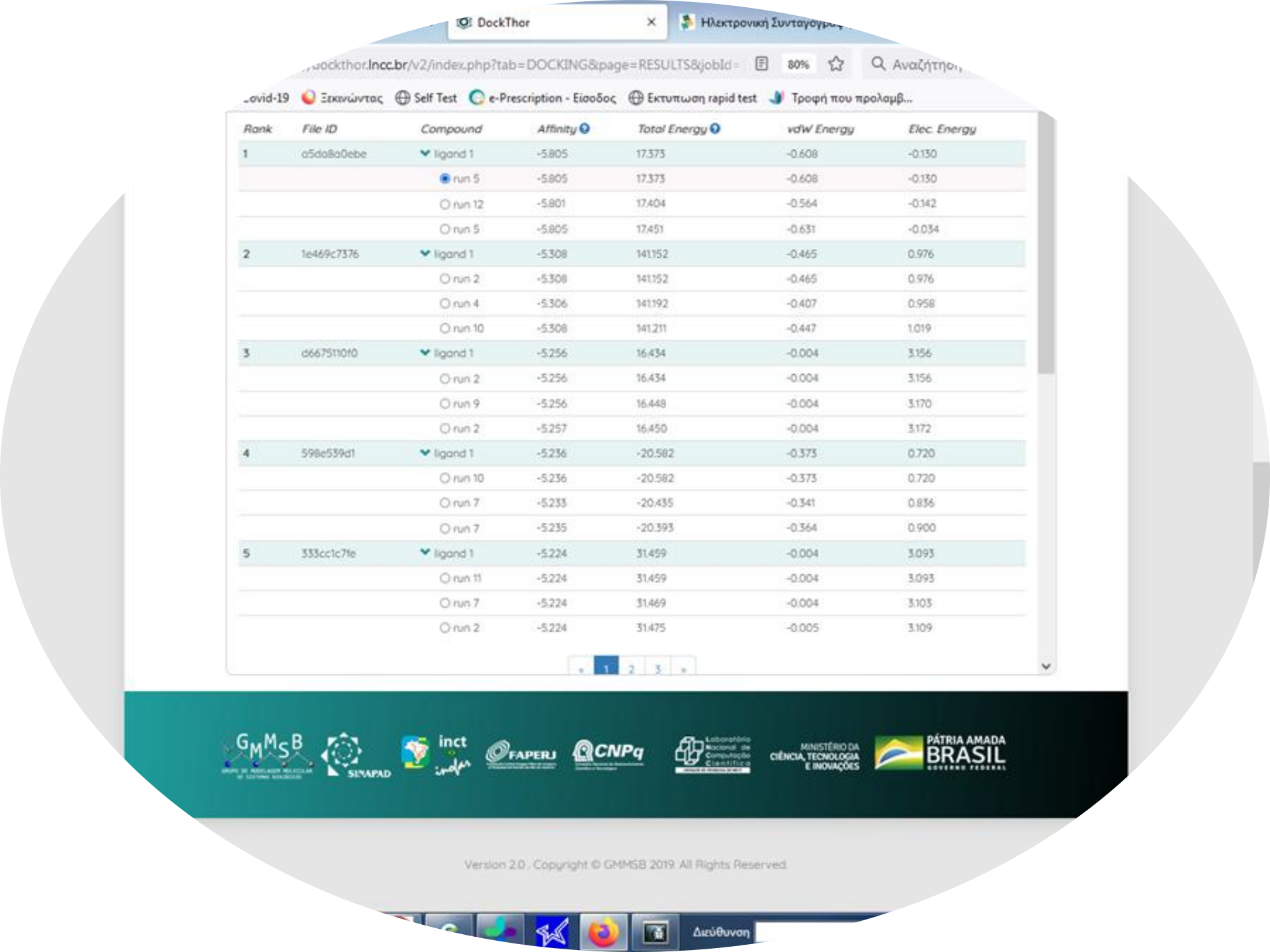
DockThor
Ηλεκτρονική Συνταγογρ
dockthor.lncc.br/v2/index.php?tab=DOCKING&page=RESULTS&jobId=
80%
Αναζήτηση
covid-19
Ξεκινώντας
Self Test
e-Prescription - Εισοδος
Εκτυπωση rapid test
Τροφή που προλαμβ...
Rank
File ID
Compound
Affinity
Total Energy
vdW Energy
Elec. Energy
1 a5da8a0ebe ligand 1 -5.805 17.373 -0.608 -0.130
run 5 -5.805 17.373 -0.608 -0.130
run 12 -5.801 17.404 -0.564 -0.142
run 5 -5.805 17.451 -0.631 -0.034
2 1e469c7376 ligand 1 -5.308 141.152 -0.465 0.976
run 2 -5.308 141.152 -0.465 0.976
run 4 -5.306 141.192 -0.407 0.958
run 10 -5.308 141.211 -0.447 1.019
3 d667511010 ligand 1 -5.256 16.434 -0.004 3.156
run 2 -5.256 16.434 -0.004 3.156
run 9 -5.256 16.448 -0.004 3.170
run 2 -5.257 16.450 -0.004 3.172
4 598e539d1 ligand 1 -5.236 -20.582 -0.373 0.720
run 10 -5.236 -20.582 -0.373 0.720
run 7 -5.233 -20.435 -0.341 0.836
run 7 -5.235 -20.393 -0.364 0.900
5 333cc1c71e ligand 1 -5.224 31.459 -0.004 3.093
run 11 -5.224 31.459 -0.004 3.093
run 7 -5.224 31.469 -0.004 3.103
