Deep Generative Models for COVID 19 Drug Discovery

VISUM 2022 - Hands-on Session

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This hands-on session will use GT4SD to generate potential new drugs for treating COVID-19. Our goal is to find molecules that i) **bind** to the desired target protein; ii) are **non-toxic**; iii) can be **easily synthesized**.

In [1]:
```
import os
disable_gpu = True
if disable_gpu:
    os.environ["CUDA_VISIBLE_DEVICES"] = ""
import tensorflow as tf
```

```
2022-07-04 14:45:05.347470: W tensorflow/stream_executor/platform/default/dso_loader.cc:55] Could not load dynamic library 'libnvinfer.so.6'; dlerror: libnvinfer.so.6: cannot open shared object file: No such file or directory; LD_LIBRARY_PATH: /usr/local/cuda/lib64
2022-07-04 14:45:05.347525: W tensorflow/stream_executor/platform/default/dso_loader.cc:55] Could not load dynamic library 'libnvinfer_plugin.so.6'; dlerror: libnvinfer_plugin.so.6: cannot open shared object file: No such file or directory; LD_LIBRARY_PATH: /usr/local/cuda/lib64
2022-07-04 14:45:05.347530: W tensorflow/compiler/tf2tensorrt/utils/py_utils.cc:30] Cannot dlopen some TensorRT libraries. If you would like to use Nvidia GPU with TensorRT, please make sure the missing libraries mentioned above are installed properly.
```

Choosing a target protein

Our first step is to choose a target protein. To find COVID-related proteins, both from human and coronavirus organisms, we can use the following site covid-19.uniprot.org. The well-known spike glycoprotein is the one that initiates the infection of host cells and so we will be using that for this tutorial. Feel free to explore other target proteins.

Note: String representation of proteins

> Protein molecules are long sequences of aminoacids. There are a total of 20 of these basic units used by the human body and so we can code each with a letter, and the whole protein as a string (sequence of letters). For more information on this code you can check here.

Exercise: Change the string below to the desired target protein.

In [6]:
```
# This is an example string for the ACE2_HUMAN Angiotensin-converting enzyme
# Change this so that this string codes for the desired target protein
string = """
MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQ
NMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSEDKSKRLNTIL
```

```
NTMSTIYSTGKVCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLY
EEYVVLKNEMARANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHL
HAYVRAKLMNAYPSYISPIGCLPAHLLGDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVDQ
AWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILM
CTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKS
IGLLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEM
KREIVGVVEPVPHDETYCDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLH
KCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAKNMNVRPLLNYFEPLFTWLKDQNK
NSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSVAYAMRQYFLKVKN
QMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDN
SLEFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENP
YASIDISKGENNPGFQNTDDVQTSF
"""
target_protein = "".join(filter(str.isalpha, (list(string))))
```

Defining metrics of interest

The following metrics will be used to quantify properties of interest in the generated molecules:

- **drug-likeness (QED)**

  > This is a quantitative measure of how close a molecule is to approved drugs, and is estimated based on different molecular properties. A similar structure to approved drugs increases the likelihood of the molecule having desirable properties.

- **aquous solubility**
- **synthetic accessibility score (SAS)**

  > Measures how synthesiable a molecule is.

- **molecular weight**
- **toxicity**

  > Measure of how toxic the molecule is to human cells. The returned value is the average of the prediction of 12 toxicicity tests by a neural network. The dataset used to train the model was Tox21. More information here.

- **affinity**

  > Prediction of affinity to the target protein, obtained with PaccMann Algorithm [1].

References:

[1] - Manica, M., Oskooei, A., Born, J., Subramanian, V. , Sáez-Rodríguez, J. , and Rodríguez Martínez, M. (2019). Toward explainable anticancer compound sensitivity prediction via multimodal attention-based convolutional encoders. Molecular pharmaceutics. https://doi.org/10.1021/acs.molpharmaceut.9b00520

In [7]:
```
from rdkit import Chem
from paccmann_generator.drug_evaluators.esol import ESOL
from paccmann_generator.drug_evaluators.sas import SAS
from paccmann_generator.drug_evaluators.scscore import SCScore
```

```
from gt4sd.algorithms.prediction.paccmann.core import PaccMann, AffinityPred
from paccmann_generator.drug_evaluators import Tox21

#descriptors
def get_drug_likeness(mol):                    # drug likeness
    try:
        return Chem.QED.qed(mol)
    except:
        return 0.0

get_solubility = ESOL()                         # solubility
get_synthesizability = SCScore()                # synthesizability
get_molecularWeight = Chem.Descriptors.MolWt    # molecular weight

path = "Tox21_model"
toxicity_model = Tox21(path)
def get_toxicity(string):
    toxicity_model(string)
    # return the average prediction 12 clinical tests
    return toxicity_model.predictions.mean().detach().numpy()

def get_affinity(strings):
    l = len(strings)
    if l == 1: # addresses the case of batch_size==1
        l = 2
        out_l = 1
    else:
        out_l = l
    config = AffinityPredictor(protein_targets=[target_protein]*l,
                               ligands=strings)
    return list(PaccMann(config).sample(out_l))
```

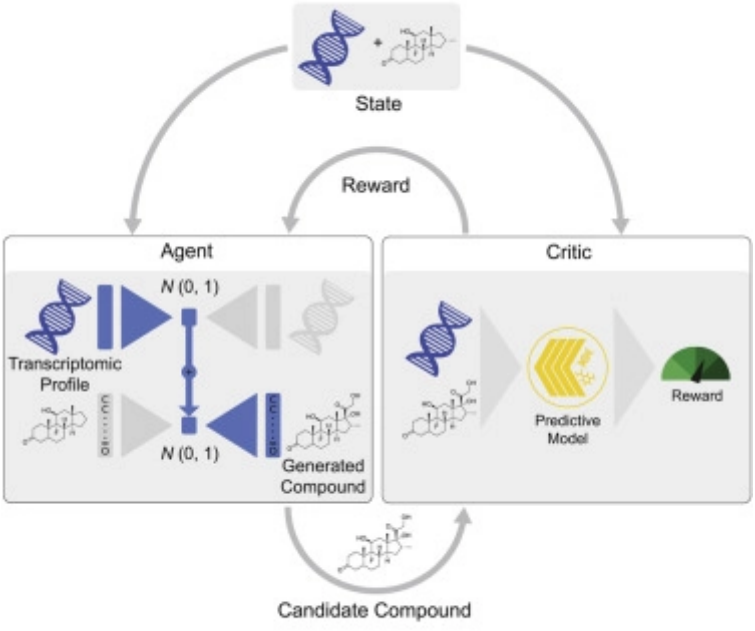
GT4SD (Generative Toolkit for Scientific Discovery)

> The GT4SD (Generative Toolkit for Scientific Discovery) is an open-source platform to accelerate hypothesis generation in the scientific discovery process. It provides a library for making state-of-the-art generative AI models easier to use.

In this tutorial we will cover two generative methods, but feel free to further explore the platform on your own (Getting started)

Generation with PaccMannRL

PaccMannRL was devised for generating molecules targeting a specific protein or biomolecular profile. In this tutorial, given a protein, we want to obtain a compound that maximizes protein-drug binding affinity.



The PaccMannRL model is composed of three basic modules:

- **Protein VAE**: creates a latent representation of the target protein;
- **Compound VAE**: generates a compound as a sequence;
- **Multimodal critic model**: given the protein and a compound, predicts the protein-drug binding affinity.

Note: Variational Autoencoder

> If you want to learn more about VAEs, you can find it here. You can also read more on sequential VAEs and Denoising VAEs.

Each of these modules are pretrained separately. The Protein VAE is trained as a denoising VAE, the Compound VAE as a sequential VAE and finally, the Multimodel critic as a regression model. Then, they are put together in the same network. Using the encoder of the Protein VAE creates a latent representation of the target protein. Then, the protein's latent representation is provided as input to the decoder of the Compound VAE, which originates a new compound. A reinforcement learning strategy is used to optimize the Protein encoder and Compount decoder, using the critic's output as reward.

References:

[2] - Born, J., Manica, M., Cadow, J., Markert, G., Mill, N. A., Filipavicius, M., Janakarajan, N., Cardinale, A., Laino, T., & Rodríguez Martínez, M. (2021). Data-driven molecular design for discovery and synthesis of novel ligands: A case study on SARS-COV-2. Machine Learning: Science and Technology, 2(2), 025024. https://doi.org/10.1088/2632-2153/abe808

[3] - Born, J., Manica, M., Oskooei, A., Cadow, J., Markert, G., & Rodríguez Martínez, M. (2021). PaccMann^RL: De novo generation of hit-like anticancer molecules from transcriptomic data via reinforcement learning. IScience, 24(4), 102269. https://doi.org/10.1016/j.isci.2021.102269

Configuring the model

Our first step is to initialize the algorithm with the target chosen in the previous step.

