

Maestro - brukinsa.prj

Quick Select: P L S ... All

Fit: AUTO

TABLE JOBS TASKS

Ligand Interaction 2D Sketcher Protein Preparation Surface (Binding Si) Minimize Selected A Quick Align Measure

Workspace Navigator

ENTRY LIST

Row	In	Title	glide gscore
		▶ OPLS4 Glide (2)	
		▶ BTK_ligands2dock_noprep (54)	
		▶ BTK_ligands2dock_set2_noprep (4)	
		▶ BTK_ligands2dock_820_patent_noprep (4)	
		▶ BTK_opls5_ligands2dock_ligprep (54)	
		▶ BTK_opls5_ligands2dock_set2_ligprep (4)	
		▶ BTK_opls5_ligands2dock_820_patent_ligprep...	
		▶ Glide Docking 2024.10.03 screen grabs (16)	
	1	▼ Glide Docking 2024.10.03 (265)	
		▶ 3GEN_c481a_ibrutinib_lib (5)	
		▶ 3GEN_c481a_ibrutinib_p-MA_lib (5)	
		▶ 3GEN_c481a_brukinsa_lib (5)	
		▶ 3GEN_c481a_W02014173289_cmpnd81_lib (5)	
		▶ 3GEN_c481a_W02016007185_cmpnd9_lib (5)	
		▶ 3GEN_c481a_W02016007185_cmpnd2_lib (5)	
		▶ 3GEN_c481a_803_patent_formulaE_struct3...	
		▶ 3GEN_c481a_803_patent_formulaE_struct4...	
		▶ 3GEN_c481a_446_patent_ex2024_cmpnd20_l...	
		▶ 3GEN_c481a_446_patent_ex2024_cmpnd30_l...	
	1	▼ 3GEN_c481a_446_patent_ex2024_cmpnd122_...	
193	●	3GEN_c481a_446_patent_ex2024_cmpnd122	-8.679
194	○	3GEN_c481a_446_patent_ex2024_cmpnd122	-8.283
195	○	3GEN_c481a_446_patent_ex2024_cmpnd122	-8.258
196	○	3GEN_c481a_446_patent_ex2024_cmpnd122	-8.052
197	○	3GEN_c481a_446_patent_ex2024_cmpnd122	-7.944
		▶ 3GEN_c481a_zhang_ex2063_cmpnd7_lib (5)	
		▶ 3GEN_c481a_zhang_ex2063_cmpnd8_lib (5)	
		▶ 3GEN_c481a_zhang_ex2063_cmpnd10_lib (5)	
		▶ 3GEN_c481a_zhang_ex2063_cmpnd11_lib (5)	
		▶ 3GEN_c481a_ghose_ex1052_cmpnd1_lib (5)	
		▶ 3GEN_c481a_ghose_ex1052_cmpnd1a_lib (5)	
		▶ 3GEN_c481a_ghose_ex1052_cmpnd2_lib (5)	
		▶ 3GEN_c481a_ghose_ex1052_cmpnd2a_lib (5)	
		▶ 3GEN_c481a_ghose_ex1052_cmpnd3_lib (5)	

STRUCTURE HIERARCHY

Current Selection

Entries: 517 total, 0 selected, 2 included

SELECTED 0 atoms 0 residues | ATOMS 4367 CHAINS 2 ENTRIES 2 |
DISPLAYED 183 of 4367 17 of 265 | RESIDUES 265 MOLS 3 CHARGE -7

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ATOMS

Quick Select:

P

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All

Invert

Expand

Fit: AUTO

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STYLE

PRESETS

BUILD

TABLE

JOBS

TASKS

Ligand Interaction

2D Sketcher

Protein Preparation

Surface (Binding Si

Minimize Selected A

Quick Align

Measure

Workspace Navigator

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▼ 1 Glide Docking 2024.10.03 (265)

▶ 3GEN_c481a_ibrutinib_lib (5)

▶ 3GEN_c481a_ibrutinib_p-MA_lib (5)

▶ 3GEN_c481a_brukinsa_lib (5)

▶ 3GEN_c481a_W02014173289_cmpnd81_lib (5)

▶ 3GEN_c481a_W02016007185_cmpnd9_lib (5)

▶ 3GEN_c481a_W02016007185_cmpnd2_lib (5)

▶ 3GEN_c481a_803_patent_formulaE_struct3...

▶ 3GEN_c481a_803_patent_formulaE_struct4...

▶ 3GEN_c481a_446_patent_ex2024_cmpnd20_l...

▶ 3GEN_c481a_446_patent_ex2024_cmpnd30_l...

▼ 1 3GEN_c481a_446_patent_ex2024_cmpnd122_...

193 3GEN_c481a_446_patent_ex2024_cmpnd122

194 3GEN_c481a_446_patent_ex2024_cmpnd122

195 3GEN_c481a_446_patent_ex2024_cmpnd122

196 3GEN_c481a_446_patent_ex2024_cmpnd122

197 3GEN_c481a_446_patent_ex2024_cmpnd122

▶ 3GEN_c481a_zhang_ex2063_cmpnd7_lib (5)

▶ 3GEN_c481a_zhang_ex2063_cmpnd8_lib (5)

▶ 3GEN_c481a_zhang_ex2063_cmpnd10_lib (5)

▶ 3GEN_c481a_zhang_ex2063_cmpnd11_lib (5)

▶ 3GEN_c481a_ghose_ex1052_cmpnd1_lib (5)

▶ 3GEN_c481a_ghose_ex1052_cmpnd1a_lib (5)

▶ 3GEN_c481a_ghose_ex1052_cmpnd2_lib (5)

▶ 3GEN_c481a_ghose_ex1052_cmpnd2a_lib (5)

▶ 3GEN_c481a_ghose_ex1052_cmpnd3_lib (5)

glide gscore

−8.679

−8.283

−8.258

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3D View

2D View

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DISPLAYED 183 of 4367 17 of 265

RESIDUES 265 MOLS 3 CHARGE −7

BeiGene Exhibit 1145.002
BeiGene v. Pharmacyclics
PGR2024-00009





