

# Библиотеки ингибиторов протеин-киназ

# Kinases Inhibitors

# Knowledge Progression & Selection

Learning

Analysis

CADD

Selection

Screening

## Reference Compounds

Thomson Integrity



ChEMBL



SciFinder



- ▶ 2D Structural similarity
- ▶ 2D Topological similarity
- ▶ Molecular docking
- ▶ Expert opinion

- ▶ Scaffold hopping
- ▶ Isosteric/Bioisosteric morphing
- ▶ Privileged fragments

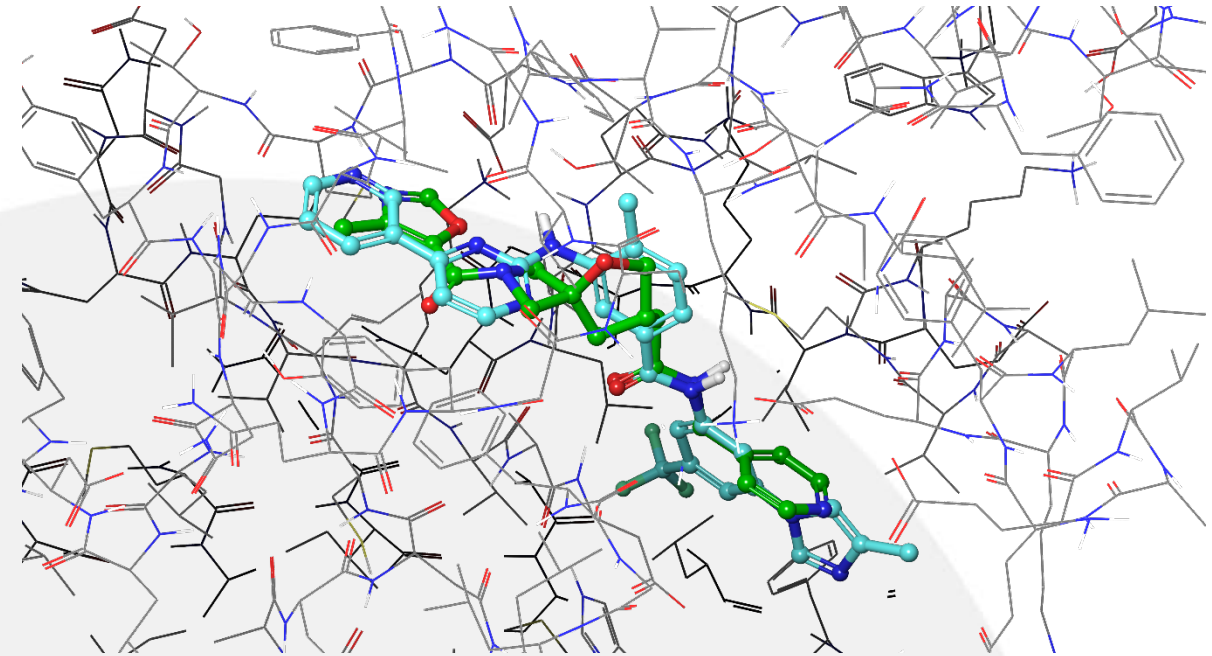
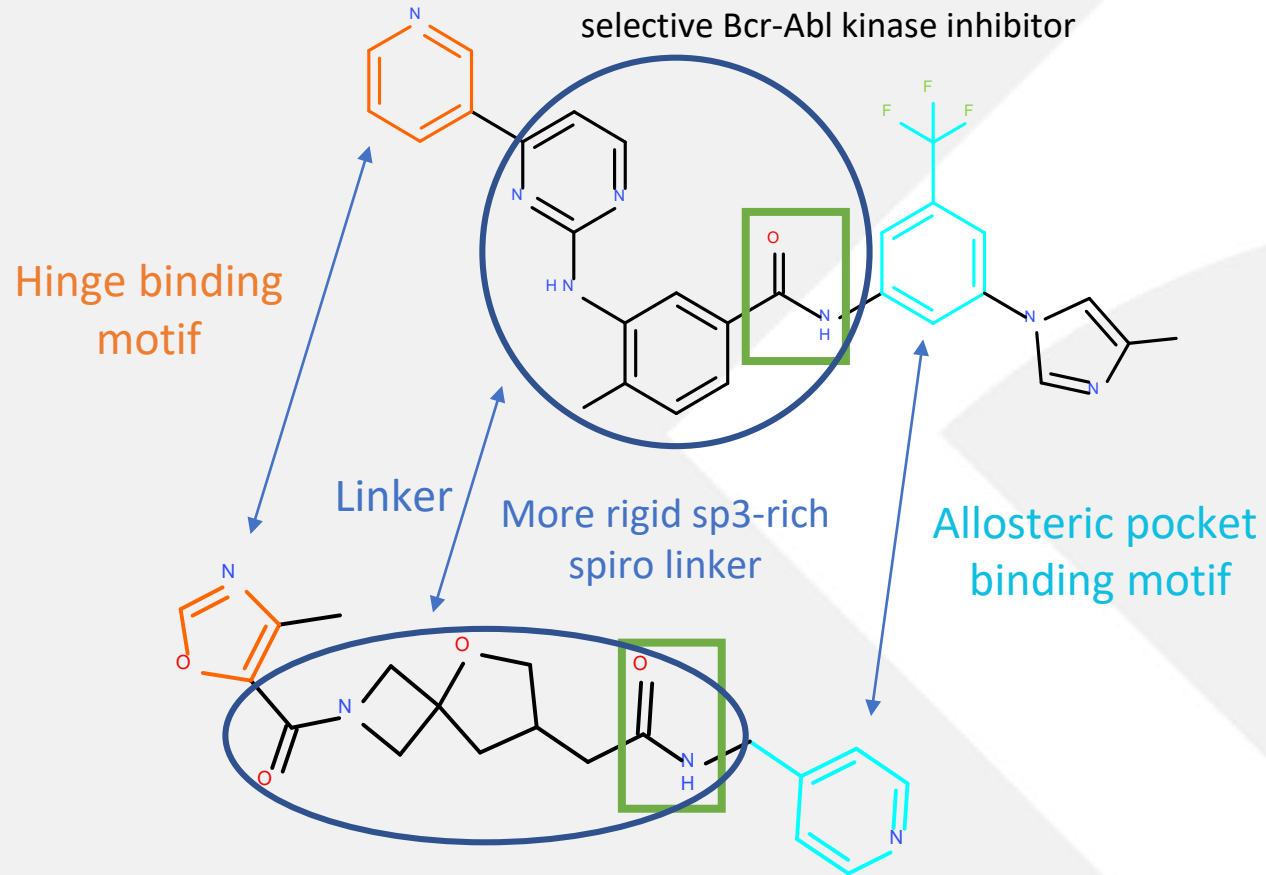
- ▶ Scaffold prioritization
- ▶ MedChem Filters
- ▶ Clustering

