

AutoPeptideML 2: An open-source library for democratizing machine learning for peptide bioactivity prediction

Speaker: **Raúl Fernández-Díaz (PhD Candidate UCD – IBM Research)**

UCD: R. Cossio-Pérez, C. Agoni, D.C. Shields

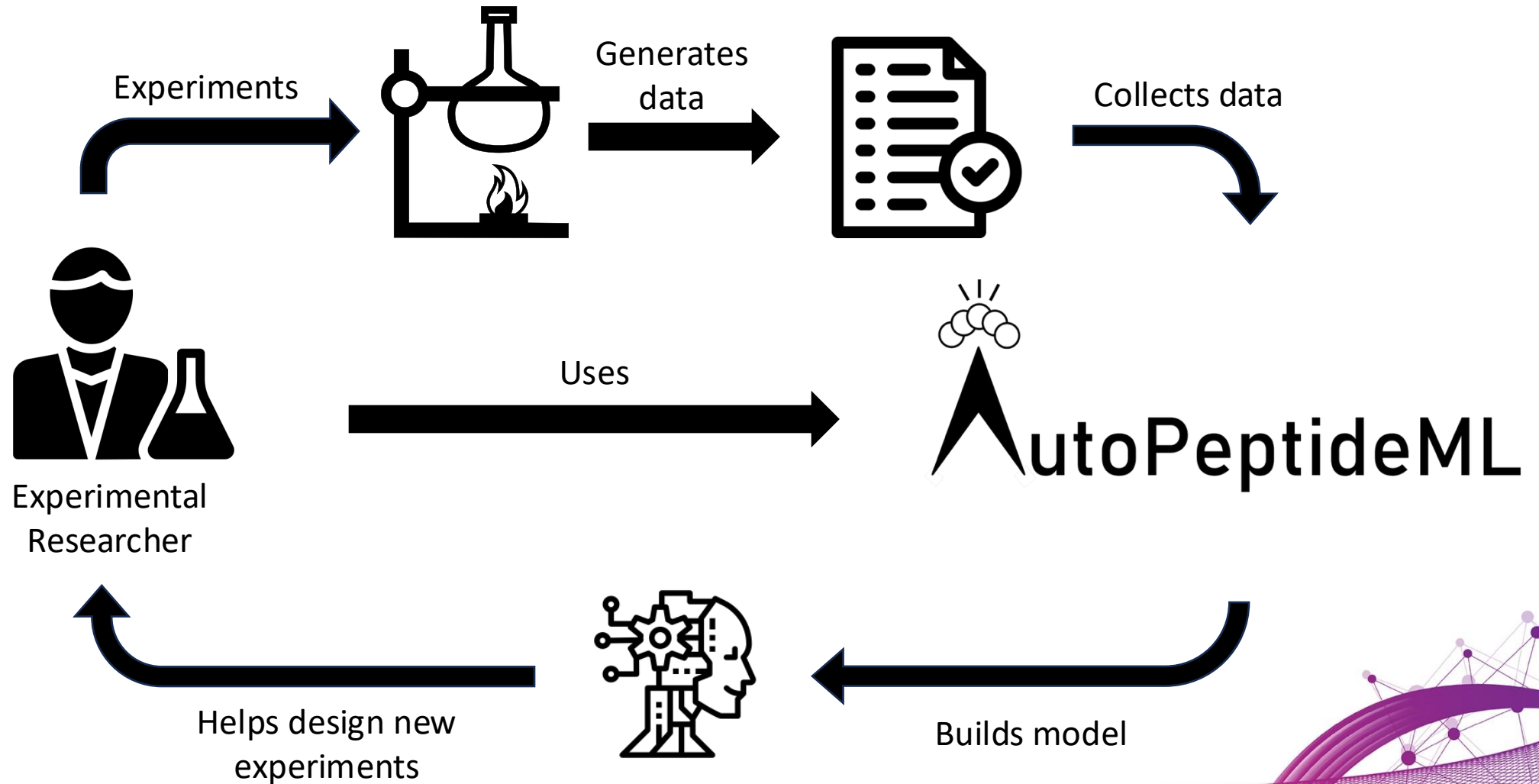
IBM Research: T.L. Hoang, V. Lopez

Novo Nordisk: R. Ochoa

More information
and contact info



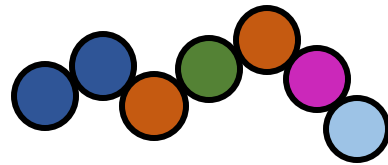
Main objective





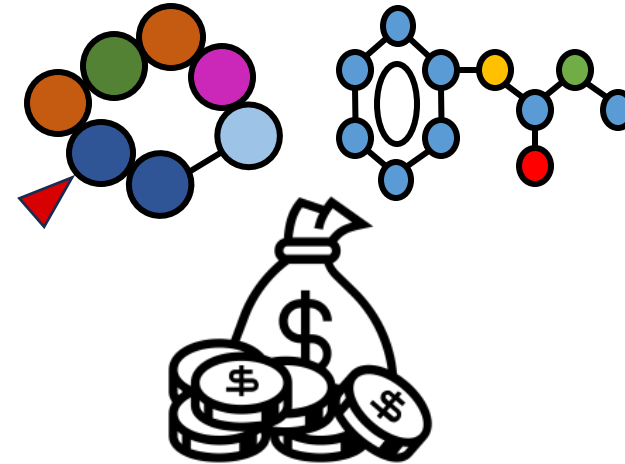
A tale of two peptides

Natural peptides
(cheap)



FOR SALE