In [8]:
```
from gt4sd.algorithms.conditional_generation.paccmann_rl.core import PaccMar


# possible arguments generated_length=100
configuration = PaccMannRLProteinBasedGenerator()
algorithm = PaccMannRL(configuration=configuration, target=target_protein)
```

```
14:57:18   runnning PaccMannRL with configuration=PaccMannRLProteinBasedGen
erator(algorithm_version='v0', batch_size=32, temperature=1.4, generated_le
ngth=100)
14:57:18   ensure artifacts for the application are present.
14:57:18   starting syncing
14:57:18   syncing complete
14:57:19   loading configuration file https://s3.amazonaws.com/songlabdata/
proteindata/pytorch-models/bert-base-config.json from cache at /home/emcast
ro/.cache/torch/protein_models/fbb05edff0ffa844a729a04850272a1f8973bc002526
f6615ad113a5f5aacd36.05edb4ed225e1907a3878f9d68b275d79e025b667555aa94a086e2
7cb5c591e0
14:57:19   Model config {
  "attention_probs_dropout_prob": 0.1,
  "base_model": "transformer",
  "finetuning_task": null,
  "hidden_act": "gelu",
  "hidden_dropout_prob": 0.1,
  "hidden_size": 768,
  "initializer_range": 0.02,
  "input_size": 768,
  "intermediate_size": 3072,
  "layer_norm_eps": 1e-12,
  "max_position_embeddings": 8192,
  "num_attention_heads": 12,
  "num_hidden_layers": 12,
  "num_labels": -1,
  "output_attentions": false,
  "output_hidden_states": false,
  "output_size": 768,
  "pruned_heads": {},
  "torchscript": false,
  "type_vocab_size": 1,
  "vocab_size": 30
}

14:57:19   loading weights file https://s3.amazonaws.com/songlabdata/protei
ndata/pytorch-models/bert-base-pytorch_model.bin from cache at /home/emcast
ro/.cache/torch/protein_models/2ed84d28db0a61af4cd2dd3f2ccdd3ee45b1533547a8
e1213840af895e2fa8d1.8206daaea9be2736b6ccde432df9dc3dbb8c3233b47f07688d6ff3
8d74258d22
```

Visualizing its components (summary)

To generate molecules we only need the protein encoder and the compound generator. In the code below:

- **Sequence Embedder**: maps the protein string into an embedding space;
- **Protein Encoder**: encodes the result of the sequence embedder into the latent representation of the Protein VAE;

- **Generator**: Compound VAE.

In [9]:
```
model = configuration.get_conditional_generator(configuration.ensure_artifac

print("\n\nLet's look at the models that will be used in the generation proc

print("Sequence Embedder")
for n, c in model.primary_sequence_embedder.named_modules():
    if n.count(".")==1:
        print("\t", n)

print("Protein Encoder")
for n, c in model.protein_embedding_encoder.named_modules():
    if n.count(".")==0 and n!="":
        print("\t", n)

print("Generator")
for n, c in model.selfies_conditional_generator.named_modules():
    if n.count(".")==0 and n!="":
        print("\t", n)
```

```
14:57:25   starting syncing
14:57:25   syncing complete
14:57:26   loading configuration file https://s3.amazonaws.com/songlabdata/
proteindata/pytorch-models/bert-base-config.json from cache at /home/emcast
ro/.cache/torch/protein_models/fbb05edff0ffa844a729a04850272a1f8973bc002526
f6615ad113a5f5aacd36.05edb4ed225e1907a3878f9d68b275d79e025b667555aa94a086e2
7cb5c591e0
14:57:26   Model config {
  "attention_probs_dropout_prob": 0.1,
  "base_model": "transformer",
  "finetuning_task": null,
  "hidden_act": "gelu",
  "hidden_dropout_prob": 0.1,
  "hidden_size": 768,
  "initializer_range": 0.02,
  "input_size": 768,
  "intermediate_size": 3072,
  "layer_norm_eps": 1e-12,
  "max_position_embeddings": 8192,
  "num_attention_heads": 12,
  "num_hidden_layers": 12,
  "num_labels": -1,
  "output_attentions": false,
  "output_hidden_states": false,
  "output_size": 768,
  "pruned_heads": {},
  "torchscript": false,
  "type_vocab_size": 1,
  "vocab_size": 30
}

14:57:26   loading weights file https://s3.amazonaws.com/songlabdata/protei
ndata/pytorch-models/bert-base-pytorch_model.bin from cache at /home/emcast
ro/.cache/torch/protein_models/2ed84d28db0a61af4cd2dd3f2ccdd3ee45b1533547a8
e1213840af895e2fa8d1.8206daaea9be2736b6ccde432df9dc3dbb8c3233b47f07688d6ff3
8d74258d22


Let's look at the models that will be used in the generation process:
Sequence Embedder
         model.embeddings
         model.encoder
         model.pooler
Protein Encoder
         activation_fn
         encoding
         encoding_to_mu
         encoding_to_logvar
Generator
         encoder
         decoder
```

Example: Generating one molecule using the Compound VAE

The code below shows how we can use the decoder of a sequential VAE to generate a compound (i.e., sequence of tokens). Notice that this is an illustrative example, since we do not condition the Compound Decoder on the protein target, as we do in PaccMannRL.

We start by defining some parameters.

The **generate_len** is the maximum size of the generated sequence. **search** defines how we decide the search strategy used after each iteration of the decoder.

In [10]:
```
import torch
from pytoda.smiles.smiles_language import SMILESLanguage
from paccmann_chemistry.utils.search import SamplingSearch

# parameters for the generation
batch_size = 1
search = SamplingSearch()
prime_input = torch.tensor([SMILESLanguage().start_index])
end_token = torch.tensor([SMILESLanguage().stop_index])
generate_len = 100

# grab the decoder model
decoder = model.selfies_conditional_generator.decoder
decoder._update_batch_size(batch_size)
```

We start by sampling a random vector in the latent representation of the compound VAE. Our initial molecule is an empty sequence, containing only the input token.

In [11]:
```
# generate latent vectors
latent_z = torch.randn(1, batch_size, decoder.latent_dim)
latent_z = latent_z.repeat(decoder.n_layers, 1, 1)

# empty sequence
generated_seq = prime_input.repeat(batch_size, 1)
prime_input = generated_seq.transpose(1, 0).unsqueeze(1)
input_token = prime_input[-1]

# first pass t=0
hidden = decoder.latent_to_hidden(latent_z)
stack = decoder.init_stack
```

In each iteration we generate an additional token. For this we first compute the probabilities of each token being the next in the sequence and then sample one based on our search strategy. We append it to the end of our sequence and set it as the input token for the next iteration. If the **end_token** is returned we exit the loop.

> In the example below, molecules_numerical is a list with all the intermediate molecules generated during the process. It serves only for visualization purposes.

In [12]:
```
smiles_language = model.smiles_language

molecules_numerical = []

for idx in range(generate_len):
    output, hidden, stack = decoder(input_token, hidden, stack)
    logits = decoder.output_layer(output).squeeze(dim=0)
    top_idx = search.step(logits)

    input_token = top_idx.view(1, -1).to(decoder.device)
    generated_seq = torch.cat((generated_seq, top_idx), dim=1)

    print(f"Step {idx} - Tokens: {smiles_language.token_indexes_to_smiles(ge

    # if we don't generate in batches, we can do early stopping.
    if batch_size == 1 and top_idx == end_token:
        break

    molecules_numerical.append(torch.cat((generated_seq, end_token.view(1,1)
```

```
Step 0 - Tokens: [C]

Step 1 - Tokens: [C][Branch2_3]

Step 2 - Tokens: [C][Branch2_3][epsilon]

Step 3 - Tokens: [C][Branch2_3][epsilon][Branch1_3]

Step 4 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C]

Step 5 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C]

Step 6 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3]

Step 7 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branch
2_3]

Step 8 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branch
2_3][C]

Step 9 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branch
2_3][C][c]

Step 10 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c]

Step 11 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c]

Step 12 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c]

Step 13 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c]

Step 14 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c]

Step 15 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1]

Step 16 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1]

Step 17 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N]

Step 18 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C]

Step 19 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3]

Step 20 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon]

Step 21 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]

Step 22 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C]

Step 23 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
```

```
[C][=C]

Step 24 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c]

Step 25 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c]

Step 26 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c]

Step 27 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c]

Step 28 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o]

Step 29 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n]

Step 30 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c]

Step 31 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c]

Step 32 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c]

Step 33 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c]

Step 34 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c][c]

Step 35 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c][c][Ring1]

Step 36 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c][c][Ring1][Branch1_1]

Step 37 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c][c][Ring1][Branch1_1][n]

Step 38 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c][c][Ring1][Branch1_1][n][Ring1]

Step 39 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c][c][Ring1][Branch1_1][n][Ring1][Branch
```

```
2_2]

Step 40 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c][c][Ring1][Branch1_1][n][Ring1][Branch
2_2][C]

Step 41 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c][c][Ring1][Branch1_1][n][Ring1][Branch
2_2][C][C]

Step 42 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c][c][Ring1][Branch1_1][n][Ring1][Branch
2_2][C][C][Ring1]

Step 43 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c][c][Ring1][Branch1_1][n][Ring1][Branch
2_2][C][C][Ring1][=N]

Step 44 - Tokens: [C][Branch2_3][epsilon][Branch1_3][C][C][Branch1_3][Branc
h2_3][C][c][c][c][c][c][c][Ring1][Branch1_1][N][C][Branch1_3][epsilon][=O]
[C][=C][c][c][c][c][o][n][c][c][c][c][c][Ring1][Branch1_1][n][Ring1][Branch
2_2][C][C][Ring1][=N]
```

We now decode the tokens in the generated sequences into the SMILES language (and clean-up) so that we can visualize the molecules. Some molecules generated intermediatly are not valid and so they are filtered.