**Kinases Inhibitors Library**  
**~32k cmpds**

# Methodology. Similarity and molecular docking. Inhibitor Type II as an example.

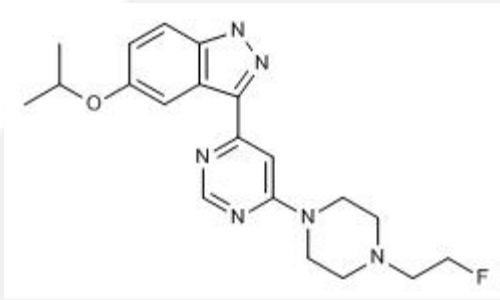
## Nilotinib

selective Bcr-Abl kinase inhibitor

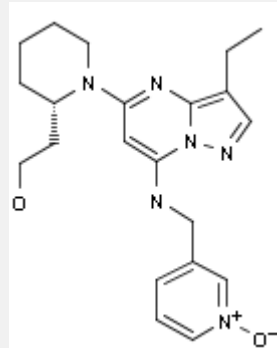


Docking results into ABL kinase (PDB 3CS9).  
Cyan – Nilotinib. Green.

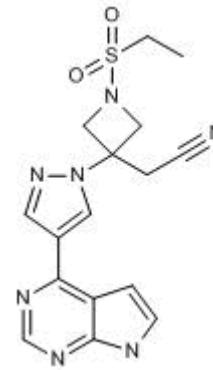
# Reference examples



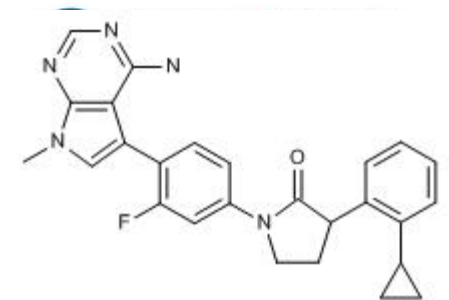
WO 2014137719  
(Merck)  
LRRK2  
Neurodegenerative



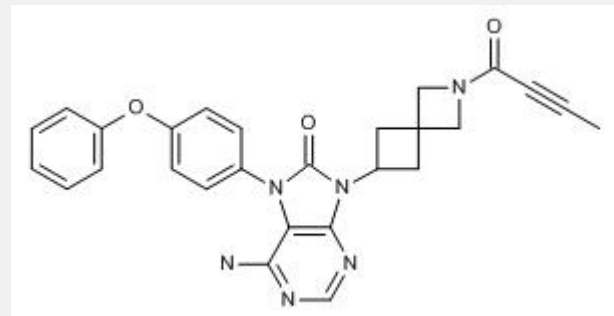
Dinaciclib  
(Merck)  
CDKs  
Neurodegenerative  
Cancer



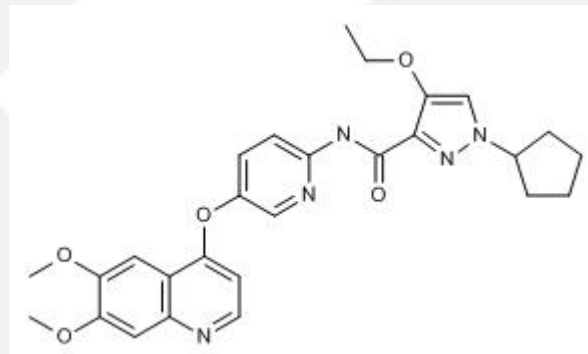
Baricitinib  
(Lilly)  
JAK1,2  
Inflammatory  
Autoimmune diseases



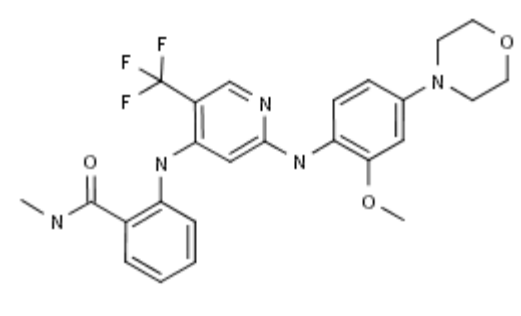
WO 2015136463  
(GSK)  
Cancer  
Macular degeneration  
Neurodegeneration



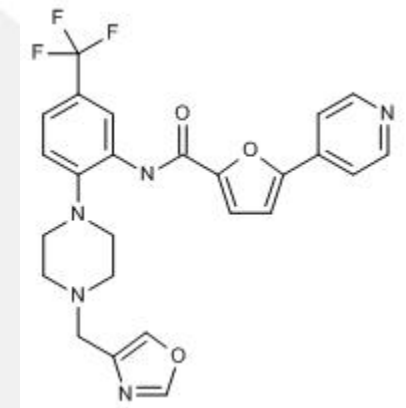
WO 2018156901 (Gilead Sciences)  
BTK Cancer  
Autoimmune diseases  
Cardiovascular Disorders  
Inflammation



