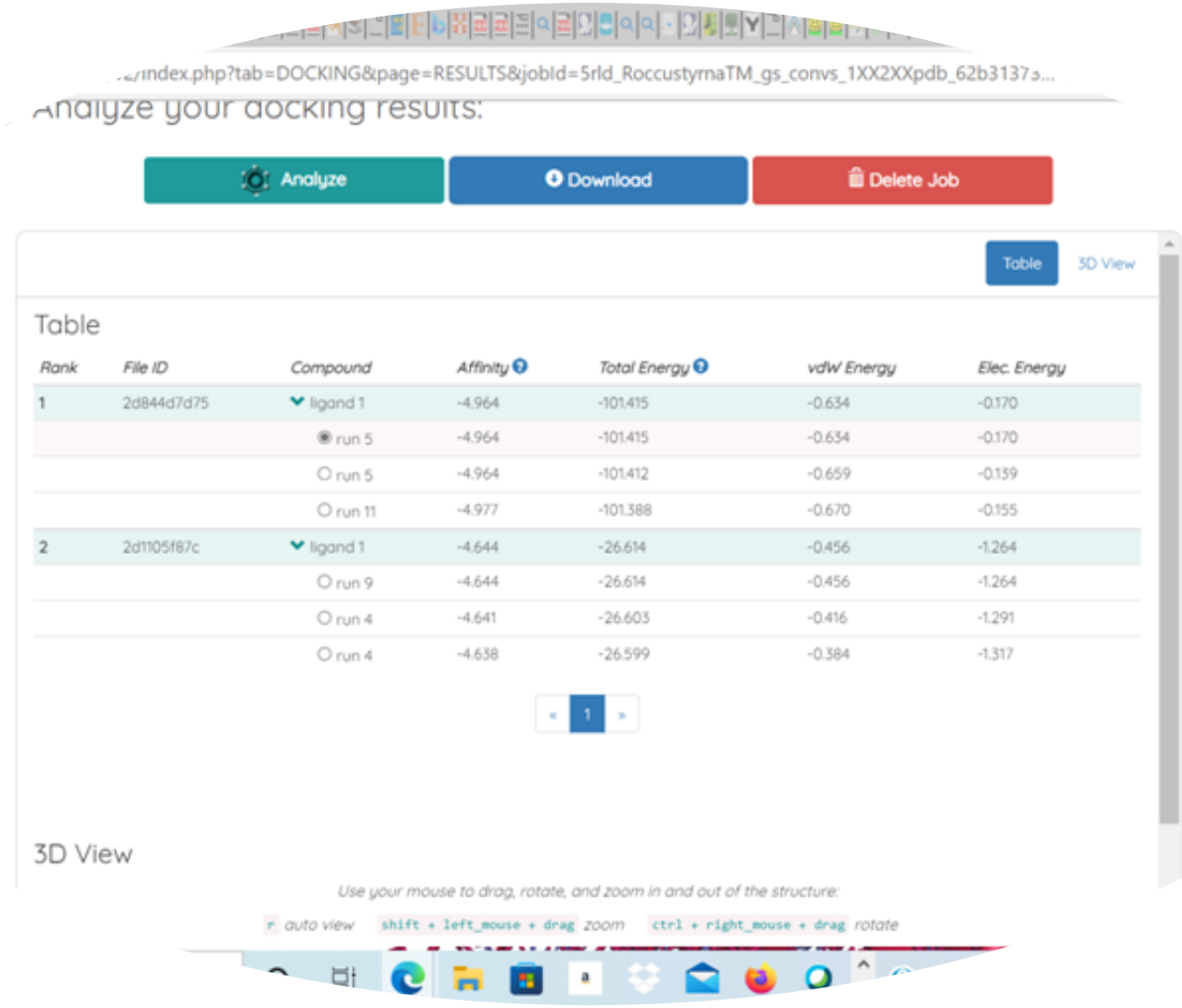
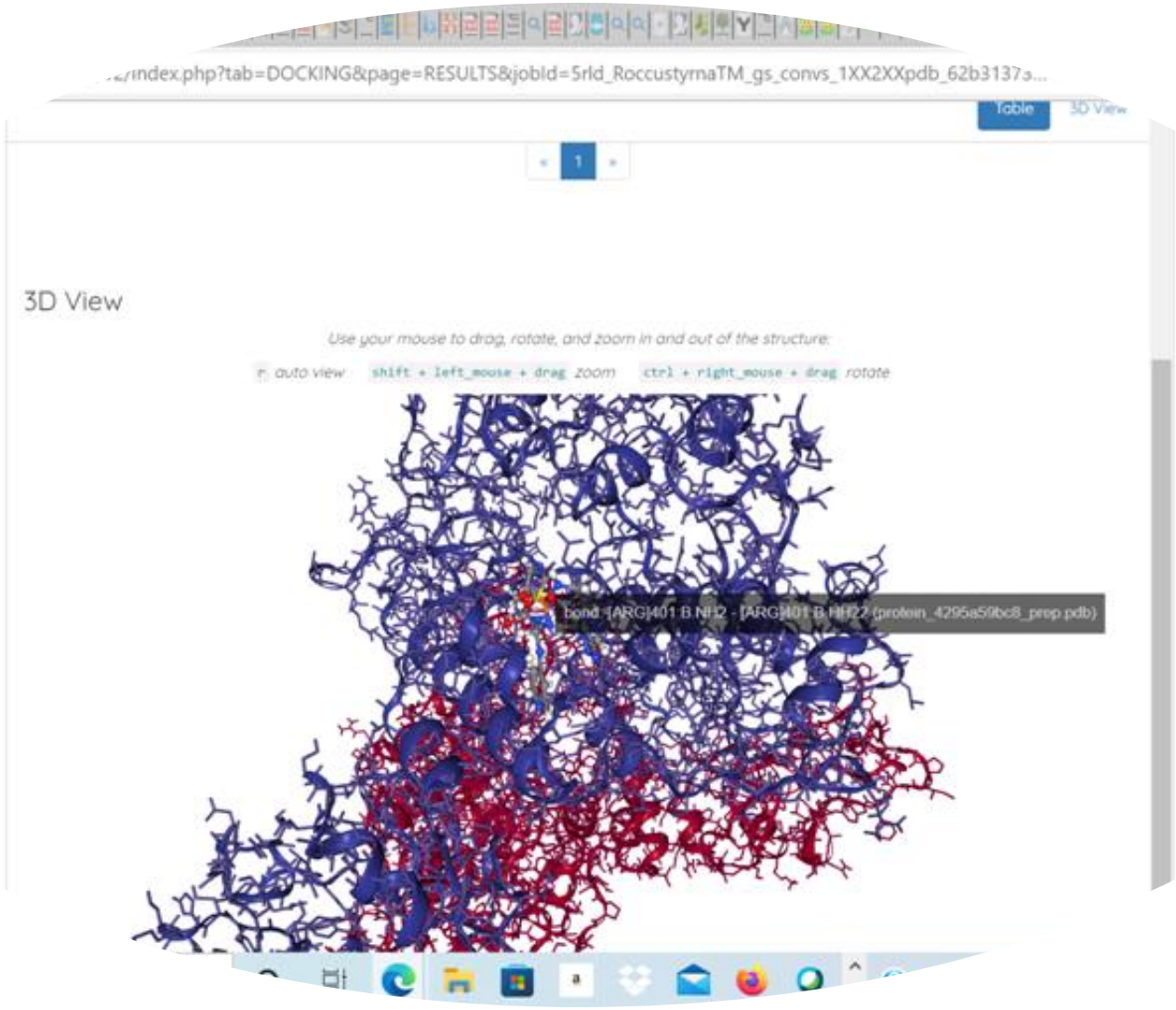
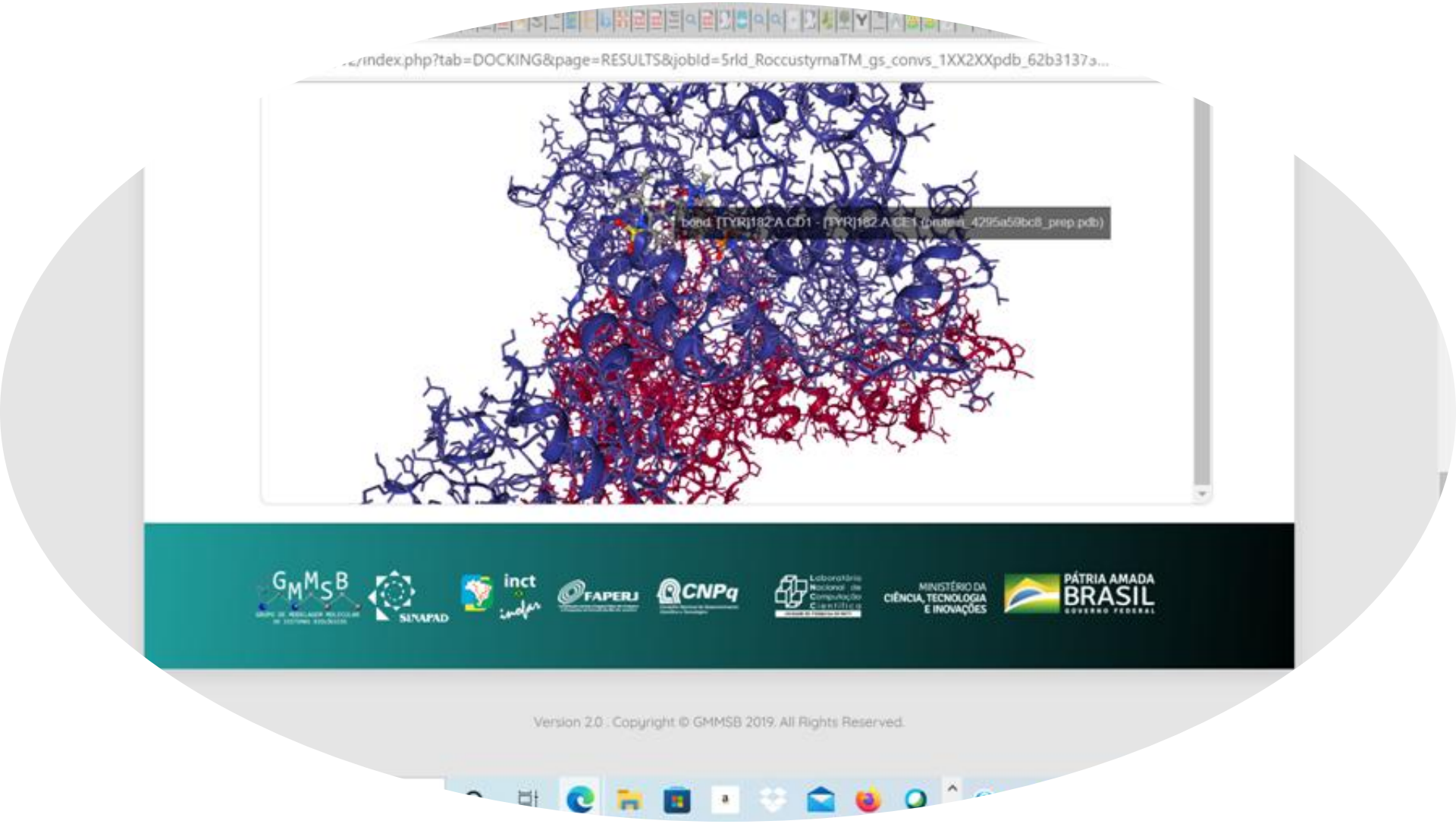

index.php?tab=DOCKING&page=RESULTS&jobId=5rld_RoccustyrnaTM_gs_convs_1XX2XXpdb_62b3137
Analyze your docking results:
Analyze
Download
Delete Job
Table
3D View
Table
Rank
File ID
Compound
Affinity
Total Energy
vdW Energy
Elec. Energy
1
2d844d7d75
ligand 1
-4.964
-101.415
-0.634
-0.170
run 5
-4.964
-101.415
-0.634
-0.170
run 5
-4.964
-101.412
-0.659
-0.139
run 11
-4.977
-101.388
-0.670
-0.155
2
2d1105f87c
ligand 1
-4.644
-26.614
-0.456
-1.264
run 9
-4.644
-26.614
-0.456
-1.264
run 4
-4.641
-26.603
-0.416
-1.291
run 4
-4.638
-26.599
-0.384
-1.317
«
1
»
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure:
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate


index.php?tab=DOCKING&page=RESULTS&jobId=5rld_RoccustyrnaTM_gs_convs_1XX2XXpdb_62b3137a...
Table
3D View
1
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond [ARG]401.B.NH2 - [ARG]401.B.HH22 (protein_4295a59bc8_prep.pdb)


index.php?tab=DOCKING&page=RESULTS&jobId=5rld_RoccustyrnaTM_gs_convs_1XX2XXpdb_62b3137a...
bond [TYR]182:A.CD1 - [TYR]182:A.CE1 (outputs_4295a58bc8_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
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