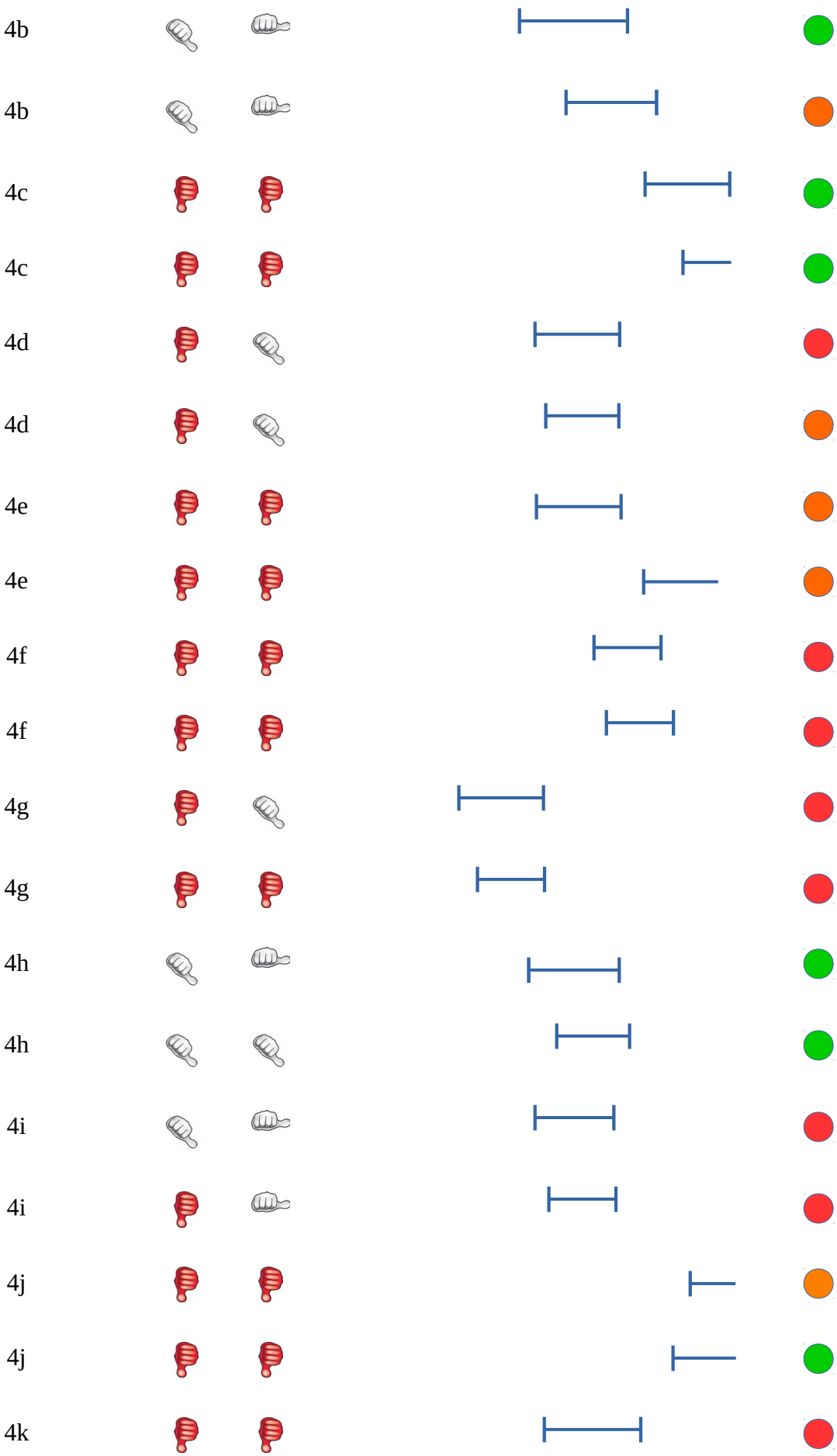
