**Molecular Design Using Signal Processing and Machine Learning: Time-Frequency-*like* Representation and Forward Design**

**Alain B. Tchagang**

alain.tchagangf@nrc-cnrc.gc.ca

**Additional File 1** 🡪 It is a 133855×19 matrix. It contains the 19 properties of all the molecules in the following order and in the respective units.

|  |  |
| --- | --- |
|  |  |
| Properties | Unit |
| g298\_atom | kcal/mol |
| h298\_atom | kcal/mol |
| u298\_atom | kcal/mol |
| u0\_atom | kcal/mol |
| cv | cal/(mol\*K) |
| g298 | kcal/mol |
| h298 | kcal/mol |
| u298 | kcal/mol |
| u0 | kcal/mol |
| zpve | kcal/mol |
| r2 | Bohr^2 |
| gap | kcal/mol |
| lumo | kcal/mol |
| homo | kcal/mol |
| alpha | Bohr^3 |
| mu | D |
| C | GHz |
| B | GHz |
| A | GHz |

**Additional File 2** 🡪 It is a 133855×29 matrix. It contains the Coulomb Eigen Spectrum of each molecule.

**Additional File 3** 🡪 Matlab script for generating the time-frequency like representation of each molecule.

**Additional File 4** 🡪 Python code for training and testing the deep convolutional neural networks for training and predictions.

**Additional File 5** 🡪 ID of the molecules.

**Running Everything.**

To run the program, you need Matlab and Python. Matlab to generate the TFL and Python for training and testing of your deep CNNs. You can also use Python to generate the TFLs if you wish.

1. Create a folder name PythonQM9. Download all the additional files in this folder.
2. Create a subfolder TFL\_WVD in the PythonQM9 folder for saving the WVD of the molecules computes using Matlab.
3. Create a subfolder TFL\_STFT in the PythonQM9 folder for saving the short time Fourier transform (Spectrogram) of molecules computes using Matlab.
4. Create a subfolder TFL\_CWT in the PythonQM9 folder for saving the continuous wavelet transform (scalogram) of molecules computes using Matlab.
5. Run the Matlab script to generate the respective TFL of the molecules. Make sure to specify in your Matlab script where they will be save by uncommenting the right folder. For this unzip Additional\_File\_2 and save as Additional\_File\_2.xlsx (excel file).
6. Once you have all the ingredients, check and install the libraries that the code is using and that your python version might not have. For example: Prettytable, tqdm, etc. Do not forget to unzip Additional\_File\_1 and leave it as Additional\_File\_1.csv
7. Run your Python script for training and testing.