

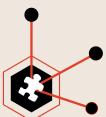




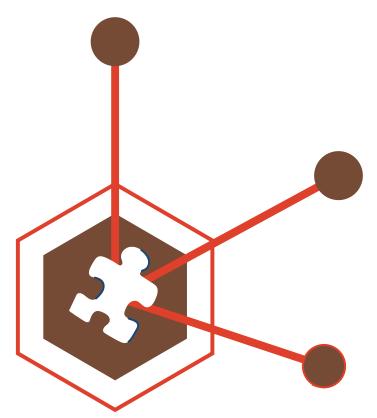
Alternative Colors







Icon of the '.exe' (Windows Version)





Software Concept v1.0

```
: C:\Users\Rêmullo Costa\Desktop\Compounds\Patente\dockme-lite.exe
                                                               X
INKkdddxkx:,,dXNNNKkxddddxOKNNNNNKkxddddxk0NXo,,:0WNNKkxxkKNKl,,ox:,c0NNO:,cxl,,oXNNNXOxxdddxk0XNNNN
NOc,,;ccc:;,,dXNXx:,,:cc:,;:kXNXk:;,,::::ckNXo,,:8WN01;,ckXNK1,,o8o,;xNXd,;d01,,1KNN01;,:clc;,;oKNNN
Kl,,:kXXXk:,,dXNk;,;o0XX01,,:ONO:,,ckKKKKXNXo,,:x0x:,;oKNNN0c,,oXO:,cK0c,c0Xo,,lKWK1,,cOXXXd;,;kNNN
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Kd;,;lxxdc;,,dXNOc,,cxOOd:,,c0W01,,;oxkkkxONXo,,:0WNOc,;l0NNO:,;xNNXxll1lkXNKd;,:OWXd;,;lxkkkkxOXNNN
ikd:;;;:1xd::dXNNOoc:;;;;:cd0NNN0dc:;;;;::xXXd::10NNN0o::10NOc:ckNNNNNNXKXX0d1:ckK0koc:;;;;::dKNNN
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Bem-vindo ao dockME!
Dual tarefa deseia realizar?
           MENU:
           [1] - Iniciar Interação COMPLETA entre Macromoleculas e ligantes
           [2] - Iniciar Interação INDIVIDUAL entre Macromoleculas e ligantes
           [3] - Sair
scolha uma opção:
```



Software Concept v1.0

```
d: C:\Users\Rêmullo Costa\Desktop\Compounds\Patente\dockme-lite.exe

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инивания в с : : dxnannannannannannannannannannannan dx : c выпинивания x c : : : c вканина в ! : : : c кинивания напинивания
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NKKdddxkx:,,dxmnNKixddddxXKNNmmNKixddddxk0NXo,,:0WmNKixxkKNKl,,ox:,c0NNO:,cxl,,oxmnXXxxdddxk0XmmN
Oc,,;ccc:;,,dxnxx:,,:cc:,;:kxnxk:;,,::::cknxxo,,:0wn01;,ckxnxl,,000,;xnxxd,;d01,,lxnnv01;,:clc;,;oknnnn
1,,:kxxxx:,,dxxk;,;eexxel,,:oxo:,,ckxxxxxxxxo,,:xex:,;oxxxxec,cxo:,cxec,cexo,,lxxxl,,cxxxxd;,;kxxx
c,,lknnno:,;dxnd,,;xnnnxd;,;xnk;,,dxnnnnnnnxo,,;::;,;oxnnnnec,;dxxo,;xd;,dxxo,,cewo:,,:looo:,,lennn
c,,cewano:,,oxnd;,;xnnaxd;,;xnk;,,oxnanaanaxo,,:kxk:,;oxnano:,;dnnk:,::,:0xxd;,cewec,,;oxxxxkoxnaan
d;,;lxxdc;,,dxNoc,,cx0od:,,ceWel,,;oxkkkxONXo,,:eWNoc,;leNNo:,;xNNXxllllkXNKd;,:OWXd;,;lxkkkkxOXNNN
Kd:;;;:lxd::dxnNooc:;;;;:cd0NNN0dc:;;;;;:xXXd::l0NNN0o::l0NOc:ckNNNNNNNXXXXXdl:ckK0kc:;;;;;::dKNNN
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Bem-vindo ao dockME!
Qual tarefa deseja realizar?
                   MENUL
                   [1] - Iniciar Interação COMPLETA entre Macromoleculas e ligantes
                    [2] - Iniciar Interação INDIVIDUAL entre Macromoleculas e ligantes
                   [3] - Sair
scolha uma opção: 2
lista de macromoleculas ['0.pdbqt', '1.pdbqt', '2.pdbqt', '3.pdbqt', '4.pdbqt', '5.pdbqt', '6.pdbqt']
Digite a ordem da macromolécula, com base na lista acima: 1
lista de ligantes ['10.pdbqt', '11.pdbqt', '12.pdbqt', '2.pdbqt', '3.pdbqt', '4.pdbqt', '5.pdbqt', '6.pdbqt', '7.pdbqt
'8.pdbqt', '9.pdbqt']
Digite a ordem do ligante, com base na lista acima: 3
```

The software were able to list the files from the macromolecules and ligands folders, show it up to the user and let him choose which one he wanted to use. Very straight forward, making all the docking process easier, with no complicated command lines