

Getting webbed with OEChem

Craig Bruce

EuroCUP IV

Why the web?



- Everyone has a browser
 - not all equal...
- Corporate environment – always available
- Plug-ins not required



How should we deploy?



PHP, Perl or Python?

- We use all 3
- OEChem via Python SWIG bindings

- PHP in MediaWiki
- Perl for in-house pages
- Python for in-house pages

Apache to Python interface

- Previously



- Now



- When using OEChem 1.7.2

- Global interpreter lock

Hivemind (current incarnation)

The screenshot shows a forum post on the OpenEye Scientific Software website. The post title is "Why is OEChem >1.7 not working with mod_python after updating web apps?". The post is by Cynthia Bancale, asked on Jan 27 at 14:59, with 23 votes and 3 answers. It has tags for "oechem", "python", and "faq". The post content asks for help with OEChem versions >1.7 not working with mod_python. There is one answer by Joe Corkery, dated Jan 27 at 15:37, with 210 votes and 8 answers. The answer explains that the problem was caused by threading support for Python in SWIG in the 1.7.0 release and recommends using *mod_wsgi* instead. The right sidebar shows statistics for the question, including 10 faq tags, 7 oechem tags, and 5 python tags. It also lists "Education" and "New Products" sections.

Craig Bruce 47 | log out | FAQ | Documentation | Training | OpenEye

OpenEye Scientific Software

Questions Tags Users Badges Unanswered Ask Question

Why is OEChem >1.7 not working with mod_python after updating web apps?

2

When I updated my web apps to work with the latest OEChem, I found that versions of OEChem >1.7 don't appear to work with mod python. Is there something I am doing wrong?

oechem python faq

retag | flag

add comment

edited Jan 27 at 15:29

asked Jan 27 at 14:59

Joe Corkery ♦♦ 210 8

Cynthia Bancale ♦♦ 23 3

1 Answer

oldest newest votes

2

The problem was caused when OpenEye turned on threading support for Python in SWIG in the 1.7.0 release. This was done as part of the ongoing push towards multi-core/multi-threading support. However, *mod_python* is an old project that doesn't use the Python global interpreter lock correctly. Newer frameworks like *mod_wsgi* have specifically worked around this [issue](#).

To give you an idea of how old *mod_python* is, nothing has been committed to its [subversion repository](#) in 15 months, which practically makes it a dinosaur in the open source world.

OpenEye recommends that you use *mod_wsgi* instead.

link | flag

answered Jan 27 at 15:37

Joe Corkery ♦♦ 210 8

tagged

faq × 10

oechem × 7

python × 5

asked

2 months ago

viewed

17 times

latest activity

2 months ago

Education

[Sign up for an OpenEye training course.](#)

New Products

- [ROCS/ROCS](#)
- [MolProp TK](#)
- [GraphSim TK](#)

Done

Internet | Protected Mode: Off

100%

Python

- Our language of choice, v2.6
- `mod_python` no longer an option
- Various web frameworks available/required



django



django

“The Web framework for perfectionists with deadlines.”

Django makes it easier to build better Web apps more quickly and with less code.”

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Monday, April 26, 2010 Markets: DJIA +19.72 NASDAQ -2.97 S&P 500 -2.15

FINANCIAL REGULATORY OVERHAUL

Two-thirds of Americans back stricter reform

WASHINGTON POST-ABC NEWS POLL | Majorities also back two main components of legislation Democrats plan to bring to a vote in Senate.
» Jon Cohen | 9:00 a.m. ET

Shelby: GOP united, for now

Top negotiator expects all 41 Senate Republicans to vote against moving forward with debate.
» Brady Dennis | 12:15 p.m. ET

- Treasury to begin selling 1.5B shares of Citigroup

Immigration on front burner?

WEST WING BRIEFING | Arizona governor may have revived a major item on Obama's agenda.
» Michael D. Shear

- Ezra Klein | Congressman: U.S. should fight law

Wanted: A justice like Stevens

Search is on for retiring justice's replacement -- one who, like him, can relate to ordinary citizens.
» Robert Barnes and Anne E. Kornblut

- Court to decide if state can regulate video games
- Supreme Court staves out of Asian car dispute



(Photo: AP) « || »

Quick end to leak depends on robots

Robot submarines used in hopes of stopping oil leak, which threatens ecosystem.
• Photos: Gulf Coast oil rig sinks | Video

OPINIONS

Obama's focus

Hiatt: The president's discipline is why so many are disappointed in him.
dot.comments: [Reader debate](#)



- Thiessen: Gov. Christie for president?
- Samuelson: Can reform prevent another panic?

Enable mod_wsgi in Django

- Add a `project.wsgi` file

```
import os, sys

# Django Version
sys.path.append('/apps/django/Django-1.1.1')

# This project
sys.path.append('/apps/djangoapps/myproj')
os.environ['DJANGO_SETTINGS_MODULE'] = 'myproj.settings'

import django.core.handlers.wsgi
application = django.core.handlers.wsgi.WSGIHandler()
```

Enable mod_wsgi in Apache

```
<VirtualHost *:80>
    DocumentRoot "/apps/djangoapps/myproj/media/"
    ServerName myproj.astrazeneca.com:80

    Alias /media/ /apps/djangoapps/myproj/media/
    Alias /docs/ /apps/djangoapps/myproj/media/docs/

    <Directory /apps/djangoapps/myproj/media>
        Options FollowSymLinks Indexes
        Order deny,allow
        Allow from all
    </Directory>
```

Enable mod_wsgi in Apache cont.

```
# Run in daemon mode, touch project.wsgi to reload
WSGIDaemonProcess myproj.astrazeneca.com processes=2 threads=15
display-name=mod_wsgi_proj python-eggs=/tmp/.python-eggs

WSGIProcessGroup myproj.astrazeneca.com

WSGIScriptAlias / /apps/djangoapps/myproj/project.wsgi

<Directory /apps/djangoapps/myproj>
    Order deny,allow
    Allow from all
</Directory>
</VirtualHost>
```

mod_wsgi

- Use daemon mode
- Avoid embedded
- Refresh files by touching project.wsgi

Apache Apache

- One Apache instance for Django
- Another to serve static files, e.g. media
- Improves performance
- Django “runserver” for dev very slow