WO 2016166250  
(Lead Discovery Center GmbH)  
TAM family  
Cancer



WO 2009105498  
(GSK)  
FAK family  
Oncolytic Drugs  
Solid Tumors Therapy

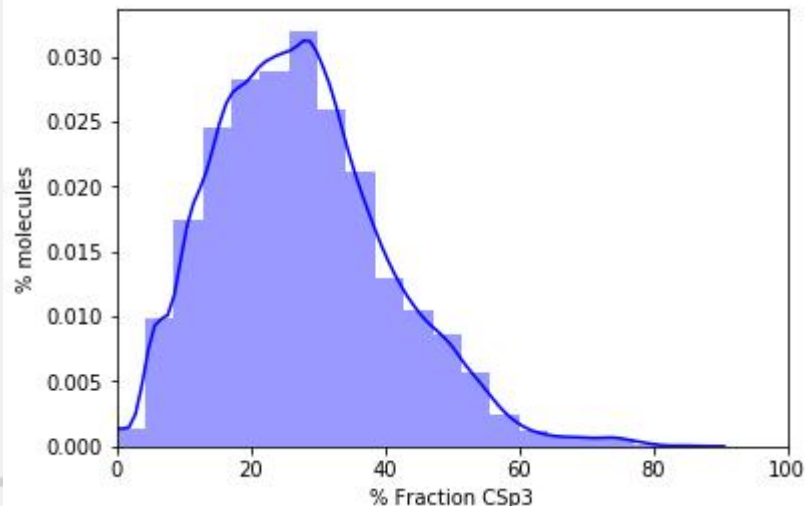
