

osmo

Digitizing smell with a principal odor map

Wesley Qian
2025-03-31 COSYNE 2025 Workshop



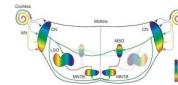
About Osmo and me

- A startup focusing on giving computers a sense of smell.
- We started at Google Brain, where we used cutting-edge machine learning to build the foundations of the principal odor map.
- We spun out in 2022 with \$60 million Series A led by Lux Capital and Google Ventures.
- We recently launched Generation by Osmo to make beautiful fragrance more accessible.

- I am leading the applied research team at Osmo focusing on AI and high throughput data collections.
- I come from a background of computer science, with a PhD focusing on machine learning for drug discovery.

Every time we digitize a sense, our society changes for the better.

Hearing



1961
von Békésy for
mechanism for hearing

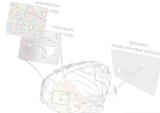
MP3 audio
Voice recognition

osmo

Vision

1967

Granit, Hartline & Wald,
for physiology of color
vision in the retina



1981
Hubel and Wiesel, for
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Digital cameras
Virtual reality

Olfaction

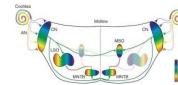
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to Buck and Axel for
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Smell "camera"?
Cooking robot?

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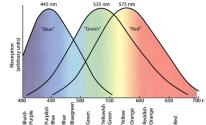
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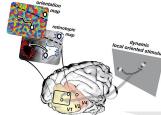
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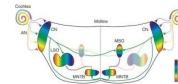
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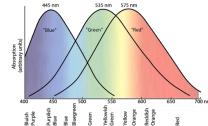
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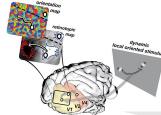
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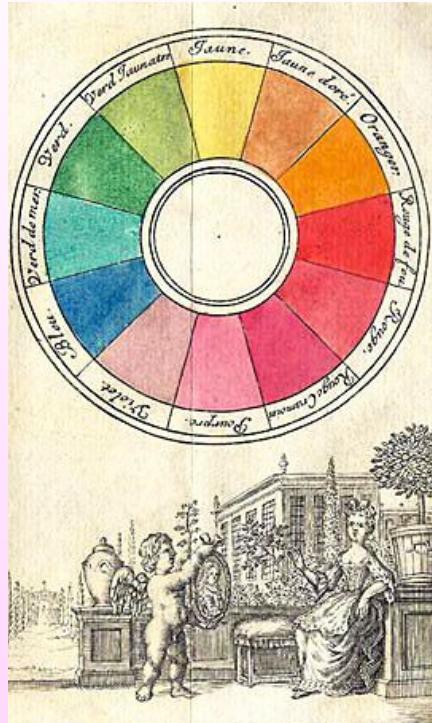
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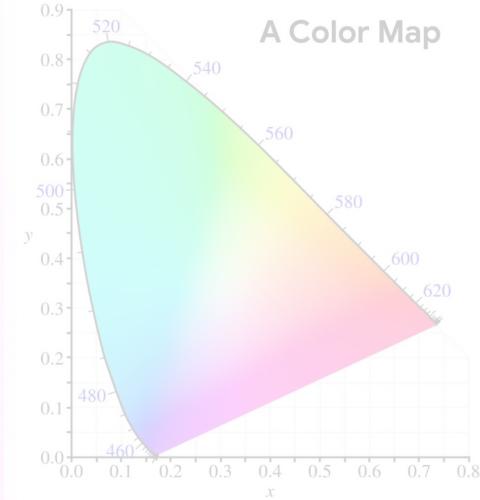


What is an odor map?

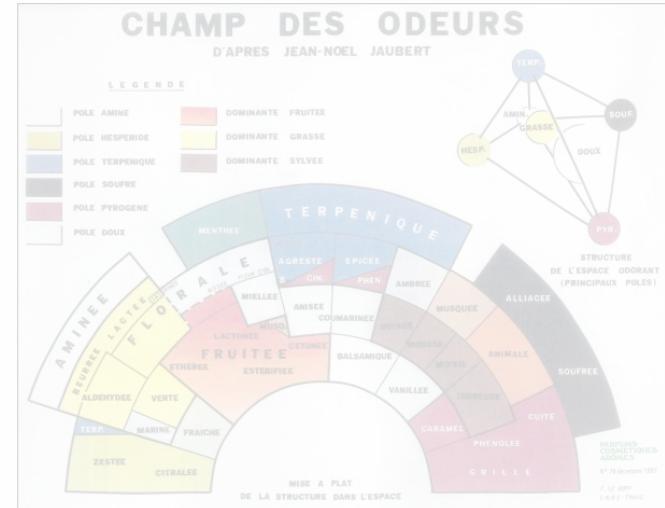
Color Wheel in ~1700



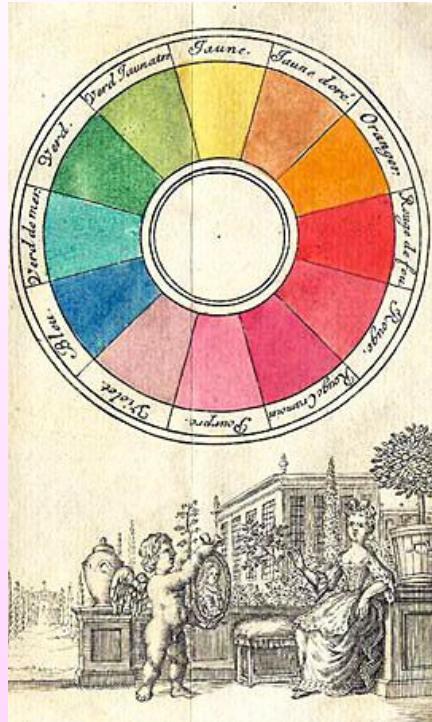
CIE 1931



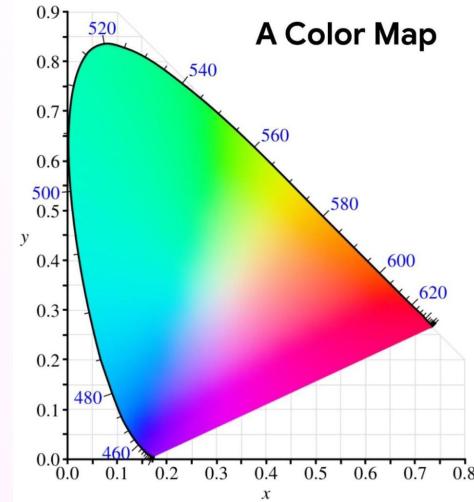
Field of Smell in 1983



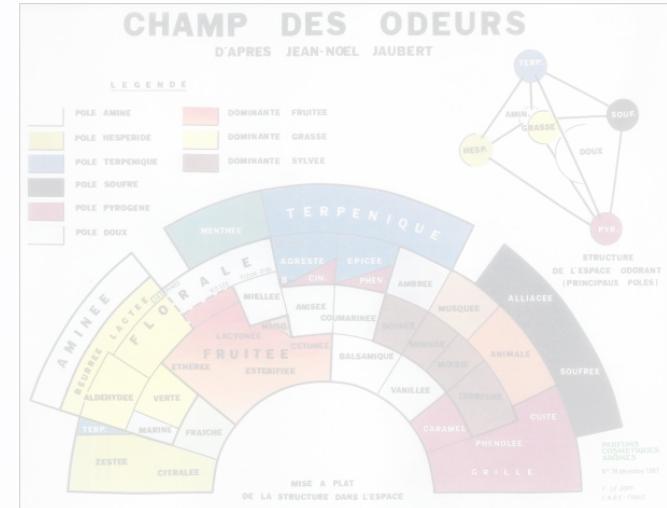
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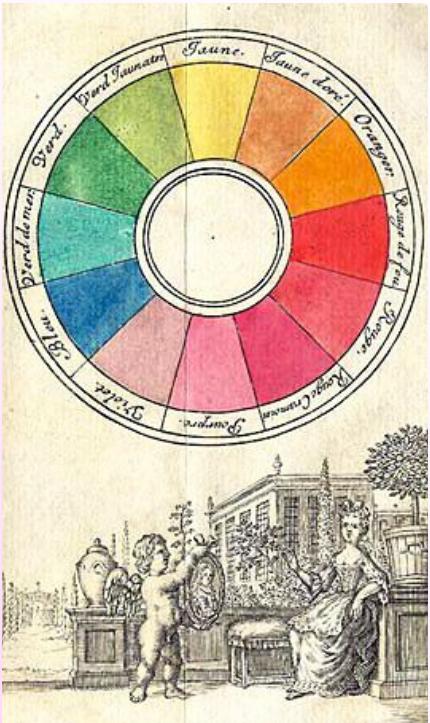
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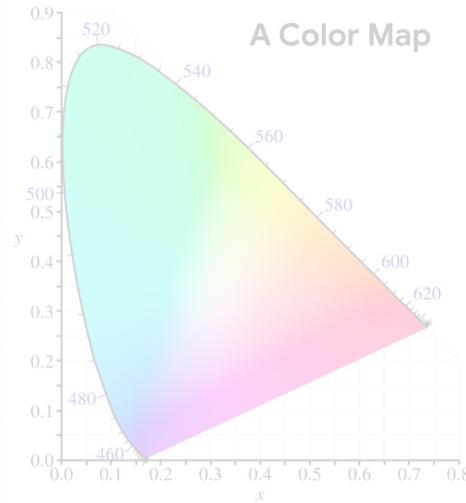
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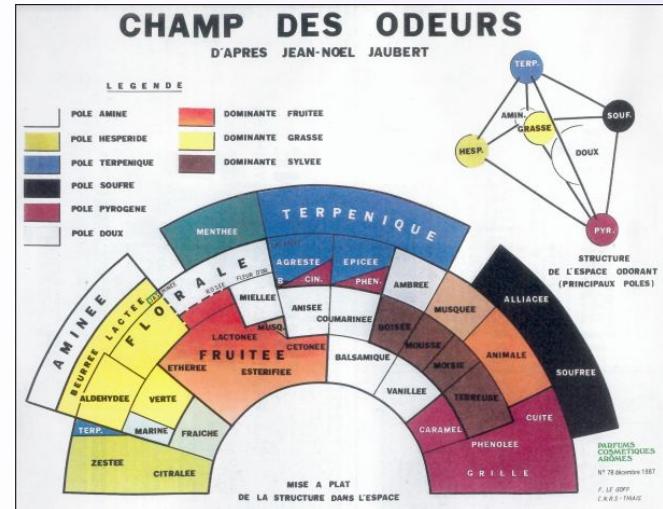
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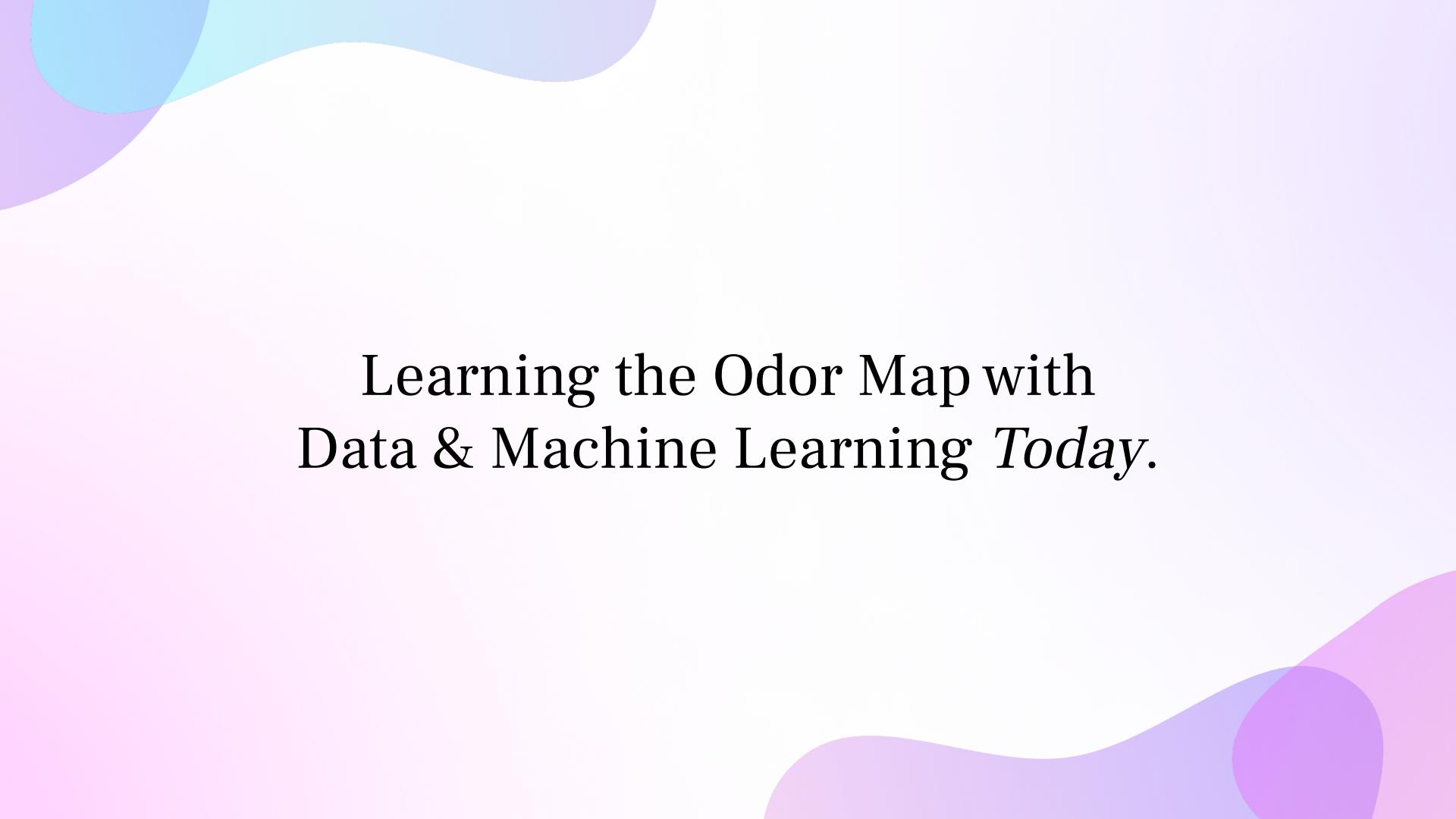


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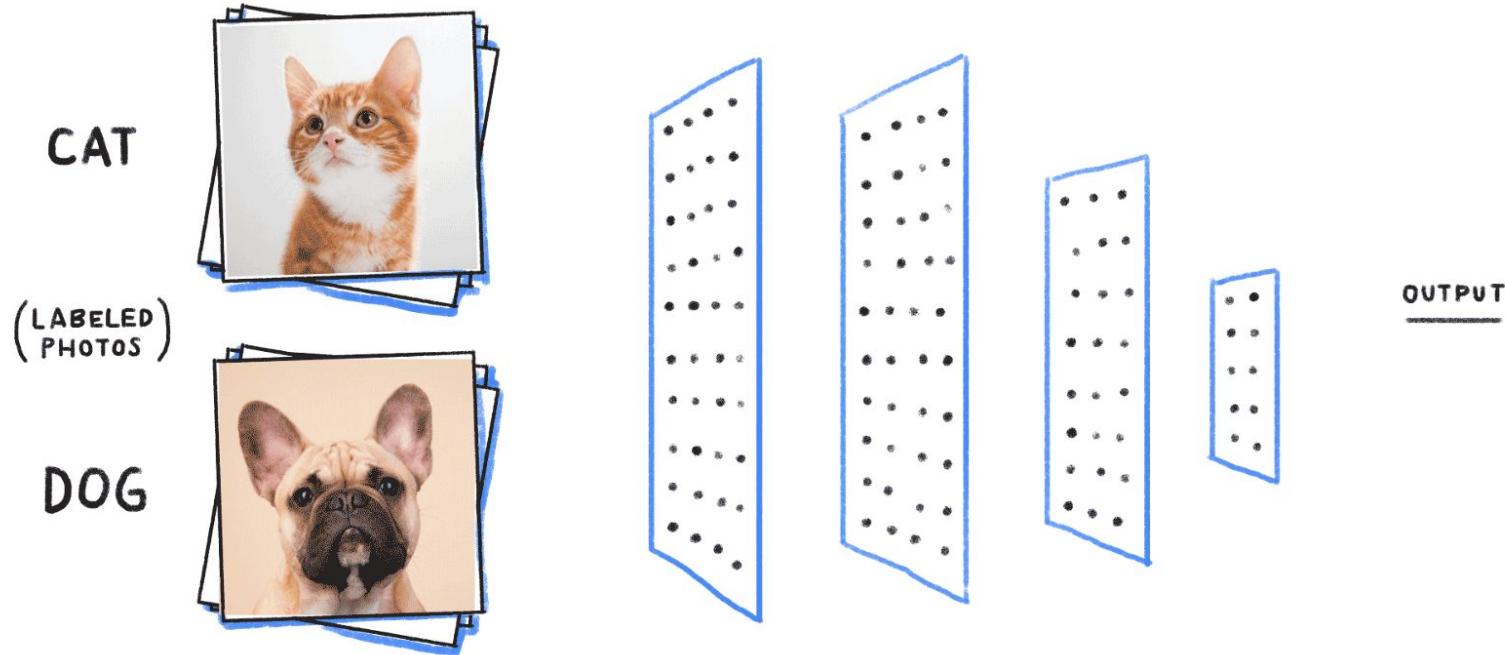
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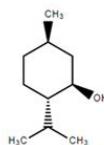
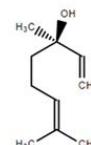
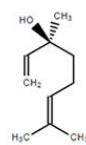
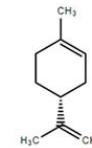
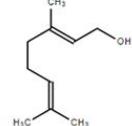
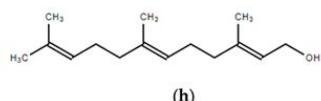
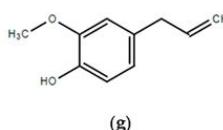
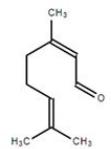
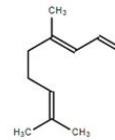
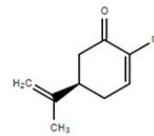
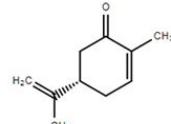
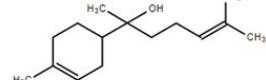
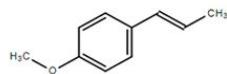


Learning the Odor Map with Data & Machine Learning *Today*.

Machine learning uses rectangles a lot

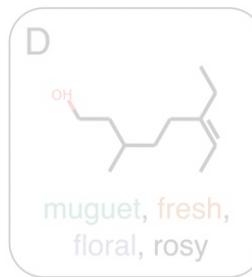
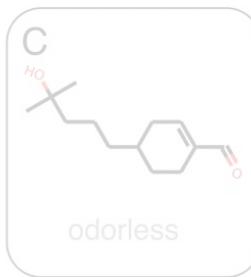
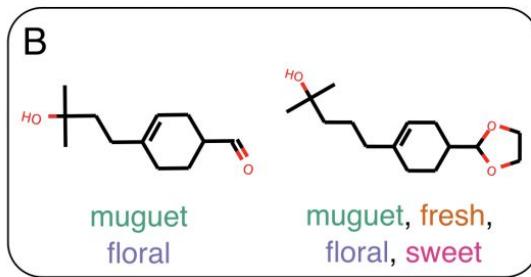
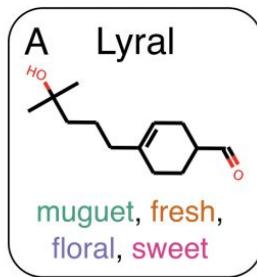


but molecules are not rectangles!



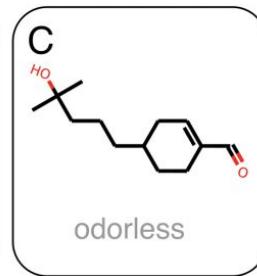
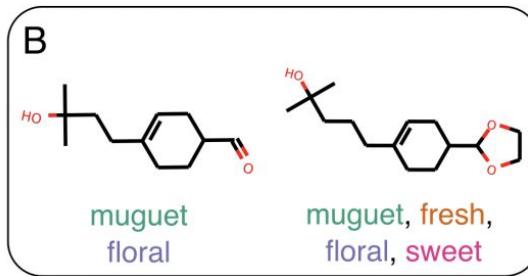
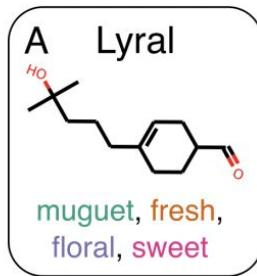
Structure ≠ Odor

Sell (2006)



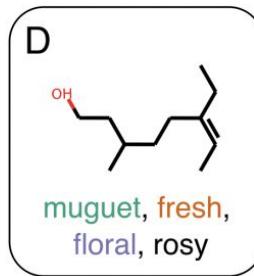
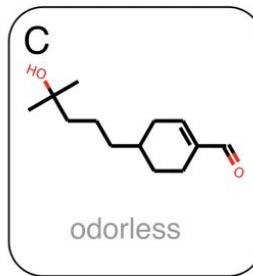
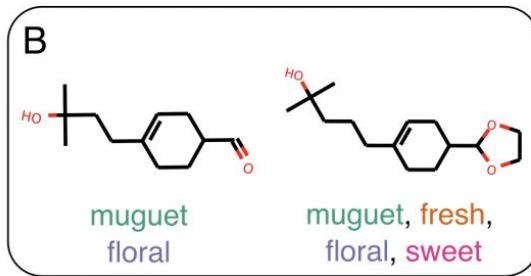
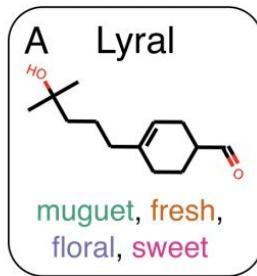
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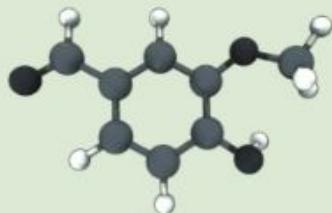
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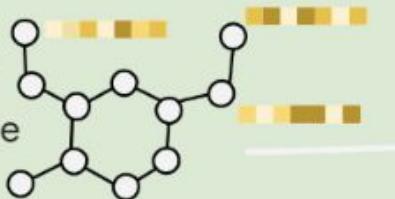


Graph Neural Network (GNN)

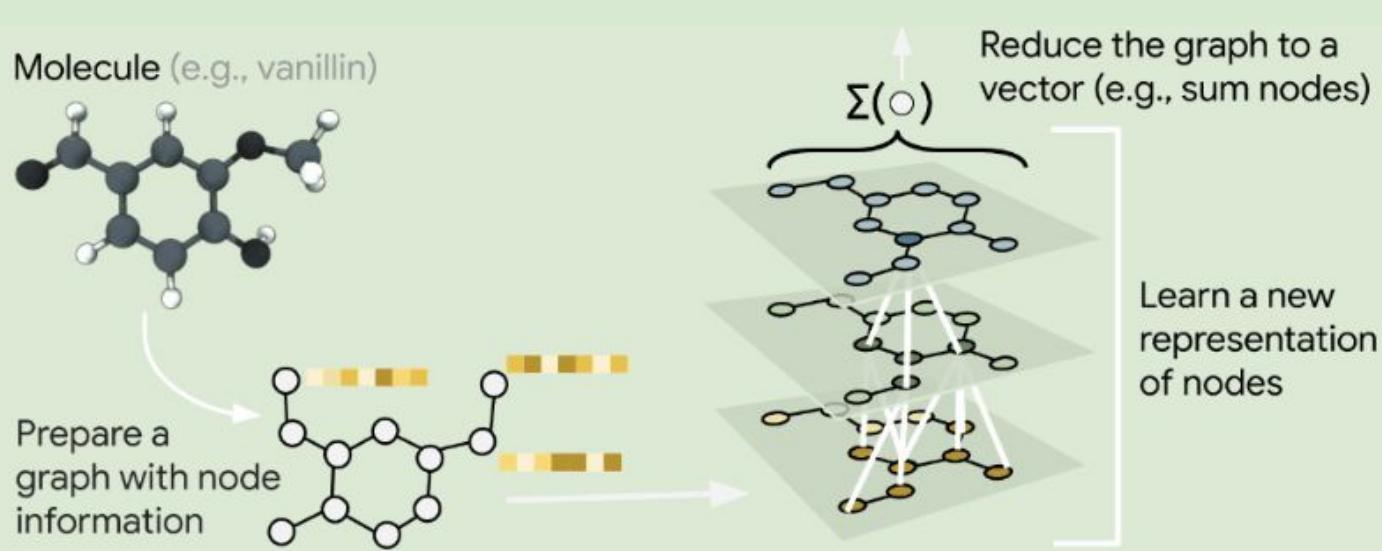
Molecule (e.g., vanillin)



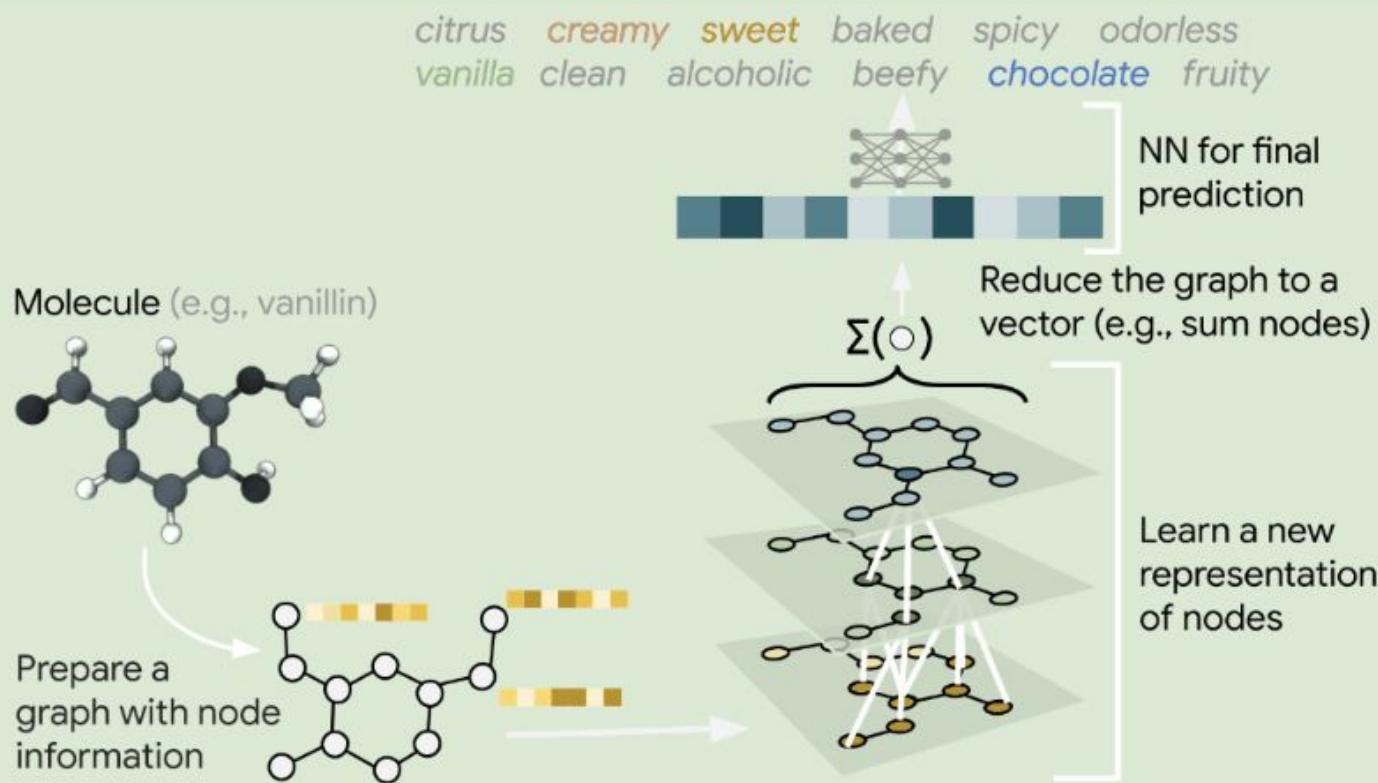
Prepare a
graph with node
information



Graph Neural Network (GNN)



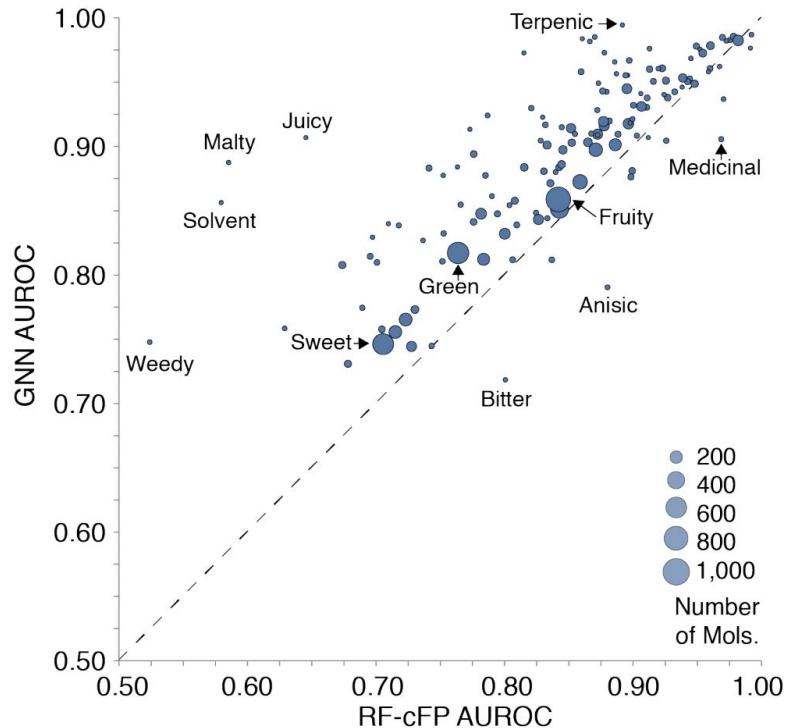
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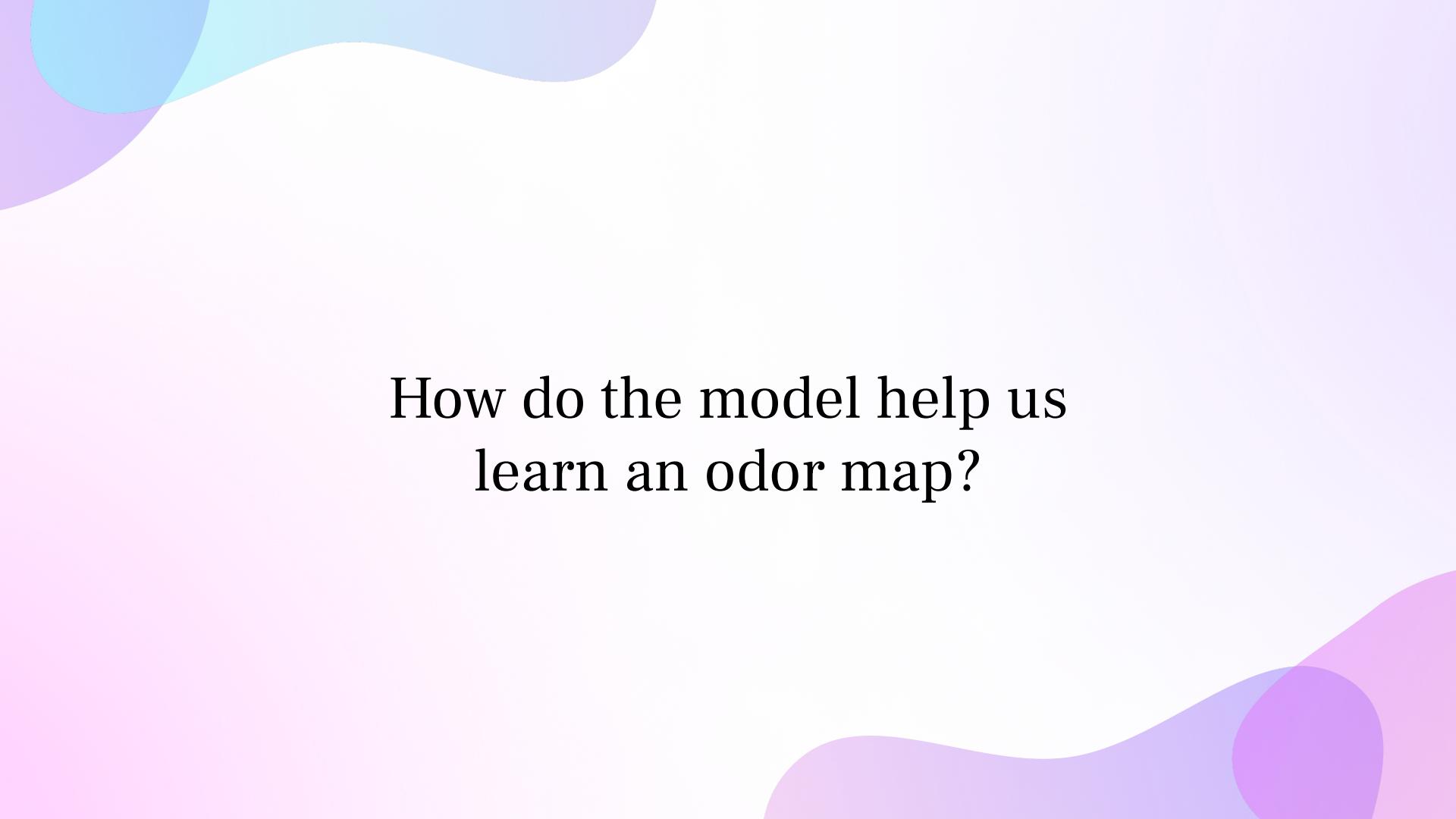


State of the art model for predicting odor labels of molecules

Sanchez-Lengeling et al. (2019)

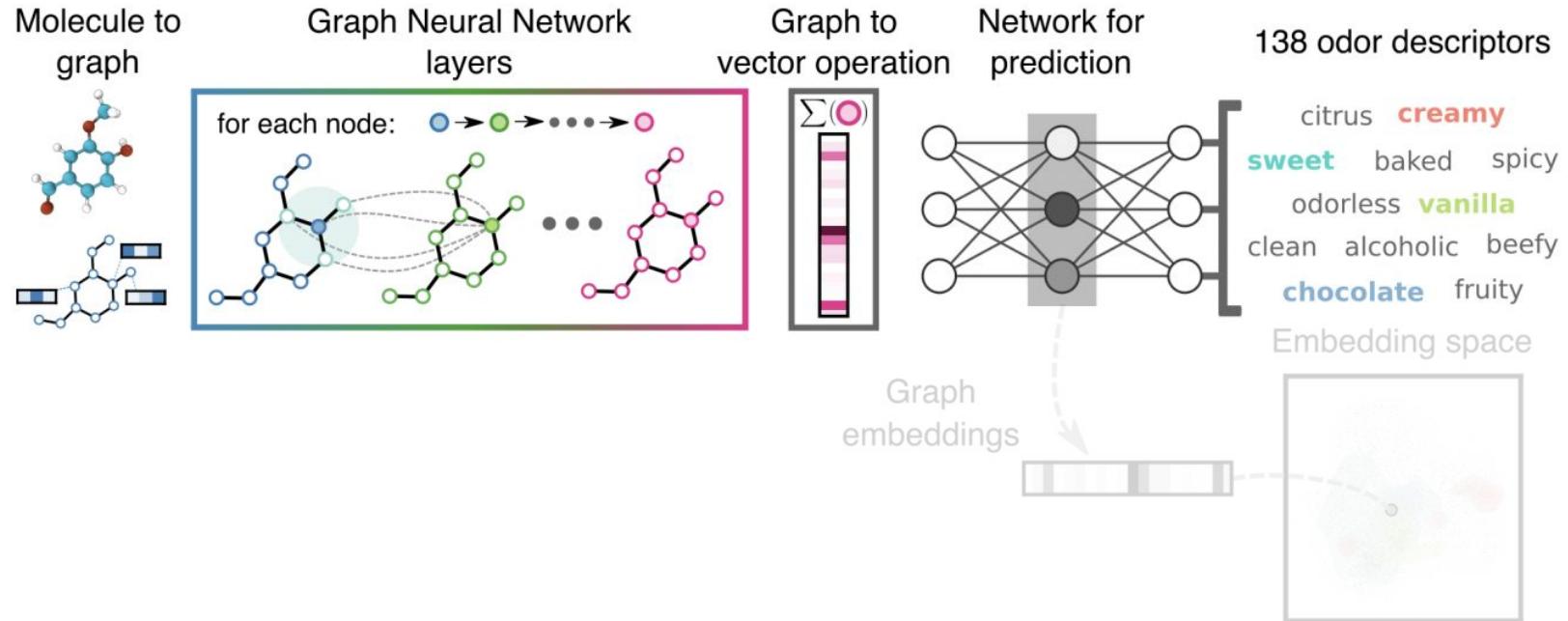
- Curated ~5000 labeled odor molecules
- Compared against traditional cheminformatic approach with structural fingerprints and random forest models.
- You can learn odor from molecular structure with GNN!



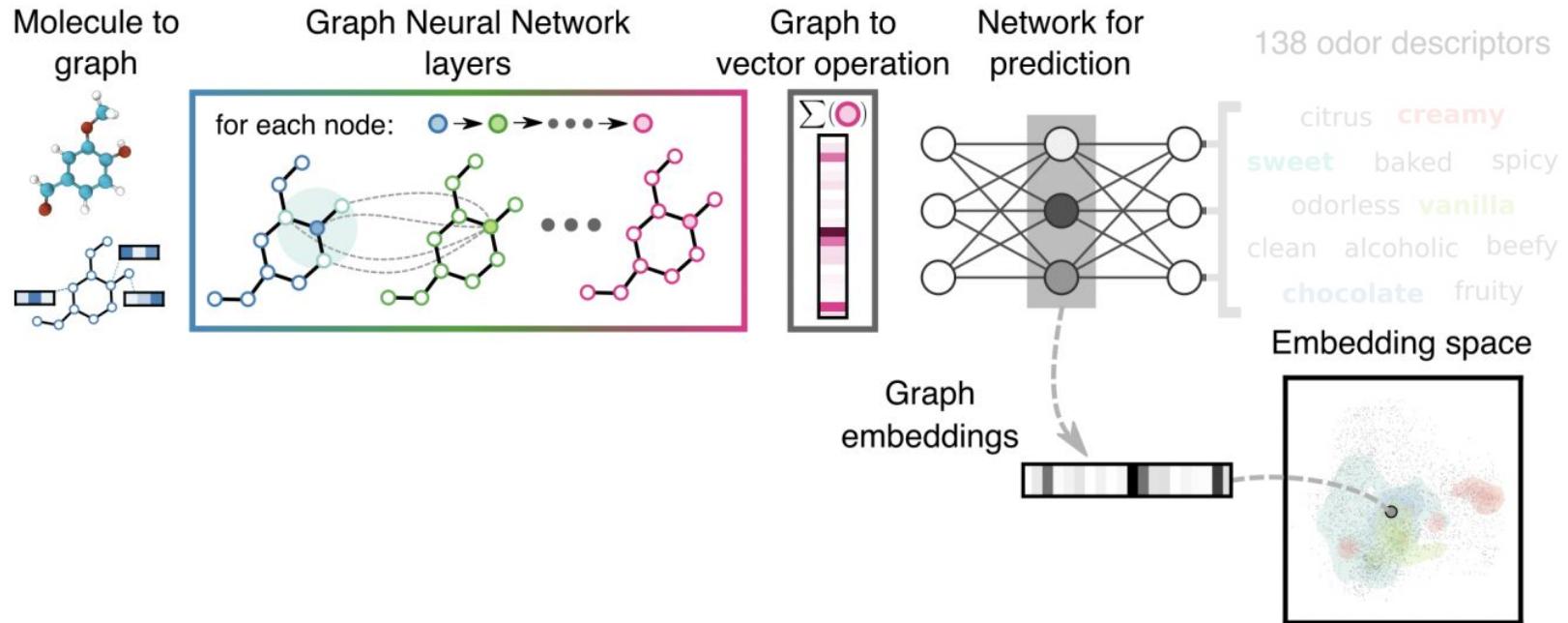


How do the model help us
learn an odor map?