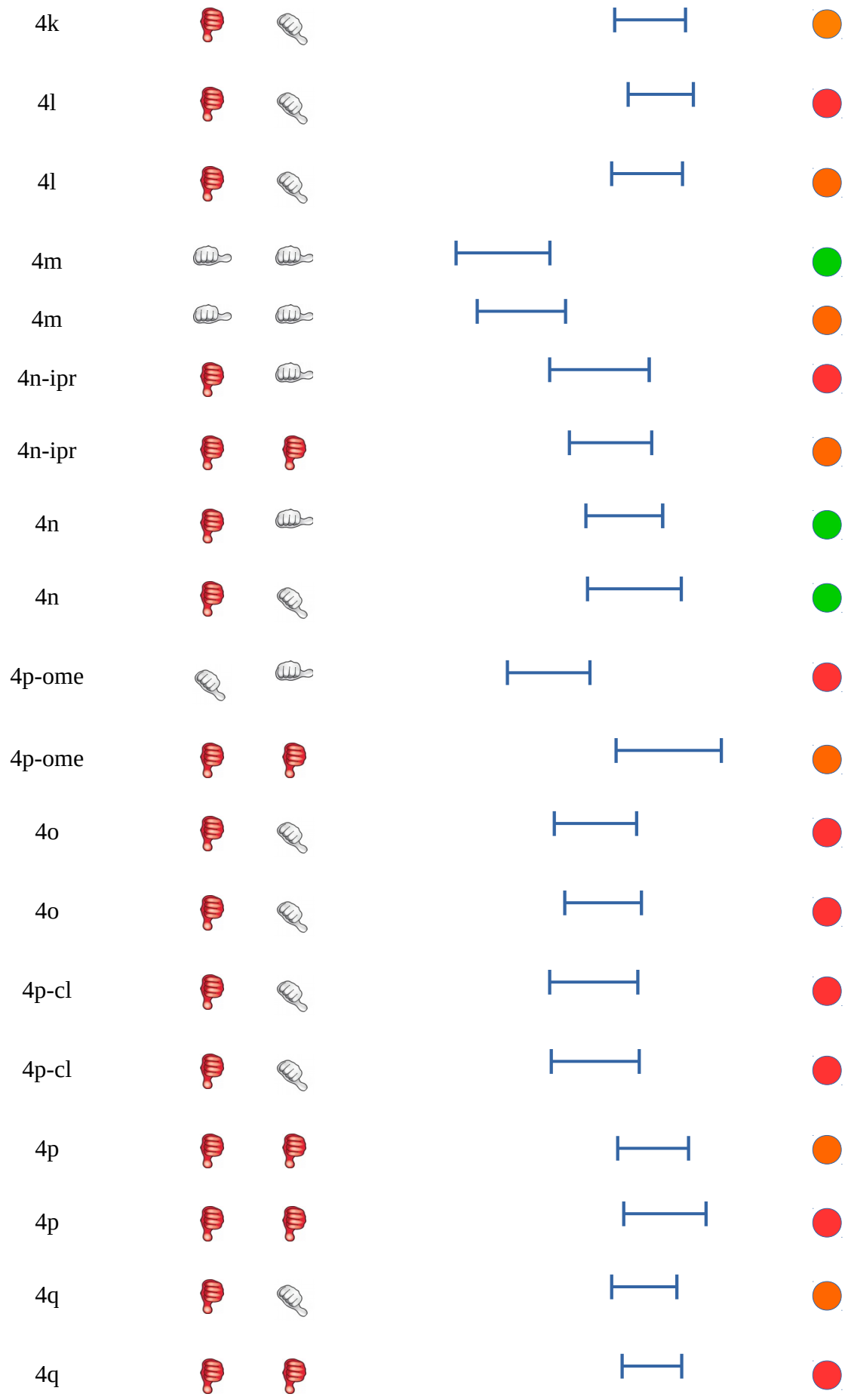
Supplementary Materials

