News

Optibrium Shows Deep Learning to Successfully Predict Human Panel-based Sensory Perception of Novel Compounds Used for Flavours and Fragrances

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Optibrium, IFF and Intellegens' joint peer-reviewed research published in Journal of Computer Aided Molecular Design.

Study demonstrates accuracy and predictive capability of proprietary deep learning method for developing flavours and fragrances, and in drug discovery.

CAMBRIDGE, UK, 09 December 2021 – Optibrium™, a leading provider of software and artificial intelligence (AI) solutions for drug discovery, today announced the publication of a peer-reviewed study in the Journal of Computer-Aided Molecular Design, "Imputation of Sensory Properties Using Deep Learning". In collaboration with International Flavors & Fragrances (IFF), a global leader in co-creating sensorial experiences, and Intellegens, an AI company, the team applied Optibrium's Augmented Chemistry® platform to predict human panel-based assessments, including sensory properties, such as odour intensity and odour detection threshold. The study demonstrated the platform's high predictive reliability and the opportunity to reduce the need for human testing when developing new flavour and fragrance ingredients, opening the potential for cost and time savings. The study also reinforced the translational ability of the method for related applications, including offering new insights into drug discovery data to identify opportunities for new drugs and streamline the drug discovery process [1].

Fragrance ingredient development currently requires human panel-based trials. Critical for the success of new fragrance ingredients are properties such as odour detection threshold, which are hard to predict reliably *in silico* as small changes in a molecule's structure can substantially impact an individual's odour perception. Furthermore, only limited data on attributes such as odour perception are available due to being assessed in trials with human panellists. Such studies are both costly and time-consuming to undertake. Leveraging the Alchemite™ deep learning imputation method developed by Intellegens, Augmented Chemistry® draws on data for the property of interest whilst also utilising measurements and data from other endpoints and assays to make predictions. This increases the predictive power for critical endpoints like the odour perception threshold by learning the relationships between different experiments and exploiting earlier-stage measurements to make robust predictions of critical downstream properties.

The study demonstrated translational capabilities that expand the applicability of computational approaches to resource-intensive late-stage discovery, including human trial data and otherwise intractable complex endpoints. The method also provides robust uncertainty estimates for each individual prediction, increasing the confidence in decisions based on the method. Consequently, Augmented Chemistry® offers unique opportunities to reduce the time and cost of developing new flavours and fragrances and in related fields like drug discovery.

Samar Mahmoud, Senior Scientist at Optibrium, said: *"We have demonstrated Augmented Chemistry's unprecedented capabilities to robustly predict otherwise intractable complex endpoints in several drug discovery collaborations with leading pharma and biotech companies. This study further underlines its translational capabilities, providing further evidence for its applicability to other related trial outcomes across fields such as drug discovery"*

Dmitriy Chekmarev, Senior Research Investigator at IFF, said: *"We were impressed by the outcomes of the collaboration. Not just because it is the first approach that offers meaningful overall predictive power, but because its reliable uncertainty estimates give us the confidence to make critical project decisions based on computational methods."*

Read the full study >

[1] Deep imputation on large-scale drug discovery data https://doi.org/10.1002/ail2.31

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