In [13]:

```
import mols2grid

def remove_none_and_duplicate(seq):
    pool = []
    result = []
    for mol in seq:
        if mol is None:
            continue
        if mol in pool:
            continue
        result.append(mol)
    return result

smiles_num = [smiles_language.token_indexes_to_smiles(molecule_numerical.to
              for molecule_numerical in iter(molecules_numerical)]

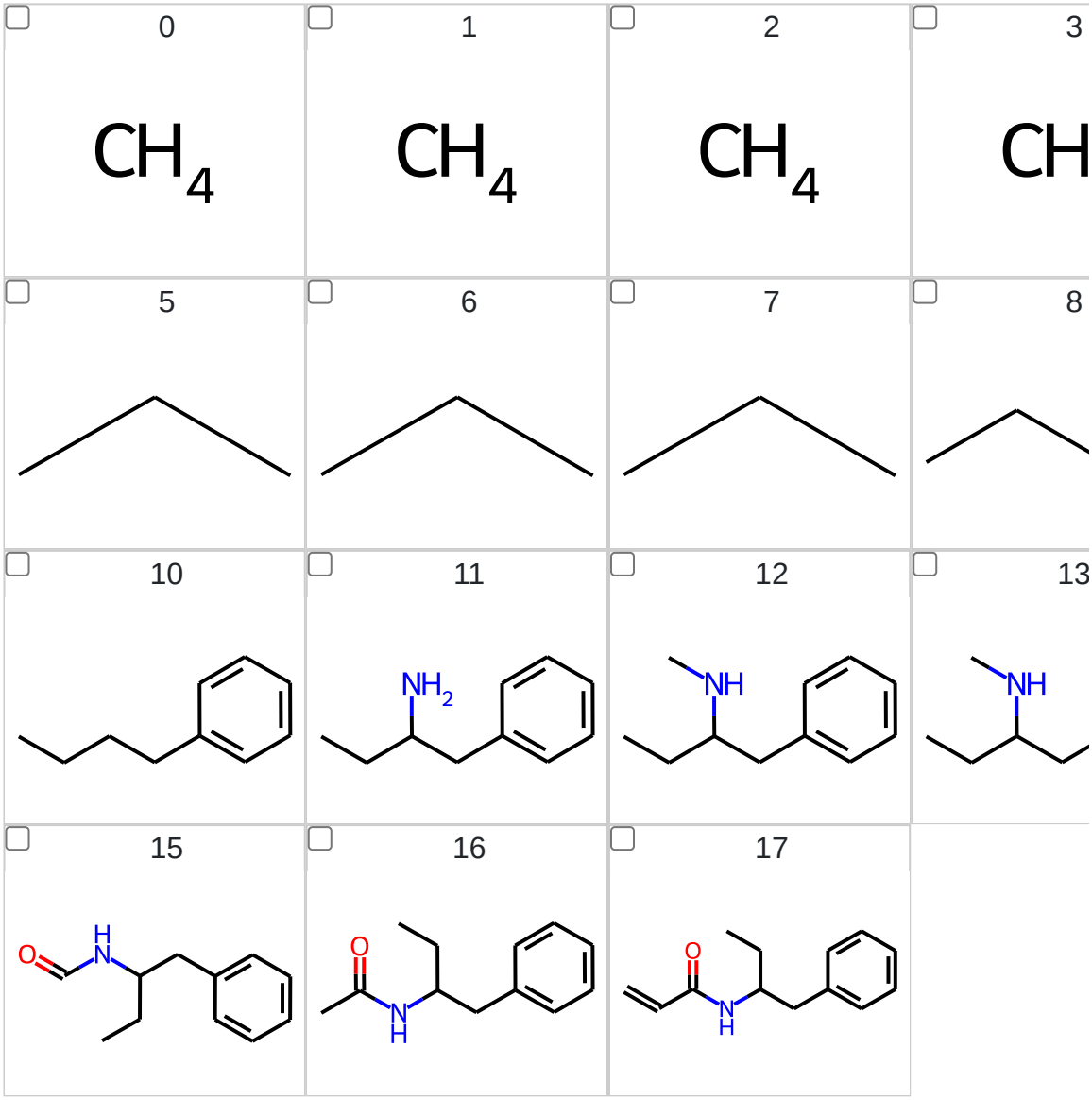
smiles = [smiles_language.selfies_to_smiles(sm) for sm in smiles_num]

molecules = []
for a_smiles in smiles:
    try:
        molecules.append(Chem.MolFromSmiles(a_smiles, sanitize=True))
        # This is used to catch errors in Chem.MolFromSmiles.
        # To debug remove from the try/except clause.

    except Exception:
        molecules.append(None)

molecules = remove_none_and_duplicate(molecules)
mols2grid.display(molecules, n_rows=10, fixedBondLength=200)
```

Out[13]:



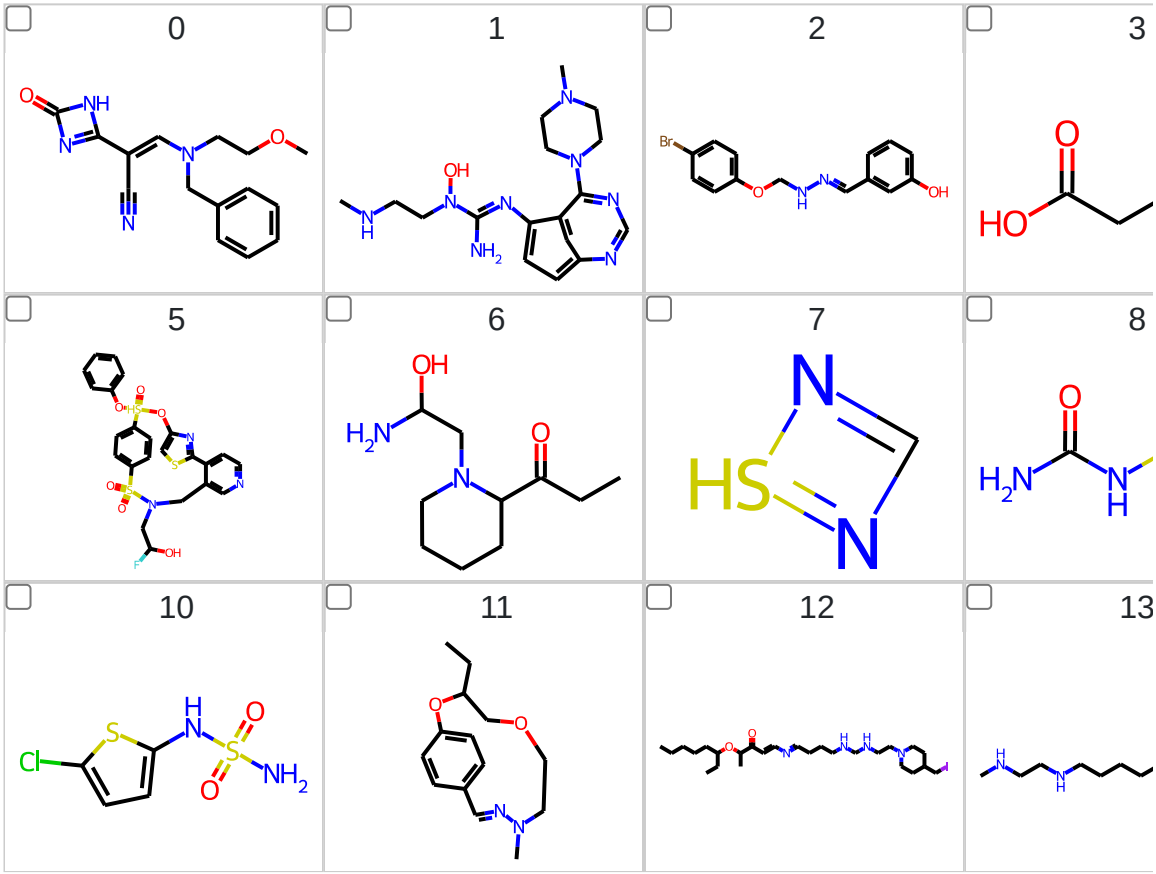
Sampling and Plotting Molecules with GT4SD

Let's go ahead and sample some molecules using the PaccMannRL algorithm. This time we will use the GT4SD interface, which greatly simplifies sampling for us. We start by sampling 15 molecules. We then convert them into a **Mol** object (**RDKit** package). Finally, we display them using the **mols2grid** package.

In [14]:
```
n_sampled_molecules = 15
molecules = list(algorithm.sample(n_sampled_molecules))
molecules = [Chem.MolFromSmiles(molecule) for molecule in molecules]
mols2grid.display(molecules, fixedBondLength=200)
```

```
14:57:35   embedding condition and getting reparametrized latent samples
14:57:36   starting generation of molecules
14:57:37   embedding condition and getting reparametrized latent samples
14:57:39   starting generation of molecules
14:57:39   embedding condition and getting reparametrized latent samples
14:57:40   starting generation of molecules
14:57:41   embedding condition and getting reparametrized latent samples
14:57:42   starting generation of molecules
```

Out[14]:



Evaluating the generated molecules

If we want to compare different algorithms, we can do so using different metrics. This next example shows how to estimate the properties of generated molecules using the PaccMannRL algorithm. We start by generating 100 new molecules. For each we compute the metrics defined in the beggining of the tutorial.

