

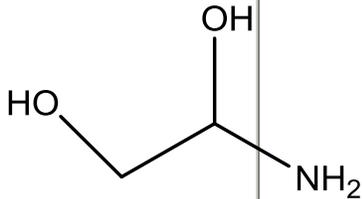
## Module 4b: Assignment

### 2.4. Exercises (Module 4b)

#### 2.4.1. Exercise 1

Fill in the following table using both ChemSpider and PubChem and indicate where answers may differ. Use the new compound identity search in PubChem (click on the hexagon for structural formula,

[https://pubchem.ncbi.nlm.nih.gov/search/#collection=compounds&query\\_type=structure&query\\_subtype=identity](https://pubchem.ncbi.nlm.nih.gov/search/#collection=compounds&query_type=structure&query_subtype=identity))

molecular formula	Structural formula	Systematic name	SMILES	InChI	CAS RN
			<chem>CC(=C)C=C</chem>		
					
		Ammonium acetate			
<chem>C6H6O</chem>					
					105-53-3



- c. Luckily, the makers of PubChem have followed some of the best practices that we've outlined above. What have they done that can help you get to the bottom of the inconsistency that you've discovered in parts (b-c)?
  
- d. Follow the clue that PubChem left you as to the source of the discrepancy and describe what might have happened with the data coming into Pubchem. (If you aren't sure, what to do, click <http://www.drugbank.ca/drugs/DB03066> and <http://www.drugbank.ca/drugs/DB04398>).