

https://vitasmlab.net

Vitas-M CNS-Focused Library

Vitas-M CNS-focused library is a curated collection of compounds specifically designed to overcome the unique challenge of traversing the blood-brain barrier (BBB) to reach therapeutic targets within the central nervous system. Unlike general screening libraries, its value lies not merely in chemical diversity, but in a pre-optimized balance of physicochemical proper- ties that prioritize brain penetrance while maintaining drug-like character. The critical barrier to CNS drug efficacy is often not a lack of target engagement, but an inability to deliver the therapeutic molecule to its site of action. The BBB selectively excludes >98% of all small molecules. Our CNS-focused library pre-filters for compounds with a high probability of brain exposure, dramatically increasing the hit rate. This library is constructed by applying a multi-parameter optimization funnel, prioritizing compounds that conform to the "Rule of CNS" principles, a refinement of broader rules like Lipinski's Rule of Five: the primary filter is a computationally predicted BBB score, indicating a high likelihood of passive diffusion across the endo- thelial cells of the BBB. Other parameters, which were accounted are: Low Molecular Weight (MW), Controlled Lipophilicity, Low Hydrogen Bonding Potential, Topological Polar Surface Area (TPSA), Number of H-bond Donors and Acceptors. The conformational restraint provided by optimal physicochemical properties reduces the entropic penalty upon binding, leading to higher selectivity and binding efficiency for neurologically relevant targets like GPCRs, ion channels, and transporters.

This library enables the direct screening of compounds against CNS targets with the increased likehood that any "hit" already possesses the fundamental blueprint required to reach that target in a living organism. It is an indispensable tool for accelerating the discovery of novel therapeutics for conditions like Alzheimer's disease, Parkinson's disease, schizophrenia, and brain cancers, where overcoming the BBB remains the single greatest hurdle.

Our CNS-Focused Library contains 6213 compounds.

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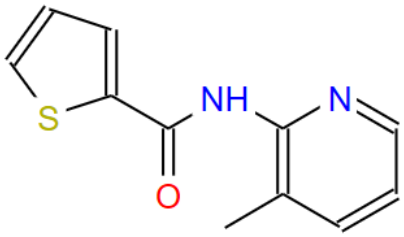

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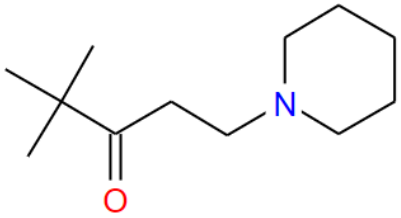

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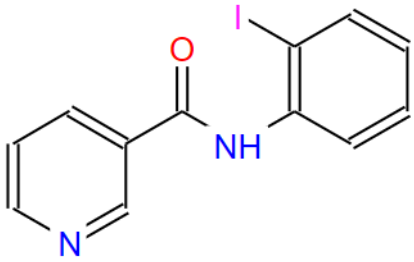

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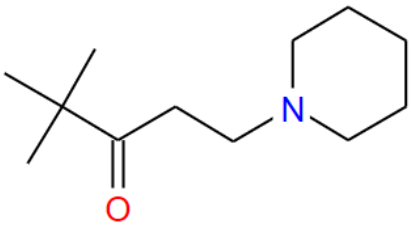

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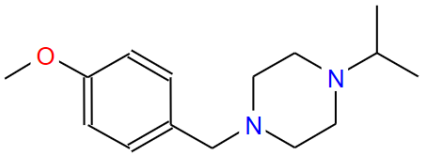

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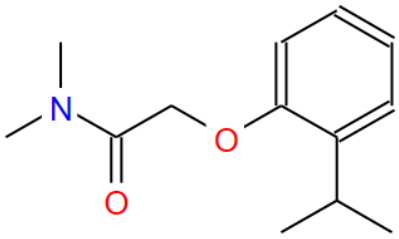

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If you have any specific needs for your project, we can provide specially tailored compound library based on your request.

Have questions or need a quote? Contact Irina Haywood (Ryabushenko) at
irina@vitasmlab.biz
Let's Connect on LinkedIn! Expand your professional network.

We look forward to collaborating with you!
Empowering Your Research, One Molecule at a Time.