

Warren DeLano and the future of PyMOL

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Abstract

This blog is old and new news. The old news is that Warren passed away at the end of last year, after having successfully shown how OpenSource cheminformatics (and/or bioinformatics) software can be developed in a commercial setting (DeLano Scientific), and PyMol was a huge success.

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This blog is old and new news. The old news is that [Warren passed away](#) at the end of last year, after having successfully shown how OpenSource cheminformatics (and/or bioinformatics) software can be developed in a commercial setting ([DeLano Scientific](#)), and [PyMol](#) was a huge success. Warren had a SourceForge account ([wdelano](#)) for almost 10 years:

About Me

Joined: 2000-02-22 (10 years ago)
User ID: 15464
Username: [wdelano \(My Site\)](#)
Public Name: Warren L. DeLano

[Send me a message](#)

My Projects

[Jmol Develop](#)
[PyMOL Molecular Graphics System Develop](#)

I had not blogged about it before as the news hit me hard. Surely, Warren knew a lot of people and I only was only one of many, but Warren's memory stuck well. I know Warren from the [Jmol](#) project, where we talked in the past of coming to an Open Specification for exchanging scenes between Jmol and PyMol. Around the end of my PhD contract we even briefly, but seriously, explored doing a post-doc in his group.

Anyway, lot's of people wrote up blogs (in arbitrary order: [Rich](#), [P212121](#), [MacResearch](#), [Jörg](#), [MMB](#), [Shirley](#), [Derek](#), [Wavefunction](#), [Dan](#), [Barry](#), and probably many more). They have set up a memorial fund which will focus on promoting the Open Source ideas of Warren, including an [Award](#).

Schrödinger

Yesterday, I was [pinged](#) about [Schrödinger acquiring PyMol](#). The press release is, as usual, short on details, but those have become clearer during the day. Schrödinger is not new to Open Source cheminformatics, and has an [product based on KNIME](#), which is now GPL, but also has a proprietary license for those who wish to license so.

But, unless I missed any other Open Source (-oriented) product, the acquisition of PyMol significantly changes the game for them: PyMol is a major Open Source product, bigger than KNIME at the moment, I'd guess. My immediate response to the acquisition is whether they acquired copyrights, and they did, according to [this commit](#):

| | revision 3885, Sat Jan 9 08:30:46 2010 UTC | revision 3886, Sat Jan 9 09:16:30 2010 UTC |
|---|--|--|
| # | Line 1 | Line 1 |
| 1 | I* | I* |
| 2 | A* | A* |
| 3 | B* This file contains source code for the PyMOL computer program | B* This file contains source code for the PyMOL computer program |
| 4 | C* copyright 1998-2000 by Warren Lyford Delano of DeLano Scientific. | C* Copyright (c) Schrodinger, LLC. |
| 5 | D* | D* |
| 6 | E* It is unlawful to modify or remove this copyright notice. | E* It is unlawful to modify or remove this copyright notice. |
| 7 | F* | F* |

Colored Diff

Legend:

| | |
|---------------------|-----------------|
| Removed from v.3885 | |
| changed lines | |
| | Added in v.3886 |

This is important as it puts Schrödinger in charge of license changes. Fortunately, they seem rather serious about the Open Source thing, and hired an active PyMol developer (Jason), and kept the existing Open Source license:

| | | |
|----|--|--|
| 10 | ----- | ----- |
| 11 | Open-Source PyMOL is Copyright (C) 1998-2003 Warren L. DeLano and Copyright (C) 2003-2008 DeLano Scientific LLC, South San Francisco, California, U.S.A. (www.delanoscientific.com). | Open-Source PyMOL is Copyright (C) Schrodinger, LLC. |
| 12 | | |
| 13 | All Rights Reserved | All Rights Reserved |
| 14 | | |
| # | Line 19 | Line 17 |
| 17 | purpose and without fee is hereby granted, provided that the above | purpose and without fee is hereby granted, provided that the above |
| 18 | copyright notice appears in all copies and that both the copyright | copyright notice appears in all copies and that both the copyright |
| 19 | notice and this permission notice appear in supporting documentation, | notice and this permission notice appear in supporting documentation, |
| 20 | and that the names of Warren L. DeLano or DeLano Scientific LLC not be | and that the name of Schrodinger, LLC not be used in advertising or |
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| 23 | | |
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| 28 | OF USE, DATA OR PROFITS, WHETHER IN AN ACTION OF CONTRACT, NEGLIGENCE | OF USE, DATA OR PROFITS, WHETHER IN AN ACTION OF CONTRACT, NEGLIGENCE |
| 29 | OR OTHER TORTIOUS ACTION, ARISING OUT OF OR IN CONNECTION WITH THE | OR OTHER TORTIOUS ACTION, ARISING OUT OF OR IN CONNECTION WITH THE |
| # | Line 36 | Line 33 |
| 33 | PyMOL Trademark Notice | PyMOL Trademark Notice |
| 34 | ===== | ===== |
| 35 | | |
| 36 | PyMOL(TM) is a trademark of DeLano Scientific LLC. Derivative | PyMOL(TM) is a trademark of Schrodinger, LLC. Derivative |
| 37 | software which contains PyMOL source code must be plainly | software which contains PyMOL source code must be plainly |

Therefore, congratulations to Schrödinger for getting seriously into the Open Source community, making them the next [Dr Who of PyMol](#), and congratulations to the family of Warren in ensuring continued development of the PyMol project! It's hearth-warming to see that despite the bad times they are going through, and all they options they had with the PyMol

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code base, they find time for and strength in supporting Warren's ideas about the future of cheminformatics. My thoughts are with them!