

Monoamine Transporter Ligands Library

As key elements of the peripheral and central nervous systems, monoamine transporter proteins have been well explored and exploited for the amelioration of **motor disorders, schizophrenia, drug addiction, dementia, sleep apnea, anxiety, and depression** to name a few. Ligands that bind to these transporters in selective and distinct ways will continue to be discovered and medical research will certainly reveal that more diseases and conditions will benefit from them. Thus, scientists at ChemDiv have designed and implemented our monoamine transporter ligand library consisting of four strategic sub-libraries:

- **Dopamine Transporter (DAT)** ligands; *3650 compounds*
- **Serotonin Transporter (SERT)** ligands; *3650 compounds*
- **Norepinephrine Transporter (NET)** ligands; *1450 compounds*
- **Vesicular Monoamine (VMAT2) and Acetylcholine (VACHT) Transporter** ligands; *800 compounds*

The **selection process** for generating this library started with the identification of known target ligands from Prous Science Integrity database:

- 1st level – all launched drugs and drugs under active development.
- 2nd level – selected drugs at preclinical up to phase III clinical trials.
- 3rd level – selected ligands from the most recently (since 2005) published patents and literature sources.

Then for each “hit”, a similarity search was conducted over the entire (>1.2 million stock compounds) ChemDiv collection. These similar compounds were then subjected to the filtering criteria: 1) $MW \leq 500$; 2) $\log P \leq 5$; 3) $N+O \leq 10$. Compounds with reactive functionalities were removed (aldehydes, methylaryl ketones, Michael acceptors, trifluoromethyl ketones, etc.) and finally, “non-drug-like” compounds were filtered out (structures overloaded with NO_2 , SO_2N , Halogens, etc. groups). The process was repeated for each of the four categories listed above resulting in their respective compound populations. **Embellishment of the library** is an ongoing effort at ChemDiv. Regular updates are being made as newly synthesized compounds become available and pass our QA specifications (>90% purity as established by LC/MS with UV and ELSD).

Statistical data for the current generation of ChemDiv's Monoamine Transporter Library.

Library	Size	Unique Heterocycles	Diversity Coefficient	Templates	Property Range
Monoamine Transporter (2009 Generation)	8700 cmpds	265	0.728	335	190 < MW < 500; 406 ave. 1 < N+O < 10; 6 ave. clogP < 5

Please **contact a ChemDiv business development professional** to discuss your specific needs.