

Collaborations Pharmaceuticals, Inc. case studies describe the safe real-world applications of AI over the past decade

Collaborations Pharmaceuticals, Inc. highlights how select case studies from a decade of using AI have positive applications for research and development.

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EINPresswire.com/ -- Collaborations Pharmaceuticals, Inc. (CPI) is a Raleigh-based company founded over a decade ago. It was built on the founder Sean Ekins' over 20 years of prior experience using computational approaches for drug discovery and toxicity predictions as well as many external collaborations applying computational approaches to

neglected and rare disease drug discovery. The company has developed its own artificial intelligence (AI) software products (e.g. [Assay Central](#), [MegaTox](#), MegaTrans, MegaSyn, MegaAChE and more) with funding from NIH grants and matching funds from the one NC small business program. We have validated these tools leveraging our own internal chemistry and biology laboratories as well as through external collaborations.

"From the beginning we have put our software to use in working with outside clients from the pharmaceutical, chemical and consumer product industries. Most of these projects have involved using our software to pursue projects that these companies did not have the capabilities to do. We have worked on a range of projects like toxicology predictions, off-target prediction, designed PROTACs, polymers, PFAS alternatives as well as developed PK/PD models. More recently we have undertaken software development projects to create bespoke software tools for clients such as for clinical trial data modeling, spectra prediction for GC/MS and clinical trial success prediction. The computational strengths of CPI compliment companies that may not have their own internal AI groups." stated Dr. Sean Ekins, CEO of Collaborations Pharmaceuticals,



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PHARMACEUTICALS, INC.**

Collaborations Pharmaceuticals logo

Inc.

As these projects are all predominantly confidential, very few of these fee-for-service projects have been publicly disclosed. We have now described these projects at a high level as a dozen brief [case studies](#).

Case Study 1: De-Risking a Large Molecule Through Predictive ADME/Tox and Metabolism Profiling.

Case Study 2: Custom Multi-Target Models and Patent Screening for a Competitive Assessment.

Case Study 3: Generative Design of Selective ADORA3 Agonists for an Anticancer Target.

Case Study 4: Understanding Off-Target Effects of Drug Candidates.

Case Study 5: Repurposing Approved Drugs as Specific Cytokine Inhibitors.

Case Study 6: Identification of dual kinase inhibitors.

Case Study 7: Determining the Kd of a molecule against PPT1.

Case Study 8: Designing new polymers for human health applications.

Case Study 9: Assessing endocrine disruption potential of consumer product ingredients.

Case Study 10: Designing new prodrugs with predicted ADME/PK properties.

Case Study 11: Improving hERG and solubility for PROTACs.

Case Study 12: Predicting off-target liabilities for a PROTAC molecule.

Case Study 13: Developing an algorithm to predict ocular bioavailability.

“The majority of these case studies illustrate the value that AI has brought to such applications addressing predominantly pharmaceutical and consumer product uses which could ultimately impact healthcare. Simultaneously these case-studies also illustrate the safe real-world applications of AI that builds on decades of experience and validation. Collaborations Pharmaceuticals, Inc. has the expertise to apply AI to bespoke projects that a client might require. We look forward to your challenging projects so we can continue to share such case studies” emphasized Dr. Ekins.

At a time when AI has a tarnished reputation for failures in large companies controlling foundation models it is worth highlighting how small companies like CPI have been using AI safely and demonstrating positive applications for human health and beyond for years.

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