

Supporting Information - Table

RESOURCE	SOURCE	IDENTIFIER
Software and Algorithms		
ModLoop	(49, 50)	https://modbase.compbio.ucsf.edu/modloop/
Gromacs 2016, 4.5.5	(52, 54, 55)	http://www.gromacs.org/
PLUMED version 2.0	(53)	https://www.plumed.org/
Maestro	(60)	https://www.schrodinger.com/maestro
Gaussian 09	(66)	https://gaussian.com/
VMD	(68)	https://www.ks.uiuc.edu/Research/vmd/
PyMol	(69)	https://pymol.org/
DSSP	(70)	https://swift.cmbi.umcn.nl/gv/dssp/
PyEMMA	(73)	http://emma-project.org/
Databases		
PDB files	Protein Data Bank	https://www.rcsb.org/