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Supporting Information

Exploring the Trimerization Process of Transmembrane Helix with Ionizable Residue by Molecular Dynamics Simulations: A Case Study of Transmembrane Domain 5 of LMP-1

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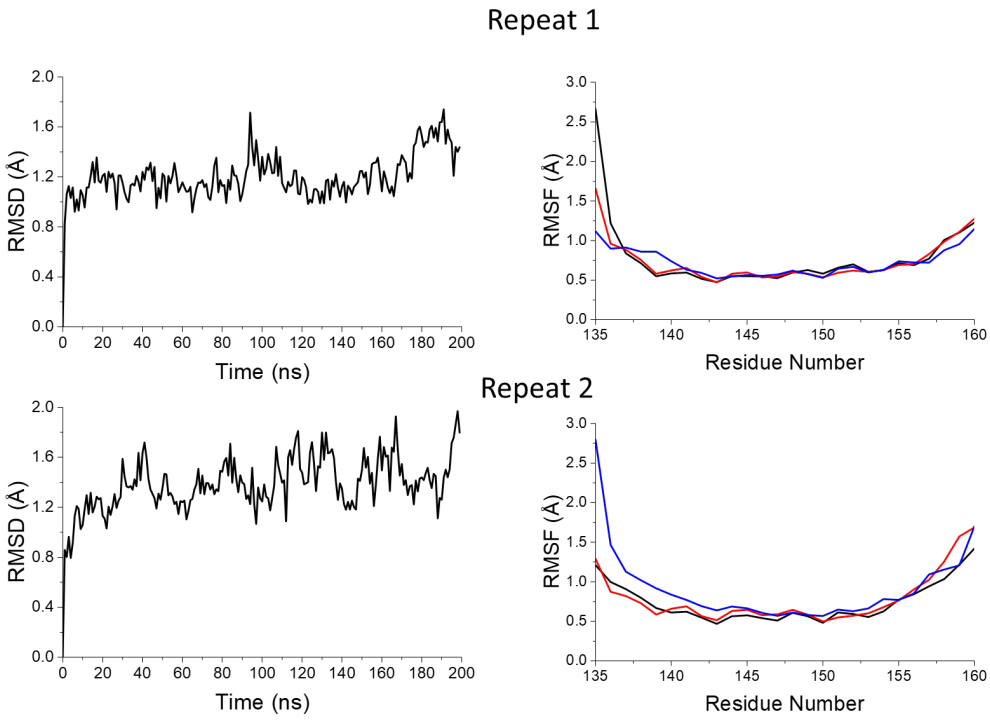

Figure S1. RMSD of the backbone of TMD5 trimer during the 200 ns molecular dynamics simulations and RMSF per residue Cα of TMD5 monomers in the trimeric state in two replicates.

