

Getting Jmol's 'cartoon on' to work in Bioclipse

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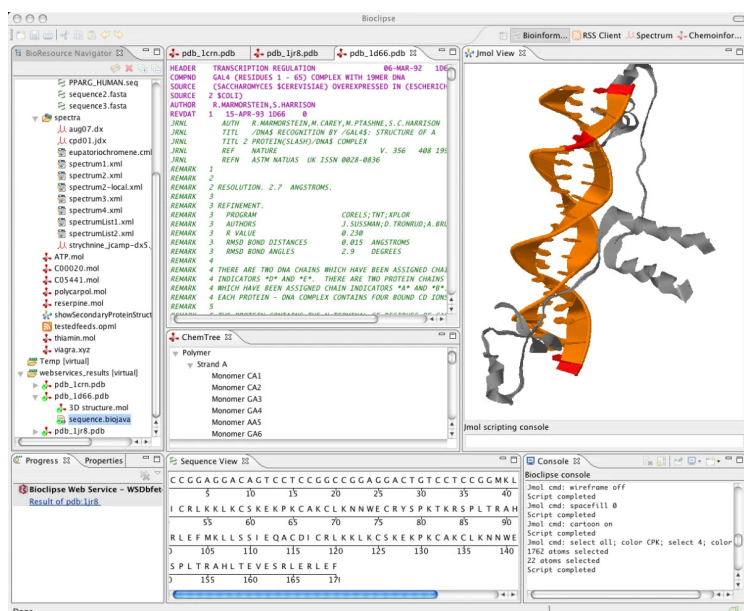
Published April 10, 2006

Citation

Willighagen, E. (2006). Getting Jmol's 'cartoon on' to work in Bioclipse. *Chem-bla-ics*. <https://doi.org/10.59350/7nz8x-a7q09>

Keywords

Bioclipse, Jmol, Protein



The screenshot displays the Bioclipse application window. On the left is the BioResource Navigator showing a tree of files including PPARC_HUMAN.fasta, spectra, and various XML files. The central Jmol View window shows a 3D model of a protein-DNA complex. The protein is represented by a grey ribbon, and the DNA is shown as an orange double helix. Below the Jmol View is a console window with a Jmol script: `Jmol cmd: wireframe off`, `Jmol cmd: spacefill 0`, `Jmol cmd: cartoon on`, `Jmol cmd: select all; color CPK; select 4; color`, and `Jmol cmd: 1762 atoms selected`. At the bottom, a sequence viewer shows the amino acid sequence: `CCGGAGCACGTCCTCCGGCCGGAGCACTGTCCTCCGGMKL` and `ICRLKLLKSKKPKKCAKCLKNWECRYSPTKRSPLTRAH`.

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chem-bla-ics

Bioclipse 1.0 is to be released in May, and the cartoon on script command is still not working in the Jmol viewer. For those who do not know yet, Bioclipse is a cool Eclipse RCP based Java chemo-and bioinformatics workbench. To have a better idea what goes on inside Bioclipse, I wrote a new BioPolymer tree to show me the strands in the protein. After Ola wrote code to show properties for IChemObject's, I extended it with PDB properties for the atoms, strands and monomers.

The contents of the ChemTree view in the middle and the Properties view below that look fine:

The screenshot displays the Bioclipse application window. The main view shows a 3D molecular model of a protein-DNA complex. The protein is represented by a grey ribbon, and the DNA is shown as an orange double helix. The interface includes several panels:

- BioResource Navigator:** A tree view on the left showing a project structure with files like 'PPARG_HUMAN.seq', 'sequence2.fasta', and 'pdb_1crn.pdb'.
- PDB View:** A window showing the PDB header and remarks for 'pdb_1crn.pdb'. The header includes: 'TRANSCRIPTION REGULATION', 'GAL4 (RESIDUES 1 - 65) COMPLEX WITH 19MER DNA', and 'SCHEMATIC OF GAL4 (SACCHAROMYCES SCEREVISIAE) OVEREXPRESSED IN (ESCHERICHIA COLI)'. Remarks include 'RESOLUTION. 2.7 ANGSTROMS.' and 'REFINEMENT. PROGRAM CORELS;TNT;XPLOR'.
- ChemTree:** A tree view showing a 'Polymer' with a 'Strand A' containing monomers CA1 through CA6.
- Properties:** A panel at the bottom left showing 'Bioclipse Web Service - WSDbfet' and a 'Result of pdb_1jr8'.
- Sequence View:** A window displaying a protein sequence in a grid format:

C	C	G	G	A	G	A	C	A	G	T	C	C	C	G	G	C	C	G	G	A	G	A	C	T	G	T	C	C	C	G	G	M	K	L					
I	C	R	L	K	K	L	K	C	S	K	E	K	P	K	C	A	K	C	L	K	N	N	W	E	C	R	Y	S	P	K	T	R	S	P	L	T	R	A	H
R	L	E	F	M	K	L	L	S	I	E	Q	A	C	D	I	C	R	L	K	K	L	K	C	S	K	E	K	P	K	C	A	K	C	L	K	N	N	W	E
S	P	L	T	R	A	H	L	T	E	V	E	S	R	L	E	R	L	E	F																				
- Console:** A window at the bottom right showing Jmol commands and their output, such as 'Jmol cmd: wireframe off', 'Script completed', and 'Jmol cmd: select all; color CPK; select 4; color 1762 atoms selected'.

So I'll have to dig a bit further.

References