run 2 -5.224 31.475 -0.005 3.109
« 1 2 3 »
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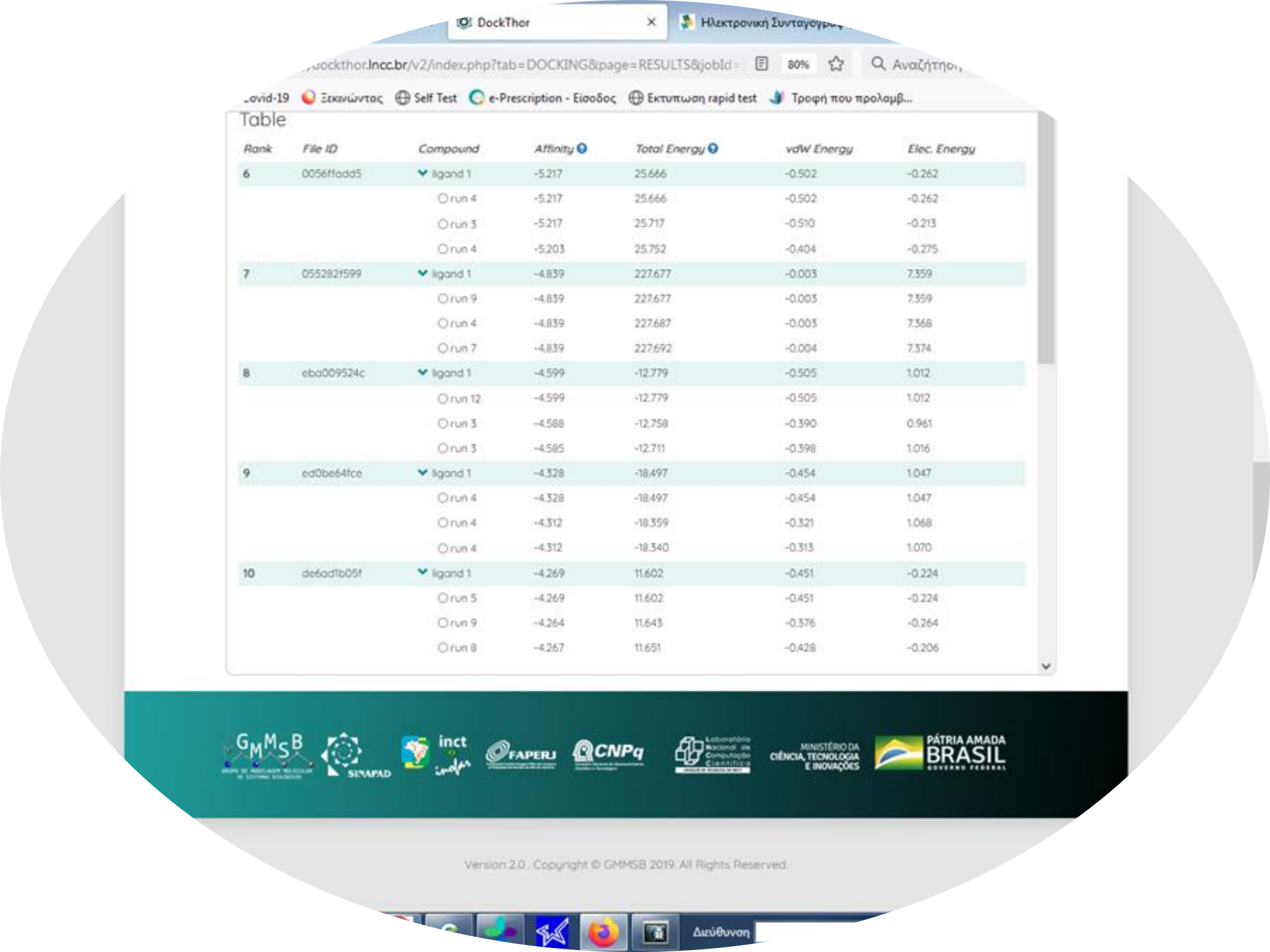
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Τροφή που προλαμβ...
Table
Rank
File ID
Compound
Affinity
Total Energy
vdW Energy
Elec. Energy
6 0056ffadd5 ligand 1 -5.217 25.666 -0.502 -0.262
run 4 -5.217 25.666 -0.502 -0.262
run 3 -5.217 25.717 -0.510 -0.213
run 4 -5.203 25.752 -0.404 -0.275
7 055282f599 ligand 1 -4.839 227.677 -0.003 7.359
run 9 -4.839 227.677 -0.003 7.359
run 4 -4.839 227.687 -0.003 7.368
run 7 -4.839 227.692 -0.004 7.374
8 eba009524c ligand 1 -4.599 -12.779 -0.505 1.012
run 12 -4.599 -12.779 -0.505 1.012
run 3 -4.588 -12.758 -0.390 0.961
run 3 -4.585 -12.711 -0.398 1.016
9 ed0be64fce ligand 1 -4.328 -18.497 -0.454 1.047
run 4 -4.328 -18.497 -0.454 1.047
run 4 -4.312 -18.359 -0.321 1.068
run 4 -4.312 -18.340 -0.313 1.070
10 de6ad1b05f ligand 1 -4.269 11.602 -0.451 -0.224
run 5 -4.269 11.602 -0.451 -0.224
run 9 -4.264 11.643 -0.376 -0.264
run 8 -4.267 11.651 -0.428 -0.206
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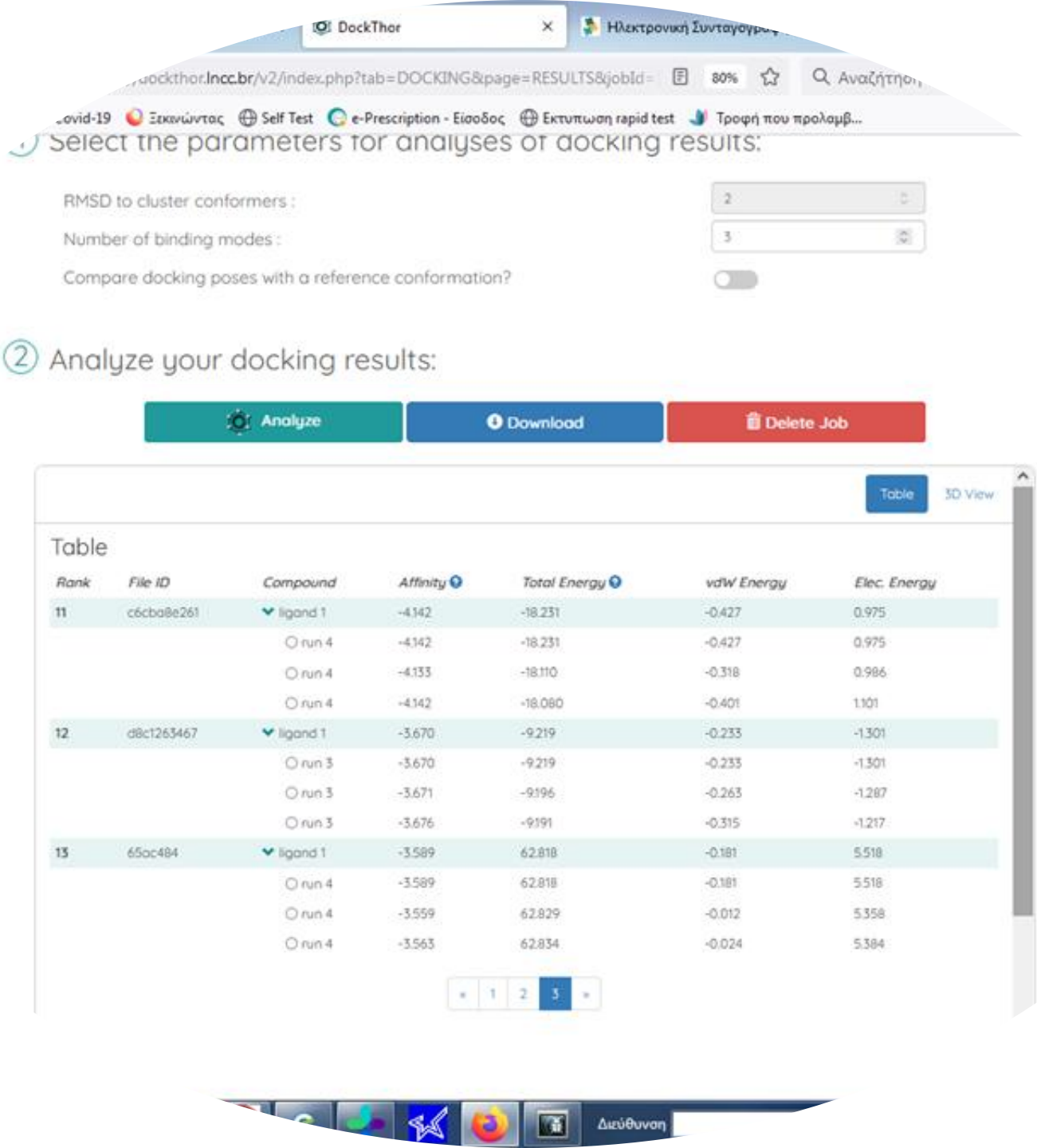
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Αναζήτηση
Covid-19
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Τροφή που προλαμβ...
Select the parameters for analyses of docking results:
RMSD to cluster conformers :
2
Number of binding modes :
3
Compare docking poses with a reference conformation?
2 Analyze your docking results:
Analyze
Download
Delete Job
Table
3D View
Table
Rank
File ID
Compound
Affinity
Total Energy
vdW Energy
Elec. Energy
11 c6cba8e261 ligand 1 -4.142 -18.231 -0.427 0.975
run 4 -4.142 -18.231 -0.427 0.975
run 4 -4.133 -18.110 -0.318 0.986
run 4 -4.142 -18.080 -0.401 1.101
12 d8c1263467 ligand 1 -3.670 -9.219 -0.233 -1.301
run 3 -3.670 -9.219 -0.233 -1.301
run 3 -3.671 -9.196 -0.263 -1.287
run 3 -3.676 -9.191 -0.315 -1.217
13 65ac484 ligand 1 -3.589 62.818 -0.181 5.518
run 4 -3.589 62.818 -0.181 5.518
run 4 -3.559 62.829 -0.012 5.358
run 4 -3.563 62.834 -0.024 5.384
« 1 2 3 »
Διεύθυνση

