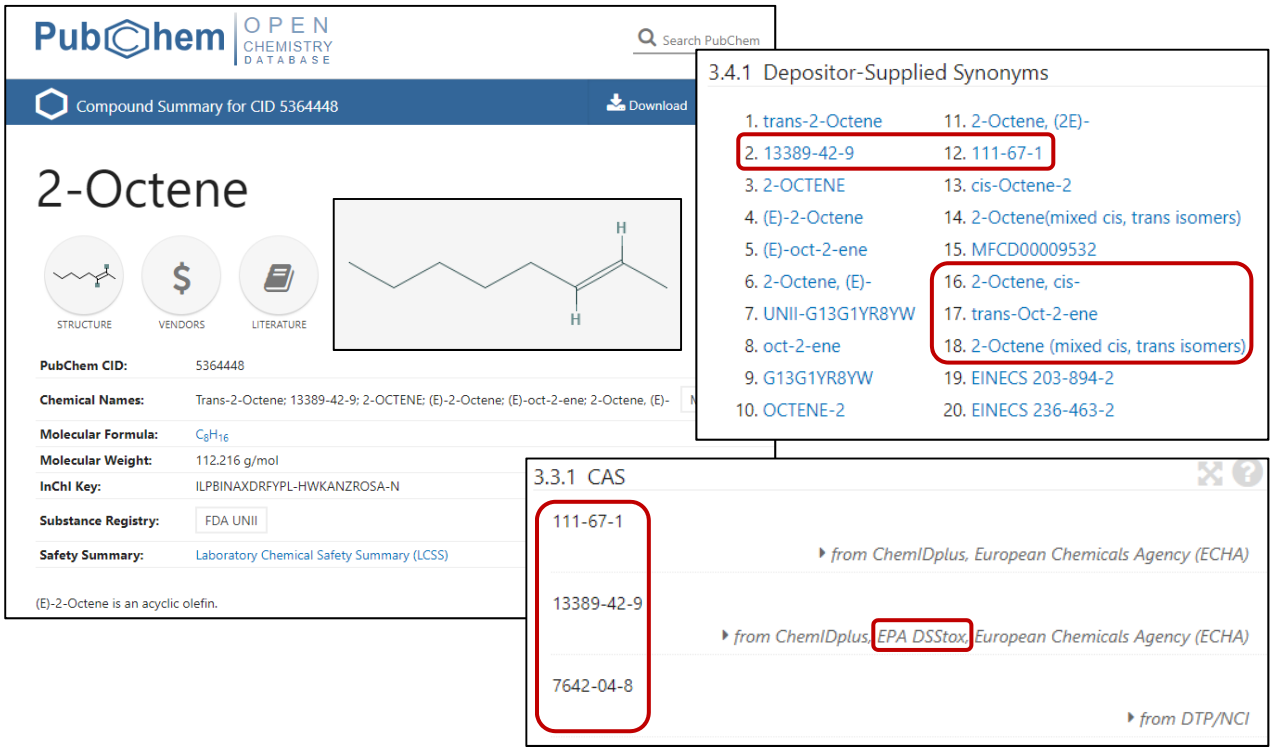
EPA's DSSTox Chemical Structure Database: A curated chemistry resource supporting computational toxicology research (Grulke et al.)

Supplemental Material:

All websites accessed on 3/6/2019.

