In Silico Substrate-Binding Profiling for SARS-CoV-2 Main Protease (M^{pro}) Using Hexapeptide Substrates

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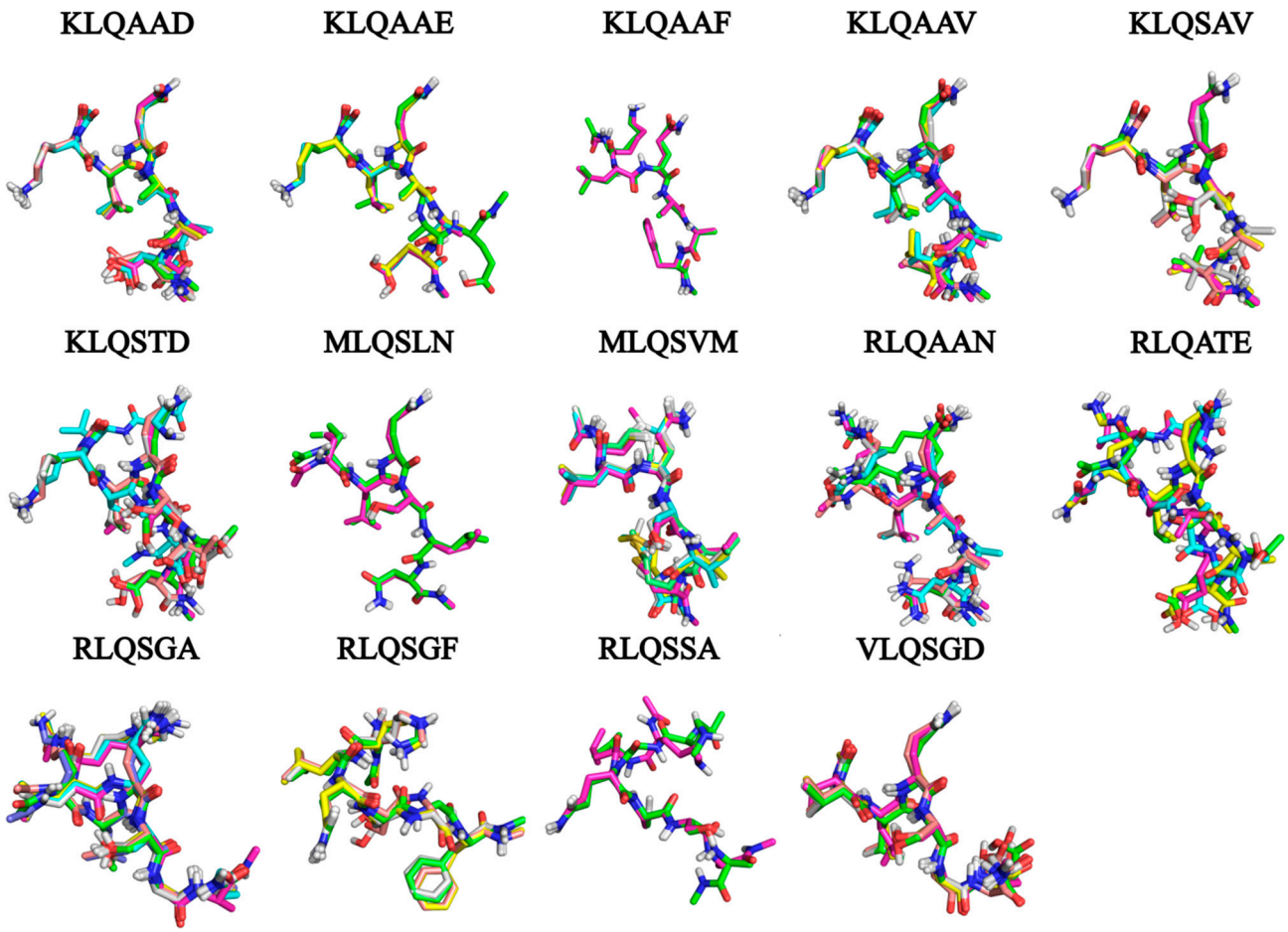
Supplementary Material

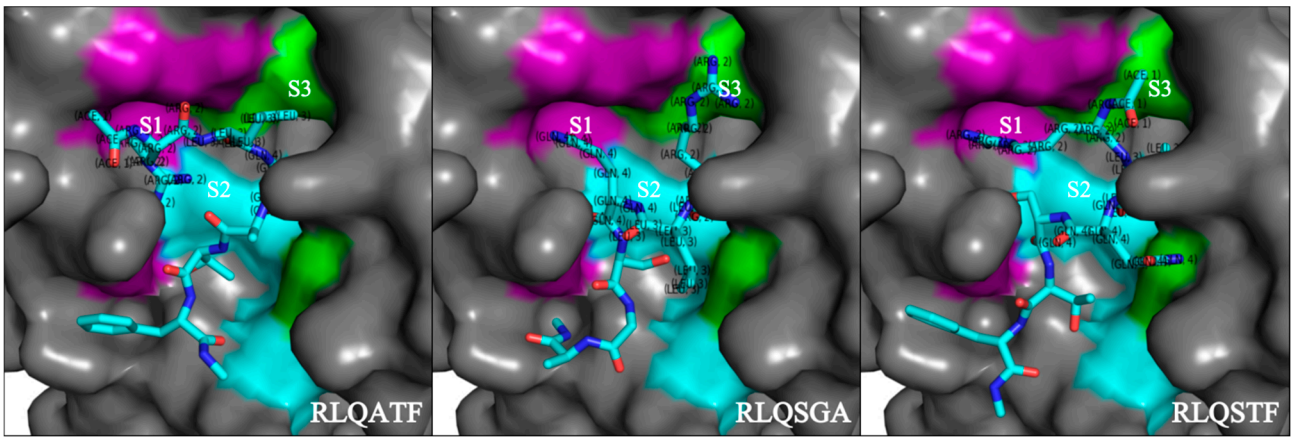


Supplementary Figure S1. Validation of reproducibility of the best poses in the docking results. The visualisation of the best poses of substrates with all 100 conformers docked. Image was generated using PyMOL.

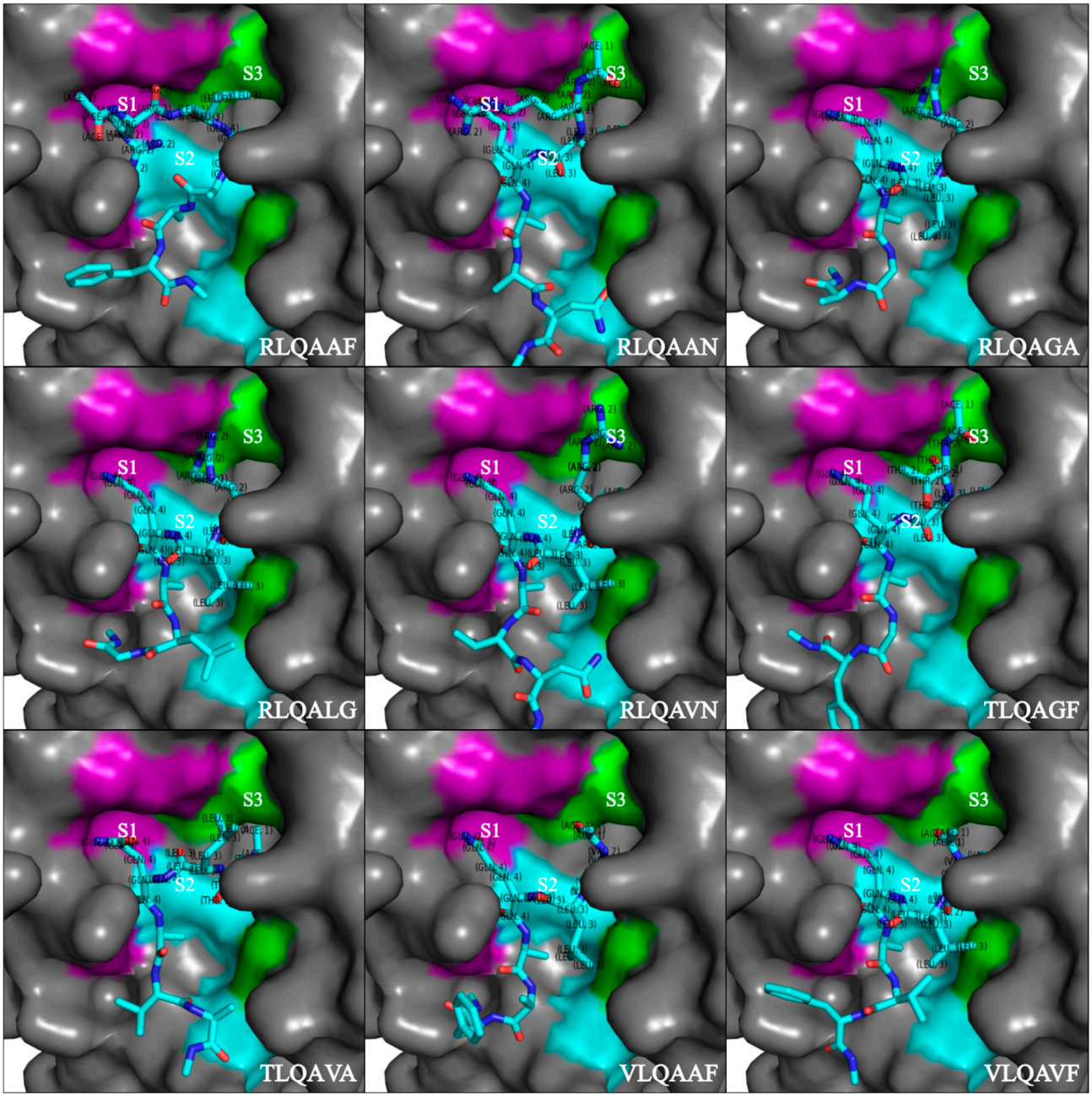
Supplementary Table S1: The ligand efficiencies of the hexapeptide substrates docked onto SARS-CoV-2 M^{pro} on basis of recognition sequence.

Sequence	Docking Score (kcal.mol^{-1})	HA	LE (kcal.mol^{-1} per atom)
LQ↓A	-8.0 ± 0.28	22	-0.4 ± 0.01
LQ↓S	-7.9 ± 0.28	23	-0.3 ± 0.01

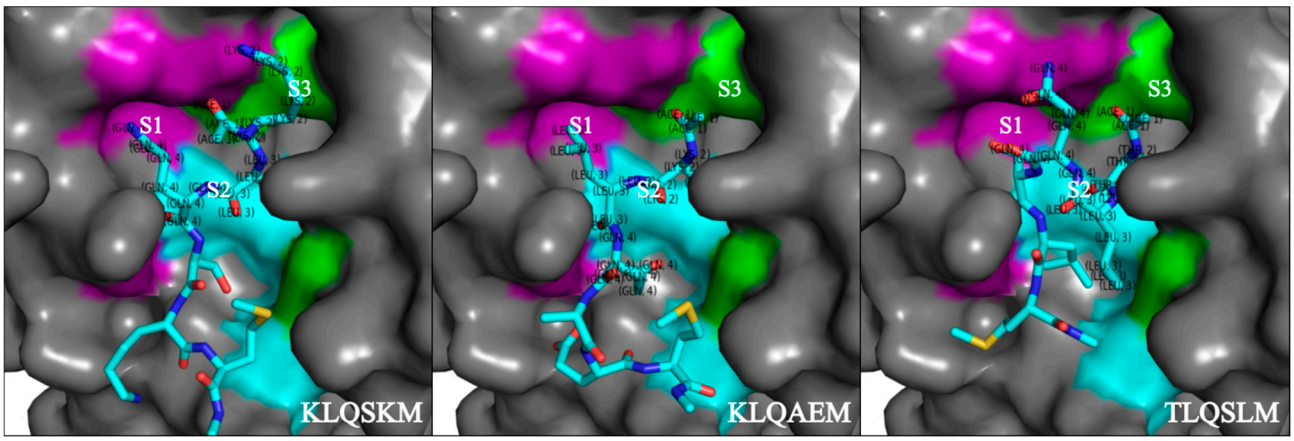
HA: heavy atoms (non-hydrogen atoms); LE: ligand efficiency.



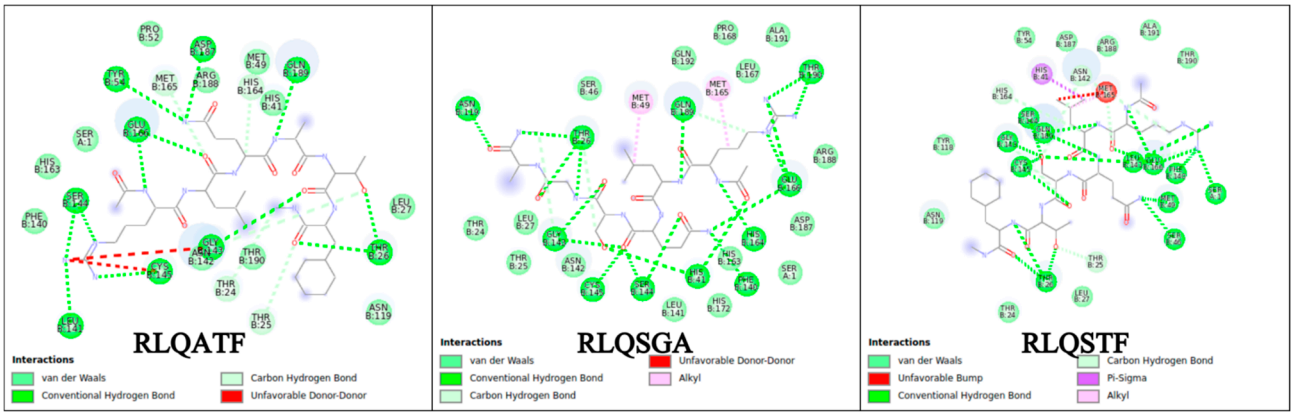
Supplementary Figure S2. Confirmation of SARS-CoV-2 M^{pro} substrate recognition in binding poses for substrates RLQATF, RLQSGA and RLQSTF. The surface of SARS-CoV-2 M^{pro} (PDB ID:6XHM) showing docked substrates and substrate binding subsites colour-coded as follows: Purple: S1, Cyan: S2; Green: S3. The substrates attained a docking score of -8.7 $kcal.mol^{-1}$. The image was generated using PyMOL.