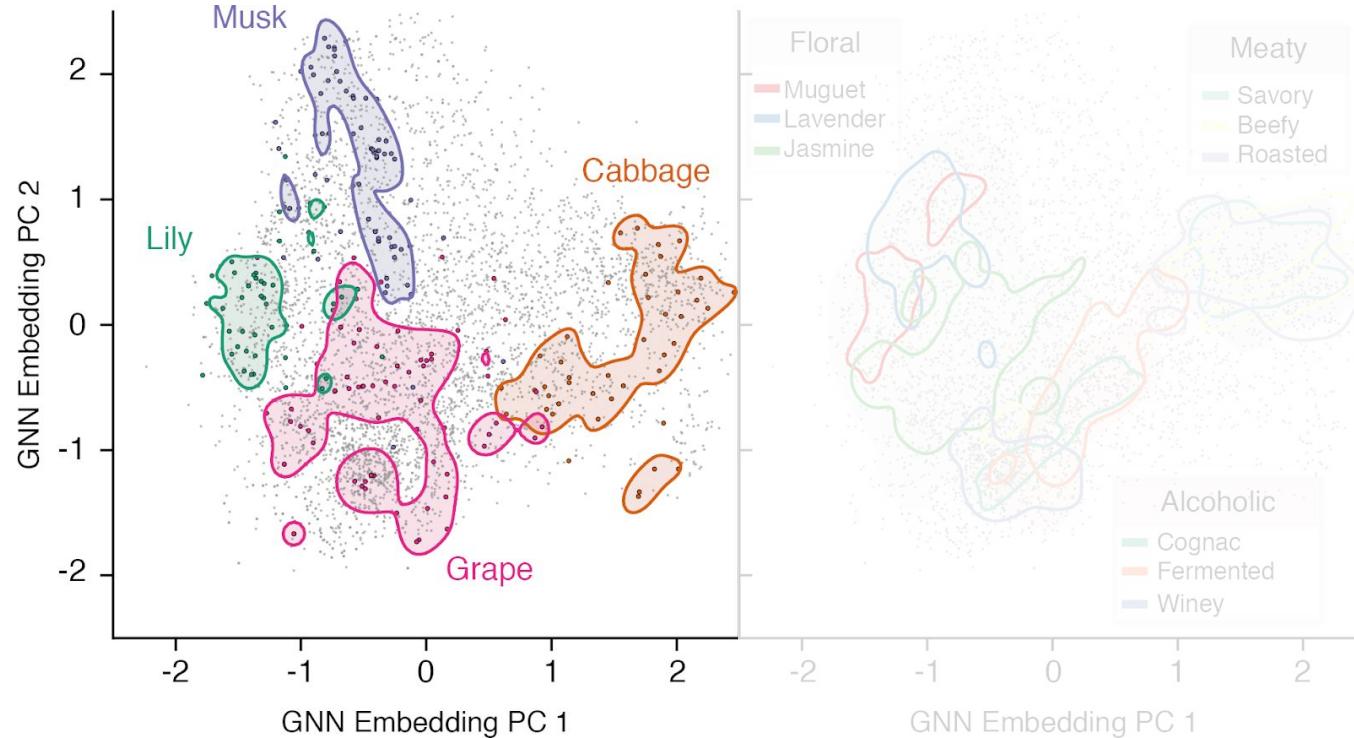
Neural Network Embedding



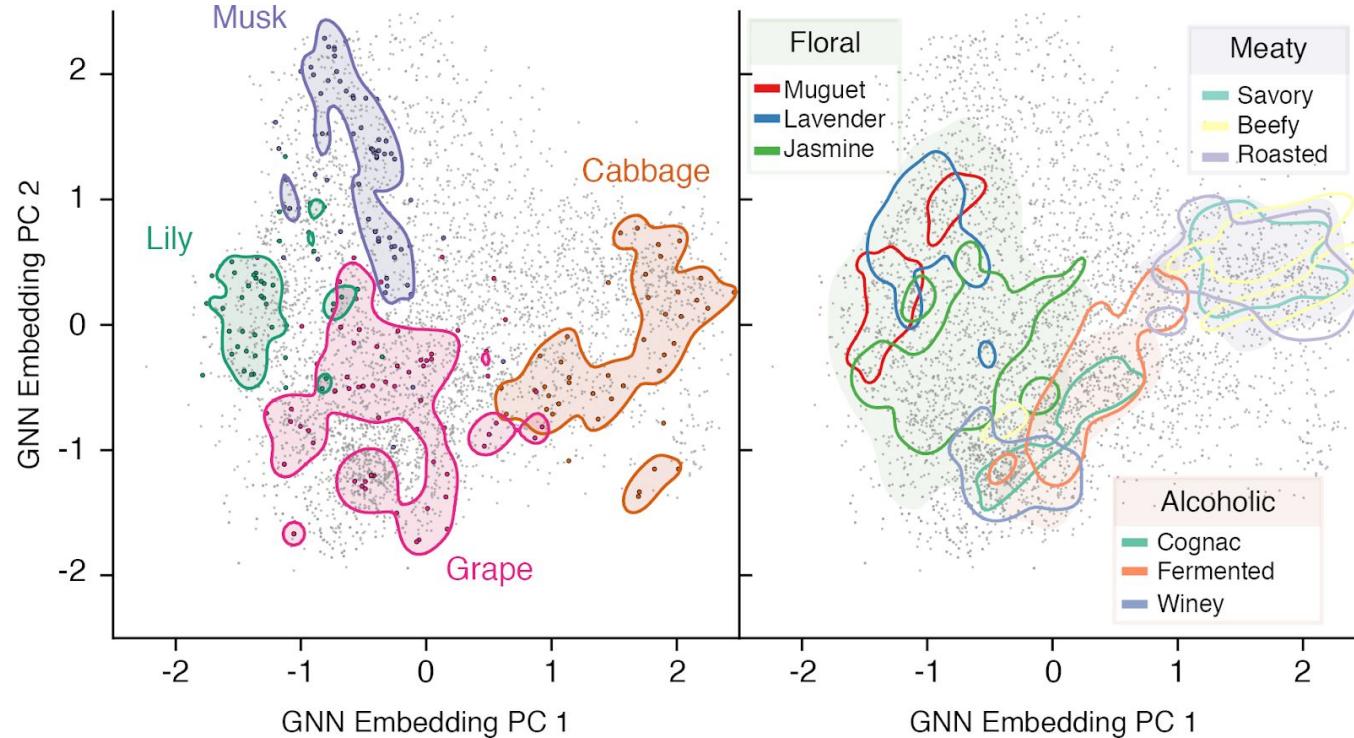
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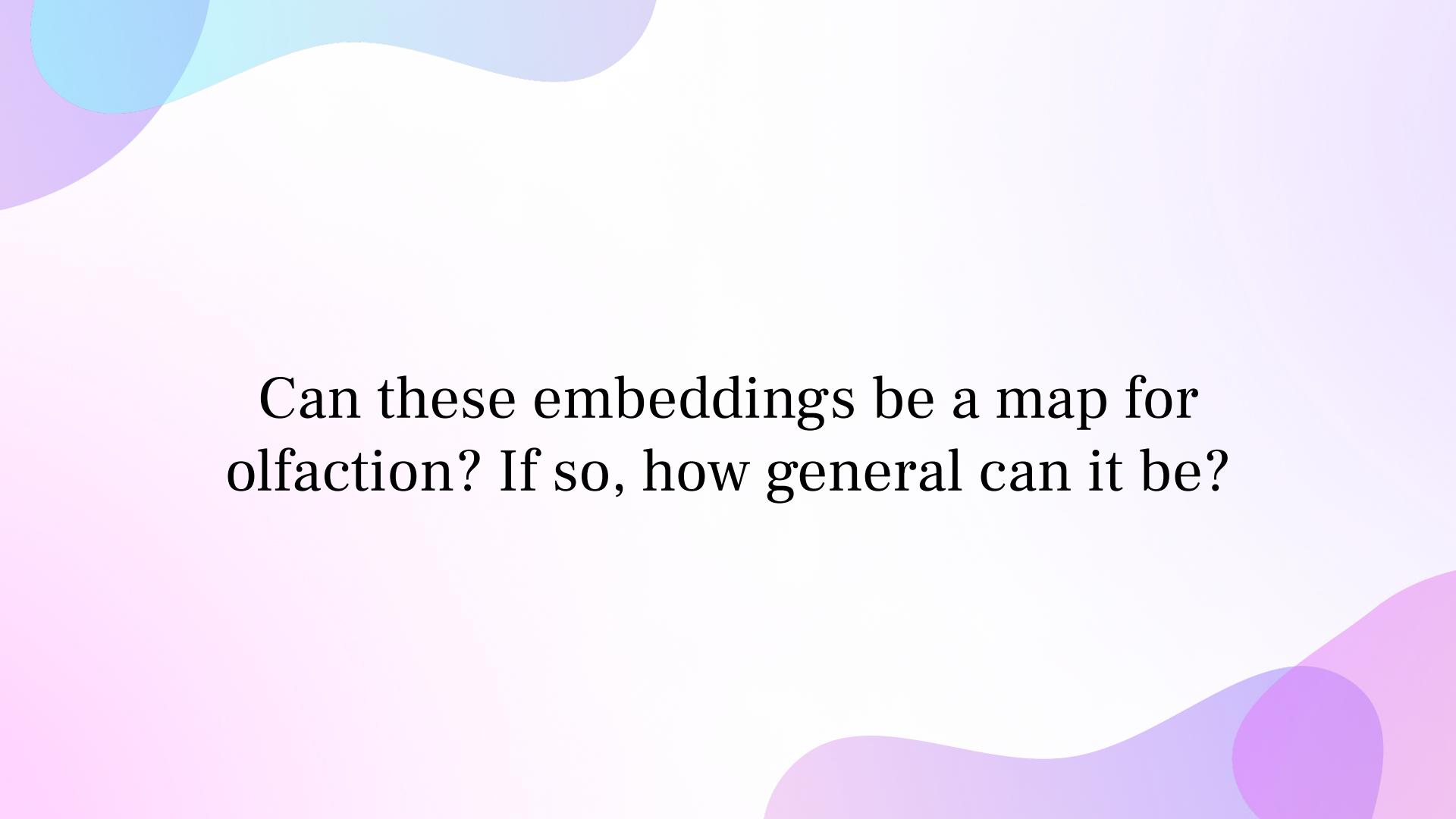


Embeddings organized molecules logically.



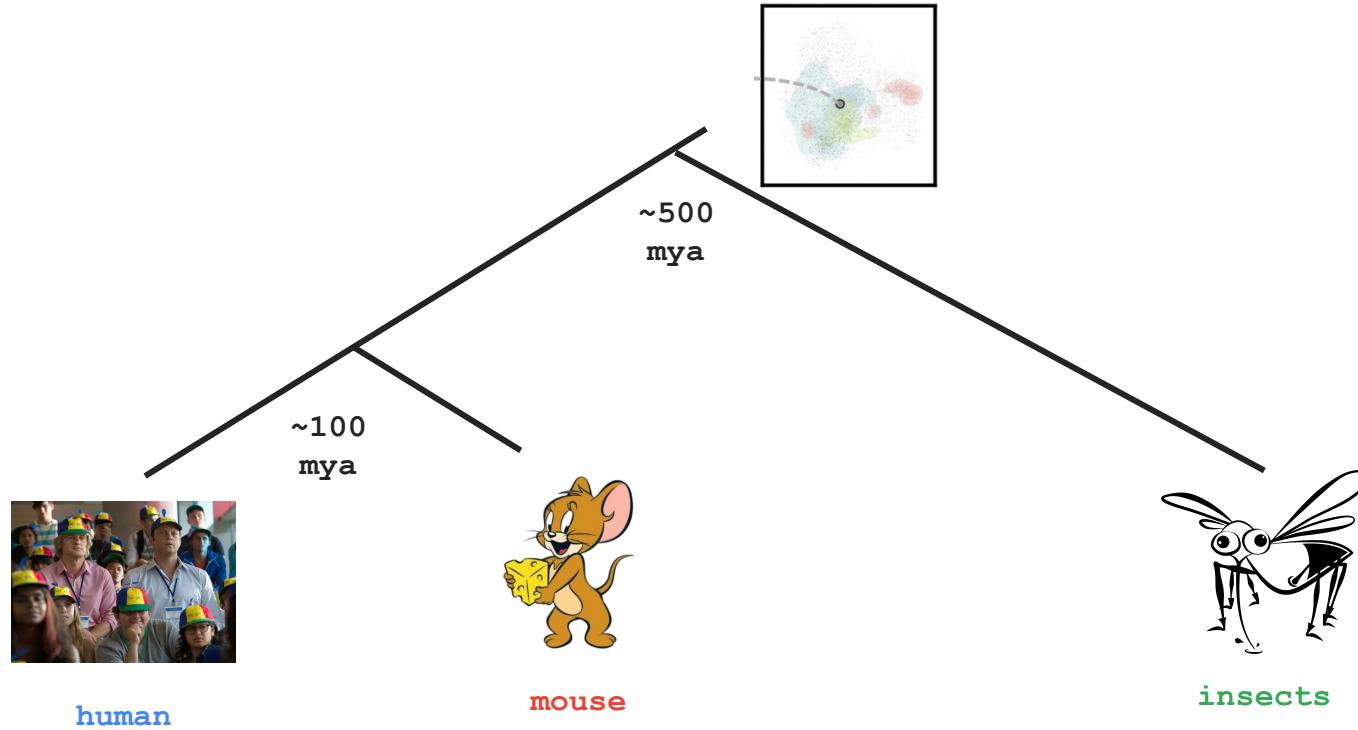
Embeddings organized molecules logically.





Can these embeddings be a map for
olfaction? If so, how general can it be?

Transfer learning across different species.



Transfer learning across different species.

Why this might NOT work?

- Biological implementations are different:
 - GPCR for mammals
 - Non-GPCR + Ion Channels for insects

Why this might work?

- Convergent evolution!

Transfer learning across different species.

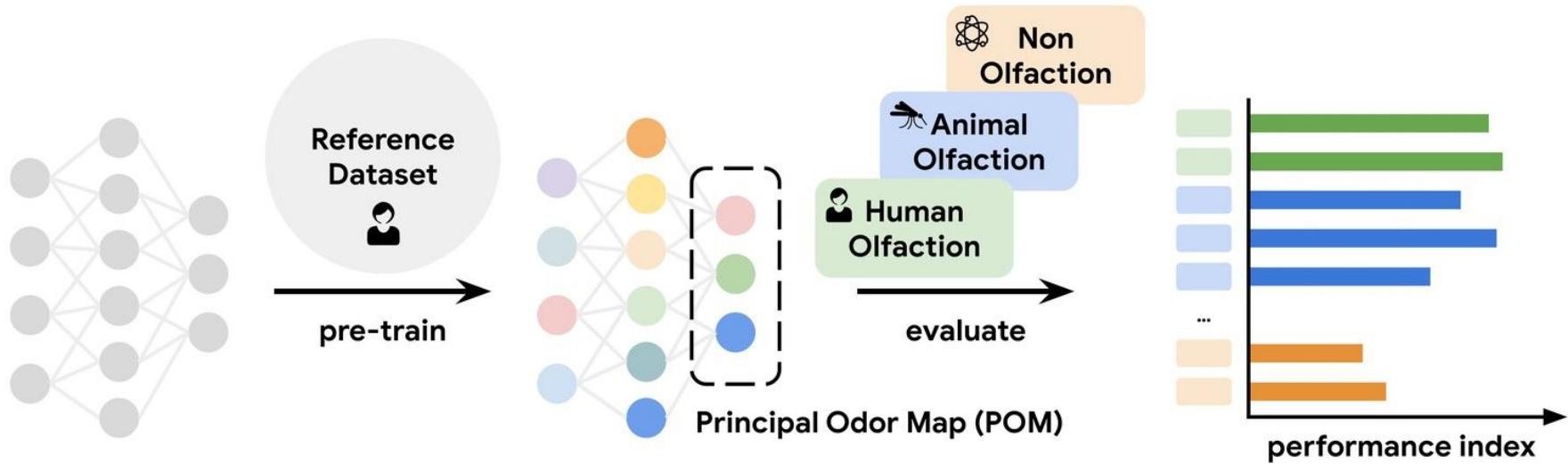
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Olfaction agnostic representations

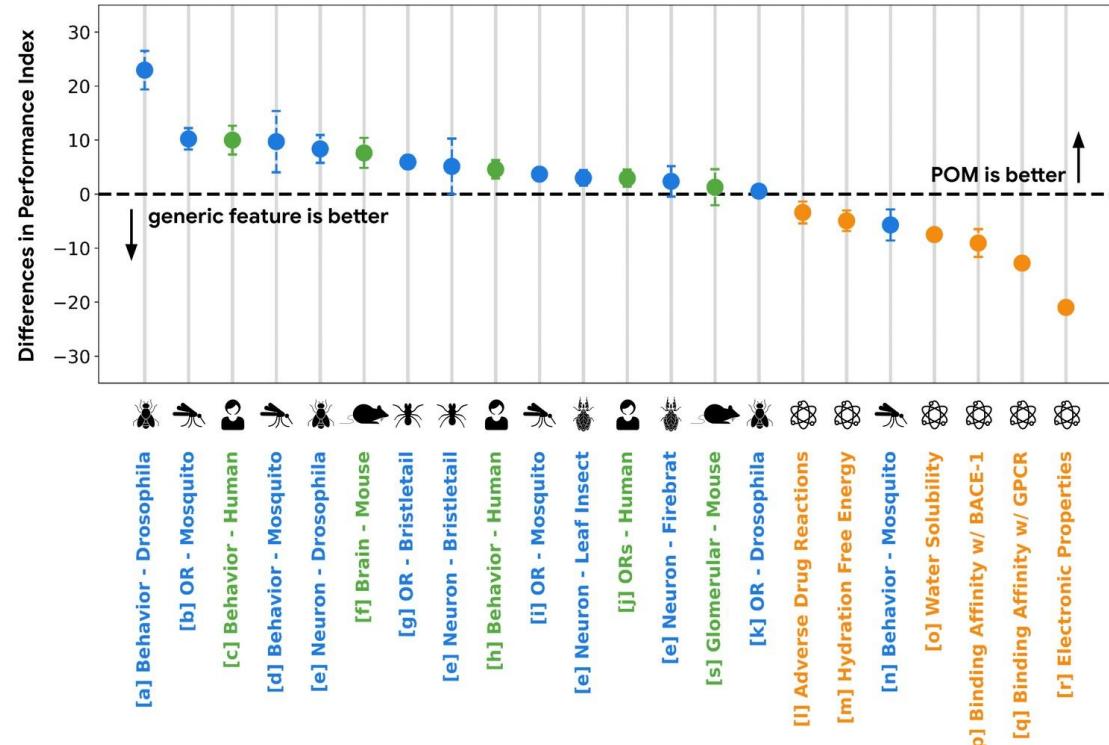
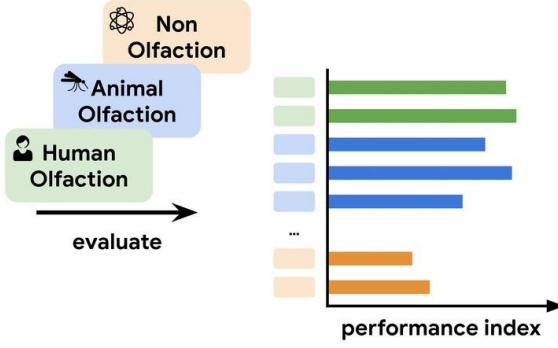
Structure Fingerprints

- N-dim vectors (cFP / bFP)
- standard tool developed to capture small motifs in the molecules
- serves as a strong baseline here

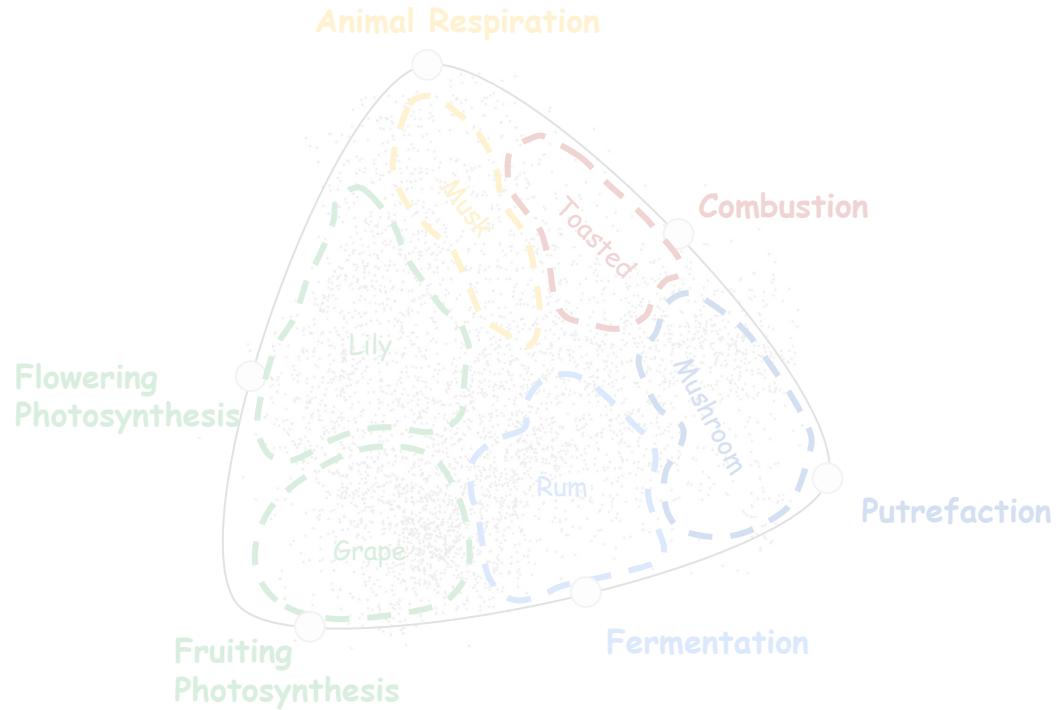
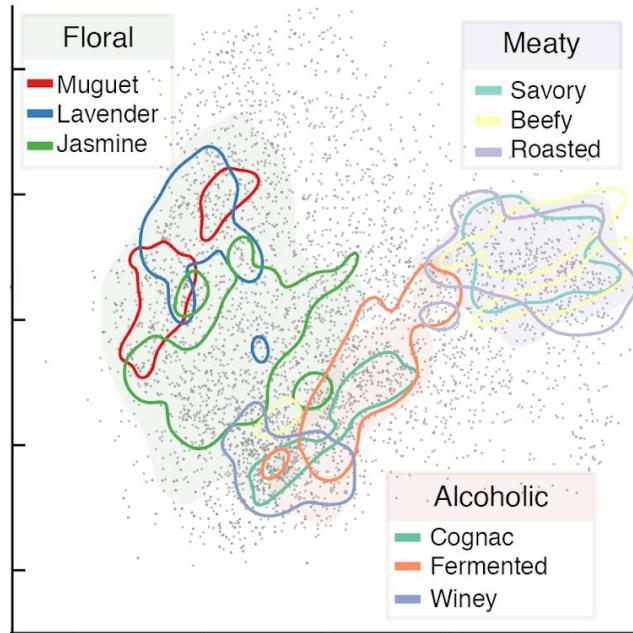
Mordred/Dragon Descriptors

- 2873-dim vectors
- common descriptors used in the field of chemoinformatics
- computed physical and chemical properties of the molecule

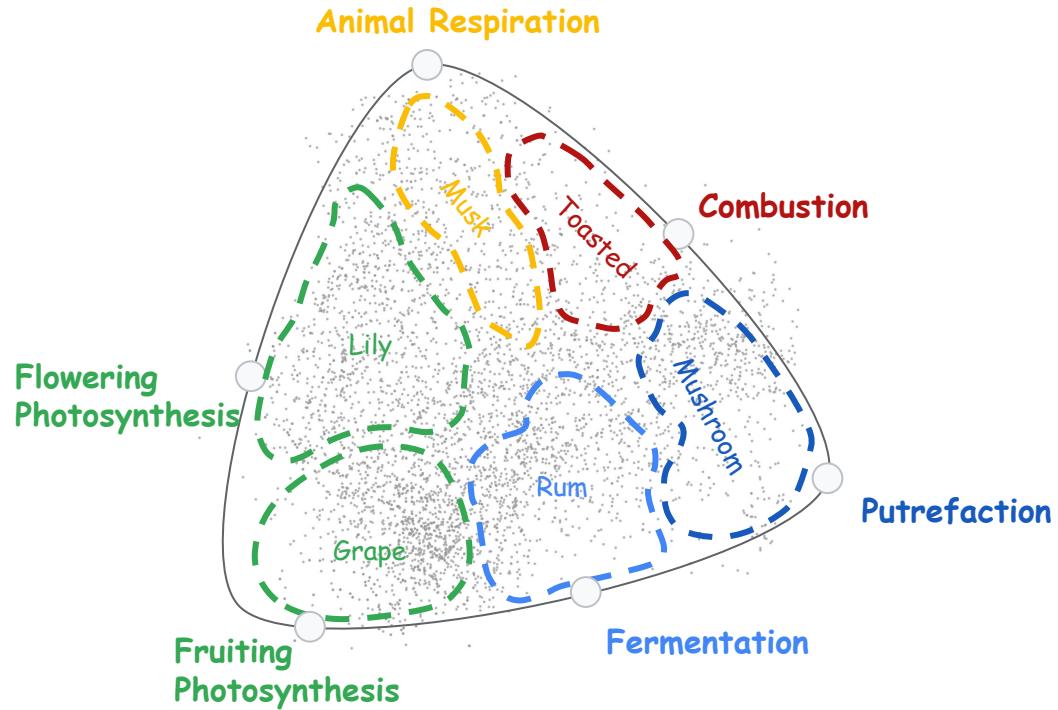
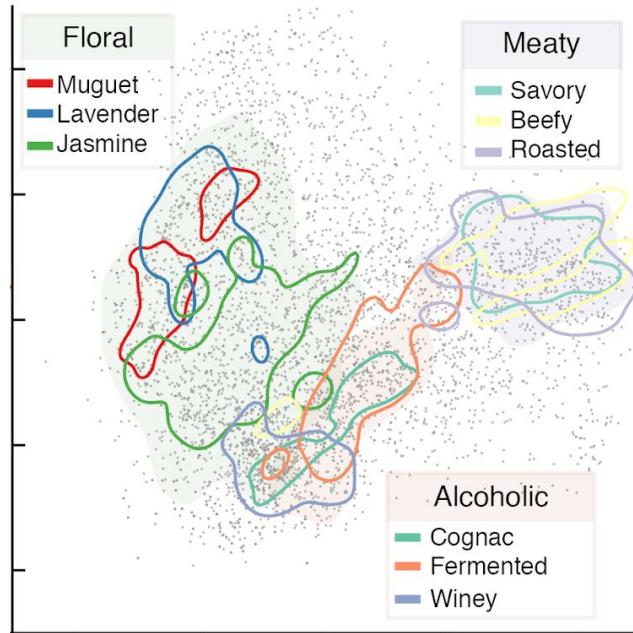
POM generalizes across 500M years of evolution.



And maybe we should look at the embedding differently?

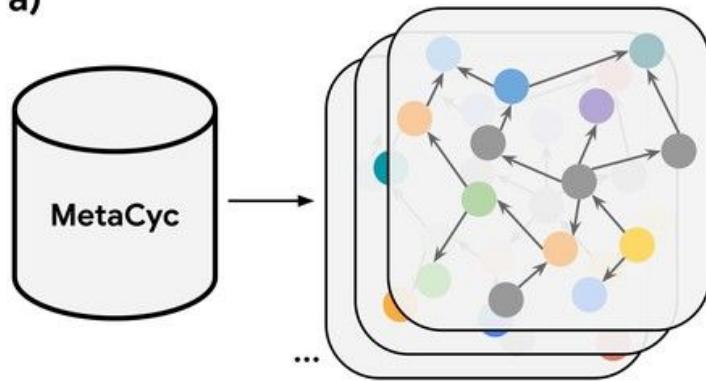


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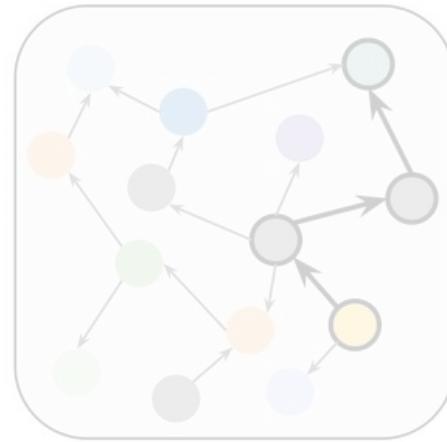
Could POM be organized by metabolic activity?

a)



construct a directed graph of metabolites with experimentally elucidated metabolic reactions

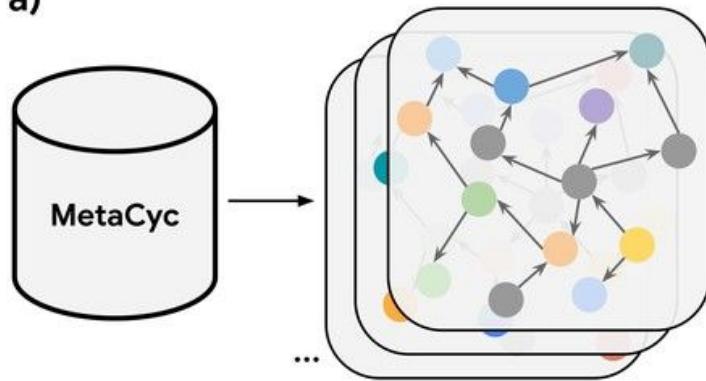
b)



metabolic distance(,) = 3

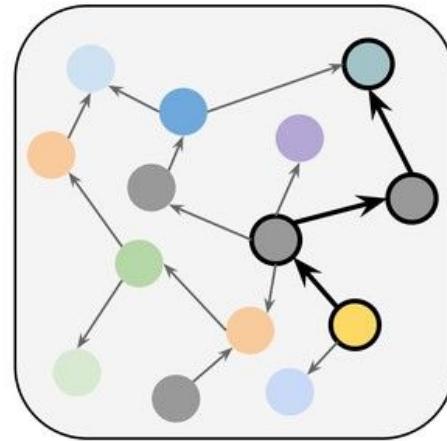
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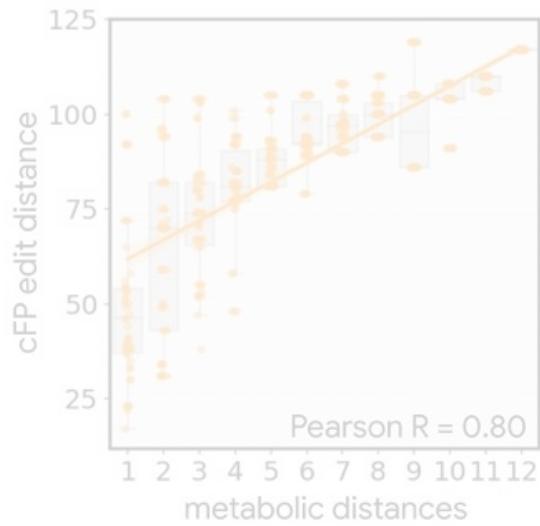
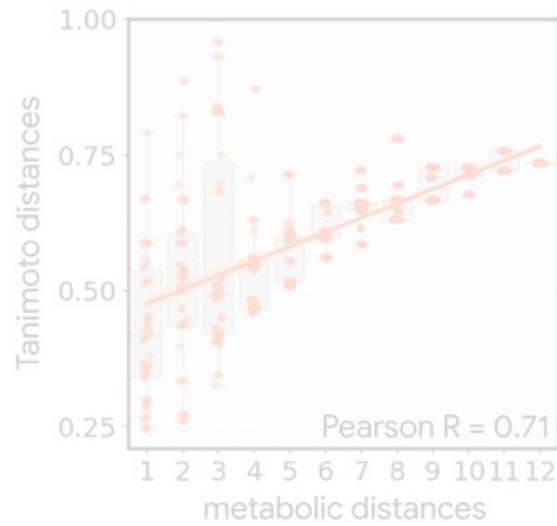
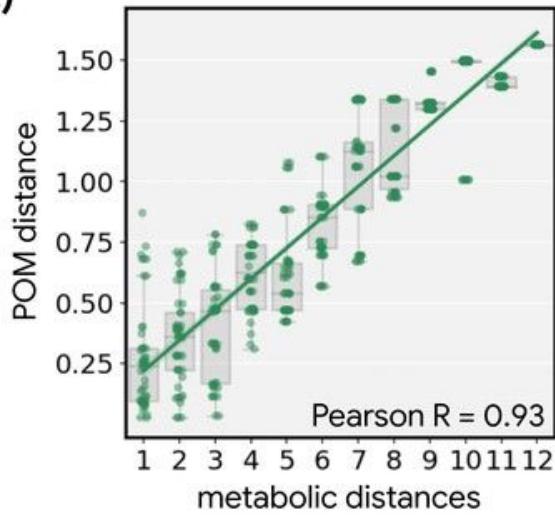
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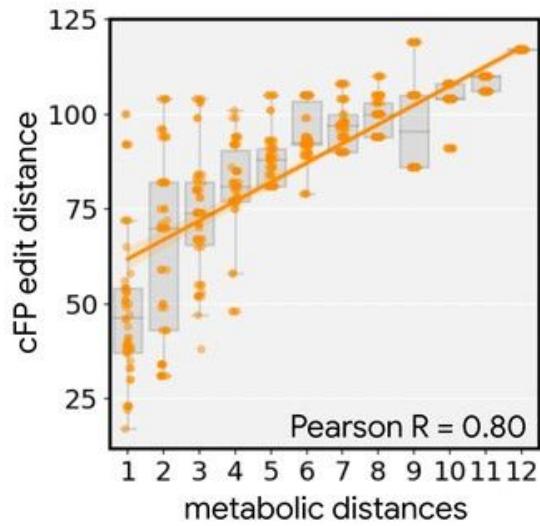
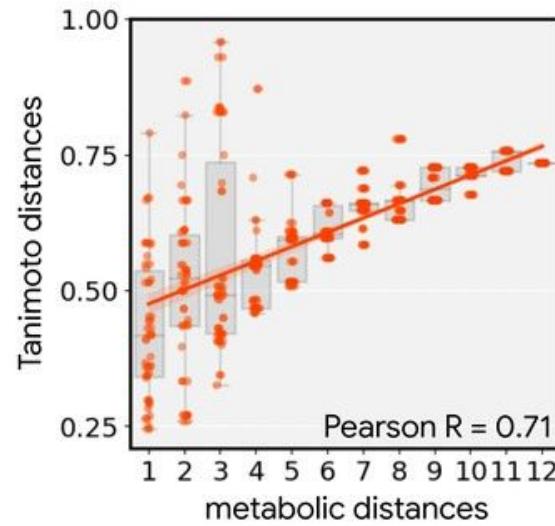
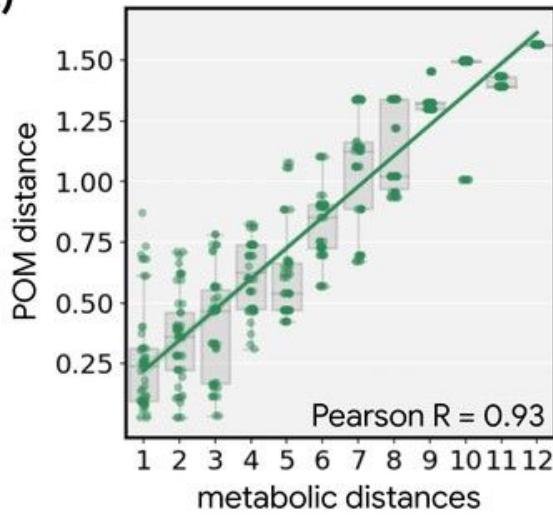
POM is strongly correlated with nature's metabolome.

c)



POM is strongly correlated with nature's metabolome.

