In this shared folder, the file "all\_test\_smiles.csv" contains the SMILES strings of the molecules, their corresponding annotation files (in the “Annotations” directory). The images of the molecules can be found in the “Image” directory. The annotation file and the image file of a molecule have the same name (except for their extensions: “csv” for the annotation file, “png” for the image file).

Each annotation file contains four columns:

1. "c\_idx": The index of the annotated carbon
2. "C": The chemical shift of the annotated carbon.
3. "H 1": The first possible hydrogen shift associated with the carbon.
4. "H 2": The second possible hydrogen shift associated with the carbon.

Note: If a carbon is associated with only one hydrogen signal, "H 1" and "H 2" will have identical values.