# Supplementary Material

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**Figure S1** Molecular Docking Results of Catechin

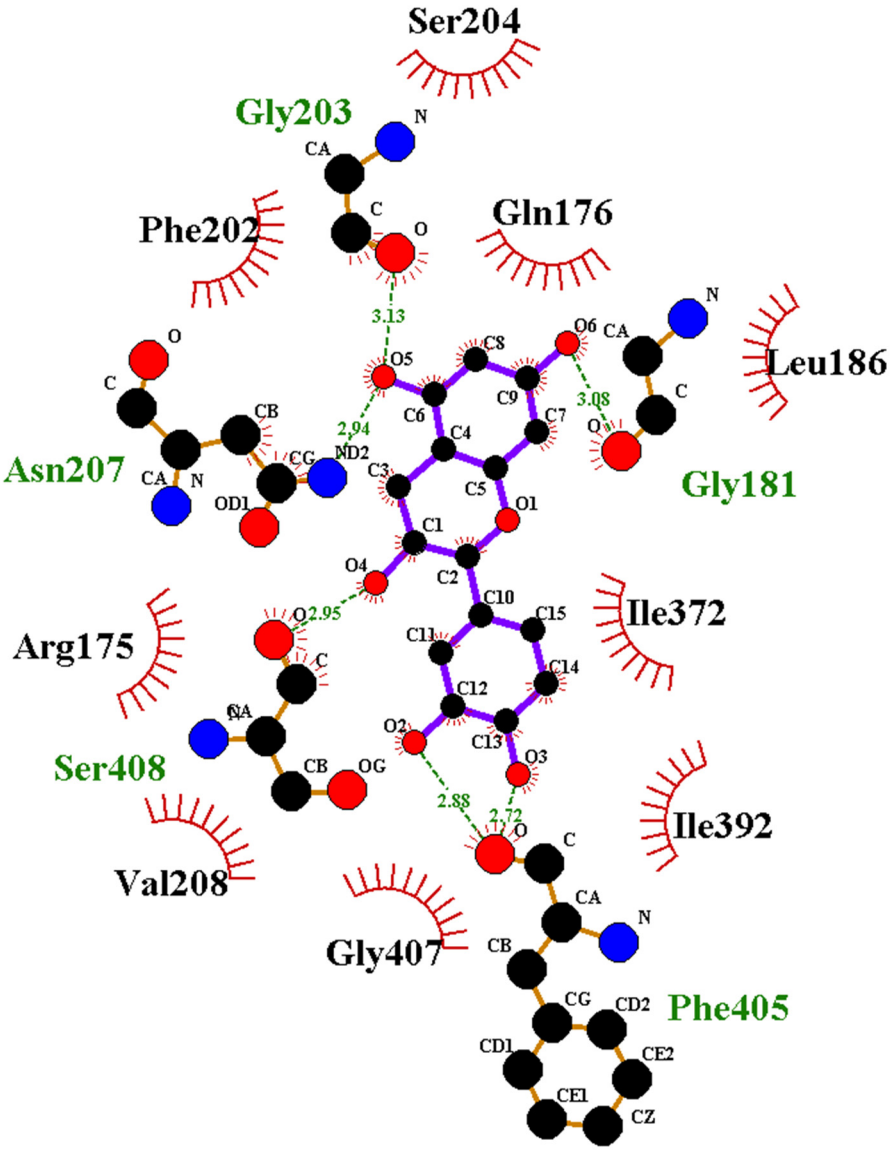


**Figure S2** Molecular Docking Results of Epicatechin

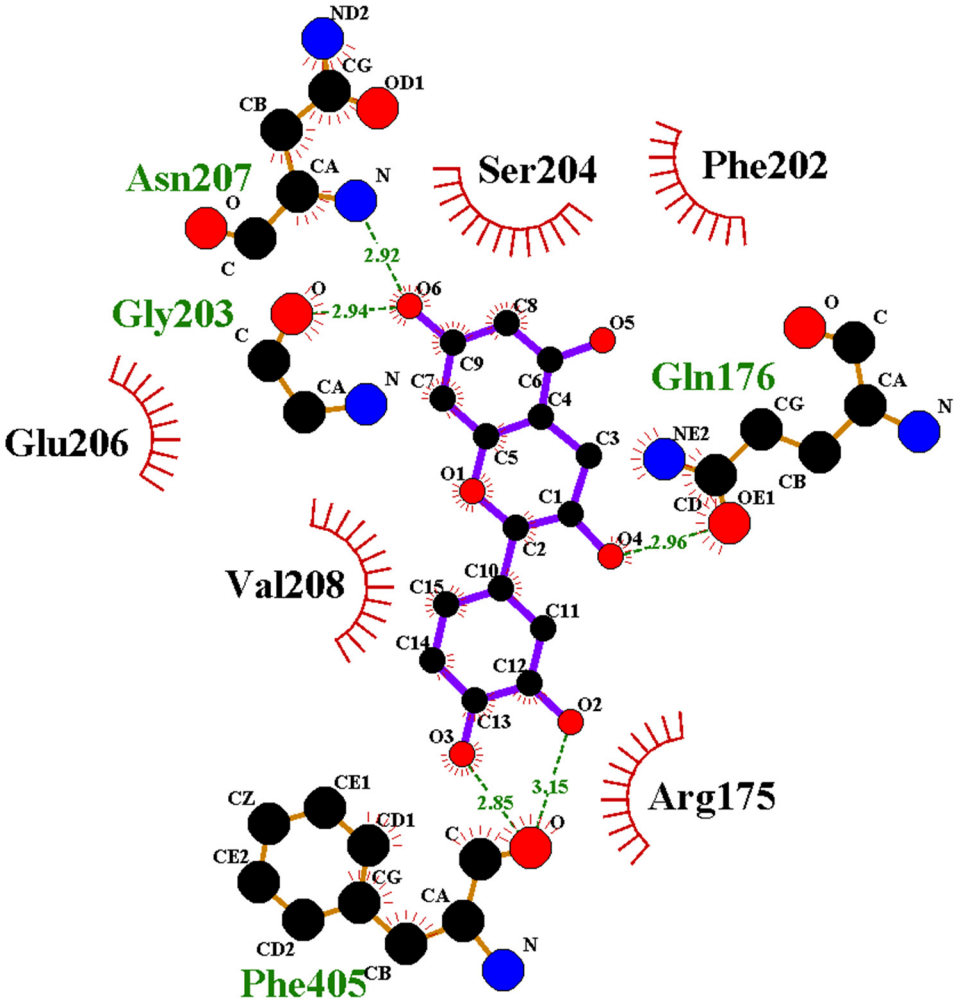


**Figure S3** Molecular Docking Results of Chlorogenic acid

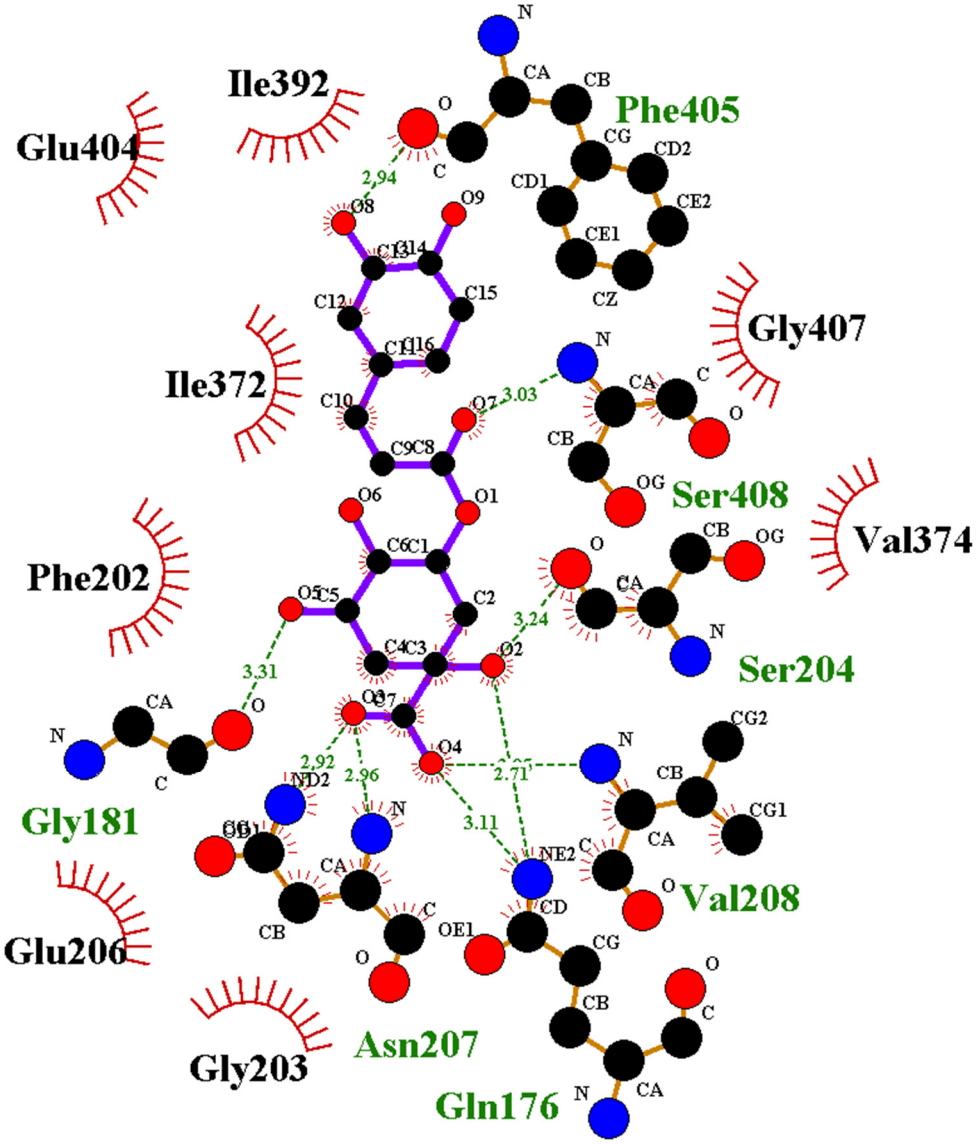


**Figure S4** Molecular Docking Results of Oxalic acid

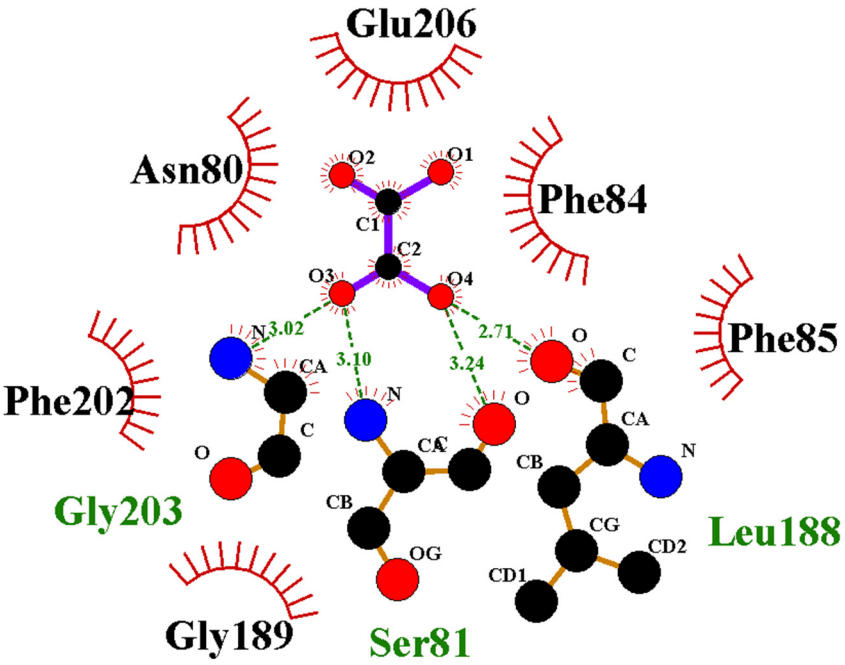
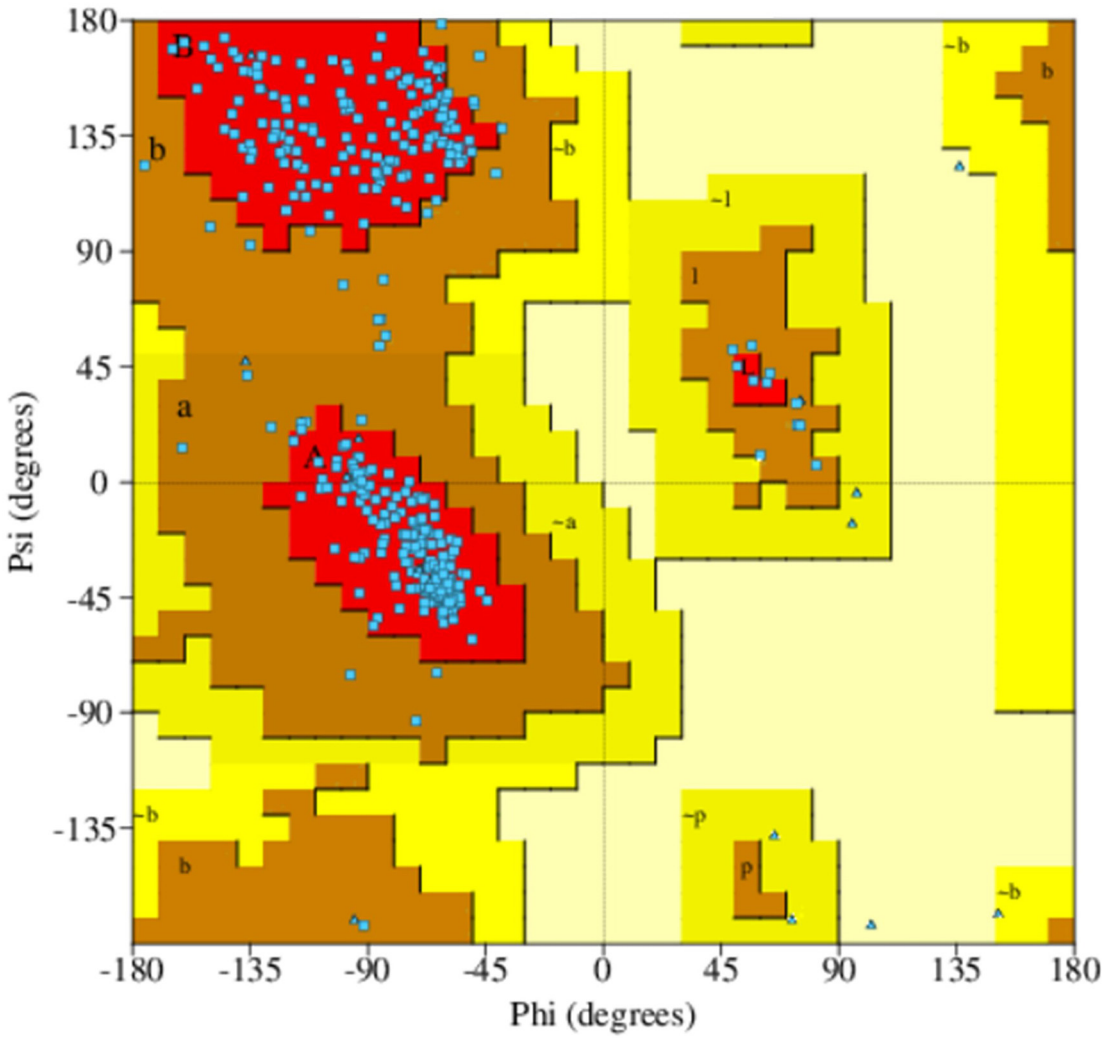


**Figure S5** Ramachandran Plot of PPO



**Specific Parameters for cMD During Pre-equilibration**

```
&cntrl
   imin = 0,
   irest = 0,
   ntx = 1,
   ioutfm = 1,
   nstlim = 25000000,
   dt = 0.002,
   ntt = 3,
   gamma_ln = 5.0,
   ig = -1,
   tempi = 300.0,
   temp0 = 300.0,
   ntp = 0,
   ntb = 1,
   ntc = 2,
   ntf = 2,
   cut = 8,
   ntwr = 50000,
   ntpr = 5000,
   ntwx = 50000,
   ntwe = 50000,
   iwrap = 1,
   ntr = 0,

   igamd = 3, iE = 1, irest_gamd = 0,
   ntcmd = 1000000, nteb = 25000000, ntave = 200000,
   ntcmdprep = 200000, ntebprep = 800000,
   sigma0P = 6.0, sigma0D = 6.0,
/
```

