

JChemPaint history: CML patches in 1999



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Keywords

Jmol, Jchempaint, Cml

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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

chem-bla-ics

>

> 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:

