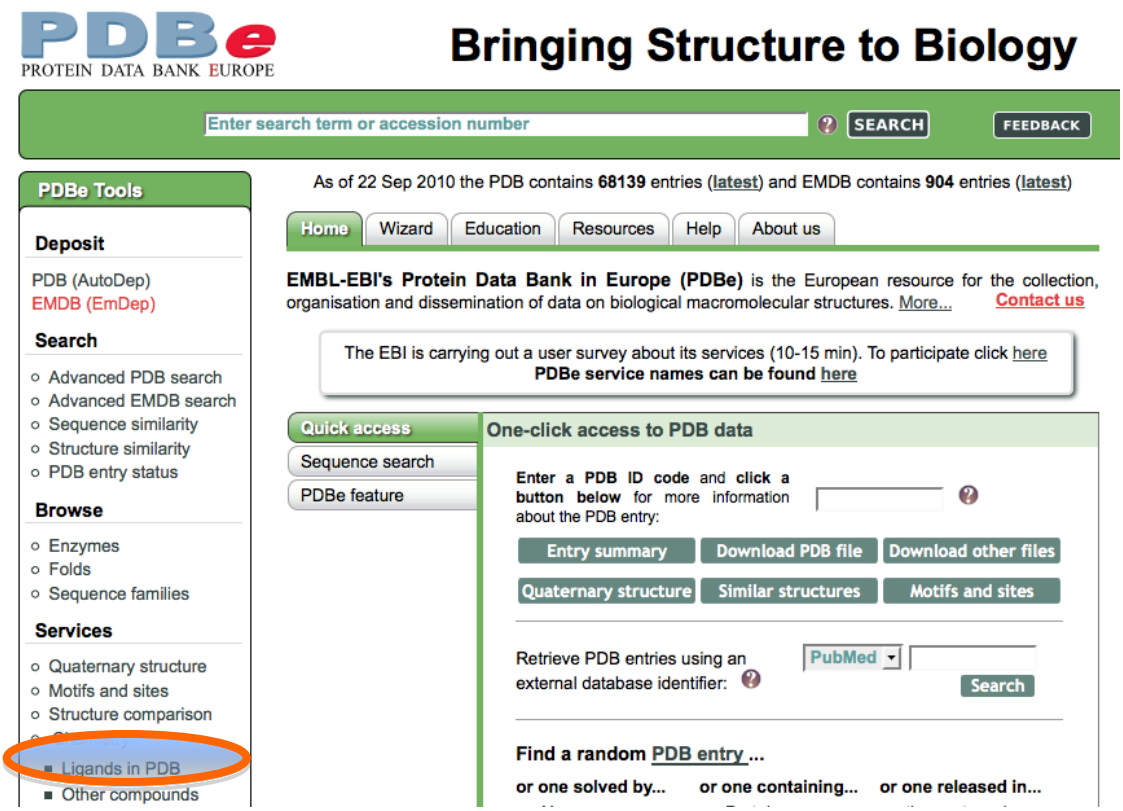
PDBeChem
http://pdbe.org/pdbechem/

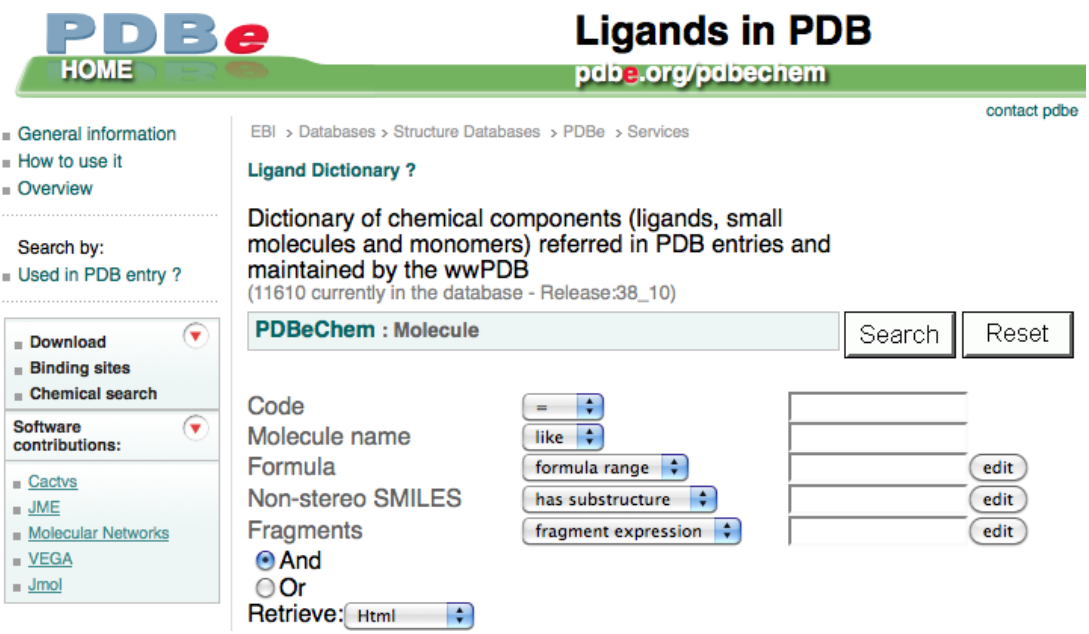
This PDBe tutorial introduces the PDBeChem Database and search engine. The PDBeChem database stores information regarding all chemical species (small molecules, ligands, metal ions, amino acids and nucleotides) found in the Protein Data Bank (PDB) archive. For every unique chemical in the PDB archive, this database contains detailed descriptions of chemical formula, formal charge, IUPAC systematic name, stereochemistry, atom names, atom types and bond information.