**Specific Parameters for GaMD**

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&cntrl
   imin = 0,
   irest = 1,
   ntx = 5,
   ioutfm = 1,
   nstlim = 250000000,
   dt = 0.002,
   ntt = 3,
   gamma_ln = 2.0,
   ig = -1,
   tempi = 300.0,
   temp0 = 300.0,
   ntp = 0,
   ntb = 1,
   ntc = 2,
   ntf = 2,
   cut = 8,
   ntwr = 50000,
   ntpr = 5000,
   ntwx = 50000,
   ntwe = 50000,
   iwrap = 1,
   ntr = 0,

   igamd = 3, iE = 1, irest_gamd = 1,
   ntcmd = 0, nteb = 0, ntave = 200000,
   ntcmdprep = 0, ntebprep = 0,
   sigma0P = 6.0, sigma0D = 6.0,
/
```

**Figure S6** RMSD Results of Parallel Trajectories

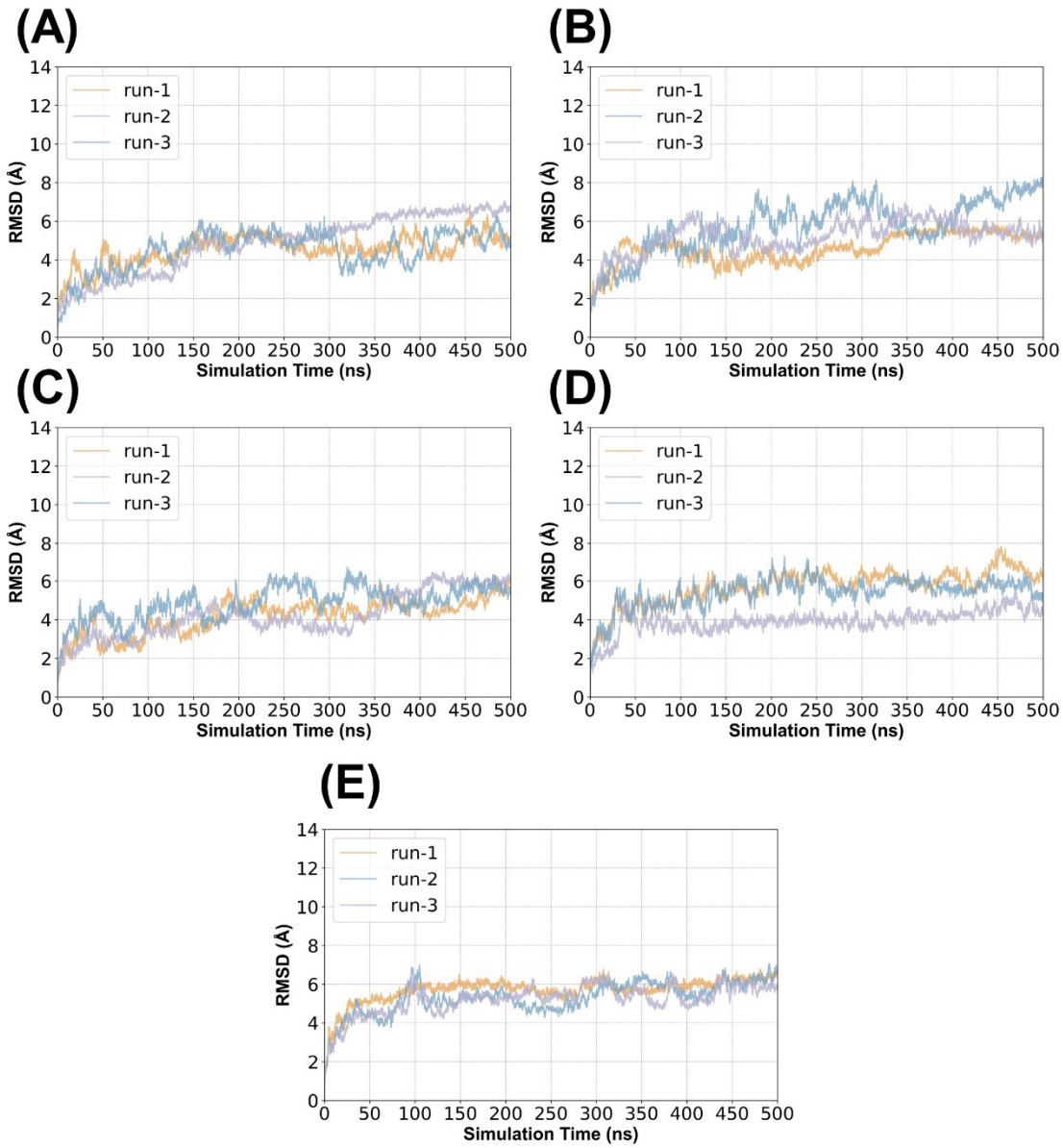


