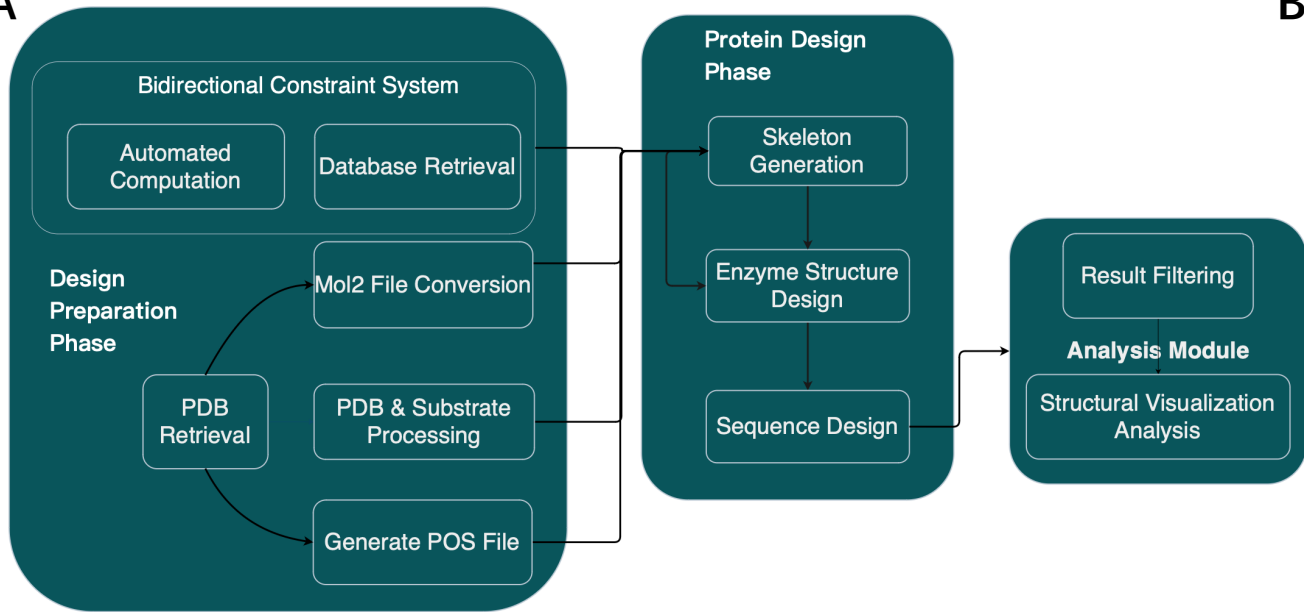


A



B

PyMOL@DL

File Edit Build Movie Display Setting Scenes Mouse Wizard Plugin Help

Residu Zoom Orient Rock resets. uilder. Scenes Draw/R...

binding_site_3.cst
binding_site_2.cst
binding_site_0.cst
binding_site_1.cst
binding_site_1.pdb.gz
binding_site_3.pdb.gz
binding_site_0.pdb.gz
binding_site_2.pdb.gz

download selected

License Expiry date: 25-mar-2050
Detected OpenGL version 4.5. Shaders available
Detected GLSL version 4.50

PyMOL > Click to type in command line

Rosetta Match Plugin@DL

prepare match enzyme_design ligand_mpnn

ligand Parameters: Select File... nyang/plugin/CADED/test/FUD.params

CST File: Select File... g/plugin/CADED/test/binding_site_1.cst

Design PDB File: Select File... /plugin/CADED/test/match_result9.pdb

Run Rosetta Design

Select ScFile bsetta_ui_temp/design_results/score.sc Analysis

	SR_3_all_cst	SR_3_interf E 1 2	SR_3_dsasa 1 2	SR_3_hbond pm/rur		description
0	15.26	29.52	0.93	0.0	...	match_result...
1	15.26	29.54	0.93	0.0	...	match_result...
2	15.26	29.54	0.93	0.0	...	match_result...
3	15.26	29.54	0.93	0.0	...	match_result...
4	15.26	31.49	0.93	0.0	...	match_result...
5	15.26	31.51	0.93	0.0	...	match_result...

Name	Size	Type	Date Modified
match...	433.20 KiB	pdb File	2025/2/25 下午5:01
match...	433.24 KiB	pdb File	2025/2/25 下午5:01
match...	433.20 KiB	pdb File	2025/2/25 下午5:01
match...	433.20 KiB	pdb File	2025/2/25 下午5:01
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match...	433.20 KiB	pdb File	2025/2/25 下午5:02

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