Isomorphism:

- Find alanine (L-alanine) in Pubchem, copy its 3D visualization and describe it by atom indexes.
- Find alanine in LigandExpo, copy its 3D visualization and describe it by atom indexes.
- Note: If problem with LigandExpo, use this link: <u>https://www.rcsb.org/ligand/ALA</u>
- Describe two isomorphic projections between them.
- How many isomorphic projections can you find?

## Planar graphs:

- Find (in Pubchem) a molecule, which molecular graph is not planar.
- Is adamantane molecule planar? If yes, prove by providing the planar drawing.

## Automorhism:

- Find in Pubchem aminomethanethiol, copy its 2D or 3D visualization and describe it by atom indexes.
- Find topologically equivalent atoms and wrote them here:
- Describe 2 automorphisms.
- How many automorphisms it has?

## Canonical indexing:

• Index the 1-chloropropane molecule using Morgan's algorithm