ChemDiv
The chemistry of cures℠

Autophagy targeted library

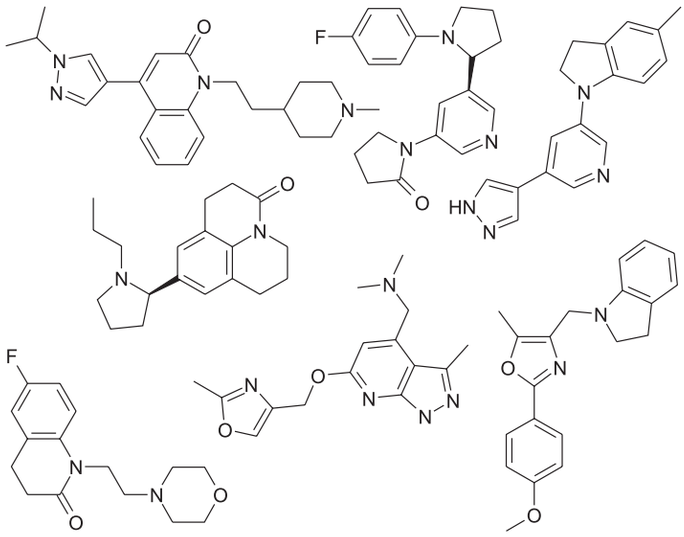
***19,190** compounds, comprised by ~ 540 templates*

Concept

There were several considerations that went into the design of this library, specifically:

1. **Published modulators (activators and blockers) of autophagy in various settings (ex., tumor cell lines, neurons, etc).**
2. **Modeling/homology modeling of several key biological molecules involed/mediating autophagy (ex., Beclin 1, Bcl2, BclXL, bCatenin/Bcl9, bCatenin/Bcl4 PPIs).**
3. **Reported key kinases (Cdk1/5, vacuolar protein sorting kinase (Vps 34), a class III PI3K, components of the IGF1R signaling cascade specifically including modulators of mTOR OTHER THAN rapamycin/ analogues, p70S6, Akt1, PDK1, IGF1R; ROCK I/II, ATM, etc).**
4. **Additional reported activators/inhibitors of targets mediating autophagy (P2X7, AMPAR, Eg5, etc).**

In general, we have procured over 50 reported/suspected targets and selected respective modulators using literature analysis or computational/modeling data.



Statistical data:

- **number of unique heterocycles: 286;**
- **diversity coefficient: 0,791;**
- **number of screens: 4591;**
- **property range**
  - **113< MW < 1295; 362 on average**
  - **0 < H-bond acceptors < 22; 5 on average**
  - **0 < H-bond donors < 10 1 on average**
  - **0 < rotatable bonds < 62; 5 on average**
  - **-12.3 < logD (pH 7.4) < 17.7; 3.3 on average**
  - **-14.6 < log of solubility in water (pH 7.4) < 10.6; -3.8 on average**

About ChemDiv

ChemDiv, Inc., is a fully Integrated Target-to-Clinic Contract Research Organization (CRO) headquartered in San Diego, CA USA. The company features multiple research and development (R&D) subsidiaries in Russia, Ukraine and China as well as business and logistic operations around the world. We engage pharmaceutical and biotech partners by offering 'one stop' drug discovery and development services based on a project- , FTE- , and risk sharing collaborative models. Today, ChemDiv is the global leader in discovery chemistry. We have built the industry largest and the most diverse collection of over 1,500,000 individually crafted, lead-like, drug-like small molecules. This collection is steadily growing at a rate of over 16,000 compounds a month, exclusively synthesized in-house. Our novel chemistry is designed by a group of experts and is finely balanced with maximal diversity, bioactivity against particular targets, template novelty and robust IP position. Being focused on discovery chemistry for over a decade, we understand our customers' needs and the peculiarities of bioscreening – the next link in the drug discovery where our libraries are used. ChemDiv is known for its high-quality customer service, flexible business models and a variety of formatting, packaging and delivery options

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LEAD TO CANDIDATE
CANDIDATE TO POC
POC TO MARKET