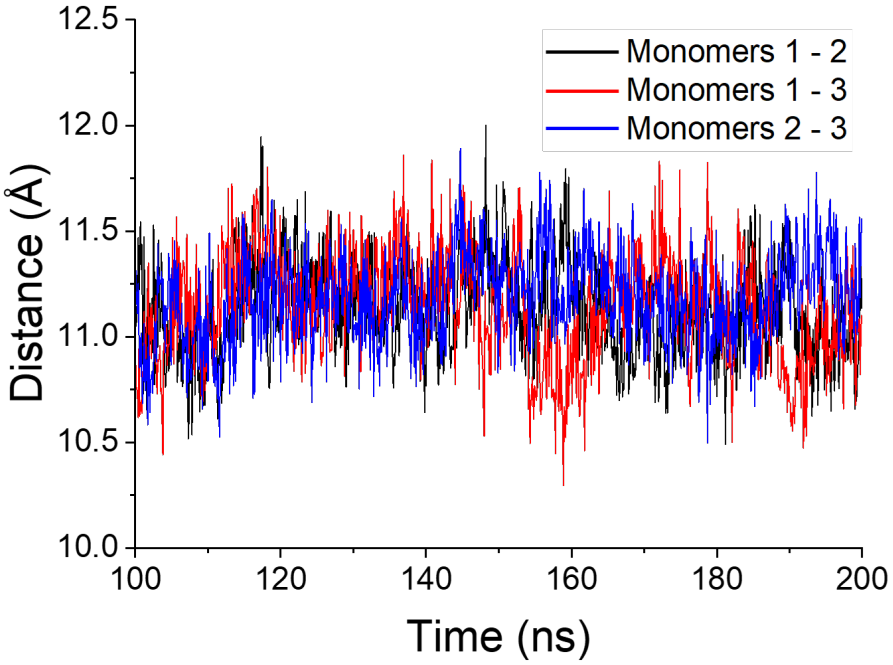

Figure S2. Distance of the center of mass of the Cα atoms of each two TMD5s in the last 100 ns simulation.

