

NPS Detection Benchmark



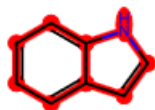
UNODC



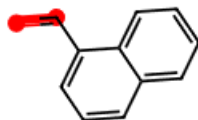
DEA

DRUGBANK

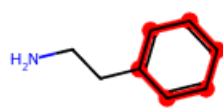
PubChem



Indole



Naphthoyl

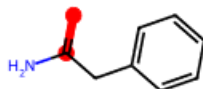
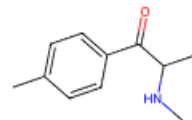


Phenethylamine

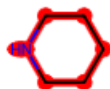
CC1=CC=C(C=C1)C(=O)C(C)NC

CID: 45266826

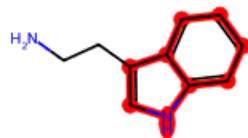
Mephedrone



β -Keto (Cathinone)



Piperidine
(Fentanyl core)

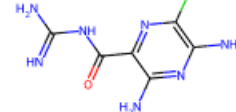


Tryptamine

NC(=N)NC(=O)C1=NC(Cl)=C(N)N=C1N

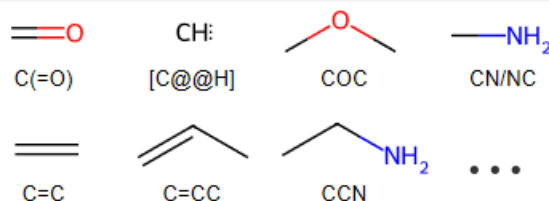
CID: 16231

Amiloride



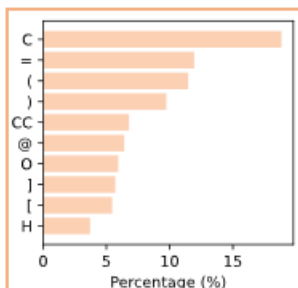
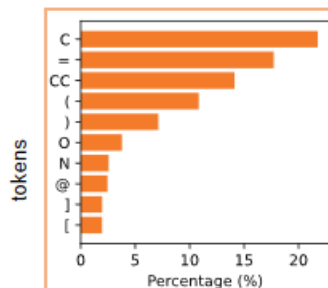
Fragment Decoding

NPS high-frequency fragments



NPS molecules

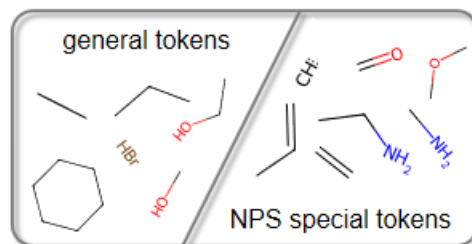
approved drugs



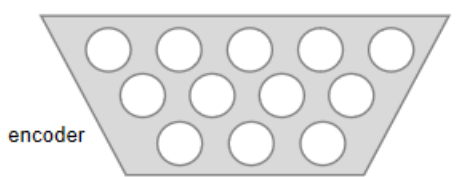
tokens distribution

Model Learning

NPS-aware tokenizer



tokens: C C 1 ... C = C 1) C ... N C

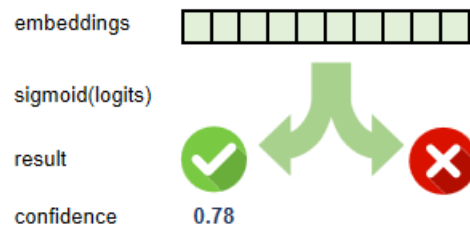


encoder

molecular representation

Confidence Analysis

NPS detection



uncertainty quantification

