NEW PSYCHOACTIVE SUBSTANCES

NPS

From EU Drug Market Trends to
Cutting-Edge Detection Methods

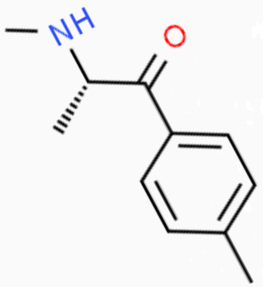
ABOUT NPS

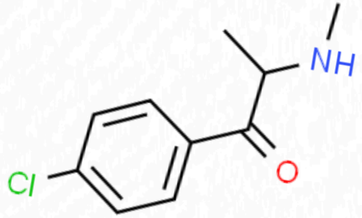
- Substances not controlled under UN drug conventions
- Mimic effects of controlled drugs
- Include stimulants, cannabinoids, opioids, and hallucinogens etc.
- Pose similar health and social risks as controlled substances

GLOBAL CONTEXT

- Over 1,200 NPS identified globally since 2008
- Industrial-scale production of precursors China and India
- Sold under “legal highs”, “research chemicals”, and “dietary supplements”
- Not monitored systematically in many parts of the world

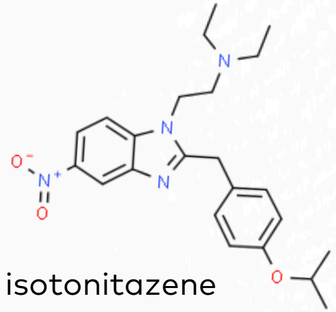
COMMON TYPES NPS

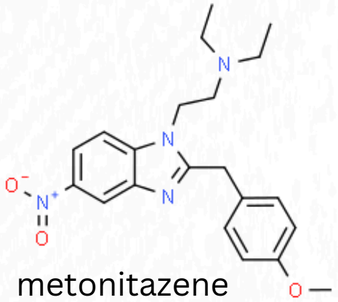


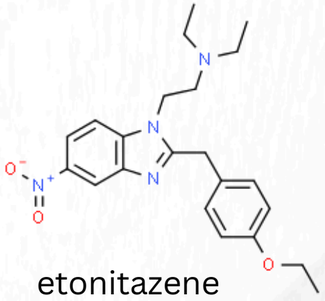


- **Synthetic cathinones**
  - Replacements for controlled stimulants such as amphetamines, cocaine and MDMA
  - 4-MMC (mephedrone), 4-CMC (clephedrone) and 3-CMC (clophedrone)
- **Synthetic Cannabinoids**
  - ‘Legal’ replacements for cannabis - some routine test cannot detect synthetic cannabinoids
  - Sprayed onto herbal material or tobacco and smoked
  - Currently monitored 247 synthetic cannabinoids, the largest group of NPS in Europe

COMMON TYPES NPS

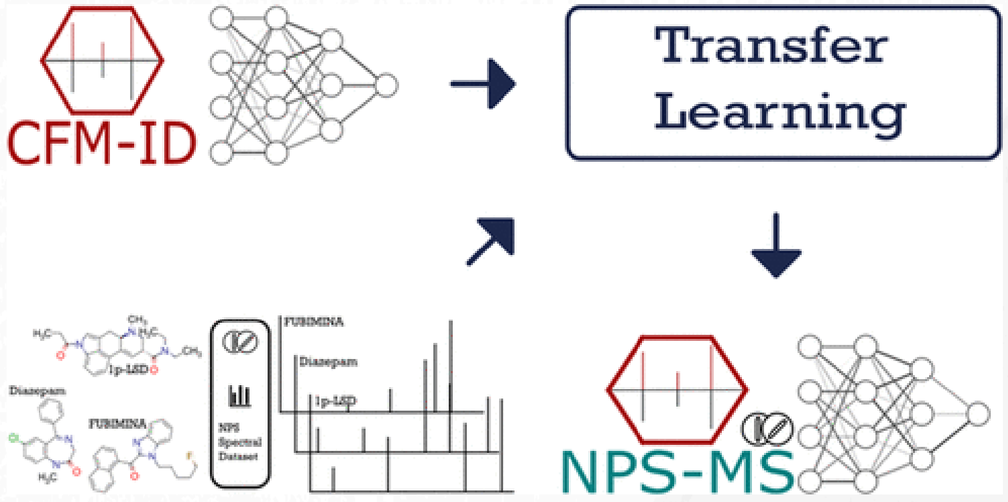






- **New Opioids**
  - Replacements for controlled opioids such as heroin, oxycodone…
  - Fentanyl, methadone, Nitazene opioids (produced in China), carfentanil (from Russia), tramadol (from India)
- **Benzodiazepines**
  - Fake versions of legitimate medicines (diazepam and alprazolam)
  - etizolam and flualprazolam (controlled in 2020), flubromazolam and clonazolam (controlled in 2021), bromazolam

AI-POWERED
NPS PREDICTION : NPS-MS



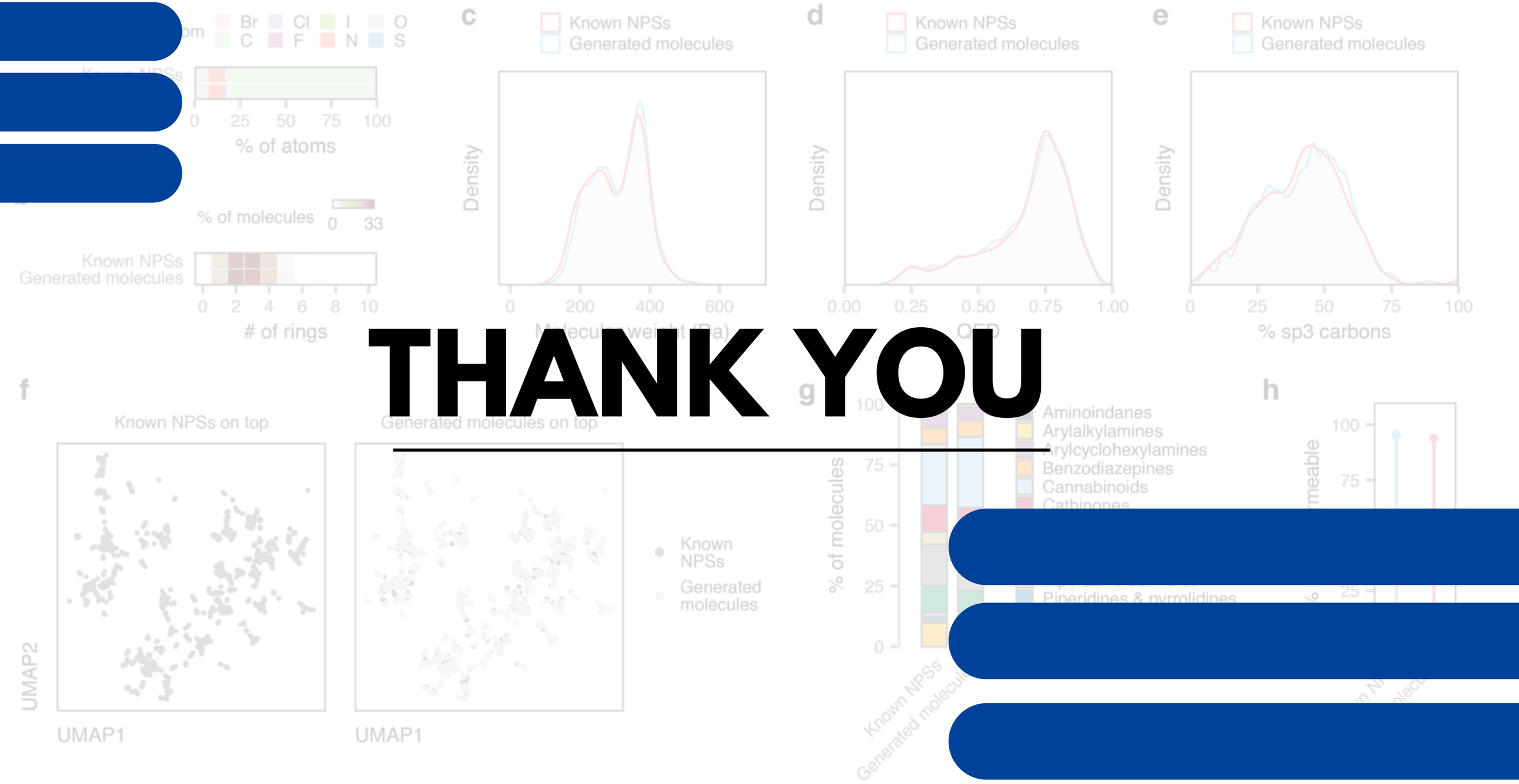
- NPS-MS: Deep learning model for MS/MS spectrum prediction
- Uses transfer learning from generic MS/MS prediction model (CFM-ID 4.0)
- Trained on 1872 MS/MS spectra from 624 NPS compounds
- Identify a previously unknown PCP derivative without the use of any reference materials
- Open the possibility of *identifying emerging NPSs for which reference MS/MS spectra are not yet available* or even never-before-seen NPS
- Available as a web server at https://nps-ms.ca/

DRAK NPS
A DEEP GENERATIVE MODEL FOR NPS PREDICTION

- Deep generative model trained on ~1,700 known NPS structures
  - training dataset of NPS chemical structures from HighResNP
- Learns statistical probability distribution over unobserved NPS structures
- Generated 8.9 million unique potential NPS molecules
- Anticipated >90% of NPSs that appeared on the market after training
- Enables structure elucidation from mass spectrometry data alone

Source Code: https://github.com/skinnider/low-data-generative-models

THANK YOU


Br
Cl
I
O
C
F
N
S
% of atoms
% of molecules
Known NPSs
Generated molecules
# of rings
c
Density
d
QED
e
% sp3 carbons
f
Known NPSs on top
Generated molecules on top
UMAP1
UMAP2
g
% of molecules
Aminoindanes
Arylalkylamines
Arylcyclohexylamines
Benzodiazepines
Cannabinoids
Cathinones
Piperidines & pyrrolidines
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