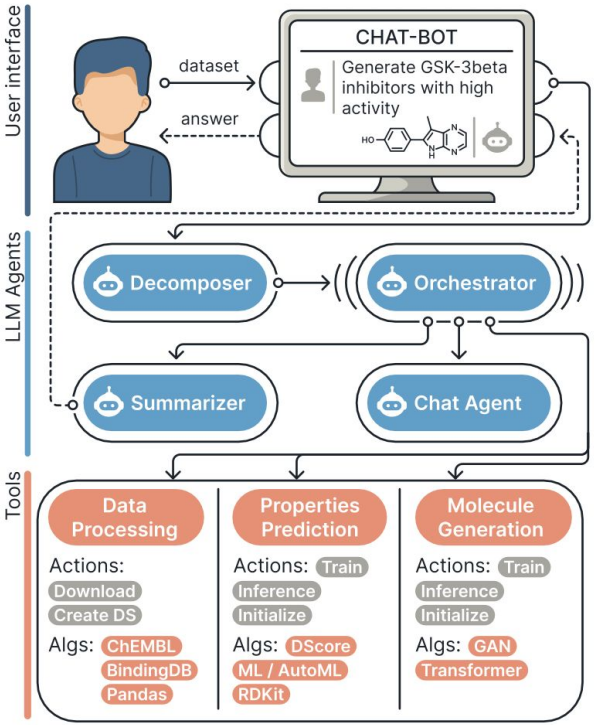
Levels of complexity

Table 2: Comparison of the Final Accuracy (%) of MADD and baseline methods on datasets of different complexity.

Dataset	S	M	L
MADD	**86.9**	**84.3**	**79.8**
ChemAgent	12.4	15.3	16.4
LlasMol	0.46	0.24	0
X-Lora-Gemma	0.44	0.12	0
ChemDFM	5.31	0.33	0

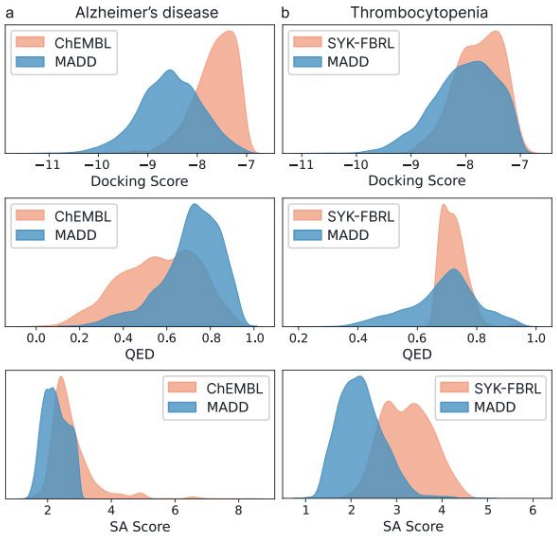
- S – only single-task queries
- M – up to 3 tasks in a query
- L – up to 5 tasks in a query

* ***Phoenix*** *from the FutureHouse Platform managed to create a single molecule that satisfied the 2/5 filter groups, but no more. The molecules produced by* ***TxGemma*** *did not pass any filters.*



Validation case studies

- Reproducing experimentally validated molecules for validation



Case	Alzheimer		Thrombocytopenia	
Model	MADD	MADD Auto	SYK-FBRL	MADD Auto
Mean DS	-7.46	**-7.57**	-7.76	**-8.02**
Novelty	**78.21**	73.47	100	100
Validity	87.47	**89.5**	**100**	90.71
GR1,%	**20.30**	15.99	0.18	**1.54**
GR2,%	**17.56**	14.43	0.07	**1.35**
GR3,%	**13.72**	13.14	0.06	**1.32**
GR4, %	**13.40**	12.34	0.06	**1.32**
GR5,%	**13.40**	12.34	0.06	**1.32**

What MADD is and isn't

Is:

- A first-of-its-kind effective *application* of multi-agent systems to early drug discovery
- A powerful *showcase* for the next-generation pharma R&D tools
- A versatile *interface* for the wet-lab researchers

Is not:

- A universal framework to solve drug design
- A commercially available product
- A definitive solution for hit identification – *a lot more to come*