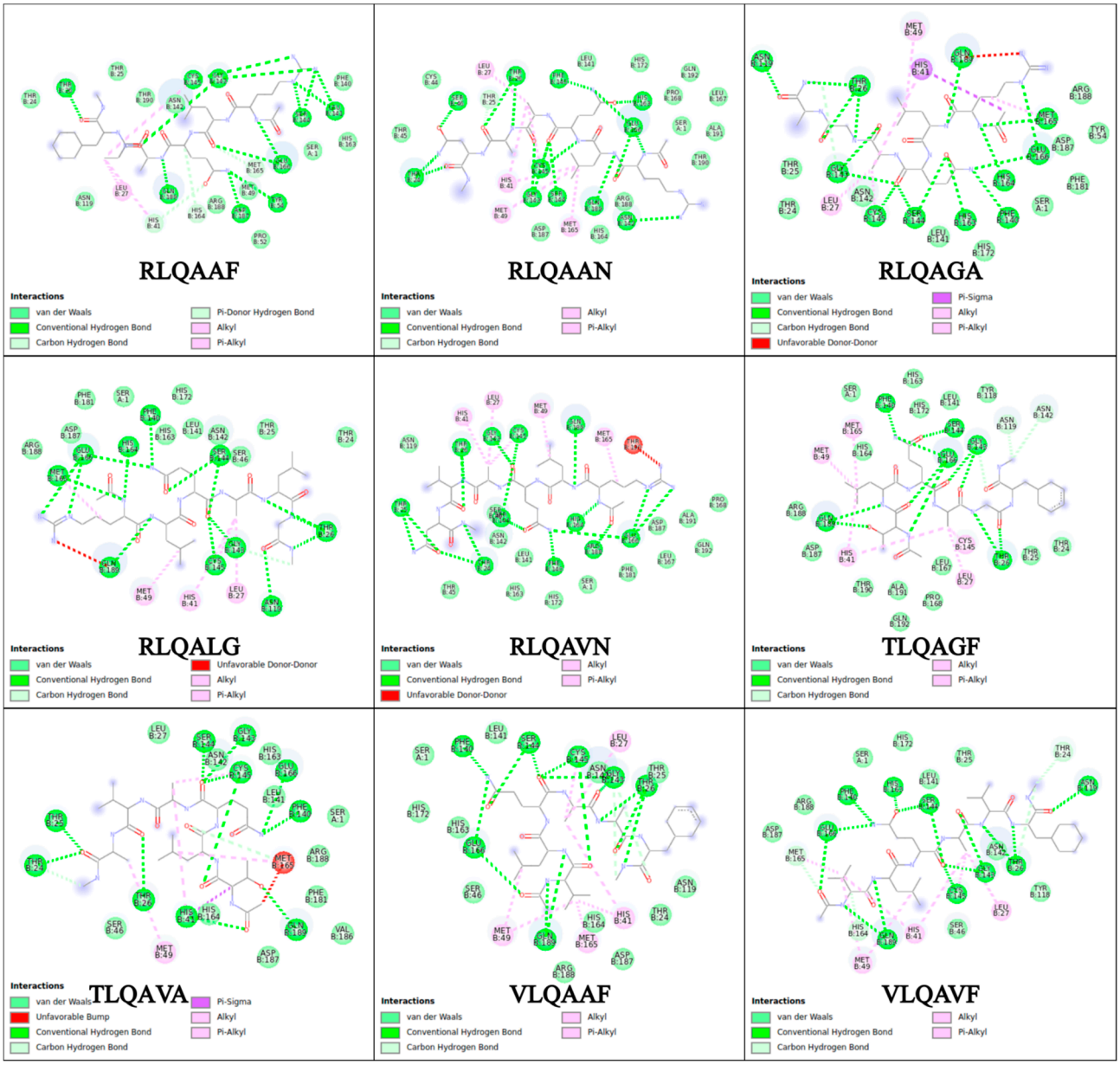
Supplementary Figure S3. Confirmation of SARS-CoV-2 M^{pro} substrate recognition in binding poses for substrates RLQAAN, RLQAAF, RLQAGA, RLQALG, RLQAVN, TLQAGF, TLQAVA, VLQAAF and VLQAVF. The surface of SARS-CoV-2 M^{pro} (PDB ID:6XHM) showing docked substrates and substrate binding subsites colour-coded as follows: Purple: S1, Cyan: S2; Green: S3. The substrates attained a docking score of -8.6 kcal.mol^{-1}. The image was generated using PyMOL.



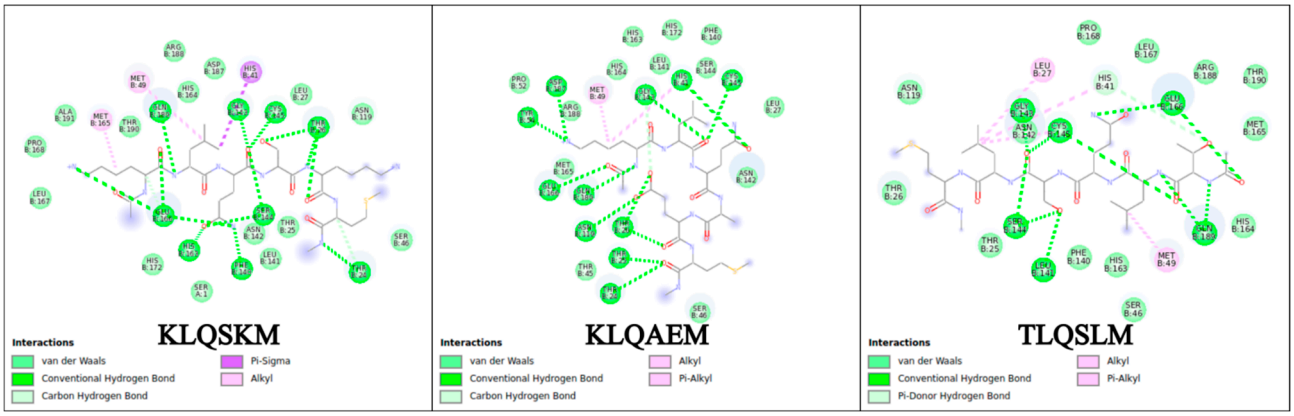
Supplementary Figure S4. Confirmation of SARS-CoV-2 M^{pro} substrate recognition in binding poses for substrates KLQSKM, KLQAEM and TLQSLM. The surface of SARS-CoV-2 M^{pro} (PDB ID:6XHM) showing docked substrates and substrate binding subsites color-coded as follows: Purple: S1, Cyan: S2; Green: S3. The substrates attained docking score of -7.0 kcal.mol^{-1} (KLQSKM) and -7.1 kcal.mol^{-1} (KLQAEM and TLQSLM). Image was generated using PyMOL



Supplementary Figure S5. Resolution of intermolecular interactions between M^{pro} and substrates at the active site. 2D representation of the protein-ligand interactions at active sites for M^{pro} complexed with RLQATF, RLQSGA and RLQSTF hexapeptides. The substrates attained a docking score of -8.6 kcal.mol^{-1}. The images were generated on BIOVIA Discovery Studio 2020 Client.

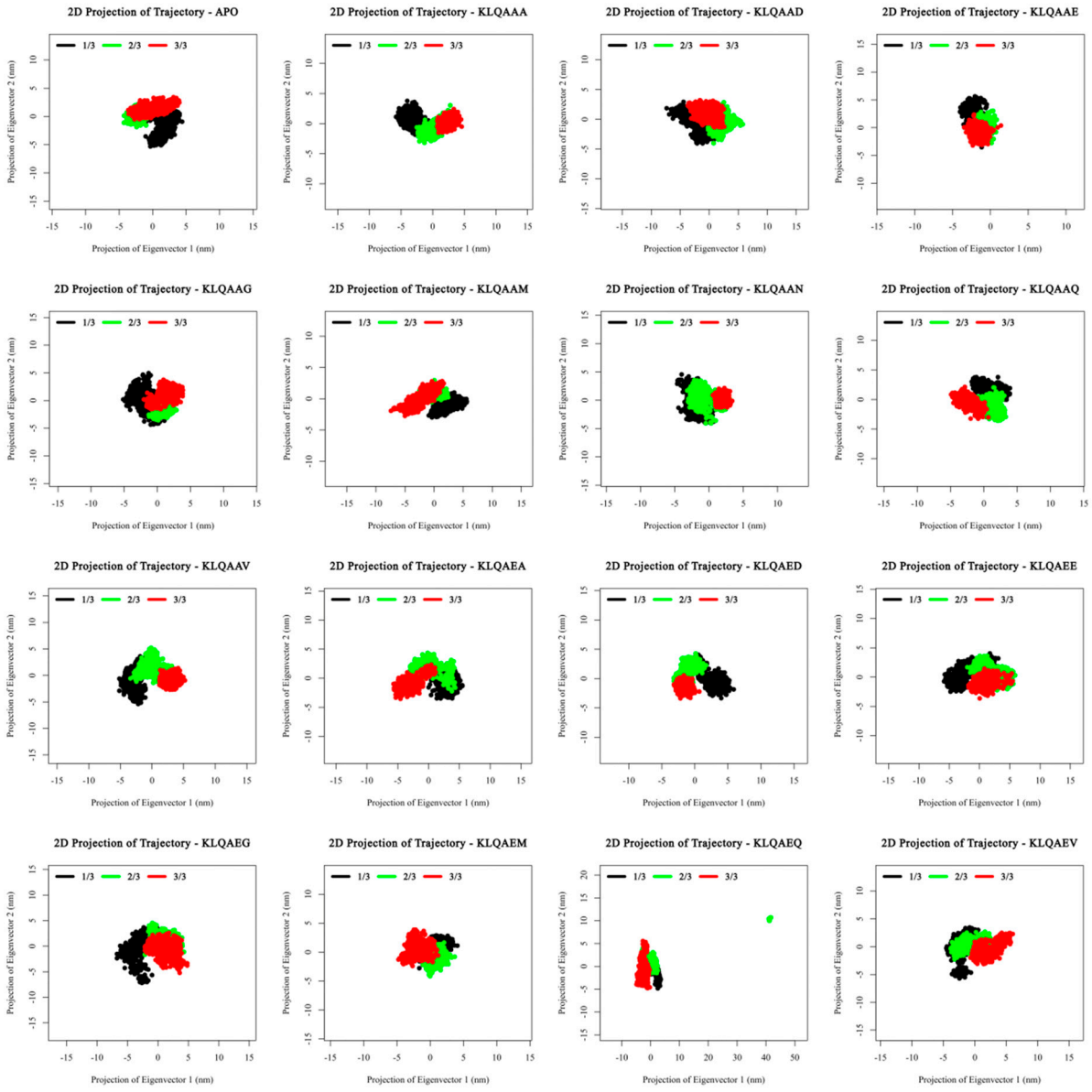


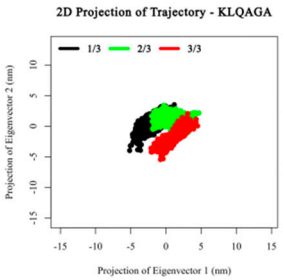
Supplementary Figure S6. Resolution of intermolecular interactions between M^{pro} and substrates at the active site. 2D representation of the protein-ligand interactions at active sites for M^{pro} complexed with RLQAAF, RLQAAN, RLQAGA, RLQALG, RLQAVN, TLQAGF, TLQAVA, VLQAAF and VLQAVF hexapeptides. The substrates attained a docking score of -8.6 $kcal.mol^{-1}$. The images were generated on BIOVIA Discovery Studio 2020 Client.

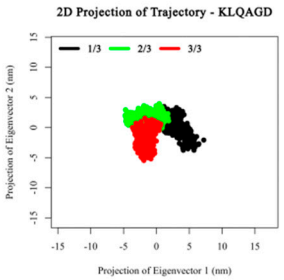


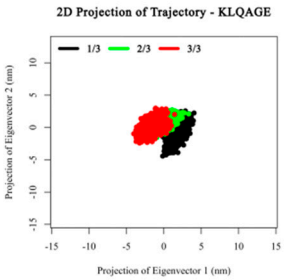
Supplementary Figure S7. Resolution of intermolecular interactions between M^{pro} and substrates at the active site. 2D representation of the protein-ligand interactions at active sites for M^{pro}

complexed with KLQSKM, KLQAEM and TLQSLM hexapeptides. The substrates attained docking score of -7.0 kcal.mol^{-1} (KLQSKM) and -7.1 kcal.mol^{-1} (KLQAEM and TLQSLM). The images were generated on BIOVIA Discovery Studio 2020 Client.




