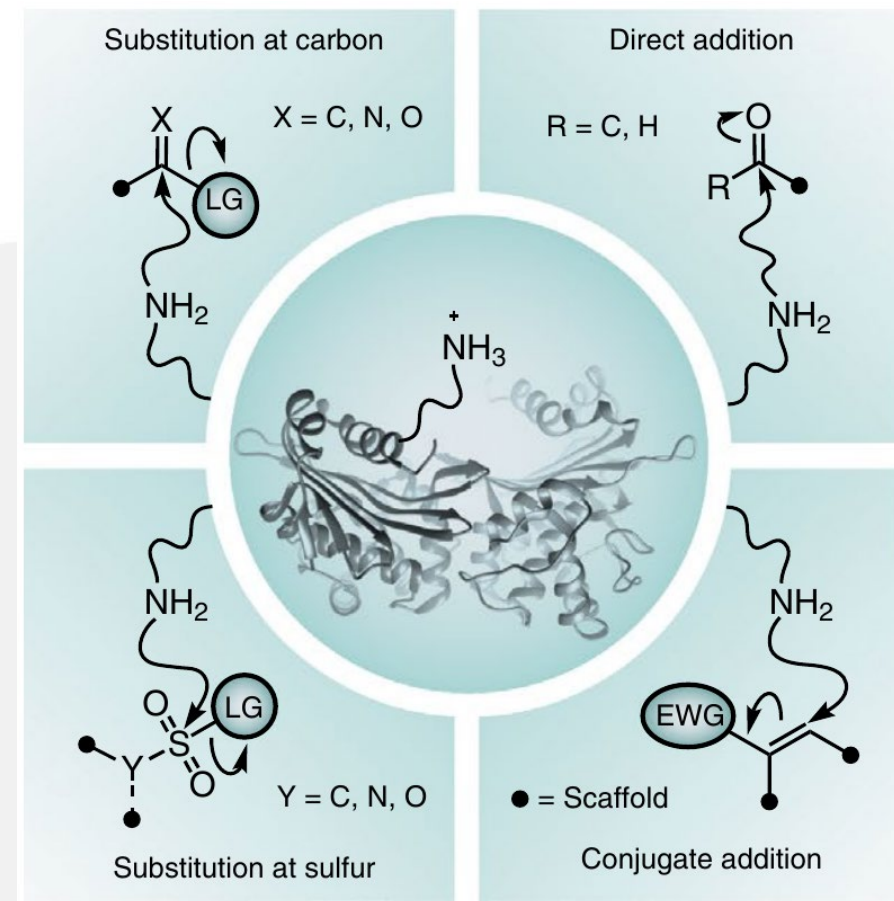


Ковалентно лизин-связывающие библиотеки

Covalent lysine binder library

21 warhead scaffolds
4 200+ compounds

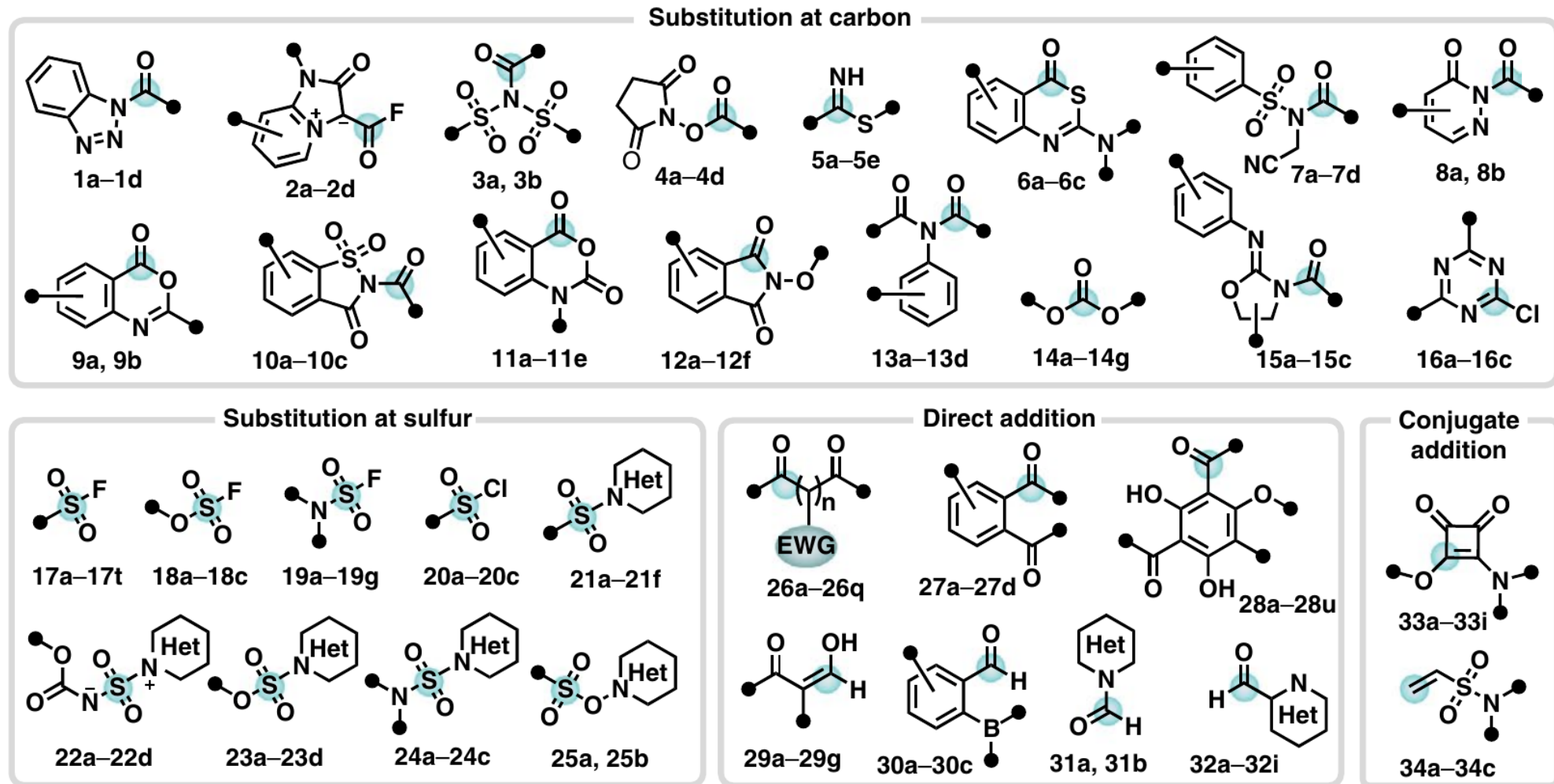
MedChem compatible



Covalent lysine binder library

The core idea of library design

Warhead scaffolds known to be rather selective to serine binding



Warhead scaffolds taken from: Abbasov, M.E. et al // Nature chemistry, (2021), 13(11), 1081-1092.

Covalent lysine binder library



1. The preparation algorithm:

2. Prepare a set of SMARTS queries that capture literature extracted warheads selective to covalent lysine binding – 34 SMARTS patterns prepared*
3. Filter entire 1.6M ChemDiv inventory using the SMARTS prepared
4. Apply MedChem filter (Rule-of-five) to rule out the most MedChemically undesirable structures

*Warhead pattern source: Abbasov, M.E. et al // Nature chemistry, (2021), 13(11), 1081-1092.

Covalent lysine binder library



The library properties:

1. In total 4215 MedChem tolerable compounds
2. 21 warhead patterns with 1 to 1500+ representative molecules in each
3. In silico calculated phys chem properties added to aid in compound selection

Pattern name	Str. count	Pat #
Thioimido_esters	1576	5
Ketoaldehydes	1482	29
Benzoxazinones	250	9
Heterocyclic_aldehydes	208	32
Chlorotriazenes	119	16
Carbonates	114	14
N_formyl_heterocycles	102	31
Acyl_benzotriazoles	95	1
Bisacetanilides	71	13
Sulfonyl_heterocycles	65	21
Sulfonyl_chlorides	56	20

Pattern name	Str. count	Pat #
Isatoic_anhydrides	23	11
N-hydroxyphthalimides	17	12
N-succinimidyl_esters	16	4
Polycarbonyls	7	26
Heterocyclic_sulfonyl_ureas	5	24
Sulfonyl_fluorides	3	17
Vinyl_sulfonamides	2	34
N_O_sulfonates	2	25
Benzothiazinones	1	6
Acyl_saccharins	1	10