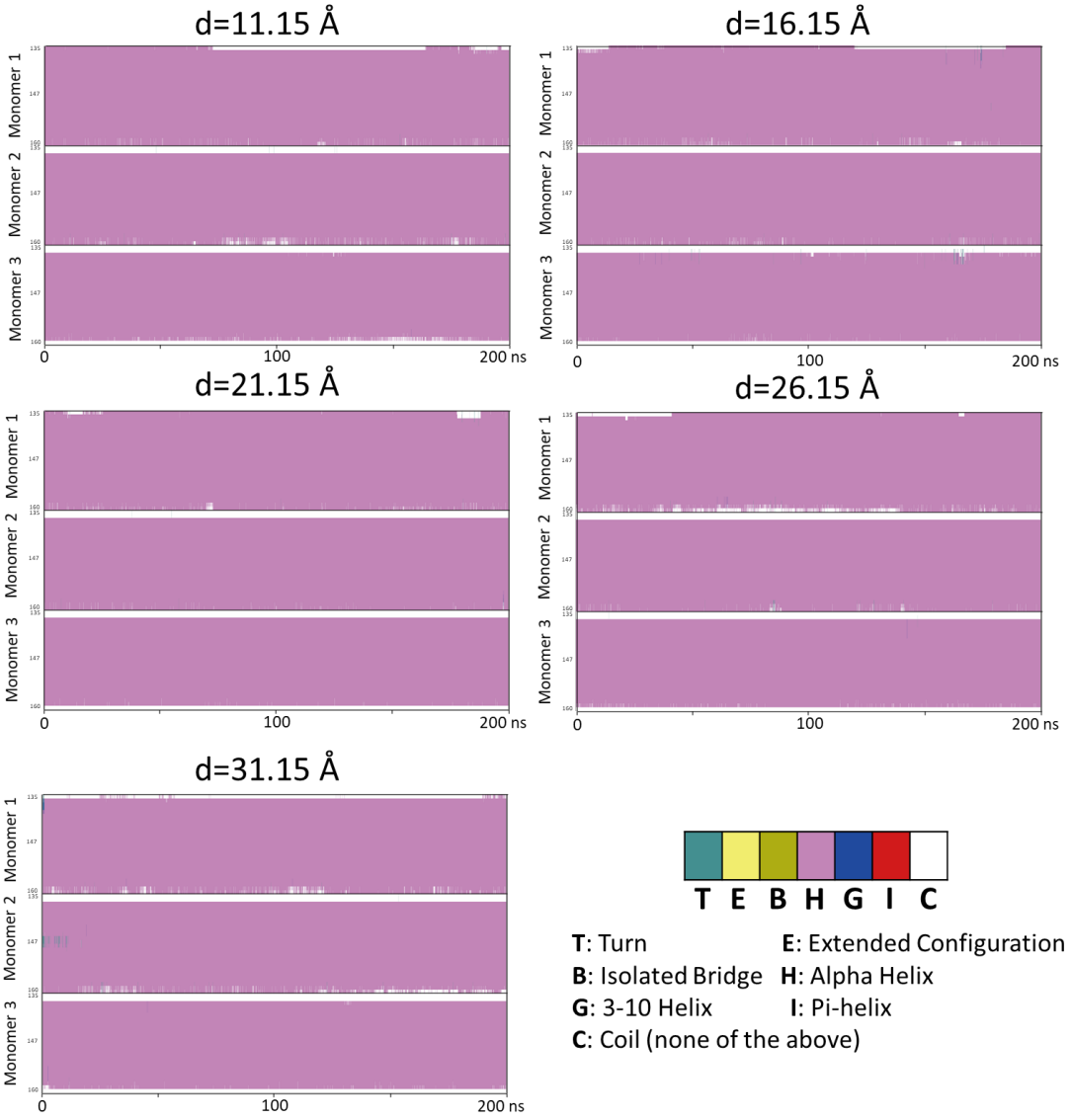

Figure S3. Protein secondary structures of TMD5 trimers with different reaction coordinates in 200 ns simulations.

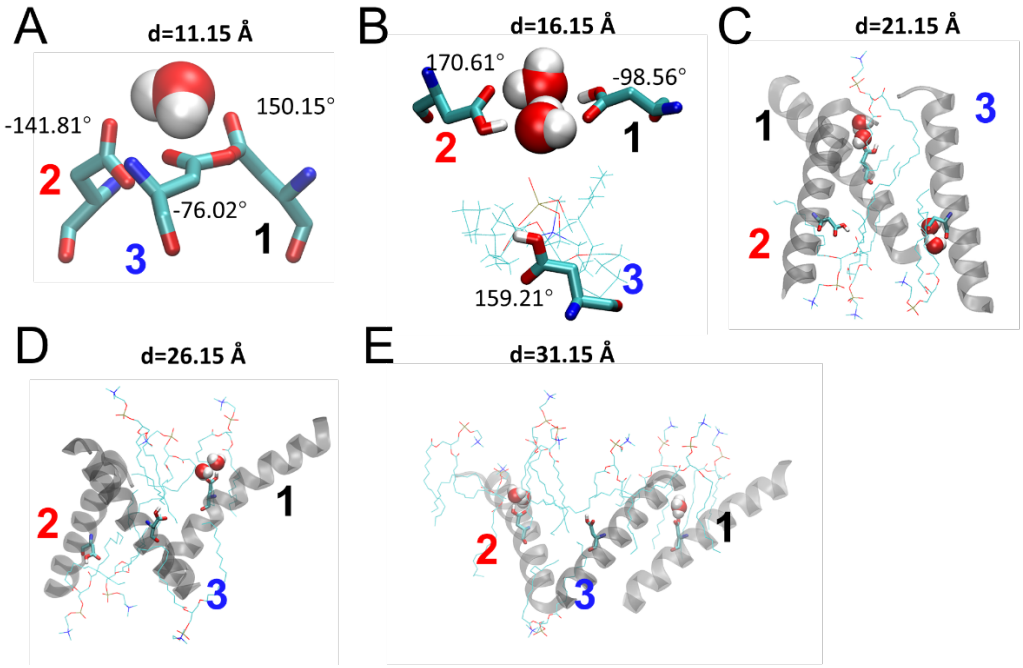

Figure S4. Interaction details of D150 along the reaction coordinate. Residue D150 is shown in cyan sticks. Representative dihedrals are labeled in (A) and (B). The transmembrane helixes are depicted with gray cartoon representation and the monomers are numbered with colors in (C), (D), and (E). The lipids within 3 Å of D150 are shown with cyan lines.

Table S1. Protonated fraction observed at each pH value at different reaction coordinates.