2D Projection of Trajectory - KLQAGA
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQAGD
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQAGE
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2/3
3/3
Projection of Eigenvector 2 (nm)
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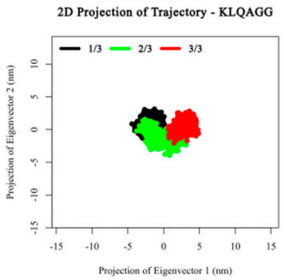
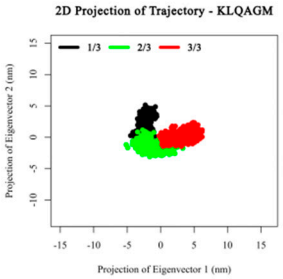

2D Projection of Trajectory - KLQAGG
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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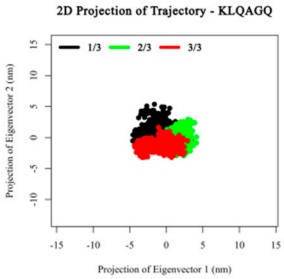
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQAGQ
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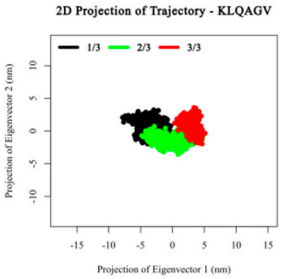
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQAGV
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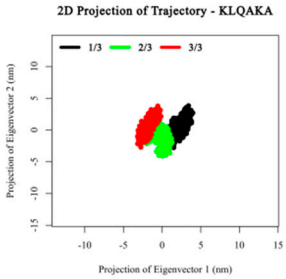
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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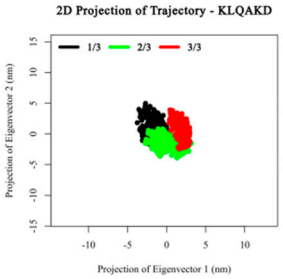
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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2/3
3/3
Projection of Eigenvector 2 (nm)
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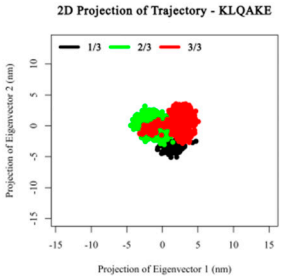
2D Projection of Trajectory - KLQAKE
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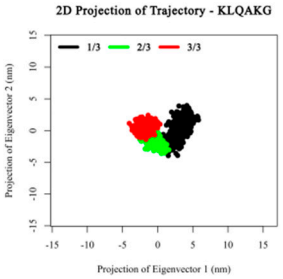
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQAKG
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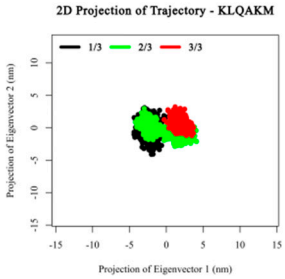
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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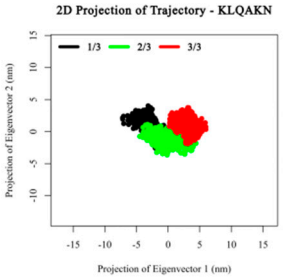
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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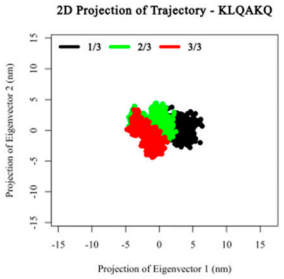
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQAKQ
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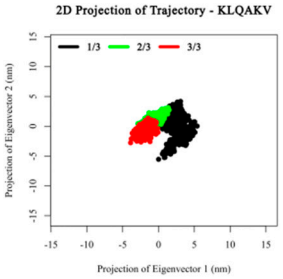
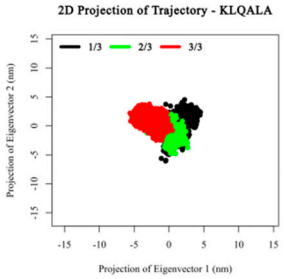
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQAKV
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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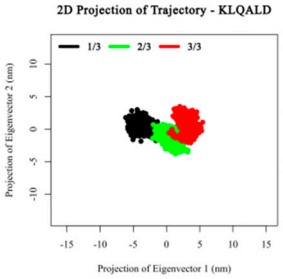
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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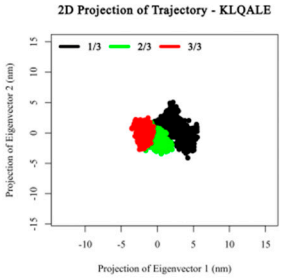
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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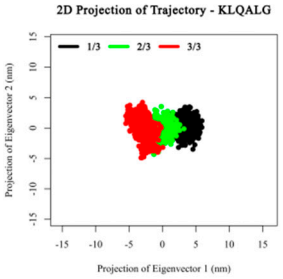
2D Projection of Trajectory - KLQALG
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2/3
3/3
Projection of Eigenvector 2 (nm)
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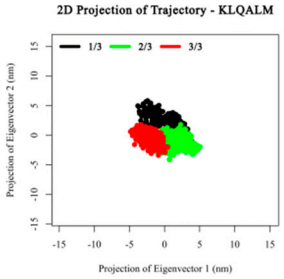
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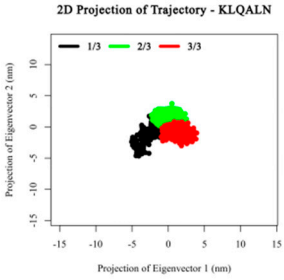
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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2/3
3/3
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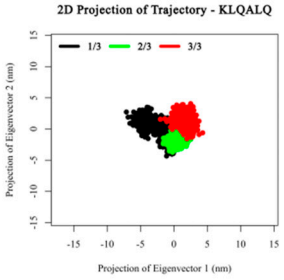
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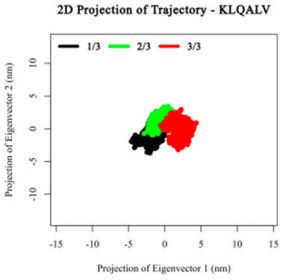
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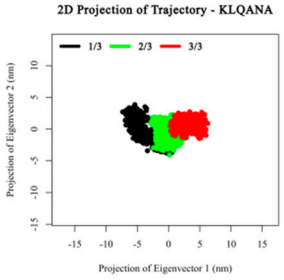
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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2/3
3/3
Projection of Eigenvector 2 (nm)
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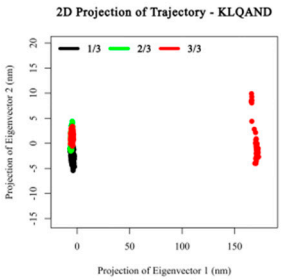
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2/3
3/3
Projection of Eigenvector 2 (nm)
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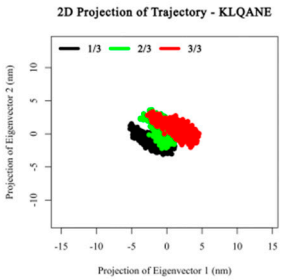
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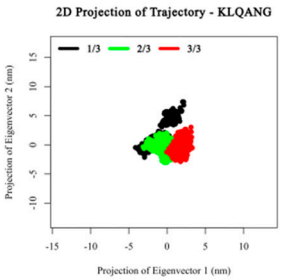
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQANG
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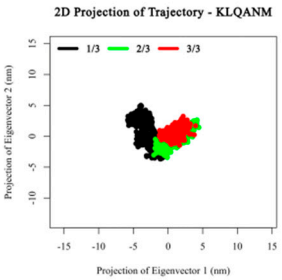
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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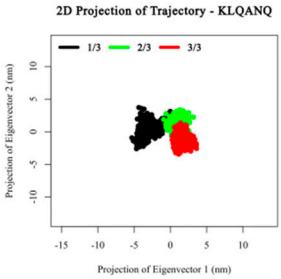
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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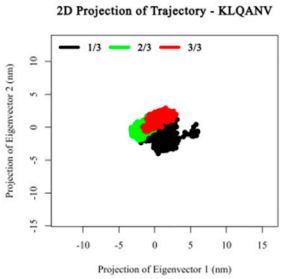
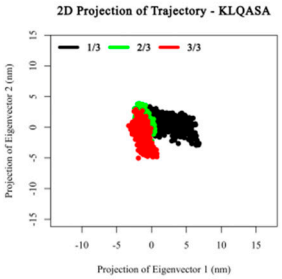
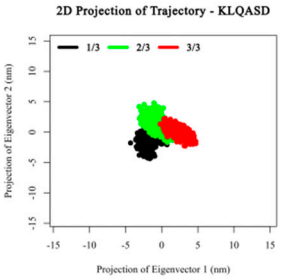
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQANV
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQASA
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQASD
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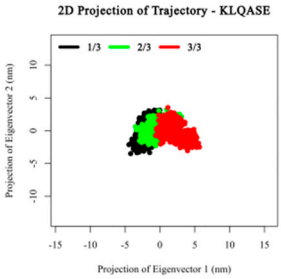
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)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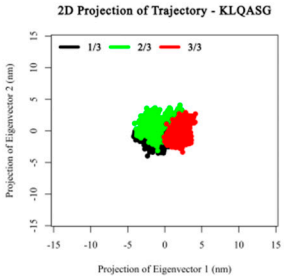
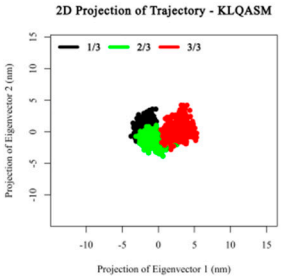
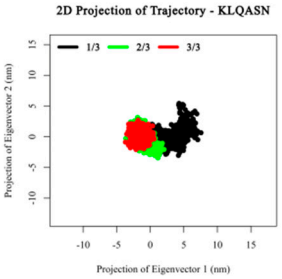
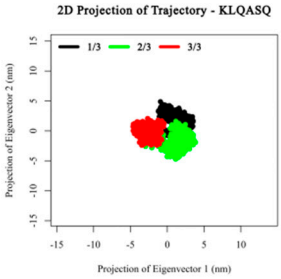
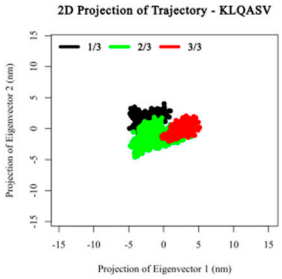
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

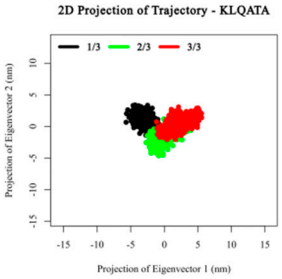

2D Projection of Trajectory - KLQASG
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

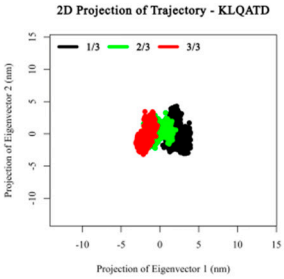

2D Projection of Trajectory - KLQASM
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

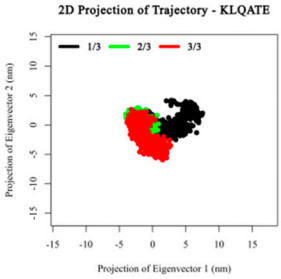

2D Projection of Trajectory - KLQASN
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

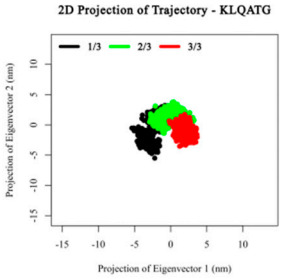

2D Projection of Trajectory - KLQASQ
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

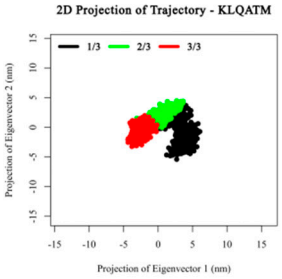

2D Projection of Trajectory - KLQASV
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

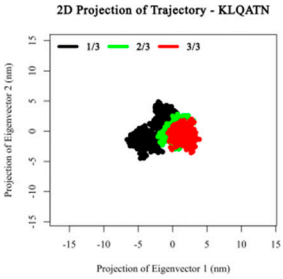

2D Projection of Trajectory - KLQATA
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

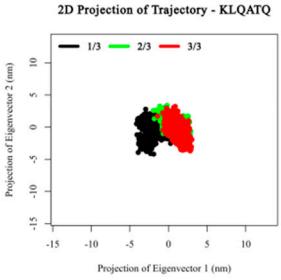

2D Projection of Trajectory - KLQATD
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

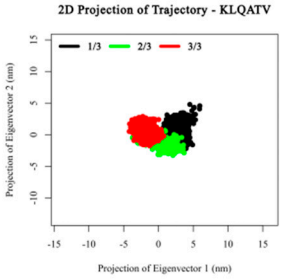

2D Projection of Trajectory - KLQATE
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

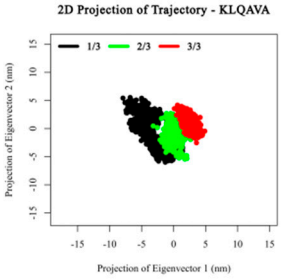

2D Projection of Trajectory - KLQATG
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

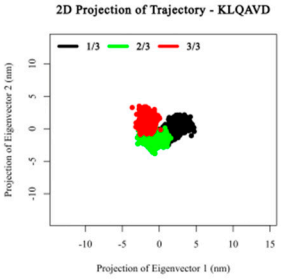

2D Projection of Trajectory - KLQATM
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

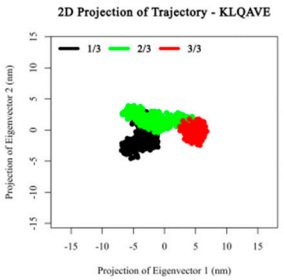

2D Projection of Trajectory - KLQATN
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

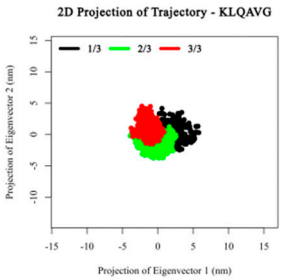

2D Projection of Trajectory - KLQATQ
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

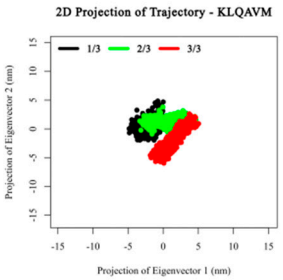

2D Projection of Trajectory - KLQATV
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

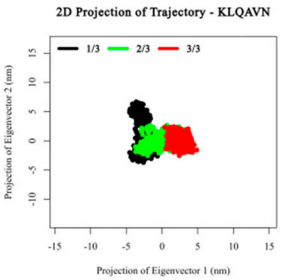

2D Projection of Trajectory - KLQAVA
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

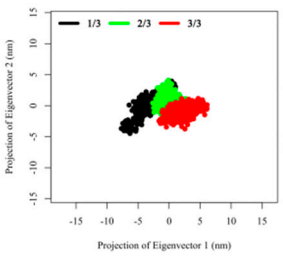

2D Projection of Trajectory - KLQAVD
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

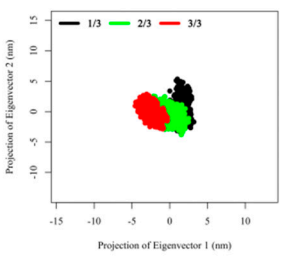

2D Projection of Trajectory - KLQAVE
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

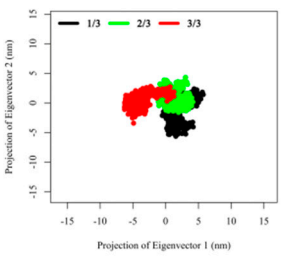

2D Projection of Trajectory - KLQAVG
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

