

chem-bla-ics

Complex PDB documents using the Bioclipse ChildResourceCreator

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Keywords

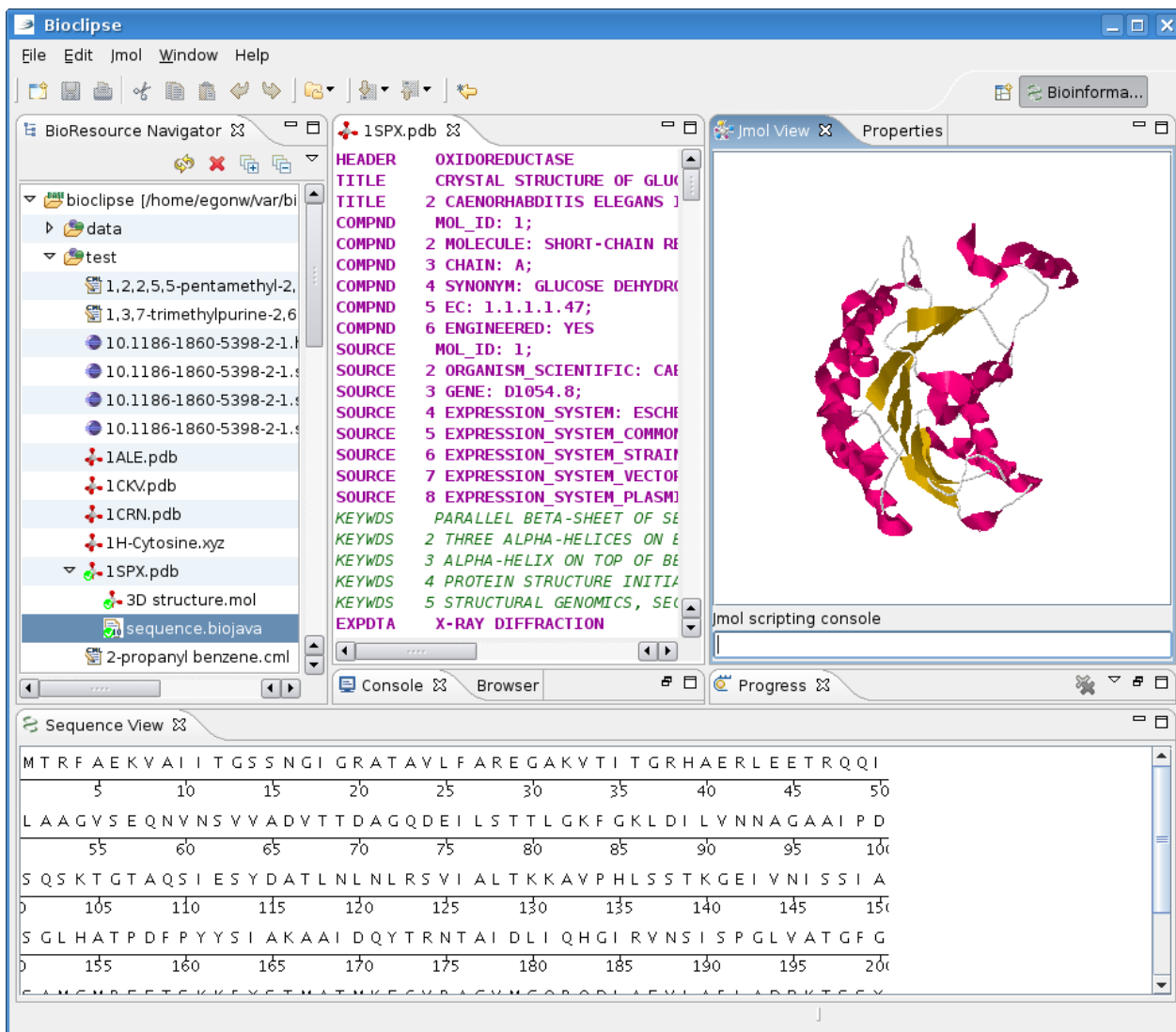
Bioclipse, Biojava, Cdk, Pdb, Jmol

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Some time ago I blogged about the [ChildResourceCreator extension point in Bioclipse](#) and hinted as using that for [PDB files](#), which contain 3D molecular models, sequences and bibliographic information. Using the new extension point, [Bioclipse](#) now treats PDB files as complex documents, creating child resources for the 3D molecular model (using the [CDK](#) plugin), and a sequence resource (using the [BioJava](#) plugin).



The screenshot displays the Bioclipse application window. The main interface is divided into several panes:

- BioResource Navigator:** Shows a tree view of resources, including a 'test' folder with various files like '1SPX.pdb' and '3D structure.mol'.
- 1SPX.pdb:** Displays the PDB header information:

```
HEADER OXIDOREDUCTASE
TITLE CRYSTAL STRUCTURE OF GLUC
TITLE 2 CAENORHABDITIS ELEGANS ]
COMPND MOL_ID: 1;
COMPND 2 MOLECULE: SHORT-CHAIN RE
COMPND 3 CHAIN: A;
COMPND 4 SYNONYM: GLUCOSE DEHYDR
COMPND 5 EC: 1.1.1.1.47;
COMPND 6 ENGINEERED: YES
SOURCE MOL_ID: 1;
SOURCE 2 ORGANISM_SCIENTIFIC: CAE
SOURCE 3 GENE: D1054.8;
SOURCE 4 EXPRESSION_SYSTEM: ESCH
SOURCE 5 EXPRESSION_SYSTEM_COMMO
SOURCE 6 EXPRESSION_SYSTEM_STRAI
SOURCE 7 EXPRESSION_SYSTEM_VECTOF
SOURCE 8 EXPRESSION_SYSTEM_PLASM
KEYWDS PARALLEL BETA-SHEET OF SE
KEYWDS 2 THREE ALPHA-HELICES ON E
KEYWDS 3 ALPHA-HELIX ON TOP OF BE
KEYWDS 4 PROTEIN STRUCTURE INITIA
KEYWDS 5 STRUCTURAL GENOMICS, SEC
EXPDTA X-RAY DIFFRACTION
```
- Jmol View:** Shows a 3D ribbon representation of the protein structure, colored in shades of pink and yellow.
- Sequence View:** Displays the amino acid sequence:

```
MTRFAEKVAII TGS SNGI GRATAVLFA REGAKVTI TGRHAERLEETRQQI
5 10 15 20 25 30 35 40 45 50
LAAGVSEQNVNSV VADVTT DAGQDEI LSTTLGKFGKLDI LVNNAGAAI PD
55 60 65 70 75 80 85 90 95 100
S Q S K T G T A Q S I E S Y D A T L N L N L R S V I A L T K K A V P H L S S T K G E I V N I S S I A
105 110 115 120 125 130 135 140 145 150
S G L H A T P D F P Y S I A K A A I D Q Y T R N T A I D L I Q H G I R V N S I S P G L V A T G F G
155 160 165 170 175 180 185 190 195 200
E A M C N R E E F T S K K E Y S T M A T M K E C Y R A G Y M C G R O D L A E V L A E L A D R K T E S Y
```