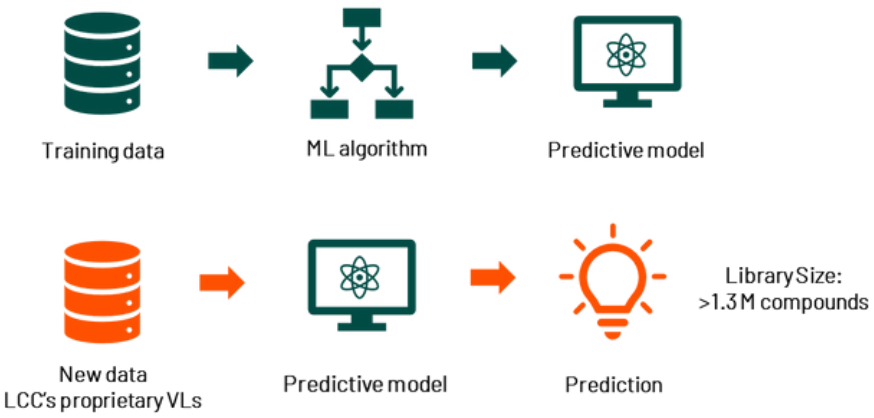
March 2024

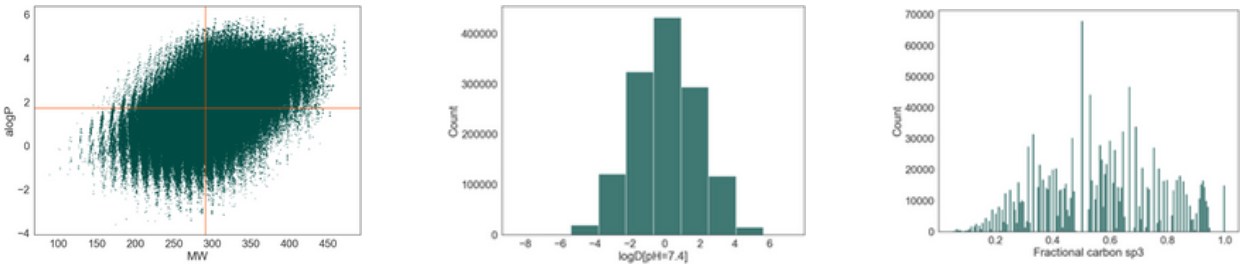
LCC'S MOLECULES OF THE MONTH

RNA Virtual Library

While classical drug discovery efforts have focused on targeting the proteome, it is estimated that only ~15% is druggable. Whereas, transcription of the human genome into RNA stands at around 75%, with only ~1% encoding for proteins.[1] This paves the way for the use of RNA-targeting molecules to target the encoded mRNA of 'undruggable' proteins, or non-coding RNA in relevant disease-regulatory mechanisms.[1] While other RNA-targeting modalities, such as antisense oligonucleotides, have been used extensively to target RNA, these can often present challenges when it comes to cell permeability and distribution.[2] Comparatively, small molecules can be advantageous due to their well-established synthetic methodologies and their tunability, enabling easier modification to improve delivery or uptake.[3]



LCC has designed and enumerated an RNA-focused virtual library. The library is based on LCC's novel, chirally pure, multi-functional scaffolds and was created by using a machine learning algorithm, trained with experimentally derived sets of RNA binders (ROBIN).[2] By design, the library is diverse and optimised for Hit-ID, while near-neighbour analogues can be found in the parent virtual space and rapidly synthesised in LCC's parallel synthesis laboratory.



If you are interested in accessing LCC's RNA Virtual Library, please get in touch!

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1 Physicochemical principles driving small molecule binding to RNA, 2024.

2 Machine learning informs RNA-binding chemical space, 2022.

3 Chemical Communications, 2020, 56, 14744–14756.