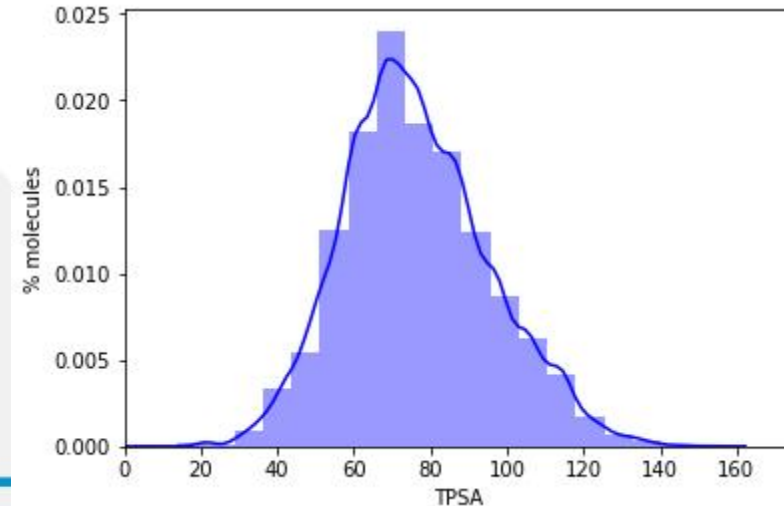
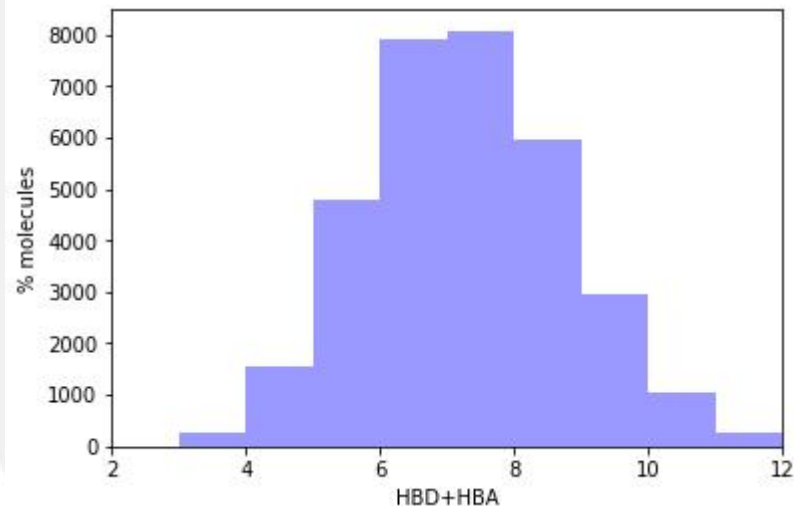
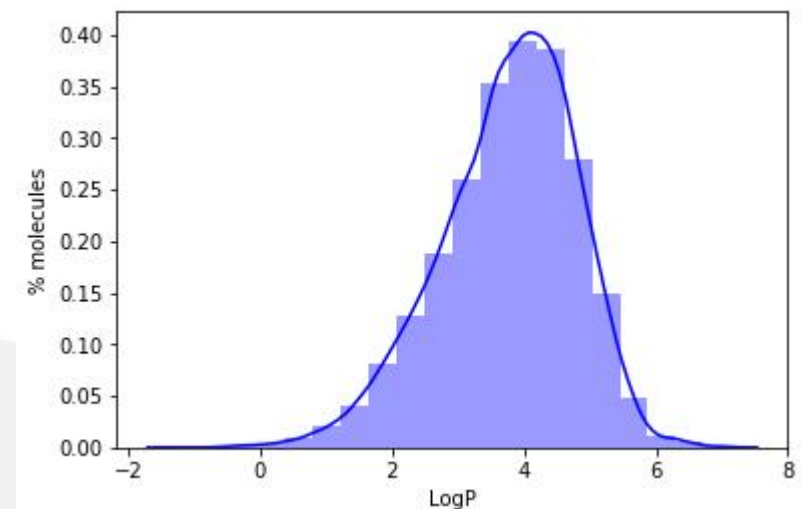
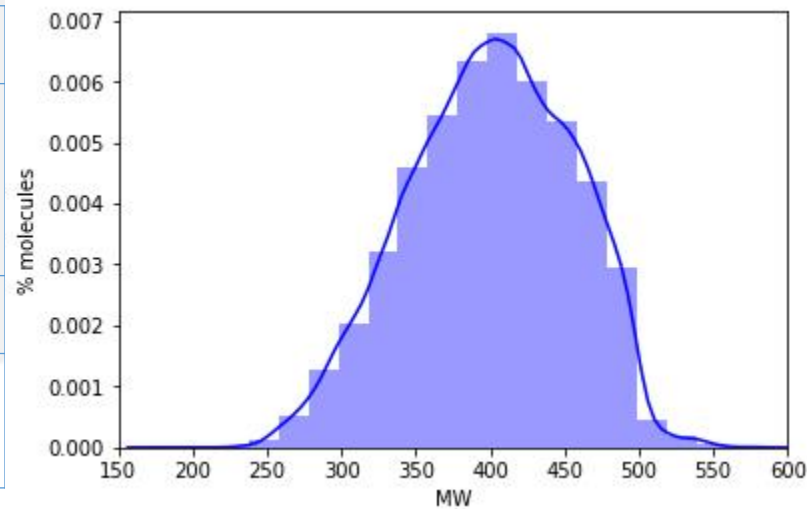