Table S1: LLE, LE, Est. Affinity, and Torsion values for *Pf*LDH with 68 molecules and CQ.

Molecules	LLE	LE	Estimated Affinity				Torsion
			pM	nM	μM	mM	
3a							
3b							
3c							
3d							
3e							
3f							
3g							
3h							
3i-ome							
3i							
3j							
3k							
3m							
3n							
4a							
4a							


4b
4b
4c
4c
4d
4d
4e
4e
4f
4f
4g
4g
4h
4h
4i
4i
4j
4j
4k


4k
4l
4l
4m
4m
4n-ipr
4n-ipr
4n
4n
4p-ome
4p-ome
4o
4o
4p-cl
4p-cl
4p
4p
4q
4q

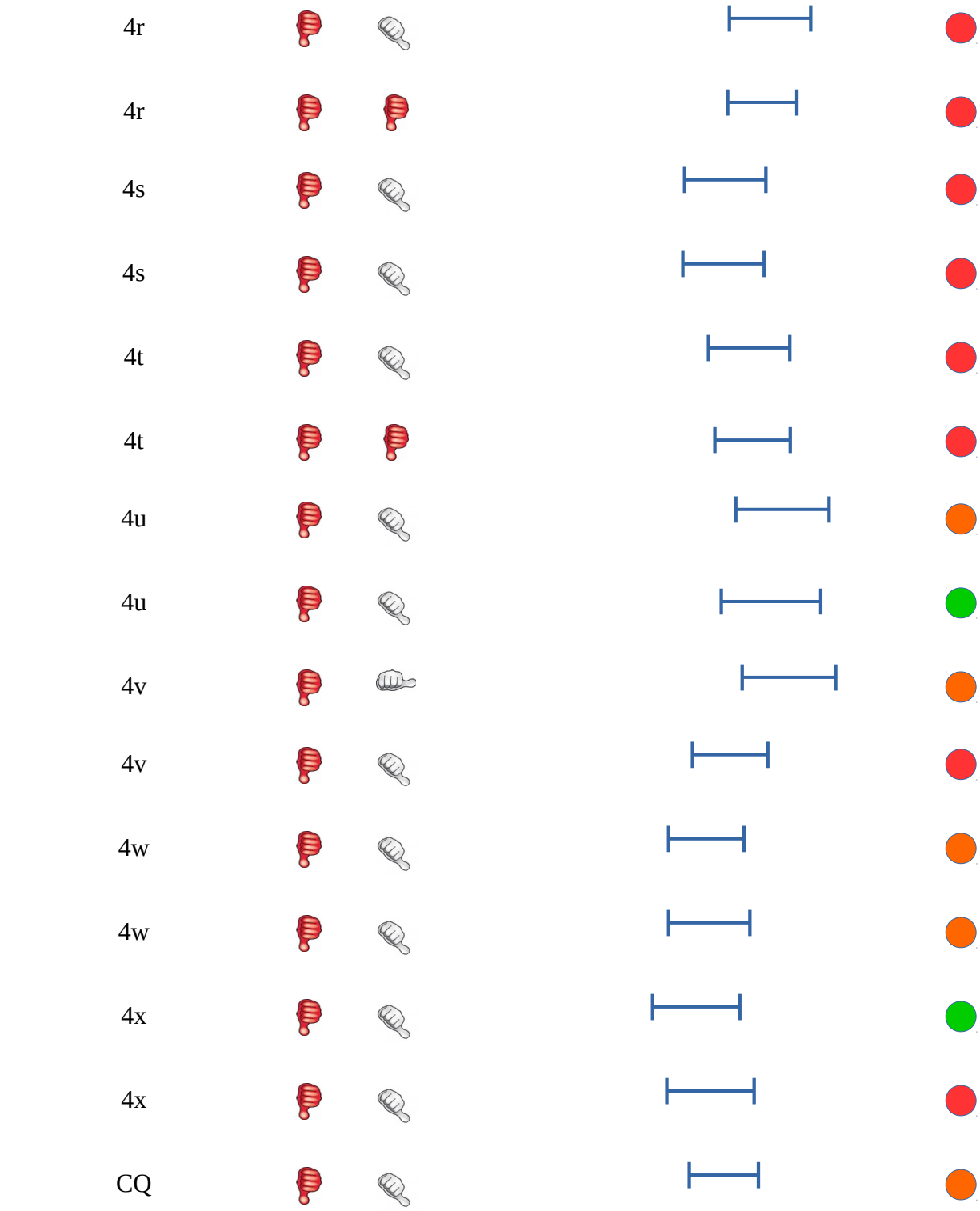
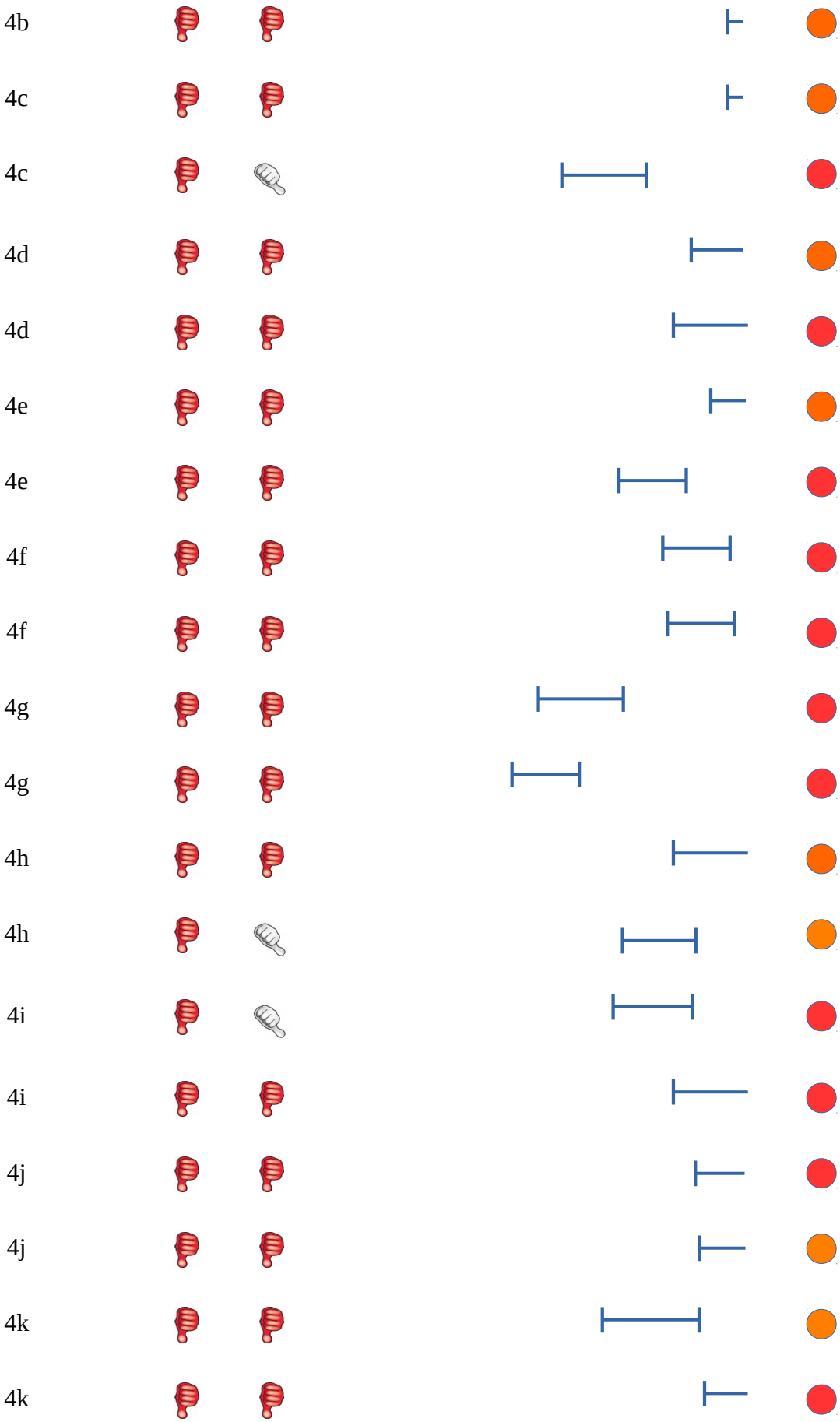
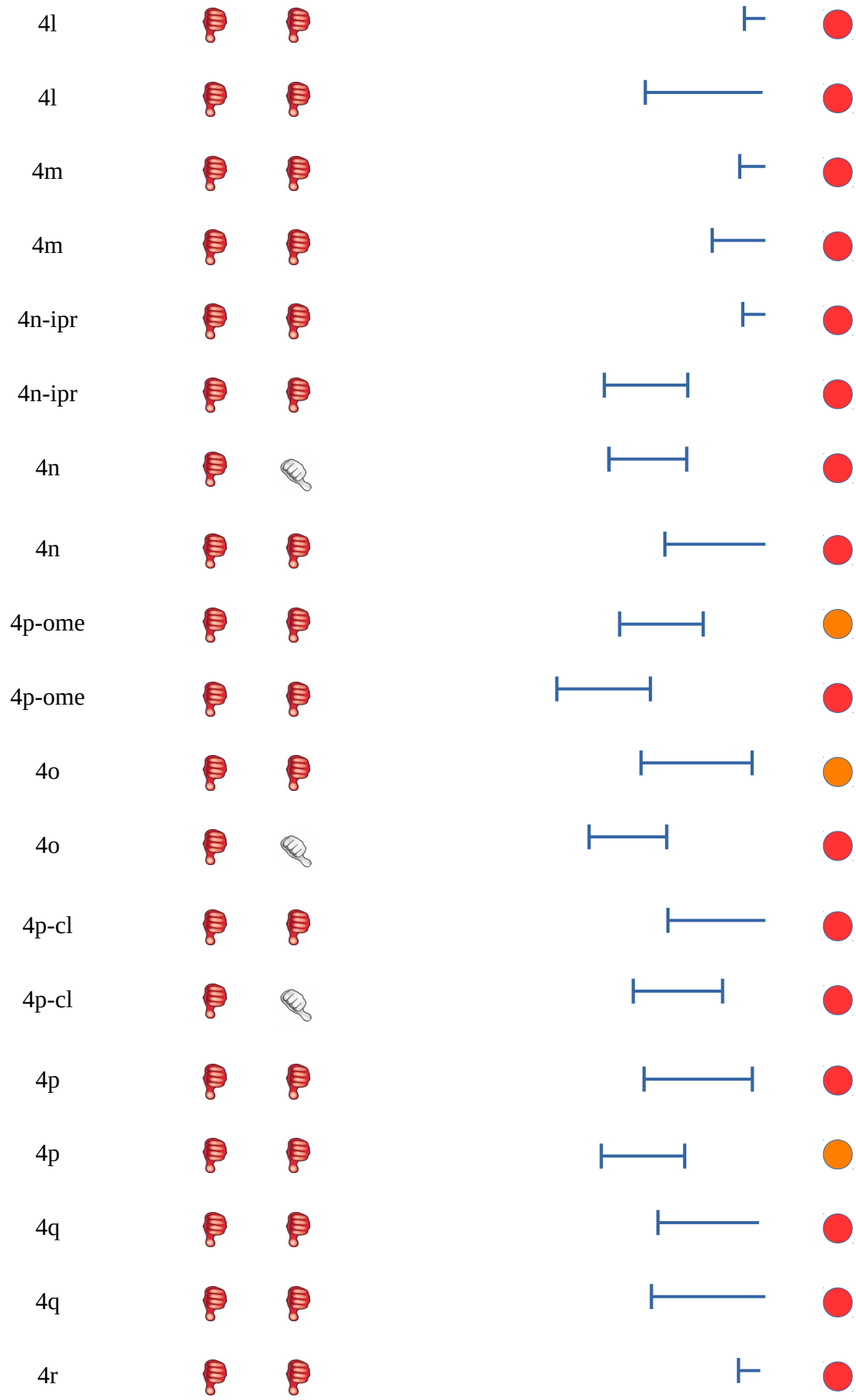

4r
4r
4s
4s
4t
4t
4u
4u
4v
4v
4w
4w
4x
4x
CQ

Table S2: LLE, LE, Est. Affinity, and Torsion values for human LDH with 68 molecules and CQ.

Molecules	LLE	LE	Estimated Affinity				Torsion
			pM	nM	µM	mM	
3a							
3b							
3c							
3d							
3e							
3f							
3g							
3h							
3i-ome							
3i							
3j							
3k							
3m							
3n							
4a							
4a							
4b							


4b
4c
4c
4d
4d
4e
4e
4f
4f
4g
4g
4h
4h
4i
4i
4j
4j
4k
4k


4l
4l
4m
4m
4n-ipr
4n-ipr
4n
4n
4p-ome
4p-ome
4o
4o
4p-cl
4p-cl
4p
4p
4q
4q
4r

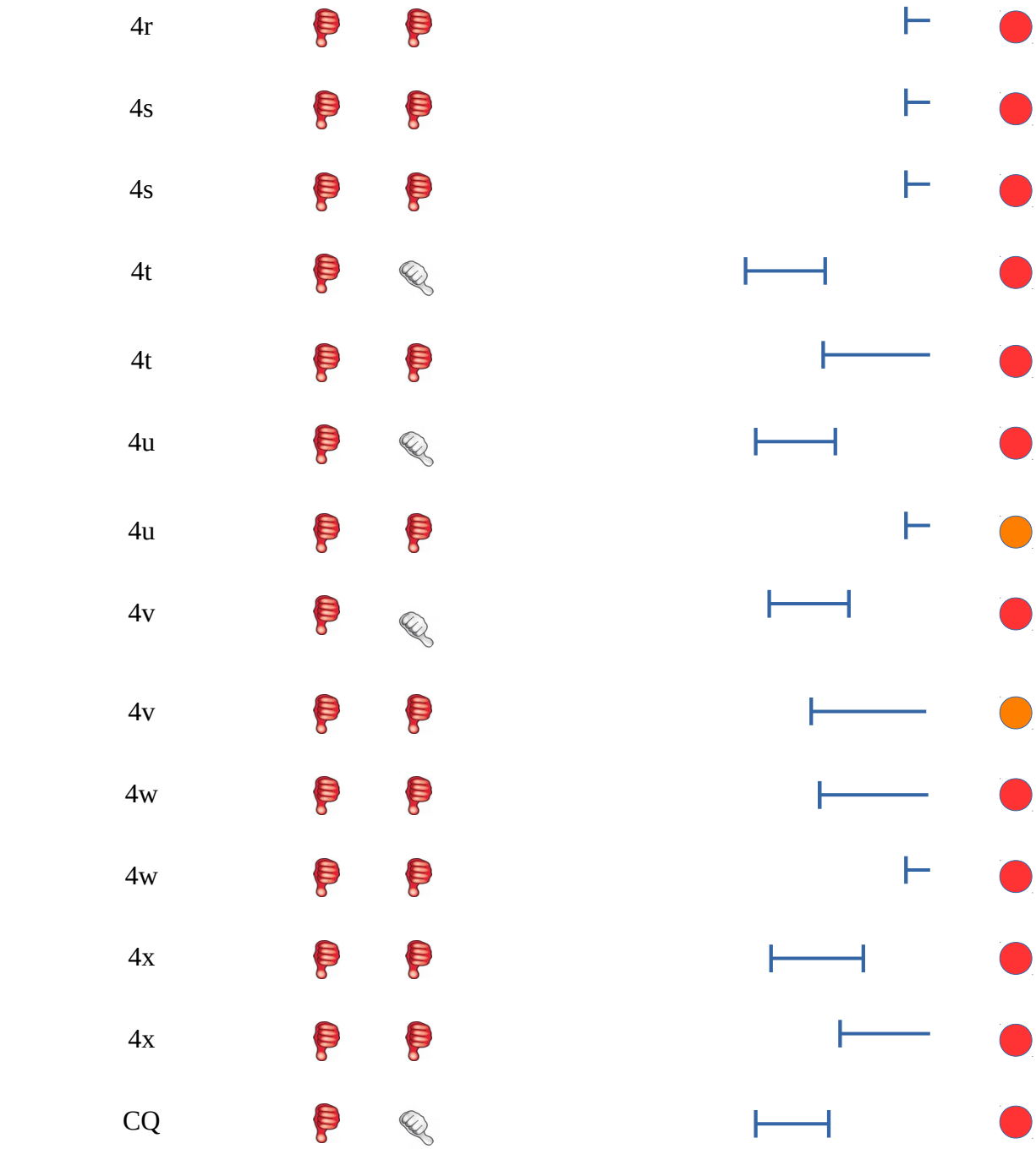

4r
4s
4s
4t
4t
4u
4u
4v
4v
4w
4w
4x
4x
CQ

Table S3: MM-PBSA internal calculations of binding energy for human LDH and *Pf*LDH complexes.

S. No.	Complexes	$\Delta E_{binding\ (kj/mol)}$	SASA	$\Delta E_{polar\ solvation}$ (kj/mol)	$\Delta E_{Electrostatic}$ (kj/mol)	$\Delta E_{Van\ der\ Waal}$ (kj/mol)
1.	1I10-CQ	-79.489	-15.110	163.974	-9.869	-218.484
2.	1I10-3j	-111.752	-12.411	32.244	-1.427	-130.158
3.	1I10-4b	-186.078	-14.971	64.235	-18.272	-217.070
4.	1I10-4h	-169.214	-15.874	83.218	-22.170	-214.389
5.	1I10-4m	-170.515	-18.838	168.094	-65.546	-254.226
6.	1LDG-CQ	-107.192	-16.283	118.347	-14.068	-195.189
7.	1LDG-3j	-161.138	-14.199	26.464	-1.804	-171.599
8.	1LDG-4b	-113.420	-12.651	57.919	-27.257	-131.431
9.	1LDG-4h	-136.928	-14.779	64.678	-31.918	-154.908
10.	1LDG-4m	-194.375	-18.495	133.251	-52.355	-256.776

Figure S1: Structure of 68 quinolines based molecules with CQ.

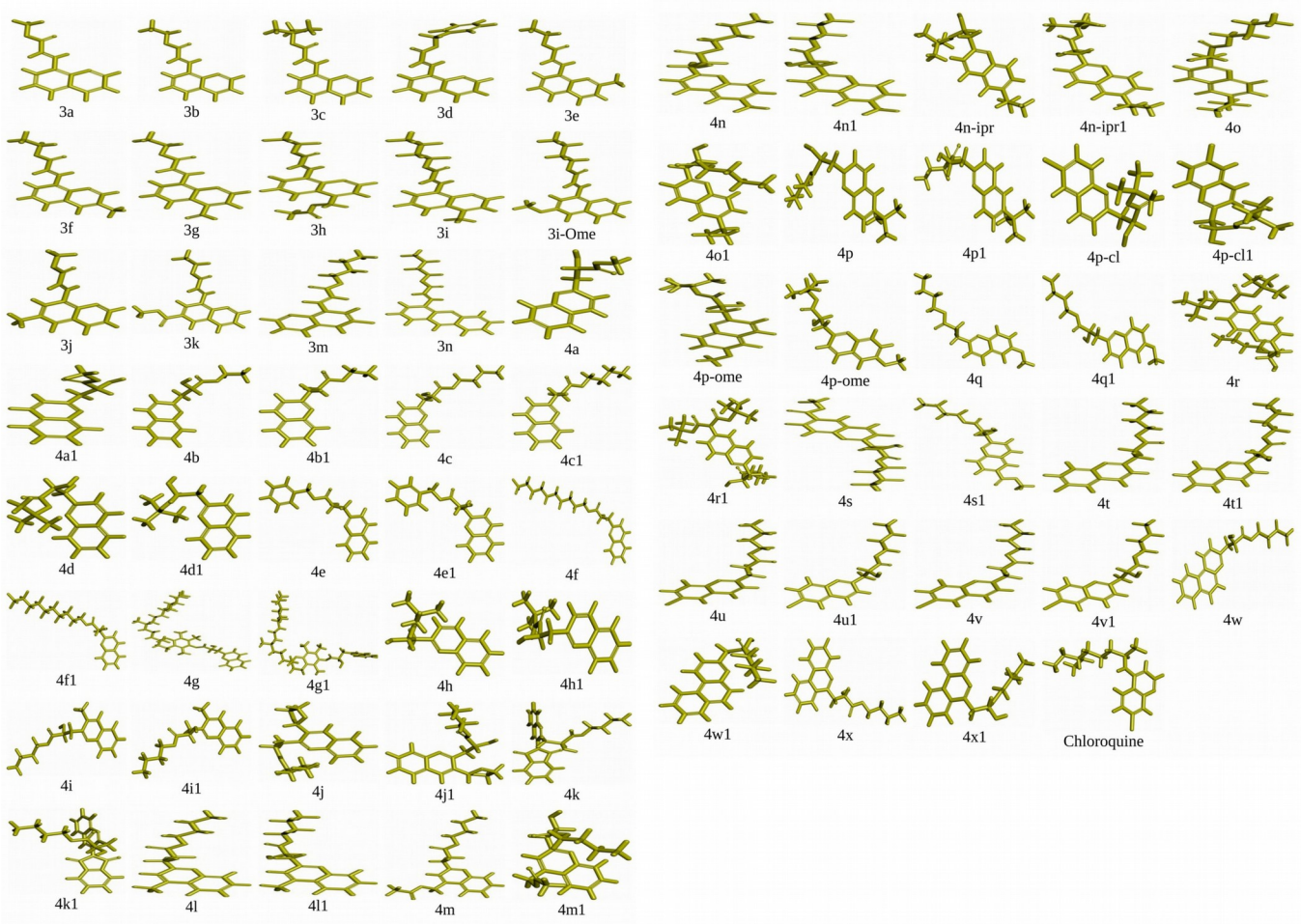


Figure S2: Superimposed protein 3-dimensional X-ray crystal structures of human LDH (brown), *Pf*LDH(blue).

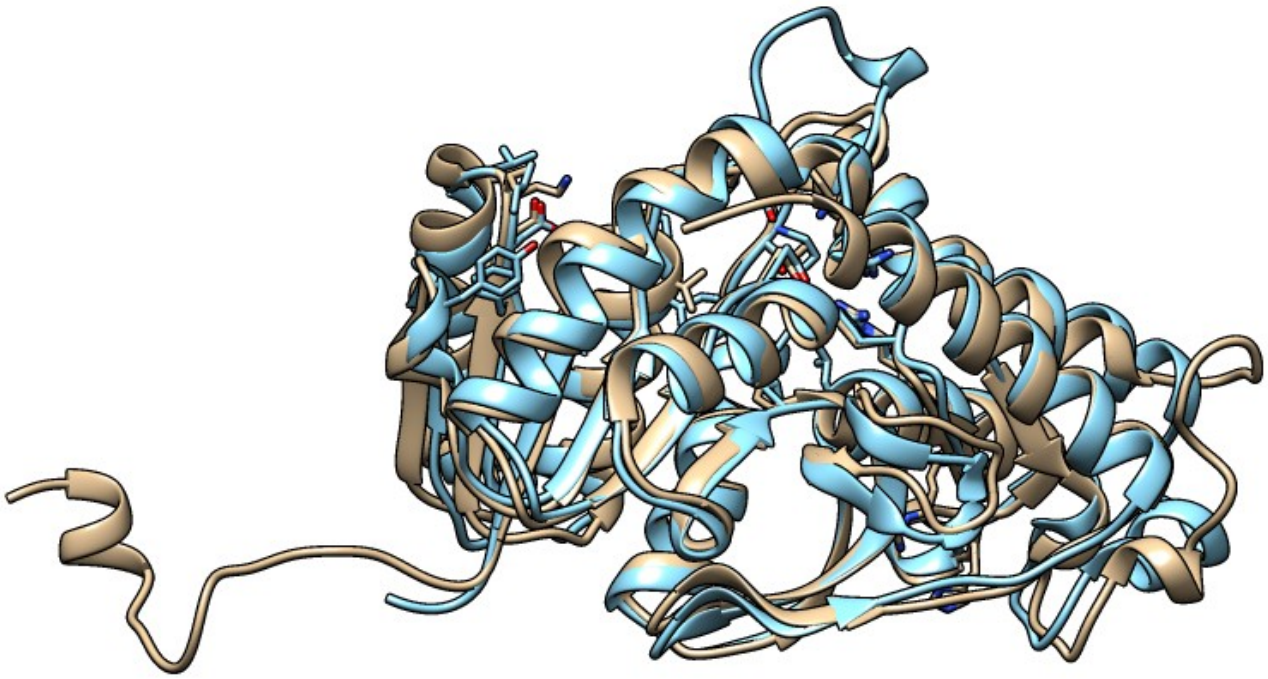


Figure S3: 3D binding poses of *Pf*LDH with molecules 4b and 4h.