

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 **BioResource Navigator** on the left shows a tree structure with a 'test' folder containing several files, including '1SPX.pdb'. The central panel displays the PDB header and keywords for '1SPX.pdb':

```

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 DEHYDRO
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: ESCHER
SOURCE      5 EXPRESSION_SYSTEM_COMMON
SOURCE      6 EXPRESSION_SYSTEM_STRAIN
SOURCE      7 EXPRESSION_SYSTEM_VECTOR
SOURCE      8 EXPRESSION_SYSTEM_PLASMI
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
  
```

The **Jmol View** window on the right shows a 3D ribbon model of the protein structure. The **Sequence View** window at the bottom displays the amino acid sequence:

```

M T R F A E K V A I I T G S S N G I G R A T A V L F A R E G A K V T I T G R H A E R L E E T R Q Q I
  5      10      15      20      25      30      35      40      45      50
L A A G V S E Q N V N S V V A D V T T D A G Q D E I L S T T L G K F G K L D I L V N N A G A A I P D
  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 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
S A M C N R E E T S K K E Y S T M A T M K E C Y R A G Y M C O R D L A E V I A E L A D R K T E S Y
  
```