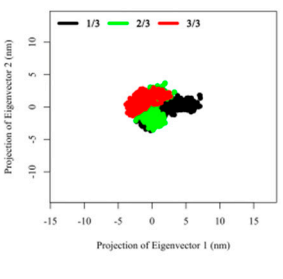

2D Projection of Trajectory - KLQAVM
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

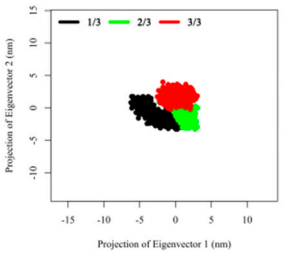

2D Projection of Trajectory - KLQAVN
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

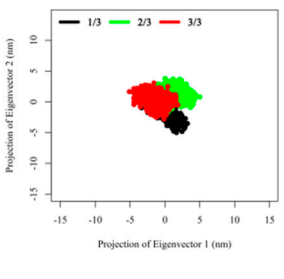

2D Projection of Trajectory - KLQAVQ
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

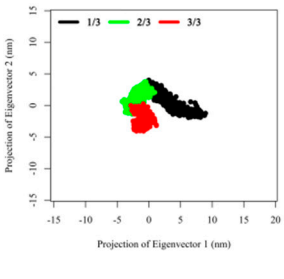

2D Projection of Trajectory - KLQAVV
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

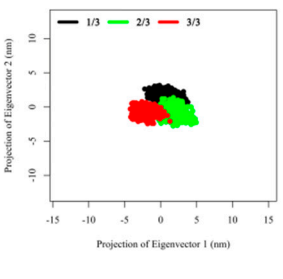

2D Projection of Trajectory - KLQSAA
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

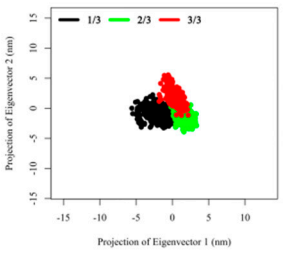

2D Projection of Trajectory - KLQSAD
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

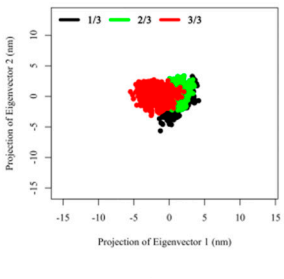

2D Projection of Trajectory - KLQSAE
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

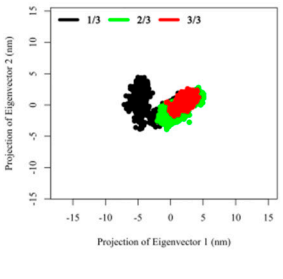

2D Projection of Trajectory - KLQSAG
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

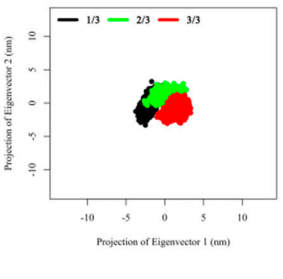

2D Projection of Trajectory - KLQSAM
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

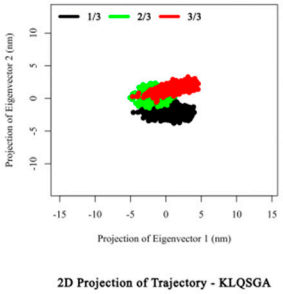

2D Projection of Trajectory - KLQSAN
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

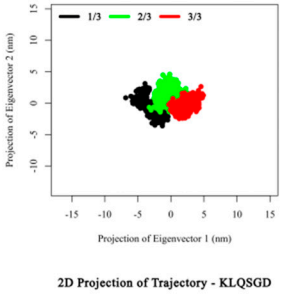

2D Projection of Trajectory - KLQSAQ
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

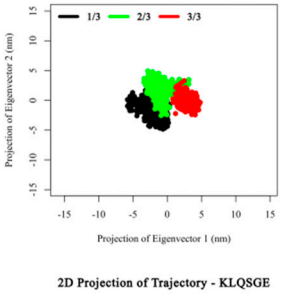

2D Projection of Trajectory - KLQSAV
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

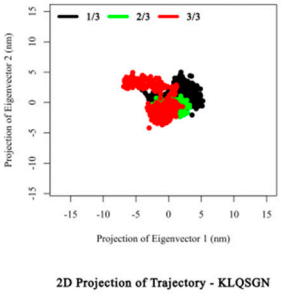

2D Projection of Trajectory - KLQSEA
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

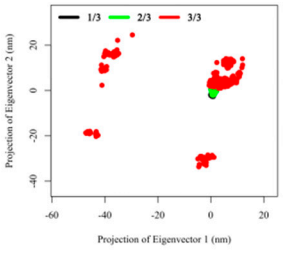

2D Projection of Trajectory - KLQSEE
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

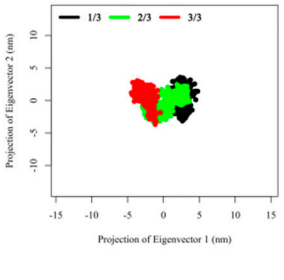

2D Projection of Trajectory - KLQSEG
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

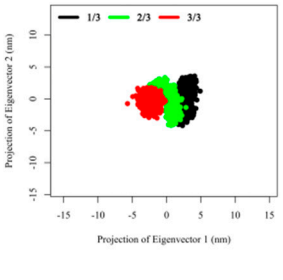

2D Projection of Trajectory - KLQSEM
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

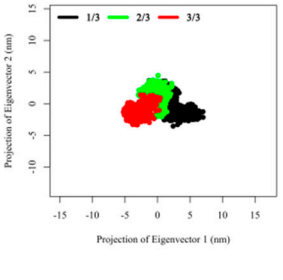

2D Projection of Trajectory - KLQSEN
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

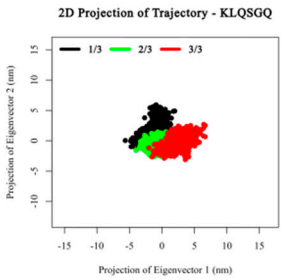

2D Projection of Trajectory - KLQSEQ
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

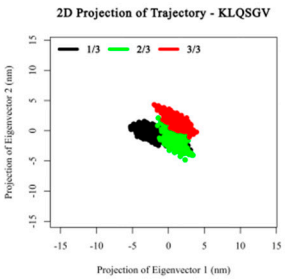

2D Projection of Trajectory - KLQSGA
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

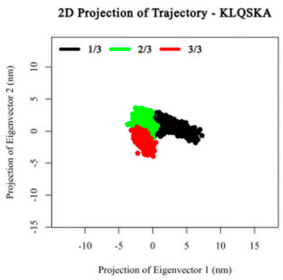

2D Projection of Trajectory - KLQSGD
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

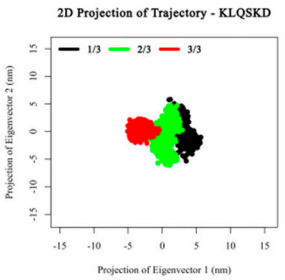

2D Projection of Trajectory - KLQSGE
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

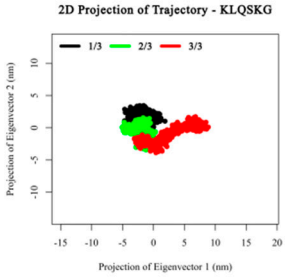

2D Projection of Trajectory - KLQSGN
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

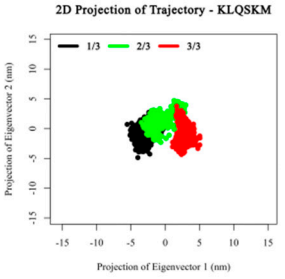

2D Projection of Trajectory - KLQSGQ
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

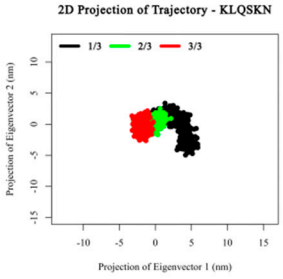

2D Projection of Trajectory - KLQSGV
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

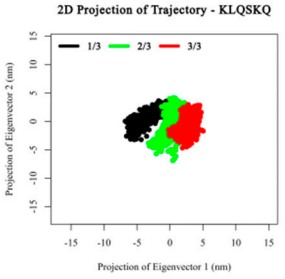

2D Projection of Trajectory - KLQSKA
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

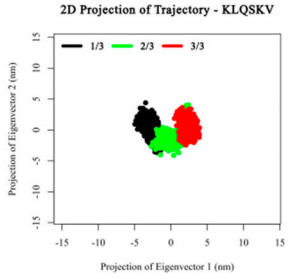

2D Projection of Trajectory - KLQSKD
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

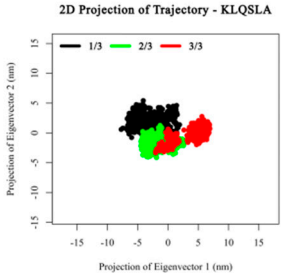

2D Projection of Trajectory - KLQSKG
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

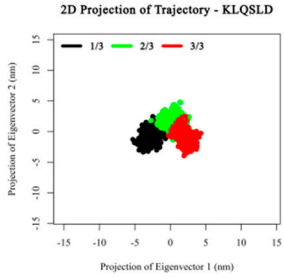

2D Projection of Trajectory - KLQSKM
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

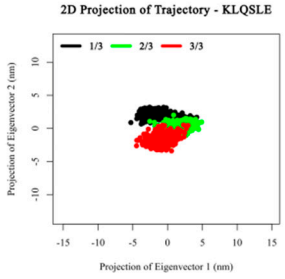

2D Projection of Trajectory - KLQSKN
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

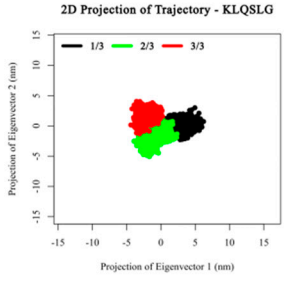

2D Projection of Trajectory - KLQSKQ
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

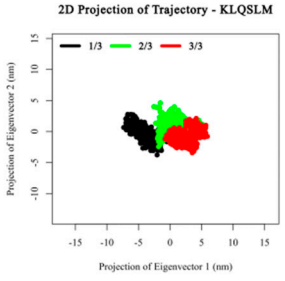

2D Projection of Trajectory - KLQSKV
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

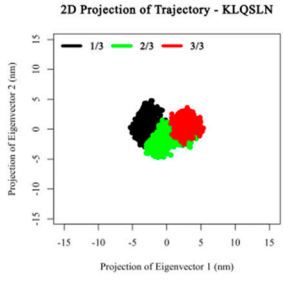

2D Projection of Trajectory - KLQSLA
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

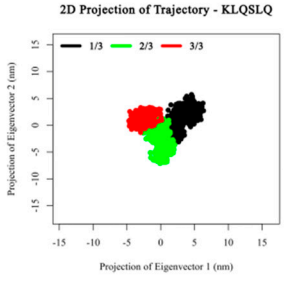

2D Projection of Trajectory - KLQSLD
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

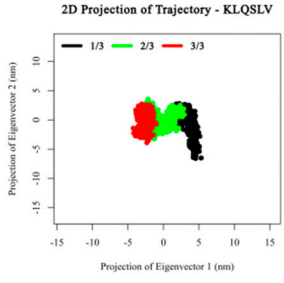

2D Projection of Trajectory - KLQSLE
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

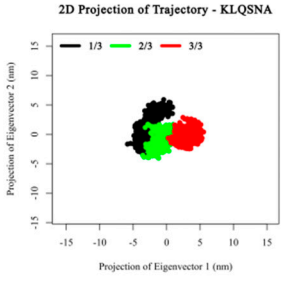

2D Projection of Trajectory - KLQSLG
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

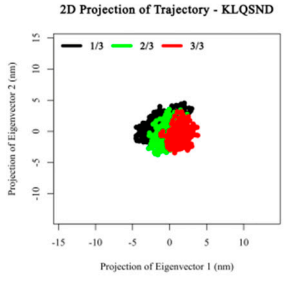

2D Projection of Trajectory - KLQSLM
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

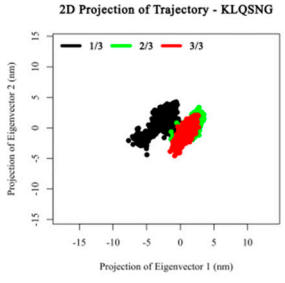

2D Projection of Trajectory - KLQSLN
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

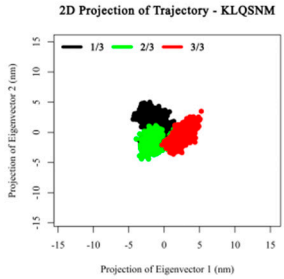

2D Projection of Trajectory - KLQSLQ
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

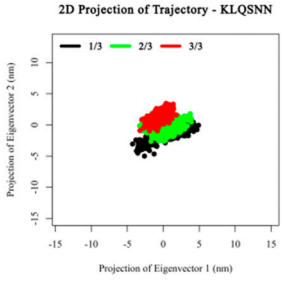

2D Projection of Trajectory - KLQSLV
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

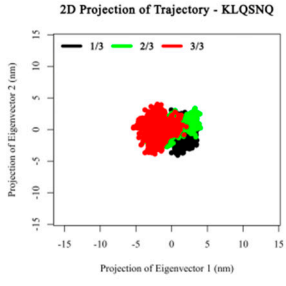

2D Projection of Trajectory - KLQSNA
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

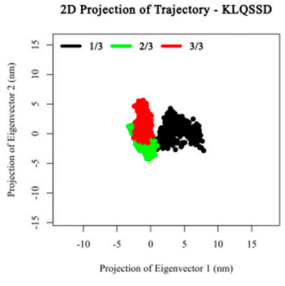

2D Projection of Trajectory - KLQSND
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

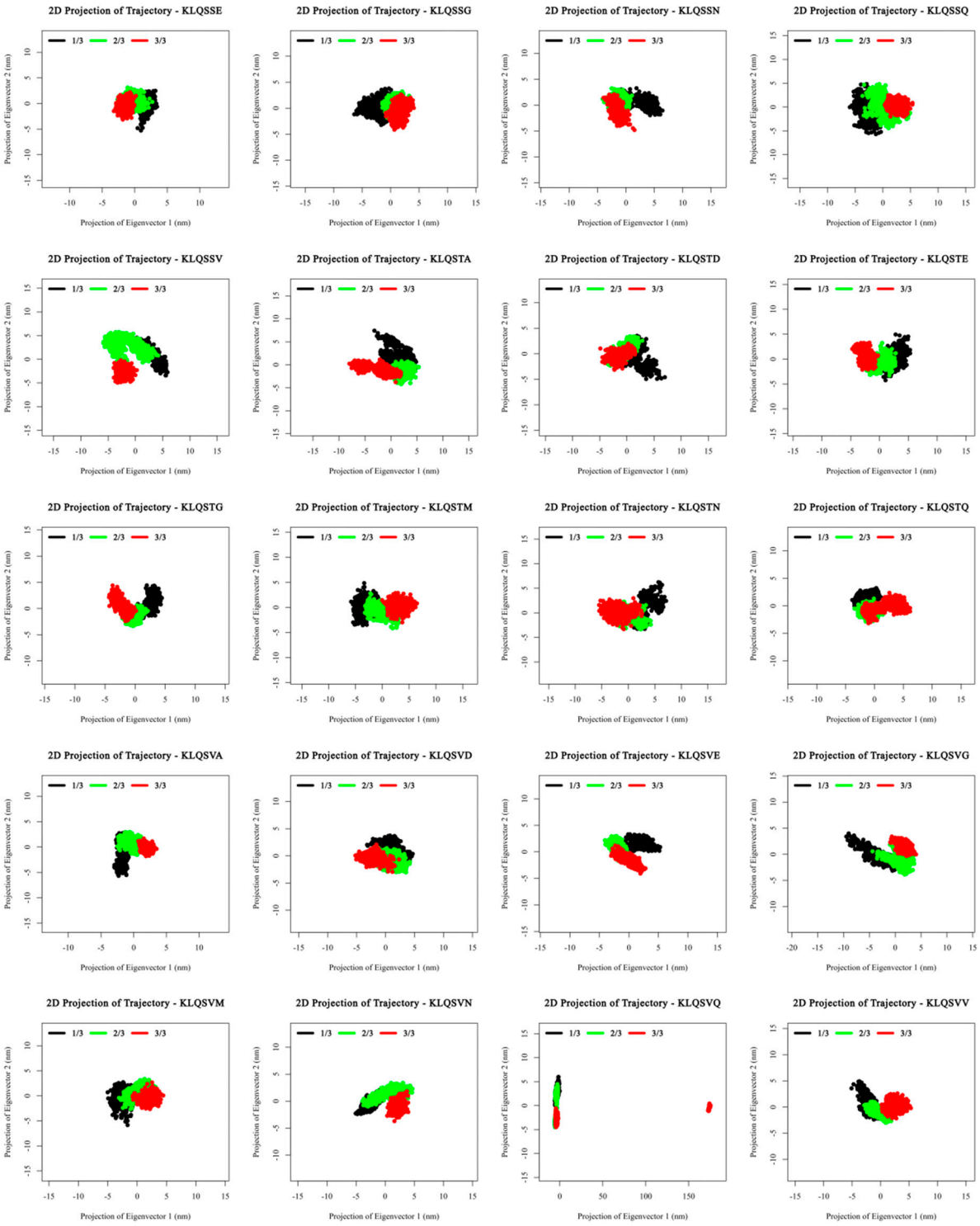

2D Projection of Trajectory - KLQSNG
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQSNM
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

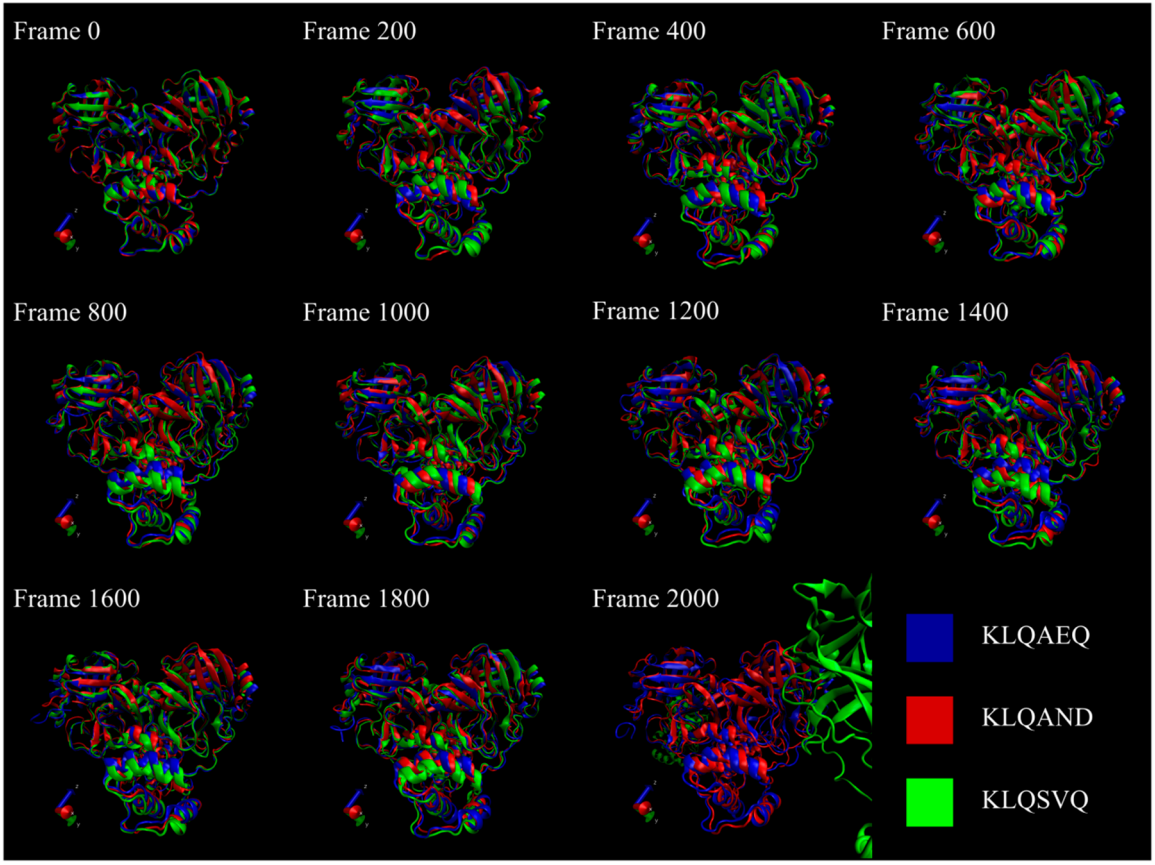

2D Projection of Trajectory - KLQSNN
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)


2D Projection of Trajectory - KLQSNQ
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)

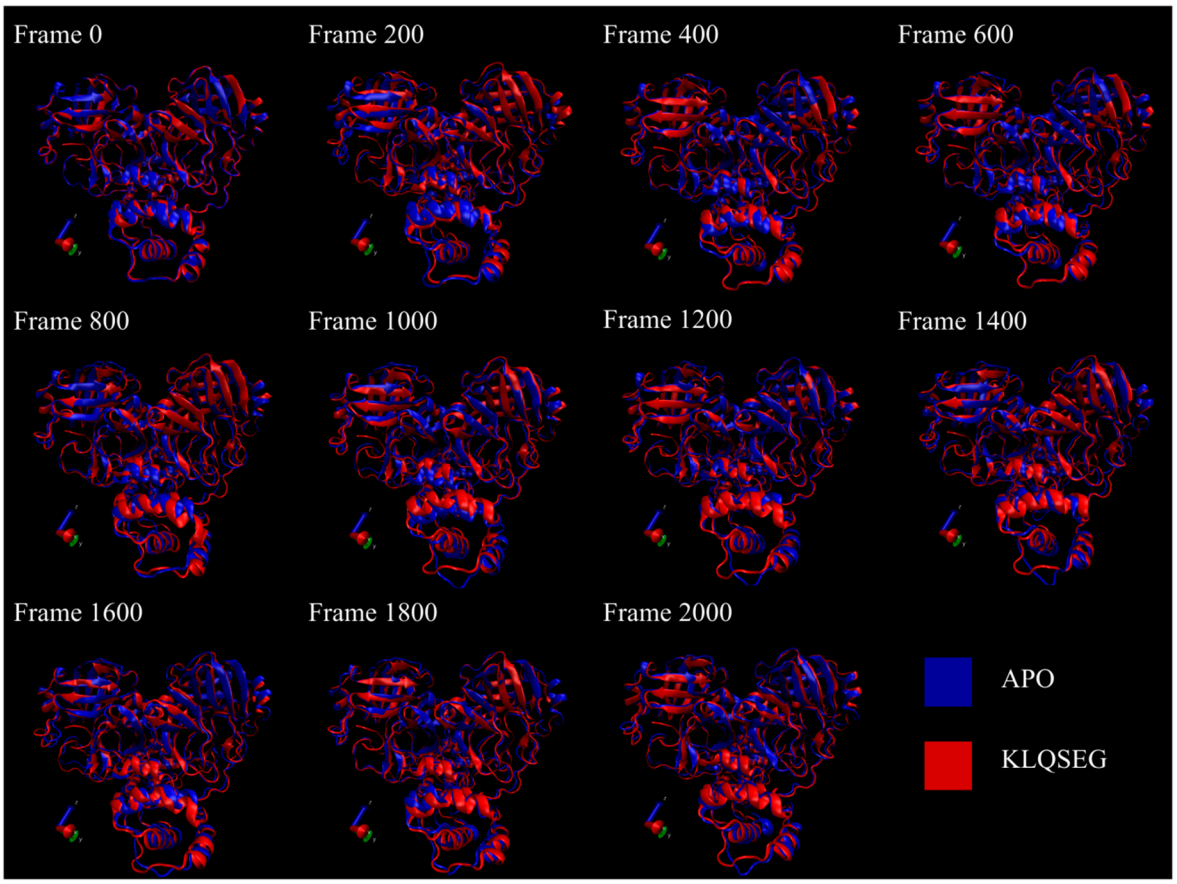

2D Projection of Trajectory - KLQSSD
1/3
2/3
3/3
Projection of Eigenvector 2 (nm)
Projection of Eigenvector 1 (nm)



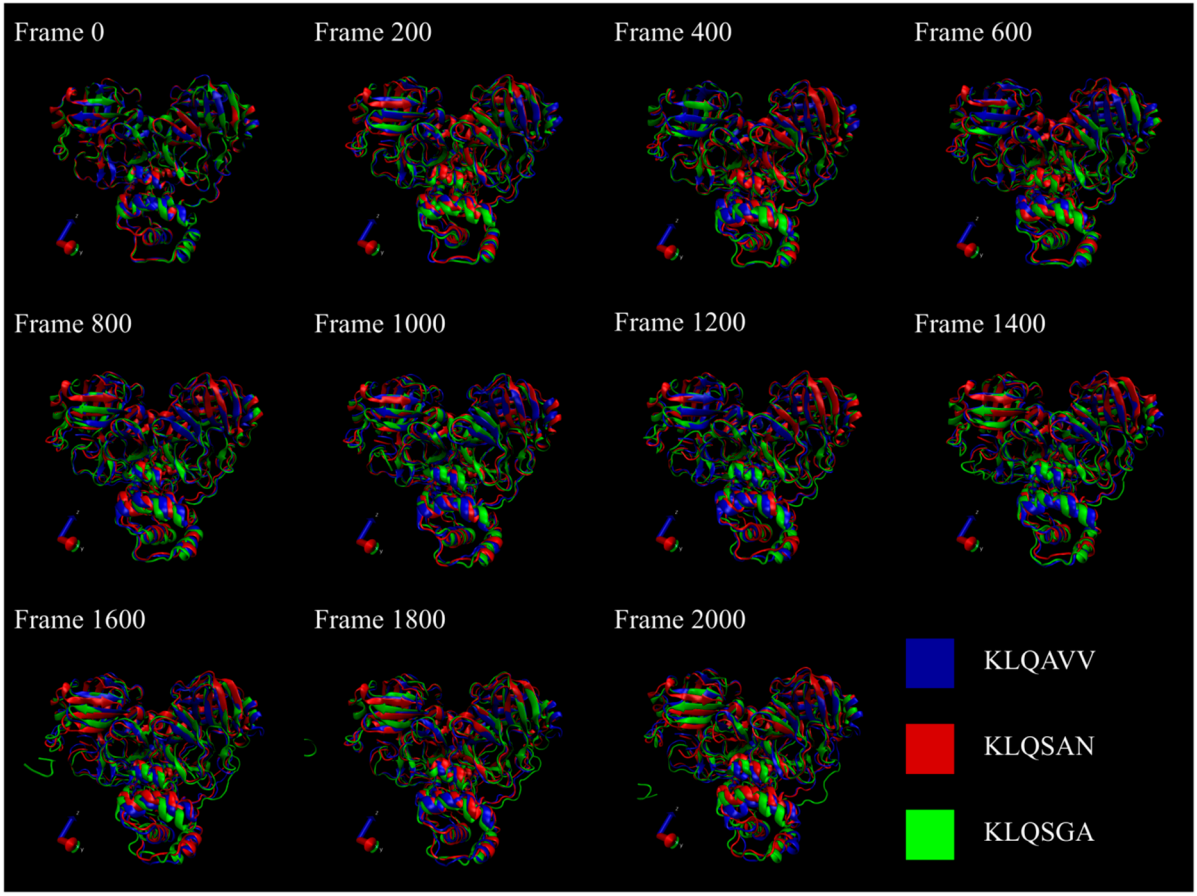
Supplementary Figure S8. The 2D projections of the principal components for M^{pro} (*apo* and KLQ***-substrate-bound) systems over the duration of the 20 ns MD simulations. The projection of the motion along phase space for PC1 and PC2 of M^{pro} *apo* and KLQ***-substrate-bound systems, showing the first third (black), second third (green) and final third (red) of the 20 ns simulation. Images were generated using Xmgrace (of Grace 5) and RStudio.