WO 2017064512  
(Exonate Ltd.)  
SRPK1  
Angiogenesis

We improve the quality of life by creating new medicines

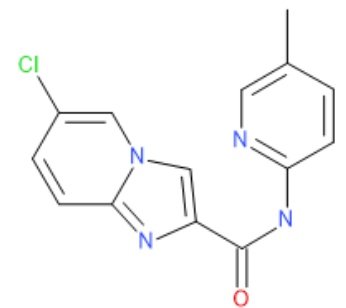
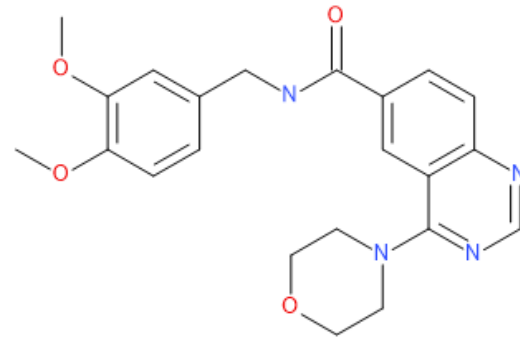
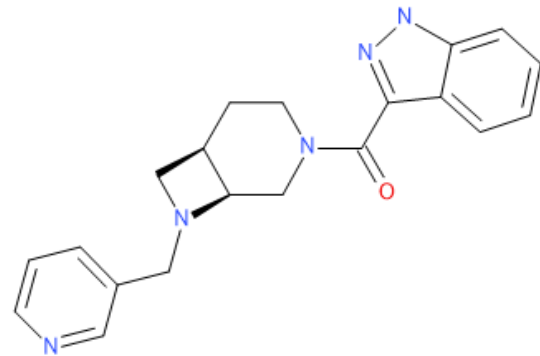
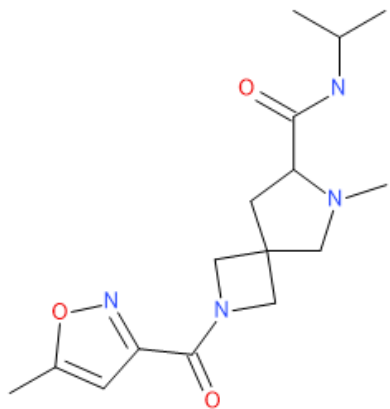
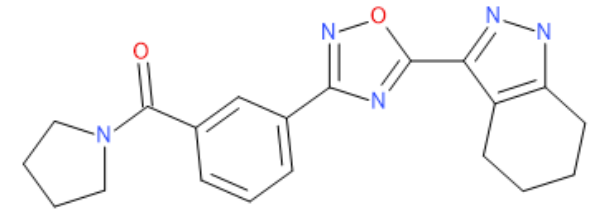
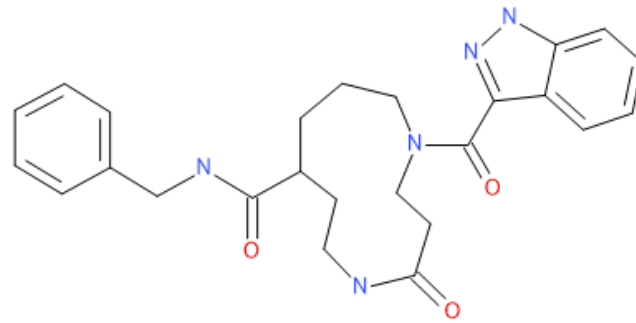
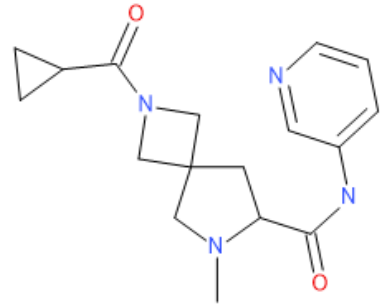
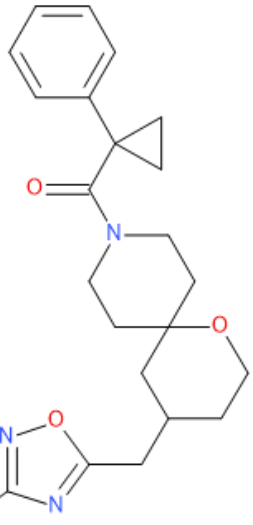
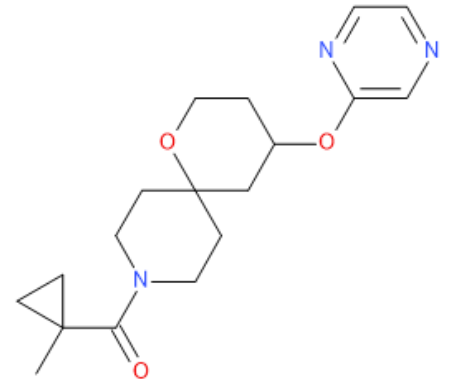
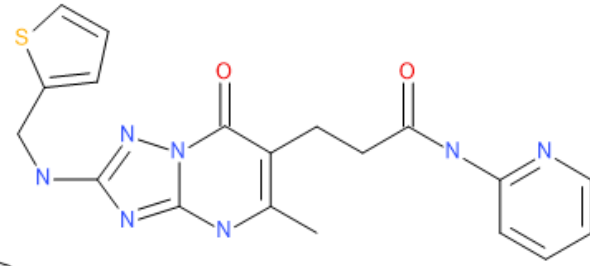
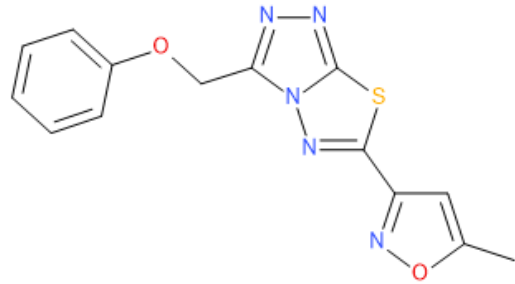
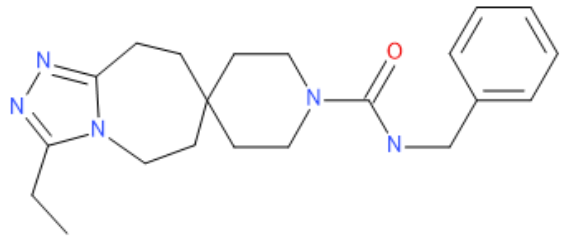
# Physicochemical description

Diversity	0.78
Clusters (Tanimoto, similarity threshold = 0.5, min cmpds per cluster = 5)	860
Singletons	1163
Avr structures in clusters	36.9

