

Entorno de conda

Crear entorno

```
conda create --name ToxTwentyCast python=3.7
```

Activar entorno

```
conda activate ToxTwentyCast
```

Paquetes necesarios

Pandas:

```
conda install pandas
```

Sklearn:

```
conda install sklearn
```

Selfies:

```
conda install selfies
```

Weights and bias:

```
conda install -c conda-forge wandb
```

Es importante usar las versiones especificadas

Pytorch with CUDA support

```
conda install pytorch>=1.6 cudatoolkit=10.2 -c pytorch
```

Simple transformers (0.48.6):

```
pip install 'simpletransformers==0.48.6'
```

Transformers (3.3.1):

```
conda install -c huggingface 'transformers==3.3.1'
```