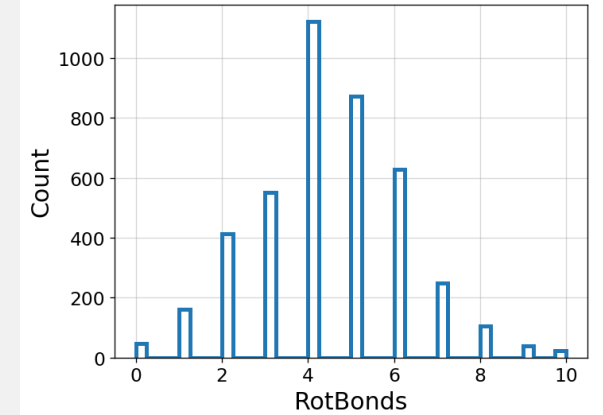
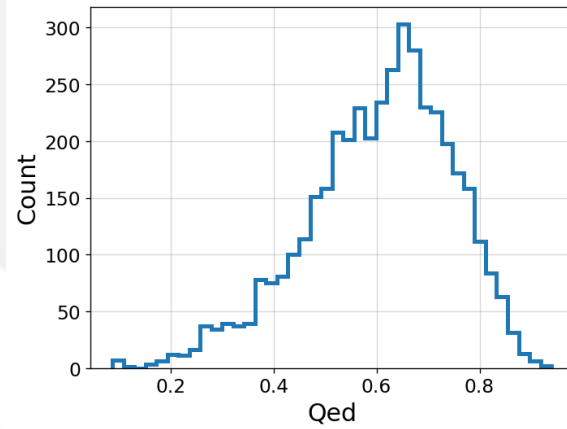
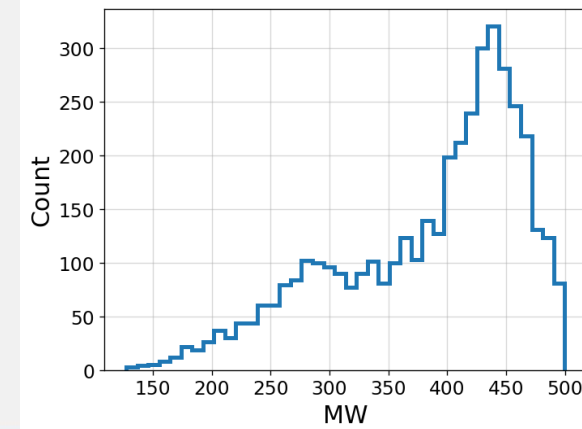
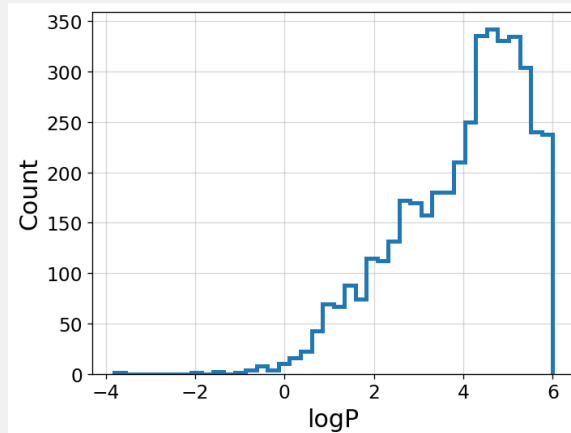
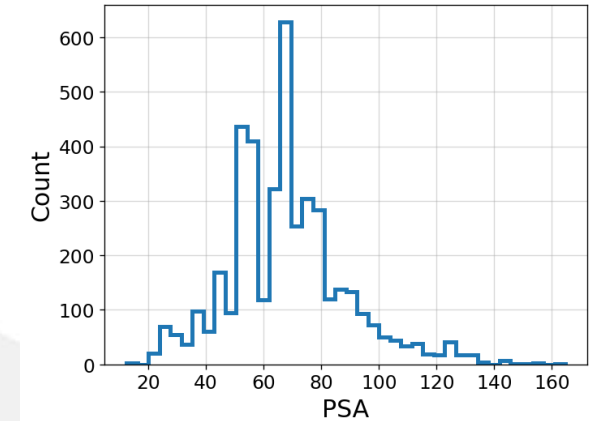
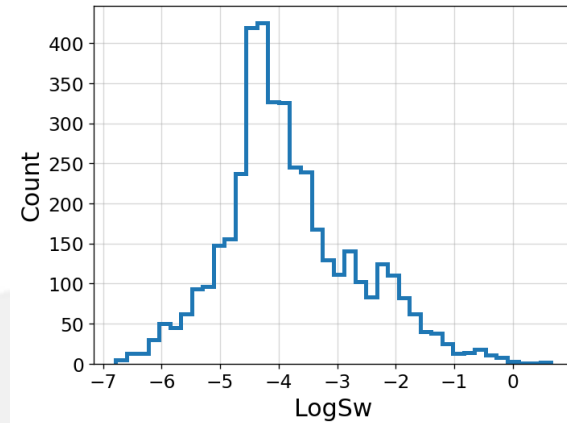
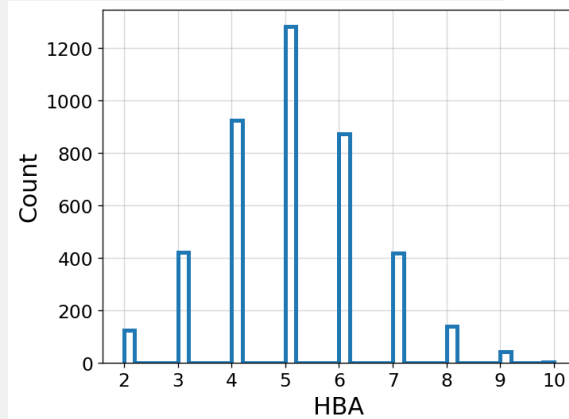
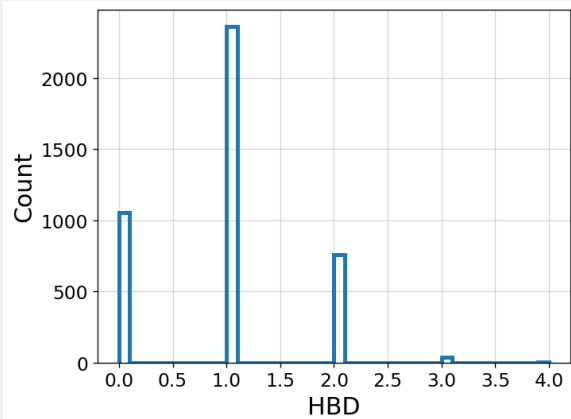
Pattern name and **Pat #** taken from: Abbasov, M.E. et al // Nature chemistry, (2021), 13(11), 1081-1092.

