Supplementary Figure 2. Script for visualization of tunnels in YASARA. Adjust text in bold to ensure correct path to generated tunnel files (from CAVER).

```
###Macro to merge tunnels generated from CAVER for visualization in YASARA###

clear

#The MacroTarget of this example is a snapshot generated from 2.1) above
LoadPDB (MacroTarget).pdb, Center = No

#Path to the output folder of CAVER tunnels, change this to your specific path
path = 'C:\Users\Asus\Desktop\caver_3.0\Out\data\clusters_timeless'

#Variables used to count the number of tunnels found
i = 001
sim = 1
while (sim != 0)
  LoadPDB (path)\tun_cl_(i)_1.pdb, Center = No
  # Join the tunnel with the simulation snapshot
  JoinObj 2,1,Center=No
  i = i+1
  sim = FileSize (path)\tun_cl_(i)_1.pdb
  if not sim
    ShowMessage 'Tunnel cluster (i) not found'
#Save the new file by adding _tunnels to the file name
SavePDB 1,(MacroTarget)_tunnels.pdb, format=PDB, Transform=YES
ShowMessage '(i) tunnels successfully merged.'
```