Chemspace Compound Libraries: CNS-Focused Library and PPI Modulators

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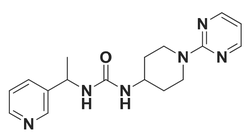
CNS-Focused Library

Compounds that affect the central nervous system are an important class of drugs. The basic requirements for the compounds that are supposed to penetrate the blood-brain barrier (BBB) are somewhat different from those utilized in the majority of drug discovery projects: small and polar compounds are not able to pass the BBB. On the other hand, large non-polar compounds do not pass through the cell membrane. We have accounted for the all aforementioned and created CNS-focused set.

Selection criteria:

- 200 ≤ MW ≤ 450
- SlogP ≤ 5
- HBD ≤ 4
- HBA ≤ 8
- Rotatable Bonds ≤ 8
- H-bonds ≤ 8
- pKa 6.5-10.5, neutral or basic compounds
- TPSA 40-100 Å^2
- No PAINS, toxic moieties



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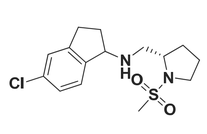

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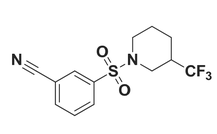

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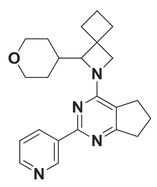

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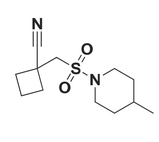

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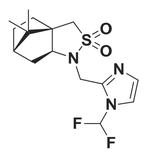

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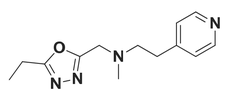

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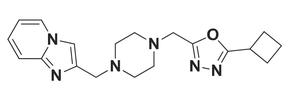

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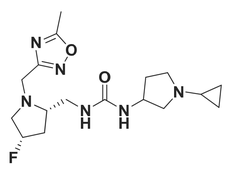

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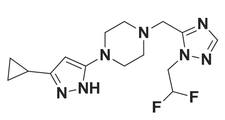

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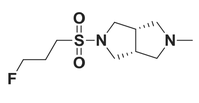

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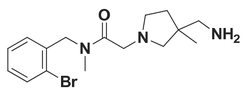

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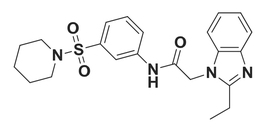
PPI Modulators

Modulation of the protein-protein interactions (PPIs) is a promising strategy in drug discovery since PPIs are involved in numerous cell processes. As promising as difficult the studying and targeting PPIs is because molecular complexes, in comparison with “simple” single-protein targeting, have remained much less explored: the surface of the proteins that are responsible for these interactions differs from that in the classical targets. We have elaborated the latest findings and created PPI modulators set.

Selection criteria:

- MW ≥ 400
- SLogP ≥ 4
- HBA ≥ 3
- Rings ≥ 3
- No PAINS, toxic moieties
- “Hot spot” paradigm: compounds with functional groups that interact with important amino acids (Arg, Trp, Tyr).



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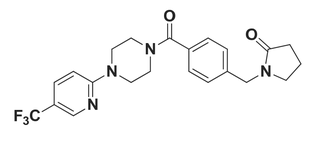

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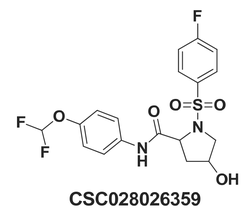

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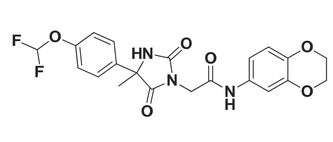

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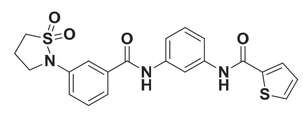

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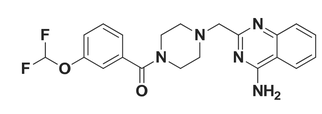

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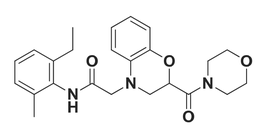

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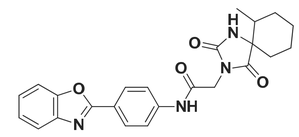

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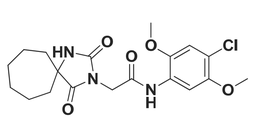

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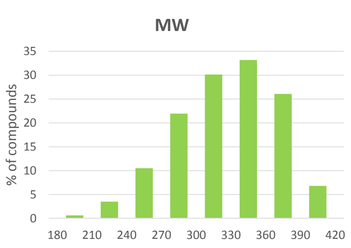
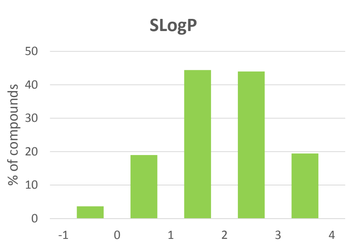
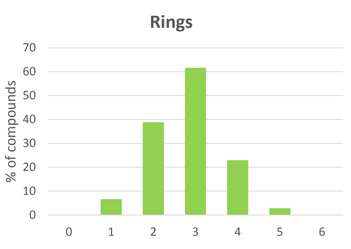
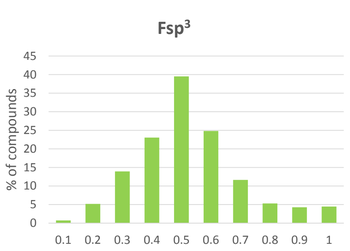
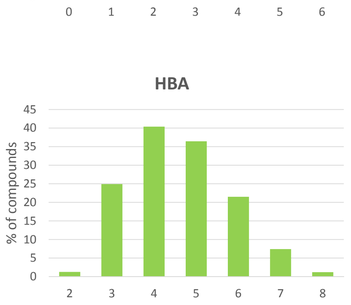


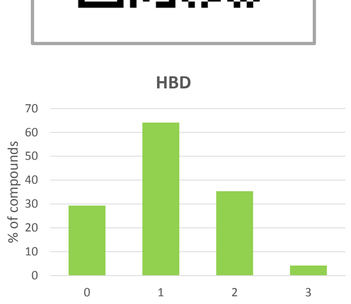


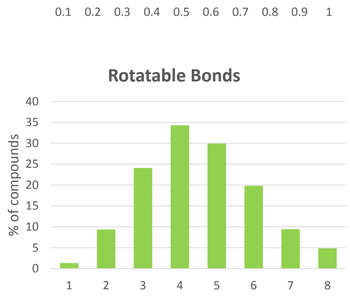


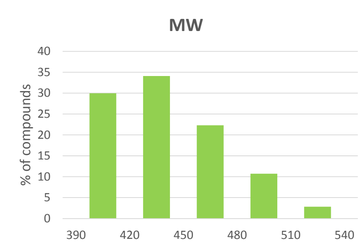
CNS-Focused Library

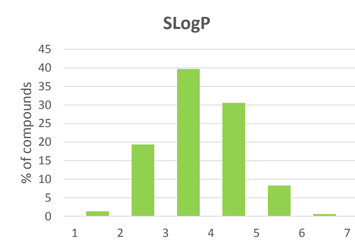


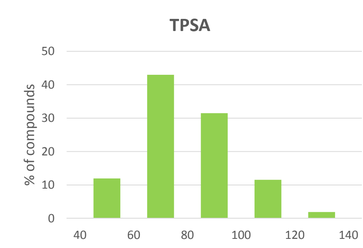


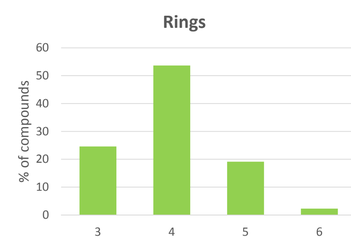




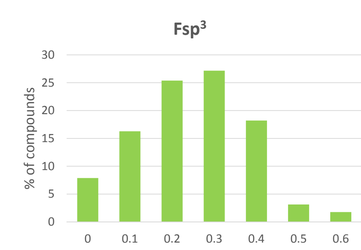


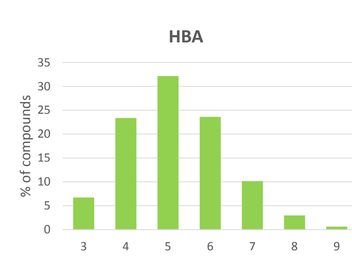


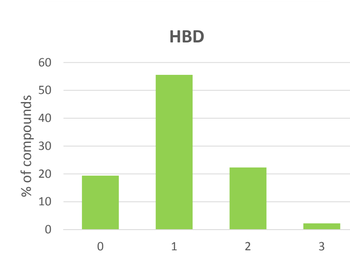


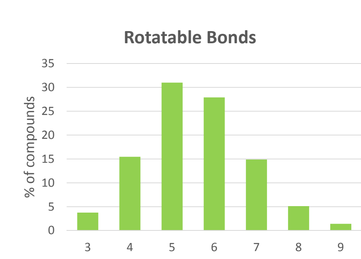


PPI Modulators









Availability

- In-stock and Make-on-demand sets are available
- Ordering options: full or cherry-picked set
- Purity, 90%+ (LC-MS)
- Various formatting: solids, DMSO solutions (96-, 384-well plates)

Contacts

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