# Informatics “Speed Talk”


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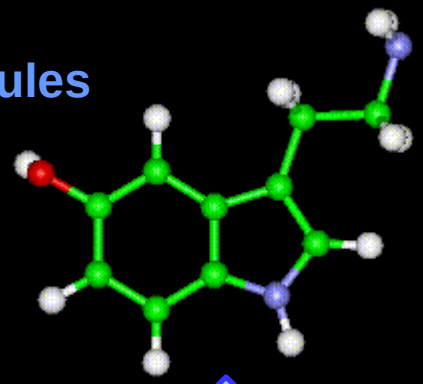
# Data / Resources

Chemistry ⟷ Cellular / Molecular Biology ⟷ Preclinical Behavioral Neuropharmacology ⟷ Clinical Behavioral Psycho-pharmacology

New Molecules



*In Vivo* Behavioral Models

*In Vitro* Assays

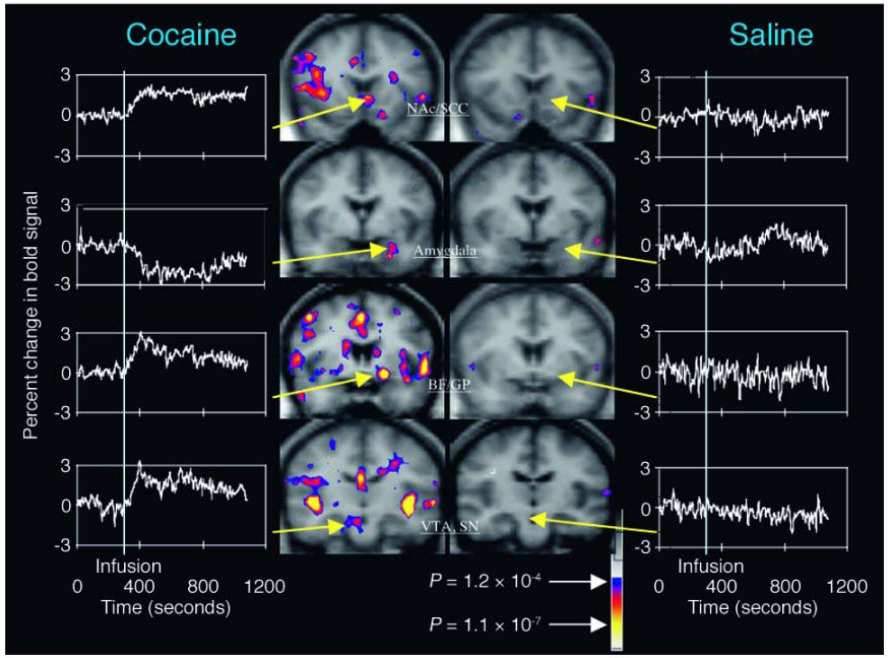
Structure-Activity Data

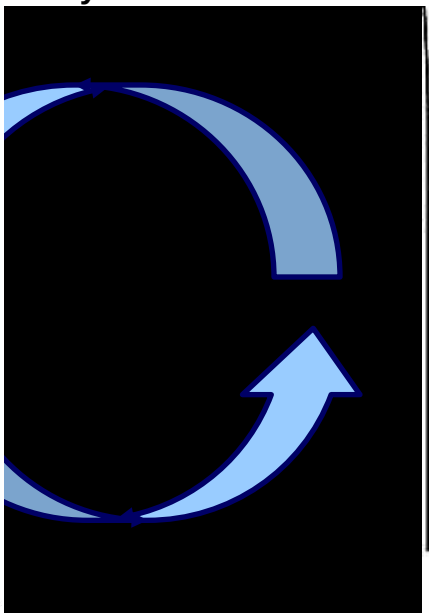
# Data / Resources

Chemistry ⟷ Cellular / Molecular Biology ⟷ Preclinical Behavioral Neuropharmacology ⟷ Clinical Behavioral Psycho-pharmacology

"at" by Robert Neubecker

## phMRI Imaging



## *In Vivo* Behavioral Models

"They took my pellets, man, I been hittin' that lever all day, they took my PELLETS!"

# External Resources Utilized

- Ki data ➡ NIMH Psychoactive Drug Screening Program
- Signaling Networks ➡ Ingenuity Pathway Analysis
- Gene/protein expression ➡ Allen Brain Atlas
- Gene sequence, SNPs, etc. ➡ UCSC genome browser
- Behavior models/data ➡ Comprehensive Database of Drug Discrimination and Self-administration Research

# Need

- mRNA/protein expression in cell lines
- Searchable behavior experiment protocols & results

# Relating Data

- **Literature Search (Pubmed & Google Scholar)**
- NIMH Psychoactive Drug Screening Program (Ki data)
- Ingenuity Pathway Analysis (signaling networks)
- Allen Brain Atlas (gene expression)
- UCSC genome browser (gene sequence, SNPs, etc)
- Comprehensive Database of Drug Discrimination and Self-administration Research (NIDA; publications search)

# Data Sharing

- Peer-reviewed publication
- Send newly synthesized molecules to PDSP for screening
- Post resource information on our Center website
  - Synthesis routes for new compounds
  - Protocols
  - Cell lines
  - Viral vectors

# Obstacles

## Relational database development

- Establish electronic lab notebooks that feed into relational databases
- Identify appropriate info to input into database
- Establish Secure Inter-University data sharing
- Effective communication with informatics specialists

## Database discovery

- What databases exist?
- What information they contain?
- How to query effectively?

# Links

- NIMH Psychoactive Drug Screening Program http://pdsp.med.unc.edu/indexR.html
- Allen Brain Atlas http://www.brain-map.org/
- UCSC genome browser http://genome.ucsc.edu/
- Ingenuity Pathway Analysis http://www.ingenuity.com
- Comprehensive Database of Drug Discrimination and Self-administration Research http://dsa-database.org/