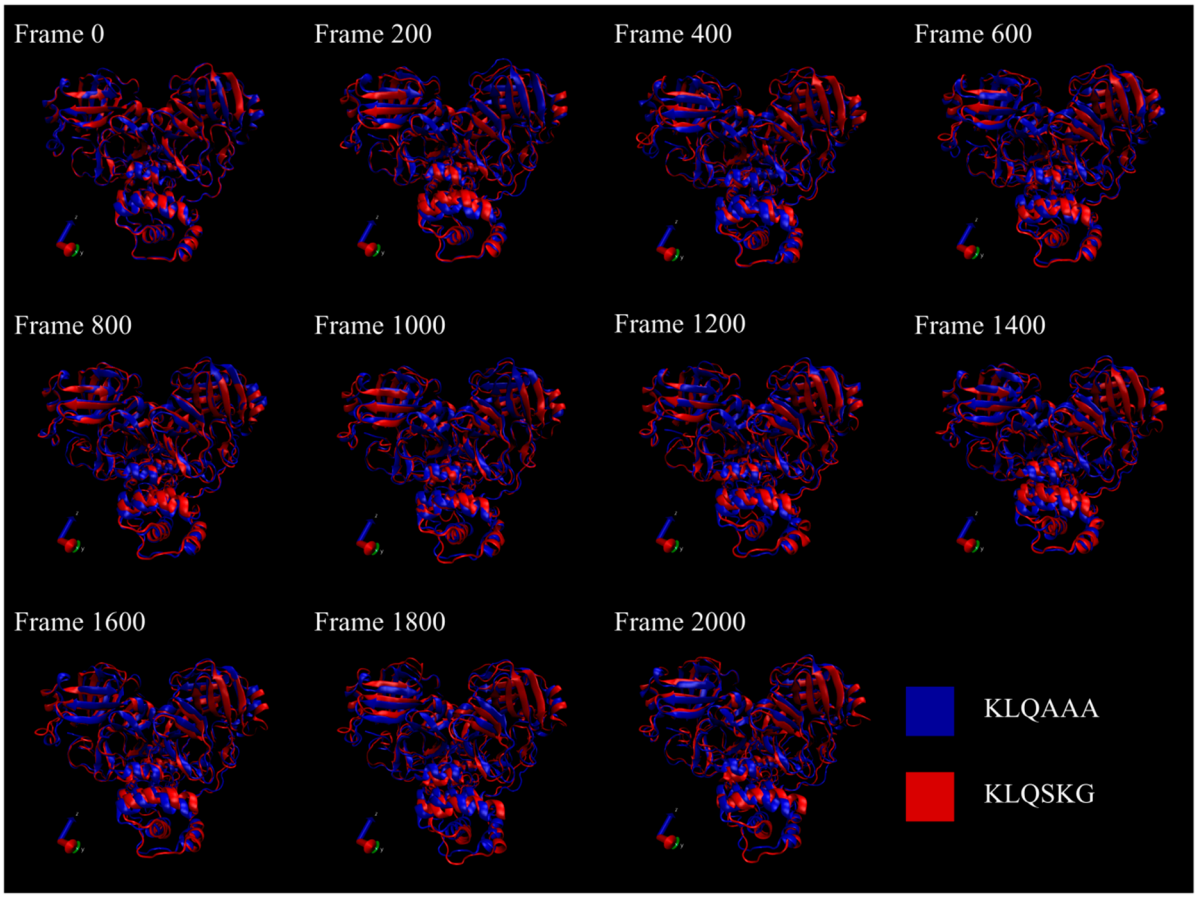
Supplementary Figure S9. Visualisation of the MD trajectories for Group 1 systems. Protein systems are shown cartoon representation, showing M^{pro}-KLQAEQ in blue; M^{pro}-KLQSVQ in red and M^{pro}-KLQAND in green. Images were generated using VMD.



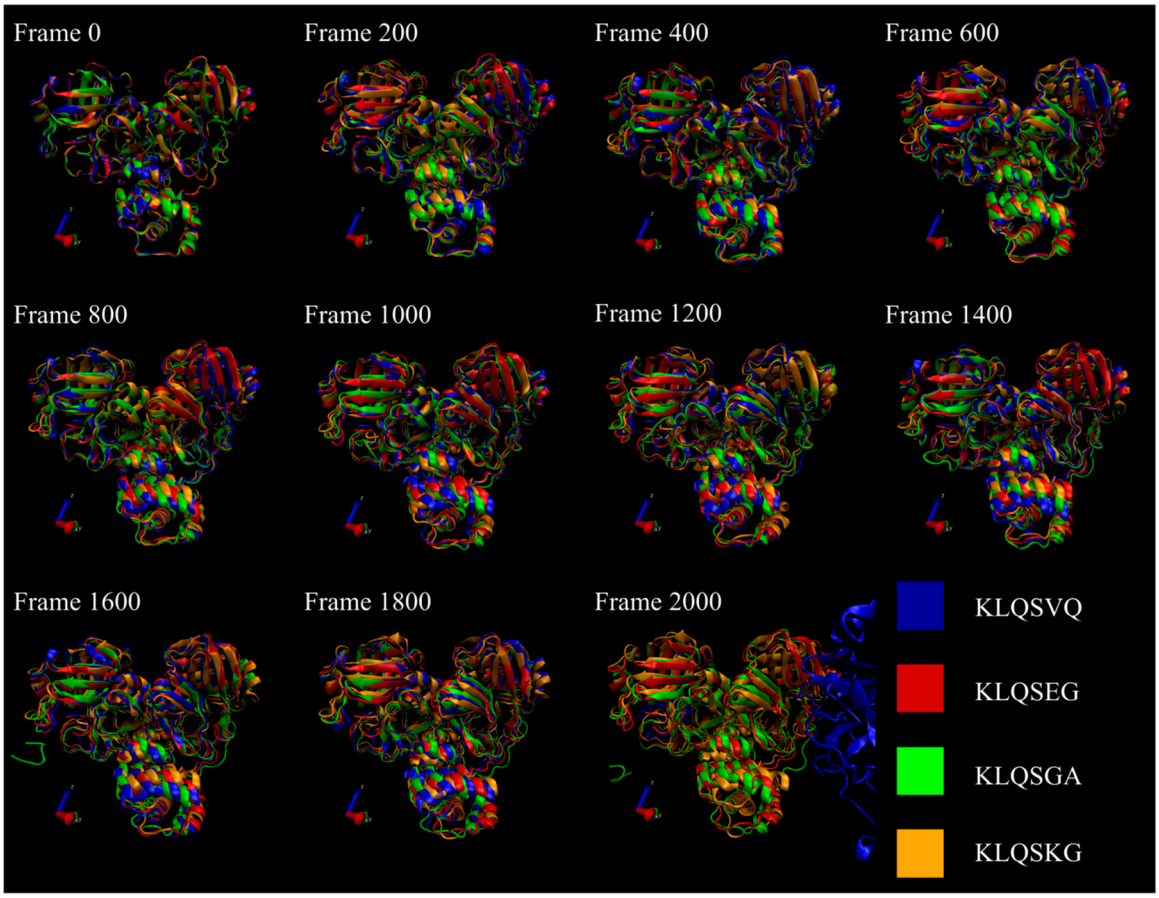
Supplementary Figure S10. Visualisation of the MD trajectories for Group 2 systems. Protein systems are shown cartoon representation, showing *apo*-M^{pro} in blue; and M^{pro}-KLQSEG in red. Images were generated using VMD.



Supplementary Figure S11. Visualisation of the MD trajectories for Group 3 systems. Protein systems are shown cartoon representation, showing M^{pro}-KLQAVV in blue; M^{pro}-KLQSAN in red and M^{pro}-KLQSGA in green. Images were generated using VMD.



Supplementary Figure S12. Visualisation of the MD trajectories for Group 4 systems. Protein systems are shown cartoon representation, showing M^{pro}-KLQAAA in blue and M^{pro}-KLQSKG in red. Images were generated using VMD.



Supplementary Figure S13. Visualisation of the MD trajectories for systems in all hierarchical groups. Protein systems are shown cartoon representation, showing M^{pro}-KLQSVQ (Group 1) in blue; M^{pro}-KLQSEG (Group 2) in red; M^{pro}-KLQSGA (Group 3) in green; and M^{pro}-KLQSKG in orange. Images were generated using VMD.

Supplementary Table S2: RMSD from substrate dynamics ordered by Mean and ordered by Standard Deviation:

RMSD sorted by mean

substrate	mean (nm)	std-dev	substrate	mean (nm)	std-dev
KLQAKA	0.169	0.016	KLQANM	0.204	0.028
KLQASG	0.171	0.018	KLQSVA	0.204	0.022
KLQSND	0.172	0.020	KLQSVD	0.204	0.022
KLQSVG	0.173	0.025	KLQSKQ	0.204	0.039
KLQSNQ	0.173	0.019	KLQAEM	0.205	0.020
KLQSSN	0.174	0.019	KLQSSD	0.205	0.023
KLQAAN	0.175	0.018	KLQAEG	0.206	0.023
KLQAAM	0.177	0.025	APO	0.206	0.023
KLQSAN	0.177	0.023	KLQSKN	0.206	0.028
KLQSTQ	0.177	0.027	KLQSGN	0.206	0.036
KLQSNM	0.179	0.026	KLQSVV	0.207	0.033
KLQASD	0.179	0.020	KLQSVN	0.207	0.025
KLQSGD	0.179	0.023	KLQATE	0.207	0.027
KLQATA	0.180	0.024	KLQSGV	0.208	0.018
KLQAAD	0.180	0.017	KLQAKV	0.209	0.022
KLQSGQ	0.181	0.023	KLQAEV	0.209	0.029
KLQATD	0.181	0.021	KLQANQ	0.209	0.025
KLQSLE	0.181	0.024	KLQAAG	0.209	0.023
KLQSGE	0.182	0.028	KLQALE	0.209	0.025
KLQSAV	0.183	0.016	KLQATM	0.209	0.024
KLQSTE	0.183	0.024	KLQSKM	0.211	0.033
KLQAGE	0.184	0.021	KLQALD	0.211	0.040
KLQAAQ	0.184	0.024	KLQSKV	0.213	0.030
KLQAEE	0.185	0.026	KLQANE	0.214	0.025
KLQASV	0.186	0.021	KLQAKN	0.214	0.036
KLQAGG	0.187	0.018	KLQASN	0.214	0.031

RMSD sorted by standard deviation

substrate	mean (nm)	std-dev	substrate	mean (nm)	std-dev
KLQSAV	0.183	0.016	KLQAAV	0.191	0.026
KLQAKA	0.169	0.016	KLQAGA	0.215	0.026
KLQAAD	0.180	0.017	KLQSNM	0.179	0.026
KLQAGG	0.187	0.018	KLQAEE	0.185	0.026
KLQASG	0.171	0.018	KLQSTQ	0.177	0.027
KLQAAN	0.175	0.018	KLQAED	0.202	0.027
KLQSGV	0.208	0.018	KLQATE	0.207	0.027
KLQSSE	0.189	0.019	KLQSTG	0.192	0.027
KLQAKD	0.217	0.019	KLQAAE	0.218	0.027
KLQSNQ	0.173	0.019	KLQAKM	0.196	0.027
KLQATQ	0.193	0.019	KLQSGE	0.182	0.028
KLQSSN	0.174	0.019	KLQANM	0.204	0.028
KLQSEE	0.190	0.019	KLQSKN	0.206	0.028
KLQSNN	0.193	0.020	KLQAVN	0.216	0.028
KLQSTD	0.203	0.020	KLQSSG	0.216	0.028
KLQATN	0.197	0.020	KLQSNG	0.228	0.028
KLQSND	0.172	0.020	KLQSLD	0.188	0.028
KLQAVD	0.187	0.020	KLQALA	0.224	0.029
KLQAEM	0.205	0.020	KLQAEV	0.209	0.029
KLQASD	0.179	0.020	KLQAKE	0.198	0.029
KLQAGE	0.184	0.021	KLQASA	0.227	0.030
KLQASE	0.192	0.021	KLQAAA	0.192	0.030
KLQATD	0.181	0.021	KLQALM	0.217	0.030
KLQASV	0.186	0.021	KLQSKV	0.213	0.030
KLQSVM	0.189	0.021	KLQSEM	0.224	0.030
KLQSEG	0.187	0.021	KLQSEN	0.225	0.030

KLQSEG	0.187	0.021		KLQAGA	0.215	0.026		KLQSVD	0.204	0.022		KLQASN	0.214	0.031
KLQSLN	0.187	0.023		KLQANV	0.215	0.023		KLQSVA	0.204	0.022		KLQSSV	0.247	0.031
KLQAVD	0.187	0.020		KLQSSG	0.216	0.028		KLQSAQ	0.201	0.022		KLQAGM	0.193	0.032
KLQSLD	0.188	0.028		KLQAVN	0.216	0.028		KLQSAE	0.195	0.022		KLQSKD	0.222	0.032
KLQSAG	0.188	0.024		KLQALM	0.217	0.030		KLQAKV	0.209	0.022		KLQALG	0.204	0.032
KLQSVM	0.189	0.021		KLQSEQ	0.217	0.033		KLQAKQ	0.194	0.023		KLQSKA	0.222	0.032
KLQSSE	0.189	0.019		KLQSSQ	0.217	0.033		KLQSGD	0.179	0.023		KLQSLV	0.232	0.032
KLQSEE	0.190	0.019		KLQAKD	0.217	0.019		KLQSGQ	0.181	0.023		KLQSAD	0.229	0.033
KLQASM	0.190	0.024		KLQSLG	0.218	0.033		KLQANV	0.215	0.023		KLQSSQ	0.217	0.033
KLQSVE	0.190	0.025		KLQAAE	0.218	0.027		KLQSLN	0.187	0.023		KLQSLG	0.218	0.033
KLQAAV	0.191	0.026		KLQANA	0.218	0.050		APO	0.206	0.023		KLQSEQ	0.217	0.033
KLQAAA	0.192	0.030		KLQSKA	0.222	0.032		KLQAAG	0.209	0.023		KLQATV	0.226	0.033
KLQASE	0.192	0.021		KLQSEA	0.222	0.041		KLQAKG	0.194	0.023		KLQSTA	0.242	0.033
KLQAGQ	0.192	0.025		KLQSKD	0.222	0.032		KLQAEG	0.206	0.023		KLQSKM	0.211	0.033
KLQSTG	0.192	0.027		KLQALV	0.223	0.024		KLQALN	0.224	0.023		KLQSVV	0.207	0.033
KLQSTM	0.193	0.040		KLQALN	0.224	0.023		KLQSAN	0.177	0.023		KLQSAM	0.230	0.035
KLQAGM	0.193	0.032		KLQSEM	0.224	0.030		KLQSSD	0.205	0.023		KLQSGN	0.206	0.036
KLQSNN	0.193	0.020		KLQALA	0.224	0.029		KLQASM	0.190	0.024		KLQAEA	0.194	0.036
KLQATQ	0.193	0.019		KLQSEN	0.225	0.030		KLQALV	0.223	0.024		KLQAKN	0.214	0.036
KLQAKQ	0.194	0.023		KLQATV	0.226	0.033		KLQATM	0.209	0.024		KLQSNA	0.226	0.036
KLQAVM	0.194	0.024		KLQSNA	0.226	0.036		KLQAVM	0.194	0.024		KLQSTN	0.244	0.037
KLQAEA	0.194	0.036		KLQASA	0.227	0.030		KLQANG	0.227	0.024		KLQSLQ	0.233	0.037
KLQAKG	0.194	0.023		KLQANG	0.227	0.024		KLQSAG	0.188	0.024		KLQSKQ	0.204	0.039
KLQSLM	0.194	0.043		KLQSNG	0.228	0.028		KLQSLE	0.181	0.024		KLQALD	0.211	0.040
KLQSAE	0.195	0.022		KLQSAD	0.229	0.033		KLQALQ	0.202	0.024		KLQAGD	0.244	0.040
KLQAKM	0.196	0.027		KLQSAM	0.230	0.035		KLQAVV	0.200	0.024		KLQSTM	0.193	0.040
KLQSKG	0.196	0.051		KLQSLV	0.232	0.032		KLQAAQ	0.184	0.024		KLQSAA	0.203	0.041
KLQATN	0.197	0.020		KLQSLQ	0.233	0.037		KLQASQ	0.199	0.024		KLQSEA	0.222	0.041
KLQAKE	0.198	0.029		KLQSGA	0.238	0.187		KLQSTE	0.183	0.024		KLQAVQ	0.240	0.042
KLQASQ	0.199	0.024		KLQAVQ	0.240	0.042		KLQATA	0.180	0.024		KLQAVA	0.267	0.043
KLQAVV	0.200	0.024		KLQSTA	0.242	0.033		KLQAGQ	0.192	0.025		KLQSLM	0.194	0.043
KLQATG	0.200	0.025		KLQAGD	0.244	0.040		KLQSVE	0.190	0.025		KLQAGV	0.259	0.049