In [15]:

```
n = 100
molecules = list(algorithm.sample(n))

drug_likeness = []
solubility = []
synthesizability = []
molecular_weight = []
toxicity = []

for molecule in molecules:
    mol = Chem.MolFromSmiles(molecule)
    drug_likeness.append(get_drug_likeness(mol))
    solubility.append(get_solubility(mol))
    synthesizability.append(get_synthesizability(mol))
    molecular_weight.append(get_molecularWeight(mol))
    toxicity.append(get_toxicity(molecule))

affinity = get_affinity(molecules)

paccmann_rl_results = dict()
paccmann_rl_results["drug_likeness"] = drug_likeness
paccmann_rl_results["solubility"] = solubility
```

```
paccmann_rl_results["synthesizability"] = synthesizability
paccmann_rl_results["molecular_weight"] = molecular_weight
paccmann_rl_results["toxicity"] = toxicity
paccmann_rl_results["affinity"] = affinity
```

```
14:57:42   embedding condition and getting reparametrized latent samples
14:57:44   starting generation of molecules
14:57:44   embedding condition and getting reparametrized latent samples
14:57:45   starting generation of molecules
14:57:46   embedding condition and getting reparametrized latent samples
14:57:47   starting generation of molecules
14:57:48   embedding condition and getting reparametrized latent samples
14:57:48   starting generation of molecules
14:57:49   embedding condition and getting reparametrized latent samples
14:57:50   starting generation of molecules
14:57:50   embedding condition and getting reparametrized latent samples
14:57:51   starting generation of molecules
14:57:52   embedding condition and getting reparametrized latent samples
14:57:53   starting generation of molecules
14:57:53   embedding condition and getting reparametrized latent samples
14:57:54   starting generation of molecules
14:57:55   embedding condition and getting reparametrized latent samples
14:57:56   starting generation of molecules
14:57:56   embedding condition and getting reparametrized latent samples
14:57:57   starting generation of molecules
14:57:57   embedding condition and getting reparametrized latent samples
14:57:58   starting generation of molecules
14:57:59   embedding condition and getting reparametrized latent samples
14:58:00   starting generation of molecules
14:58:00   embedding condition and getting reparametrized latent samples
14:58:01   starting generation of molecules
14:58:02   embedding condition and getting reparametrized latent samples
14:58:03   starting generation of molecules
14:58:03   embedding condition and getting reparametrized latent samples
14:58:04   starting generation of molecules
14:58:04   embedding condition and getting reparametrized latent samples
14:58:05   starting generation of molecules
14:58:06   embedding condition and getting reparametrized latent samples
14:58:07   starting generation of molecules
14:58:08   no parameters validation
14:58:08   runnning PaccMann with configuration=AffinityPredictor(algorithm
_version='v0', protein_targets=['MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQ
SSLASWNYNTNITEENVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSEDKSKRLN
TILNTMSTIYSTGKVCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMAR
ANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLL
GDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKA
VCHPTAWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKH
LKSIGLLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVP
HDETYCDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWT
LALENVVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYL
FRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRL
NDNSLEFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPYASIDISKGENN
PGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEEN
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NPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYEDYGDYWRGDYE
VNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLLGDMWGRFWTNLYSLTV
PFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRI
LMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDNE
TEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPASLFHVSN
DYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAKNMNVRP
LLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSVAYAMRQYFLKV
KNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSLEFLGIQPTLGP
PNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPYASIDISKGENNPGFQNTDDVQTSF',
'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMNNAGDKWSAFLK
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EIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIE
DVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLLGDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVD
QAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILMCTKVTMDDFLTAHH
EMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDNETEINFLLKQALTIVGT
LPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPASLFHVSNDYSFIRYYTRTLYQFQ
```

```
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RDRKKKNKARSGENPYASIDISKGENNPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDK
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VLSEDKSKRLNTILNTMSTIYSTGKVCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYE
EYVVLKNEMARANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYI
SPIGCLPAHLLGDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENS
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IMSLSAATPKHLKSIGLLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMK
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MLRLGKSEPWTLALENVVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDK
AYEWNDNEMYLFRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRM
SRSRINDAFRLNDNSLEFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPY
ASIDISKGENNPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLAS
WNYNTNITEENVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSEDKSKRLNTILNT
MSTIYSTGKVCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYE
DYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLLGDMWG
RFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPT
AWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIG
LLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETY
CDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALEN
VVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSV
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TDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMN
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QECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYEDYGDYWRGDYEVNGVD
GYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLLGDMWGRFWTNLYSLTVPFGQK
PNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILMCTK
VTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDNETEINF
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RYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAKNMNVRPLLNYF
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QRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILMCTKVTMDDFLTAHHEMGHI
QYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDNETEINFLLKQALTIVGTLPFTY
MLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPASLFHVSNDYSFIRYYTRTLYQFQFQEAL
CQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFV
GWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRI
SFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSLEFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIV
VGIVILIFTGIRDRKKKNKARSGENPYASIDISKGENNPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQST
IEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKL
QLQALQQNGSSVLSEDKSKRLNTILNTMSTIYSTGKVCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRS
EVGKQLRPLYEEYVVLKNEMARANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVR
AKLMNAYPSYISPIGCLPAHLLGDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGL
PNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNG
ANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPK
DQWMKKWWEMKREIVGVVEPVPHDETYCDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDIS
```

```
NSTEAGQKLFNMLRLGKSEPWTLALENVVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKV
RISLKSALGDKAYEWNDNEMYLFRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDII
PRTEVEKAIRMSRSRINDAFRLNDNSLEFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKK
KNKARSGENPYASIDISKGENNPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEA
EDLFYQSSLASWNYNTNITEENVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSED
KSKRLNTILNTMSTIYSTGKVCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVL
KNEMARANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGC
LPAHLLGDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDP
GNVQKAVCHPTAWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLS
AATPKHLKSIGLLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVG
VVEPVPHDETYCDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLG
KSEPWTLALENVVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWN
DNEMYLFRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRI
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FQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPAS
LFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAK
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QYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSLEFLGI
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VVEPVPHDETYCDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLG
KSEPWTLALENVVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWN
DNEMYLFRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRI
NDAFRLNDNSLEFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPYASIDI
SKGENNPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNT
NITEENVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSEDKSKRLNTILNTMSTIY
STGKVCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYEDYGDY
WRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLLGDMWGRFWTN
LYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLG
KGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIGLLSPD
FQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPAS
LFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAK
NMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSVAYAMR
QYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSLEFLGI
QPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPYASIDISKGENNPGFQNTDDVQ
TSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMNNAGDK
WSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSEDKSKRLNTILNTMSTIYSTGKVCNPDNPQECLL
LEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYEDYGDYWRGDYEVNGVDGYDYS
RGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLLGDMWGRFWTNLYSLTVPFGQKPNIDV
TDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILMCTKVTMDD
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LTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPASLFHVSNDYSFIRYYTR
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DVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSLEFLGIQPTLGPPNQPPVSIWL
IVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPYASIDISKGENNPGFQNTDDVQTSF', 'MSSSSWLLL
SLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMNNAGDKWSAFLKEQSTLAQMYP
LQEIQNLTVKLQLQALQQNGSSVLSEDKSKRLNTILNTMSTIYSTGKVCNPDNPQECLLLEPGLNEIMANSLDYN
ERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIK
PLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLLGDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFK
EAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMA
YAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKW
RWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAK
HEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTD
WSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFF
VTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSLEFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVI
LIFTGIRDRKKKNKARSGENPYASIDISKGENNPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQA
KTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQAL
QQNGSSVLSEDKSKRLNTILNTMSTIYSTGKVCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQ
LRPLYEEYVVLKNEMARANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMN
AYPSYISPIGCLPAHLLGDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQ
GFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGF
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KWWEMKREIVGVVEPVPHDETYCDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEA
GQKLFNMLRLGKSEPWTLALENVVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLK
SALGDKAYEWNDNEMYLFRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEV
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SGENPYASIDISKGENNPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFY
QSSLASWNYNTNITEENVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSEDKSKRL
NTILNTMSTIYSTGKVCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMA
RANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHL
LGDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQK
AVCHPTAWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPK
HLKSIGLLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPV
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TLALENVVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMY
LFRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFR
LNDNSLEFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPYASIDISKGEN
NPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEE
```

```
NVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSEDKSKRLNTILNTMSTIYSTGKV
CNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYEDYGDYWRGDY
EVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLLGDMWGRFWTNLYSLT
VPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFR
ILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDN
ETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPASLFHVS
NDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAKNMNVR
PLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSVAYAMRQYFLK
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PPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPYASIDISKGENNPGFQNTDDVQTS
F'], ligands=['C1OcC=CN1(C(C(=O)N(C)NNC)O)', 'O1C(=O)cc(Br)cc(Ncnn2c(N3C(CO
C3=N)N(O)O)c2s1)', 'FC(F)', 'O1ON2C(=O)C3CCOC(C3)N(Cc3cscc3)OC12c1cccs1',
 'OC(=O)C(F)(F)F', 'CCCCCC(=C(CN(C)O))C(C)CN(CC1CCOCC1)C#N', 'CN(C1CCCCC1)C
(=CC(C=C=C1C=CC=N1)S)O', 'CCc1cccc(Sc2ccccc2)c1-c1ccccc1C', 'C1ONC2cccc3C4C
Oc5ccccc5C3C=Nc4Sc12', 'C12CCCC(C)CC(C3C4)oncN(C)C1(Cc2cc34C)', 'O=CS(=O)(=
O)c1cccc2c1Sccc(cccnccc2N(O)O)', 'C1C(=O)Nc(c1OC)NCC(COC)NNC(=O)C(CC)(C(O)=
O)O', 'OCCOC(CCc1ccccc1O)C(CNC(Cl)OC)C(c1ccccc1)c1ccccc1', 'COC(=O)C=C(OCNC
=C=N)CN(Cc1ccco1)C=N', 'CS1SCCN1C(=O)C(CCC1N(CCC=C1))NNC(=O)C1CCCN1S(=O)(=
O)c1cccs1', 'NC=NN1C2(CO)C(O)C1OC(OC)C2O', 'Cl', 'COC(=O)NS(=O)(=O)O', 'FC
(F)(F)c1ccc(Cl)cc1F', '[O-]Oc1cccc(c1S)OO', 'CN(C(NC1CC(nn1)C(F)(F)C(C)CNC
(CC(N)=O)C(=O)c1ccccc1NC))F', 'CS(=O)([O-])N=C(NC(=O)c1c[nH]c2nccccc12)C(N)=
O', 'N1C=NC(=O)N(C=Cc2ccccc2Cl)-c2ccc(F)cc12', 'Brc1ccc(cc1)S(=O)(=O)NNNc1c
ccs1', 'SCC(N)', 'C12COC(=O)C1(N=C1NC#COC1)Ccc(C)ccO2', 'CN(C(CC=C(C)CC))
O', 'NC(=Nc1cccc2c(cccc12)C=C)OC=C1c2ncc3ccccc3c21', 'Cl[C-]=C(N=CN(O)Oc1cc
c(Cl)cc1)N=CC', 'Oc1ccc(cc1)C=COC=NC=O', 'CS(=O)(=O)c1ccc(cn1)S(=O)(=O)N1CC
N(CC1)O', 'CC(C)CC[P+]', 'CN(C)C(=O)CNC(N)CCNS(=O)#N', 'CNC(N)=Nc1ccc2OCOc2
c1', 'COC(=O)c1nnc(s1)N', 'CNCC(=O)COC(=Cc1ccccn1)c1cccs1', 'C1OC=CC(C)C(CC
Cl)=C(OC(N))C(=O)O1', 'O=NCCNS1=CC(N2CCCc2CN=1)', 'C1CN(C(NC(=O)NC2=O)ccs2C
1(F)C(=O)NS)', 'COc1ccc2cc1CNC=Nc1cccn1[nH]2', 'CCC(C=CN(C)C(C)=O)', 'O=C(N
CCCNCC1cnccs1)', 'C1SC1=O', 'O=CC1=CN(CN1)O', 'O1C(C1(NCSS(Br)=O))', 'O=COC
(COP(O)(O)=O)OO', 'C1Occccc(C=O)c1N1CC2CC1(SC2)c1cccs1', 'CC1ncc(c(c1C(=O)c
1ccccc1N))=O', 'CN(SC(C)N1CCNC(=O)N1Cc1ccc2(c1)C=CN)C2=O', 'O=NO', 'O=C(Nc1
ccc(cc1)C#Cc1)ccccc1', 'COc1cc(ccc1C)NC(C)=O', 'C1CN(CCOCCCC)COOCC(OC(C=O))
C(OOC(C))OC1C=CCC(OC)C(C=Cc1cc(O)cc(Br)c1C(=O)C(OC))CCOC(C)=O', 'O=C(Cc1ccn
2n(c1S(=O)(=O))O2)F', 'CCOC(SCCC1CCC=CC1C)c1c(Br)cccc1OCCCNC(C)c1ccccc1OCc1
ccc(cn1)-c1cccnc1', 'NC(=O)OCC(=O)CCCC(NC(=O)C(C)C(C)C)CCOP(O)(O)=O', 'Cl1c
ccnc1(C(=S)NC(=O)SCC(=NC(=O)NC=CC(=O)c1ccccc1CNC))=O', 'C(NCC(O)=NCNCCCC)',
'C(CC1C2CCCCC2)NC(COCc2cccc(Cl)c2)NC1=O', 'CC(O)CN=C1(NC1=O)', 'O=NCO', 'CC
(=C)C=COc1cccc(c1)COC=C', 'O=C(OCCNC=C1CCCl)ccc(NC(=O)NC=O)c1', 'OC(=O)C=C1
NccncccccS1[O-]', 'CC1CNC(=O)SC=NC1', 'C1NCC(cccncc1C)N=C=CC=CC', 'Fc1ccc(c
c1)S(=O)(=O)NC1CCCCC1', 'O=C(C)C=C1NCCC(C1)C(=N)NCCCCCNC=N', 'C(N(CCCl)C
C)', 'CCN=CCNC(=O)c1[nH]c2ccccc2s1CC', 'C(N1CCN(CC1)S)O', 'O=C(c1ccccc1CC)c
1cccc2cccnc12', 'C1Ocnc(cc(c1)N)Cl', 'O=C(Nc1cccc(c1)N(O))O', 'O=C(NS(=O)(=
O)CNcnc(-n1nc2nc1C1)ccc3c(F)cccc3n1)n2c1cccnc1', 'FC(F)(F)ON1CCN(CC1)C(=O)c
1ccc(Cl)c(c1)S(=O)(=O)N(C)C', 'C1C(N=C1Cc1cccc(F)c1)c1ccco1', 'CC(C)c1ccc(c
c1)-c1cc(oc1)', 'CN1CC(CCC11)c2ccc(cn2)C(=O)Nc2nccnc12', 'O=SNC=O', 'ON(CC1
nc(Cl)C=NC(CC2))C1OC([O-])C2=O', 'FC(F)(F)Cl', 'COCC1CN(C(=O)NCc2ccccc2)CC1
1CCOC1', 'C1Occcc(CNCc2ccccc2C1)NOO', 'Fc1cccc(Ccc2[nH]ccc2c1C)#N', 'CCCC',
'O=Cc1ccc(cc1)C(=NOCCF)S', 'OC(CNC(CN1CCN(Cc1)c1ccccc1COC(=O)C)C)C(C)(C)C',
'CC(N(CCcc(c1ccccc1)OC(=S)N1)C)CN(CC1)c1ccccc1', 'CCN(CCN(Cc1ccc2cc1)c1cccc
c1C)-cccccc2', 'Cl12CCNccccc(NC(CN(F)Ic1C)Ccccc(CC2))=O', 'Brc1ccccc1C(=O)O
Nc1ccc(cc1)N(O)O', 'CC(=O)OP(O)(=O)c1ccccc1Cl', 'COC(=O)C(C)C(=O)Nc1cccc2cc
ccc12', 'O=C(NC=CC(N)=NN)NC(Sc1c2cccc1)S(=O)(O2)c1ccccc1', 'CCOc1c(Cl)c(CO)
c(o1)C(O)CC(=Cc1cc(Cl)c(Cl)cc1)F', 'C1COS(=O)(=O)c2ccc(F)cc2NC(=O)Nccc(CC2N
(N)C#C)nnc12', 'CC(NN(OC(OCC)NP(=O)))O', 'CCCCCN(CNS(=O)(=O))Cc1ccc(cc1)S
(N)(=O)=O', 'C12COcccc(C)c1(-c1cc[nH]c1C=NCOC(C)=O)C(=O)NCC2=O'], confidenc
e=False)
14:58:08   ensure artifacts for the application are present.
14:58:08   starting syncing
14:58:09   syncing complete
```