PDBeChem can be accessed from the main PDBe home page (http://pdbe.org/) as shown below or by directly going to http://pdbe.org/pdbechem in your internet browser.



Please begin this tutorial by opening a new browser window and going to http://pdbe.org and choosing the link as shown above. Please keep this tutorial document open in order to follow the instructions.

Tutorial

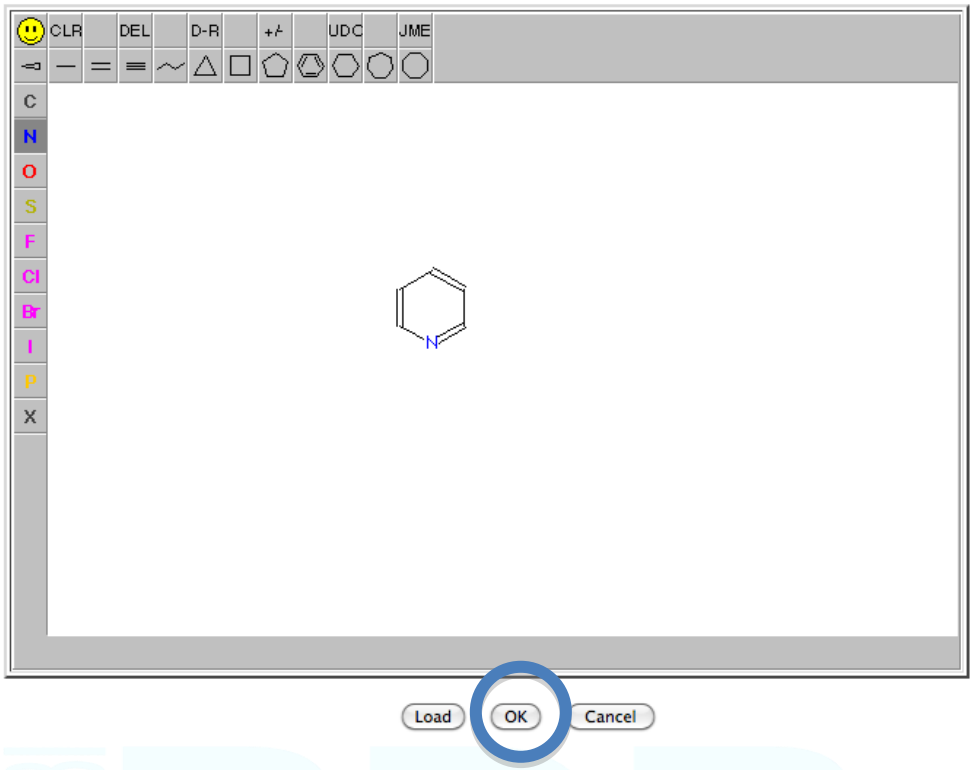


The main page for PDBeChem contains many different search options. One may search for a chemical of interest based on any of the following criteria:

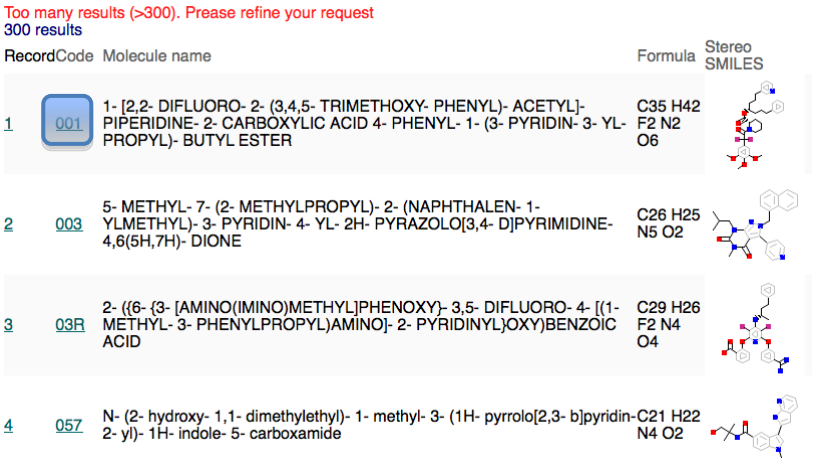
- 3 letter code for the ligand
- Name of the ligand
- Chemical formula
- Substructure (both stereo and non-stereo)
- Typical chemical fragment pattern present in the ligand of choice.

In order to search for any chemical in the PDB based on a substructure search, click on the edit button next to the "Non-Stereo SMILES" option on this search page. This will bring up a new window where you can use various drawing tools (single bond, double bond, benzene ring etc.) to construct the substructure present in your ligand of interest.

Draw the ligand structure (Pyridine C5 N1) as shown below and click on the "OK" button to go back to the main search page.



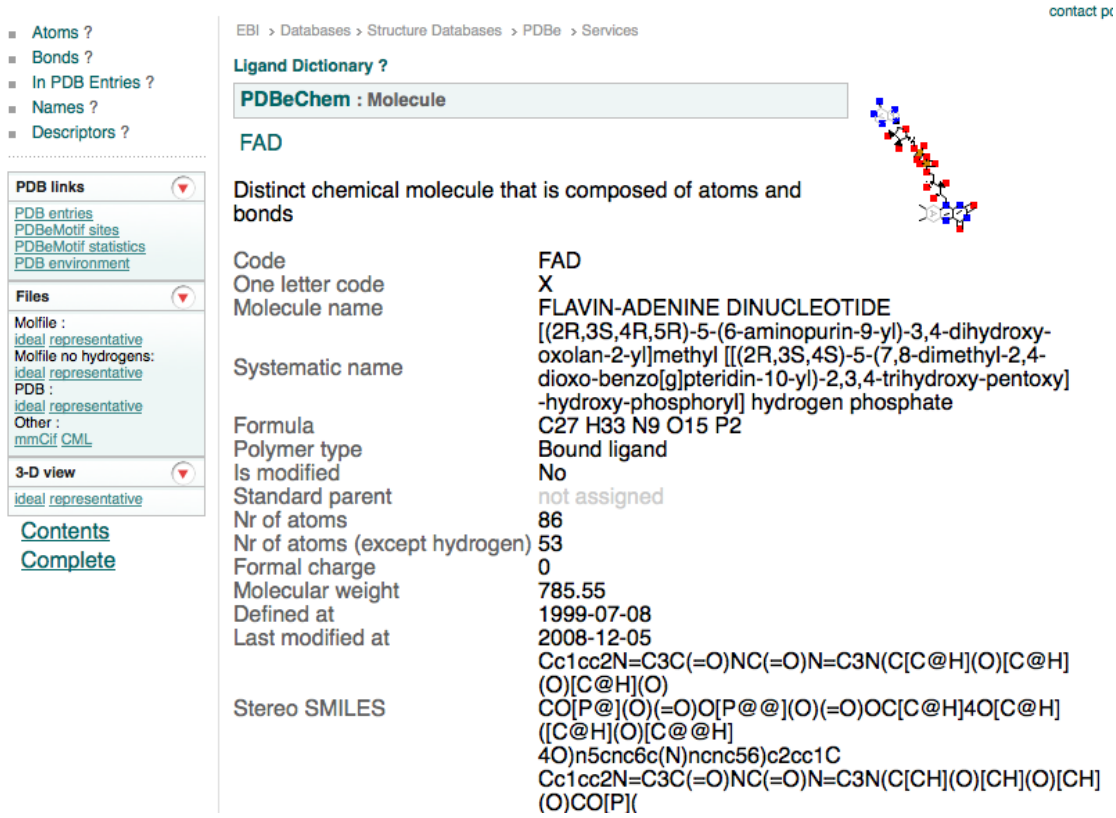
On the main page you will see that the input field box for the non-stereo smile has been populated with the smile notation of the structure drawn. Now click on the "Search" button on the PDBeChem page to search for all compounds in the PDB that contain this fragment.