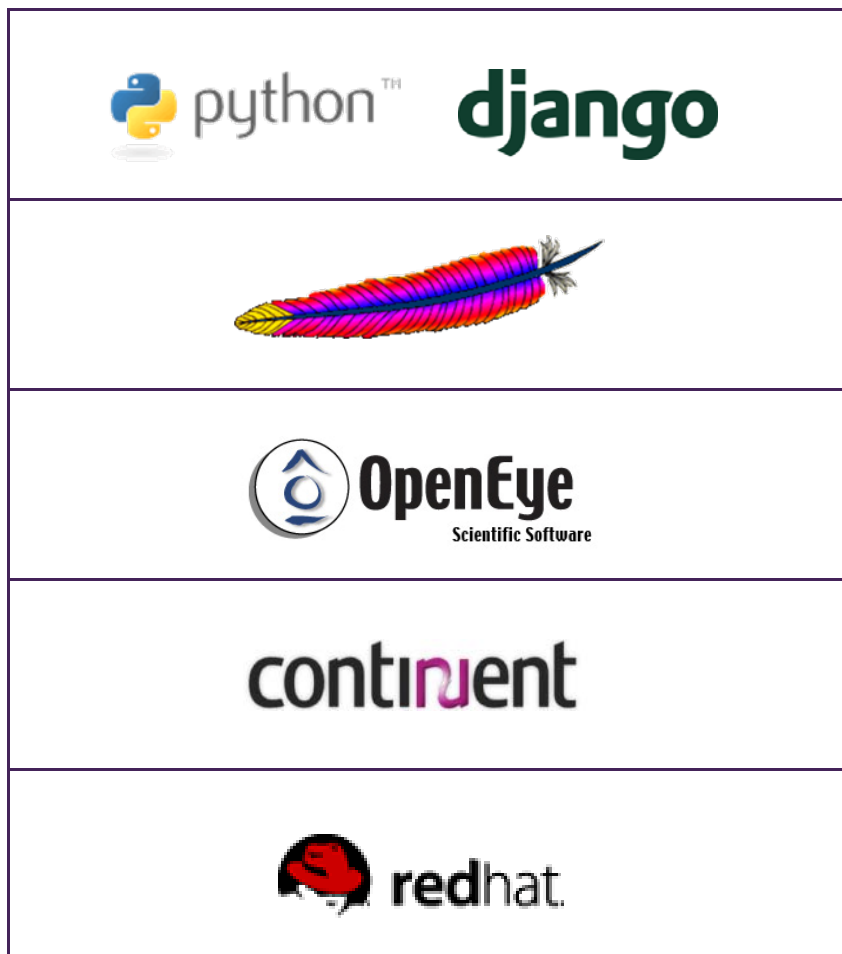
Open source software stack

- LAMP
 - Linux
 - Apache
 - MySQL
 - Python
- Django

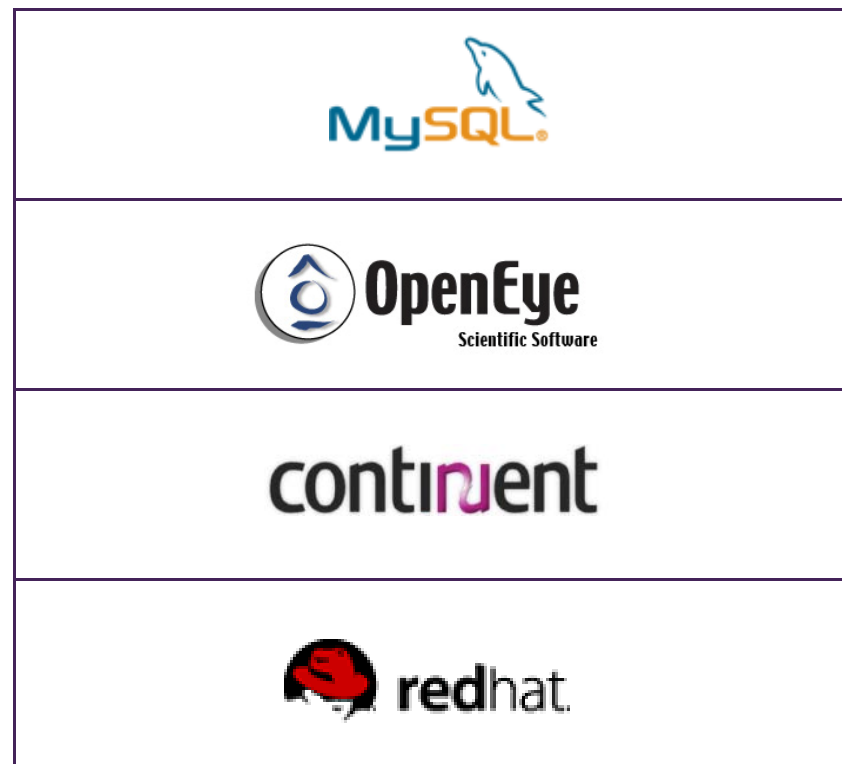


Clustered software stack

Application layer



Database layer



continent

- Data Management
 - High Availability
 - Performance
 - Data protection
-
- Components: Replicator, Connector
 - Master-slave replication

CoDD – Compound Design Database

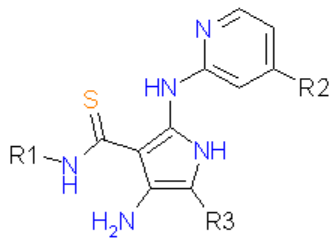
■ Design, Make, Test Cycle

The screenshot shows a Microsoft Internet Explorer browser window displaying the Pretend Project Compound Design Database. The browser title is "Pretend Project Compound Design Database - Cc_wiki - Microsoft Internet Explorer provided by AstraZeneca". The address bar shows the URL: http://apcc1.1.astrazeneca.net/cc_wiki/index.php/Pretend_Project. The browser interface includes a menu bar (File, Edit, View, Favorites, Tools, Help) and a search bar with the Google logo. The website content features a navigation menu on the left with links like "Main Page", "Community portal", "Current events", "Recent changes", "Random page", "Help", and "Donations". The main content area is titled "Pretend Project Compound Design Database" and includes a "Compound Design Database Feedback" link. Below this, there are three columns of links: "CONTENT SUMMARY", "VIRTUAL COMPOUND LIST", "PROGRESS CHART", and "INTERACTIVE VIEW" (all in a green box); "Tracking Summary", "User-Defined Cmpd Matches", "CoDD Training Manual", and "Pretend matchable cmpds" (all in a purple box); and "Pretend Design Team Output", "Install Canvas", "DMT Tool", and "Testing Schedule" (all in a pink box). A paragraph of text explains that the page contains synthesis target ideas and provides instructions on how to add or edit ideas, including a link to Graeme Robb. Below this, there are two bullet points: "Linked files are all stored here" and "Excluding remakes, the highest target ID used so far is: 0 1 7 9 (caution, updated hourly)". At the bottom, there is a "Contents" section with a "hide" link and a list of items: "1 Ideas Addressing Potency" and "1.1 Explore P1 market".

Why a wiki?