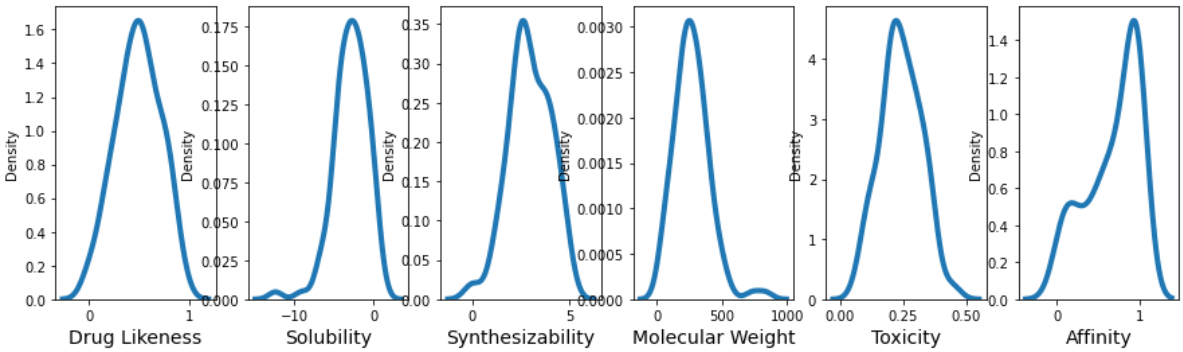
In [16]:

```
from matplotlib import pyplot as plt
import seaborn as sns
%matplotlib inline
plt.rcParams["figure.figsize"] = (10,7)
```

```
n_subplots = 6
def plot_density(values, x_axis="", subplot=1):
    plt.subplot(1, n_subplots, subplot)
    g = sns.distplot(values, hist=False, kde_kws={"linewidth": 4})
    plt.xlabel(x_axis, size=14)

plt.gcf().set_size_inches(15,4)
plot_density(paccmann_rl_results["drug_likeness"], "Drug Likeness", subplot=
plot_density(paccmann_rl_results["solubility"], "Solubility", subplot=2)
plot_density(paccmann_rl_results["synthesizability"], "Synthesizability", su
plot_density(paccmann_rl_results["molecular_weight"], "Molecular Weight", su
plot_density(paccmann_rl_results["toxicity"], "Toxicity", subplot=5)
plot_density(paccmann_rl_results["affinity"], "Affinity", subplot=6)
plt.show()

threshold = 0.75
number_of_potential_molecules = len([qed for qed in drug_likeness if qed>=th
print(f"Out of the {n} generated molecules, {number_of_potential_molecules}
```




```
Out of the 100 generated molecules, 15 have a drug likeness equal or greate
r than 0.75.
```

One of the most important metrics is drug likeness. We define the threshold of 0.75 and are "satisfied" with molecules that surpass that value. We will use the number of molecules that surpass this level to compare different algorithms.

