

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

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Published April 10, 2006

Citation

Willighagen, E. (2006, April 10). Getting Jmol's 'cartoon on' to work in Bioclipse. *Chem-bla-ics*. <https://doi.org/10.59350/7nz8x-a7q09>

Keywords

Bioclipse, Jmol, Protein

Abstract

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.

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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 top-left pane, 'BioResource Navigator', shows a hierarchical tree of files including sequences (PPARG_HUMAN.seq, sequence2.fasta, sequence3.fasta) and spectra (aug07.dx, cpd01.jdx, eupatoriochromene.cml, spectrum1.xml, spectrum2.xml, spectrum2-local.xml, spectrum3.xml, spectrum4.xml, spectrumList1.xml, spectrumList2.xml, strychnine_jcamp-dx5). The top-middle pane, 'pdb_1crn.pdb', displays PDB file details: HEADER, COMPND (TRANSCRIPTION REGULATION), SOURCE (GAL4 (RESIDUES 1 - 65) COMPLEX WITH 19MER DNA), REVSTAT (1 15-APR-93 1066 0), JRNAL (AUTH R.MARMORSTEIN,M.CAREY,M.PTASHNE,S.C.HARRISON), JRNAL (TITL /DNAS RECOGNITION BY /GAL45: STRUCTURE OF A), JRNAL (TITL 2 PROTEIN(SLASH)/DNAS COMPLEX), JRNAL (REF NATURE V. 356 408 195), JRNAL (REFN ASTM NATUAS UK ISSN 0028-0836), REMARK 1, REMARK 2, REMARK 3 (RESOLUTION. 2.7 ANGSTROMS.), REMARK 4, REMARK 5 (REFINEMENT), REMARK 6 (PROGRAM CORELS;TNT;XPLOR), REMARK 7 (AUTHORS J.SUSSMAN;D.TRONRUD;A.BR), REMARK 8 (R VALUE 0.230), REMARK 9 (RMSD BOND DISTANCES 0.015 ANGSTROMS), REMARK 10 (RMSD BOND ANGLES 2.9 DEGREES), REMARK 11, REMARK 12 (THERE ARE TWO DNA CHAINS WHICH HAVE BEEN ASSIGNED CHAIN INDICATORS *D* AND *E*. THERE ARE TWO PROTEIN CHAINS WHICH HAVE BEEN ASSIGNED CHAIN INDICATORS *A* AND *B*.), REMARK 13 (EACH PROTEIN - DNA COMPLEX CONTAINS FOUR BOUND CD IONS), REMARK 14. The top-right pane, 'Jmol View', shows a 3D ribbon model of a protein-DNA complex. The bottom-left pane, 'Progress', shows 'Bioclipse Web Service - WSDbfet' and 'Result of pdb:1jr8'. The bottom-middle pane, 'Sequence View', shows a sequence alignment: CCGGAGGACAGTCTCCGGCCGGAGGACTGTCTCCGGMKL, I CRLKKLKCSKEPKCAKCLKNNWECRYSPTKRSPLTRAH, RLEFMKLLSSI EQACDI CRLKKLKCSKEPKCAKCLKNNWE, SPLTRAHLTEVESRLERLEF. The bottom-right pane, 'Console', shows Jmol script commands and output: Jmol cmd: wireframe off, Script completed, Jmol cmd: spacefill 0, Script completed, Jmol cmd: cartoon on, Script completed, Jmol cmd: select all; color CPK; select 4; color 1762 atoms selected, 22 atoms selected, Script completed.

So I'll have to dig a bit further.