Supplementary Data

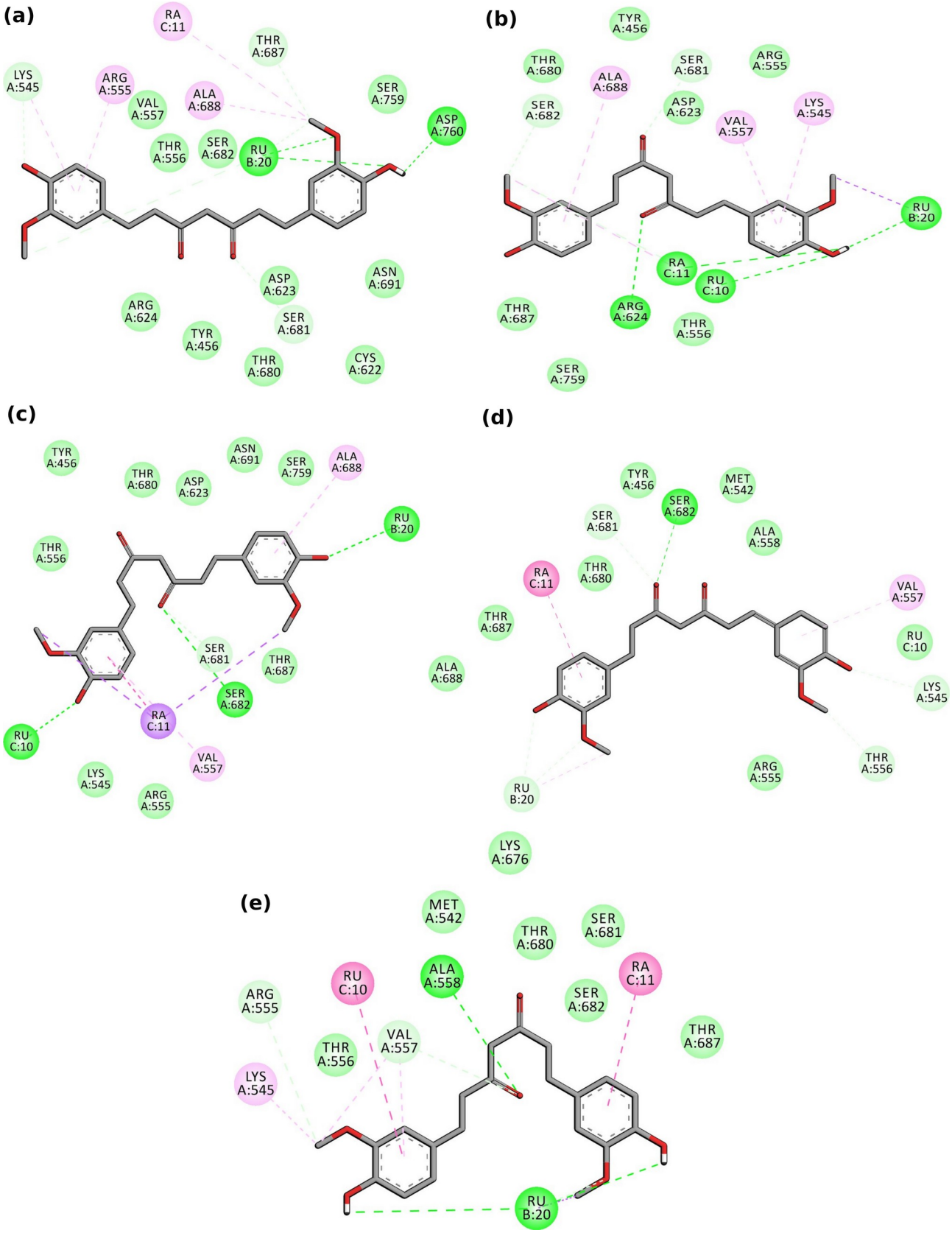

Figure S1. Molecular docking 2D interaction poses of the RdRp-RNA of SARS-CoV-2 in complex with curcumin at different time intervals. (a) 5 ns, (b) 25 ns, (c) 50 ns, (d) 75 ns, and 100 ns.