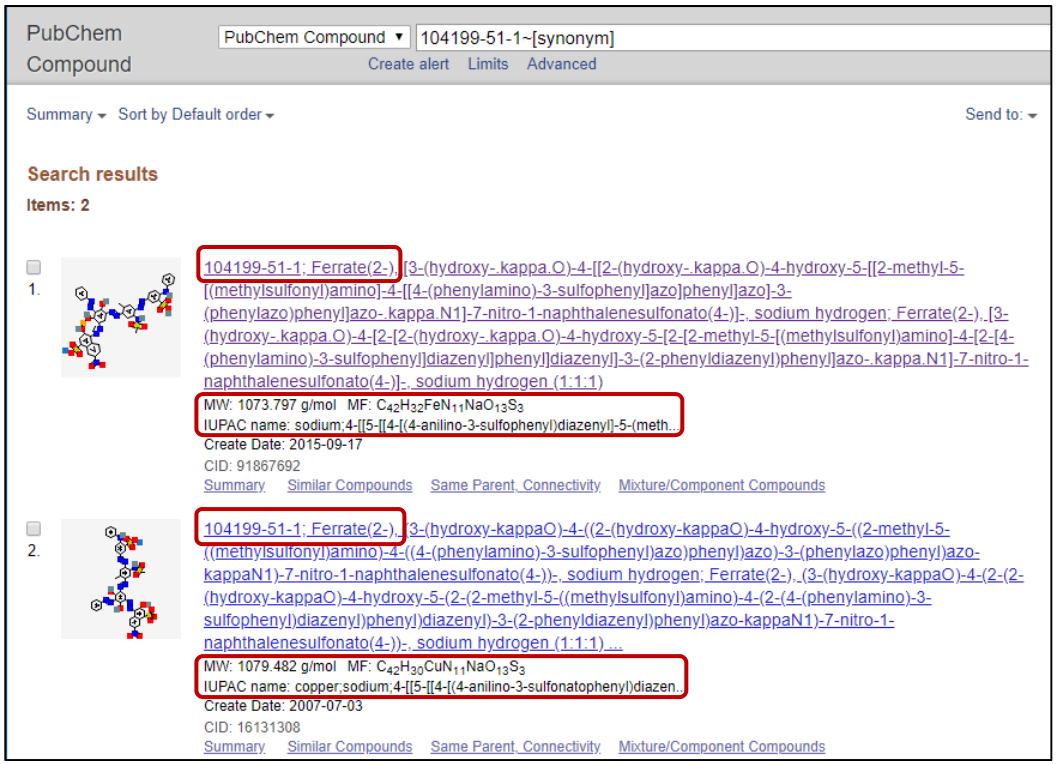
Example 1. PubChem record with multiple CAS RN and names synonyms assigned to "2-Octene". The trans (E) form of 2-Octene structure is shown, but three forms are listed as synonyms (cis, trans, mixture of cis/trans). DSSTox assigns each of these three forms to different substance records, each with its own substance name, CAS RN and structure.

https://pubchem.ncbi.nlm.nih.gov/compound/5364448

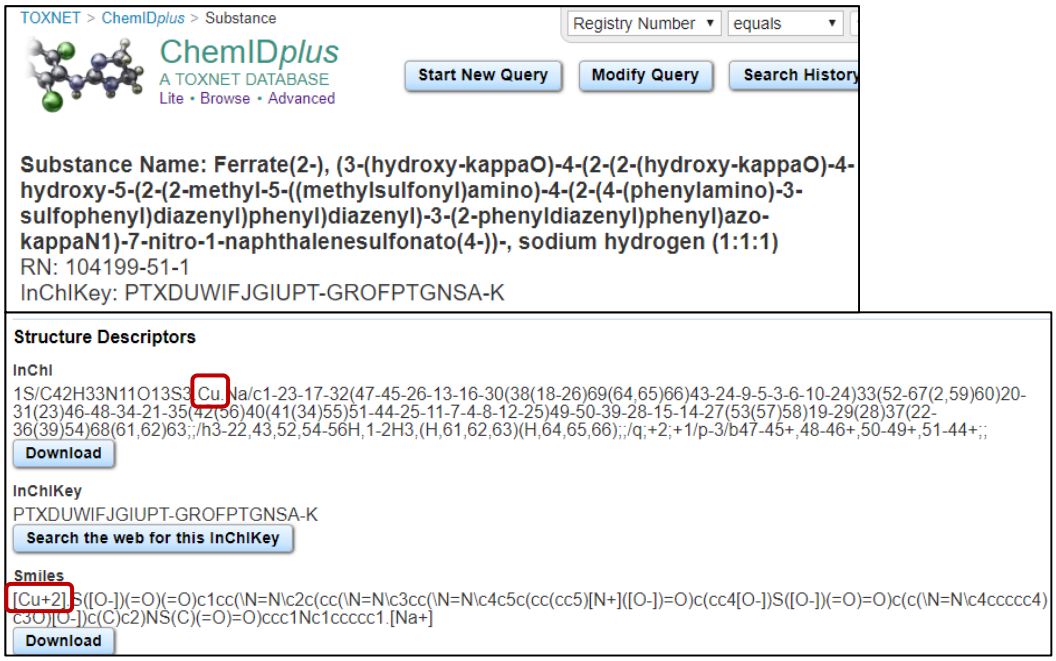


Example 2. PubChem and ChemID records with incorrect metal assigned to structure.

https://www.ncbi.nlm.nih.gov/pccompound?term=104199-51-1~%5Bsynonym%5D

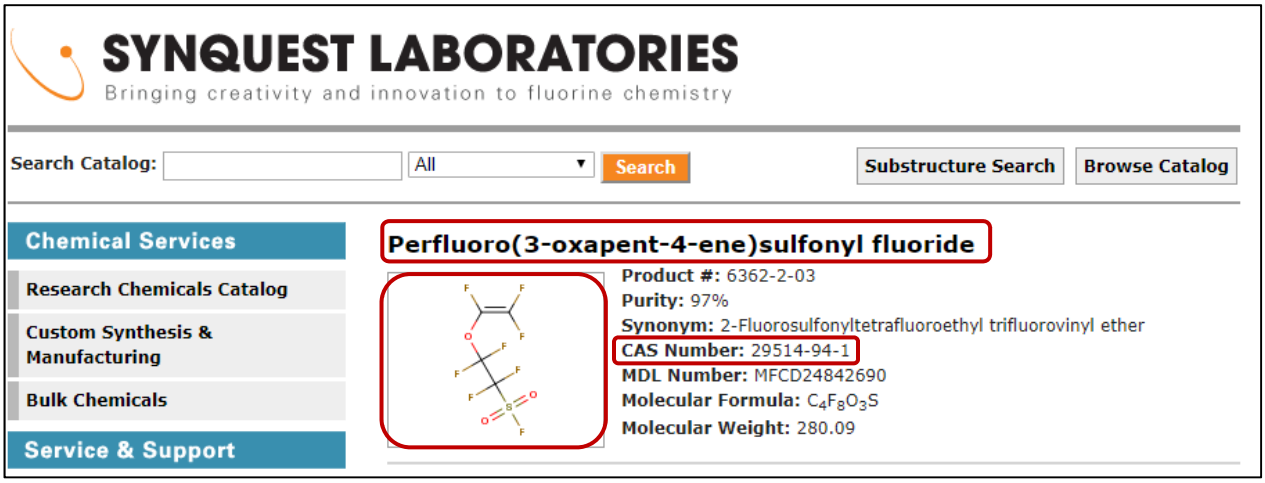


https://chem.nlm.nih.gov/chemidplus/rn/104199-51-1

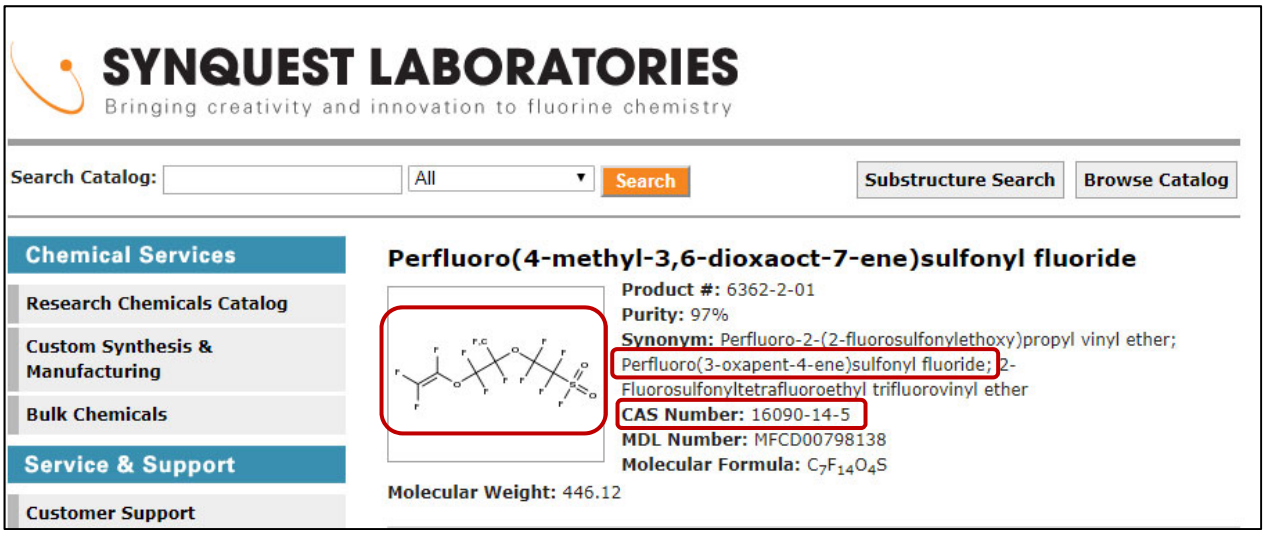


Example 3. Sample public supplier website listing both the correct structure-name-CAS and a mismapped synonym-structure-CAS.

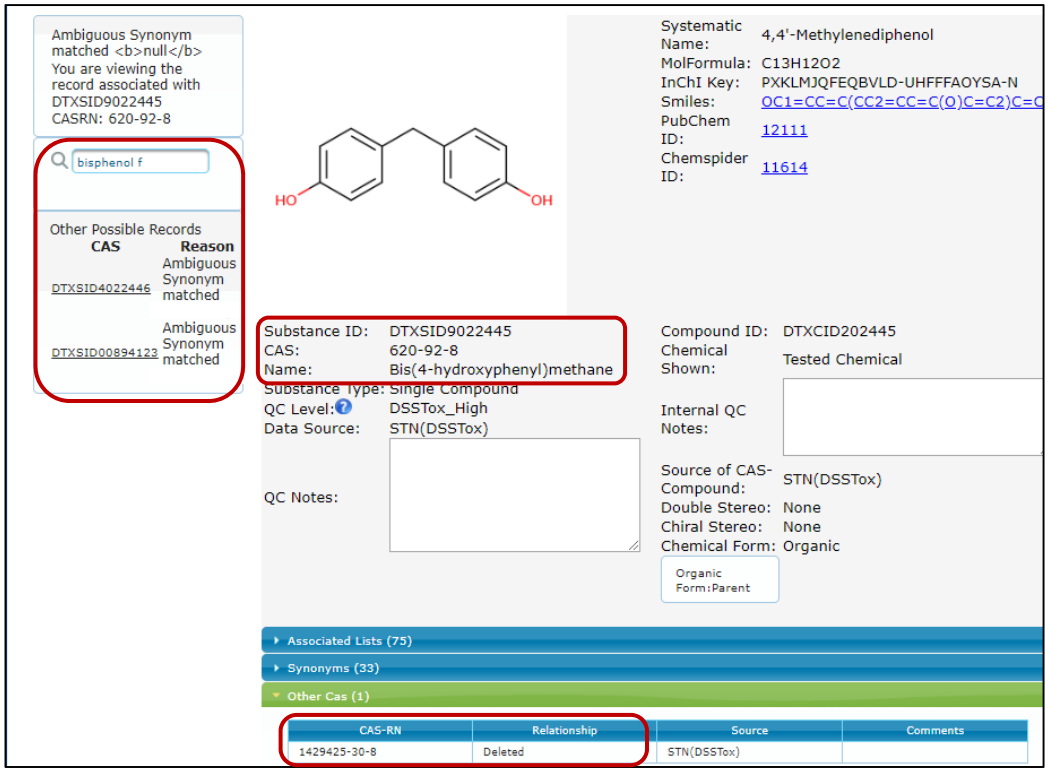
http://www.synquestlabs.com/product/id/72359.html

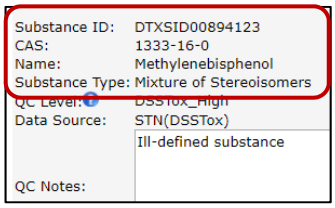


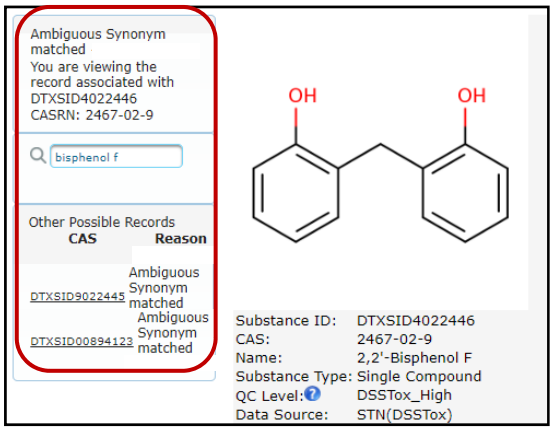
http://www.synquestlabs.com/product/id/27815.html



Example 4. Sample DSSTox substance record with ambiguous synonyms and how they are mapped within DSSTox, also showing instance of mapped deleted CAS RN.

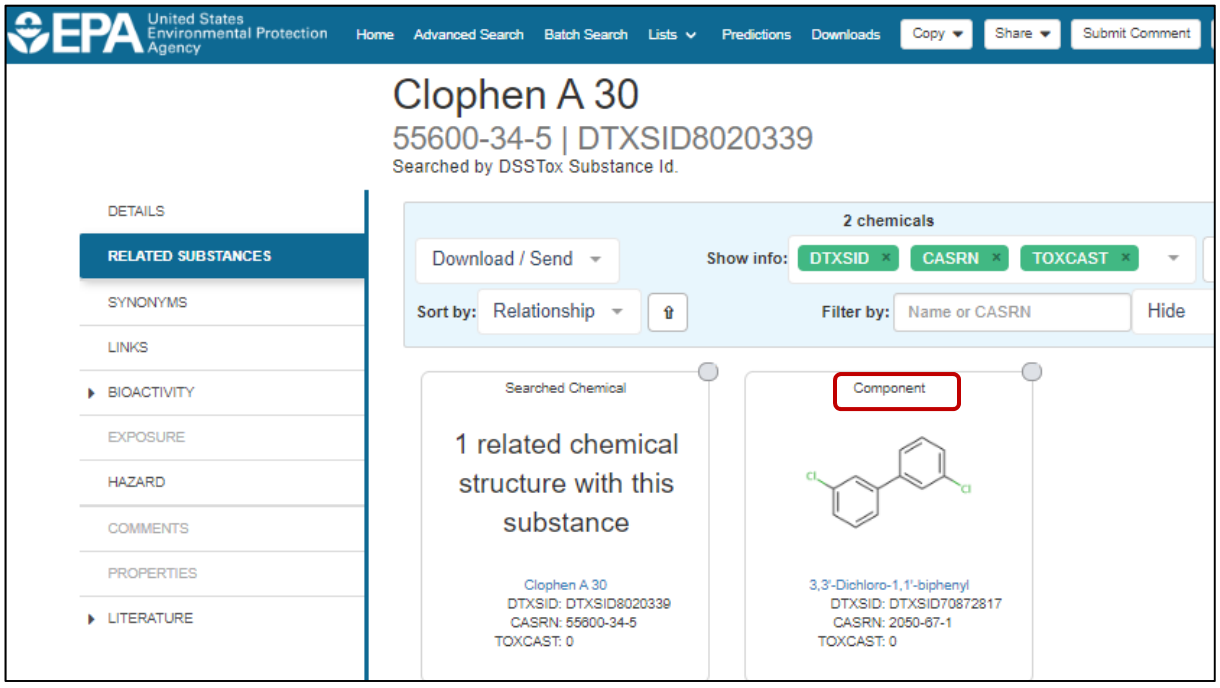




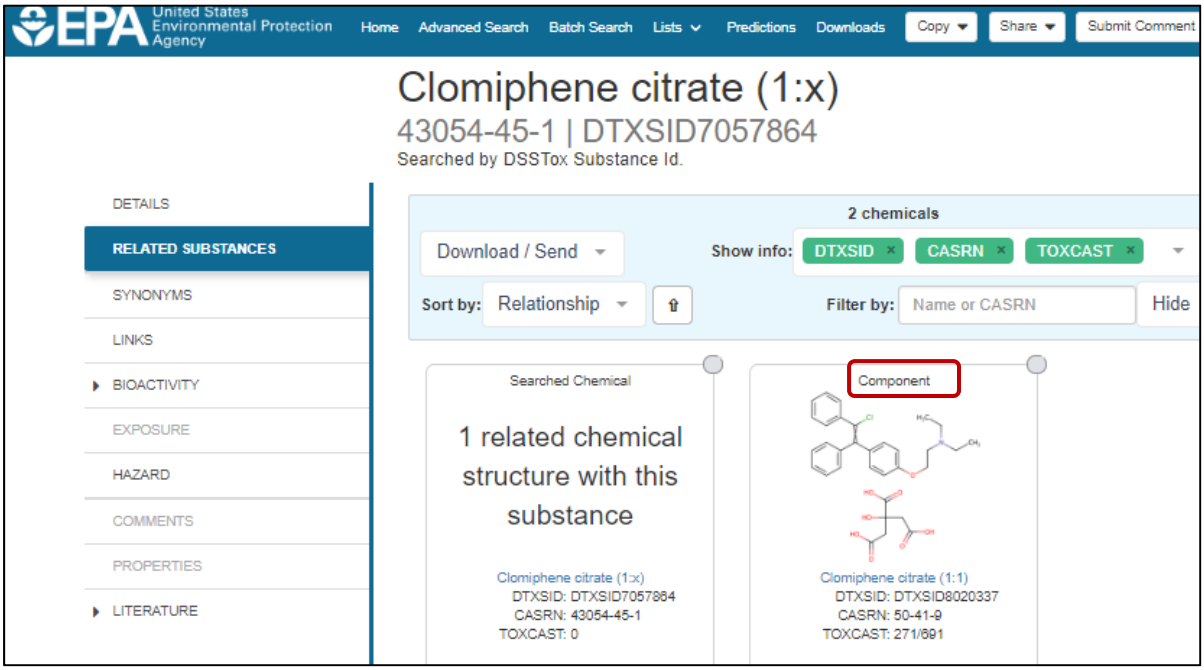


Example 5: Sample relationship mappings in DSSTox for mixtures mapped to a component.

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID8020339#related-substances

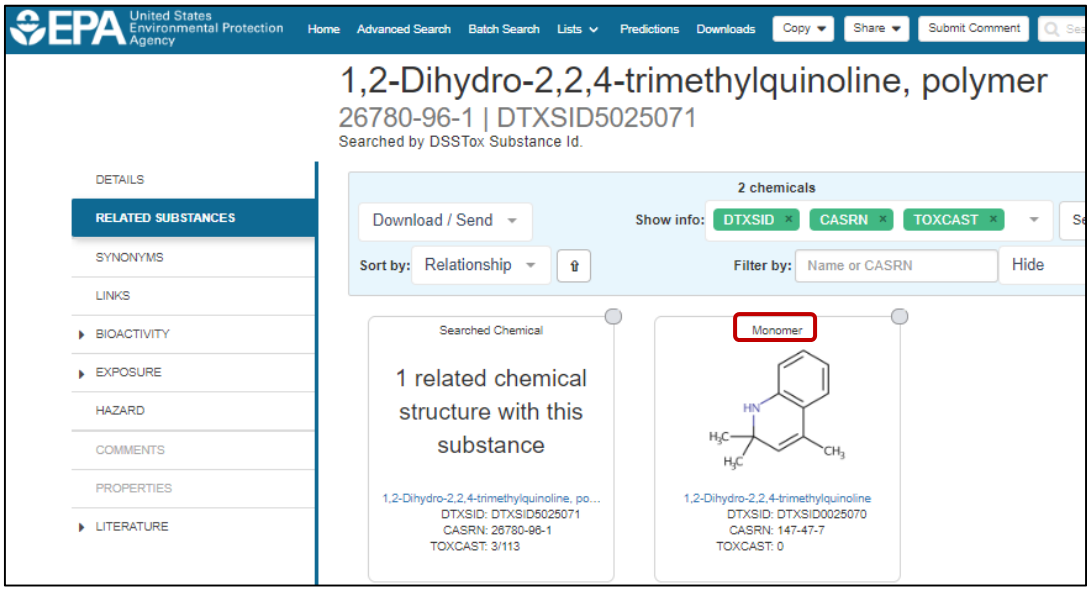


https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID7057864#related-substances

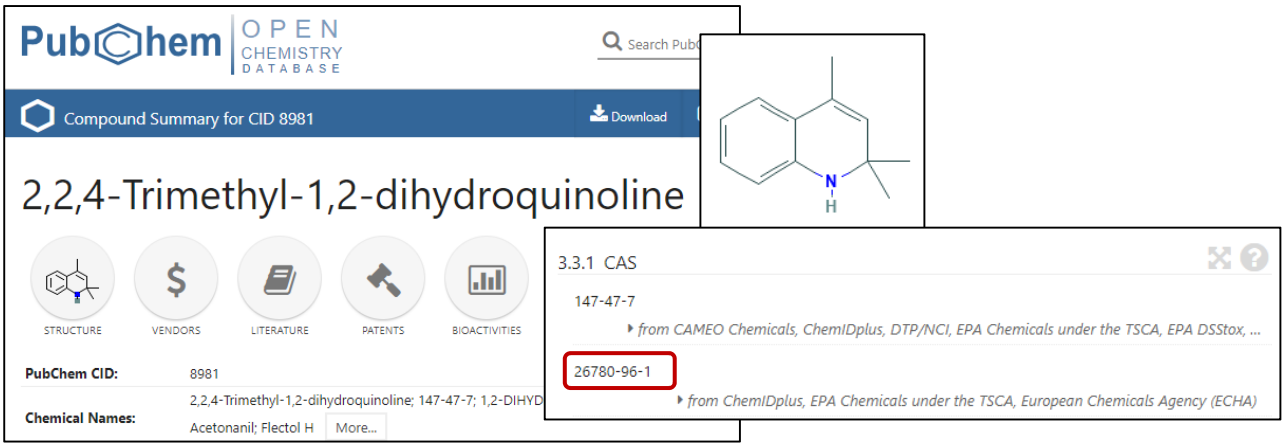


Example 6: Sample relationship mappings in DSSTox for polymer mapped to a monomer, also showing representative structures provided for the non-structurable record on 2 public websites.

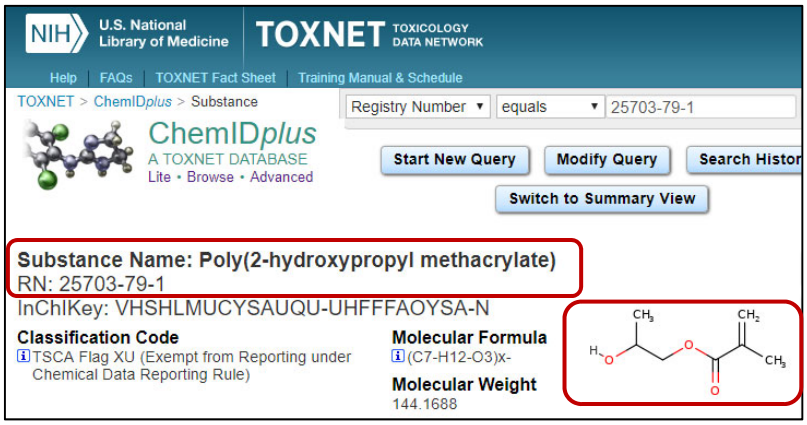
https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID5025071#related-substances



https://pubchem.ncbi.nlm.nih.gov/compound/8981#section=2D-Structure

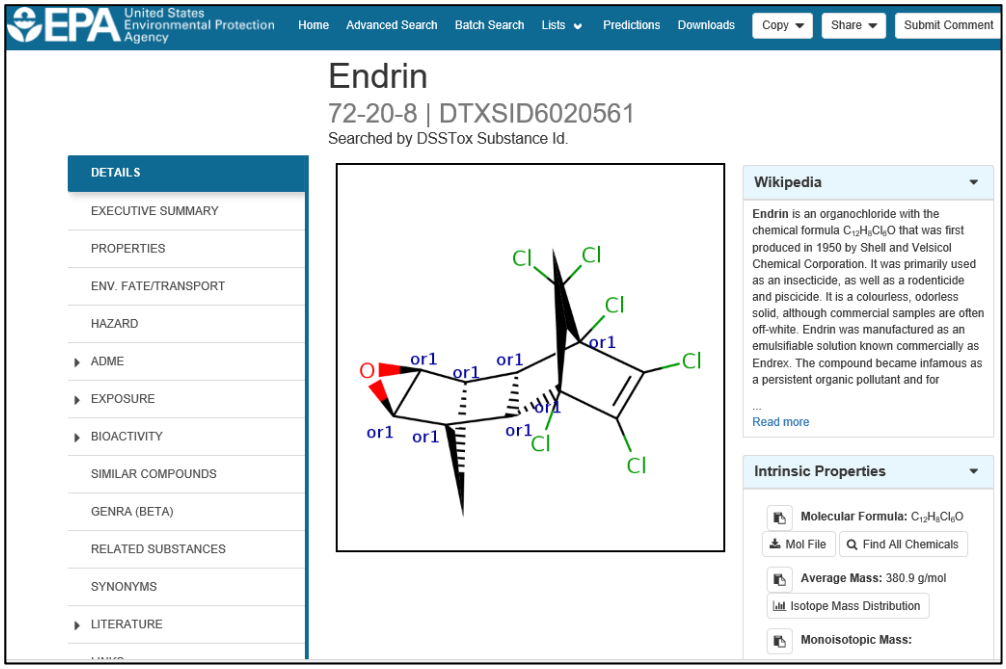


https://chem.nlm.nih.gov/chemidplus/rn/25703-79-1

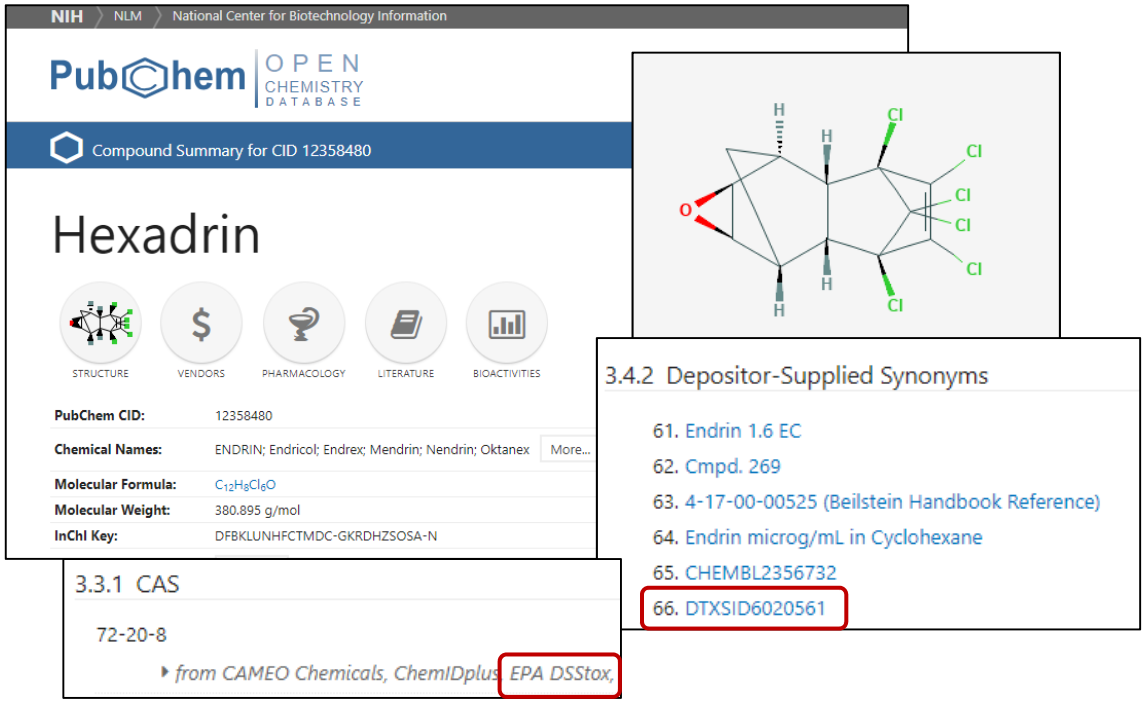


Example 7. Two sample DTXSID structures with advanced relative stereochemistry supported by v3000 mol files that are mapped by PubChem to v2000 structures in which the relative stereochemistry information is lost.

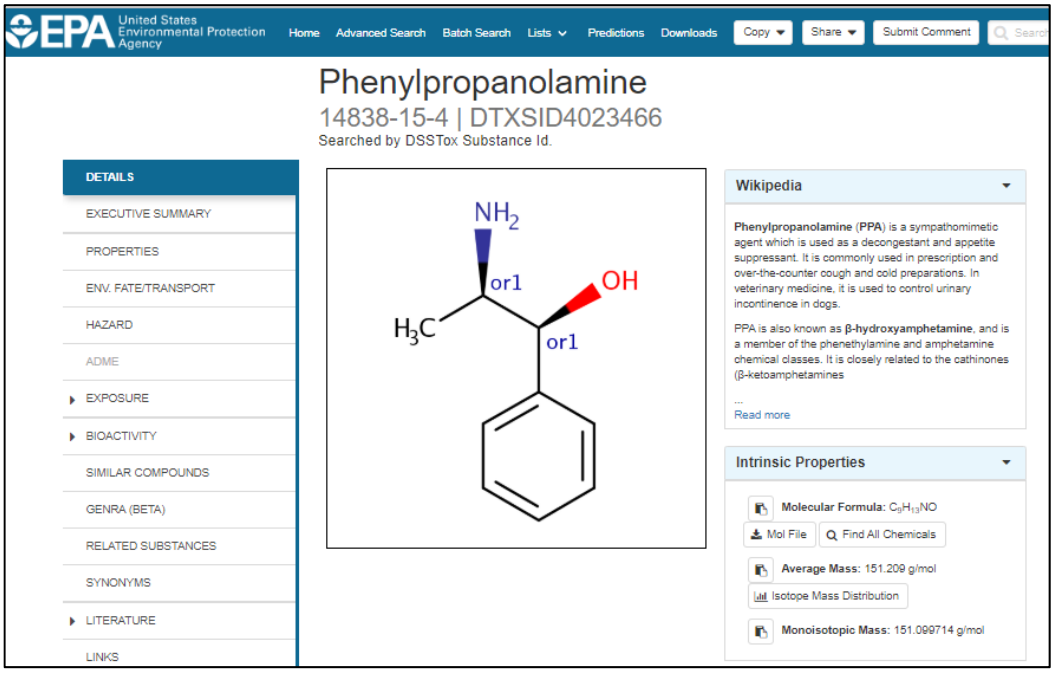
https://comptox.epa.gov/dashboard/DTXSID6020561



https://pubchem.ncbi.nlm.nih.gov/compound/12358480#section=2D-Structure



https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID4023466



https://pubchem.ncbi.nlm.nih.gov/compound/26934#section=Depositor-Supplied-Synonyms