

## 3.11: Assignments

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1. Read these articles and answer the following questions.

- What is the difference between a substance and a compound in PubChem?  
(<https://pubchemblog.ncbi.nlm.nih.gov/2014/06/19/what-is-the-difference-between-a-substance-and-a-compound-in-pubchem/>)
- Compound Summary Page Redesigned  
(<https://pubchemblog.ncbi.nlm.nih.gov/2014/10/20/compound-summary-page-redesigned/>)
- Substance Record Page Released  
(<https://pubchemblog.ncbi.nlm.nih.gov/2015/04/09/substance-record-page-released/>)
- PubChem adds a “legacy” designation for outdated data  
(<https://pubchemblog.ncbi.nlm.nih.gov/2015/11/16/pubchem-adds-a-legacy-designation-for-outdated-data/>)
- “§2.4. Availability of compounds for subsequent experiments” in “Getting the most out of PubChem for virtual screening”  
(<http://www.tandfonline.com/doi/full/10.1080/17460441.2016.1216967>) [If you don’t have access to this article, Author’s original manuscript for this paper is available as an attachment at the end of Module 4.]

(a) Explain the difference between the PubChem Substance and Compound databases in two or three sentences.

(b) Explain what the Compound Summary page of a compound is.

(c) Explain what the Substance Record page of a substance is.

(d) Explain the reason why the “legacy” designation was introduced in PubChem in two or three sentences.

(e) Among the menus available on the top of the PubChem home page (<https://pubchem.ncbi.nlm.nih.gov>) is “Today’s Statistics”. The number of compounds/substances/assays shown under this menu does not include “non-live” records. What does “non-live” mean here?

2. While the PubChem Substance database is an archive in nature, data providers often want to update their substance information archived in PubChem. For this reason, PubChem keeps all different “versions” of a substance record and shows the most recent version on its Substance Record page by default (Click [here](#) to read about what the Substance Record page is). Go to the PubChem home page (<https://pubchem.ncbi.nlm.nih.gov>) and follow the steps described below.

(a) After selecting the “Compound” tab above the search box, type “60823” in the search box and click the “Go” button. This will direct you to the Compound Summary page for CID 60823 (atorvastatin). (Click [here](#) to read about what the Compound Summary page is.) [You will learn how to search PubChem in much more detail for next two modules (Modules 5 and 6).]

(b) Scroll down until you see “Contents” on the left column. Expand this table of contents by clicking the “+” sign before “Contents”. Locate the “Related Substances” section and click the record count for the “Same” item under that section.

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