

JChemPaint history: CML patches in 1999

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Keywords

Jmol, Jchempaint, Cml

Abstract

There was some talk about the history of chemoinformatics toolkits by Noel and Andrew, which made me wonder on the exact history of Jmol and JChemPaint.

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chem-bla-ics

There was some talk about the history of chemoinformatics toolkits by [Noel](#) and [Andrew](#), which made me wonder on the exact history of [Jmol](#) and [JChemPaint](#). Below is the email [Christoph](#) dug up from his archives:

X-Mozilla-Status: 1011
X-Mozilla-Status2: 00000000
Message-ID: <372ECD5E.53A49584@ice.mpg.de>
Date: Tue, 04 May 1999 12:35:10 +0200
From: Christoph Steinbeck
Reply-To: steinbeck@ice.mpg.de
Organization: Max-Planck-Institute of Chemical Ecology
X-Mailer: Mozilla 4.51 [en] (WinNT; I)
X-Accept-Language: en
MIME-Version: 1.0
To: Egon Willighagen
Subject: Re: Participating in JChemPaint
References: <000701be9613\$34cf52e0\$8e74ae83@catv6142.extern.kun.nl>
Content-Type: text/plain; charset=us-ascii
Content-Transfer-Encoding: 7bit

> Egon Willighagen wrote:
>
> Dear Christoph Steinbeck,
>
> Yesterday I visited your site on JChemPaint. I like to contribute some
> of my expertise on
> Java and CML (1).
>
> CML is a markup language that is able to contain chemical information.
> It can contain for example physical properties, for which I use CML in
> my Dictionary on Organic Chemistry (2).
> But is also might contain spectra, bibliographic references etc. And
> of course 2D and 3D
> structural information.
>
> Therefore I propose to write both CML-input and -output procedures for
> the JChemPaint project.
>
> I hope to hear from you soon.
>
> Yours sincerely,
>
> Egon Willighagen

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>

> 1. <http://www.xml-cml.org/>

> 2. <http://www.sci.kun.nl/sigma/Chemisch/Woordenboek/>

Dear Egon,

thanks very much for your mail and your offer to write CML-input and output routines for JChemPaint.

That really sounds great to me and I will give you access to our CVS tree as soon as we have discussed the details.

Cheers,

Chris

--C. S.

Dr. Christoph Steinbeck (<http://www.ice.mpg.de/~stein>)

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What is man but that lofty spirit - that sense of enterprise.

.. Kirk, "I, Mudd," stardate 4513.3..

Now, my email must have been triggered by the [announcement of JChemPaint on FreshMeat.net](#), which is the oldest public record of JChemPaint I have found so far:

