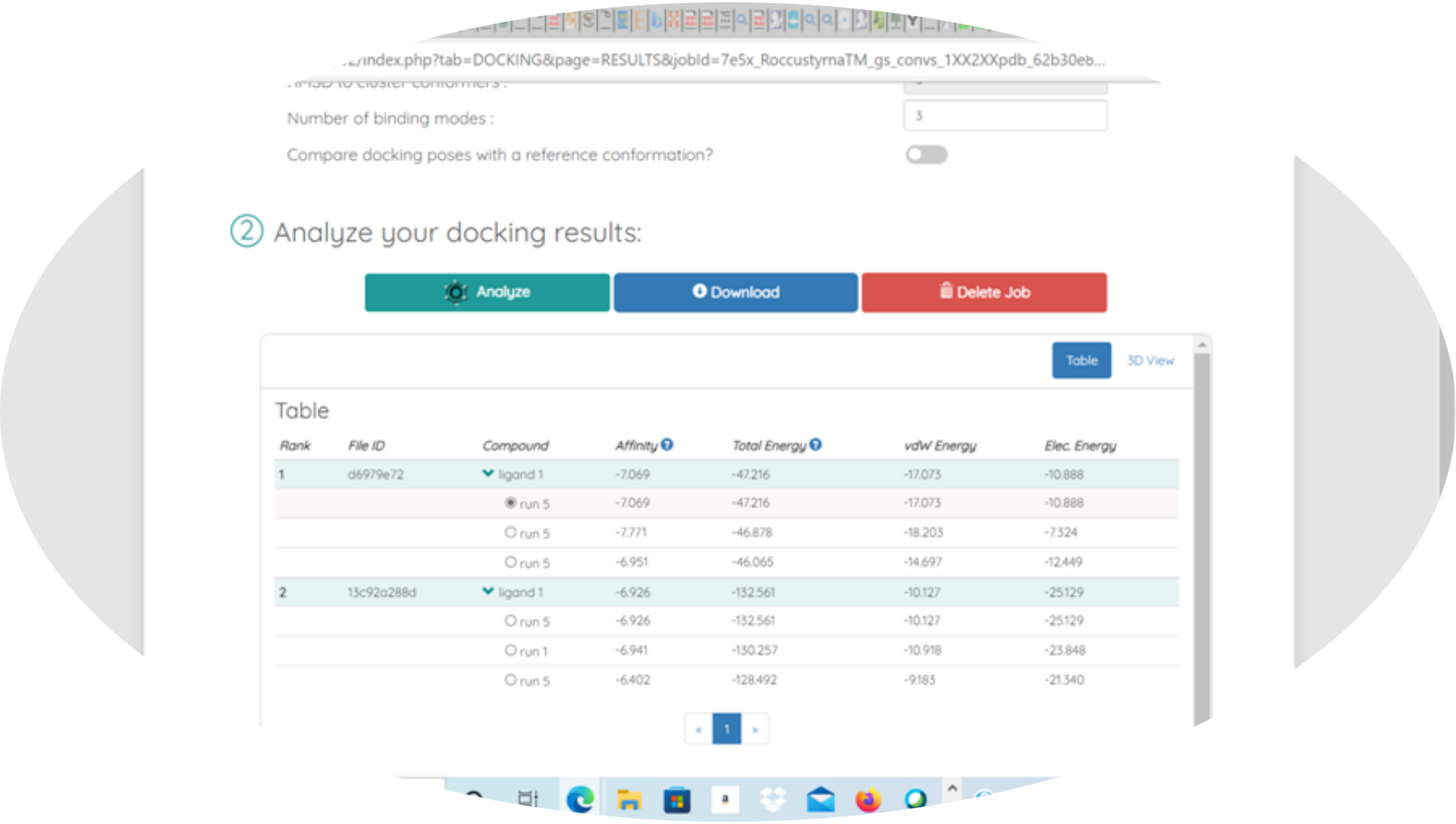
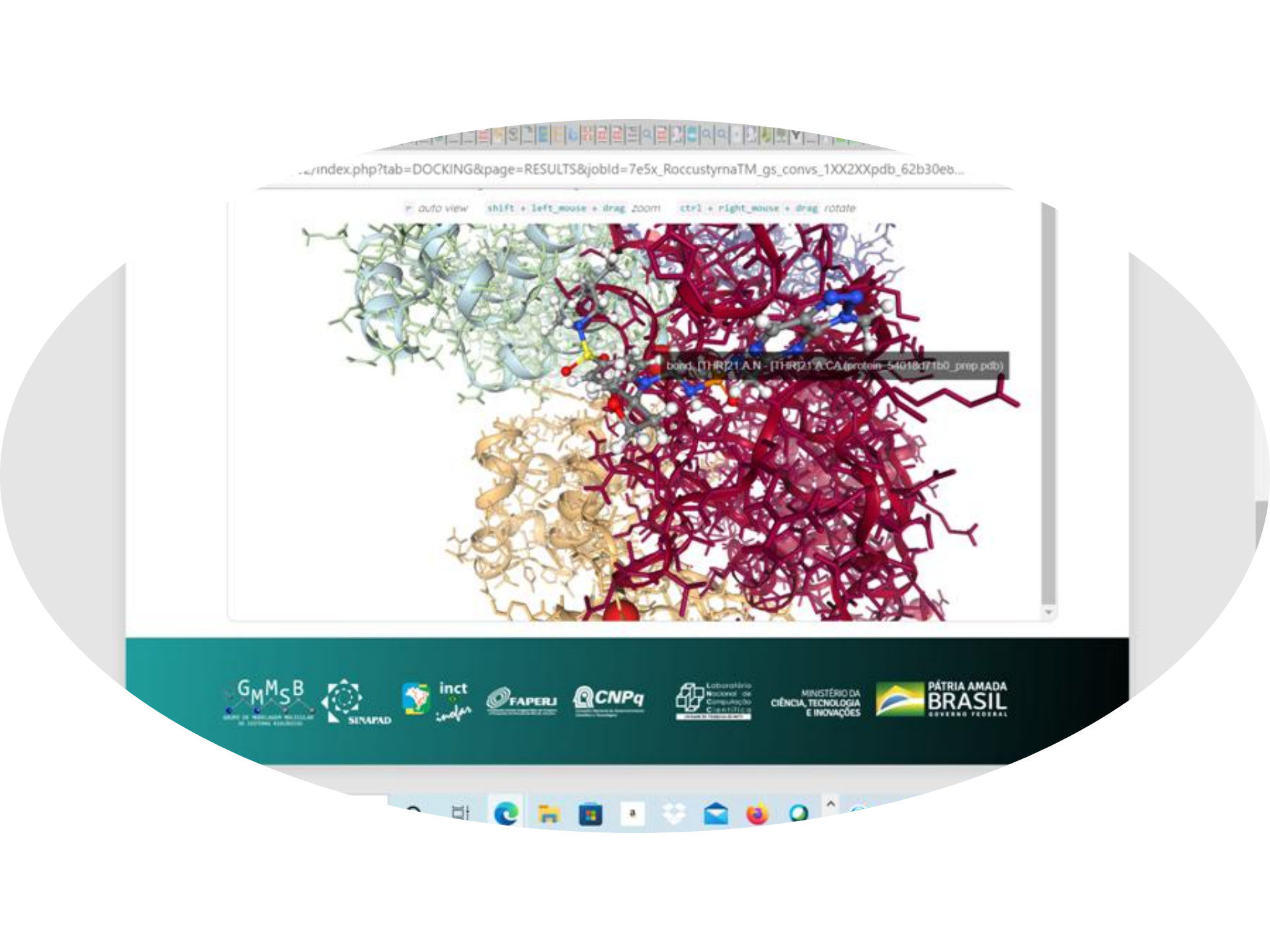
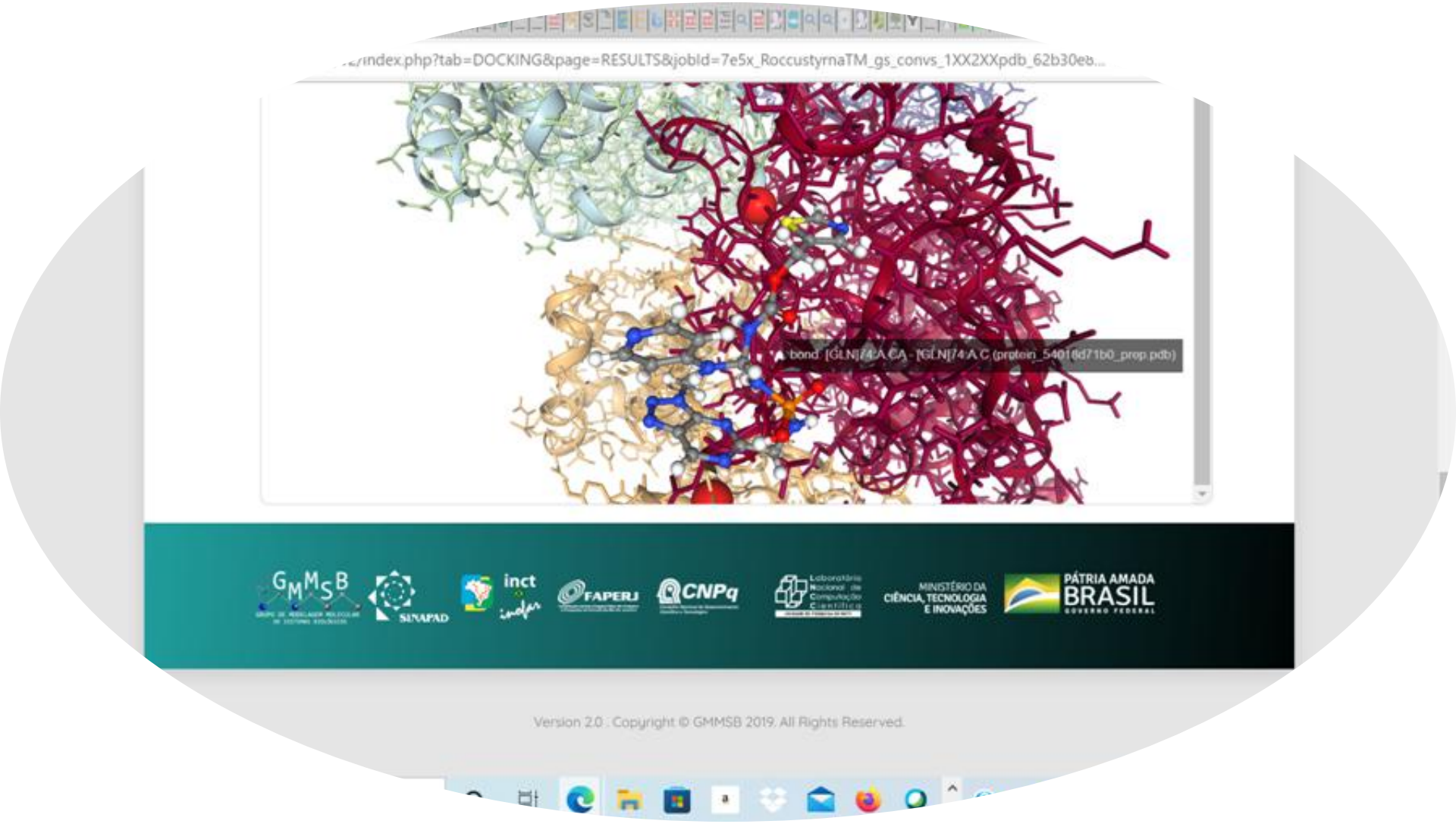

index.php?tab=DOCKING&page=RESULTS&jobId=7e5x_RoccustyrnaTM_gs_convs_1XX2XXpdb_62b30eb...
Number of binding modes :
3
Compare docking poses with a reference conformation?
2 Analyze your docking results:
Analyze
Download
Delete Job
Table
3D View
Table
Rank File ID Compound Affinity Total Energy vdW Energy Elec. Energy
1 d6979e72 ligand 1 -7.069 -47.216 -17.073 -10.888
run 5 -7.069 -47.216 -17.073 -10.888
run 5 -7.771 -46.878 -18.203 -7.324
run 5 -6.951 -46.065 -14.697 -12.449
2 13c92a288d ligand 1 -6.926 -132.561 -10.127 -25.129
run 5 -6.926 -132.561 -10.127 -25.129
run 1 -6.941 -130.257 -10.918 -23.848
run 5 -6.402 -128.492 -9.183 -21.340
1


index.php?tab=DOCKING&page=RESULTS&jobId=7e5x_RoccustyrnaTM_gs_convs_1XX2XXpdb_62b30eb...
auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [THR]21:A:N - [THR]21:A:CA (protein: 54018d71b0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
GOVERNO FEDERAL



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