

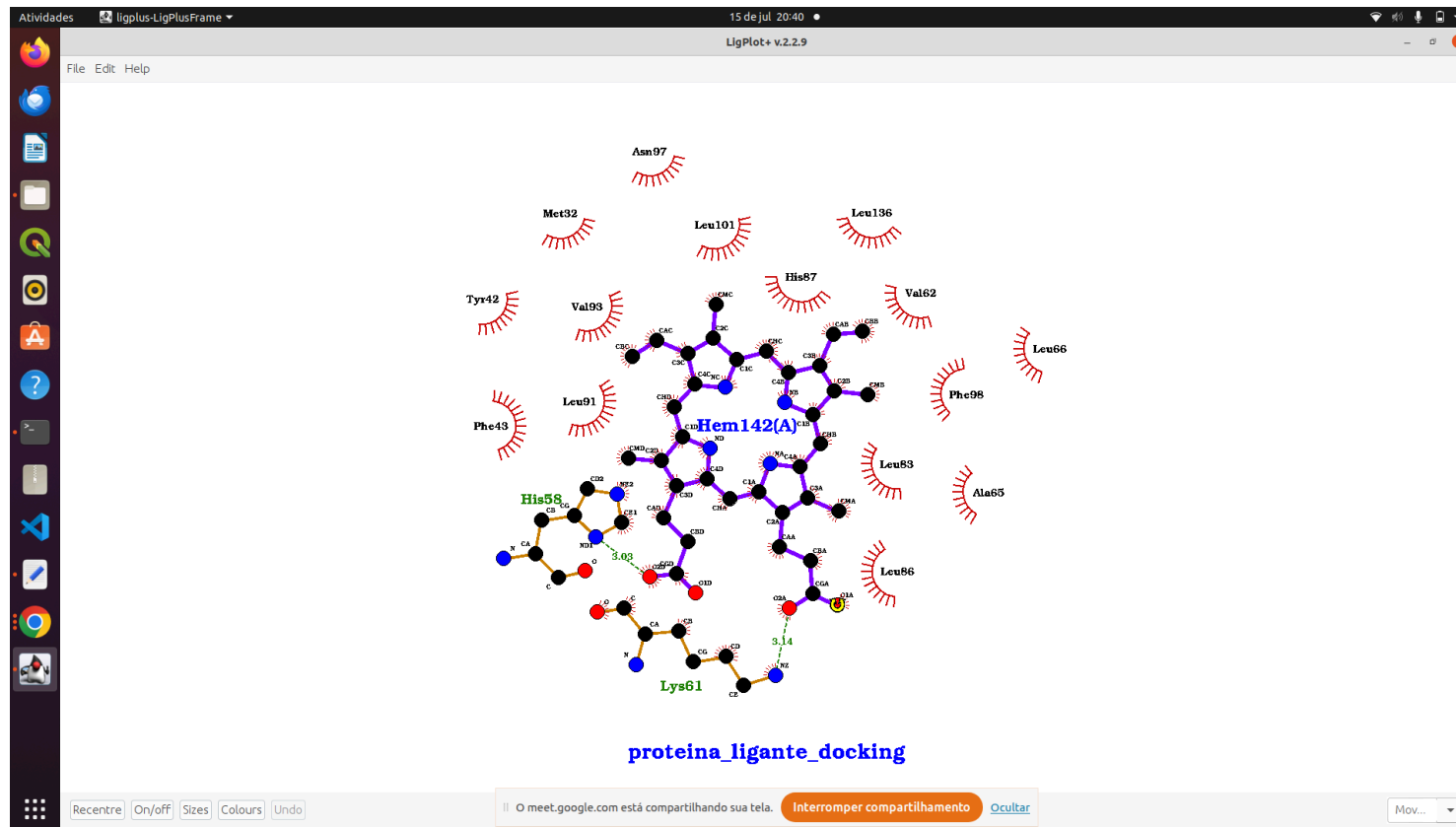
**Table 1. Parameters affinity of the molecular docking Vina.**

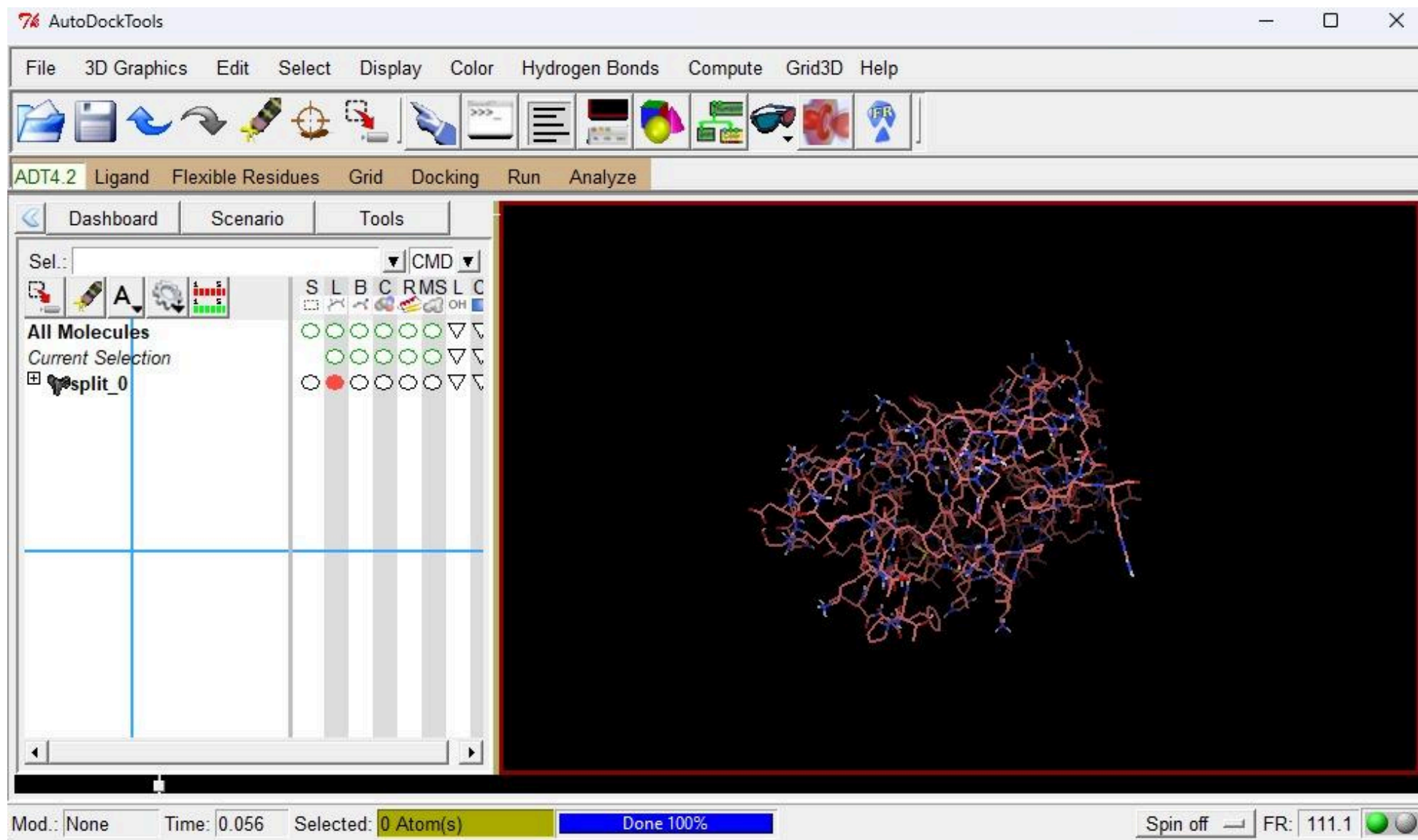
**Proteína: hemoglobina humana desoxigenada**

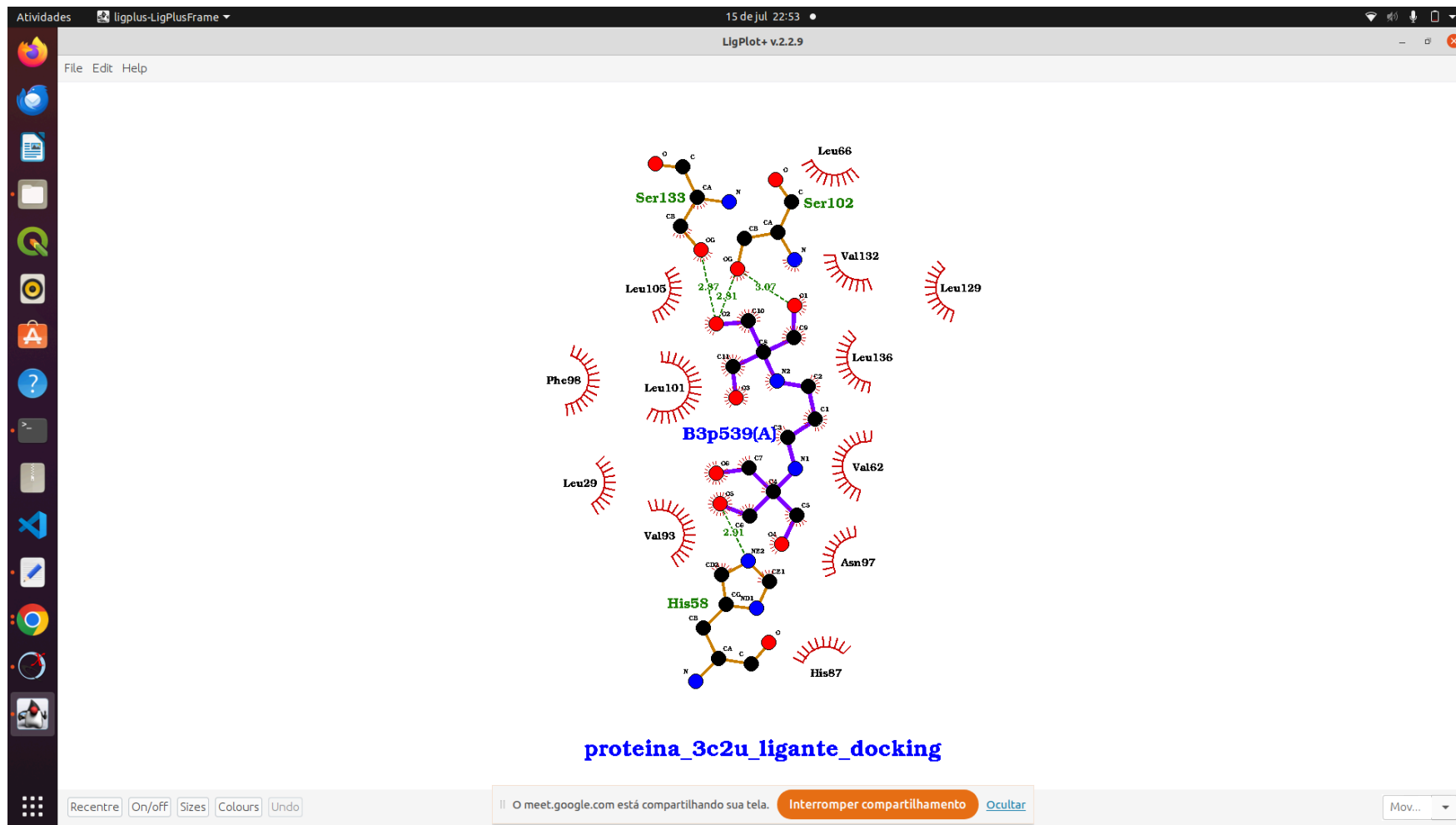
<b>Complex (Protein-ligand)</b>	<b><math>\Delta G_{\text{bind}}</math> (kcal/mol)</b>	<b>Amino acids that interact through hydrogen bonds (distance Angstrom)</b>	<b>Amino acids that make hydrophobic interactions</b>
1a3n_hem	-12.4	<b>His58</b> – distância: 3.03 Å <b>Lys61</b> – distância: 3.14 Å	<b>-Tyr42, Phe43, Val93, Leu101, Asn97, Met32, Leu136, His87, Val62, Leu66, Phe98, Leu83, Leu86, Ala65, Leu91</b>
1a3n_1eqg	-5.2	O aminoácido que interage com o ligante por ligação de hidrogênio é <b>Ser102 (2.92 Å)</b> .	Os aminoácidos que fazem interações hidrofóbicas com o ligante são: <b>Leu101, Leu105, Leu136, Leu66, Leu83, Val62, His87, Ala65, Lys61, Ser133 e Phe98.</b>
1a3n_3c2u	-5.4	<b>Ser138</b> – ligação de hidrogênio com distância 2.78 Å <b>Ser102</b> – ligação de hidrogênio com distância 2.91 Å <b>His58</b> – ligação de hidrogênio com distância 3.14 Å	Os aminoácidos que participam de interações hidrofóbicas com o ligante são: <b>Leu105, Leu129, Leu136, Val62, Val93, Val132, Phe98, Leu101, Asn97, His87, Leu66 e Val29.</b>

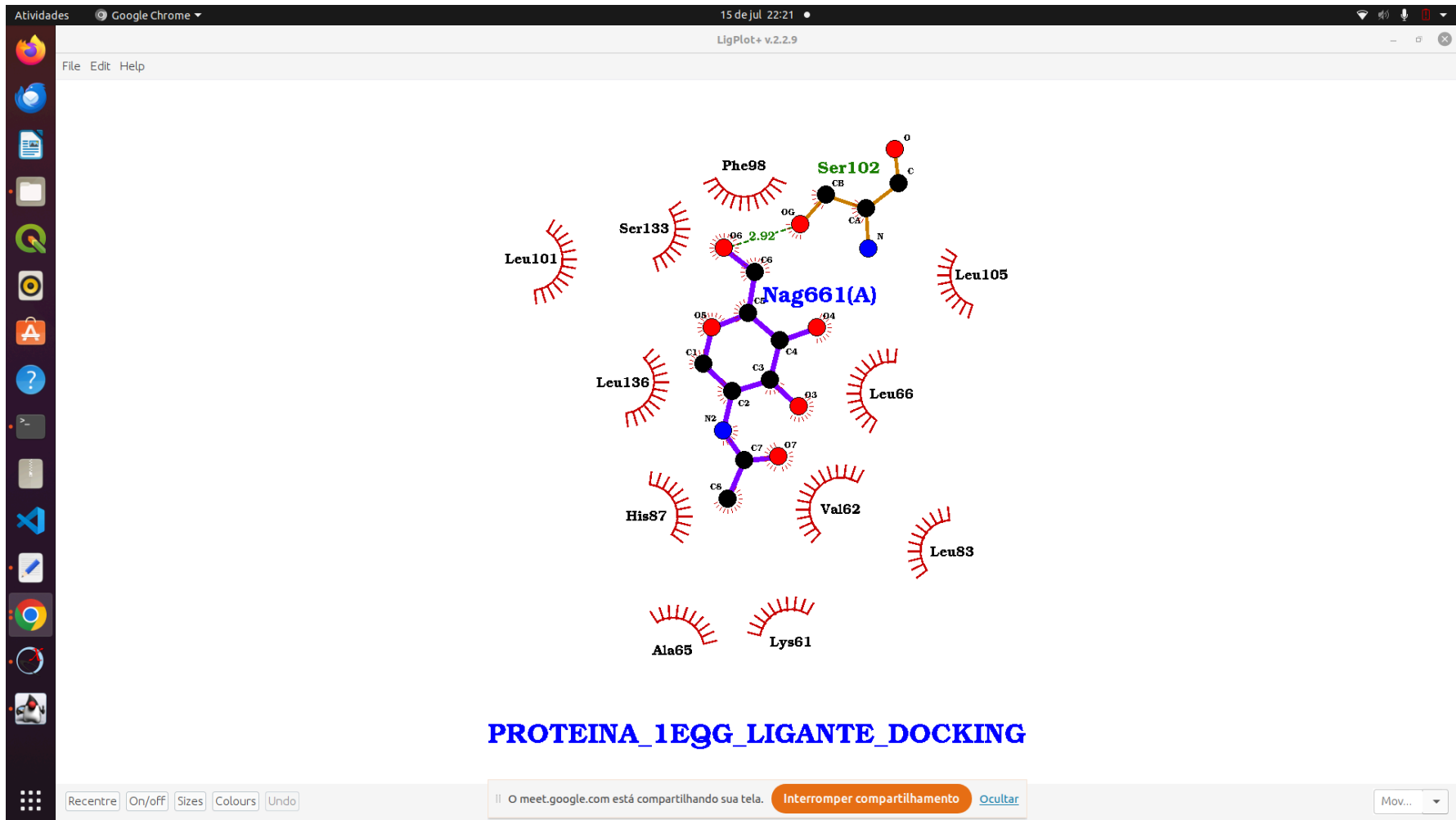
E inserir uma imagem do complexo (proteína e o ligante) com menor energia de ligação.

Proteína e o ligante com melhor energia de ligação (-12.4)  
Captura de tela após o ancoramento no LigPlot









```
Atividades Terminal 15 de jul 22:39
oliveiras@Oliveiras: ~/Downloads/trabalho ricardo

Reading input ...
Error: could not open "ligante_3c2u.pdbqt" for reading.
oliveiras@Oliveiras:~/Downloads/trabalho ricardo$ vina --config config.txt
#####
# If you used AutoDock Vina in your work, please cite: #
# #
# O. Trott, A. J. Olson, #
# AutoDock Vina: improving the speed and accuracy of docking #
# with a new scoring function, efficient optimization and #
# multithreading, Journal of Computational Chemistry 31 (2010) #
# 455-461 #
# DOI 10.1002/jcc.21334 #
# #
# Please see http://vina.scripps.edu for more information. #
#####
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -810637376
Performing search ...
0% 10 20 30 40 50 60 70 80 90 100%
|----|----|----|----|----|----|----|----|----|
*****
done.
Refining results ... done.

mode | affinity | dist from best mode
| (kcal/mol) | rmsd l.b. | rmsd u.b.
-----+-----+-----+-----
1 | -5.4 | 0.000 | 0.000
2 | -5.4 | 1.095 | 6.228
3 | -5.2 | 0.768 | 2.123
4 | -5.2 | 1.057 | 1.721
5 | -5.1 | 1.270 | 2.683
6 | -5.0 | 0.987 | 6.415
7 | -5.0 | 1.653 | 6.893
8 | -4.9 | 1.665 | 6.744
9 | -4.9 | 1.463 | 2.366
10 | -4.8 | 1.836 | 7.008
11 | -4.8 | 1.701 | 2.416
12 | -4.8 | 1.478 | 6.495
13 | -4.7 | 1.707 | 6.763
14 | -4.5 | 5.095 | 9.437
15 | -4.4 | 10.144 | 11.608
16 | -4.4 | 4.903 | 8.983
17 | -4.3 | 4.916 | 9.275
18 | -4.3 | 4.922 | 9.119
19 | -4.3 | 5.291 | 9.314
20 | -4.2 | 5.570 | 8.275

Writing output ... done.
oliveiras@Oliveiras:~/Downloads/trabalho ricardo$
```

```
Atividades Terminal 15 de jul 22:36
oliveiras@Oliveiras: ~/Downloads/trabalho ricardo

oliveiras@Oliveiras:~/Downloads/LigPlus$ ^C
oliveiras@Oliveiras:~/Downloads/LigPlus$ cd ..
oliveiras@Oliveiras:~/Downloads$ cd trabalho\ ricardo/
oliveiras@Oliveiras:~/Downloads/trabalho ricardo$ vina --config config.txt
#####
# If you used AutoDock Vina in your work, please cite: #
# #
# O. Trott, A. J. Olson, #
# AutoDock Vina: improving the speed and accuracy of docking #
# with a new scoring function, efficient optimization and #
# multithreading, Journal of Computational Chemistry 31 (2010) #
# 455-461 #
# DOI 10.1002/jcc.21334 #
# #
# Please see http://vina.scripps.edu for more information. #
#####
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1328055295
Performing search ...
0% 10 20 30 40 50 60 70 80 90 100%
|-----|-----|-----|-----|-----|-----|-----|
*****
done.
Refining results ... done.

mode | affinity | dist from best mode
| (kcal/mol) | rmsd l.b. | rmsd u.b.
-----+-----+-----+-----
1 | -5.2 | 0.000 | 0.000
2 | -5.2 | 4.437 | 5.896
3 | -5.1 | 1.869 | 5.532
4 | -5.1 | 2.125 | 5.061
5 | -5.1 | 5.169 | 5.945
6 | -5.1 | 4.865 | 6.983
7 | -4.9 | 5.818 | 7.954
8 | -4.9 | 1.860 | 3.145
9 | -4.9 | 1.578 | 2.648
10 | -4.9 | 2.760 | 4.341
11 | -4.8 | 4.357 | 5.873
12 | -4.7 | 2.945 | 5.191
13 | -4.7 | 3.814 | 5.868
14 | -4.6 | 2.693 | 4.405
15 | -4.6 | 7.075 | 9.337
16 | -4.5 | 3.561 | 5.190
17 | -4.4 | 2.820 | 5.103
18 | -4.4 | 2.422 | 3.141
19 | -4.4 | 4.988 | 7.546
20 | -4.3 | 7.975 | 9.432

Writing output ... done.
oliveiras@Oliveiras:~/Downloads/trabalho ricardo$
```

```
Atividades Terminal 15 de jul 20:11
oliveiras@Oliveiras: ~/Downloads/trabalho ricardo

oliveiras@Oliveiras:~/Downloads$ cd ..
oliveiras@Oliveiras:~$ vina.exe --config config.txt
bash: vina.exe: comando não encontrado
oliveiras@Oliveiras:~$ vina --version
AutoDock Vina 1.1.2 (May 11, 2011)
oliveiras@Oliveiras:~$ vina --config config.txt

Error: could not open "config.txt" for reading.
oliveiras@Oliveiras:~$ cd Downloads/
oliveiras@Oliveiras:~/Downloads$ cd trabalho\ ricardo/
oliveiras@Oliveiras:~/Downloads/trabalho ricardo$ vina.exe --config config.txt
bash: vina.exe: comando não encontrado
oliveiras@Oliveiras:~/Downloads/trabalho ricardo$ vina --config config.txt
#####
# If you used AutoDock Vina in your work, please cite:      #
#                                                           #
# O. Trott, A. J. Olson,                                    #
# AutoDock Vina: improving the speed and accuracy of docking #
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# multithreading, Journal of Computational Chemistry 31 (2010) #
# 455-461                                                    #
#                                                           #
# DOI 10.1002/jcc.21334                                     #
#                                                           #
# Please see http://vina.scripps.edu for more information.   #
#####
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1569418907
Performing search ...
0% 10 20 30 40 50 60 70 80 90 100%
|---|---|---|---|---|---|---|---|---|
*****
done.
Refining results ... done.

mode | affinity | dist from best mode
      | (kcal/mol) | rmsd l.b. | rmsd u.b.
-----+-----+-----+-----
1      -12.4      0.000      0.000
2      -11.4      3.332      7.334
3      -10.9      3.321      7.275
4      -10.6      4.008      7.852
5      -10.4      1.324      6.056
6      -10.3      4.151      9.778
7      -10.3      2.353      6.599
8      -10.1      1.403      5.863
9       -9.6      4.084      9.686
10     -9.5      2.187      6.481

Writing output ... done.
oliveiras@Oliveiras:~/Downloads/trabalho ricardo$
```