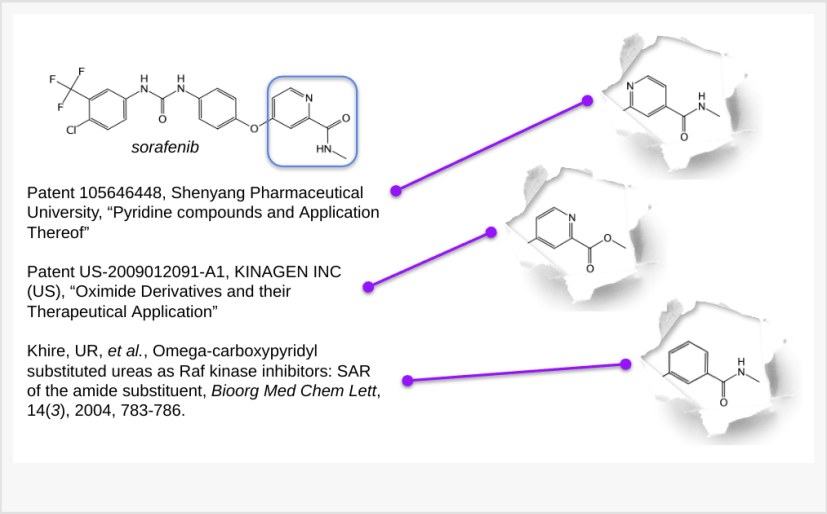
Quantum-Aided Drug Design from POLARISqb Demonstrates Best-in-Class Capabilities

POLARISqb released a white paper on their Best-in-Class mode., which identifies novel molecules that are just outside published IP of a given template ligand.



DURHAM, NC, USA, November 1, 2023 /EINPresswire.com/ -- Polaris Quantum Biotech (POLARISqb), the leader in quantum computing-based drug design, announced the development of Quantum-Aided Drug Design (QuADD) for molecular library optimization in April 2023. QuADD runs on quantum computers that solve problems with unprecedented speed and power, allowing users to search a chemical space of more than 10^30 molecules for those that complement their specific binding pocket. This Software-as-a-Service platform builds custom, enriched molecular libraries, and it is currently available to customers. As a part of a series of white papers detailing how QuADD works, POLARISqb released a white paper concerning Best-in-Class mode. This new feature identifies novel molecules that are just outside the published intellectual property of a given template ligand.

> Best-In-Class allows QuADD to examine areas very close to a known drug patent by searching an enormous chemical space and recovering subtly novel structures that still resemble the template."
>
> *Dr. Kendall Byler, Director of Computational Chemistry*

The white paper reports the results for the test case of sorafenib in complex with p38 MAP kinase. QuADD's Best-In-Class mode was able to generate a library of molecules with optimal drug-like properties and similar binding profiles as the template but with distinct structural characteristics that maintain an appropriate degree of diversity. With this approach, Best-In-Class mode is ideal for searches in the periphery of intellectual property. Dr. Kendall Byler, Director of Computational Chemistry for POLARISqb, said, "Best-In-Class allows QuADD to examine areas very close to a known drug patent by searching an enormous chemical space and recovering subtly novel structures that still resemble the template."

The figure below shows sorafenib with three alternate groups generated by QuADD's Best-In-Class mode. Patent and literature searches revealed that these groups are known actives. This example demonstrates that QuADD's Best-In-Class mode discovers small molecule libraries with strong candidates for drug design. For more details, find the white paper at their website here.

Quantum-Aided Drug Design, a new SaaS from POLARISqb, generates optimized molecular libraries at quantum speed.

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