Visualizing the embedding space

We can visualize the embedding space of the Variational Autoencoder. It can give us an idea of how this space is organized, and hint at how the VAE may be encoding different molecules.

For this, we:

- randomly generate points in the latent space;
- keep the points that correspond to valid molecules;
- plot those points using a 2D approximation;

We visualize how different chemical properties are distributed in the latent space.

Notice that we are compacting a high dimensional subspace into a 2D plot, and thus, necessarily loosing information.

In [17]:
```
from tqdm import tqdm

# generate randomly points in the latent space
number_of_latent_points = 2048
```

```
latent_points = torch.randn(number_of_latent_points,
                            model.encoder_latent_size,
                            device=model.device)

# keep points which correspond to valid molecules
molecules = []
for latent_point in tqdm(torch.unsqueeze(latent_points, 1)):
    smiles_list = model.get_smiles_from_latent(latent_point)
    generated_molecules = [Chem.MolFromSmiles(smiles) for smiles in smiles_l
    molecules.extend(generated_molecules)
valid_indexes = [index for index, molecule in enumerate(molecules) if molecu
molecules = [molecules[index] for index in valid_indexes]
latent_points = latent_points[valid_indexes]
```

```
100%|████████████████████████████████████████████████████████████████
████████████████| 2048/2048 [02:46<00:00, 12.34it/s]
```

Exercise: comment/uncomment the code below to display different properties in the latent space

Exercise: comment/uncomment the code below to use different algorithms for dimentionality reduction (TSNE/PCA)

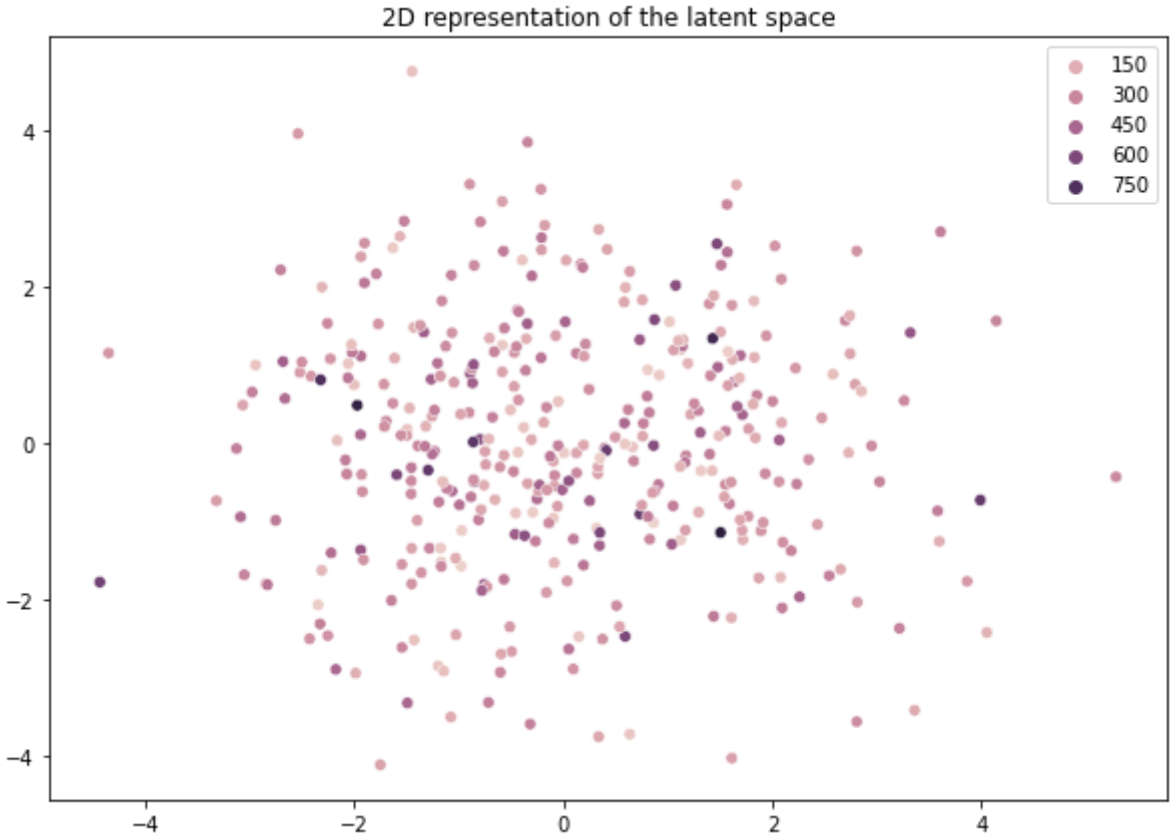
In [18]:

```
# Visualization
from sklearn.decomposition import PCA
from sklearn.manifold import TSNE
import seaborn as sns
%matplotlib inline
plt.rcParams["figure.figsize"] = (10,7)

def render_latent_points(latent_points, values):
    decomposed_points = PCA(n_components=2).fit_transform(latent_points)
    #decomposed_points = TSNE(n_components=2).fit_transform(latent_points)
    sns.scatterplot(x=decomposed_points[:, 0], y=decomposed_points[:, 1], hu

values=[]
for molecule in molecules:
    try:
        #values.append(get_drug_likeness(molecule))
        #values.append(get_solubility(molecule))
        #values.append(get_synthesizability(molecule))
        #values.append(get_molecularWeight(molecule))
    except:
        values.append(0.0)

_ = render_latent_points(latent_points.cpu(), values=values)
_ = plt.title("2D representation of the latent space")
```



Generation with PaccMannGP

The goal of the PaccMannGP method is to generate new molecules that optimize predefined parameters, such as drug likeness.

The model used in PaccMannGP is a standard Variational Autoencoder for molecular design, trained with the standard reconstruction and regularization losses. The encoder of the VAE maps a molecule into a latent space with a Gaussian distribution, where it is possible to sample new data points. The decoder performs the reverse operation by translating data points from the latent space into the original data space.

The method performs Bayesian Optimization with Gaussian Processes to explore the latent space of the VAE, aiming to find a compound that maximizes drug likeness. Then, the method uses the decoder of the VAE to obtain the compound that was found to maximize drug likeness in the latent space.

References:

[1] - Born J., Huynh T., Stroobants A., Cornell W. D. , and Manica M. (2022). Active Site Sequence Representations of Human Kinases Outperform Full Sequence Representations for Affinity Prediction and Inhibitor Generation: 3D Effects in a 1D Model. Journal of Chemical Information and Modeling 2022 62 (2), 240-257
https://doi.org/10.1021/acs.jcim.1c00889

Configuring the model

In [38]:
```
from gt4sd.algorithms.controlled_sampling.paccmann_gp.core import PaccMannGP
```

```
# maximizing drug likeness and synthesizability
target = {"qed": {"weight": 1.0},
          "sa": {"weight": 1.0}}

configuration = PaccMannGPGenerator(number_of_optimization_rounds=1)
algorithm = PaccMannGP(configuration=configuration, target=target)
```

```
15:34:09   runnning PaccMannGP with configuration=PaccMannGPGenerator(algor
ithm_version='v0', batch_size=32, temperature=1.4, generated_length=100, li
mit=5.0, acquisition_function='EI', number_of_steps=32, number_of_initial_p
oints=16, initial_point_generator='random', seed=42, number_of_optimization
_rounds=1, sampling_variance=0.1, samples_for_evaluation=4, maximum_number_
of_sampling_steps=32)
15:34:09   ensure artifacts for the application are present.
15:34:09   starting syncing
15:34:09   syncing complete
```

Sampling and Plotting Molecules with GT4SD

Let's go ahead and sample some molecules using the PaccMannRL algorithm. This time we will use the GT4SD interface, which greatly simplifies sampling for us. We start by sampling 15 molecules. We then convert them into a **Mol** object (**RDKit** package). Finally, we display them using the **mols2grid** package.

