BlueObelisk StackExchange: summary of the first month

Egon Willighagen ⬤

Published December 21, 2009

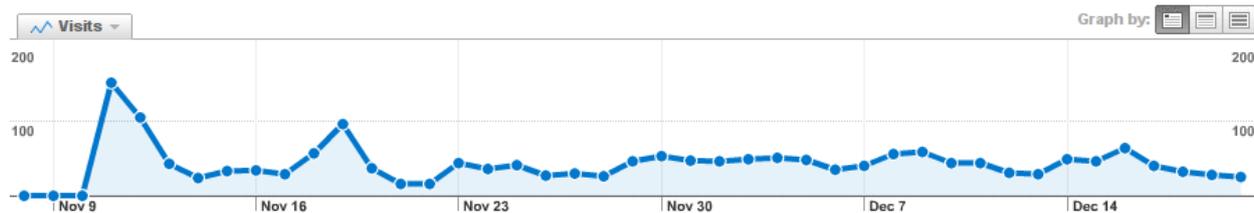**Citation**

Willighagen, E. (2009). BlueObelisk StackExchange: summary of the first month. In *chem-bla-ics*. chem-bla-ics. https://doi.org/10.59350/x958j-0xm21

Copyright

chem-bla-ics

The Blue Obelisk StackExchange (BO$_x$) has seen a relatively good start, but the number of questions is dropping. The average number of unique visits is about 23-30 now:

The number of registered users is not insignificant but also has not been growing much lately:

At the same time, the quality of the questions are high, and have real users questions:

· Good way to produce a table of R-groups (yet unanswered!)
· Is there an open source pKa or LogD tool available
· Easiest way to align two molecules from the command line?

The overall state is 37 questions with about 50 different tags :

howto × 7	python × 2	logd	bioclipse	graphics
cdk × 6	structure × 2	logp	alignment	gromacs
cheminformatics × 5	terminology	mdl	analysis	
blueobelisk × 5	visualization	member	cinfony	
opendata × 5	web-service	info	cluster	
opensource × 5	what-odosos-cannot-do	bodr	copyright	
meta × 5	xml	boiling-point	crystal	
openstandards × 4	rgroup	mol-file	design	
cml × 3	science	ontologies	dinner	
automation × 2	sdf	openbabel	discussions	
pka × 2	smiles	proteins	docking	
molecules × 2	moleculardynamics	psa	drug	
inchi × 2	jnati	publishing	dynamics	
java × 2	license	benzene	forum	

chem-bla-ics

To the make progress with BO$_x$, we primarily need to promote it more as central point of entry to people who want to know what *free* tools they can use to perform there need, and to the people who want to contribute to *ODOSOS cheminformatics*, by pointing out the unsolved problems.