InnoMatch

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EIC INNOVATION PROCUREMENT PROGRAMME

BDocker & BQChem

case study



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molecure

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PILOT: BEIT sp. z o.o. & Molecure SA

BDocker & BQChem | Life Sciences, Oncology, and Quantum Drug Discovery

6 CANDIDATES

MUTANT SELECTIVE MOLECULES

Identified 6 selective drug candidates for complex oncology targets

≥30% GAIN

SELECTIVITY PREDICTION BOOST

Over 30% higher accuracy in predicting target selectivity over classical tools

6,000 to 2-5

LIBRARY FILTERING SCALE

Filtered a 6,000-compound library down to 2-5 high-probability molecules

5 OUT OF 5

PROJECT KPIS MET

100% on-schedule completion within pre-agreed project budget

PILOT PROFILE

EIC Awardee: BEIT sp. z o.o.

Solution: BDocker & BQChem

Partner: Molecure SA (Biotechnology Company, Poland)

Testing Ground: Cloud and virtual machine computational infrastructure integrated into Molecure's drug discovery pipeline

Sector & Challenge Focus: Life Sciences, Oncology, and Quantum Drug Discovery

The Challenge

Developing targeted cancer drugs requires finding small molecules that bind specifically to mutated protein targets in cancer cells without binding to healthy cells. Traditional computer simulation software (classical molecular docking) is computationally slow, expensive, and struggles to predict molecule binding accurately, forcing biopharma companies to spend millions synthesising and testing weak candidates in wet labs.

The Solution

BDocker and BQChem are high-performance computational platforms that combine quantum-inspired algorithms with classical computing. By simulating atomic interactions with quantum-level accuracy, the platforms screen chemical libraries rapidly, identifying highly selective drug candidates for physical lab synthesis.

Objectives

The pilot aimed to filter a 6,000-compound library, identify selective drug candidates for a complex cancer target, and demonstrate superior prediction accuracy over conventional docking software within a €59,400 budget.

Constrains

Establishing data security protocols before sharing proprietary protein structure data required careful intellectual property agreements.

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Performance

The platform met all five project targets on schedule at Technology Readiness Level 8. It filtered 6,000 compounds down to 2-5 molecules for synthesis, identified six selective cancer drug candidates, and improved selectivity prediction accuracy by over 30% compared to standard docking tools.

Partner Operational Improvements

Accelerated drug discovery timeline, reduced wet-lab synthesis expenses, and successful identification of selective cancer drug candidates.

SUCCESSFUL PILOT VALIDATION

Molecure expanded its partnership with BEIT into an advanced scientific collaboration to model covalent drug binding and generate AI training data for oncology pipelines.

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