- Web-based, so no client software to develop
- Easy to prototype
- Fast and easy to use
- Easy to customise for our requirements
- Can handle multiple simultaneous edits
- Always up-to-date
- Has all the history/version features needed
- Can plug in OEChem for added functionality
- It's free

CoDD entry

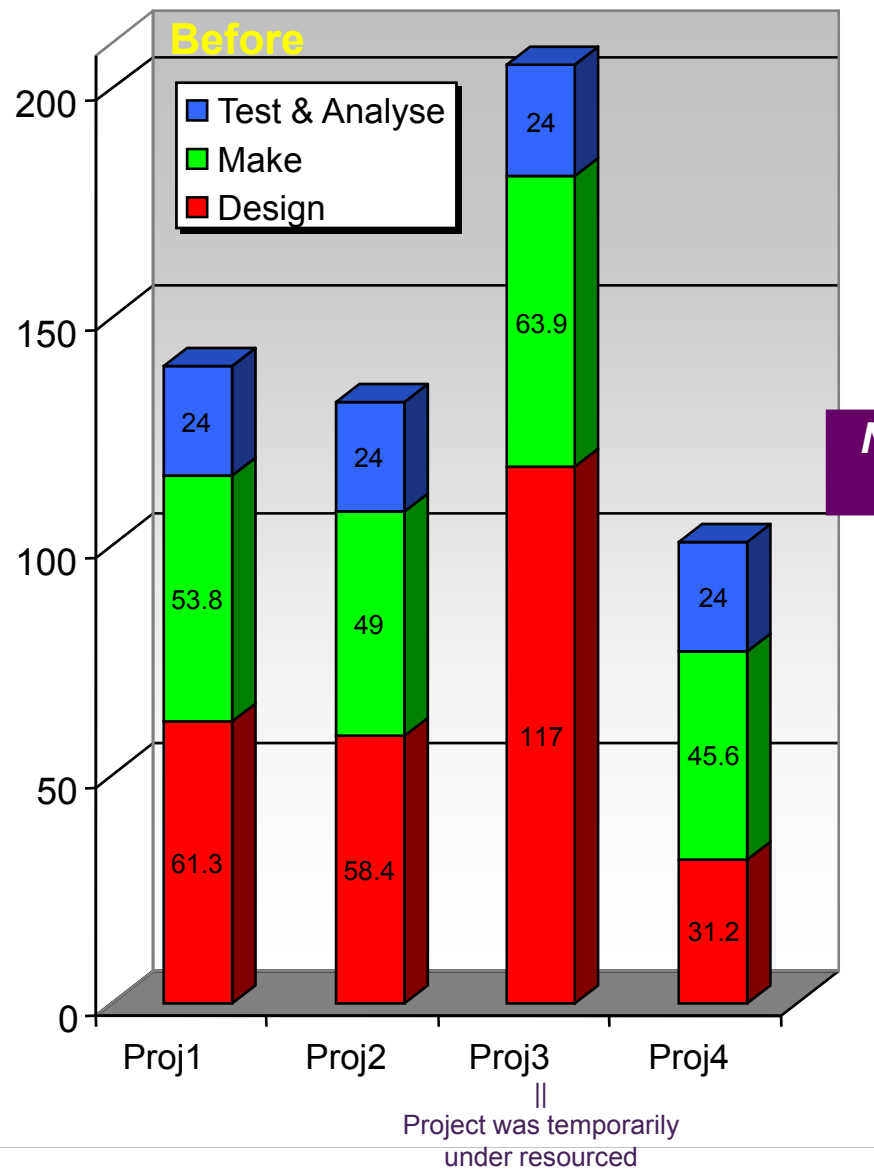
Ideas Addressing Potency [edit]			
Explore P1 pocket [edit]			
DesignSet Number One [edit]			
<i>Project Aim: Increase in-vitro potency</i>			
DBview Link for ID=1			
Date <small>(xx/xx/xx)</small>	Generic Structure	Rationale	Status/Outcome
CONCEPT 10/11/2008	 <p>Where R1 and R2 are small or polar groups.</p>	Docking shows that there is a largely unexplored P1 pocket close to the ligand. Small increases in the size of the groups at R1 or R2 may better fill this pocket to give greater potency. {J.Bloggs}	Priority = 2
STARTED 15/11/2008		Polar groups may be preferred as these may pick up an additional interaction in the P1 pocket while keeping physprops in the right area. {C.Smith}	Status = In Progress
COMPLETION		This is all pretend and just an example of what you might write in order to share your ideas and form a basis for discussion. You can also include links to supporting data.	Chemist = Geoff
Upload SMILES			Chemist comments

