Docket #: S17-150

Novel Ligands with Affinity for Opioid Receptors

Researchers at Stanford have discovered new, chemically distinct opioid receptor ligands that may be used to develop safer opioid therapeutics. Opioids are ligands that bind to the mu, delta, and/or kappa opioid receptors. They are used to treat pain, diarrhea, and for overdose reversal. Current opioid therapeutics have severe side effects including respiratory depression and addiction. Thus, it would be highly beneficial to develop safer opioid therapeutics without such severe side effects. To help achieve this goal the inventors have used a new computational method, which leverages crystallography and molecular modeling with machine learning (see Stanford Docket S17-431), to explore a new chemical space of molecules active at opioid receptors. This technology describes the discovery of three fundamentally new chemical scaffolds that bind the mu, delta, and kappa opioid receptors. The novelty of these scaffolds will serve as the basis for further lead optimization that can generate a new family of opioids with varying receptor selectivity and agonism. This technology may aid in the development of safer, next generation opioid therapeutics.

Stage of research
Validation studies have been conducted and additional development is ongoing.

If interested in this technology, please contact team by November 25, 2018.

Applications

- Novel opioid therapeutics for:
  - Pain
  - Diarrhea
  - Overdose reversal

Advantages

- Aid in the development of safer opioid therapeutics
- Novel use of compounds:
    - Molecules have new chemical scaffolds- may help reduce side effects
    - May serve as the basis for analogues with selectivity for a specific opioid receptor subtype
- Pan-opioid binding activity

Publications

- Evan N. Feinberg, Amir Barati Farimani, Rajendra Uprety, Amanda Hunkele, Gavril W. Pasternak, Susruta Majumdar, Vijay S. Pande. Machine Learning Harnesses Molecular Dynamics to Discover New ? Opioid Chemotypes arXiv:1803.04479v1 [q-bio.BM]. 2018 Mar 12.

Patents

- Published Application: WO2019099573
- Published Application: 20200345715
- Issued: 11,213,518 (USA)

Innovators

- Evan Feinberg
- Vijay Pande
- Susruta Majumdar
- Gavril Pasternak

Licensing Contact

Cheryl Cathey

Senior Licensing and Strategic Alliance Manager

Email