FUJITSU

Biodrug Design Accelerator: Software Solution for Peptide Drug Discovery

Product release planned for April 2023

Biodrug Design Accelerator solves the data management and workflow coordination challenges of the peptide design process.

In current peptide drug discovery, tools and data tend to be scattered across several teams, making it difficult for teams to coordinate, and for management to get a clear picture of progress. Unfortunately, poor coordination and visibility ultimately slows down the drug design process, highlighting a need to improve the sharing of data and to speed up decision-making among drug discovery chemists, biological researchers, pharmacokinetic researchers, and computational chemists.

Connecting drug discovery scientists with data and workflows

In collaboration with PeptiDream, Fujitsu has developed a Software-as-a-service (Saas) solution for the hit-to-lead and lead-optimization stages of peptide drug discovery.

Technical Benefits

- Manage data centrally
- View project history & progress
- Discuss data, criteria & next steps
- Share & utilize researcher know-how
- Co-ideate path forward
- Be peptide-centric
- HELM support

Business Benefit

- Accelerate drug discovery

Primary functions

Project Management

DMTA
Design Make Test Analyze

1 **Generation management**
- Creation and management of generations
- Selection of hit and lead peptides

2 **Design board**

- Hypothesis
- Designset
- Library Enumeration
- Synthesis
- Analysis

- Progress management for each peptide, tagging function for grouping, and structure comparison of selected peptide
- Peptide design hypothesis, target setting, slide production
- Construction of peptide database, presentation of combination list, simulation of property and activity data
- Comparison of peptide candidates from 'Designset' combinations, instructions for synthesis (export of order sheets)
- Synthesis, assay progress management, incorporation of assay result data, confirmation of assay result listings
- Aggregation, comparison and analysis of peptides with assay results

3 **Peptide/Monomer search**
- Search for peptides that meet cross-project conditions
- Search for monomers with various conditions

4 **Communication**
- Chat with members within each project and design board

Learn more about how we are innovating drug discovery

www.youtube.com/watch?v=SKTmSN0YtRg

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