CoDD

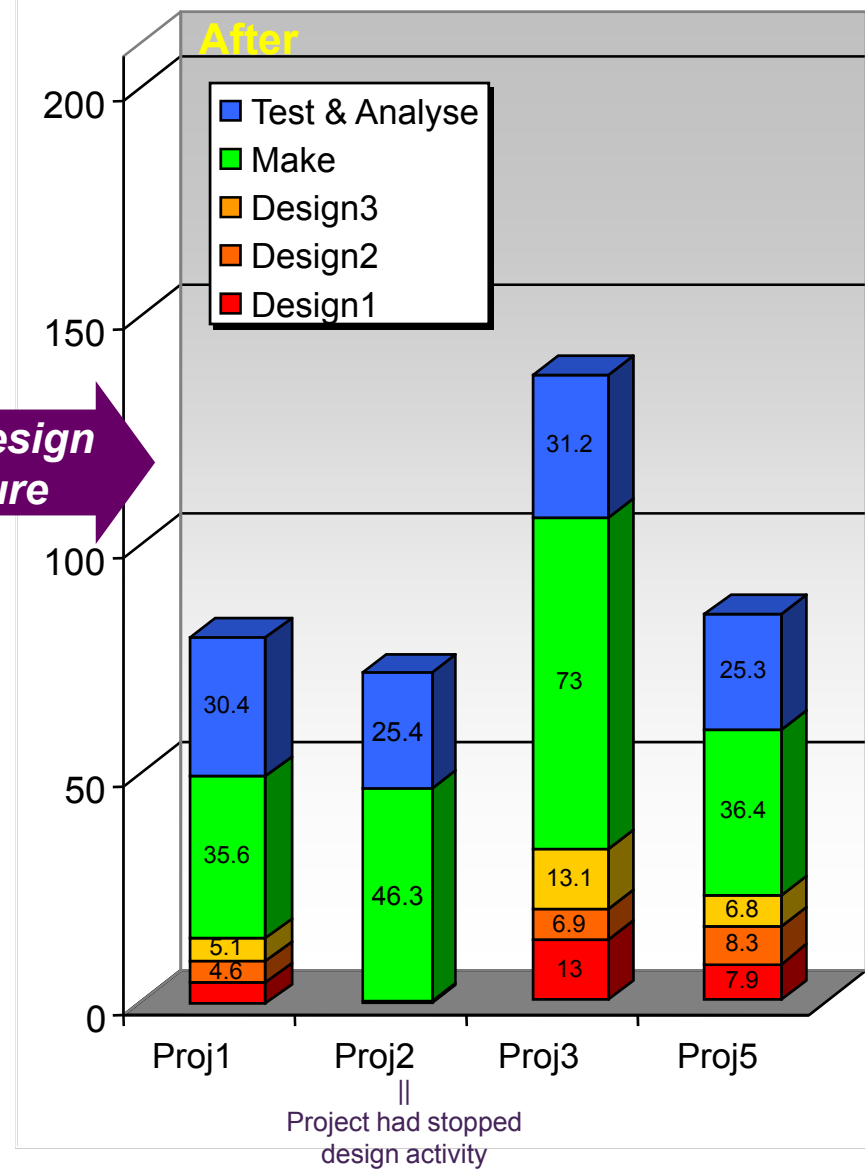
- Collaboration between designers and chemists
- More than a wiki (external reports)
- Keeps track and organises
- Crucially, does not **design** for you
- Time spent on design reduces

Real value

- Mean Time spent on each DesignSet (set of compounds) for 5 projects in LO



New Design Culture →



CoDD - Perl

System CoDD Progress Chart

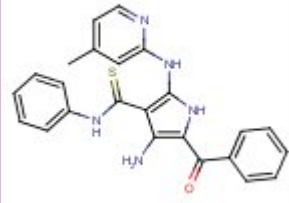
DesignSet Synthesis Completion Rate: last month = 1.4 / week, previous month = 0.9 / week.