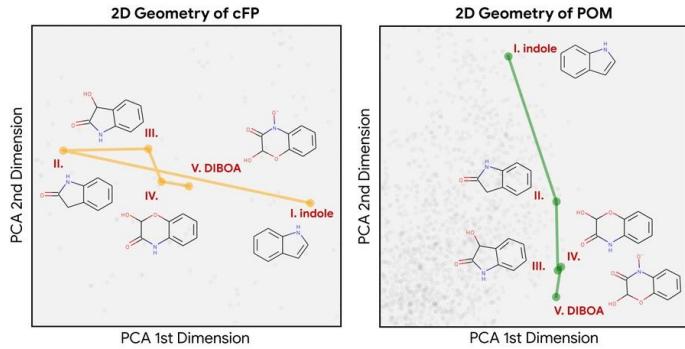
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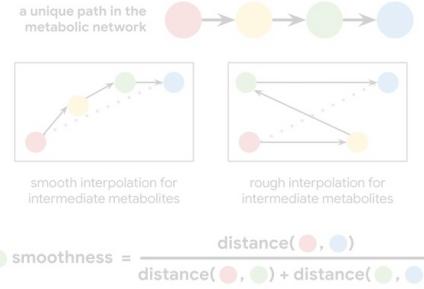
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a)

DIBOA-Glucoside Biosynthesis

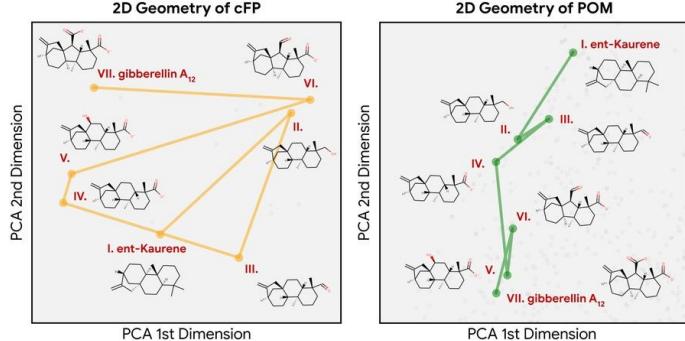


c)

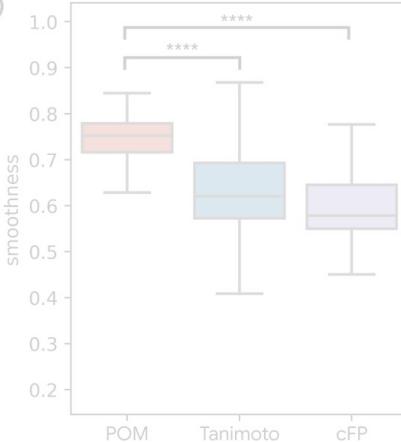


b)

Gibberellin Biosynthesis



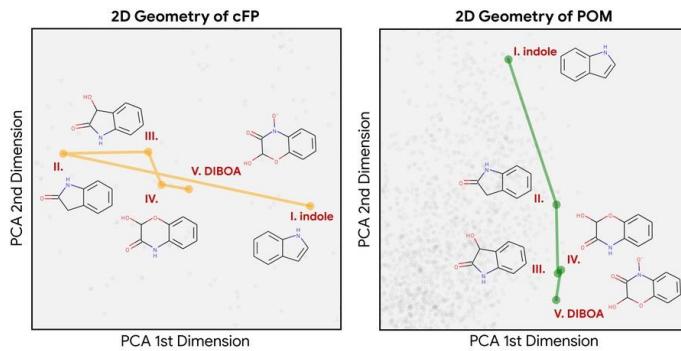
d)



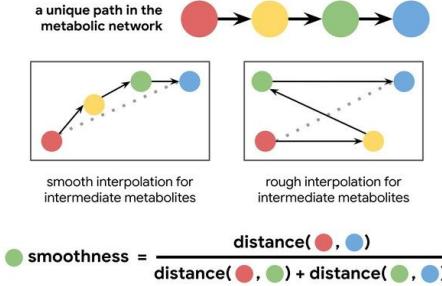
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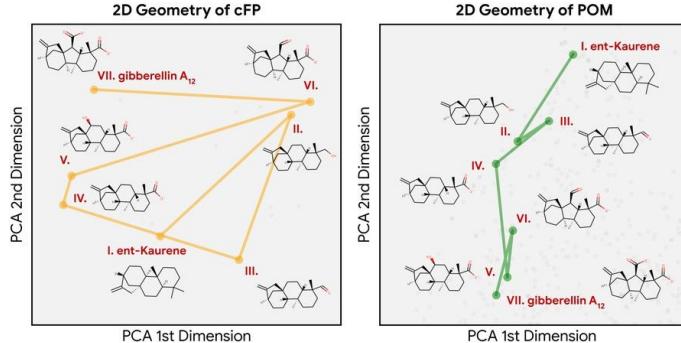


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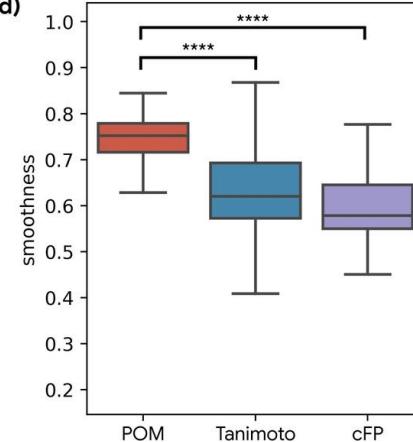


b)

Gibberellin Biosynthesis

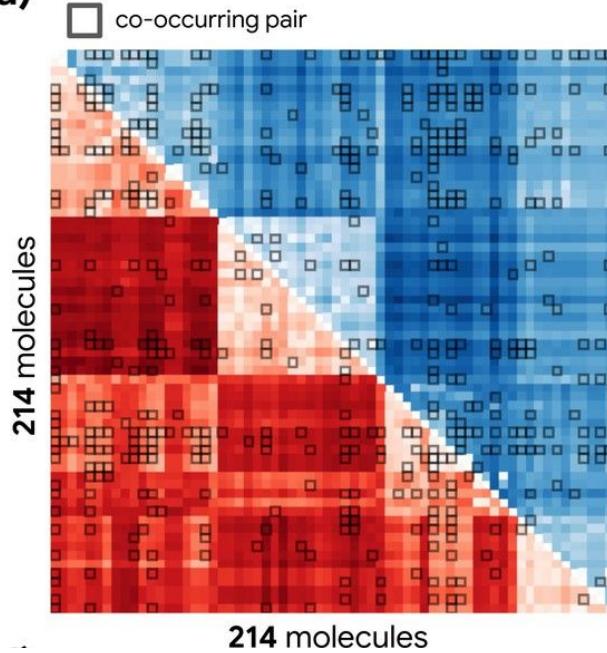


d)



Co-occurring natural molecules should also be nearby in POM?

a)



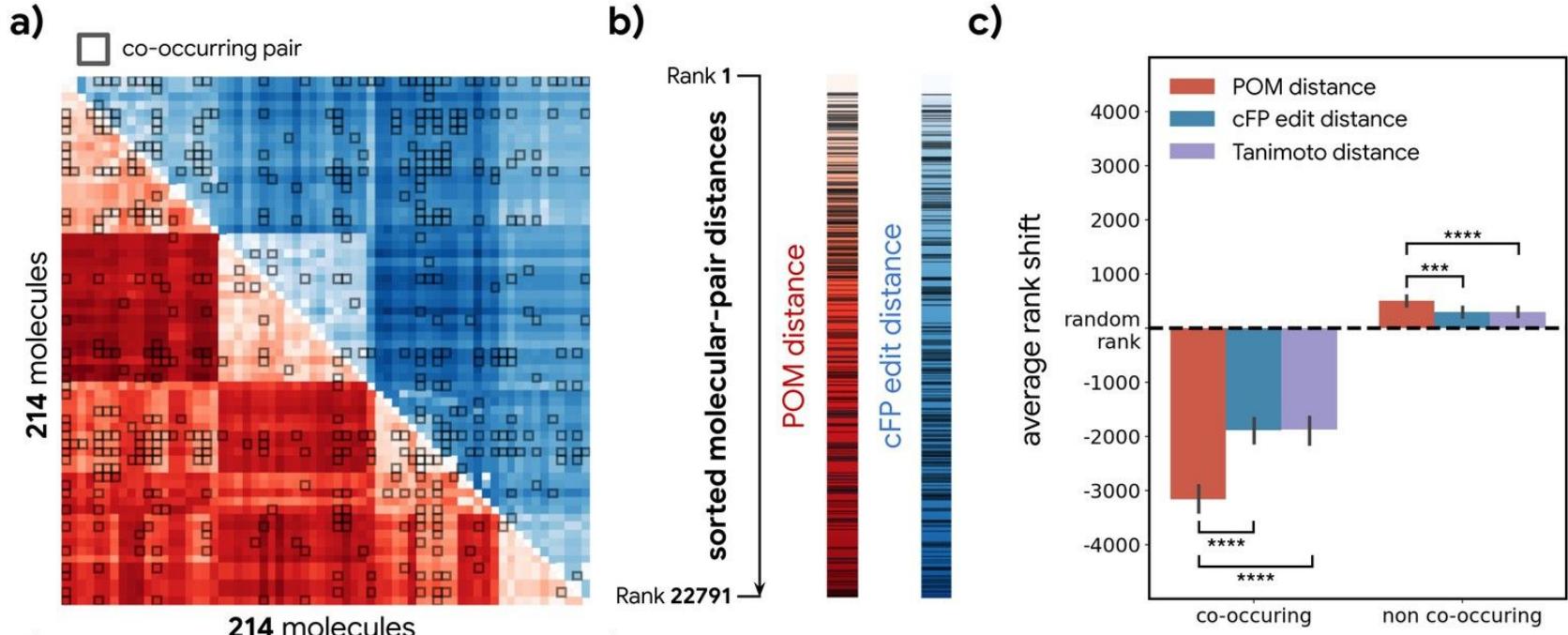
b)

Rank 1
sorted molecular-pair distances
POM distance
Rank 22791

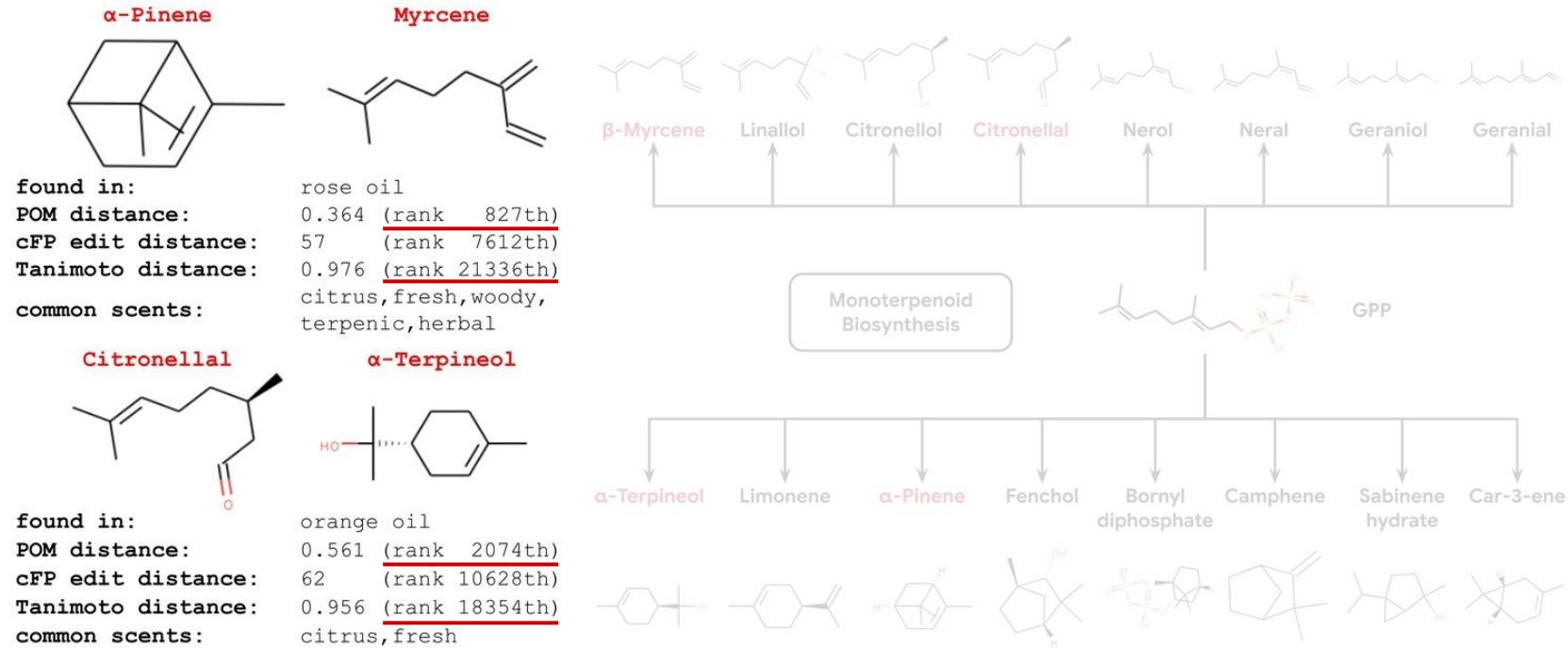
c)



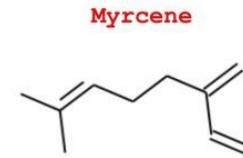
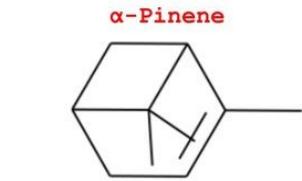
POM is tuned by the odor statistics of nature.