index.php?tab=DOCKING&page=RESULTS&jobId=5rlg_1xakXRoccustyrna_1gs5X1Xfr8pdb_62b361538c
atom: [GLU]106:B:CD (protein_8cb8a53_prep.pdb)
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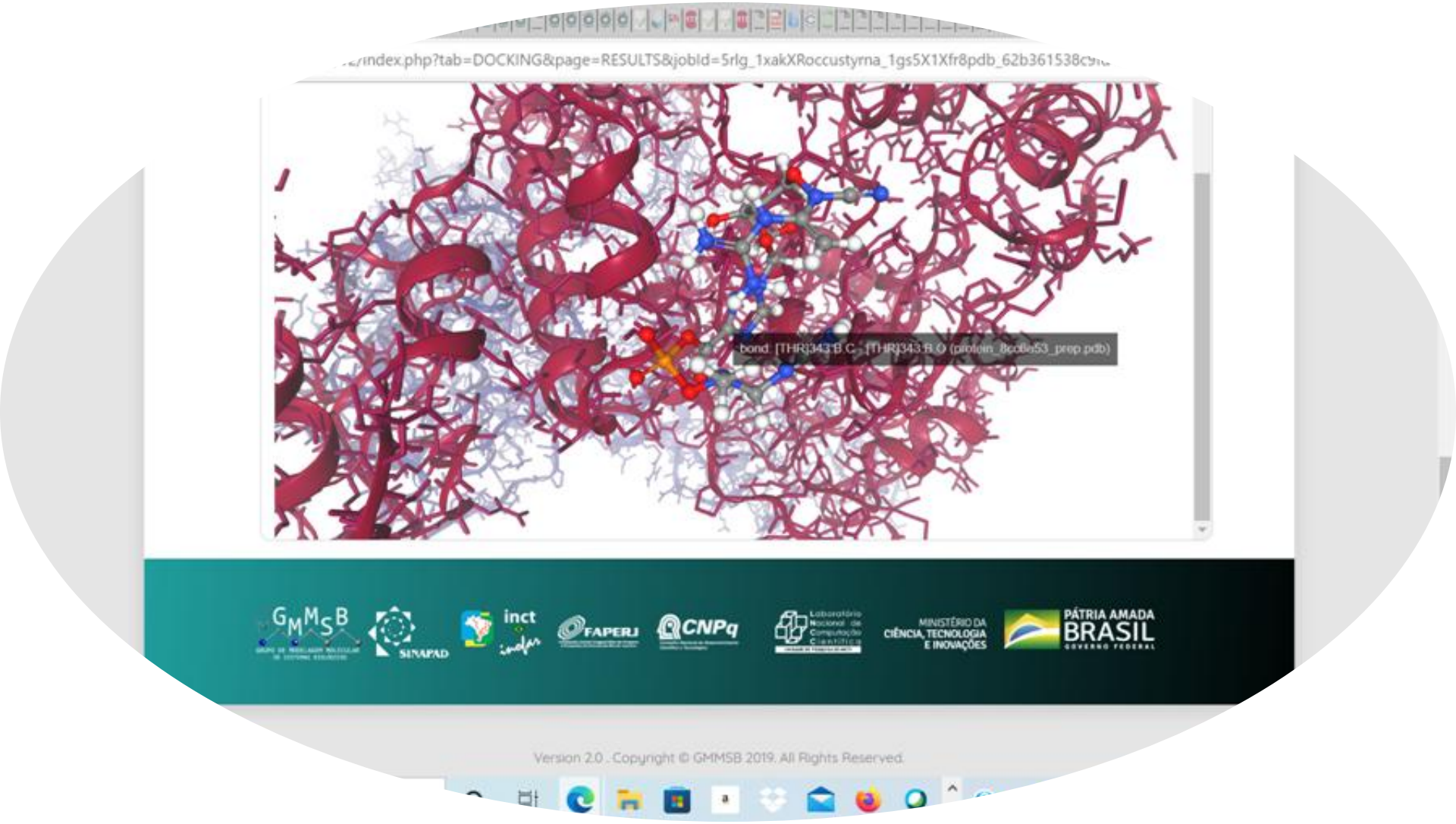
index.php?tab=DOCKING&page=RESULTS&jobId=5rlg_1xakXRoccustyrna_1gs5X1Xfr8pdb_62b361538c
bond: [THR]343:B.C - [THR]343:B.O (protein_8cc8e53_prep.pdb)
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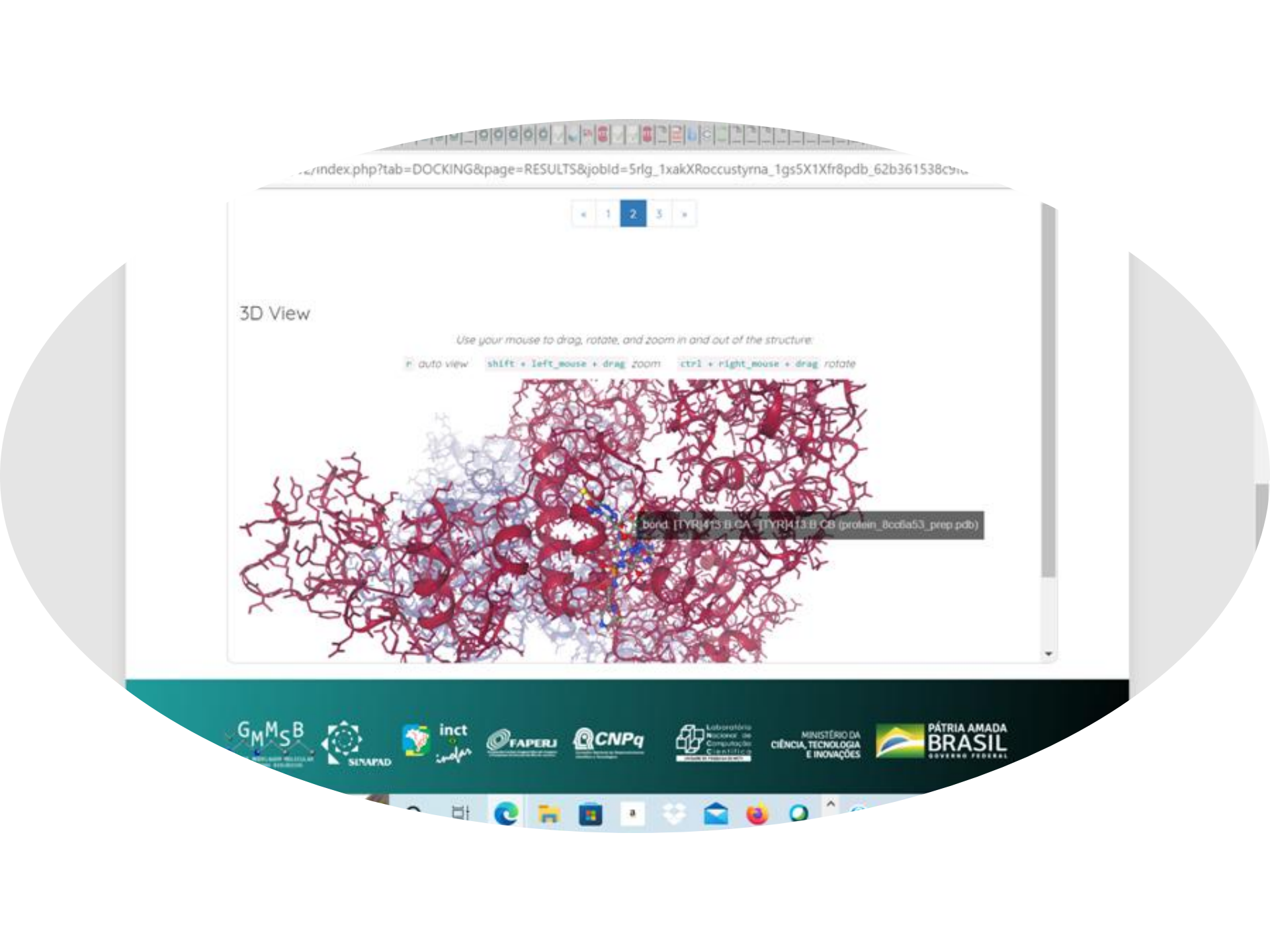
index.php?tab=DOCKING&page=RESULTS&jobId=5rlg_1xakXRoccustyrna_1gs5X1Xfr8pdb_62b361538c
« 1 2 3 »
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [TYR]413:B.CA - [TYR]413:B.CB (protein_8ccdia53_prep.pdb)
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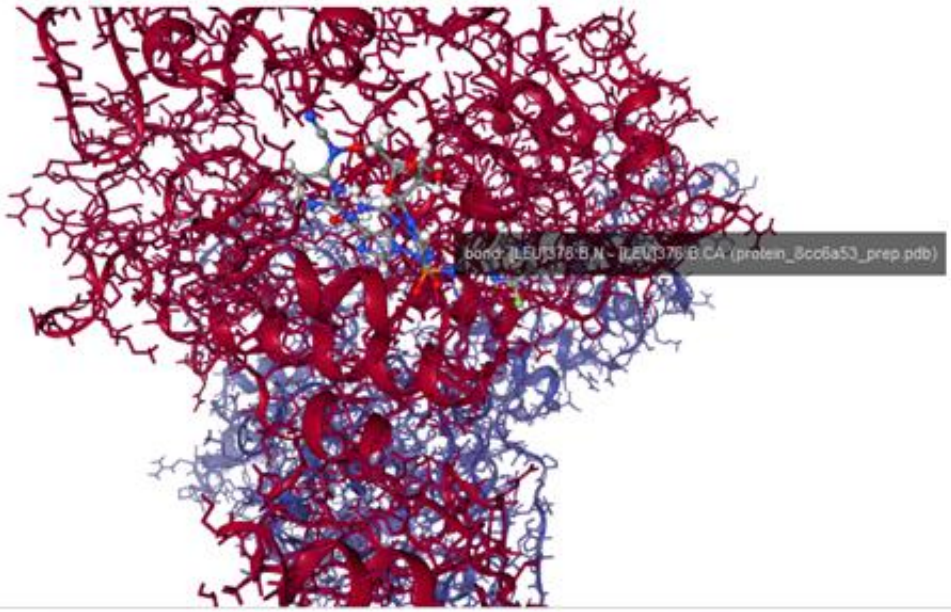
3D View

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



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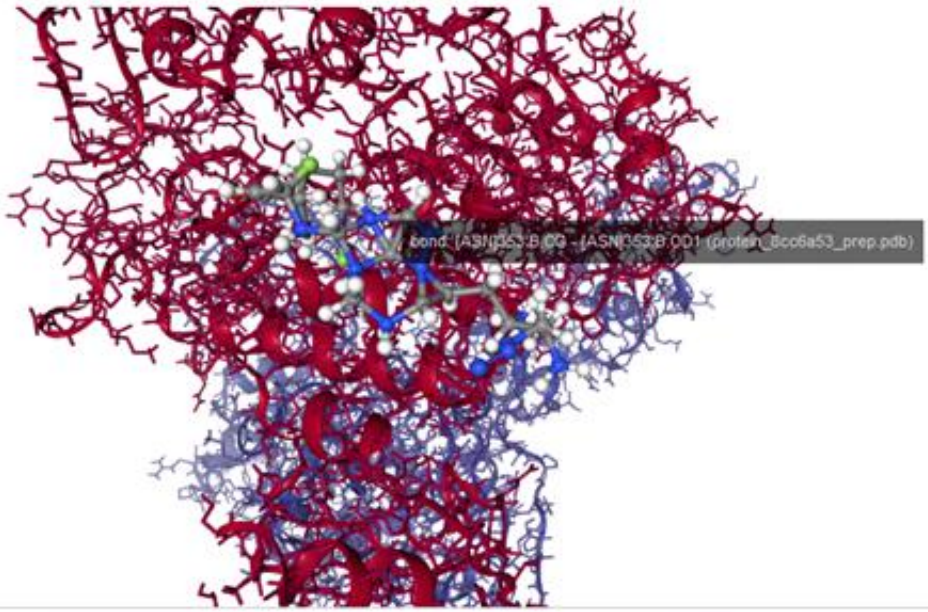
3D View

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



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Αναζήτηση
Covid-19
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Self Test
e-Prescription - Είσοδος
Εκτυπωση rapid test
Τροφή που προλαμβ...
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure:
auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
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Table 3D View

« 1 2 3 »

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: [SER]216:A.N - [SER]216:A.H (protein_8cc6a53_prep.pdb)

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Αναζήτηση

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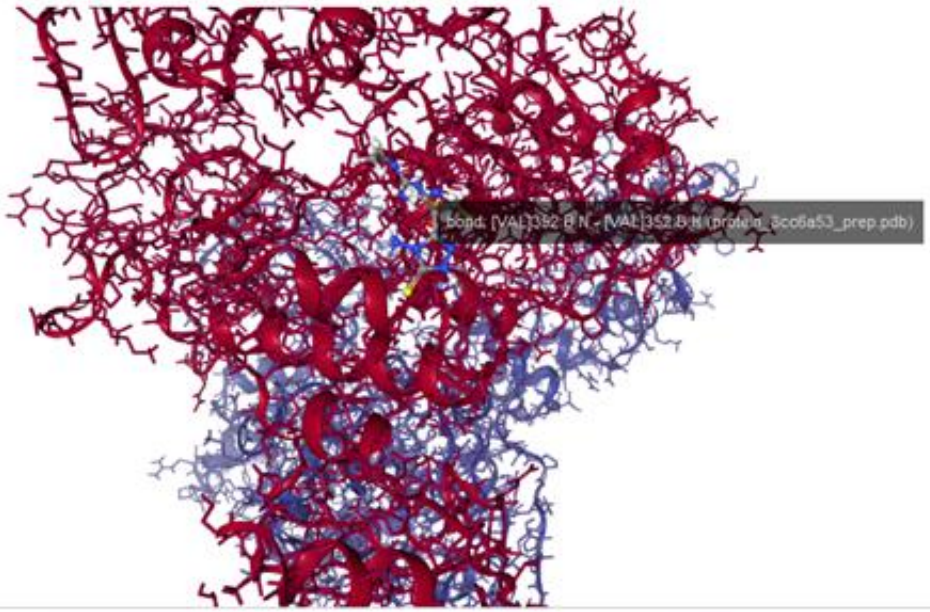
3D View

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



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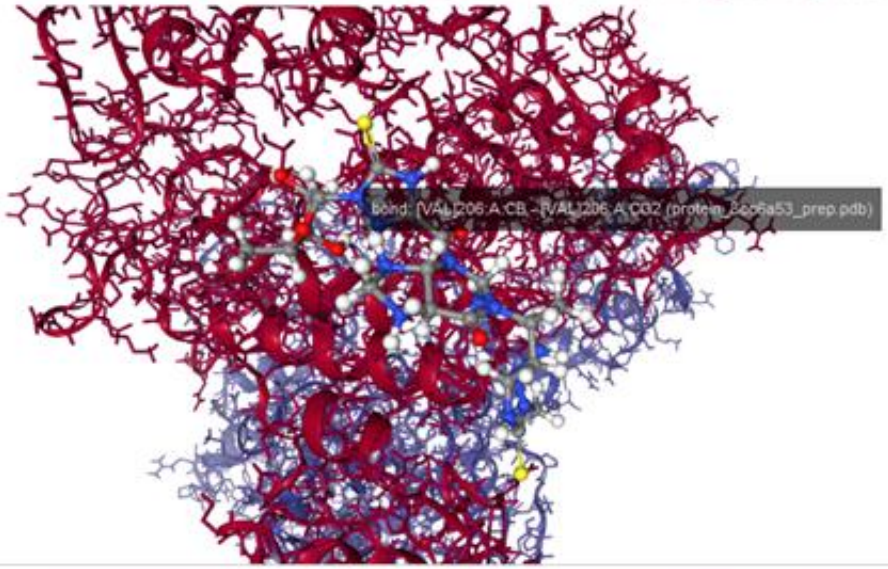
« 1 2 3 »

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



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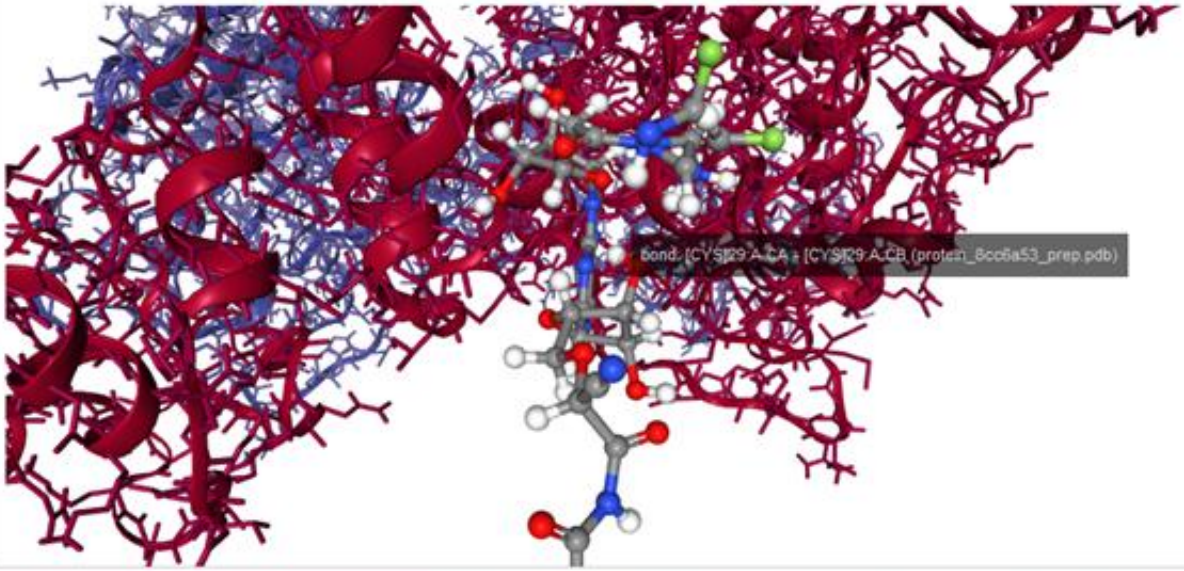
« 1 2 3 »

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



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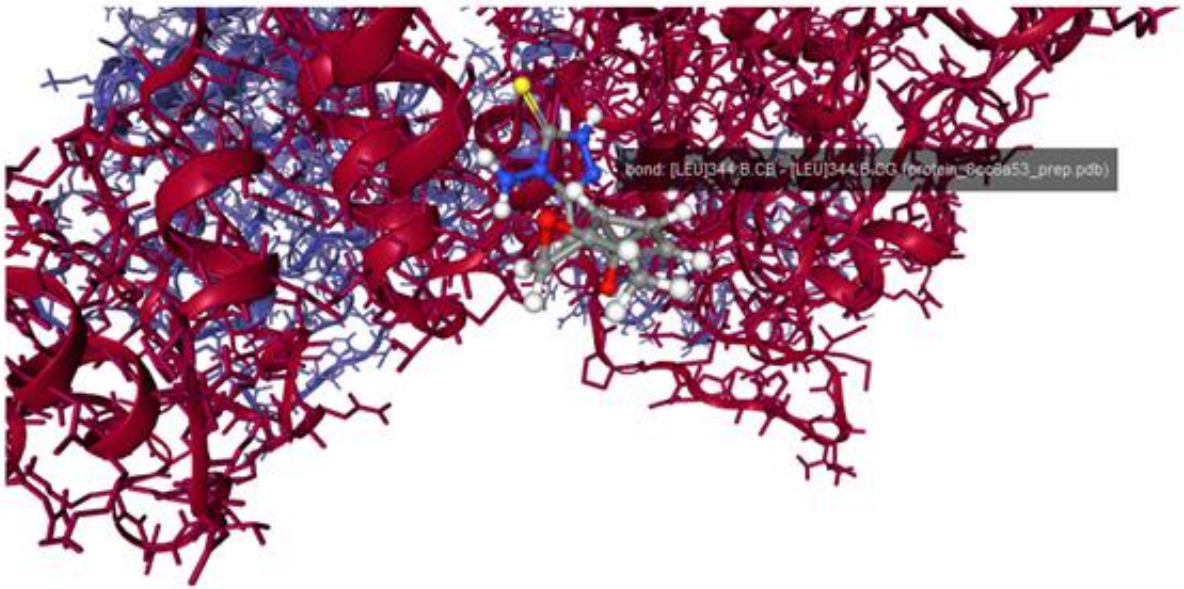
3D View

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



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