ChemSpaceScanner: A platform for virtual screening of HUGE chemical libraries at high resolution

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The drug design process involves multiple screening steps, coupled with trial and error. During the past decade various computational drug design tools have been developed, yet these have not lived up to expectations to become the main driver of drug design. In part, this is due to the fact that the most powerful of the tools are highly computation-intensive and thus can be applied to small numbers of compounds (generally < 10^6). The size of the universe of possible drug-like molecules is estimated to be at least 10^{50} molecules, and space, and therefore powerful computations can only be applied to a very minute subset of the relevant chemical space.

HQL is developing a computational drug design platform based on a unique representation of small molecule chemical space that obviates the need for enumerating all molecules in the library, and efficient screening algorithms that together enable screening 7-8 orders of magnitude higher than what is possible today using high-resolution drug models.