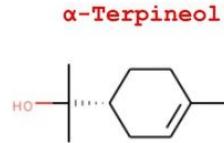
POM is tuned by the odor statistics of nature.



POM is tuned by the odor statistics of nature.

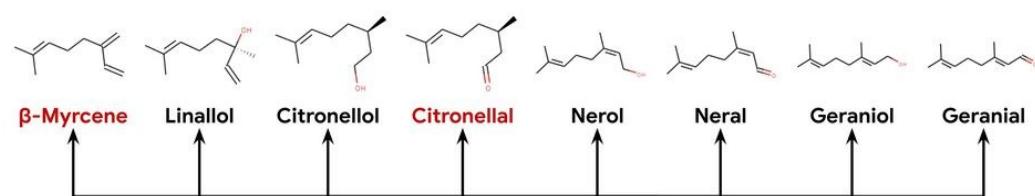


rose oil
0.364 (rank 827th)
57 (rank 7612th)
0.976 (rank 21336th)
citrus, fresh, woody,
terpenic, herbal

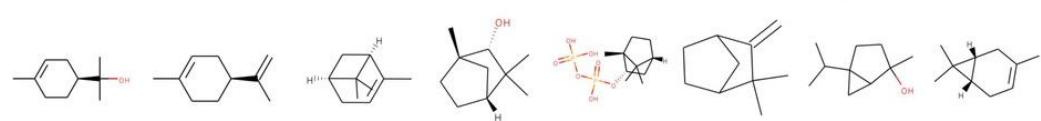
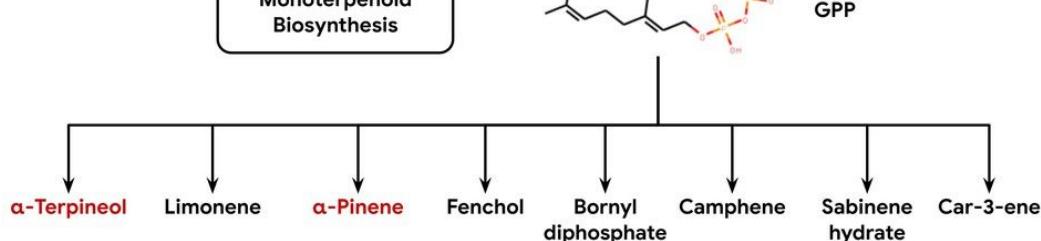
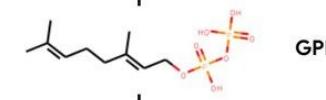


found in:
POM distance:
cFP edit distance:
Tanimoto distance:
common scents:

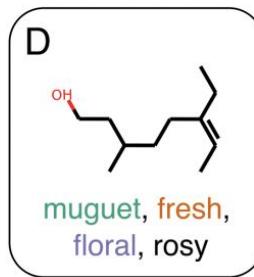
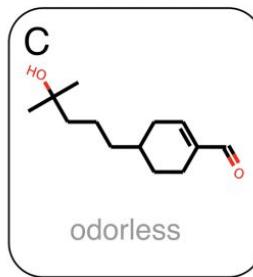
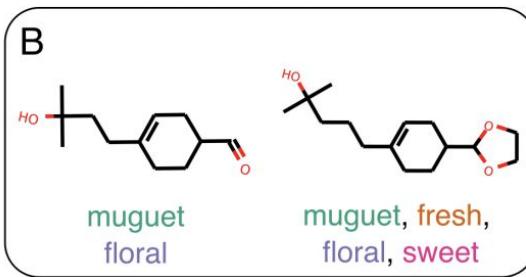
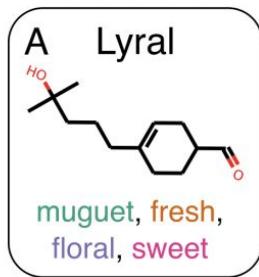
orange oil
0.561 (rank 2074th)
62 (rank 10628th)
0.956 (rank 18354th)
citrus, fresh

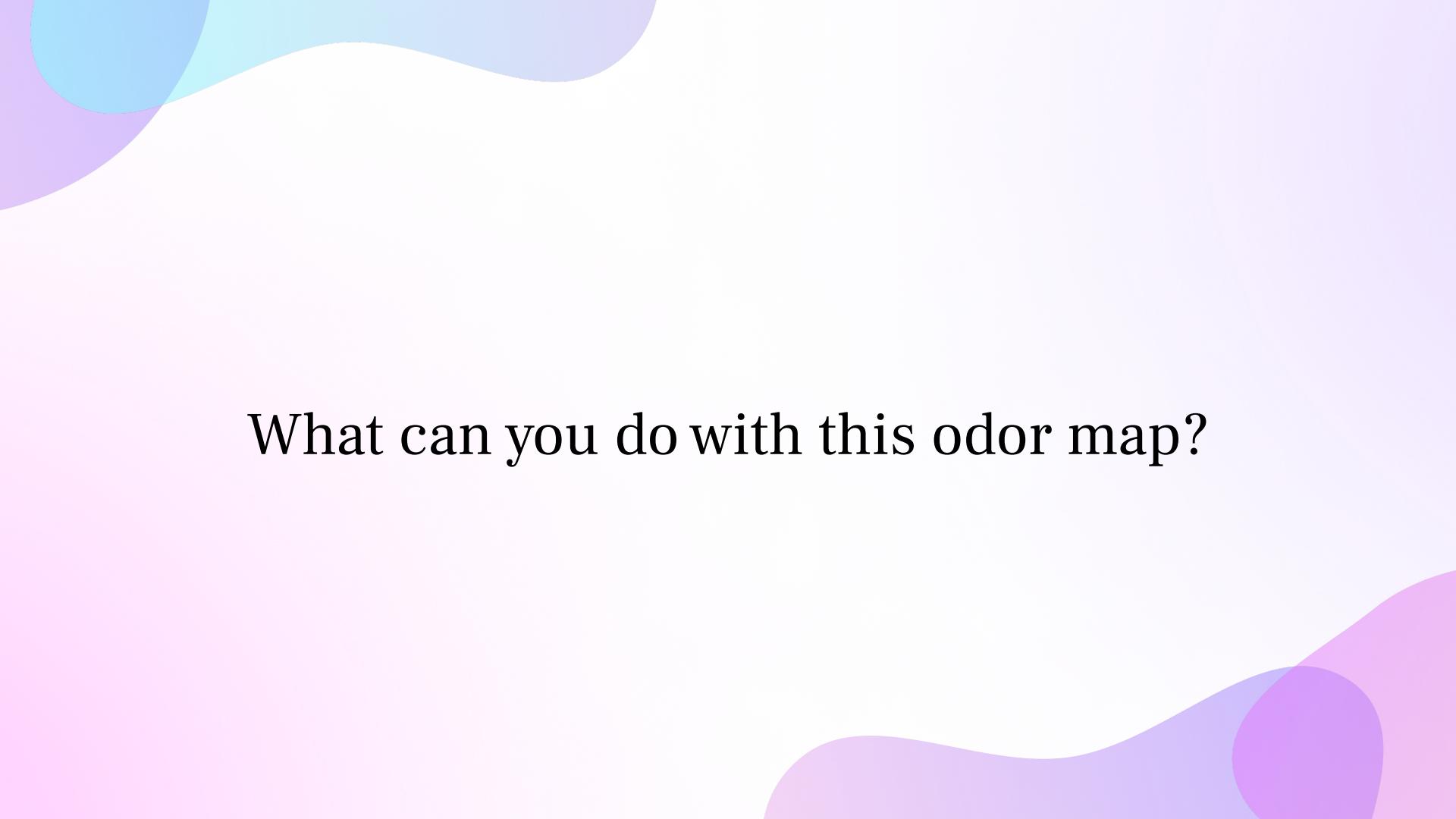


Monoterpene Biosynthesis



which could also explain why structure ≠ odor



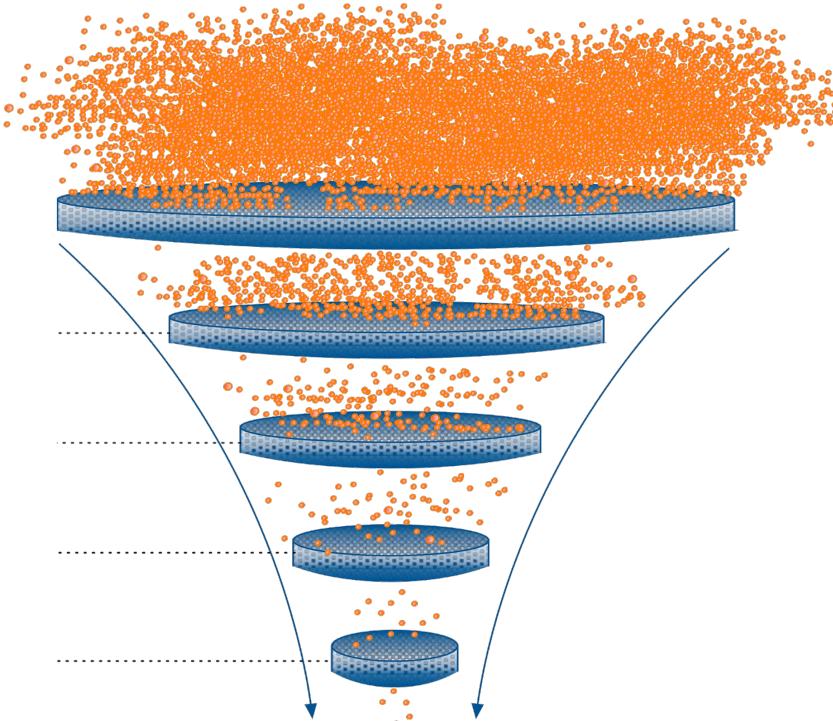


What can you do with this odor map?

Molecular discovery for new fragrance ingredients

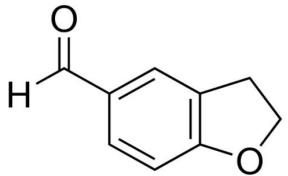
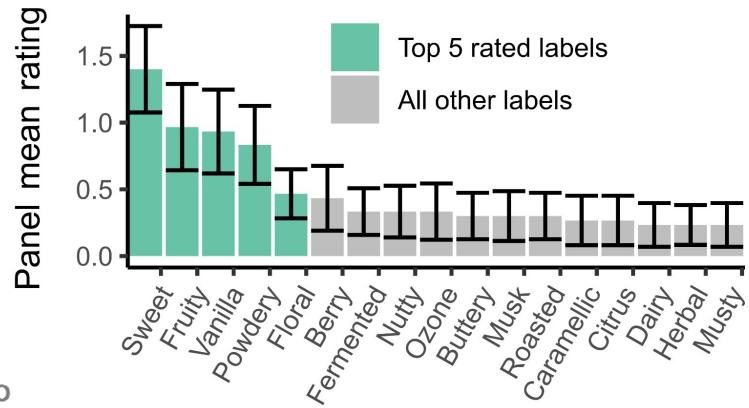
A prospective validation study

Molecule can be ordered	7 M
"Likely" to be odorous	4 M
Price < \$1k per 10 g	90K
Safe (non-toxic)	89K
Testable Quickly	400



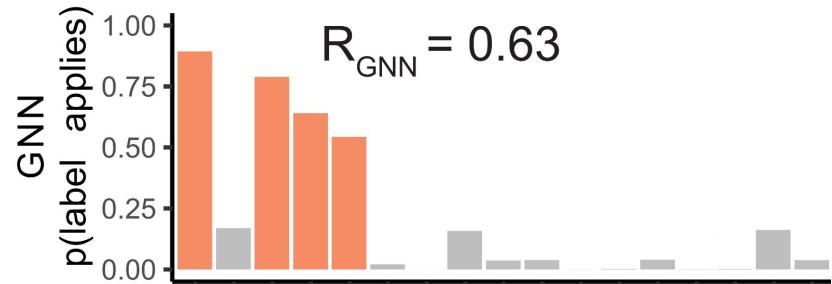
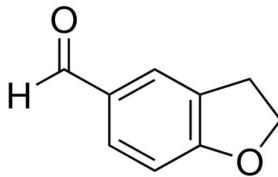
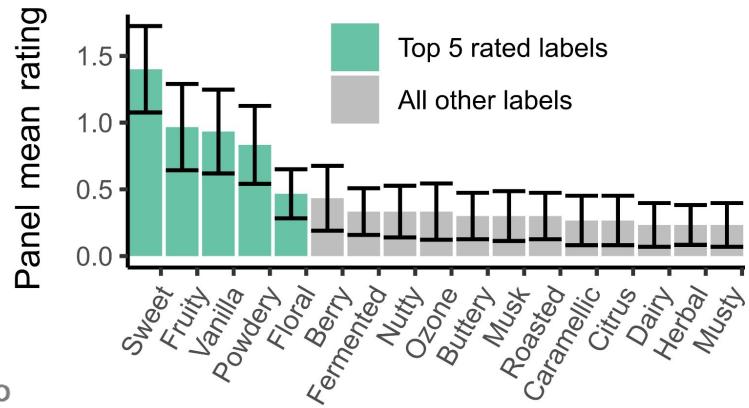
Molecular discovery for new fragrance ingredients

A prospective validation study



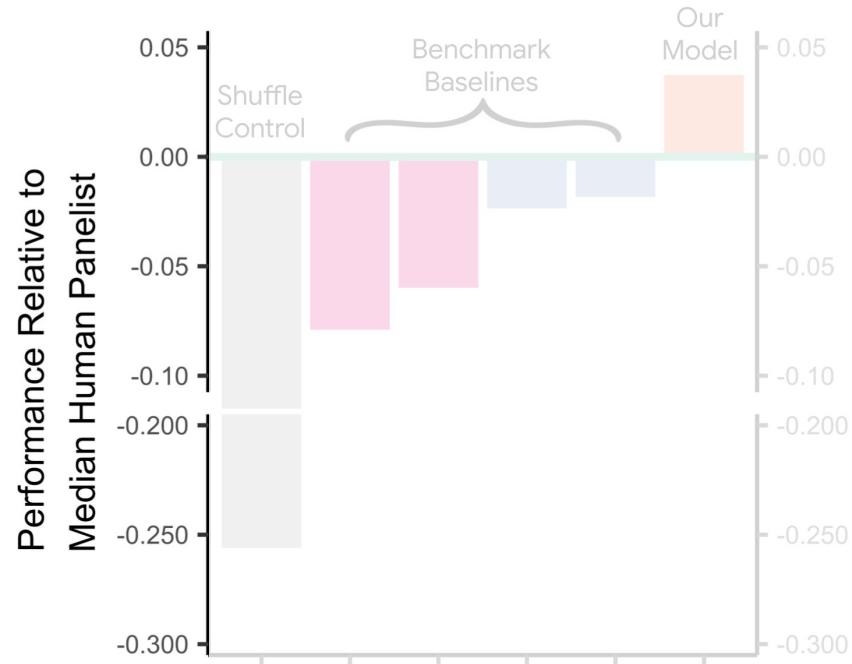
Molecular discovery for new fragrance ingredients

