

1. Save Gold complex with highest HSC conformation or top SHB conformation according to the manuscript into the pdb file.
2. Open the GaussView and delete ligand and two heme groups from the complex.
3. Open 'R' program and write EXACTLY the following:

```
library(bio3d)
```

```
t<-
```

```
read.pdb('B:/Ozren/COCONUT/Gold_izabr/Gold_izabr_fileovi/To_MD  
_simul/prot/Only_protein_gold_soln_CNP0406621_27_HBGlu272.pd  
b') #route to the only_protein_file
```

```
FE<-as.matrix(t$atom)
```

```
FEsort<-FE[order(FE[,7]),]
```

```
FEsort2<-FEsort[,-16]
```

```
FEsort2<-FEsort2[,-8]
```

```
FEsort2<-FEsort2[,-4]
```

```
FE3<-FEsort2
```

```
for (i in 1:nrow(FE3)) {
```

```
  if (FE3[i,1]=='HETATM')
```

```
    FE3[i,1]<-'ATOM'
```

```
    FE3[i,2]<-i
```

```
    FE3[i,10]<-1.00
```

```
    FE3[i,11]<-0.00
```

```
    FE3[i,12]<-'CP1'
```

```
  }
```

```
write.table(FE3,
```

```
'B:/Ozren/COCONUT/Gold_izabr/Gold_izabr_fileovi/To_MD_simul/prot/output_166.pdb'  
,quote=FALSE,sep = " ",col.names=FALSE,row.names=FALSE)
```

q()

n

4. Open the python and write exactly the following:

python

s=""

with open('output_166.pdb','r') as f:

for line in f:

data=line.split()

s+= '{0[0]:<5}{0[1]:>6}'.format(data)+'
'+'{0[2]:<5}{0[3]:<4}{0[4]:<2}{0[5]:>3}{0[6]:>12}{0[7]:>8}{0[8]:>8}{0[9]:>6}{0[10]:>6}
{0[11]:>9}{0[12]:>3}'.format(data)+'\n'

f6=open('w166.pdb','w')

f6.write(s)

f6.close()

exit()

5. Add at the beginning of the file "REMARK original generated coordinate pdb file" and add at the end of the file: "END". Rename the file according to the docked ligand name.

6. Open the finally obtained file with the GaussView to check it.