	pH	D150 in Monomer 1		D150 in Monomer 2		D150 in Monomer 3	
		f	Error	f	Error	f	Error
d = 11.15 Å	5	0.9745	0.0008	0.9999	0	0.9888	0.0005
	5.5	0.917	0.0024	0.9981	0.0001	0.9585	0.0015
	6	0.7171	0.0058	0.956	0.0014	0.813	0.0046
	6.5	0.2458	0.0056	0.6065	0.0068	0.3315	0.0067
	7	0.0248	0.0009	0.1936	0.0045	0.0421	0.0014
	7.5	0.0021	0.0001	0.0569	0.0017	0.004	0.0002
	8	0.0002	0	0.0175	0.0006	0.0004	0
	8.5	0	0	0.0055	0.0002	0	0
	9	0	0	0.0017	0.0001	0	0
d = 16.15 Å	4.5	0.9966	0.0002	0.9994	0.0001	0.9996	0
	5	0.9892	0.0005	0.9961	0.0002	0.997	0.0001
	5.5	0.9635	0.0016	0.9683	0.0011	0.9721	0.0009
	6	0.8465	0.004	0.744	0.0061	0.7597	0.0059
	6.5	0.4887	0.0061	0.1899	0.005	0.215	0.0053
	7	0.2033	0.0044	0.0193	0.0008	0.0321	0.0014
	7.5	0.0738	0.0019	0.0025	0.0002	0.0072	0.0005
	8	0.0246	0.0007	0.0005	0.0001	0.0021	0.0002
	8.5	0.0079	0.0002	0.0001	0	0.0006	0
	9	0.0025	0.0001	0	0	0.0002	0
d = 21.15 Å	3	0.9999	0	0.9986	0.0001	0.9889	0.0003
	3.5	0.9996	0.0001	0.9957	0.0002	0.9656	0.0008
	4	0.9989	0.0002	0.9868	0.0006	0.899	0.0021
	4.5	0.9968	0.0004	0.96	0.0014	0.7388	0.0045
	5	0.9878	0.0008	0.8828	0.0029	0.4738	0.0056
	5.5	0.9208	0.0021	0.6726	0.0055	0.2149	0.004
	6	0.6319	0.0061	0.2942	0.0056	0.0598	0.0018
	6.5	0.2624	0.0051	0.0579	0.0016	0.0095	0.0005
	7	0.0863	0.0022	0.0076	0.0003	0.0013	0.0001
	7.5	0.0273	0.0007	0.001	0.0001	0.0002	0
	8	0.0086	0.0002	0.0002	0	0	0
	8.5	0.0027	0.0001	0	0	0	0
d = 26.15 Å	2.5	1	0	0.9992	0	0.9989	0
	3	1	0	0.9975	0.0001	0.9966	0.0001
	3.5	1	0	0.9921	0.0002	0.9893	0.0003
	4	1	0	0.9758	0.0007	0.9674	0.0008
	4.5	0.9999	0	0.9304	0.0017	0.9068	0.0021
	5	0.9986	0.0001	0.8274	0.0035	0.772	0.0041
	5.5	0.9864	0.0005	0.6588	0.0049	0.5664	0.0052
	6	0.8988	0.0025	0.4318	0.0054	0.3348	0.005
	6.5	0.5949	0.0060	0.174	0.0038	0.1188	0.0029
	7	0.2498	0.0048	0.0391	0.0013	0.021	0.0007
	7.5	0.0845	0.0020	0.0077	0.0004	0.0025	0.0001
	8	0.0271	0.0007	0.0018	0.0001	0.0003	0
	8.5	0.0086	0.0002	0.0005	0	0	0
	9	0.0027	0.0001	0.0002	0	0	0
d = 31.15 Å	2.5	1	0	1	0	0.9978	0
	3	1	0	1	0	0.9931	0.0002
	3.5	0.9999	0	0.9999	0	0.9784	0.0005
	4	0.9996	0.0001	0.9997	0.0001	0.9348	0.0014
	4.5	0.9985	0.0002	0.9988	0.0002	0.819	0.0034
	5	0.9931	0.0004	0.9944	0.0004	0.5867	0.0055
	5.5	0.9574	0.0014	0.9624	0.0013	0.3008	0.0047
	6	0.7378	0.0057	0.7516	0.0055	0.0953	0.0021
	6.5	0.2523	0.0055	0.2665	0.0057	0.0132	0.0007
	7	0.0443	0.0014	0.0503	0.0016	0.0015	0.0002
	7.5	0.0084	0.0004	0.0104	0.0004	0.0003	0.0001
	8	0.002	0.0001	0.0027	0.0001	0.0001	0
	8.5	0.0006	0	0.0008	0	0	0