Str. Count – is the count of structures containing a specific scaffold in the lysine library

Covalent lysine binder library



Distribution of Phys-Chem Properties

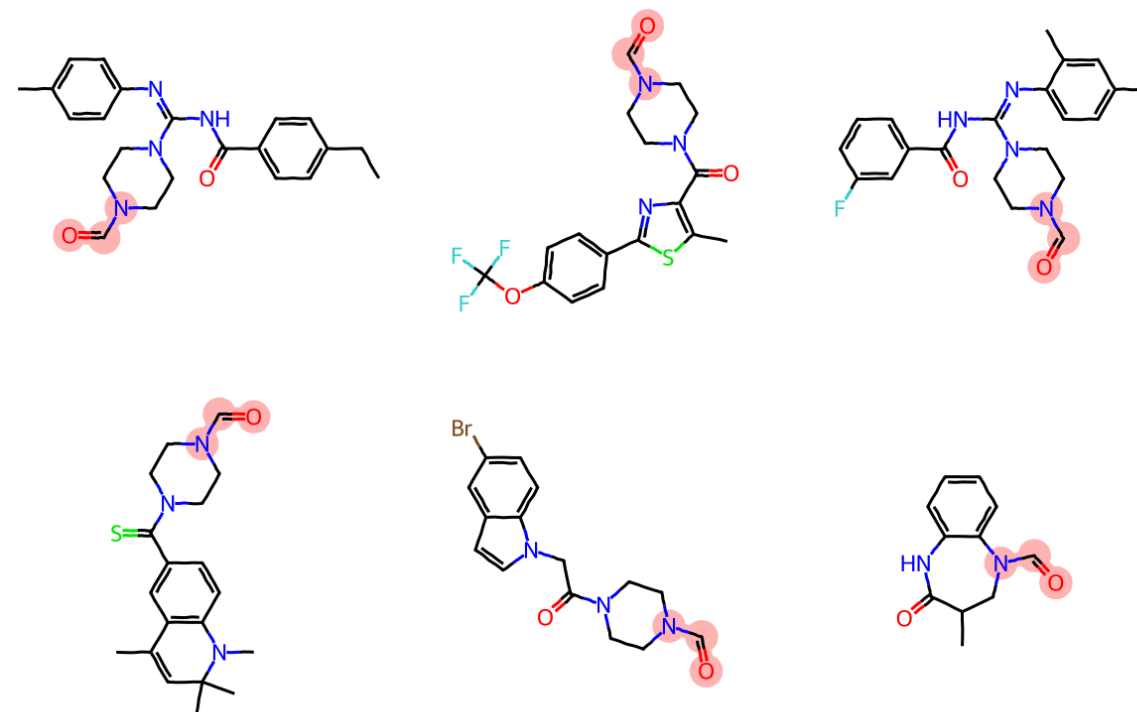
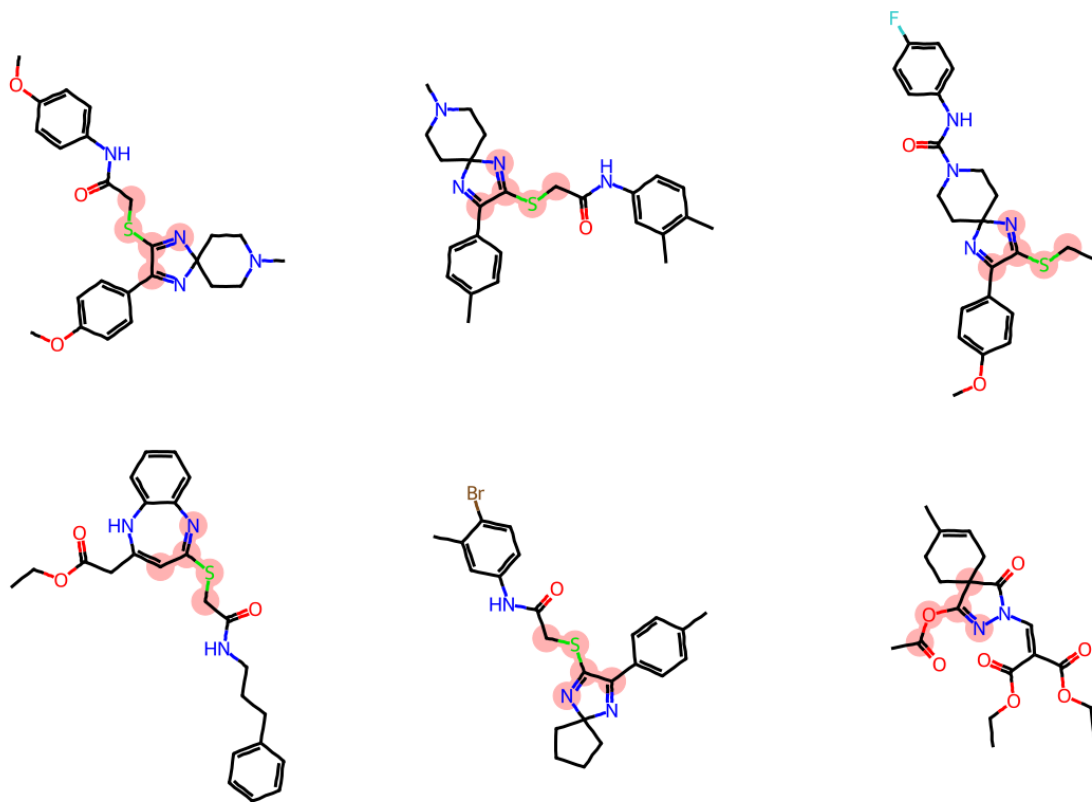


We improve the quality of life by creating new medicines

Covalent lysine binder library

Examples of Structures with warheads

(Thio)imido esters



N-formyl heterocycles



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

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.