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Thank you

Work & collaboration:
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Appendix: molecule generation

		GR1	GR2	GR3	GR4	GR5	Diversity
Drug resistance	GAN	0.23	0.15	0.10	0.10	0.10	0.39
	Transformer	**8.32**	**6.92**	**6.14**	**6.05**	**6.05**	0.77
	RL	0.63	0.52	0.40	0.38	0.38	0.13
	MTDD-EF	0.00	0.00	0.00	0.00	0.00	0.11
	ChemTSv2	0.14	0.14	0.09	0.09	0.09	0.43
Dyslipidemia	GAN	7.27	6.15	4.92	4.72	4.72	0.34
	Transformer	**28.87**	**28.27**	**25.07**	**24.50**	**13.16**	0.21
	RL	0.02	0.02	0.02	0.02	0.02	0.05
	MTDD-EF	0.00	0.00	0.00	0.00	0.00	0.06
	ChemTSv2	0.12	0.12	0.06	0.06	0.06	0.44
Lung cancer	GAN	5.53	4.41	3.43	3.31	3.31	0.39
	Transformer	6.12	5.72	**4.97**	**4.76**	**4.76**	0.8
	RL	0.57	0.53	0.51	0.51	0.51	0.09
	MTDD-EF	1.00	1.00	1.00	1.00	1.00	0.11
	ChemTSv2	**6.65**	**6.65**	4.06	3.53	3.53	0.43

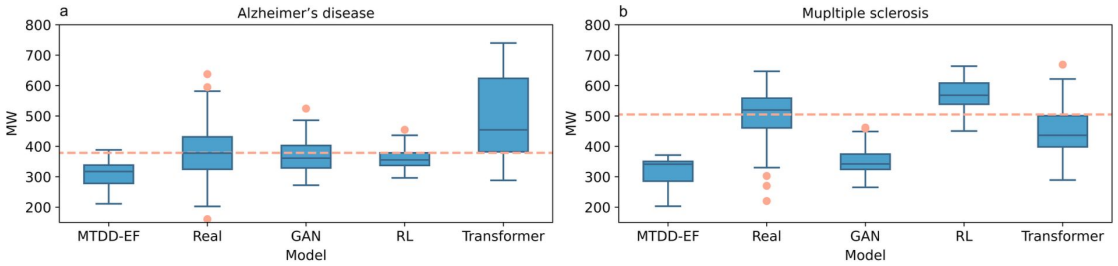

Figure 11: Comparison of the molecular mass of experimentally validated molecules ("Real") with generated molecules using MTDD-EF and integrated models for: a) Alzheimer's disease, b) Multiple sclerosis.

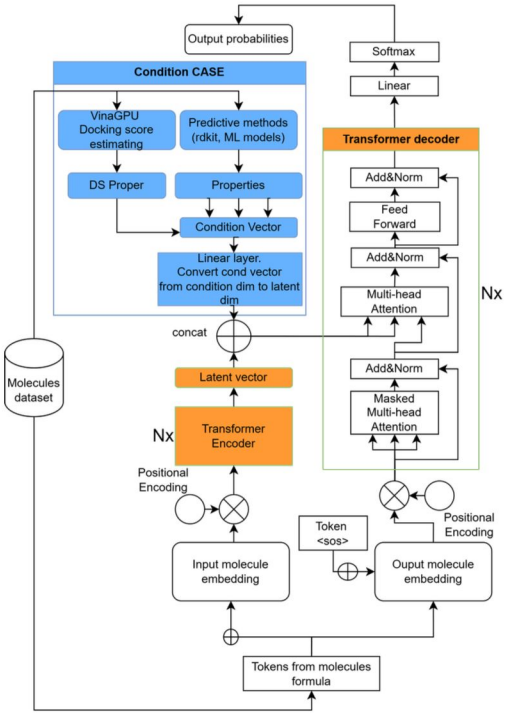

Figure 10: Our CVAE transformer architecture

Model	GAN	Transformer
GPU memory (GB)	**6.40**	8.43
Training time (hours)	**2.82**	23.73
Generation time (ms/molecule)	**0.19**	295.00