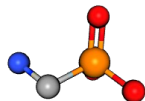


INPUTS

FINGERPRINTS DESCRIPTORS

1 0 1 ... 1 0 0.7 0.1 ...

= TABULAR

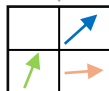


CHEMICAL
REPRESENTATION

NC P(O)(O)=O
SMILES

= SEQUENTIAL

Latent Space:



SMILES EMBEDDING



0.1 0.5 0.7 ...

SPECIES TRAITS

MODELS

**RANDOM
FOREST
&
MLP**

**Bi-GRU
&
TRANS-
FORMER**

P
R
E
D
I
C
T

E
X
P
L
A
I
N

OUTPUT

**LC50
Toxicity**

GENERAL

SPECIES-SPECIFIC

