Links to software used:

Phosphorylation site prediction

GPS 3.0 http://gps.biocuckoo.org/online.php

NetPhos3.1 http://www.cbs.dtu.dk/services/NetPhos/

Scansite 3.0 https://scansite4.mit.edu/

Molecular Simulation and analysis

NAMD 2.12 https://www.ks.uiuc.edu/Research/namd/

UCSF Chimera 1.14 https://www.cgl.ucsf.edu/chimera/

ClusPro 2.0 web server (https://cluspro.bu.edu/)

VMD 1.9.3- https://www.ks.uiuc.edu/Research/vmd/

Sequence Analysis

Clustal Omega 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.)