In [39]:
```
n_sampled_molecules = 15
molecules = list(algorithm.sample(n_sampled_molecules))
molecues = [Chem.MolFromSmiles(molecule) for molecule in molecules]
mols2grid.display(molecues, fixedBondLength=200)
```

```
15:34:10   configuring optimization for target: {'qed': {'weight': 1.0}, 's
a': {'weight': 1.0}}
15:34:11   running optimization with the following parameters: {'dimension
s': [(-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.
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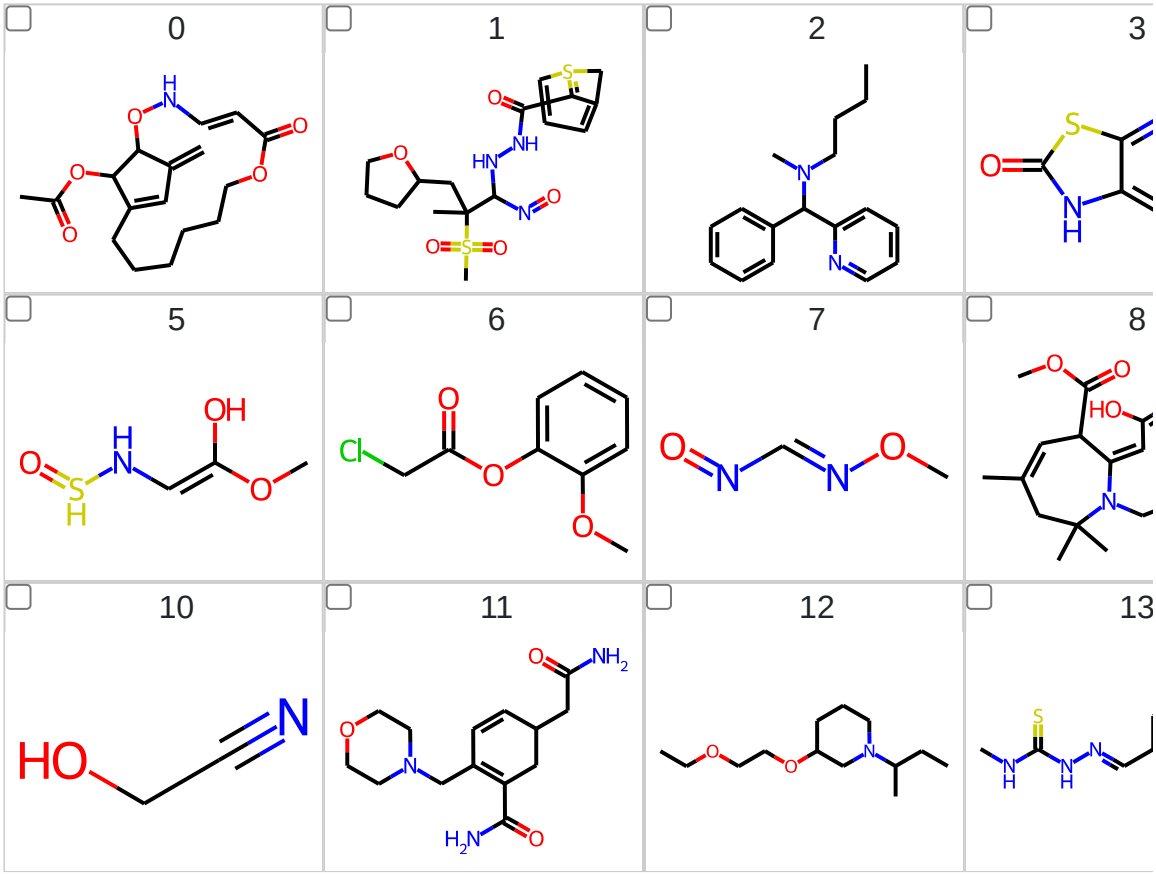
32, 'n_initial_points': 16, 'initial_point_generator': 'random', 'random_st
ate': 4112119562}
15:34:11   running at most 1 optmization rounds
15:34:11   starting round 1
15:34:53   starting sampling for 1
15:35:13   completing round 1
15:35:13   generated 229 molecules in the current run
```

Out[39]:



Evaluating the generated molecules

If we want to compare different algorithms, we can do so using different metrics. This next example shows how to estimate the properties of generated molecules using the PaccMannRL algorithm. We start by generating 100 new molecules. For each we compute the metrics defined in the beggining of the tutorial.

In [40]:

```
n = 100
molecules = list(algorithm.sample(n))

drug_likeness = []
solubility = []
synthesizability = []
molecular_weight = []
toxicity = []

for molecule in molecules:
    mol = Chem.MolFromSmiles(molecule)
    drug_likeness.append(get_drug_likeness(mol))
    solubility.append(get_solubility(mol))
    synthesizability.append(get_synthesizability(mol))
    molecular_weight.append(get_molecularWeight(mol))
    toxicity.append(get_toxicity(molecule))

affinity = get_affinity(molecules)
paccmann_gl_results = dict()
paccmann_gl_results["drug_likeness"] = drug_likeness
paccmann_gl_results["solubility"] = solubility
paccmann_gl_results["synthesizability"] = synthesizability
```

```
paccmann_gl_results["molecular_weight"] = molecular_weight
paccmann_gl_results["toxicity"] = toxicity
paccmann_gl_results["affinity"] = affinity
```

```
15:35:13   configuring optimization for target: {'qed': {}, 'sa': {}}
15:35:13   running optimization with the following parameters: {'dimension
s': [(-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.
0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0),
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(-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.
0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0,
5.0), (-5.0, 5.0), (-5.0, 5.0), (-5.0, 5.0)], 'acq_func': 'EI', 'n_calls':
32, 'n_initial_points': 16, 'initial_point_generator': 'random', 'random_st
ate': 4225599466}
15:35:13   running at most 1 optmization rounds
15:35:13   starting round 1
```

```
2022-07-04 15:35:15.896 | WARNING  | paccmann_gp.qed_minimization:evaluate:
48 - QED calculation failed.
```

```
15:36:01   starting sampling for 1
15:36:22   completing round 1
15:36:22   generated 206 molecules in the current run
15:36:23   no parameters validation
15:36:23   runnning PaccMann with configuration=AffinityPredictor(algorithm
_version='v0', protein_targets=['MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQ
SSLASWNYNTNITEENVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSEDKSKRLN
TILNTMSTIYSTGKVCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMAR
ANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLL
GDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKA
VCHPTAWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKH
LKSIGLLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVP
HDETYCDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWT
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FRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRL
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LMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDNE
TEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPASLFHVSN
DYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAKNMNVRP
LLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSVAYAMRQYFLKV
KNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSLEFLGIQPTLGP
PNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPYASIDISKGENNPGFQNTDDVQTSF',
'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMNNAGDKWSAFLK
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EIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIE
DVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLLGDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVD
QAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILMCTKVTMDDFLTAHH
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FQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAKNMNVRPLLNYFEPLFTWLKDQN
KNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSVAYAMRQYFLKVKNQMILFGEEDVRVAN
LKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSLEFLGIQPTLGPPNQPPVSIWLIVFGVV
MGVIVVGIVILIFTGIRDRKKKNKARSGENPYASIDISKGENNPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVT
AAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQN
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VSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPF
LLRNGANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFK
GEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLH
KCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYAD
QSIKVRISLKSALGDKAYEWNDNEMYLFRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKN
VSDIIPRTEVEKAIRMSRSRINDAFRLNDNSLEFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGI
RDRKKKNKARSGENPYASIDISKGENNPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDK
FNHEAEDLFYQSSLASWNYNTNITEENVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSS
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EYVVLKNEMARANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYI
SPIGCLPAHLLGDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENS
MLTDPGNVQKAVCHPTAWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGE
IMSLSAATPKHLKSIGLLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMK
REIVGVVEPVPHDETYCDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFN
MLRLGKSEPWTLALENVVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDK
AYEWNDNEMYLFRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRM
SRSRINDAFRLNDNSLEFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPY
ASIDISKGENNPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLAS
WNYNTNITEENVQNMNNAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSEDKSKRLNTILNT
MSTIYSTGKVCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYE
DYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLLGDMWG
RFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPT
AWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIG
```

```
LLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETY
CDPASLFHVSNDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALEN
VVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSV
AYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSL
EFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPYASIDISKGENNPGFQN
TDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMN
NAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSEDKSKRLNTILNTMSTIYSTGKVCNPDNP
QECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYEDYGDYWRGDYEVNGVD
GYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGCLPAHLLGDMWGRFWTNLYSLTVPFGQK
PNIDVTDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILMCTK
VTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDNETEINF
LLKQALTIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPASLFHVSNDYSFI
RYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQKLFNMLRLGKSEPWTLALENVVGAKNMNVRPLLNYF
EPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSVAYAMRQYFLKVKNQMI
LFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSLEFLGIQPTLGPPNQPP
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VVGAKNMNVRPLLNYFEPLFTWLKDQNKNSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSV
AYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFFVTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSL
```

```
EFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVILIFTGIRDRKKKNKARSGENPYASIDISKGENNPGFQN
TDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMN
NAGDKWSAFLKEQSTLAQMYPLQEIQNLTVKLQLQALQQNGSSVLSEDKSKRLNTILNTMSTIYSTGKVCNPDNP
QECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYEDYGDYWRGDYEVNGVD
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PNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKGDFRILMCTKVTMDDFLTAHHEMGHIQYDMAYAAQPFLLRNG
ANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDNETEINFLLKQALTIVGTLPFTYMLEKWRWMVFKGEIPK
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KNEMARANHYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPSYISPIGC
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WSPYADQSIKVRISLKSALGDKAYEWNDNEMYLFRSSVAYAMRQYFLKVKNQMILFGEEDVRVANLKPRISFNFF
VTAPKNVSDIIPRTEVEKAIRMSRSRINDAFRLNDNSLEFLGIQPTLGPPNQPPVSIWLIVFGVVMGVIVVGIVI
LIFTGIRDRKKKNKARSGENPYASIDISKGENNPGFQNTDDVQTSF', 'MSSSSWLLLSLVAVTAAQSTIEEQA
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F'], ligands=['C1CCOC2Ccc(F)c1(Nc1c(Cl)cncc1F)Cnc(Ccc2)c1cccc(Cl)c1Cl', 'OO
C(C)=O', 'COc1c(cccc1NC(C)=O)', 'OC(CC)(O)Oc1cccOccc(Cl)c1Cl', 'CN(Cc1c(Cl)
cccc1C)C=C', 'COC(=O)C(OCCCCN(C)C)c1c[nH]cn1', 'C1OCCOC(F)Cc2c1c1c=NCOc1c
2', 'C=NO', 'COP(O)(O)=O', 'O=S(=O)(OP(O)(O)=O)N=Nc1ccc(o1)-c1ccc2OCOc2c1',
'C1C(NCc2cnc3ccccc23C)OC=Cc2ccccc12', 'COCCCN1CCOCC1=O', 'CC(NS=SC1CCC11)=N
cnc(Nc2ccccc2)nncC1=O', 'CCc1cccc(c2(Ncc(Cl)c1C2=O)NS(=O)(=O)N1CCOCC1N(O)
O)', 'OC(NC(F)(F)F)OO', 'CC(CC=NN(C1OCC(O)(O)C1))C#N', 'CCOCc1c(Br)ccc2c1NO
C(=O)O2', 'O1cc2[nH]cccc2S1(=O)=O', 'C(O)C(NC(Cc1ccccc1)C(NC(=S)NC(Cc1ccccc
1)C)OO)', 'N1=CC2=CN(C(=O)N1)c2C(=O)NC', 'CNC(COP(=O)OCC(OCc1ccccc1)c1ccncc
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c1)CSc1ccccc1F', 'CC(=CN=Cc1cncsccccc1)', 'C1N(C2(SCC#CCcc3))ccOC3cc2cccc1
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1cc(Oc2c4C(C)(O))=O', 'CC(NCCCl)[n+]1cccc2c1N=NN(NCc1ccc3ccccc3c1)C(=O)N2',
'O1CC(NCOc2ccc(F)cc2)-cccnc2(Sc3cc([nH]c4ccccc4cc2)Cl)c3-c1', 'C12=COC(C(=
O)N1CCC)CNC2NC1(CON(C11)COC1=O)c1ccc(cc11)N(CCC1)C(O)=O', 'OC(=O)CCCSNC(=O)
N(O)N=NSc1ccnc2ccc(cc12)NCc1ccccc1', 'C(F)', 'CCCP', 'O1CCC=C1CCCC(C)=C(c1c
cccc1)c1ccco1', 'COCC(=O)C1CN(CC(N)C2CC3SN2O2)N(C)Ccc(NN2F)C(F)=CC3c1', 'CO
C1=CC(C=C1c1cccc(c1)-c1c2cccc1C2)S=O', 'COc1cccc(C)c1Cl', '[O-]OC1COC(CN)C1
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N(c1ccccc1)C(C)(C)C(Cl)(F)F', 'COC', 'O=C(CCc1ccccc1)N=CNC(N=Cc1ccco1)',