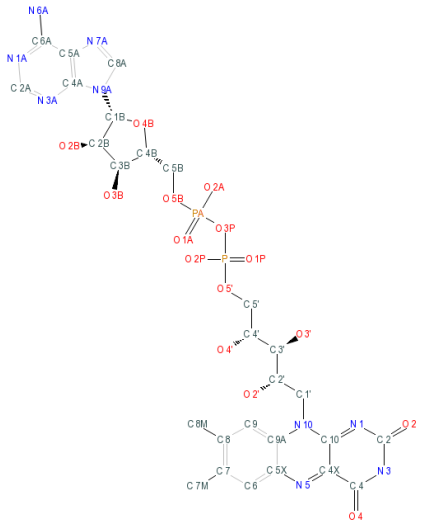
Each row in this result list contains the pyridine fragment as used for search. You can click on the ligand code to find out more about this compound.

Let us now take a look as a well known ligand FAD (Flavin adenine dinucleotide or vitamin B2) as an example to explore PDBeChem.

Go back to the main PDBeChem page and press the “Reset” button to clear the previous search. Now type in “FAD” in the Code box and press Search. Now click on the ligand code link (called FAD) to see details of this compound as stored in the PDBeChem database.



The summary page displays information about FAD including:



- Molecular Name
- Total number of atoms (and non-hydrogen atoms)
- Charge
- Molecular Weight
- IUPAC systematic name
- Stereo and non-stereo smiles.
- Schematic image of the compound showing atom names, stereochemistry and bond types.

The summary page also provides an option to download the coordinates for the ligand. Both ideal and the experimental coordinates are available for download for ligand docking and analysis purposes.

On the left hand side of the summary page there is supplementary information about the ligand. For example, clicking on the “atoms” link will take you to the page which has description for each and every atom present in the ligand including their elementary and stereochemical properties, charge, if it participates in ring formation, or functions as a leaving atom.

FAD Atoms

Atom of a chemical element, that composes a molecule

Record	Atom name	Element symbol	PDB name	Atom stereochemistry	Is aromatic	Is leaving atom	Charge	X coordinate	Y coordinate	Z coordinate
1	PA	P	AP	R	N	N	0	-1.648	-.629	-3.229
2	O1A	O	AO1	N	N	N	0	-3.035	-1.088	-2.992
3	O2A	O	AO2	N	N	N	0	-.678	-1.906	-3.378
4	O5B	O	AO5*	N	N	N	0	-1.595	.245	-4.58
5	C5B	C	AC5*	N	N	N	0	-2.036	-.605	-5.64
6	C4B	C	AC4*	R	N	N	0	-2.009	.169	-6.959
7	O4B	O	AO4*	N	N	N	0	-.665	.583	-7.256
8	C3B	C	AC3*	S	N	N	0	-2.476	-.741	-8.111
9	O3B	O	AO3*	N	N	N	0	-3.639	-.203	-8.744
10	C2B	C	AC2*	R	N	N	0	-1.277	-.748	-9.095
11	O2B	O	AO2*	N	N	N	0	-1.728	-.672	-10.449
12	C1B	C	AC1*	R	N	N	0	-.518	.541	-8.692
13	N9A	N	AN9	N	Y	N	0	.895	.449	-9.063
14	C8A	C	AC8	N	Y	N	0	1.889	-.118	-8.322
15	N7A	N	AN7	N	Y	N	0	3.023	-.024	-8.953
16	C5A	C	AC5	N	Y	N	0	2.83	.606	-10.136
17	C6A	C	AC6	N	Y	N	0	3.663	.979	-11.205
18	N6A	N	AN6	N	N	N	0	5.018	.698	-11.178
19	N1A	N	AN1	N	Y	N	0	3.119	1.607	-12.242
20	C2A	C	AC2	N	Y	N	0	1.827	1.878	-12.277
21	N3A	N	AN3	N	Y	N	0	1.01	1.549	-11.299
22	C4A	C	AC4	N	Y	N	0	1.462	.914	-10.223

Similarly the “bonds” link provides detailed information of the bond order, bond types (single, double, triple, aromatic) and bond distances for every bond in the compound.

Ligand Dictionary ?

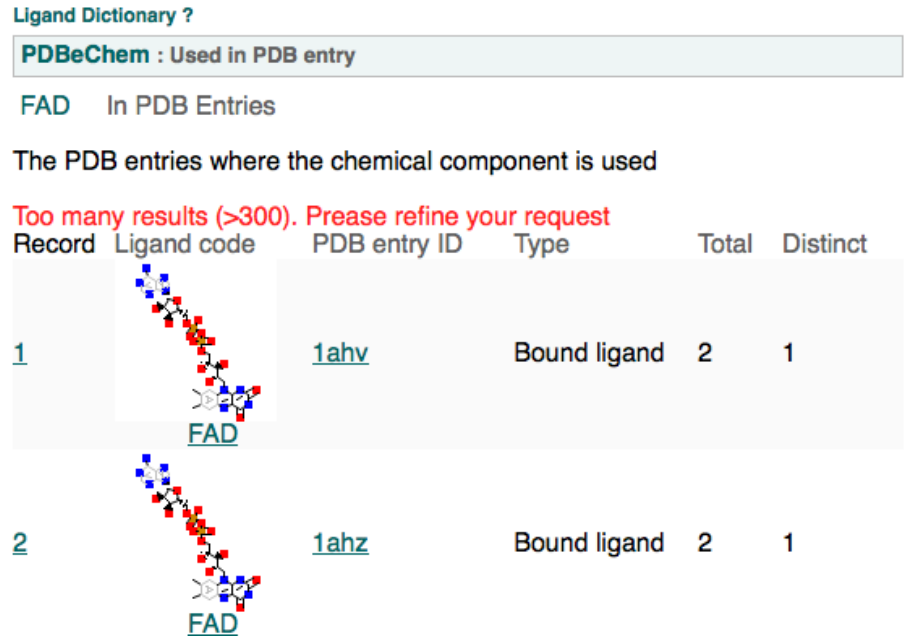
PDBeChem : Chemical bond

FAD Bonds

A bond between two atoms of the molecule

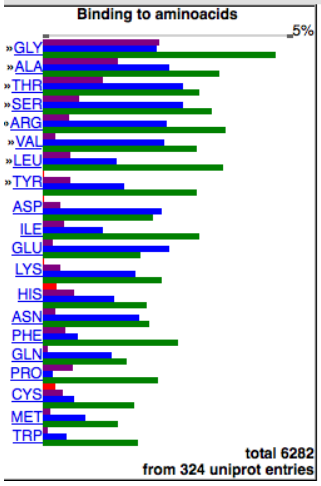
Record	First atom	Second atom	First element	Second element	Bond order type	Bond length	Bond stereochemistry	Is aromatic
1	PA	O1A	P	O	doub	1.48	N	N
2	PA	O2A	P	O	sing	1.611	N	N
3	PA	O5B	P	O	sing	1.61	N	N
4	PA	O3P	P	O	sing	1.609	N	N
5	O2A	HOA2	O	H	sing	.966	N	N
6	O5B	C5B	O	C	sing	1.428	N	N
7	C5B	C4B	C	C	sing	1.53	N	N
8	C5B	H51A	C	H	sing	1.09	N	N
9	C5B	H52A	C	H	sing	1.09	N	N
10	C4B	O4B	C	O	sing	1.437	N	N
11	C4B	C3B	C	C	sing	1.541	N	N
12	C4B	H4B	C	H	sing	1.09	N	N
13	O4B	C1B	O	C	sing	1.444	N	N
14	C3B	O3B	C	O	sing	1.429	N	N
15	C3B	C2B	C	C	sing	1.551	N	N

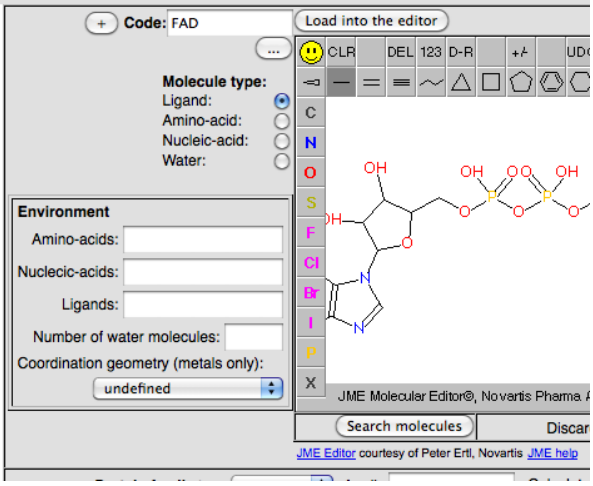
The “in PDB entries” link returns a list of PDB entries that contain the ligand FAD.



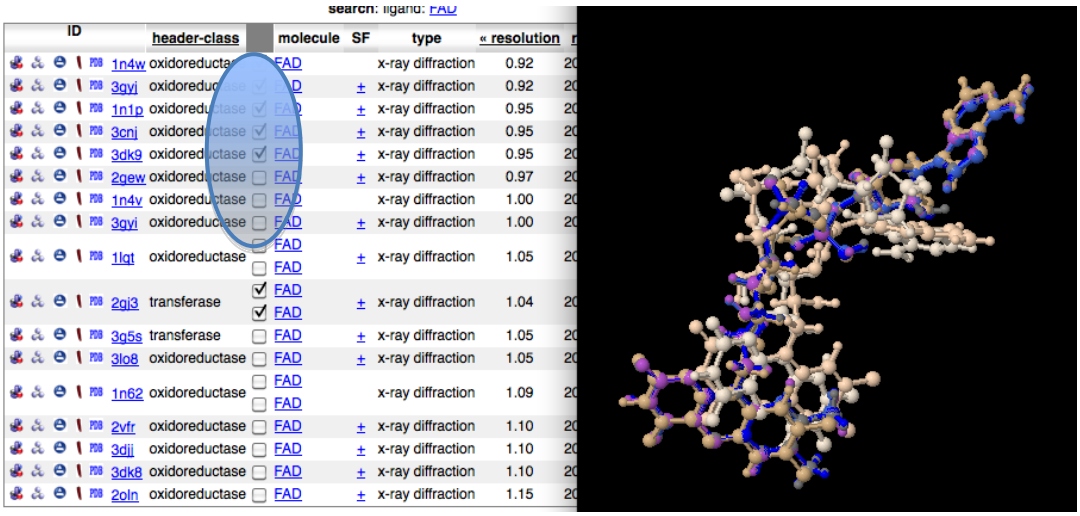
The "PDB entry ID" links on this page will take you to the details of that PDB entry which contains the ligand.

The PDBeChem summary page also provides interactions statistics (PDBeMotif statistics) for different amino acids with the ligand of interest using the PDBeMotif service (http://pdbe.org/motif/). Click on this link to see all the interactions between FAD and amino acids in the whole of the PDB archive.

