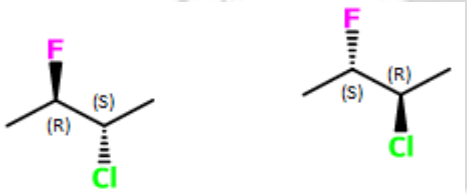
# Stereochemistry Relationship Between Molecules:

## How to Determine if Compounds are Constitutional Isomers, Enantiomers, Diastereomers, the Same, or Different Molecules

**The types of comparisons between two compounds:**

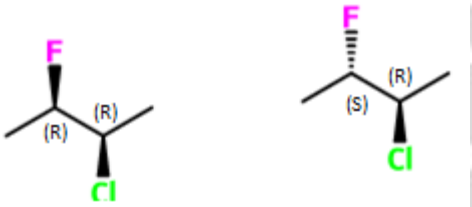
When comparing two compounds in organic chemistry, they are often categorized into one of the following groups:

(i) **Enantiomers**: Molecules have the same configuration and chemical formula but all (S) stereocenters change to (R) conformation and all (R) to (S) conformation. For example, the following pair are enantiomers:



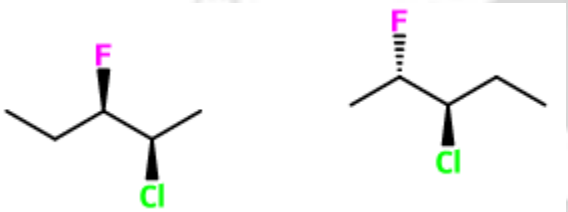

- ***Chemical formula:*** Both $C_4H_8ClF$
- ***Same configuration (connectivity of elements)***
- ***Stereocenters both change***

**(ii) Diasteriomers:** Molecules have the same configuration and chemical formula but at least one (but not all) stereocenters change (S) to (R) conformation or (R) to (S) conformation. For example, the following pair are diasteriomers:



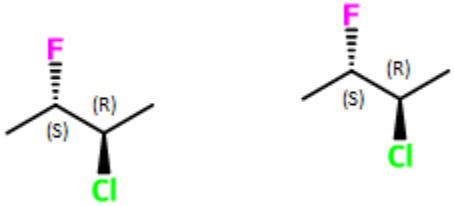

- ***Chemical formula:*** Both $C_4H_8ClF$
- ***Same configuration (connectivity of elements)***
- ***Only the carbon with the F substituent changed stereocenter conformation***

**(iii) Constitutional Isomers**: Molecules have the same chemical formula but a different configuration (they are arranged differently). For example, the following are constituational iomers**.**



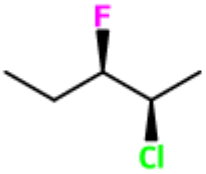

- **Chemical formula:** Both $C_5H_{10}ClF$
- **Different configuration. The connectivity of the elements is different. Cl has one carbon to the right on the first compound and two carbons to the right on the second compound**

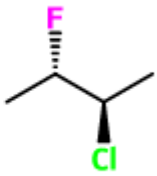
**(iv) Same Molecules**: Molecules have the same chemical formula, same conformation, and the same (R) and (S) conformations of stereocenters. For example, the following are the same molecule:




- ***Chemical formula: Both $C_4H_8ClF$***
- ***Same conformation (connectivity)***
- ***No stereocenters change***

**(v)** **Different Molecules:** Molecules have a different chemical formula. The following pair is an example of different molecules.




- ***The molecule on the right has a chemical formula of $C_4H_8ClF$ while the molecule on the left has a chemical formula of $C_5H_{10}ClF$***

**Schematic for problem solving:**

Although there are multiple ways to determine which category a set of two molecules fits into, the following schematic shows an organized way to go about determining how two molecules compare.

*Note: This method works if compounds are <u>not</u> both perfectly symmetrical, or* ***meso*** *(see example 3 in practice problems). In the case of two meso compounds with identical chemical formulas, the compounds are the same molecule.*

**Step 1:** Label each carbon in each compound numerically.

**Step 2:** Determine if the substituents coming off of each similarly numbered carbon is the same.

Are they the same??

No! Yes!

**Step 3a:**
Are the chemical formulas the same?

Yes! No!

Constitutional Isomers Different Molecules

**Step 3b:**
Determine whether each stereocenter is (R) or (S) conformation.

Do the stereocenters switch conformation R to S (or S to R)?

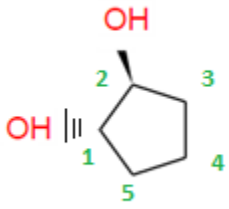
No stereocenters switch — Same Molecule

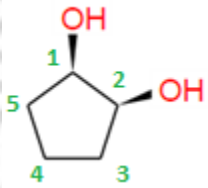
One or more stereocenters switch — Diastereomers

All stereocenters switch — Enantiomers

**Example problem using schematic approach:**

**Step 1:** Label each carbon in each compound numerically.




**Compound 1** **Compound 2**

**Step 2:** Determine if the substituents coming off of each similarly numbered carbon is the same. Are they the same??

Yes!
Carbons 1 and 2 have –OH substituents in both compounds

**Step 3b. Determine whether each stereocenter is (R) or (S) conformation**

Compound 1 has an (S) stereocenter at position 1; compound 2 has an (R) stereocenter at position 1.
Both compounds have an (R) stereocenter at position 2

Do the stereocenters switch conformation R to S (or S to R)?

One out of two stereocenters (some but not all) switched conformation. **These compounds are diastereomers!**

**References**

Meso Compounds. (n.d.). Retrieved December 1, 2014, from http://chemwiki.ucdavis.edu/Organic_Chemistry/Chirality/Meso_Compounds

Shimizu, K. (n.d.). HOW TO: Determine the stereochemical relationship Between two Molecules. Retrieved December 1, 2014, from http://www.chem.sc.edu/faculty/shimizu/333/Chem_333/5a.vi.html

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