A prospective validation study



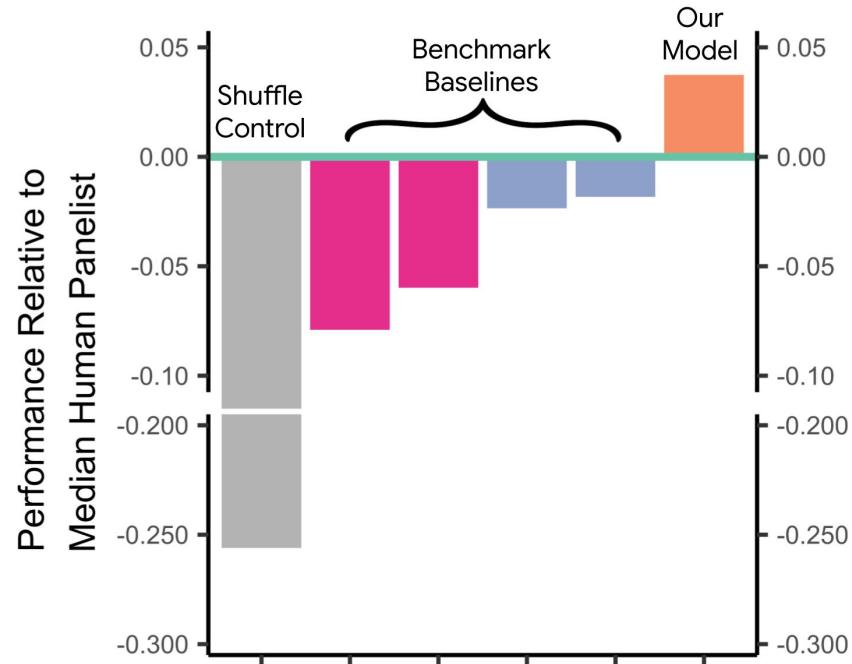
Molecular discovery for new fragrance ingredients

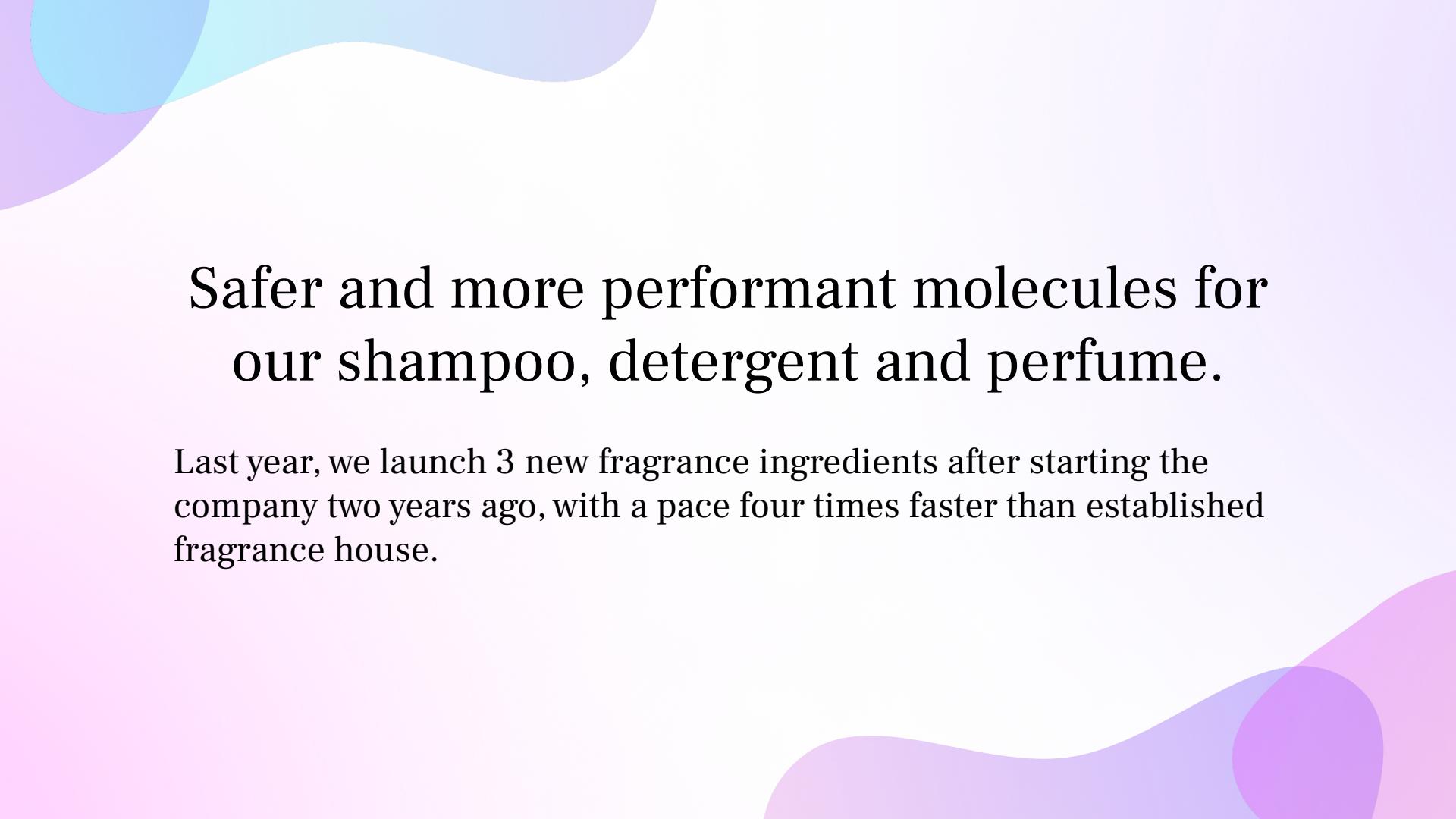
Outperform existing methods and average annotator



Molecular discovery for new fragrance ingredients

Outperform existing methods and average annotator



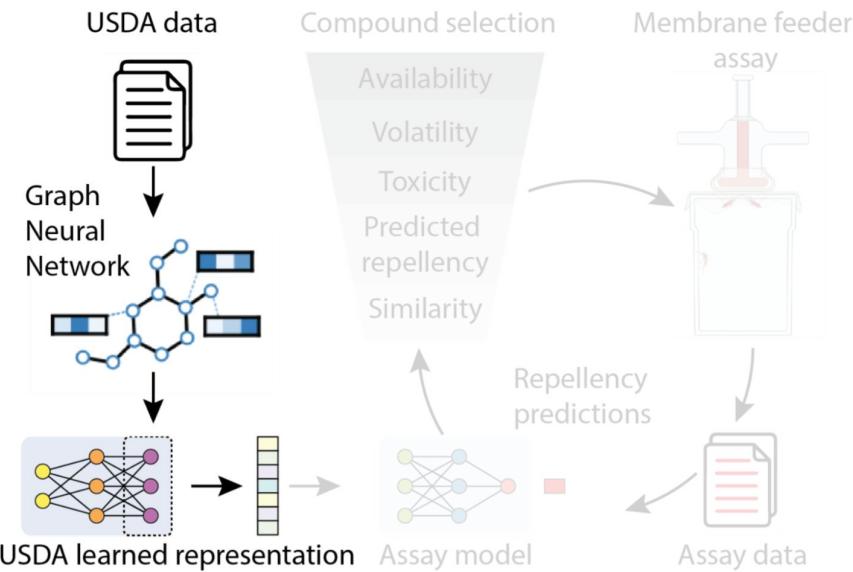


Safer and more performant molecules for our shampoo, detergent and perfume.

Last year, we launch 3 new fragrance ingredients after starting the company two years ago, with a pace four times faster than established fragrance house.

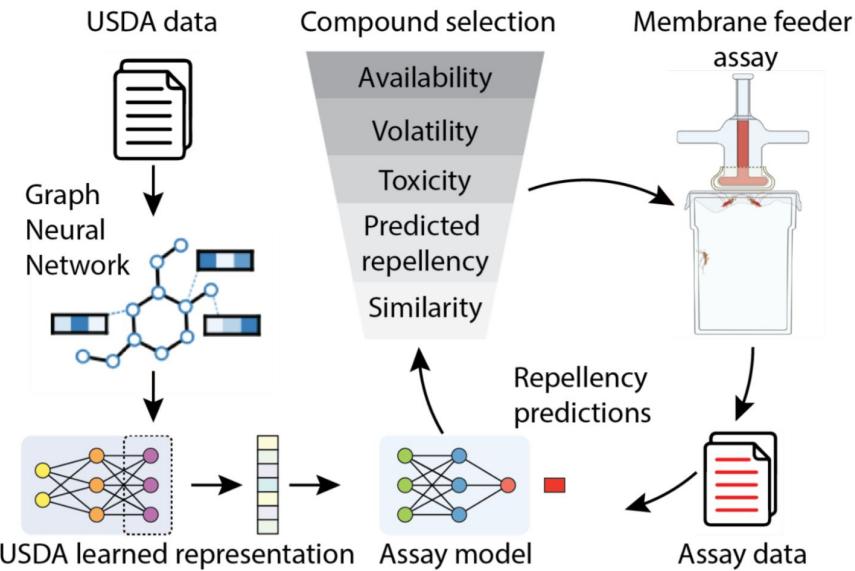
Targeting olfactory system in other animals

Developing mosquito repellent



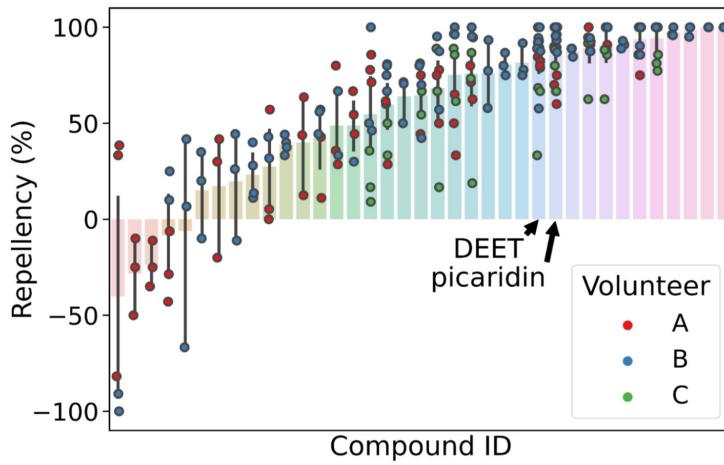
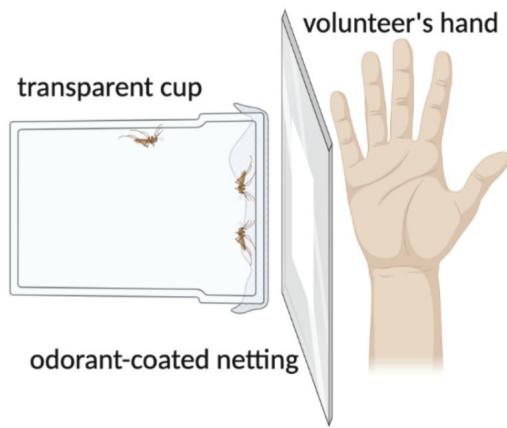
Targeting olfactory system in other animals

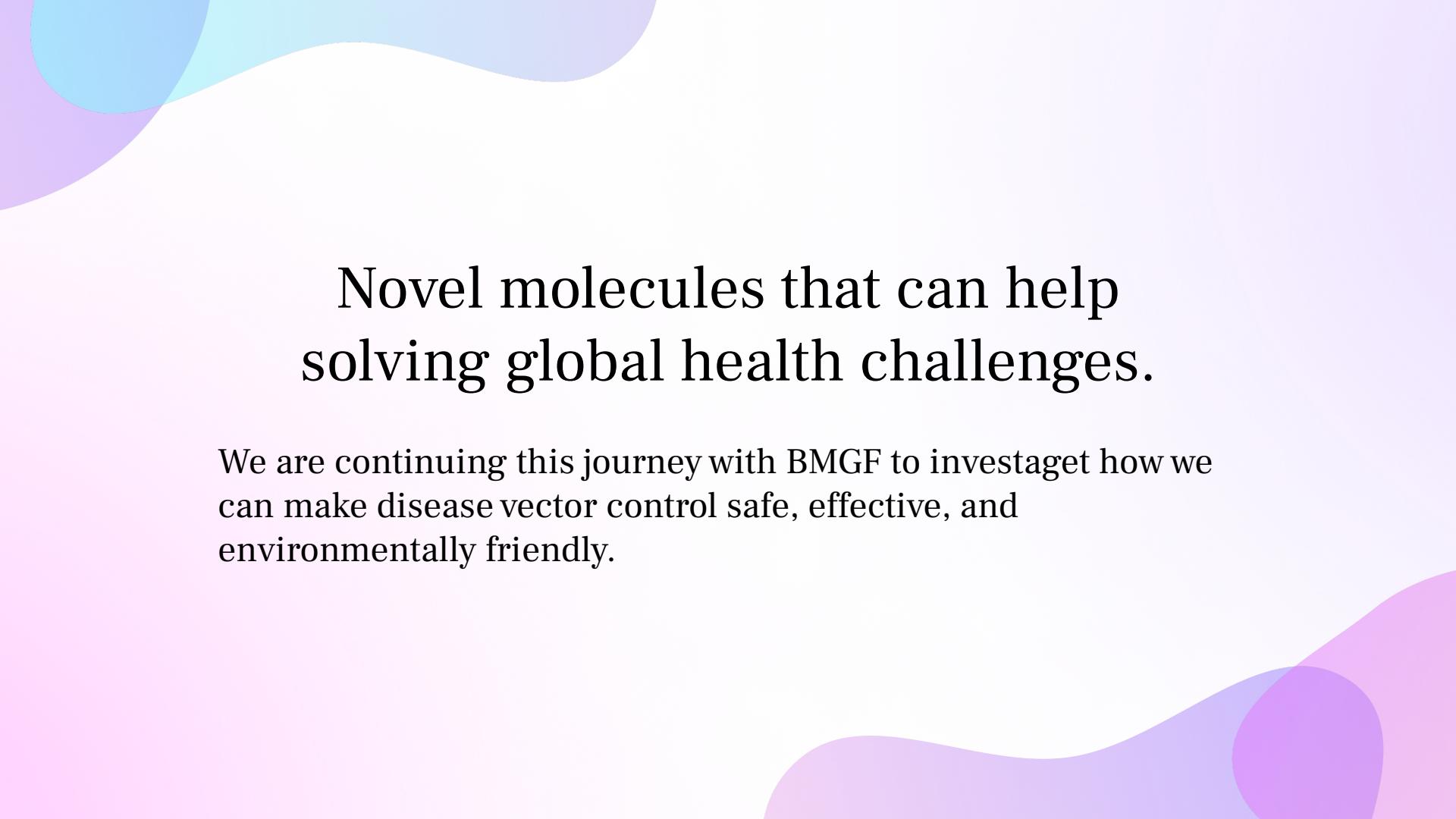
Developing mosquito repellent



Targeting olfactory system in other animals

Found 10 novel candidate compounds that are more potent than known molecules





Novel molecules that can help solving global health challenges.

We are continuing this journey with BMGF to investigate how we can make disease vector control safe, effective, and environmentally friendly.

Huge thank you to the Osmo team, former Google colleagues, and collaborators at Monell / TropIQ!



Thank you!

Q@osmo.ai