COLOUR BY: SECTION / TECHNICAL RISK / PRIORITY

NON-DESIGN TARGETS: INCLUDE / EXCLUDE

RETURN TO: CoDD PROJECT PAGE

New (20)	In Design (0<= 3 =>5)	Design Locked (1<= 2 =>3)	Work in Progress (6)	Synthesis Complete (7)	Analysis Complete (73)
<p>100: 100% complete</p> <p>101: 100% complete</p> <p>102: 100% complete</p> <p>103: 100% complete</p> <p>104: 100% complete</p> <p>105: 100% complete</p> <p>106: 100% complete</p> <p>107: 100% complete</p> <p>108: 100% complete</p> <p>109: 100% complete</p> <p>110: 100% complete</p> <p>111: 100% complete</p> <p>112: 100% complete</p> <p>113: 100% complete</p> <p>114: 100% complete</p> <p>115: 100% complete</p> <p>116: 100% complete</p> <p>117: 100% complete</p> <p>118: 100% complete</p> <p>119: 100% complete</p> <p>120: 100% complete</p>	<p>121: 100% complete</p> <p>122: 100% complete</p> <p>123: 100% complete</p> <p>124: 100% complete</p> <p>125: 100% complete</p> <p>126: 100% complete</p> <p>127: 100% complete</p> <p>128: 100% complete</p> <p>129: 100% complete</p> <p>130: 100% complete</p> <p>131: 100% complete</p> <p>132: 100% complete</p> <p>133: 100% complete</p> <p>134: 100% complete</p> <p>135: 100% complete</p> <p>136: 100% complete</p> <p>137: 100% complete</p> <p>138: 100% 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Amide isosteres (27/6)</p> <p>169: Amide isosteres (28/6)</p> <p>170: Amide isosteres (29/6)</p> <p>171: Amide isosteres (30/6)</p>	<p>172: Amide isosteres (31/6)</p> <p>173: Amide isosteres (32/6)</p> <p>174: Amide isosteres (33/6)</p> <p>175: Amide isosteres (34/6)</p> <p>176: Amide isosteres (35/6)</p> <p>177: Amide isosteres (36/6)</p> <p>178: Amide isosteres (37/6)</p> <p>179: Amide isosteres (38/6)</p> <p>180: Amide isosteres (39/6)</p> <p>181: Amide isosteres (40/6)</p> <p>182: Amide isosteres (41/6)</p> <p>183: Amide isosteres (42/6)</p> <p>184: Amide isosteres (43/6)</p> <p>185: Amide isosteres (44/6)</p> <p>186: Amide isosteres (45/6)</p> <p>187: Amide isosteres (46/6)</p> <p>188: Amide isosteres (47/6)</p> <p>189: Amide isosteres (48/6)</p> <p>190: Amide isosteres (49/6)</p> <p>191: Amide isosteres (50/6)</p> <p>192: Amide isosteres (51/6)</p> <p>193: Amide isosteres (52/6)</p> <p>194: Amide isosteres (53/6)</p> <p>195: Amide isosteres (54/6)</p> <p>196: Amide isosteres 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Amide isosteres (84/6)</p> <p>226: Amide isosteres (85/6)</p> <p>227: Amide isosteres (86/6)</p> <p>228: Amide isosteres (87/6)</p> <p>229: Amide isosteres (88/6)</p> <p>230: Amide isosteres (89/6)</p> <p>231: Amide isosteres (90/6)</p> <p>232: Amide isosteres (91/6)</p> <p>233: Amide isosteres (92/6)</p> <p>234: Amide isosteres (93/6)</p> <p>235: Amide isosteres (94/6)</p> <p>236: Amide isosteres (95/6)</p> <p>237: Amide isosteres (96/6)</p> <p>238: Amide isosteres (97/6)</p> <p>239: Amide isosteres (98/6)</p> <p>240: Amide isosteres (99/6)</p> <p>241: Amide isosteres (100/6)</p>	<p>242: Amide isosteres (101/6)</p> <p>243: Amide isosteres (102/6)</p> <p>244: Amide isosteres (103/6)</p> <p>245: Amide isosteres (104/6)</p> <p>246: Amide isosteres (105/6)</p> <p>247: Amide isosteres (106/6)</p> <p>248: Amide isosteres (107/6)</p> <p>249: Amide isosteres (108/6)</p> <p>250: Amide isosteres (109/6)</p> <p>251: Amide isosteres (110/6)</p> <p>252: Amide isosteres (111/6)</p> <p>253: Amide 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(167/6)</p> <p>309: Amide isosteres (168/6)</p> <p>310: Amide isosteres (169/6)</p> <p>311: Amide isosteres (170/6)</p> <p>312: Amide isosteres (171/6)</p> <p>313: Amide isosteres (172/6)</p> <p>314: Amide isosteres (173/6)</p> <p>315: Amide isosteres (174/6)</p> <p>316: Amide isosteres (175/6)</p> <p>317: Amide isosteres (176/6)</p> <p>318: Amide isosteres (177/6)</p> <p>319: Amide isosteres (178/6)</p> <p>320: Amide isosteres (179/6)</p> <p>321: Amide isosteres (180/6)</p> <p>322: Amide isosteres (181/6)</p> <p>323: Amide isosteres (182/6)</p> <p>324: Amide isosteres (183/6)</p> <p>325: Amide isosteres (184/6)</p> <p>326: Amide isosteres (185/6)</p> <p>327: Amide isosteres (186/6)</p> <p>328: Amide isosteres (187/6)</p> <p>329: Amide isosteres (188/6)</p> <p>330: Amide isosteres (189/6)</p> <p>331: Amide isosteres (190/6)</p> <p>332: Amide isosteres (191/6)</p> <p>333: Amide isosteres (192/6)</p> <p>334: Amide isosteres (193/6)</p> <p>335: Amide isosteres (194/6)</p> <p>336: Amide isosteres (195/6)</p> <p>337: Amide isosteres (196/6)</p> <p>338: Amide isosteres (197/6)</p> <p>339: Amide isosteres (198/6)</p> <p>340: Amide isosteres (199/6)</p> <p>341: Amide isosteres (200/6)</p>	



