

Synple Chem and Alipheron Collaborate to Unlock Ultra-Large Tractable Chemical Space

- Utilizing Alipheron's Hyperspace technology for rapid screening of over 30 trillion Synple-accessible molecules
- Leveraging Alipheron's Pharos3D search for close analogues in pharmacophore space from Synple-accessible molecules

Kemptthal/Dornach, Switzerland, September 9, 2024: Synple Chem, an innovative developer of integrated automated chemical synthesis solutions and provider of hit identification services, and Alipheron, a leading company specializing in cheminformatics solutions for searching ultra-large chemical spaces, are pleased to announce their collaboration. This partnership will make Synple Chem's multi-trillion-member, highly tractable chemical space accessible through Alipheron's advanced Hyperspace and Pharos3D search technologies.

Alipheron's Hyperspace technology allows for the rapid search of ultra-large combinatorial chemical spaces based on substructure or similarity, in just seconds. This tool is readily available through [DataWarrior](#) or can be integrated into in-house solutions. Additionally, Alipheron's three-dimensional pharmacophore search tool, Pharos3D, is available on demand. Synple Chem's virtual chemical space is a key component of their Discovery Platform, enabling users to explore a vast chemical space filled with highly tractable molecules that can be synthesized directly by Synple, with a four-week lead time.

"Leveraging our highly standardized reaction outcome data, we have developed predictive models for Synple-compatible reactions," said Dr. Benedikt Wanner, CEO of Synple Chem. "Based on building blocks predicted to yield successful outcomes in Synple-enabled reactions, we have enumerated a new, highly diverse chemical space that is both tractable and rapidly accessible using an automated approach. Collaborating with Alipheron will allow our customers to explore all the Synple-accessible space, accelerating hit discovery."

Modest von Korff, CEO of Alipheron AG, added: "We are excited about the collaboration with Synple Chem. Through the Synple Space, we can now make over thirty trillion molecules searchable with our technology, greatly enhancing drug discovery. The ability to search such ultra-large libraries for compounds that can be immediately ordered and synthesized is a game changer in the field."

About Alipheron:

Alipheron AG is a private Swiss company founded in November 2023 by former key members of the Drug Discovery IT team at Actelion Pharmaceuticals Ltd. The company specializes in cheminformatics software and database solutions for drug discovery, focusing on 2D and 3D searches of ultra-large combinatorial molecular spaces. Alipheron also maintains open-source projects such as DataWarrior and OpenChemLib and offers custom extensions for clients.

About Synple Chem:

Founded in 2016 as a spin-off from ETH Zürich, Synple Chem aims to provide easy-to-use, safe, and efficiency-enhancing organic synthesis solutions that accelerate discovery research. The company has developed a unique automated synthesis platform, recently enhanced by predictive AI tools.

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