**Links to software used:**

*Phosphorylation site prediction*

- GPS 3.0 [http://gps.biocuckoo.org/online.php](http://gps.biocuckoo.org/online.php)
- Scansite 3.0 [https://scansite4.mit.edu/](https://scansite4.mit.edu/)

*Molecular Simulation and analysis*

- NAMD 2.12 [https://www.ks.uiuc.edu/Research/namd/](https://www.ks.uiuc.edu/Research/namd/)
- UCSF Chimera 1.14 [https://www.cgl.uchc.edu/chimera/](https://www.cgl.uchc.edu/chimera/)
- ClusPro 2.0 web server (https://cluspro.bu.edu/)
- VMD 1.9.3- [https://www.ks.uiuc.edu/Research/vmd/](https://www.ks.uiuc.edu/Research/vmd/)

*Sequence Analysis*

- Clustal Omega [https://www.ebi.ac.uk/Tools/msa/clustalo/](https://www.ebi.ac.uk/Tools/msa/clustalo/)

*NAMD script files*

- 2VBC_wb_equil.namd - Minimization stage preparing the system for MD simulations is energy minimization
- 2VBC_wb_heat.amd - Heating stage, the temperature of the system is linearly increased from 0K to the desired value. Usually, this temperature corresponds to normal physiological conditions, such as 300K.
- 2VBC_wb_min.namd - Equilibration stage
- 2VBC_wb_quench.namd - Simulation stage, This stage of MD trajectory.

- psfgen_phosphorylation137.pgn – file with protein phosphorylated at S137
- psfgen_phosphorylation189.pgn – file with protein phosphorylated at T189

*NAMD trajectory files*

- WT.pdb – file with Wild Type (WT) protein coordinates regarding protein structures
WT.psf - file with Wild Type (WT) protein structure file

WT_quenchRun2.dcd - file with Wild Type (WT) protein trajectories

137.pdb - file with protein phosphorylated at S137 coordinates regarding protein structures
137.psf - file with protein phosphorylated at S137 structure file
137_quenchRun2.dcd - file with protein phosphorylated at S137 trajectories

189.pdb - file with protein phosphorylated at T189 coordinates regarding protein structures
189.psf - file with protein phosphorylated at T189 structure file
189_quenchRun2.dcd - file with protein phosphorylated at T189 trajectories

namd_run2.R - the R code that has been used to analyze the data and to produce the graphs in the paper.

File extensions

.pdb extension = Protein Data Bank (PDB) file (plain text that store coordinates regarding protein structures.)

.psf extension = Protein structure file (contains all the molecule-specific information needed to apply a particular force field to a molecular system.)

dcd extension = single-precision binary FORTRAN files (the binary trajectory file format used by CHARMM, NAMD.)