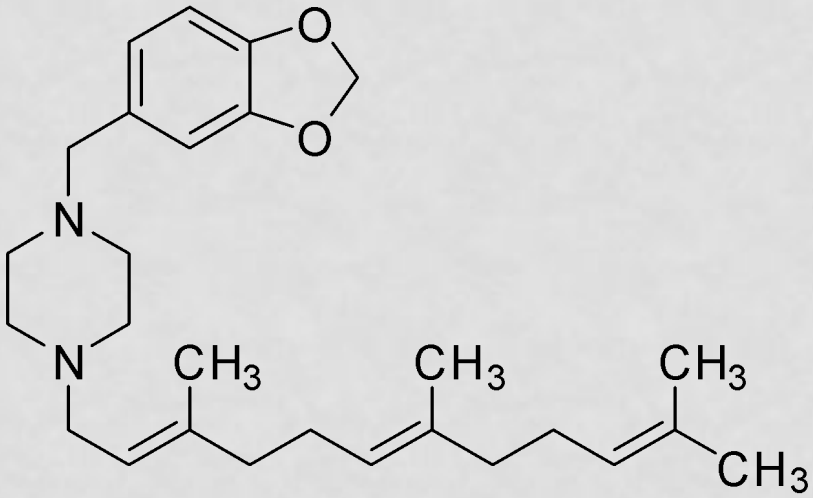
ПИФАРНИН

RIBAVIRIN

ПИФАРНИН

ИЮПАК	4-Farnesyl-1-(3,4-methylenedioxybenzyl)piperazine
MW	424,629
MF	$C_{27}H_{40}N_2O_2$

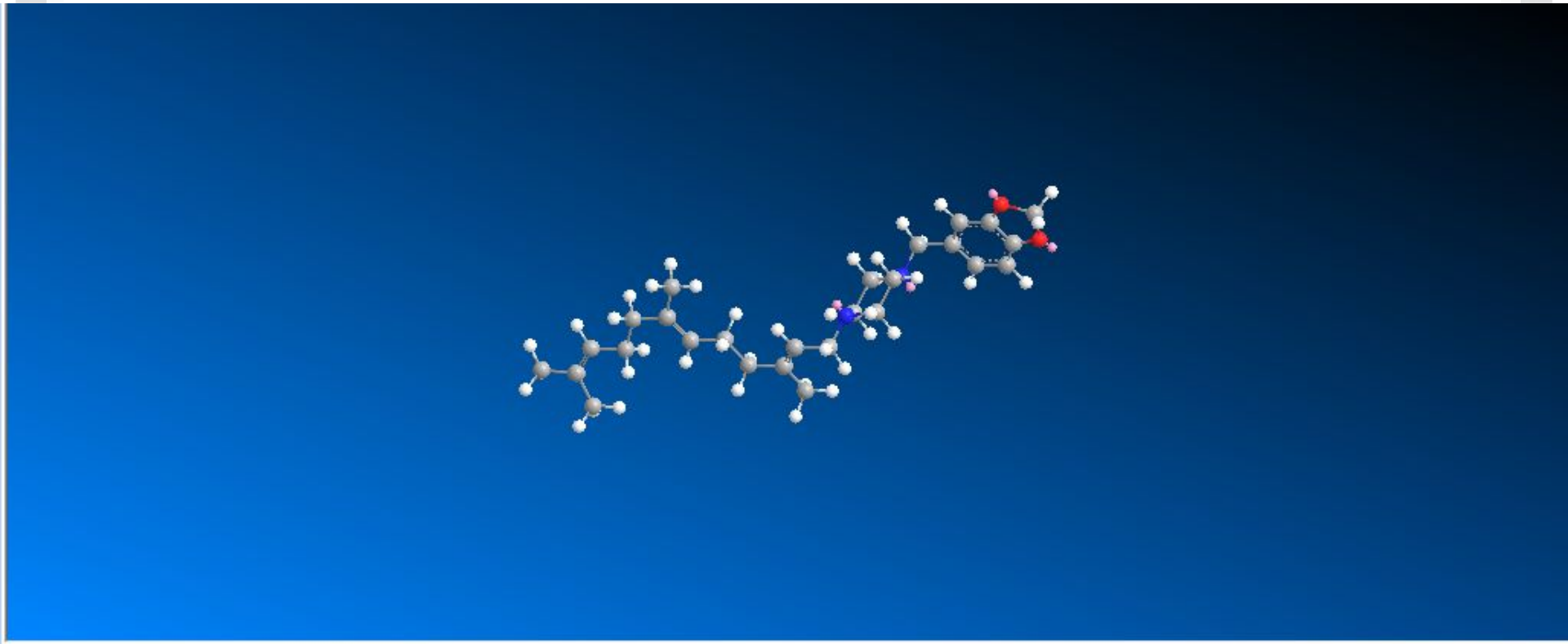


ЦЕЛИ И ЗАДАЧИ РАБОТЫ:

- Изучение биологической активности пифарнина, поиск новых мишеней для данного соединения.

- Освоить программу для создания химических формул в графическом виде – ChemBioDraw Ultra
- познакомится с работой в системе для предсказания химической активности - Pass
- познакомится с докинг-анализом.

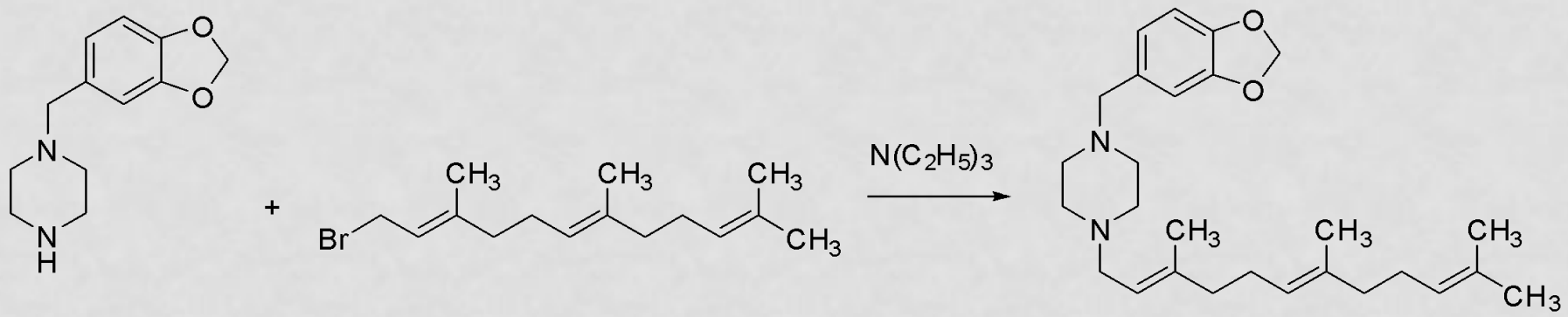
MM2 MINIMIZATION



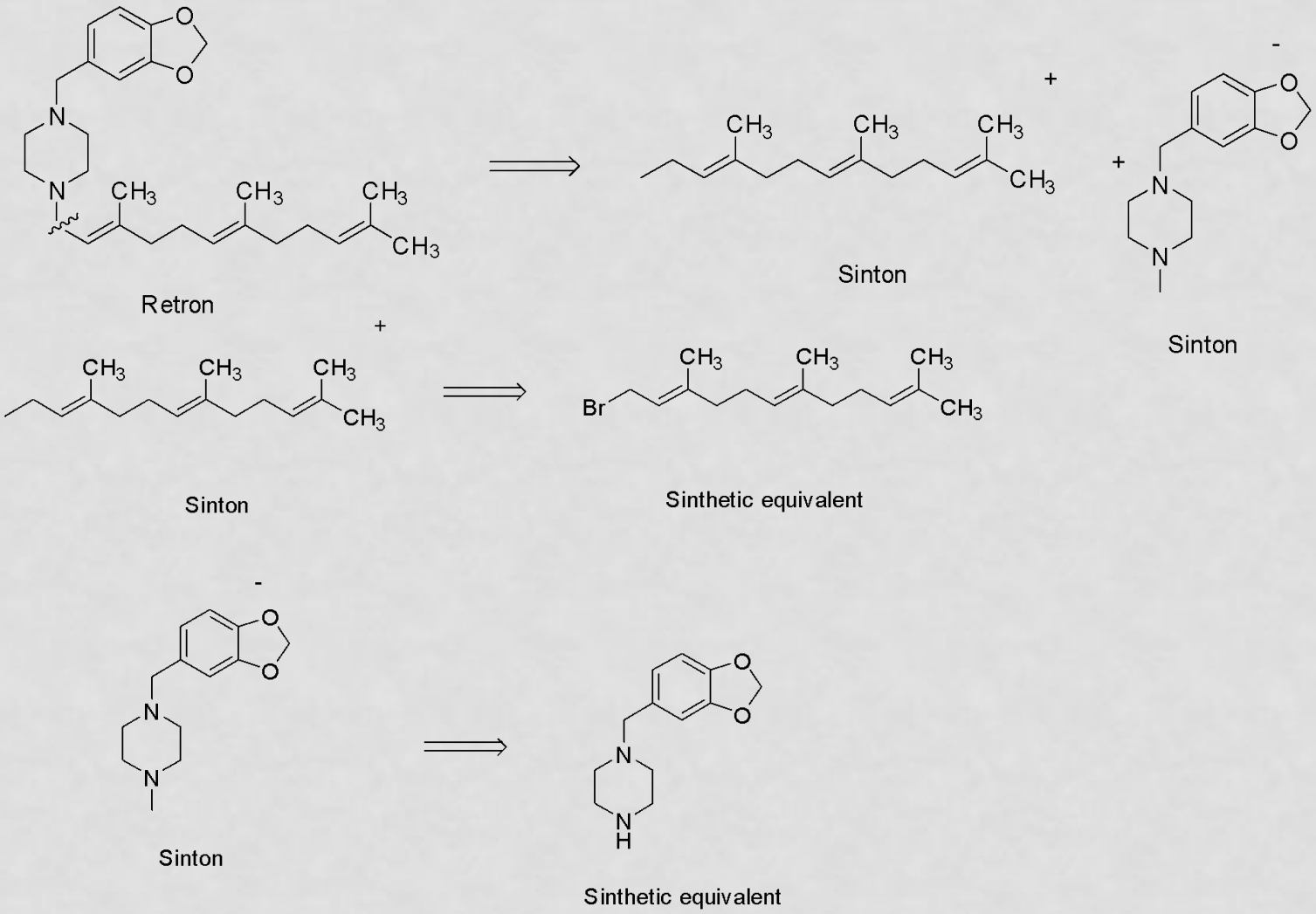
Output

```
  Dipole/Dipole:          2.5114
Total Energy:            26.0822 kcal/mol
Calculation ended
-----------------------------------------
```

СХЕМА СИНТЕЗА ПИФАРНИНА



РЕТРОСИНТЕТИЧЕСКИЙ АНАЛИЗ

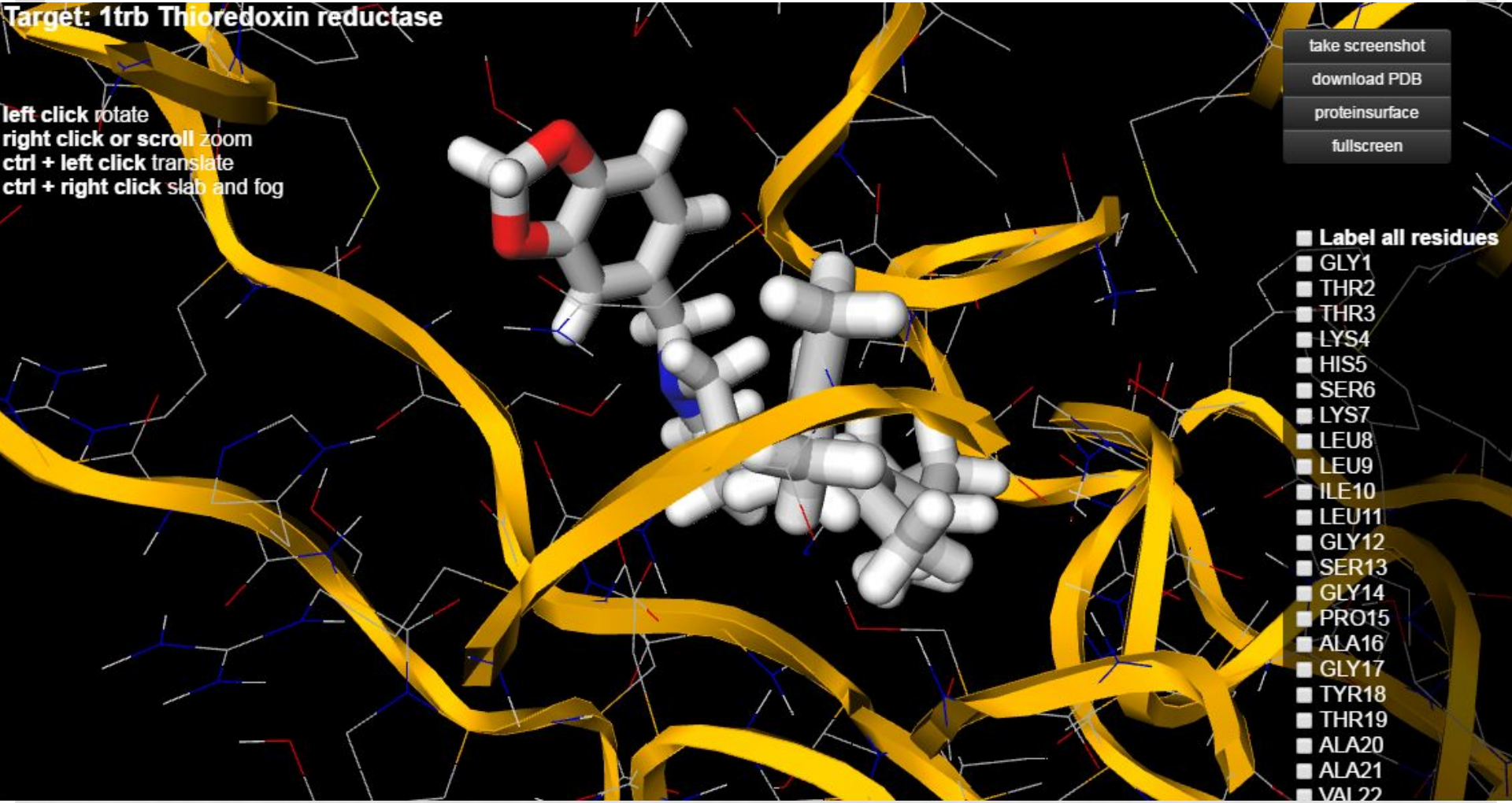


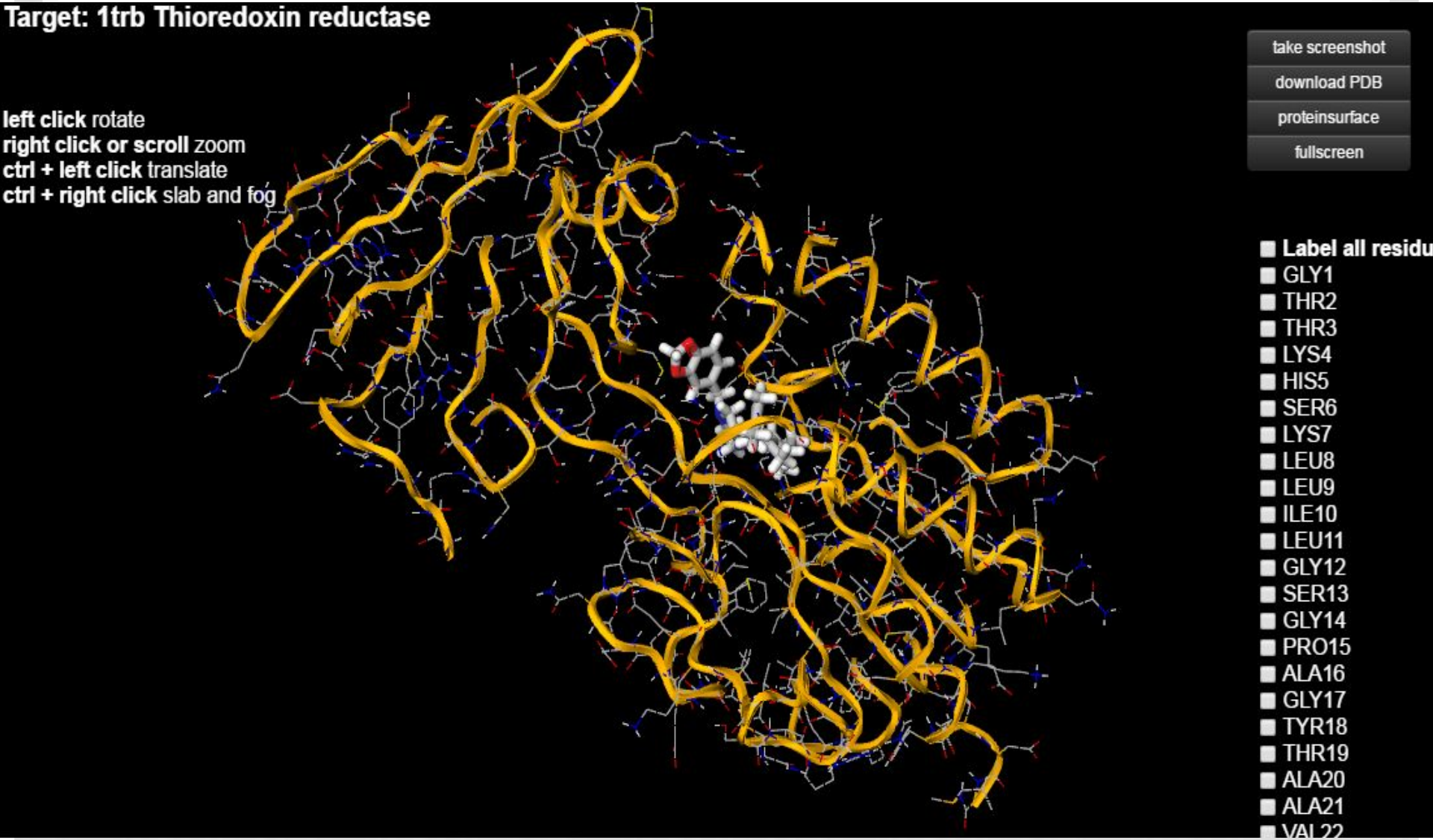
РЕЗУЛЬТАТ РАБОТЫ В PASS

Mechanisms of Action	Pi	Pa
Thioredoxin reductase inhibitor	0,119	0,122
Ribonucleoside diphosphate reductase inhibitor	0,023	0,118
Phosphofructokinase-1 inhibitor	0,006	0,346

РЕЗУЛЬТАТ РАБОТЫ В DOKING THIOREDOXIN REDUCTASE INHIBITOR

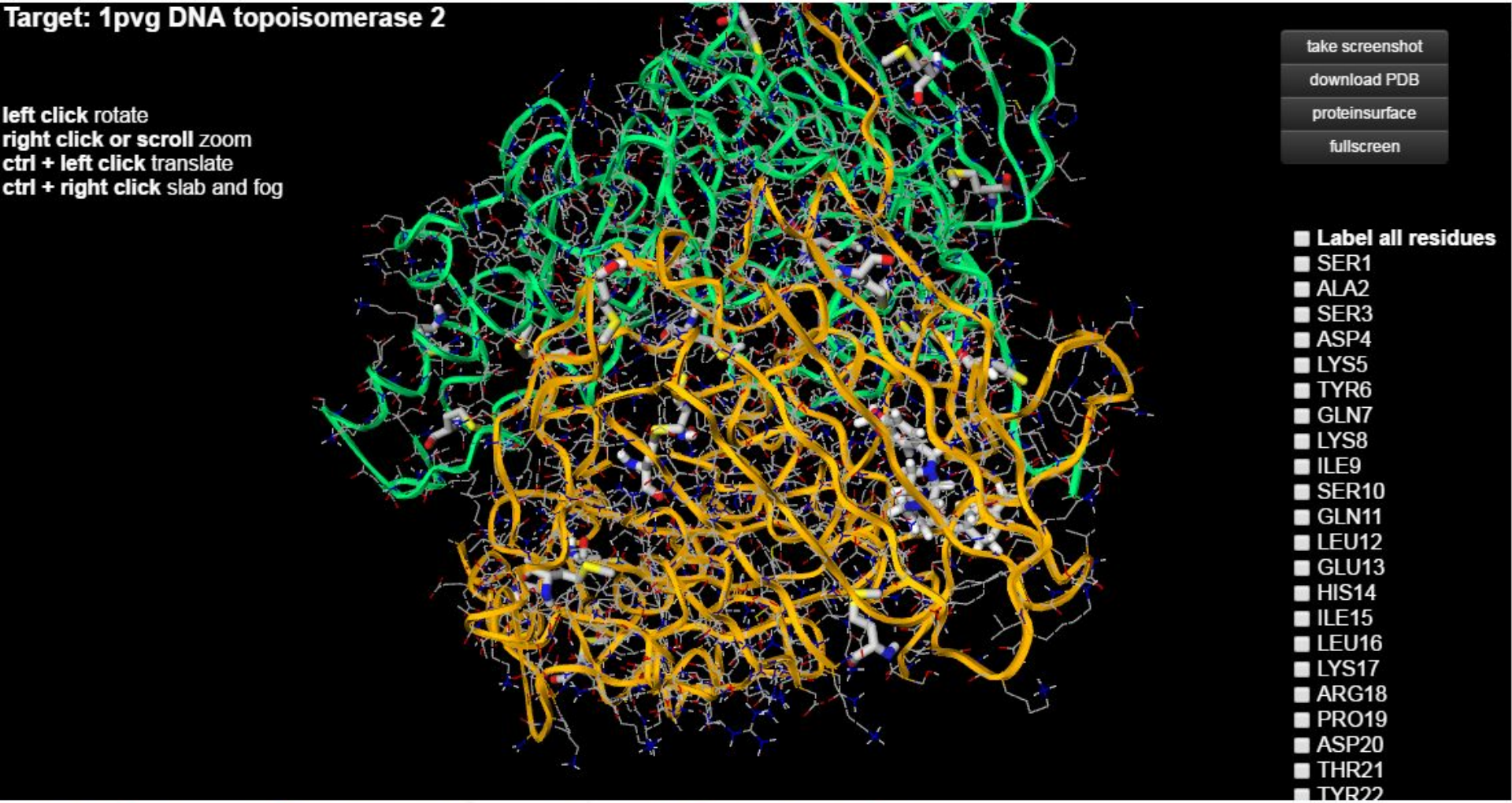
Docking pose	Docking score		
#1	-7.4	VISUALIZE POSE	DOWNLOAD POSE
#2	-6.9	VISUALIZE POSE	DOWNLOAD POSE
#3	-6.3	VISUALIZE POSE	DOWNLOAD POSE
#4	-6.3	VISUALIZE POSE	DOWNLOAD POSE

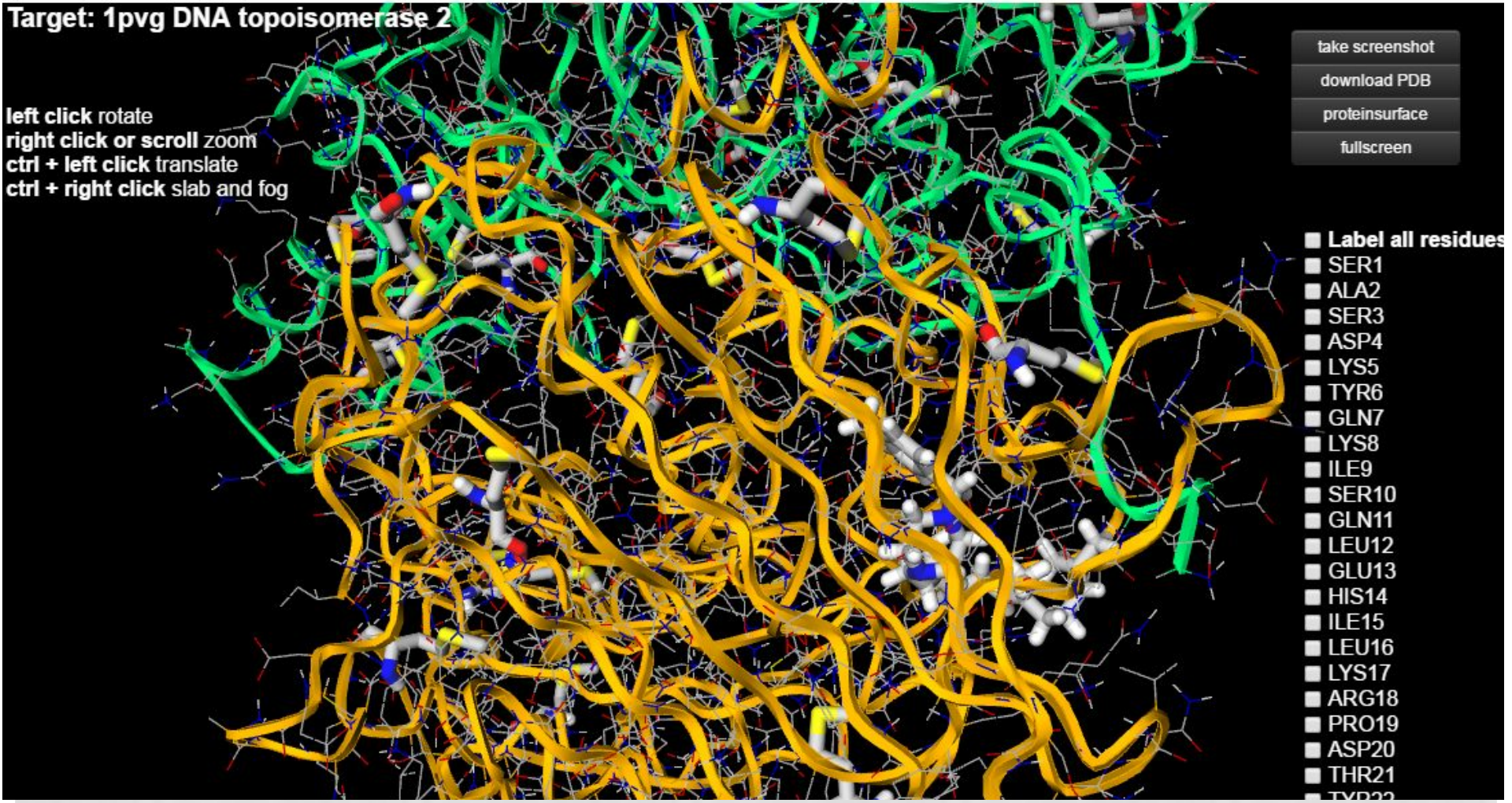

Target: 1trb Thioredoxin reductase
left click rotate
right click or scroll zoom
ctrl + left click translate
ctrl + right click slab and fog
take screenshot
download PDB
proteinsurface
fullscreen
Label all residues
GLY1
THR2
THR3
LYS4
HIS5
SER6
LYS7
LEU8
LEU9
ILE10
LEU11
GLY12
SER13
GLY14
PRO15
ALA16
GLY17
TYR18
THR19
ALA20
ALA21


Target: 1trb Thioredoxin reductase
left click rotate
right click or scroll zoom
ctrl + left click translate
ctrl + right click slab and fog
take screenshot
download PDB
proteinsurface
fullscreen
Label all residu
GLY1
THR2
THR3
LYS4
HIS5
SER6
LYS7
LEU8
LEU9
ILE10
LEU11
GLY12
SER13
GLY14
PRO15
ALA16
GLY17
TYR18
THR19
ALA20
ALA21

РЕЗУЛЬТАТ РАБОТЫ В DOKING TOPOISOMERASE II INHIBITOR

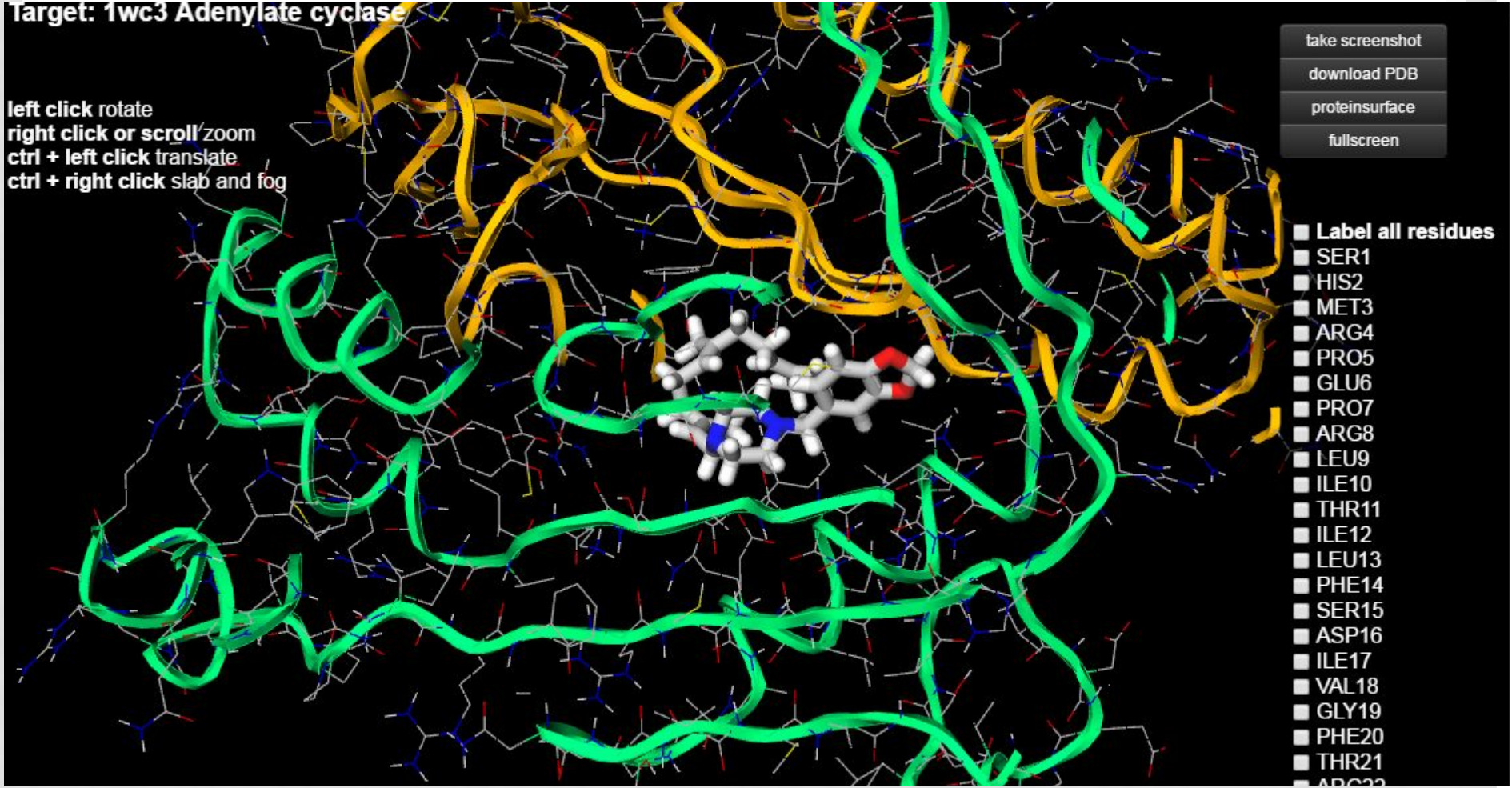
Docking pose	Docking score		
#1	-9.1	VISUALIZE POSE	DOWNLOAD POSE
#2	-9.0	VISUALIZE POSE	DOWNLOAD POSE
#3	-8.7	VISUALIZE POSE	DOWNLOAD POSE
#4	-8.6	VISUALIZE POSE	DOWNLOAD POSE

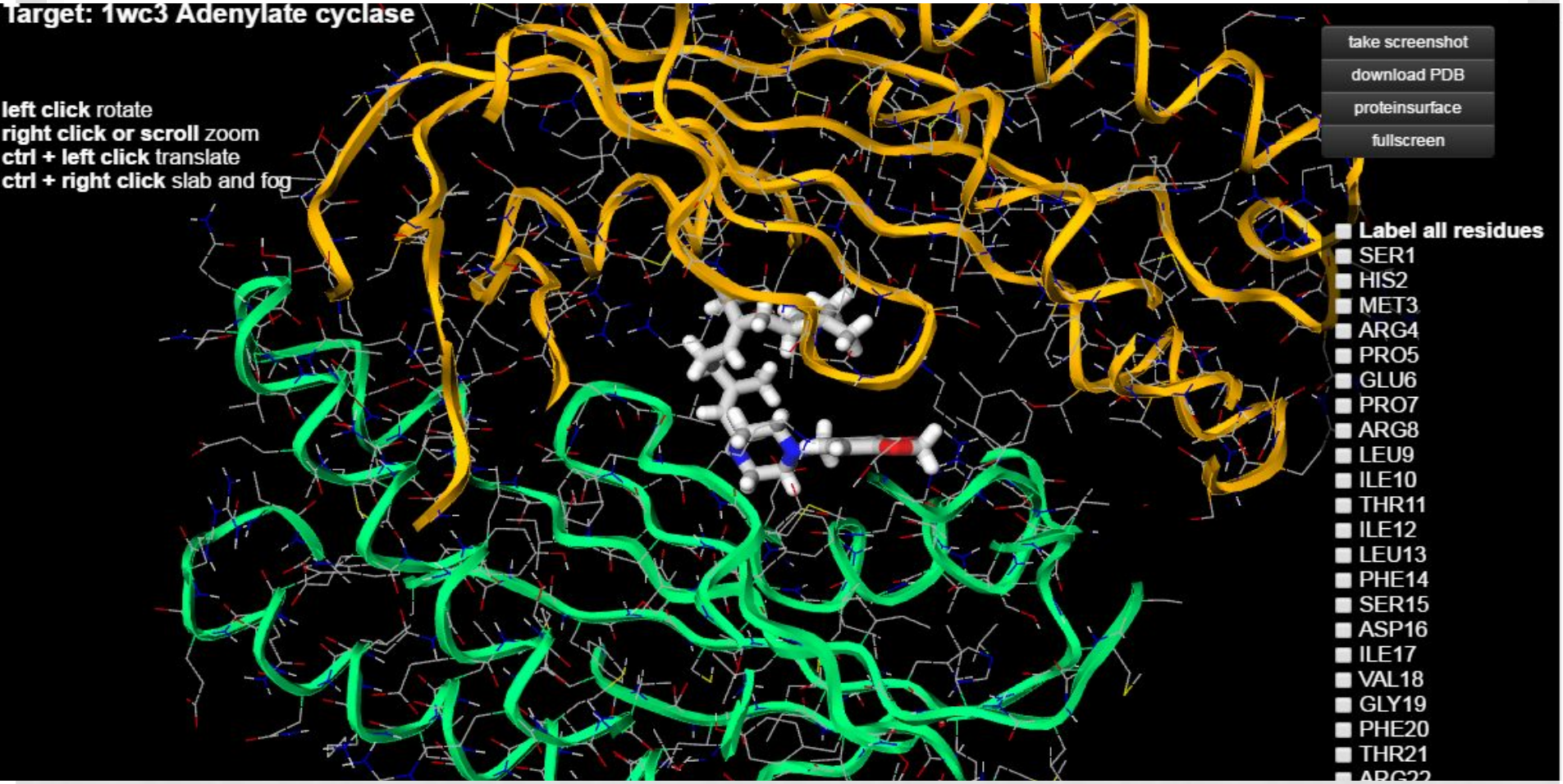

Target: 1pvg DNA topoisomerase 2
left click rotate
right click or scroll zoom
ctrl + left click translate
ctrl + right click slab and fog
take screenshot
download PDB
proteinsurface
fullscreen
Label all residues
SER1
ALA2
SER3
ASP4
LYS5
TYR6
GLN7
LYS8
ILE9
SER10
GLN11
LEU12
GLU13
HIS14
ILE15
LEU16
LYS17
ARG18
PRO19
ASP20
THR21


Target: 1pvg DNA topoisomerase 2
left click rotate
right click or scroll zoom
ctrl + left click translate
ctrl + right click slab and fog
take screenshot
download PDB
proteinsurface
fullscreen
Label all residues
SER1
ALA2
SER3
ASP4
LYS5
TYR6
GLN7
LYS8
ILE9
SER10
GLN11
LEU12
GLU13
HIS14
ILE15
LEU16
LYS17
ARG18
PRO19
ASP20
THR21

РЕЗУЛЬТАТ РАБОТЫ В DOKING ADENYLATE CYCLASE STIMULANT

Docking pose	Docking score		
#1	-7.3	VISUALIZE POSE	DOWNLOAD POSE
#2	-7.3	VISUALIZE POSE	DOWNLOAD POSE
#3	-7.2	VISUALIZE POSE	DOWNLOAD POSE
#4	-7.0	VISUALIZE POSE	DOWNLOAD POSE


Target: 1wc3 Adenylate cyclase
left click rotate
right click or scroll zoom
ctrl + left click translate
ctrl + right click slab and fog
take screenshot
download PDB
proteinsurface
fullscreen
Label all residues
SER1
HIS2
MET3
ARG4
PRO5
GLU6
PRO7
ARG8
LEU9
ILE10
THR11
ILE12
LEU13
PHE14
SER15
ASP16
ILE17
VAL18
GLY19
PHE20
THR21


Target: 1wc3 Adenylate cyclase
left click rotate
right click or scroll zoom
ctrl + left click translate
ctrl + right click slab and fog
take screenshot
download PDB
proteinsurface
fullscreen
Label all residues
SER1
HIS2
MET3
ARG4
PRO5
GLU6
PRO7
ARG8
LEU9
ILE10
THR11
ILE12
LEU13
PHE14
SER15
ASP16
ILE17
VAL18
GLY19
PHE20
THR21

ВЫВОДЫ ПО РАБОТЕ

- Результат биологической активности получены с помощью программы Pass показали что Пифарнин является препаратом, обладающим спазмалитическим и обезболивающим действием.
- В результате докинг-анализа рассматриваемого вещества для 3-х мишеней, были расчитаны энергии на основании которых можно сделать вывод, что наибольшее взаимодействие Пифарнин проявляет с Topoisomerase II.