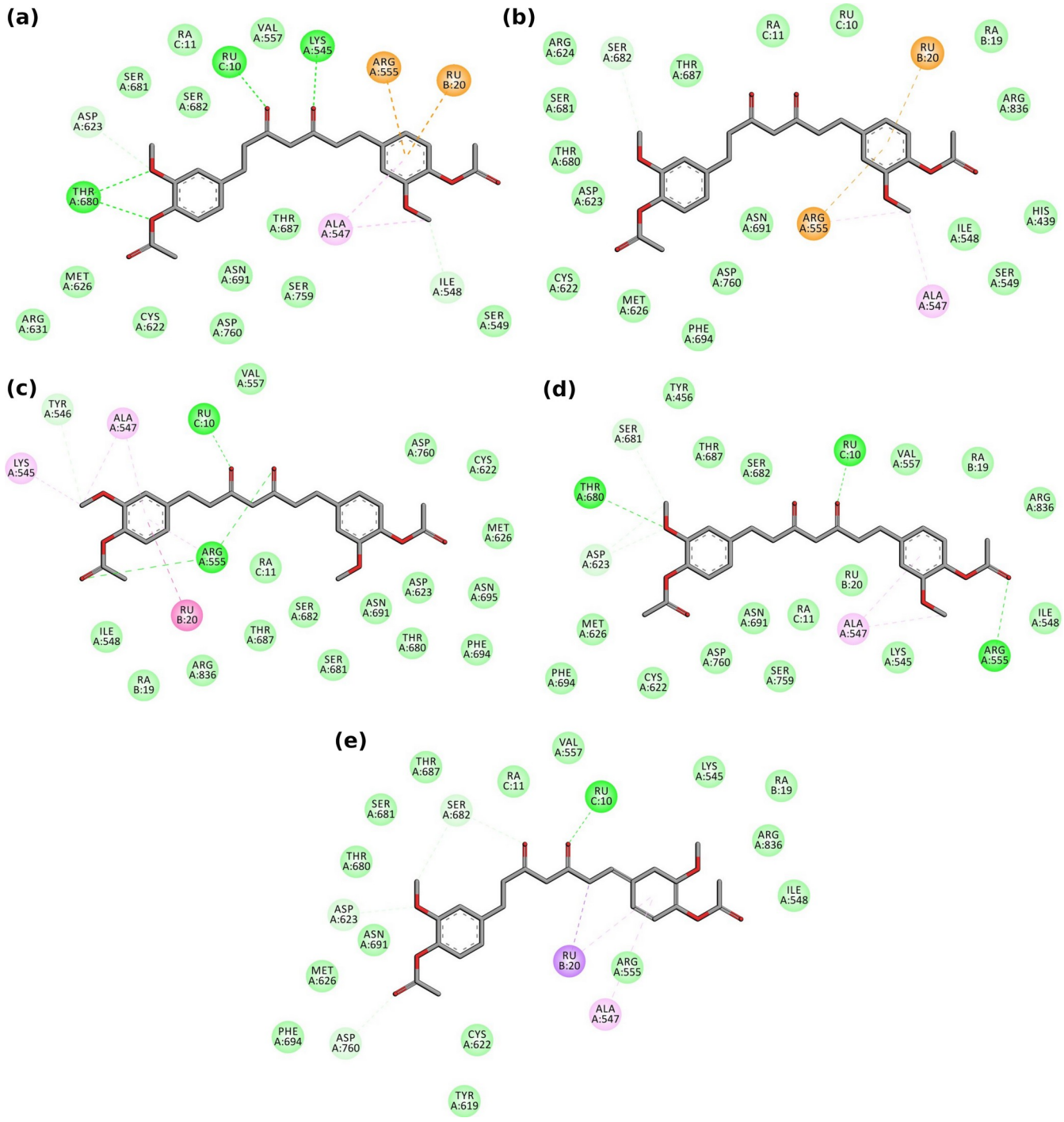

Figure S2. Molecular docking 2D interaction poses of the RdRp-RNA of SARS-CoV-2 in complex with diacetylcurcumin at different time intervals. (a) 5 ns, (b) 25 ns, (c) 50 ns, (d) 75 ns, and 100 ns.

Table S1. Comparative binding free energy in individual terms for FDA-approved drugs and selected compounds bound to RdRp-RNA generated by MM-PBSA method.

S. No.	RdRp-RNA-Ligand Complexes	$\Delta E_{binding}$ (kJ/mol)	$\Delta E_{polar\ solvation}$ (kJ/mol)	SASA (kJ/mol)	$\Delta E_{Electrostatic}$ (kJ/mol)	$\Delta E_{Van\ der\ Waals}$ (kJ/mol)
1.	RdRp-curcumin	-42.162	101.798	-13.496	-18.137	-112.327
2.	RdRp-diacetylcurcumin	-71.964	116.315	-19.107	-14.698	-154.474
3.	**RdRp-Remdesivir**	**107.346**	**437.201**	**-12.356**	**-248.406**	**-69.093**
4.	**RdRp-Favipiravir**	**248.378**	**977.029**	**-12.653**	**-657.208**	**-58.790**
5.	RNA-curcumin	-40.306	27.351	-6.539	-11.487	-49.631
6.	RNA-diacetylcurcumin	-80.718	31.556	-8.498	-31.535	-72.242
7.	**RNA-Favipiravir**	**2091.712**	**-18.286**	**-6.780**	**2168.615**	**-51.572**
8.	**RNA-Remdesivir**	**1311.862**	**- 30.025**	**- 7.045**	**1387.624**	**-40.383**