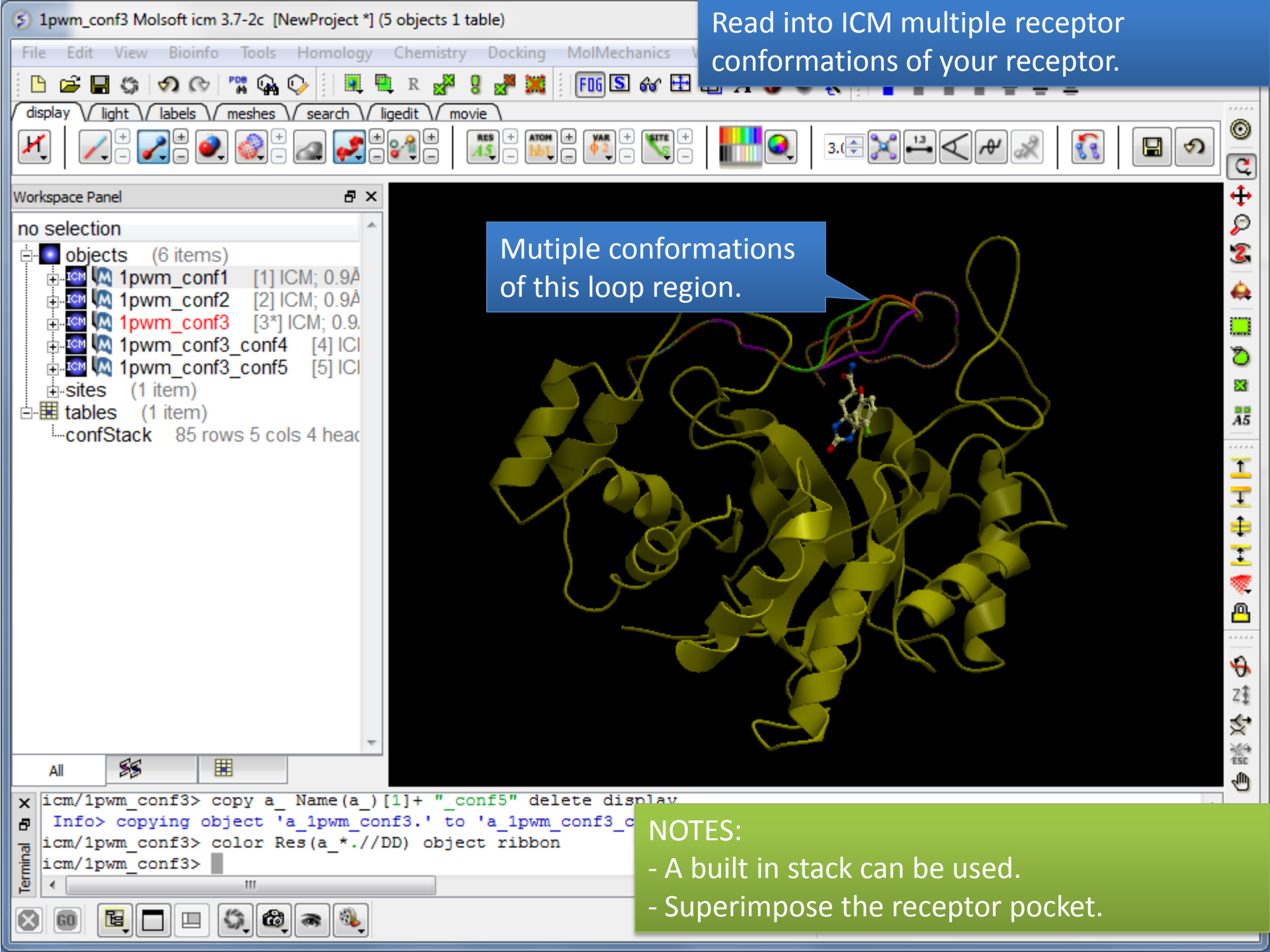
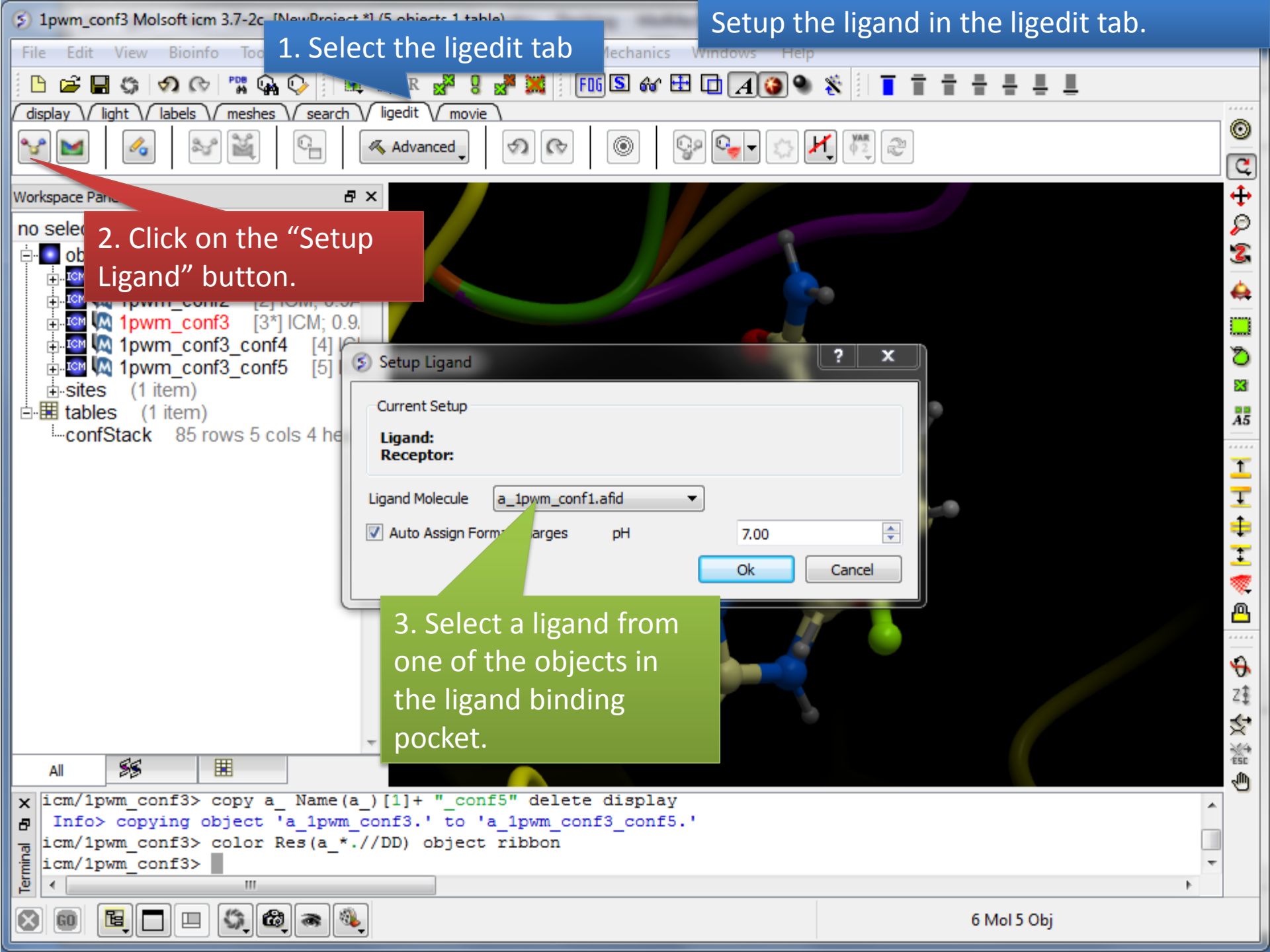
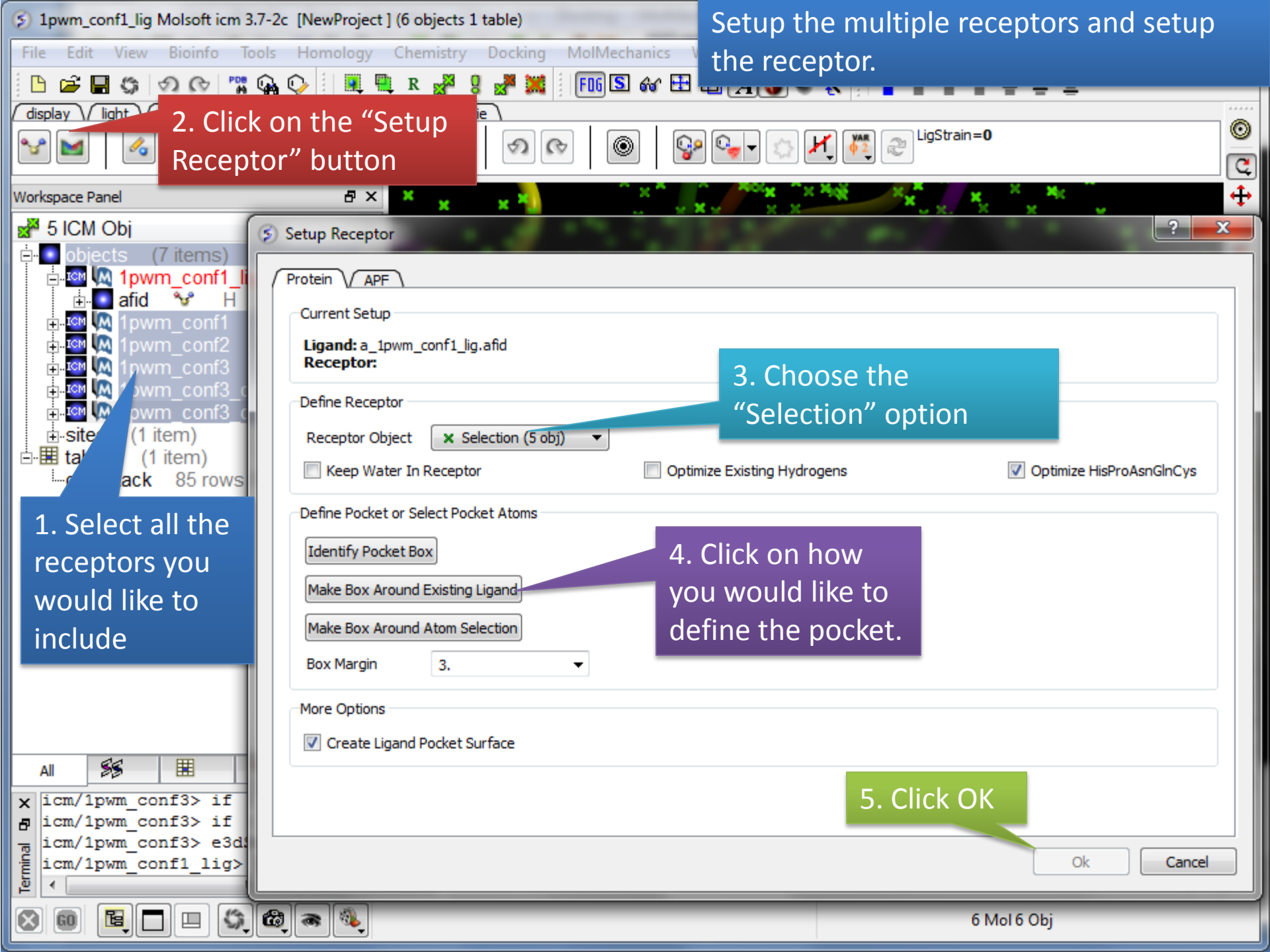
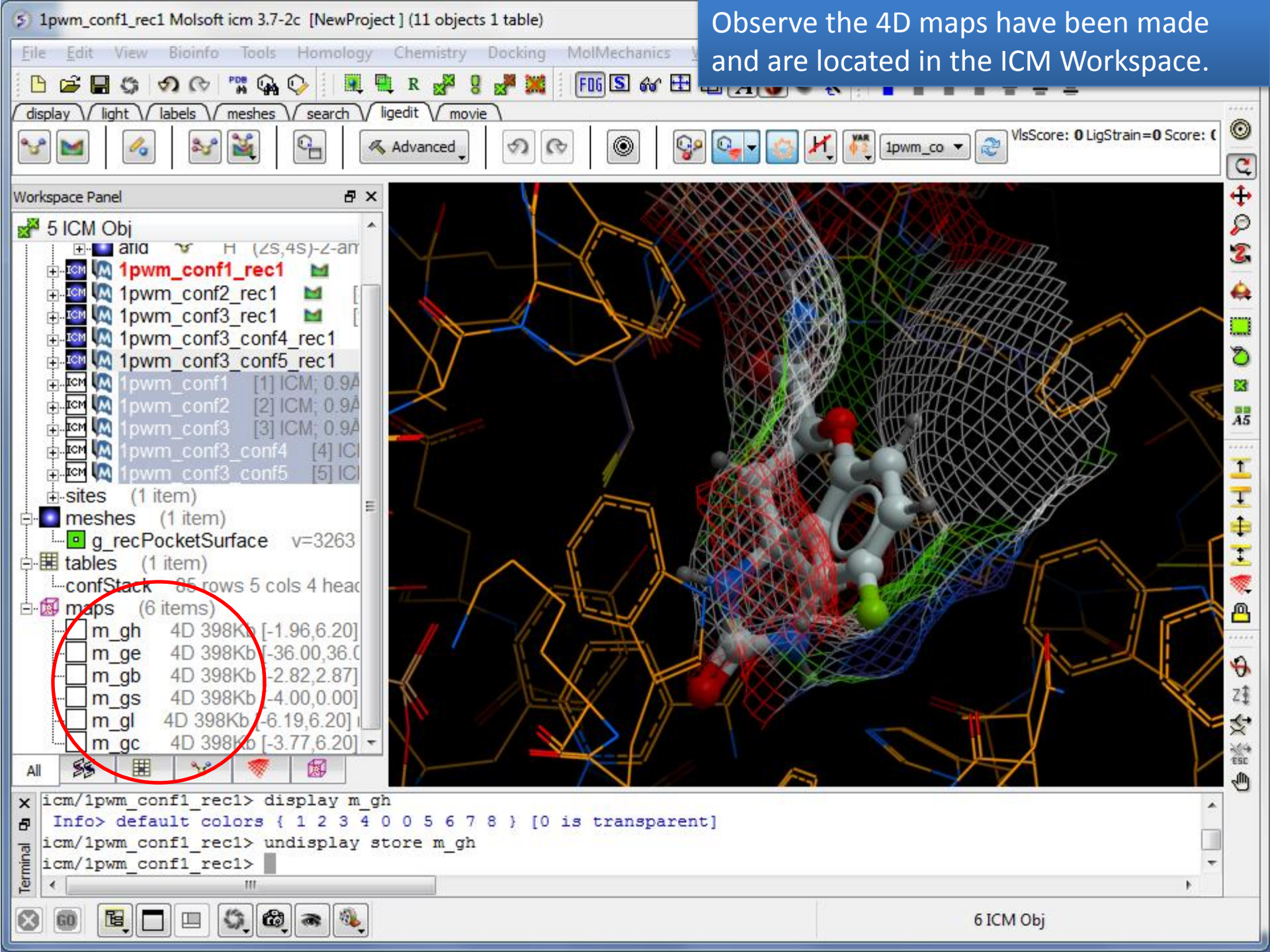
Read into ICM multiple receptor conformations of your receptor.

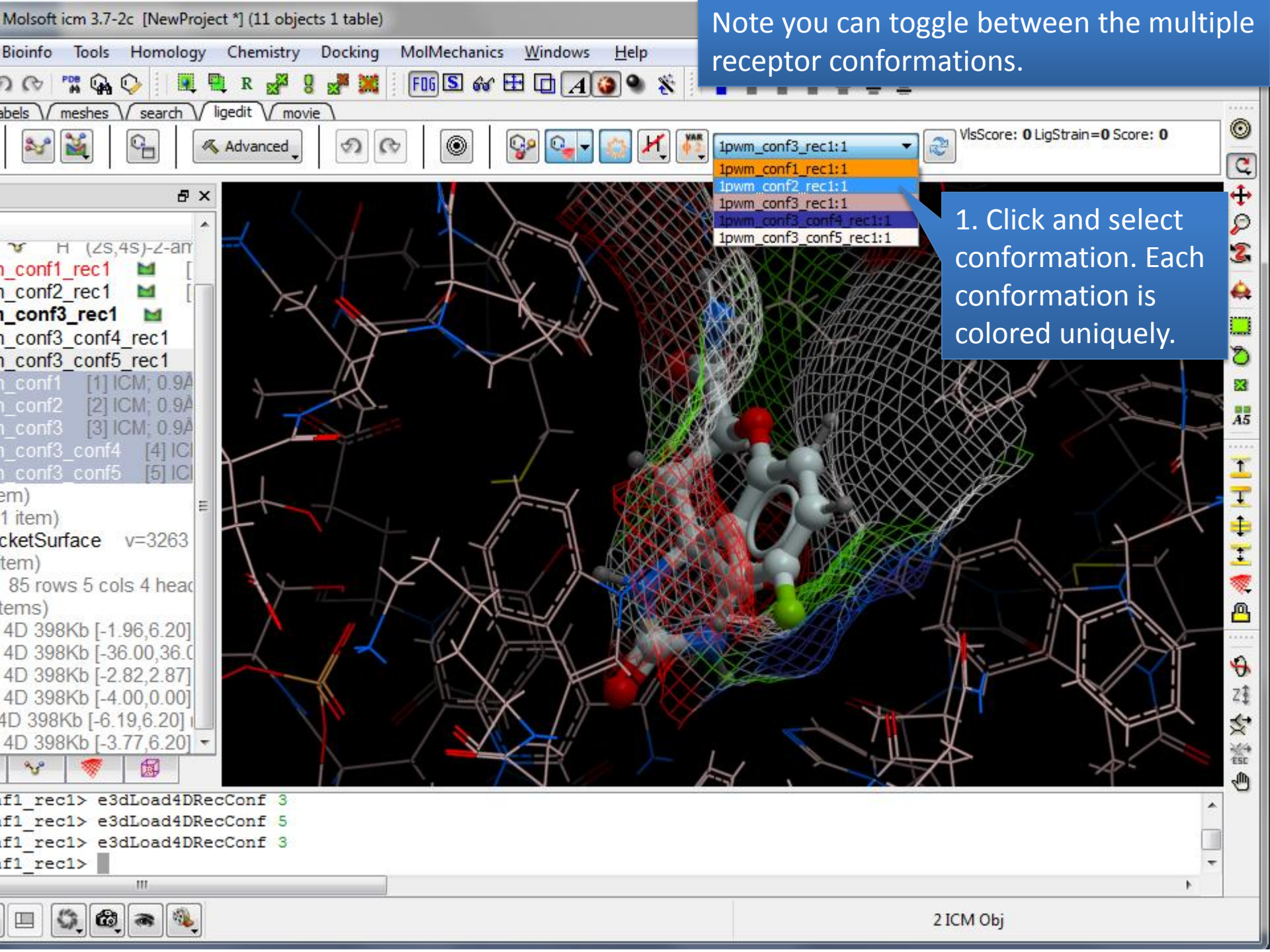


NOTES:
- A built in stack can be used.
- Superimpose the receptor pocket.

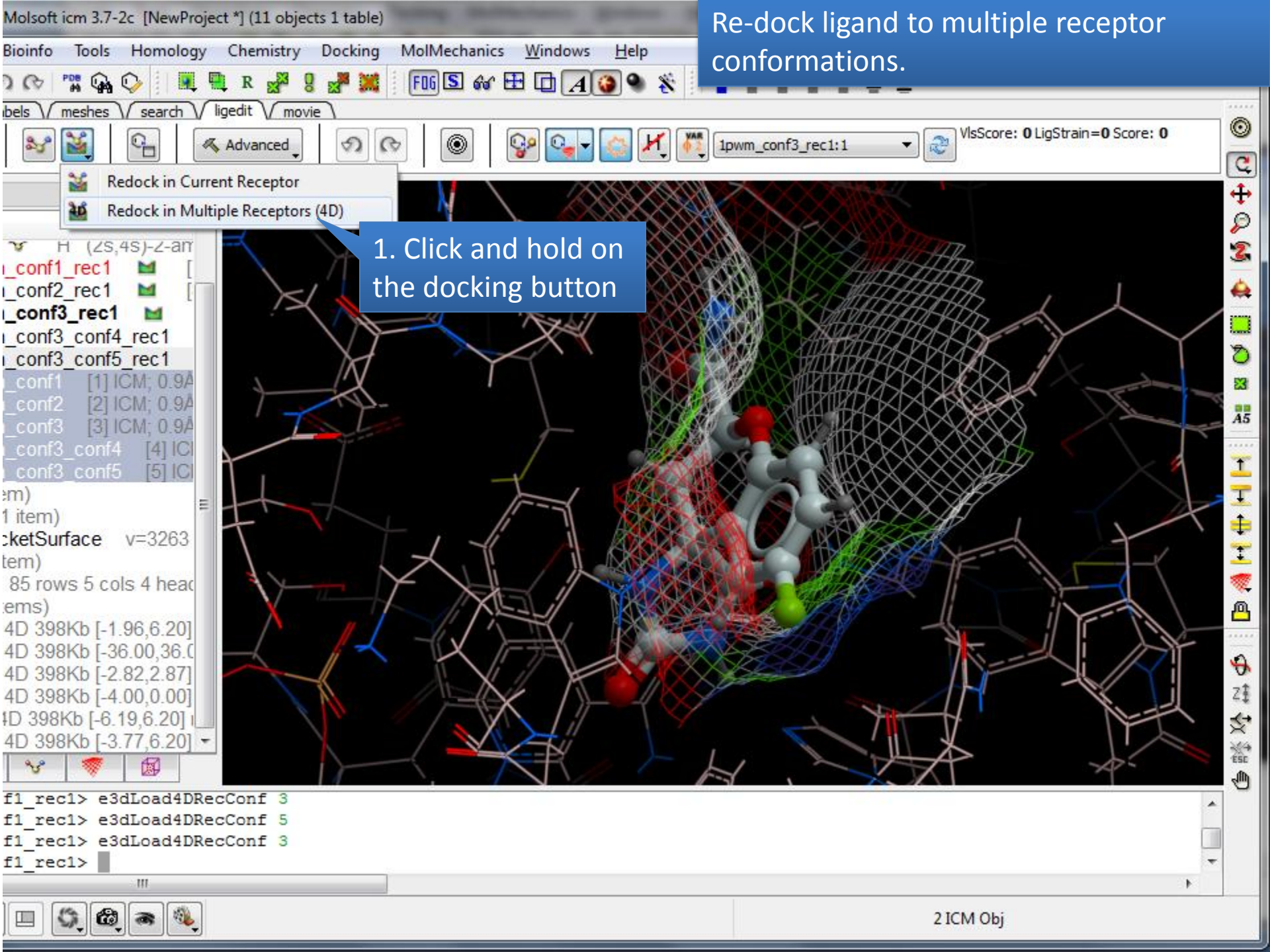

Setup the ligand in the ligedit tab.
1. Select the ligedit tab
2. Click on the “Setup Ligand” button.
3. Select a ligand from one of the objects in the ligand binding pocket.
Setup Ligand
Current Setup
Ligand:
Receptor:
Ligand Molecule
a_1pwm_conf1.afid
pH
7.00
Ok
Cancel
1pwm_conf3
1pwm_conf3_conf4
1pwm_conf3_conf5
sites (1 item)
tables (1 item)
confStack
icm/1pwm_conf3> copy a_ Name(a_)[1]+ "_conf5" delete display
Info> copying object 'a_1pwm_conf3.' to 'a_1pwm_conf3_conf5.'
icm/1pwm_conf3> color Res(a_*.//DD) object ribbon
icm/1pwm_conf3>
6 Mol 5 Obj

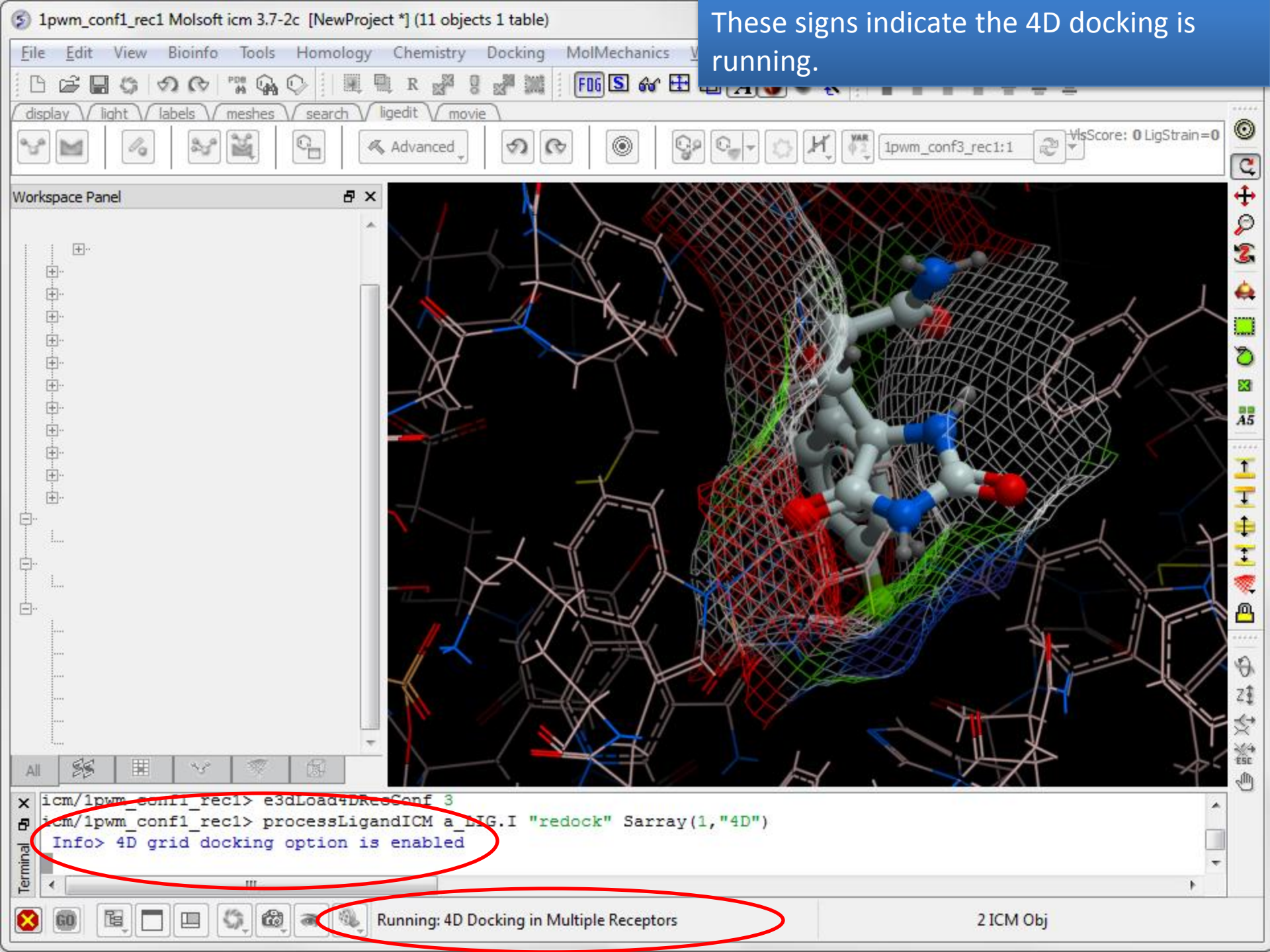

Setup the multiple receptors and setup the receptor.
2. Click on the “Setup Receptor” button
1. Select all the receptors you would like to include
3. Choose the “Selection” option
4. Click on how you would like to define the pocket.
5. Click OK
Setup Receptor
Protein
APF
Current Setup
Ligand: a_1pwm_conf1_lig.afid
Receptor:
Define Receptor
Receptor Object
Selection (5 obj)
Keep Water In Receptor
Optimize Existing Hydrogens
Optimize HisProAsnGlnCys
Define Pocket or Select Pocket Atoms
Identify Pocket Box
Make Box Around Existing Ligand
Make Box Around Atom Selection
Box Margin
3.
More Options
Create Ligand Pocket Surface
Ok
Cancel
Workspace Panel
5 ICM Obj
objects (7 items)
1pwm_conf1_lig
afid
1pwm_conf1
1pwm_conf2
1pwm_conf3
site (1 item)
(1 item)
85 rows
LigStrain=0
icm/1pwm_conf3> if
icm/1pwm_conf3> if
icm/1pwm_conf3> e3d
icm/1pwm_conf1_lig>
Terminal
6 Mol 6 Obj

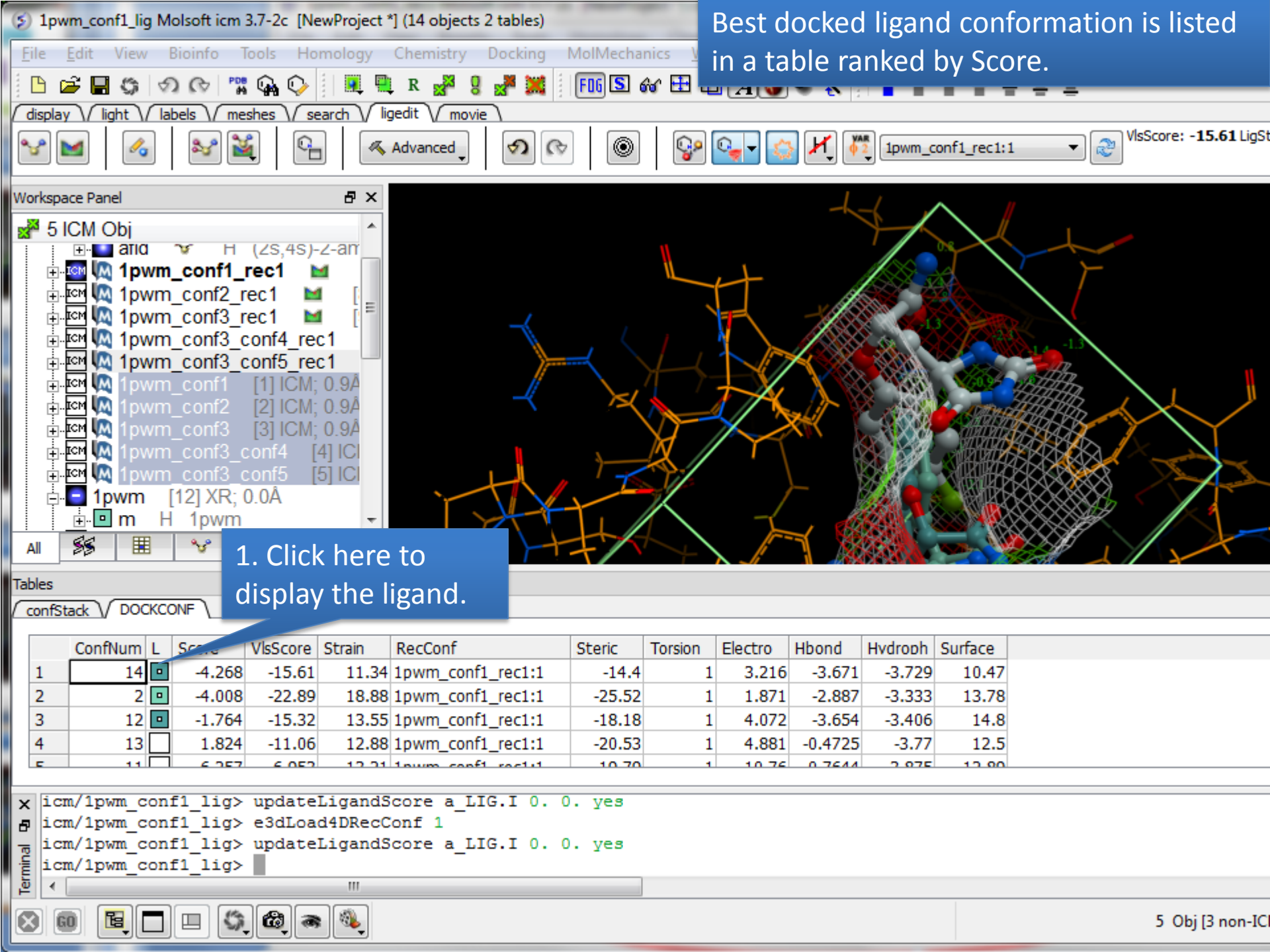

Observe the 4D maps have been made and are located in the ICM Workspace.
1pwm_conf1_rec1 Molsoft icm 3.7-2c [NewProject] (11 objects 1 table)
File Edit View Bioinfo Tools Homology Chemistry Docking MolMechanics
display light labels meshes search ligedit movie
Advanced
1pwm_co
VlsScore: 0 LigStrain=0 Score:
Workspace Panel
5 ICM Obj
1pwm_conf1_rec1
1pwm_conf2_rec1
1pwm_conf3_rec1
1pwm_conf3_conf4_rec1
1pwm_conf3_conf5_rec1
1pwm_conf1 [1] ICM; 0.9
1pwm_conf2 [2] ICM; 0.9
1pwm_conf3 [3] ICM; 0.9
1pwm_conf3_conf4 [4] IC
1pwm_conf3_conf5 [5] IC
sites (1 item)
meshes (1 item)
g_recPocketSurface v=3263
tables (1 item)
confStack
maps (6 items)
m_gh 4D 398Kb [-1.96,6.20]
m_ge 4D 398Kb [-36.00,36.0
m_gb 4D 398Kb [-2.82,2.87]
m_gs 4D 398Kb [-4.00,0.00]
m_gl 4D 398Kb [-6.19,6.20]
m_gc 4D 398Kb [-3.77,6.20]
All
icm/1pwm_conf1_rec1> display m_gh
Info> default colors { 1 2 3 4 0 0 5 6 7 8 } [0 is transparent]
icm/1pwm_conf1_rec1> undisplay store m_gh
icm/1pwm_conf1_rec1>
Terminal
6 ICM Obj

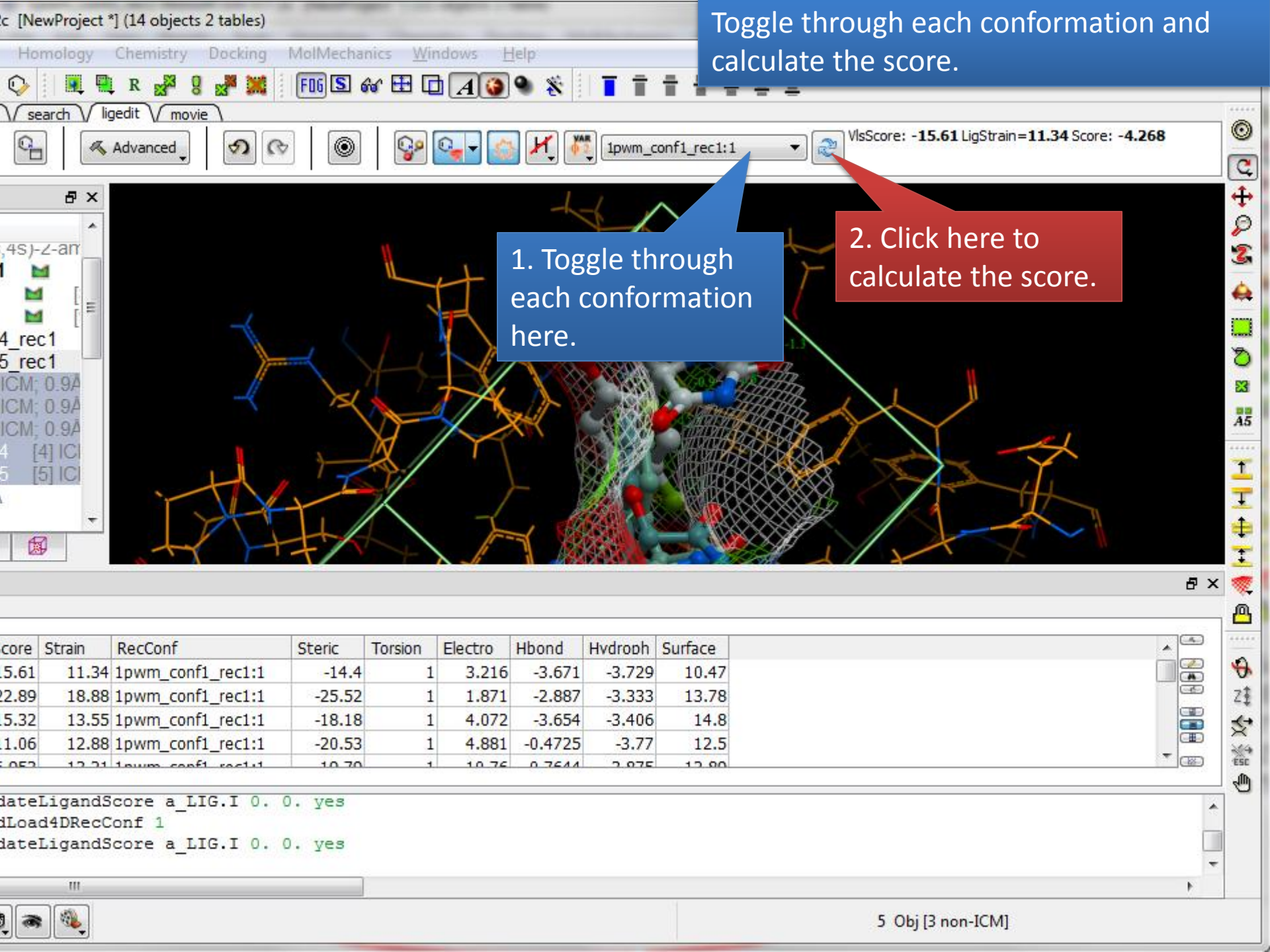

Note you can toggle between the multiple receptor conformations.
Molsoft icm 3.7-2c [NewProject *] (11 objects 1 table)
Bioinfo Tools Homology Chemistry Docking MolMechanics Windows Help
labels meshes search ligedit movie
Advanced
1pwm_conf3_rec1:1
1pwm_conf1_rec1:1
1pwm_conf2_rec1:1
1pwm_conf3_rec1:1
1pwm_conf3_conf4_rec1:1
1pwm_conf3_conf5_rec1:1
VlsScore: 0 LigStrain=0 Score: 0
1. Click and select conformation. Each conformation is colored uniquely.
_conf1_rec1
_conf2_rec1
_conf3_rec1
_conf3_conf4_rec1
_conf3_conf5_rec1
_conf1 [1] ICM; 0.9Å
_conf2 [2] ICM; 0.9Å
_conf3 [3] ICM; 0.9Å
_conf3_conf4 [4] IC
_conf3_conf5 [5] IC
cketSurface v=3263
85 rows 5 cols 4 head
4D 398Kb [-1.96,6.20]
4D 398Kb [-36.00,36.0
4D 398Kb [-2.82,2.87]
4D 398Kb [-4.00,0.00]
4D 398Kb [-6.19,6.20]
4D 398Kb [-3.77,6.20]
f1_rec1> e3dLoad4DRecConf 3
f1_rec1> e3dLoad4DRecConf 5
f1_rec1> e3dLoad4DRecConf 3
f1_rec1>
2 ICM Obj

Re-dock ligand to multiple receptor conformations.




These signs indicate the 4D docking is running.
1pwm_conf1_rec1 Molsoft icm 3.7-2c [NewProject *] (11 objects 1 table)
File Edit View Bioinfo Tools Homology Chemistry Docking MolMechanics
display light labels meshes search ligedit movie
Advanced
1pwm_conf3_rec1:1
VisScore: 0 LigStrain=0
Workspace Panel
All
icm/1pwm_conf1_rec1> e3dLoad4DRecConf 3
icm/1pwm_conf1_rec1> processLigandICM a_LIG.I "redock" Sarray(1,"4D")
Info> 4D grid docking option is enabled
Terminal
Running: 4D Docking in Multiple Receptors
2 ICM Obj


1pwm_conf1_lig Molsoft icm 3.7-2c [NewProject *] (14 objects 2 tables)
Best docked ligand conformation is listed in a table ranked by Score.
File Edit View Bioinfo Tools Homology Chemistry Docking MolMechanics
display light labels meshes search ligedit movie
Advanced
1pwm_conf1_rec1:1
VlsScore: -15.61 LigSt
Workspace Panel
5 ICM Obj
1pwm_conf1_rec1
1pwm_conf2_rec1
1pwm_conf3_rec1
1pwm_conf3_conf4_rec1
1pwm_conf3_conf5_rec1
1pwm_conf1 [1] ICM; 0.9Å
1pwm_conf2 [2] ICM; 0.9Å
1pwm_conf3 [3] ICM; 0.9Å
1pwm_conf3_conf4 [4] ICM
1pwm_conf3_conf5 [5] ICM
1pwm [12] XR; 0.0Å
m H 1pwm
All
1. Click here to display the ligand.
Tables
confStack DOCKCONF
ConfNum L Score VlsScore Strain RecConf Steric Torsion Electro Hbond Hydroph Surface
1 14 -4.268 -15.61 11.34 1pwm_conf1_rec1:1 -14.4 1 3.216 -3.671 -3.729 10.47
2 2 -4.008 -22.89 18.88 1pwm_conf1_rec1:1 -25.52 1 1.871 -2.887 -3.333 13.78
3 12 -1.764 -15.32 13.55 1pwm_conf1_rec1:1 -18.18 1 4.072 -3.654 -3.406 14.8
4 13 1.824 -11.06 12.88 1pwm_conf1_rec1:1 -20.53 1 4.881 -0.4725 -3.77 12.5
icm/1pwm_conf1_lig> updateLigandScore a_LIG.I 0. 0. yes
icm/1pwm_conf1_lig> e3dLoad4DRecConf 1
icm/1pwm_conf1_lig> updateLigandScore a_LIG.I 0. 0. yes
icm/1pwm_conf1_lig>
Terminal
GO
5 Obj [3 non-IC


Toggle through each conformation and calculate the score.
[NewProject *] (14 objects 2 tables)
Homology Chemistry Docking MolMechanics Windows Help
search ligedit movie
Advanced
1pwm_conf1_rec1:1
VlsScore: -15.61 LigStrain=11.34 Score: -4.268
1. Toggle through each conformation here.
2. Click here to calculate the score.
core Strain RecConf Steric Torsion Electro Hbond Hydroph Surface
15.61 11.34 1pwm_conf1_rec1:1 -14.4 1 3.216 -3.671 -3.729 10.47
22.89 18.88 1pwm_conf1_rec1:1 -25.52 1 1.871 -2.887 -3.333 13.78
15.32 13.55 1pwm_conf1_rec1:1 -18.18 1 4.072 -3.654 -3.406 14.8
11.06 12.88 1pwm_conf1_rec1:1 -20.53 1 4.881 -0.4725 -3.77 12.5
dateLigandScore a_LIG.I 0. 0. yes
dLoad4DRecConf 1
dateLigandScore a_LIG.I 0. 0. yes
5 Obj [3 non-ICM]