Synthetic peptides and peptidomimetics
(expensive but better drugs)

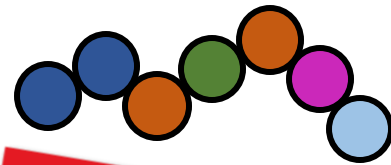




Why AutoPeptideML 2?

v 1.0

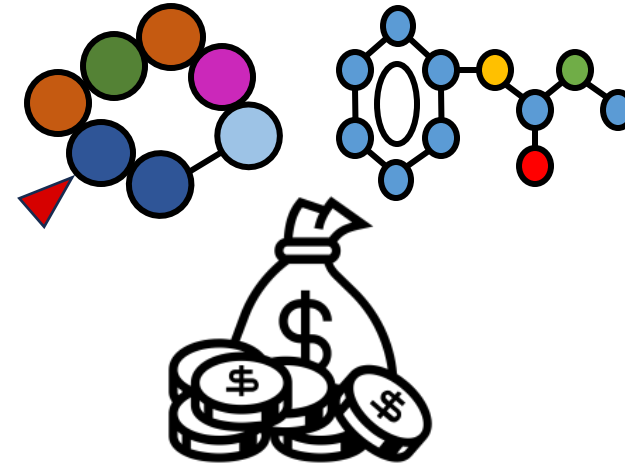
Natural peptides
(cheap)



FOR SALE

v 2.0

Synthetic peptides and peptidomimetics
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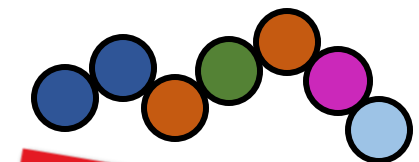


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Can we leverage data on cheaper experiments to prioritise more expensive experiments?

Natural peptides
(cheap)



FOR SALE

Train

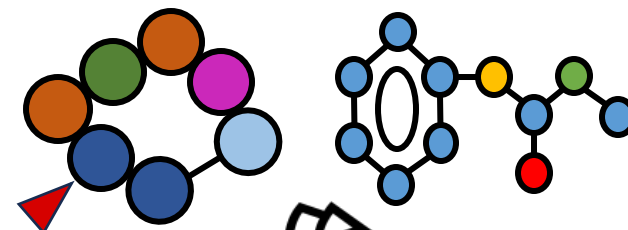


AutoPeptideML

Predict

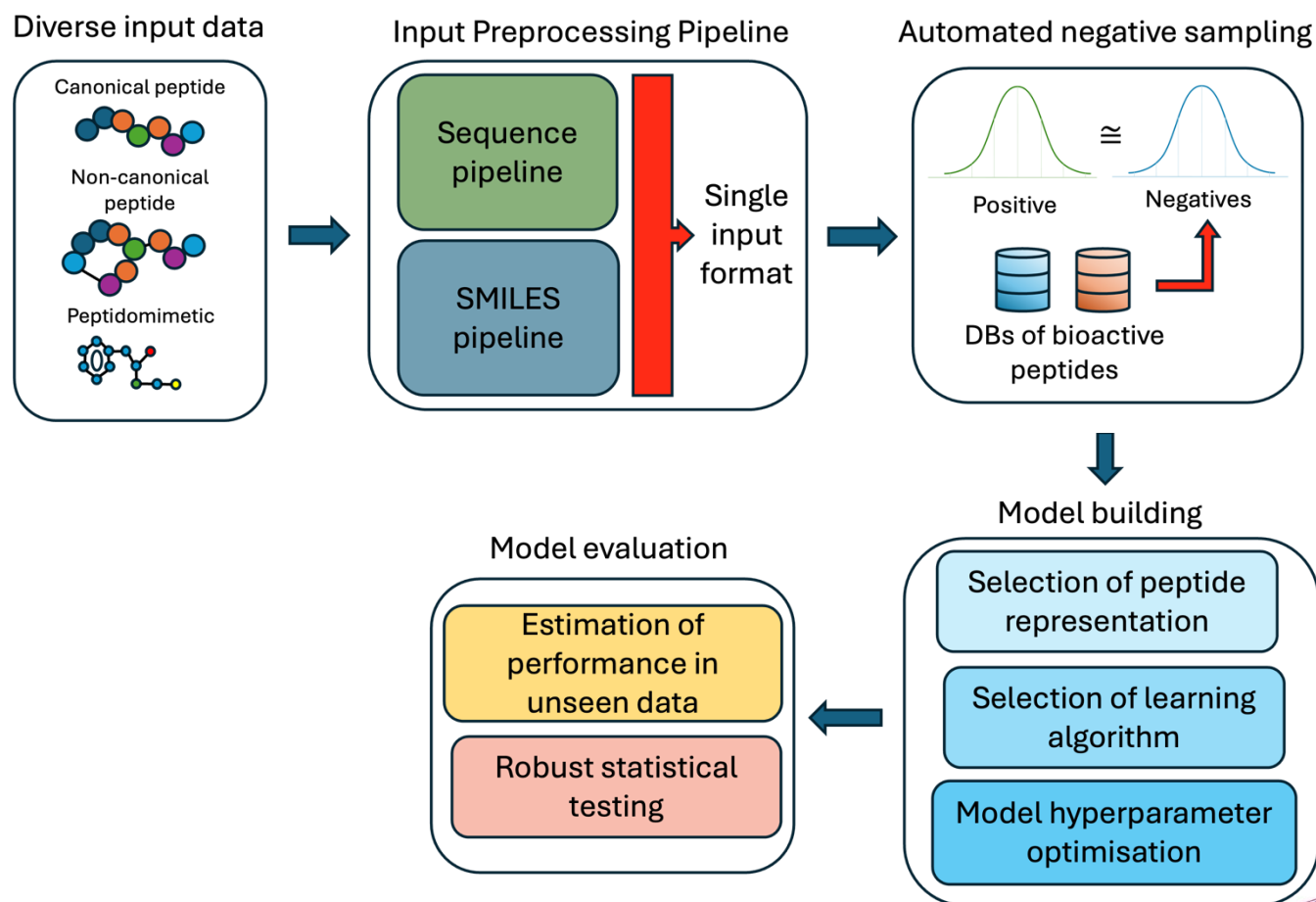


Synthetic peptides and peptidomimetics
(expensive but better drugs)





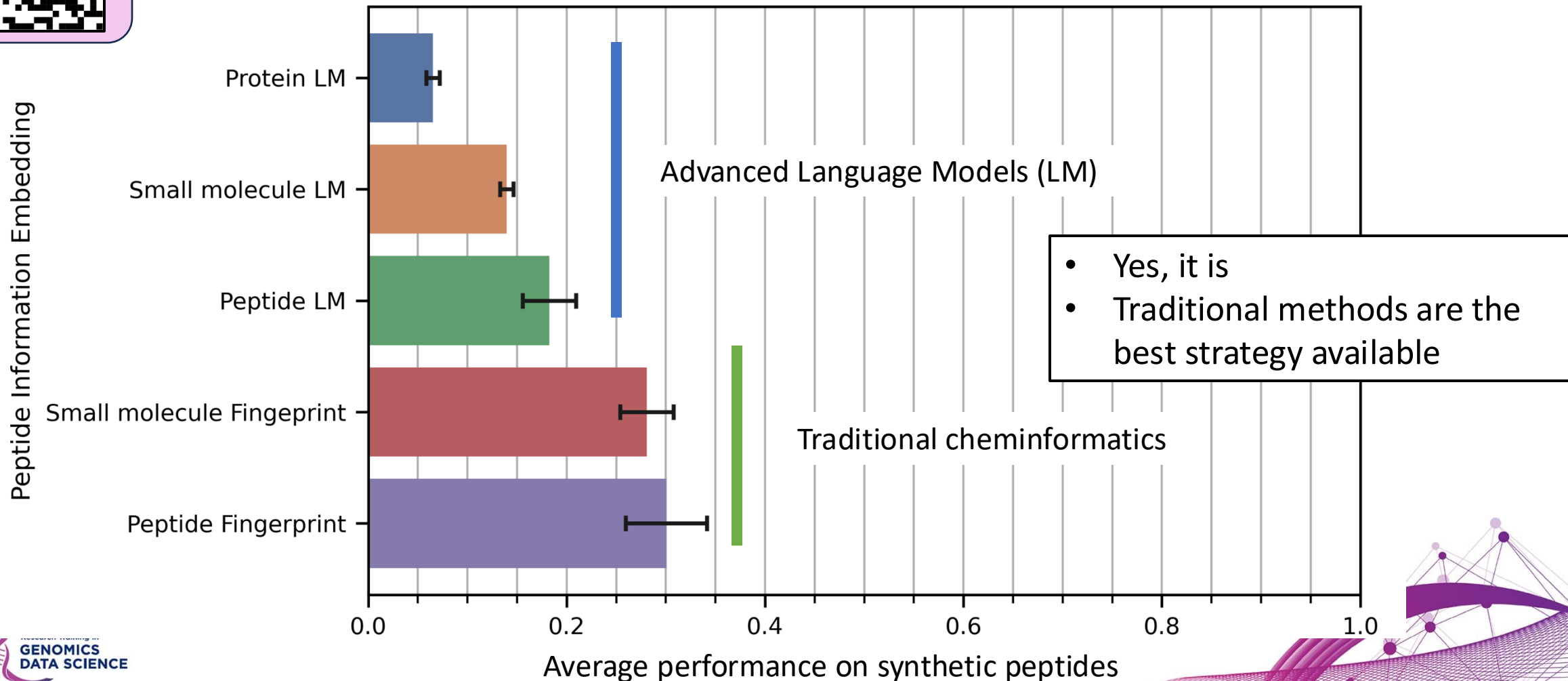
Pipeline to handle natural peptides (sequences) and synthetic ones (molecular graphs)



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Can we leverage data on natural peptides to predict the properties of synthetic peptides?



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Conclusions

1. AutoPeptideML **empowers** experimental scientist to build their own models
2. Version 2.0 extends support to **synthetic peptides and peptidomimetics**
3. **CLI** and **Webserver GUI** facilitate compliance with **FAIR principles**
4. Aims to **reduce costs** associated with experimenting with **synthetic peptides** by identifying the most promising candidates



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A lightning talk is lightning fast,
so if want to learn more,
feel free to reach out



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Centre for
Research
Training



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