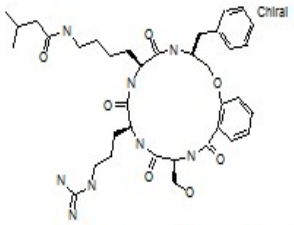
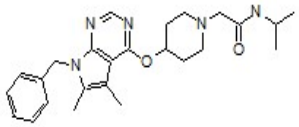
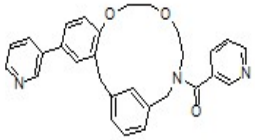
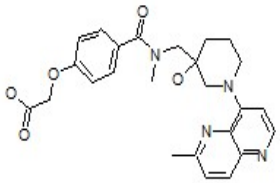
Immuno-Oncology Library

ASINEX

Small molecule therapeutic agents for modulating immune response in oncology provides several advantages over alternative modalities such as antibodies, proteins or peptides [1]. Protein-protein interaction is a fundamental a mechanism underlining immunological recognition in cells [2]. Leveraging our 7+ years of experience in the design of PPI-focused screening collections we have developed 4 distinct compound libraries to address several specific immunological targets involving PPI:

- Cell-cell adhesion proteins: CD2/CD58; LFA-1/ICAM-1
- Immunoglobulin-like receptors: KIRs
- Integrin-associated protein CD47/SIRPa
- PD-1/PD-L1 interaction
- Chemokines
- Ubiquitin-proteasome system (UPS)

Library 1	Library 2	Library 3	Library 4
			
Binding surface epitopes	**Ligand-based design**	**Scaffold selection**	**Ligand-based design**
CD2/CD58; LFA-1/ICAM-1 Immunoglobulin-like receptors KIRs Integrin-associated protein CD47/SIRPa	PD-1/PD-L1	Chemokines	E3 ligase

The design platform incorporates a careful selection of appropriate chemical space compatible with selected targets and extensive pharmacophore and structrure-based approaches for selection of the best small molecule candidates. The molecular diversity of the library expands beyond traditional “Rule of-5” domain by incorporating macrcyclic entities in order to address extracellular targets.

1.Adams J., Smothers J., Srinivasan R., Hoos A. Big opportunities for small molecules in immuno-oncology, Nat Rev Drug Discov. 2015 Sep;14(9):603-22.