KLQSAQ	0.201	0.022		KLQSTN	0.244	0.037		KLQALE	0.209	0.025		KLQAEQ	0.201	0.050
KLQAEQ	0.201	0.050		KLQAVE	0.245	0.063		KLQSVN	0.207	0.025		KLQANA	0.218	0.050
KLQALQ	0.202	0.024		KLQSSV	0.247	0.031		KLQAVG	0.203	0.025		KLQSKG	0.196	0.051
KLQAED	0.202	0.027		KLQSLA	0.251	0.057		KLQSVG	0.173	0.025		KLQSLA	0.251	0.057
KLQSTD	0.203	0.020		KLQAGV	0.259	0.049		KLQANE	0.214	0.025		KLQAVE	0.245	0.063
KLQSAA	0.203	0.041		KLQAVA	0.267	0.043		KLQAAM	0.177	0.025		KLQSGA	0.238	0.187
KLQAVG	0.203	0.025		KLQSVQ	0.271	0.564		KLQATG	0.200	0.025		KLQSVQ	0.271	0.564
KLQALG	0.204	0.032		KLQAND	0.320	0.636		KLQANQ	0.209	0.025		KLQAND	0.320	0.636

Supplementary Table S3: Rg from substrate dynamics ordered by Mean and ordered by Standard Deviation:

Rg sorted by mean							Rg sorted by standard deviation						
substrate	mean (nm)	std-dev		substrate	mean (nm)	std-dev	substrate	mean (nm)	std-dev		substrate	mean (nm)	std-dev
KLQSAM	2.5704	0.0146		KLQALD	2.5923	0.0082	KLQAAG	2.5911	0.0072		KLQAAM	2.5885	0.0093
KLQAAD	2.5740	0.0125		APO	2.5924	0.0089	KLQAGG	2.5856	0.0072		KLQAVN	2.5898	0.0093
KLQANG	2.5743	0.0095		KLQAVV	2.5925	0.0084	KLQSVD	2.5940	0.0073		KLQSAV	2.5913	0.0094
KLQSEA	2.5749	0.0127		KLQSVM	2.5925	0.0083	KLQSVV	2.5995	0.0073		KLQSKG	2.5973	0.0094
KLQALV	2.5752	0.0102		KLQASE	2.5925	0.0078	KLQSKV	2.5928	0.0074		KLQSGN	2.5939	0.0094
KLQSLA	2.5760	0.0154		KLQSVE	2.5927	0.0078	KLQAGA	2.5895	0.0074		KLQAEM	2.5885	0.0094
KLQSEN	2.5764	0.0104		KLQSKV	2.5928	0.0074	KLQSND	2.5962	0.0074		KLQSTD	2.5852	0.0094
KLQSSN	2.5788	0.0102		KLQASM	2.5928	0.0090	KLQSNN	2.5936	0.0075		KLQALM	2.5987	0.0094
KLQAKN	2.5798	0.0118		KLQSTN	2.5930	0.0091	KLQAKG	2.5905	0.0075		KLQANG	2.5743	0.0095
KLQAGQ	2.5804	0.0083		KLQAAQ	2.5934	0.0079	KLQAKV	2.5905	0.0076		KLQSLD	2.5905	0.0095
KLQAKE	2.5812	0.0093		KLQAKA	2.5934	0.0086	KLQAVG	2.6046	0.0077		KLQAEA	2.5895	0.0096
KLQATG	2.5813	0.0101		KLQATD	2.5935	0.0082	KLQASE	2.5925	0.0078		KLQATV	2.5854	0.0097
KLQSLE	2.5817	0.0101		KLQSSV	2.5936	0.0116	KLQSVE	2.5927	0.0078		KLQSLQ	2.5956	0.0099
KLQAGD	2.5821	0.0110		KLQSNN	2.5936	0.0075	KLQATQ	2.5973	0.0078		KLQATG	2.5813	0.0101
KLQAGM	2.5821	0.0112		KLQSLV	2.5936	0.0102	KLQSGD	2.6039	0.0078		KLQSLE	2.5817	0.0101
KLQANE	2.5826	0.0091		KLQAKD	2.5937	0.0091	KLQAAQ	2.5934	0.0079		KLQSSD	2.5953	0.0101
KLQAKQ	2.5828	0.0117		KLQAEG	2.5938	0.0089	KLQSAG	2.6001	0.0080		KLQSLV	2.5936	0.0102
KLQALQ	2.5830	0.0092		KLQSGN	2.5939	0.0094	KLQASG	2.6034	0.0080		KLQSTE	2.5915	0.0102
KLQSEM	2.5831	0.0084		KLQSVD	2.5940	0.0073	KLQSEE	2.5984	0.0080		KLQSSN	2.5788	0.0102
KLQANM	2.5839	0.0087		KLQAAA	2.5940	0.0121	KLQSGE	2.6007	0.0081		KLQAKM	2.6036	0.0102
KLQATN	2.5842	0.0132		KLQSGV	2.5951	0.0087	KLQSNG	2.5953	0.0082		KLQALV	2.5752	0.0102
KLQSNA	2.5842	0.0110		KLQSNG	2.5953	0.0082	KLQAED	2.5889	0.0082		KLQSVN	2.5845	0.0103
KLQSAD	2.5845	0.0087		KLQSSD	2.5953	0.0101	KLQATD	2.5935	0.0082		KLQSNQ	2.5958	0.0103
KLQSVN	2.5845	0.0103		KLQSKM	2.5954	0.0127	KLQALG	2.6041	0.0082		KLQASA	2.5979	0.0103
KLQAVM	2.5845	0.0116		KLQSKQ	2.5955	0.0093	KLQALD	2.5923	0.0082		KLQSEN	2.5764	0.0104
KLQSKA	2.5845	0.0083		KLQATA	2.5955	0.0109	KLQAGQ	2.5804	0.0083		KLQANA	2.5986	0.0105

KLQALE	2.5847	0.0129		KLQSLQ	2.5956	0.0099		KLQSKA	2.5845	0.0083		KLQAEV	2.5884	0.0105
KLQANV	2.5847	0.0086		KLQSAN	2.5958	0.0084		KLQSVM	2.5925	0.0083		KLQSLG	2.5871	0.0105
KLQALN	2.5848	0.0083		KLQSNQ	2.5958	0.0103		KLQALN	2.5848	0.0083		KLQAGV	2.5915	0.0107
KLQSTD	2.5852	0.0094		KLQSND	2.5962	0.0074		KLQSSE	2.6050	0.0083		KLQAEQ	2.6043	0.0108
KLQATV	2.5854	0.0097		KLQSNM	2.5963	0.0130		KLQAVV	2.5925	0.0084		KLQATA	2.5955	0.0109
KLQAGG	2.5856	0.0072		KLQSKD	2.5967	0.0118		KLQSTG	2.5865	0.0084		KLQSEG	2.5993	0.0110
KLQATM	2.5860	0.0090		KLQASQ	2.5968	0.0085		KLQANQ	2.5991	0.0084		KLQAGD	2.5821	0.0110
KLQAVE	2.5862	0.0125		KLQSVG	2.5971	0.0125		KLQSAN	2.5958	0.0084		KLQSNA	2.5842	0.0110
KLQSTG	2.5865	0.0084		KLQSKG	2.5973	0.0094		KLQSEM	2.5831	0.0084		KLQSTQ	2.5976	0.0112
KLQAEE	2.5867	0.0087		KLQATQ	2.5973	0.0078		KLQASQ	2.5968	0.0085		KLQAGM	2.5821	0.0112
KLQSLG	2.5871	0.0105		KLQSTQ	2.5976	0.0112		KLQSAA	2.5913	0.0085		KLQSLM	2.5884	0.0112
KLQSAE	2.5876	0.0117		KLQASA	2.5979	0.0103		KLQASD	2.5918	0.0085		KLQSLN	2.6006	0.0112
KLQSLM	2.5884	0.0112		KLQSEE	2.5984	0.0080		KLQAKA	2.5934	0.0086		KLQSSQ	2.6017	0.0113
KLQAEV	2.5884	0.0105		KLQANA	2.5986	0.0105		KLQANV	2.5847	0.0086		KLQAVM	2.5845	0.0116
KLQSVA	2.5885	0.0091		KLQALM	2.5987	0.0094		KLQSGQ	2.6045	0.0086		KLQSKN	2.5889	0.0116
KLQAAM	2.5885	0.0093		KLQANQ	2.5991	0.0084		KLQAVD	2.5999	0.0086		KLQSSV	2.5936	0.0116
KLQAEM	2.5885	0.0094		KLQSEG	2.5993	0.0110		KLQALA	2.5903	0.0086		KLQAKQ	2.5828	0.0117
KLQAGE	2.5887	0.0093		KLQSVV	2.5995	0.0073		KLQSAD	2.5845	0.0087		KLQSAE	2.5876	0.0117
KLQSKN	2.5889	0.0116		KLQAVD	2.5999	0.0086		KLQSSG	2.6106	0.0087		KLQAAV	2.6148	0.0118
KLQAED	2.5889	0.0082		KLQSAG	2.6001	0.0080		KLQANM	2.5839	0.0087		KLQAKN	2.5798	0.0118
KLQAVQ	2.5891	0.0122		KLQSTA	2.6005	0.0092		KLQAEE	2.5867	0.0087		KLQSKD	2.5967	0.0118
KLQAGA	2.5895	0.0074		KLQSLN	2.6006	0.0112		KLQSGV	2.5951	0.0087		KLQAAA	2.5940	0.0121
KLQAEA	2.5895	0.0096		KLQSGE	2.6007	0.0081		KLQAAN	2.6061	0.0088		KLQAVQ	2.5891	0.0122
KLQAAE	2.5898	0.0174		KLQSSQ	2.6017	0.0113		KLQSAQ	2.5907	0.0088		KLQAAD	2.5740	0.0125
KLQAVN	2.5898	0.0093		KLQASG	2.6034	0.0080		KLQAVA	2.6272	0.0088		KLQAVE	2.5862	0.0125
KLQALA	2.5903	0.0086		KLQAKM	2.6036	0.0102		APO	2.5924	0.0089		KLQSVG	2.5971	0.0125
KLQASV	2.5903	0.0138		KLQSGD	2.6039	0.0078		KLQAEG	2.5938	0.0089		KLQSEA	2.5749	0.0127
KLQSLD	2.5905	0.0095		KLQALG	2.6041	0.0082		KLQASN	2.5909	0.0090		KLQSKM	2.5954	0.0127
KLQAKG	2.5905	0.0075		KLQAEQ	2.6043	0.0108		KLQASM	2.5928	0.0090		KLQSEQ	2.6187	0.0128
KLQAKV	2.5905	0.0076		KLQSGQ	2.6045	0.0086		KLQATM	2.5860	0.0090		KLQALE	2.5847	0.0129
KLQSAQ	2.5907	0.0088		KLQAVG	2.6046	0.0077		KLQSTM	2.5914	0.0090		KLQSNM	2.5963	0.0130
KLQASN	2.5909	0.0090		KLQSSE	2.6050	0.0083		KLQANE	2.5826	0.0091		KLQATN	2.5842	0.0132

KLQAAG	2.5911	0.0072		KLQAAN	2.6061	0.0088		KLQSTN	2.5930	0.0091		KLQASV	2.5903	0.0138
KLQSAV	2.5913	0.0094		KLQSGA	2.6071	0.0256		KLQSVA	2.5885	0.0091		KLQSAM	2.5704	0.0146
KLQSAA	2.5913	0.0085		KLQSSG	2.6106	0.0087		KLQAKD	2.5937	0.0091		KLQATE	2.5917	0.0146
KLQSTM	2.5914	0.0090		KLQAAV	2.6148	0.0118		KLQSTA	2.6005	0.0092		KLQSLA	2.5760	0.0154
KLQAGV	2.5915	0.0107		KLQSEQ	2.6187	0.0128		KLQALQ	2.5830	0.0092		KLQAAE	2.5898	0.0174
KLQSTE	2.5915	0.0102		KLQAVA	2.6272	0.0088		KLQAGE	2.5887	0.0093		KLQSGA	2.6071	0.0256
KLQATE	2.5917	0.0146		KLQSVQ	2.6596	0.3865		KLQAKE	2.5812	0.0093		KLQSVQ	2.6596	0.3865
KLQASD	2.5918	0.0085		KLQAND	2.6605	0.4222		KLQSKQ	2.5955	0.0093		KLQAND	2.6605	0.4222

Supplementary Table S4: RMSD and Rg from substrate dynamics ordered by substrate

RMSD sorted by residue

substrate	mean (nm)	std-dev		substrate	mean (nm)	std-dev
APO	0.206	0.023		KLQAVM	0.194	0.024
KLQAAA	0.192	0.030		KLQAVN	0.216	0.028
KLQAAD	0.180	0.017		KLQAVQ	0.240	0.042
KLQAAE	0.218	0.027		KLQAVV	0.200	0.024
KLQAAG	0.209	0.023		KLQSAA	0.203	0.041
KLQAAM	0.177	0.025		KLQSAD	0.229	0.033
KLQAAN	0.175	0.018		KLQSAE	0.195	0.022
KLQAAQ	0.184	0.024		KLQSAG	0.188	0.024
KLQAAV	0.191	0.026		KLQSAM	0.230	0.035
KLQAEA	0.194	0.036		KLQSAN	0.177	0.023
KLQAED	0.202	0.027		KLQSAQ	0.201	0.022
KLQAEE	0.185	0.026		KLQSAV	0.183	0.016
KLQAEG	0.206	0.023		KLQSEA	0.222	0.041
KLQAEM	0.205	0.020		KLQSEE	0.190	0.019
KLQAEQ	0.201	0.050		KLQSEG	0.187	0.021
KLQAEV	0.209	0.029		KLQSEM	0.224	0.030
KLQAGA	0.215	0.026		KLQSEN	0.225	0.030
KLQAGD	0.244	0.040		KLQSEQ	0.217	0.033
KLQAGE	0.184	0.021		KLQSGA	0.238	0.187
KLQAGG	0.187	0.018		KLQSGD	0.179	0.023
KLQAGM	0.193	0.032		KLQSGE	0.182	0.028
KLQAGQ	0.192	0.025		KLQSGN	0.206	0.036
KLQAGV	0.259	0.049		KLQSGQ	0.181	0.023
KLQAKA	0.169	0.016		KLQSGV	0.208	0.018
KLQAKD	0.217	0.019		KLQSKA	0.222	0.032
KLQAKE	0.198	0.029		KLQSKD	0.222	0.032

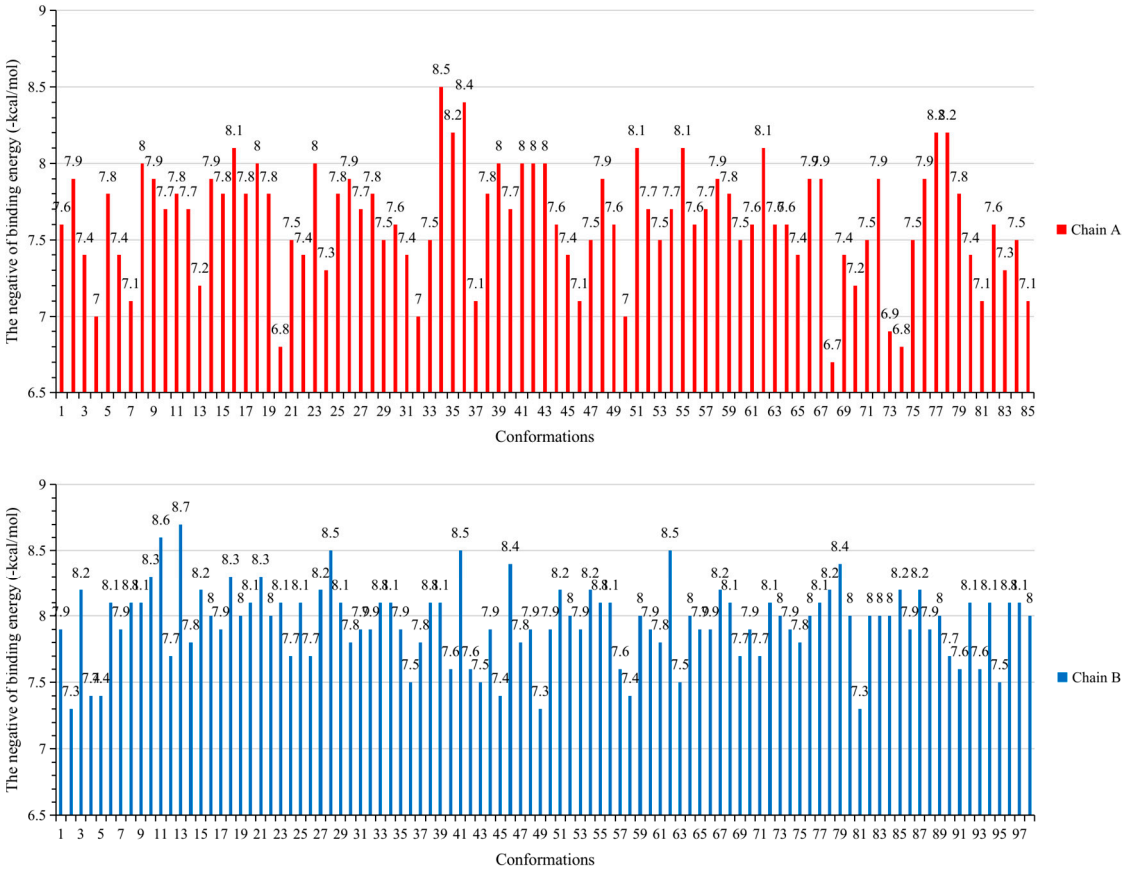
Rg sorted by residue

substrate	mean (nm)	std-dev		substrate	mean (nm)	std-dev
APO	2.5924	0.0089		KLQAVM	2.5845	0.0116
KLQAAA	2.5940	0.0121		KLQAVN	2.5898	0.0093
KLQAAD	2.5740	0.0125		KLQAVQ	2.5891	0.0122
KLQAAE	2.5898	0.0174		KLQAVV	2.5925	0.0084
KLQAAG	2.5911	0.0072		KLQSAA	2.5913	0.0085
KLQAAM	2.5885	0.0093		KLQSAD	2.5845	0.0087
KLQAAN	2.6061	0.0088		KLQSAE	2.5876	0.0117
KLQAAQ	2.5934	0.0079		KLQSAG	2.6001	0.0080
KLQAAV	2.6148	0.0118		KLQSAM	2.5704	0.0146
KLQAEA	2.5895	0.0096		KLQSAN	2.5958	0.0084
KLQAED	2.5889	0.0082		KLQSAQ	2.5907	0.0088
KLQAEE	2.5867	0.0087		KLQSAV	2.5913	0.0094
KLQAEG	2.5938	0.0089		KLQSEA	2.5749	0.0127
KLQAEM	2.5885	0.0094		KLQSEE	2.5984	0.0080
KLQAEQ	2.6043	0.0108		KLQSEG	2.5993	0.0110
KLQAEV	2.5884	0.0105		KLQSEM	2.5831	0.0084
KLQAGA	2.5895	0.0074		KLQSEN	2.5764	0.0104
KLQAGD	2.5821	0.0110		KLQSEQ	2.6187	0.0128
KLQAGE	2.5887	0.0093		KLQSGA	2.6071	0.0256
KLQAGG	2.5856	0.0072		KLQSGD	2.6039	0.0078
KLQAGM	2.5821	0.0112		KLQSGE	2.6007	0.0081
KLQAGQ	2.5804	0.0083		KLQSGN	2.5939	0.0094
KLQAGV	2.5915	0.0107		KLQSGQ	2.6045	0.0086
KLQAKA	2.5934	0.0086		KLQSGV	2.5951	0.0087
KLQAKD	2.5937	0.0091		KLQSKA	2.5845	0.0083
KLQAKE	2.5812	0.0093		KLQSKD	2.5967	0.0118

KLQAKG	0.194	0.023		KLQSKG	0.196	0.051		KLQAKG	2.5905	0.0075		KLQSKG	2.5973	0.0094
KLQAKM	0.196	0.027		KLQSKM	0.211	0.033		KLQAKM	2.6036	0.0102		KLQSKM	2.5954	0.0127
KLQAKN	0.214	0.036		KLQSKN	0.206	0.028		KLQAKN	2.5798	0.0118		KLQSKN	2.5889	0.0116
KLQAKQ	0.194	0.023		KLQSKQ	0.204	0.039		KLQAKQ	2.5828	0.0117		KLQSKQ	2.5955	0.0093
KLQAKV	0.209	0.022		KLQSKV	0.213	0.030		KLQAKV	2.5905	0.0076		KLQSKV	2.5928	0.0074
KLQALA	0.224	0.029		KLQSLA	0.251	0.057		KLQALA	2.5903	0.0086		KLQSLA	2.5760	0.0154
KLQALD	0.211	0.040		KLQSLD	0.188	0.028		KLQALD	2.5923	0.0082		KLQSLD	2.5905	0.0095
KLQALE	0.209	0.025		KLQSLE	0.181	0.024		KLQALE	2.5847	0.0129		KLQSLE	2.5817	0.0101
KLQALG	0.204	0.032		KLQSLG	0.218	0.033		KLQALG	2.6041	0.0082		KLQSLG	2.5871	0.0105
KLQALM	0.217	0.030		KLQSLM	0.194	0.043		KLQALM	2.5987	0.0094		KLQSLM	2.5884	0.0112
KLQALN	0.224	0.023		KLQSLN	0.187	0.023		KLQALN	2.5848	0.0083		KLQSLN	2.6006	0.0112
KLQALQ	0.202	0.024		KLQSLQ	0.233	0.037		KLQALQ	2.5830	0.0092		KLQSLQ	2.5956	0.0099
KLQALV	0.223	0.024		KLQSLV	0.232	0.032		KLQALV	2.5752	0.0102		KLQSLV	2.5936	0.0102
KLQANA	0.218	0.050		KLQSNA	0.226	0.036		KLQANA	2.5986	0.0105		KLQSNA	2.5842	0.0110
KLQAND	0.320	0.636		KLQSND	0.172	0.020		KLQAND	2.6605	0.4222		KLQSND	2.5962	0.0074
KLQANE	0.214	0.025		KLQSNG	0.228	0.028		KLQANE	2.5826	0.0091		KLQSNG	2.5953	0.0082
KLQANG	0.227	0.024		KLQSNM	0.179	0.026		KLQANG	2.5743	0.0095		KLQSNM	2.5963	0.0130
KLQANM	0.204	0.028		KLQSNN	0.193	0.020		KLQANM	2.5839	0.0087		KLQSNN	2.5936	0.0075
KLQANQ	0.209	0.025		KLQSNQ	0.173	0.019		KLQANQ	2.5991	0.0084		KLQSNQ	2.5958	0.0103
KLQANV	0.215	0.023		KLQSSD	0.205	0.023		KLQANV	2.5847	0.0086		KLQSSD	2.5953	0.0101
KLQASA	0.227	0.030		KLQSSE	0.189	0.019		KLQASA	2.5979	0.0103		KLQSSE	2.6050	0.0083
KLQASD	0.179	0.020		KLQSSG	0.216	0.028		KLQASD	2.5918	0.0085		KLQSSG	2.6106	0.0087
KLQASE	0.192	0.021		KLQSSN	0.174	0.019		KLQASE	2.5925	0.0078		KLQSSN	2.5788	0.0102
KLQASG	0.171	0.018		KLQSSQ	0.217	0.033		KLQASG	2.6034	0.0080		KLQSSQ	2.6017	0.0113
KLQASM	0.190	0.024		KLQSSV	0.247	0.031		KLQASM	2.5928	0.0090		KLQSSV	2.5936	0.0116
KLQASN	0.214	0.031		KLQSTA	0.242	0.033		KLQASN	2.5909	0.0090		KLQSTA	2.6005	0.0092
KLQASQ	0.199	0.024		KLQSTD	0.203	0.020		KLQASQ	2.5968	0.0085		KLQSTD	2.5852	0.0094
KLQASV	0.186	0.021		KLQSTE	0.183	0.024		KLQASV	2.5903	0.0138		KLQSTE	2.5915	0.0102
KLQATA	0.180	0.024		KLQSTG	0.192	0.027		KLQATA	2.5955	0.0109		KLQSTG	2.5865	0.0084
KLQATD	0.181	0.021		KLQSTM	0.193	0.040		KLQATD	2.5935	0.0082		KLQSTM	2.5914	0.0090
KLQATE	0.207	0.027		KLQSTN	0.244	0.037		KLQATE	2.5917	0.0146		KLQSTN	2.5930	0.0091

KLQATG	0.200	0.025		KLQSTQ	0.177	0.027
KLQATM	0.209	0.024		KLQSVA	0.204	0.022
KLQATN	0.197	0.020		KLQSVD	0.204	0.022
KLQATQ	0.193	0.019		KLQSVE	0.190	0.025
KLQATV	0.226	0.033		KLQSVG	0.173	0.025
KLQAVA	0.267	0.043		KLQSVM	0.189	0.021
KLQAVD	0.187	0.020		KLQSVN	0.207	0.025
KLQAVE	0.245	0.063		KLQSVQ	0.271	0.564
KLQAVG	0.203	0.025		KLQSVV	0.207	0.033

KLQATG	2.5813	0.0101		KLQSTQ	2.5976	0.0112
KLQATM	2.5860	0.0090		KLQSVA	2.5885	0.0091
KLQATN	2.5842	0.0132		KLQSVD	2.5940	0.0073
KLQATQ	2.5973	0.0078		KLQSVE	2.5927	0.0078
KLQATV	2.5854	0.0097		KLQSVG	2.5971	0.0125
KLQAVA	2.6272	0.0088		KLQSVM	2.5925	0.0083
KLQAVD	2.5999	0.0086		KLQSVN	2.5845	0.0103
KLQAVE	2.5862	0.0125		KLQSVQ	2.6596	0.3865
KLQAVG	2.6046	0.0077		KLQSVV	2.5995	0.0073



Supplementary Figure S14. Preliminary docking studies to determine the protein chain to prioritise for docking studies. The negative of the docking scores of the Arg-Leu-Gln-Ala-Ala-Asn (RLQAAN) conformers were plotted on bar graphs, showing the docking scores of chain A (red) and chain B (blue). The image was generated using WPS Spreadsheet 2019.