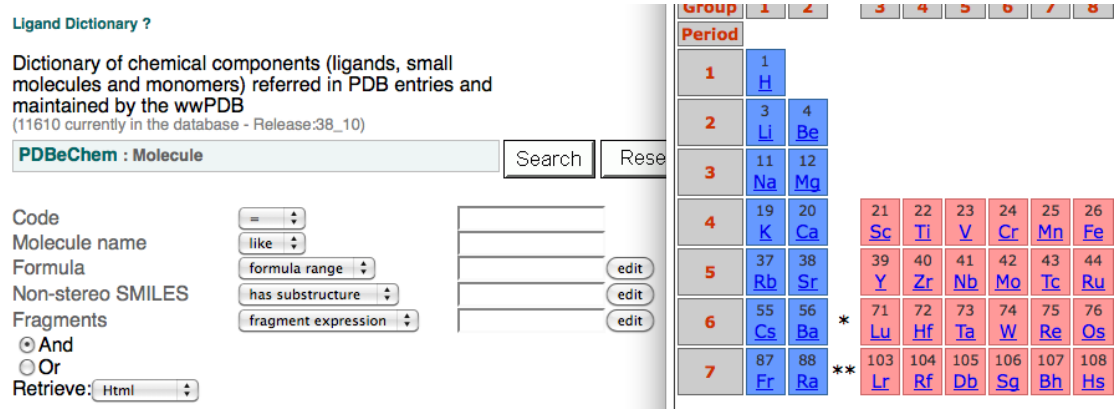




If you click on "PDBeMotif sites" it will return a list of PDB entries containing the FAD ligand. You can view these superposed FAD molecules from this list of PDB entries and explore further.

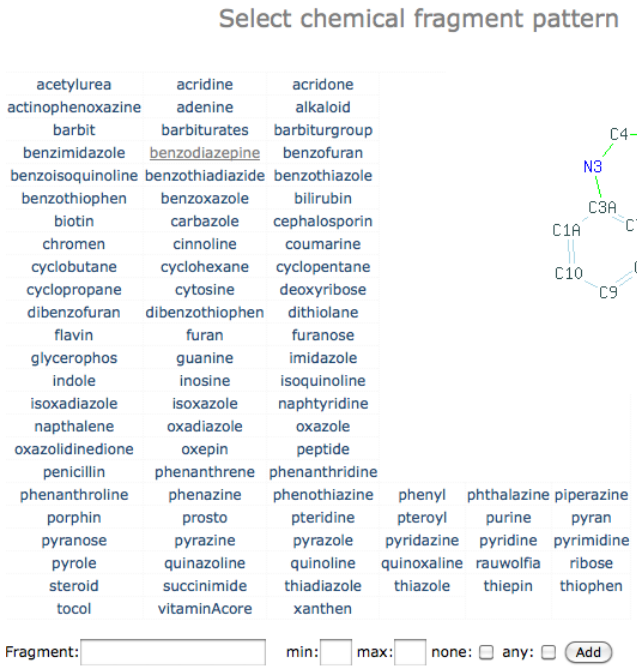


Go back to the main PDBeChem search page (http://pdbe.org). Some of the other search options that are available allow searching for all chemical components by formula or formula range.



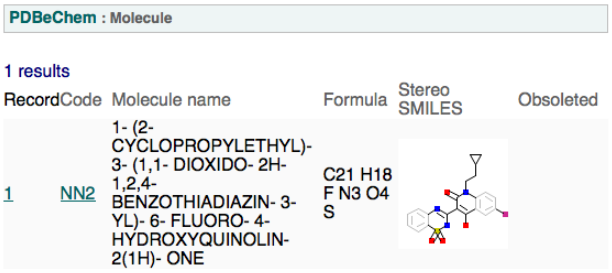
You can either graphically input the formula using the periodic table (use the edit button on the formula search option), or by typing in a formula range into the search box directly (like C1-6 O3 N1-5 to search for all compounds that contain between 1 and 6 carbons, three oxygens and 1 to 5 nitrogens). To exclude an element from the search use the number 0 after the element name (for example C1-6 O3 P0 N1-5 to find all compounds like above but without any phosphorus atoms).

Another useful search option is to use the fragment library to find all entries that contain one of the known chemical fragments. Choose the edit box on the "Fragments" option of the search form.



Choose your fragment of interest and click "OK" to close this window and return to the main search page. Now click on the "Search" button on the PDBeChem page.

The results will contain all known compounds that contain this fragment.



This ends our tutorial on PDBeChem. We hope you found this useful and will be able to use this tool in your future research and analysis. Feel free to explore this service with compounds of your interest. If you need to get in touch with the PDBe regarding any aspect of this service, please email pdbehelp@ebi.ac.uk and we will try to assist you in any way possible.