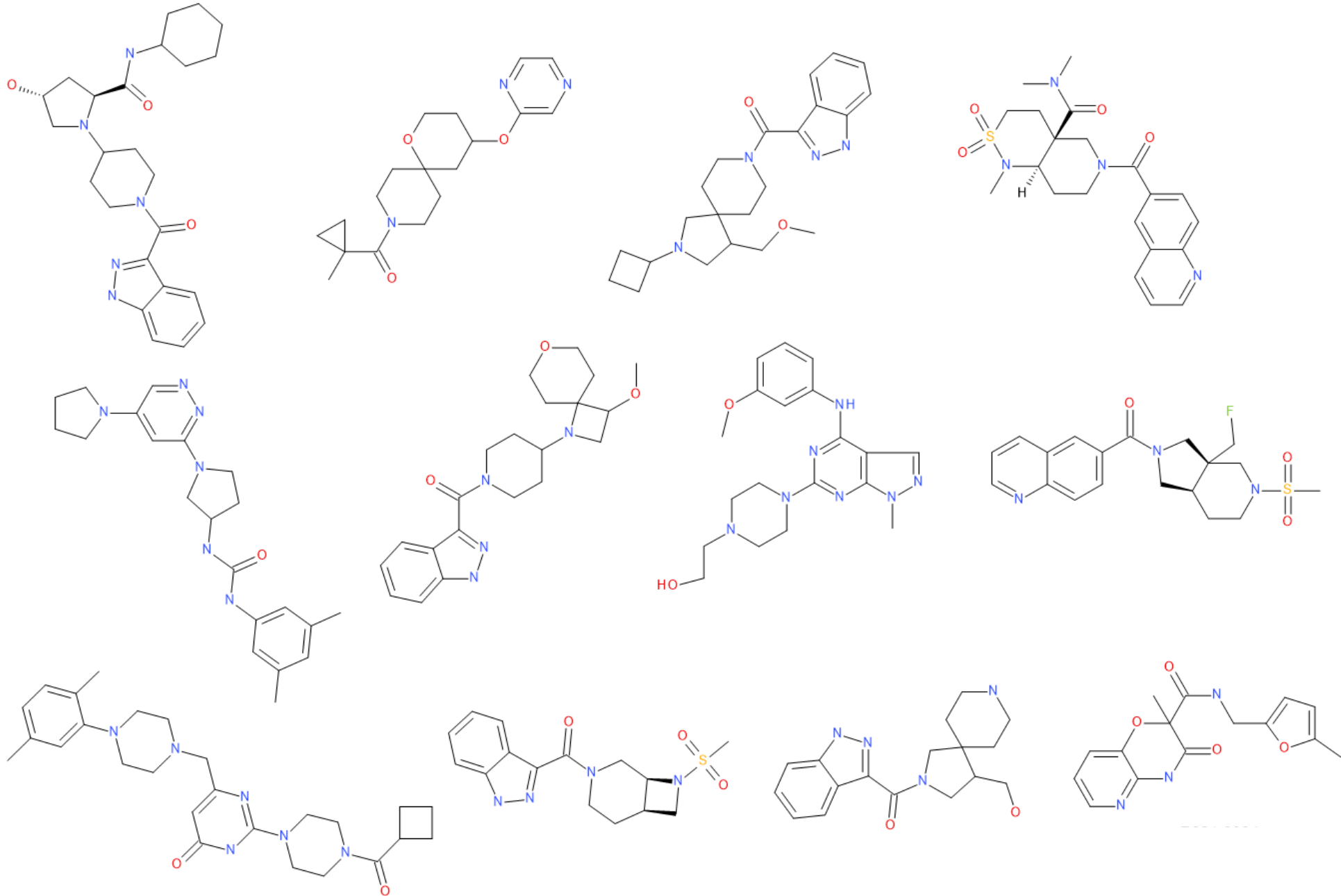


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# Representative examples



# Representative examples







# Благодарим за внимание

Инструкция по заказу соединений из библиотеки «ХимРар»:

Наш сайт: <https://chemrar.ru/library-full-list/>

Направьте список интересующих соединений на email: [vvk@chemrar.ru](mailto:vvk@chemrar.ru)

В соответствии с вашим запросом менеджер выполнит подборку соединений и направит информацию о наличии. Имеется возможность сделать поиск по структуре/буквенному идентификатору (ID, CAS, MFCD), а также импортировать файл в различных форматах: SMILE, sdf, txt.