```
 '[O-]C(=CC(NS(O)))NOc1cccc(c1)N=N', 'C1cccc2OC(=O)N(C)Nc(c12)N(O)O', 'O=CC
1C(cc[nH]cccc1)', 'C1Sc2cc3c=CC(=Cc3[n+]2n1Cl)O', 'C1N(C)S(CC1(=COc1cccncccc
nc1))', 'NC1(C)CC2CC(=O)OC2=S1', 'CCc1ccc(cc1)C(=O)NC(Nc1ccccc1N(C)C=O)S(=
O)(=O)c1ccco1', '[O-]C(C#N)', 'O=CC(NCc1cnc2ccccc12N1CC)OCC1', 'CNC=NC(=O)C
1Ncccc(N(C2CC3CC(C2)C(CN))C2CCCC)C2c3Oc1F', 'N1C(N(S)Oc2cccc(c2)C(F)=N)C1',
'C1ccC(O)=C(SCCC(=O)C#COC1)N(C)F', 'NC1(OCCOCCC1)C(=O)c1ccc(cc1C)N(O)O', 'C
(NC(=O)Oc1ccccc1)C(=S1)NCc2ccc(nc12)N(O)O', 'O=C(c1c2cccc1)n1ccnc2O1', 'O=
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 'CSC', 'COCCN(C1CC)CC(=CC1CC(=O)NCc1cc2c(C)c(c1)CCC2NCC(OCC1)cc(NC(=CCC))c
ccccc1C)C=O', 'C1C(C)=NC(CNCCC2(NOCN2)CC1=O)O', 'C1COcc(ccc1(NC(=O)NCc1cccc
c1OC)(CCC(COC)))', 'COCCOP(O)OP([O-])(=O)OP(O)(O)=O', 'COc1cccc(c1)-c1nn2nc
1C=NOC(C(C)C)c1ccccc21', 'COc1cc(OC(=O)c2cc3(ccc2NC))(C)C11c2[nH]c4cncnc4N
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N', 'CN=CN=C(SSBr)Cc1ccc[nH]1', 'CC(NC1nccn1)CCS1Cc2cccc(OC)c2S1(=O)=O', 'N
1C(N=CC1)', 'C1Occc2cCNc3cc4ccccc4n3c2n1', 'O1C(F)C(Oc2ccc(o2)NCCC=O)O1',
 'C1CCCN(C=NP(=O)(C1)c1ccccc11)nnc(n1)C(C)C', 'COC(=O)C(=C)c1ccccc1C(=NC1CC
1(N)NS(C)(=O)=O)', 'COCCOCCO', 'C(c1ccccc1NC)', 'COP([O-])(=O)=O', 'COc1ccc
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c1cc(ccc1-c1cnncc1)CC(F)(F)F', 'O1C(CCCCC2OCCO2)N1Nc1n[nH]c2cnccc12', 'C1Oc
2cccc([O-])c2C=NOcc1(CC(O)=O)', 'COc1ccc(c2n1)C(=N)NC2(=C1C(c2)cc(OCccc2)[n
H]cccccc1)', 'OCCc1cccc2cccnc12', 'O=C(Nc1ncno1)NC', 'OC(O)CCN(Cc1ccsc1)C#
N', 'C=C(F)F', 'Cl1cccc(NC(=O)c2cncnc2)cc1', 'CCCN=NNC=N', 'CCCNC(=Nc1ccncc
1)Cc1ccc2ccccc2c1', 'O=CC(CC=Cc1cc2ccc1)C(=O)C2c1cnc(N)nc1', 'N(=C=Nc1cccc
(c1)N)O'], confidence=False)
15:36:23   ensure artifacts for the application are present.
15:36:23   starting syncing
15:36:23   syncing complete
```

In [37]:

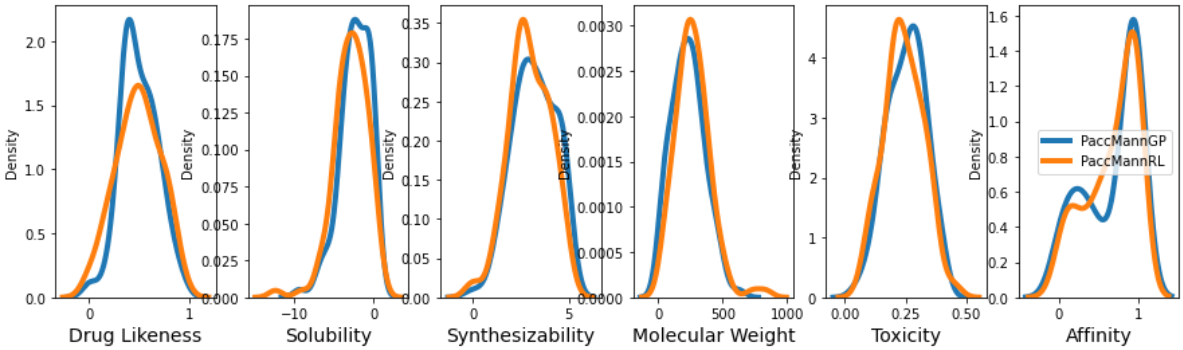
```
n_subplots = 6
def plot_density(values, x_axis="", subplot=1, legend=""):
    plt.subplot(1, n_subplots, subplot)
    g = sns.distplot(values, hist=False, kde_kws={"linewidth": 4}, label=leg
    plt.xlabel(x_axis, size=14)

plt.gcf().set_size_inches(15,4)
plot_density(paccmann_gl_results["drug_likeness"], "Drug Likeness", subplot=
plot_density(paccmann_gl_results["solubility"], "Solubility", subplot=2, leg
plot_density(paccmann_gl_results["synthesizability"], "Synthesizability", su
plot_density(paccmann_gl_results["molecular_weight"], "Molecular Weight", su
plot_density(paccmann_gl_results["toxicity"], "Toxicity", subplot=5, legend=
plot_density(paccmann_gl_results["affinity"], "Affinity", subplot=6, legend=

plot_density(paccmann_rl_results["drug_likeness"], "Drug Likeness", subplot=
plot_density(paccmann_rl_results["solubility"], "Solubility", subplot=2, leg
plot_density(paccmann_rl_results["synthesizability"], "Synthesizability", su
plot_density(paccmann_rl_results["molecular_weight"], "Molecular Weight", su
plot_density(paccmann_rl_results["toxicity"], "Toxicity", subplot=5, legend=
plot_density(paccmann_rl_results["affinity"], "Affinity", subplot=6, legend=

plt.legend()
plt.show()

threshold = 0.75
number_of_potential_molecules = len([qed for qed in drug_likeness if qed>=th
print(f"Out of the {n} generated molecules, {number_of_potential_molecules}
```




```
Out of the 100 generated molecules, 9 have a drug likeness equal or greater
than 0.75.
```

In [ ]: