Cycle repeated for *n* BLUES iterations

Take in system and identify the water and protein residues

Generate a uniform random point inside the user defined radius

Perform a NCMC move: scale off the interactions, propose a translational water move to that new location, scale on the interactions

Select a random water within the user defined radius

Is the water molecule still inside the area defined by the original radius?

No → The NCMC move is rejected

Yes

The NCMC move is accepted or rejected and the positions are updated

Run an interval of traditional MD