Thermo Fisher

Bringing Chemistry to Life podcast series

Season 1: The 2019 C&EN's Talented 12 Episode 10: Nanometric mega-libraries



Episode abstract

For decades the pharmaceutical industry has synthesized millions of molecular entities in the pursuit of novel biological activities. These huge compound libraries have always been considered a treasure trove of potential new drugs for a plethora of new therapeutic targets. With the huge progress in laboratory automation and high-throughput technology over the last decade, library screening remains a key drug discovery strategy. The size of these libraries and their handling present however multiple challenges, starting from the synthesis and screening speed, storage space, and annotation required when working with Singleton compounds. A clever alternative finds inspiration from biology and leverages the DNA information storage power. This is known as DNA Encoded Libraries, or DELs. Dr. Katelyn Billings is a pioneer of this technology that offers a number of advantages, starting from the possibility of working on the nanoscale in as little as a few microliters to make and screen millions of molecules as a pool. In this episode we learn about how DELs work and discuss their advantages, challenges and the promise of combining data from DEL screens with machine learning to disrupt modern drug discovery.

About our guest

Katelyn J. Billings, PhD

Director of Discovery Chemistry, ZebiAl Therapeutics, now part of Relay Therapeutics

Katelyn's company site: https://relaytx.com/

C&EN Talented 12 profile of Katelyn::

https://cen.acs.org/pharmaceuticals/Katelyn-Billings/97/i33

Recent Publications from Katelyn:

- Multifunctional Building Blocks Compatible with Photoredoxdiated Alkylation for DNA-Encoded Library Synthesis
- Open-Air Alkylation Reactions in Photoredox-Catalyzed DNA-Encoded Library Synthesis
- Small-molecule studies identify CDK8 as a regulator of IL-10 in myeloid cells
- 2019 National Organic Chemistry Symposium (NOS) lecture video

Katelyn's Content Recommendations:

- Machine Learning on DNA-Encoded Libraries (a journal article by McCloskey et al.)
- Merging C(sp3)—H activation with DNA-encoding (a journal article by Fan et al.)
- Expanding Reactivity in DNA-Encoded Library Synthesis via Reversible Binding of DNA to an Inert Quaternary Ammonium Support (a journal article by Flood et al.)
- <u>Nanoscale synthesis and affinity ranking</u> (a journal article by Gesmundo et al.)
- Practical Cheminformatics (a blog by Pat Walters)
- In the Pipeline (a drug discovery and pharma blog by Derek Lowe)

This podcast series is available via the following links













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