

Who says Java is not fast?!?

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Published December 4, 2008

Citation

Willighagen, E. (2008). Who says Java is not fast?!?. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/j9em9-aad11>

Keywords

Java, Cdk

Abstract

While performance tests actually show that for even core numerical calculations Java is at par with C in terms of speeds, and sometimes even hits Fortran-like speeds, people keep think that Java is not fast. I only invite you to test that yourself.

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chem-bla-ics

While performance tests actually show that for even core numerical calculations Java is at par with C in terms of speeds, and sometimes even hits Fortran-like speeds, people keep think that Java is not fast. I only invite you to test that yourself.

Meanwhile, I would like to take the opportunity to advertise [Noel's cinfony](#) paper in [CCJ](#) (doi:[10.1186/1752-153X-2-24](https://doi.org/10.1186/1752-153X-2-24)) which features these speed measurements (from the paper, CC-BY license):

Table 3 – Performance of Cinfony modules compared to a native Java or C++ implementation.

	Iterate over SDF		Iterate and calculate molecular weight	
	Time (s)	Normalised	Time (s)	Normalised
CDK				
Native Java	21.2	1.00	36.8	1.00
<i>cdkjython</i>	23.1	1.09	41.6	1.13
<i>cdkjpype</i>	33.0	1.57	69.5	1.89
OpenBabel				
Native C++	31.9	1.00	43.0	1.00
<i>pybel</i>	34.1	1.07	45.1	1.05
<i>pybel</i>	38.0	1.19	49.6	1.15
RDKit				
Native C++	99.7	1.00	100.7	1.00
<i>rdkit</i>	99.9	1.00	101.0	1.00

The times reported are wallclock times from the best of three runs on a dual-core Intel Pentium 4 3.2 GHz machine with 1GB RAM.

I have to say that these numbers surprised me, as the [CDK](#) is hardly optimized for speed at al...