CoDD v2 – Design Tracker

- MediaWiki base not suitable
- Developed by a sole computational chemist over 6 months
- Dedicated Django application is now in global use
- 500 users
- Something for everybody

Internal Wiki - PHP

- `<smiles>O[C@@H](/C=C/c1c(nc(nc1c1ccc(F)cc1)N(C)S(=O)(=O)C)C(C)C)[C@@H](O)CC(=O)O|400|Crestor</smiles>`

- MediaWiki Extension
- Via Python
- Internal database links

The screenshot shows a MediaWiki page titled "Test" with a sub-header "Crestor". The page features a navigation bar with tabs for "article", "discussion", "edit", "history", "protect", "delete", "move", and "watch". Below the navigation bar is a chemical structure of Crestor (rosuvastatin calcium). The structure is a complex molecule with a pyrimidine ring system, a piperidine ring, and a carboxylic acid group. The chemical structure is rendered in a 3D-like perspective with various colors (blue, red, black) for different atoms and bonds. To the left of the main content area, there is a sidebar with a "navigation" section containing links to "Main Page", "Community portal", "Current events", "Recent changes", "Categories", "Random page", and "Help". Below the navigation section is a "search" section with a search input field and "Go" and "Search" buttons. At the bottom of the sidebar is a "toolbox" section with links to "What links here", "Related changes", "Upload file", "Special pages", "Printable version", and "Permanent link".

Hash Codes for the Identification and Classification of Molecular Structure Elements

WOLF DIETRICH IHLENFELDT

Department of Knowledge-Based Information Engineering, Toyohashi University of Technology, Tempaku, Toyohashi 441, Japan

JOHANN GASTEIGER*

Institut für Organische Chemie, Technical University Munich, 85748 Garching, Germany

Received 15 July 1993; accepted 12 August 1993

- Implemented as MySQL UDF
- C Toolkit
- Now available as Python web service as well
- Speed comparable

OEHash python wrapper

```
from openeye.oechem import *
from oehashnum import *

mol1=OEGraphMol()
OEParseSmiles( mol1 , "BrC1CCCCC1CCBr" )

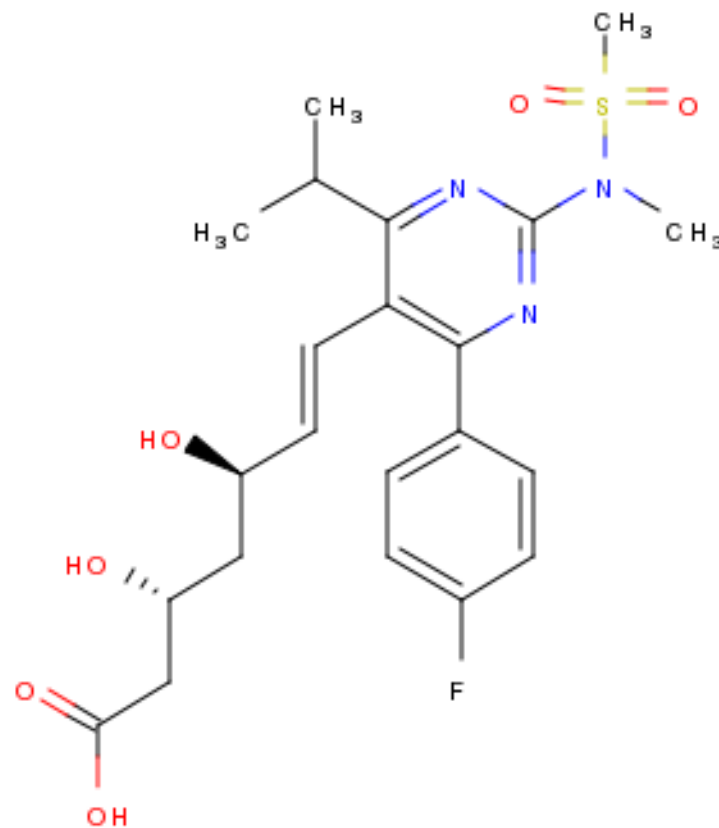
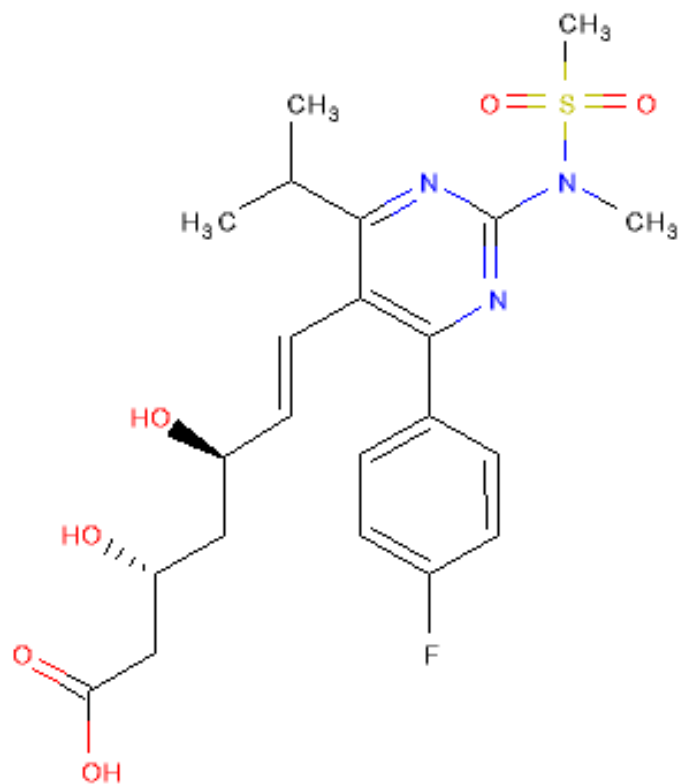
mol2=OEGraphMol()
OEParseSmiles( mol2 , "BrCCCc1CCCCC1Br" )

oehashnum1 = OEHashNum( mol1 , Normalize )
oehashnum2 = OEHashNum( mol2 , Normalize )

>>> They're the same : 3049543336433740395
```

Improved depictions

- Currently GIFs, PNG available via



Hivemind to the rescue

The screenshot shows a forum post on the OpenEye Scientific Software website. The post title is "Increase the thickness of bonds in depictions". The question asks if it's possible to increase the thickness of bonds/atoms, as the user can't find a method in either API. The post is tagged with "oedepict", "python", "c++", and "ogham". It was asked by Craig Bruce on Feb 19 at 18:47. There is one answer by Bob Tolbert on Feb 22 at 18:23. The answer explains that in C++, using Ogham 1.*, there is no way to increase the thickness of the lines, but a new implementation in Python (with PyCairo) or in Java (using the built-in Graphics2D) can adjust line thickness. It also provides an example in Java in v1.7.2 and mentions that Ogham 2.0 will include line thickness among other new features. The right sidebar shows the post is tagged with python (5), oedepict, c++, and ogham. It was asked 2 months ago, viewed 27 times, and has latest activity 2 months ago. There are also links for education (sign up for an OpenEye training course) and new products (ROCS/MROCS, MolProp TK, GraphSim TK).

Craig Bruce 47 | log out | FAQ | Documentation | Training | OpenEye

OpenEye Scientific Software

Questions Tags Users Badges Unanswered Ask Question

Increase the thickness of bonds in depictions

Is it possible to increase the thickness of bonds/atoms? I can't find a method in either API to allow this.

1

oedepict python c++ ogham

edit | delete | flag

add comment

asked Feb 19 at 18:47

Craig Bruce 47 | 3

1 Answer

oldest newest votes

2

In C++, using Ogham 1.*, there is no way to increase the thickness of the lines. However, if you derive a new implementation in Python (with PyCairo for example) or in Java (using the built-in Graphics2D), you can adjust line thickness in your DrawLine functions.

There is an example in Java in v1.7.2 in both Mol2Img.java and JavaDepict.java. These use a class called Java2DDepiction.java that derives from OEDepictBase and provides native Java drawing that includes thicker lines, Java fonts and anti-aliasing.

In Ogham 2.0, due out later this year, we are re-writing the core classes to include line thickness among many other new features.

link

answered Feb 22 at 18:23

Bob Tolbert 36 | 1

tagged

python x 5

oedepict

c++

ogham

asked

2 months ago

viewed

27 times

latest activity

2 months ago

Education

[Sign up for an OpenEye training course.](#)

New Products

- ROCS/MROCS
- MolProp TK
- GraphSim TK

Internet | Protected Mode: Off 100%

Conclusions

- OEChem/Python toolkit opens web door
- Build your own Python wrappers to C code
- Flexible across multiple programming languages
- Scalable over high availability clusters and hundreds of users

Acknowledgements

- Richard Hall
- Huw Jones
- Dave Cosgrove
- Andrew Grant

Questions?