



Grid Application Portal

Logged in user: gn

Virtual Screening

Job Management

User Information

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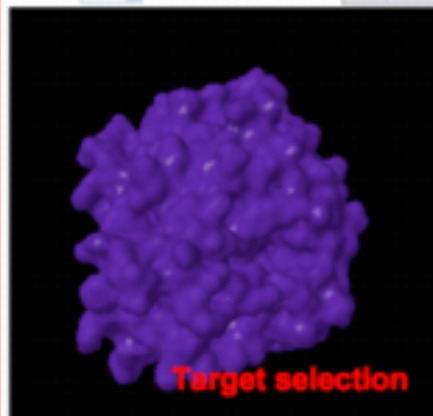
Description

Parameter: AutoSubDockParameter (qt/tygh/and)

view parameter

Mass of file: 101.000

view parameter



Target selection

Compound selection

No filter rule

filter

select all

deselect all

submit to Grid

Legend Table

select

file_name

script

101.000

101.000



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Initial Translation, Quaternion and Torsion Step Sizes

Translation step (Å):

1.0

Quaternion stepping:

50.0

Torsion stepping:

10.0

Translation reduction factor / per cycle:

1

Quaternion reduction factor / per cycle:

1

Torsion reduction factor / per cycle:

1

Docked Conformation Clustering Parameters for "analysis" command

Cluster tolerance (Angstroms):

1.0

External grid energy:

1000

Maximum allowable initial energy:

0

maximum number of retries: 10000

Genetic Algorithm (GA) and Lamarckian Genetic Algorithm Parameters

Number of individuals in population:

50

Maximum number of energy evaluations:

210000

Maximum number of generations:

27000

Number of top individuals that automatically survive:

1

Rate of Gene mutation:

0.02

Rate of Crossover:

0.80

Job Details

id	submittedTime	startedTime	finishedTime	completing element	status	view results	output sandbox	resultant	energy	pdf
de2ee3cb1115494a007	2007-03-15 07:51:47 GMT	2007-03-15 07:52:28 GMT	2007-03-15 07:59:03 GMT	querts grid once reduce	DONE	Please drop down	download	resultant	-9.44	view
de2ee3cb1115494a005	2007-03-15 07:51:47 GMT	2007-03-15 07:52:29 GMT	2007-03-15 07:59:30 GMT	querts grid once reduce	DONE	Please drop down	download	resultant	-10.29	view
de2ee3cb1115494a006	2007-03-15 07:51:48 GMT	2007-03-15 07:52:08 GMT	2007-03-15 07:59:36 GMT	querts grid once reduce	DONE	Please drop down	download	resultant	-11.19	view
de2ee3cb1115494a004	2007-03-15 07:51:45 GMT	2007-03-15 07:52:09 GMT	2007-03-15 07:59:31 GMT	querts grid once reduce	DONE	Please drop down	download	resultant	-7.41	view

Job history table

Complex visualization

Docking parameter setter

GA or LGA rule

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