

Chemoinformatics Approach

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**NIDA Informatics for Data and Resource
Discovery in Addition Research
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Multidisciplinary Research Advances the CDD Vision

- **Develop platform methodologies** for drug discovery and development that: (a) integrate chemistry and biology; (b) are applicable to a variety of biological targets/systems with an emphasis on endocannabinoid system.
- **Apply these technologies experimentally and translationally** to drugable targets to discover new medications with an emphasis on drug addiction disorders.
- **Collaborate** with the biotechnology and pharmaceutical industries and leading clinical centers

Metabolic Disorders /Addiction

*diabetes
obesity
steatosis*

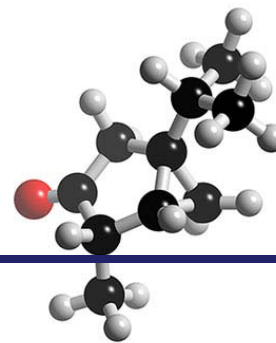
Neuropathic Pain

diabetes, shingles

Neuroprotection

*multiple sclerosis
Alzheimer's
stroke*

CDD Chemotype ADMET Portal



web-based workflow

CDD
database

Empirical drug-
like rules

Physicalchemical
properties

Public available
ADMET models

CDD literature
chemotype
ADMET models

CDD in-house
chemotype
ADMET models

Consensus drug-
like model

Computer
assisted drug
design

CDD Compound Profiling

- Chemical structures can be characterized by numerous descriptors, including topological, geometric, electronic, pharmacophoric, and physicochemical.
- **Develop systematic approaches** for modeling, visualization and global comparison of large in-house sets of biological activity target data.
- **Derive global and local relationships and predictive models** that can be used for identification of novel scaffolds, large-scale virtual screening, efficient follow-up on screening results, library design, and chemical probe and lead optimization.