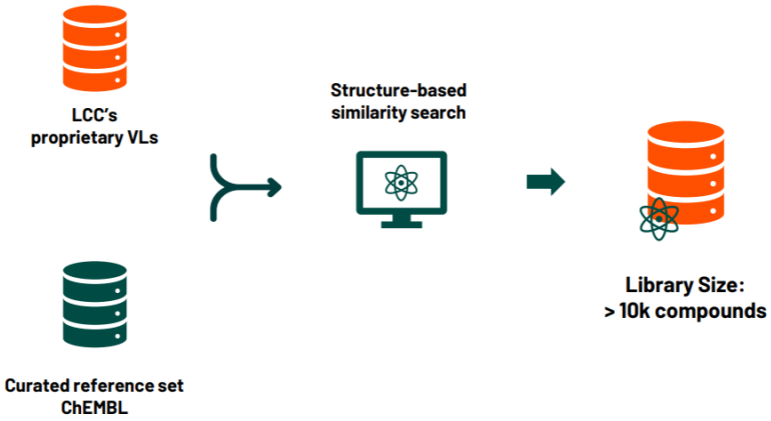
February 2024

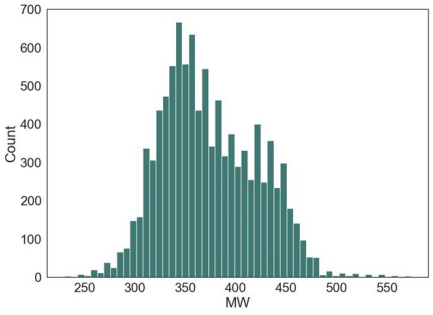
LCC'S MOLECULES OF THE MONTH

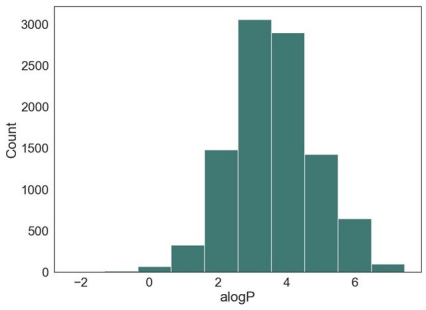
GPCR-Focused Virtual Library

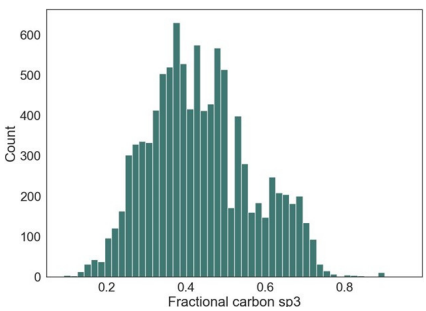
G-Protein Coupled Receptors (GPCR) are key pharmacological targets within drug discovery, with at least 92% of FDA-approved drugs for GPCRs being small molecules.[1] While traditional drug discovery programmes have focused on targeting the GPCRs orthosteric binding site, in more recent times, research efforts have shifted towards exploring the potential therapeutic benefits exhibited from targeting the topographically distinct allosteric ligand-binding sites.[2]



LCC has designed and enumerated a >10K member GPCR-focused virtual library. The library is based on LCC's novel, chirally pure, multi-functional scaffolds and was created by structure-based similarity searching of LCC's proprietary ultra-large virtual chemical space (>1.4B compounds) against a curated reference set of known GPCR binders, extracted from ChEMBL database. 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 want to learn more about how LCC's GPCR-focused Virtual Library can accelerate your drug discovery efforts and provide rapid access to novel and highly developable compounds, please get in touch!

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1 SLAS Discovery, 2024, 29, 1–22.

2 Frontiers in Endocrinology, 2023, 14.