**Figure S7** $R_g$ Results of Parallel Trajectories

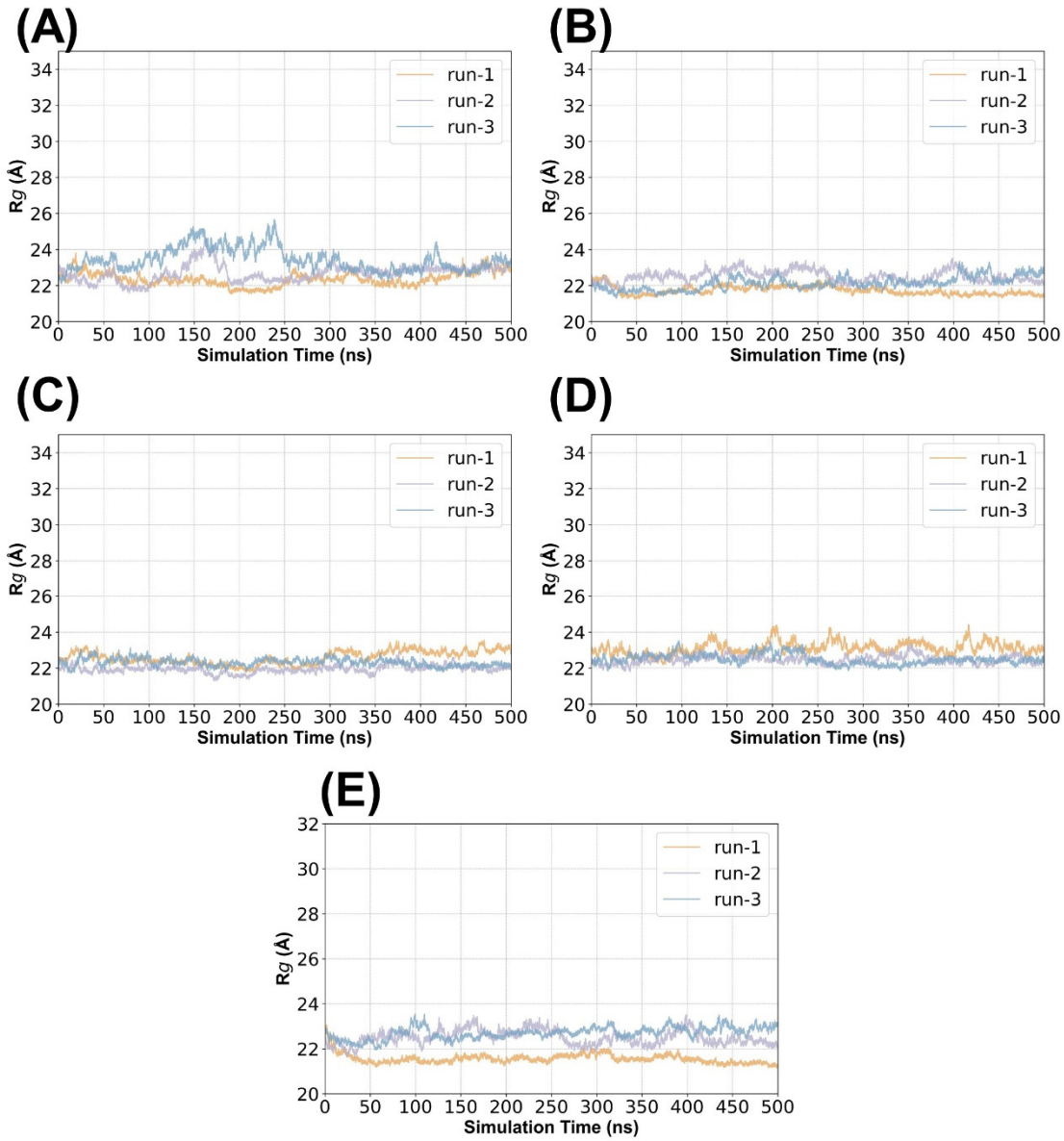


**Figure S8** SASA Results of Parallel Trajectories

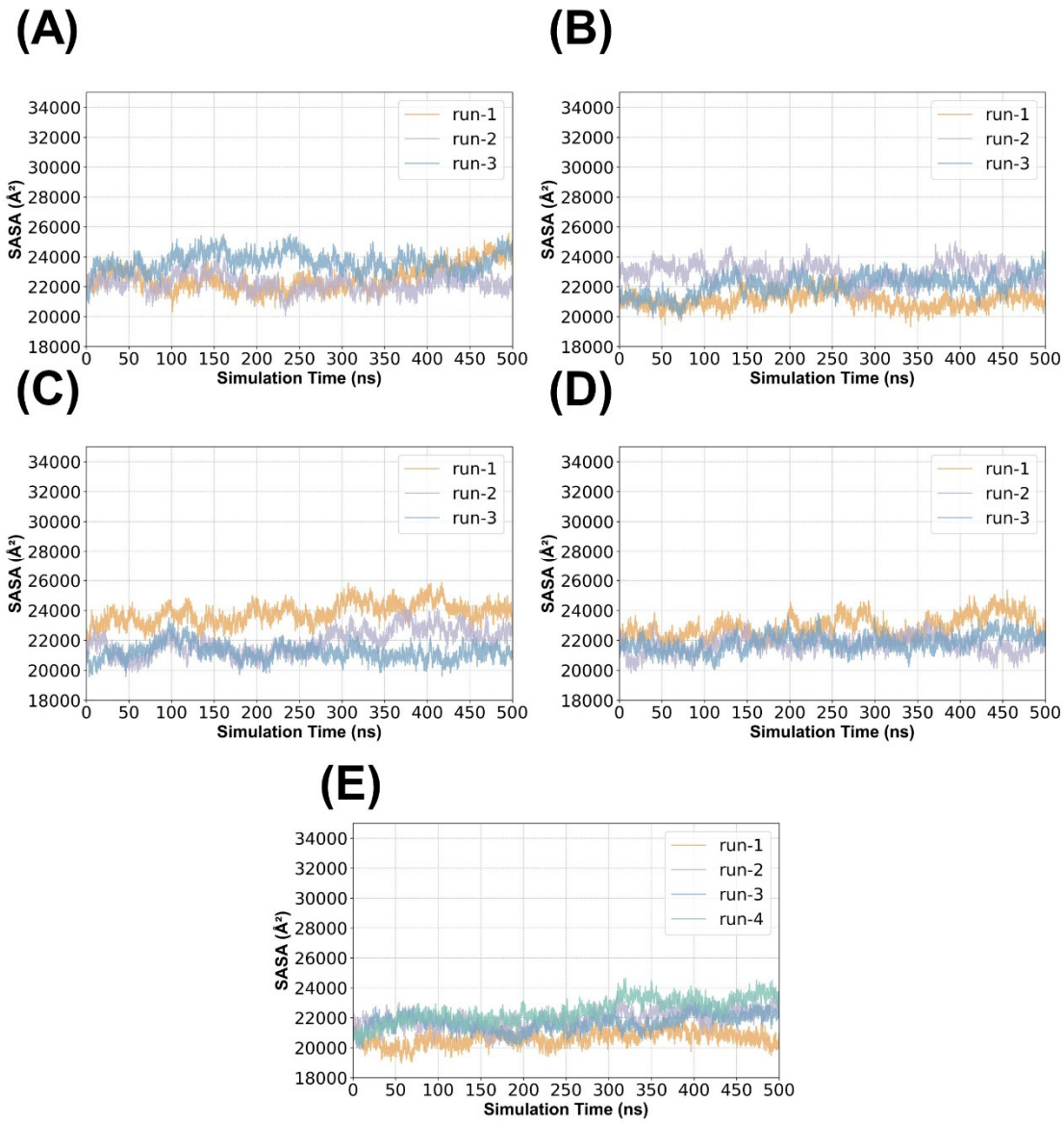


**Table S1** Probability of α-Helix Formation in Residue Ranges D53-Q63 and F350-V378 Across Five Systems with Three Parallel Trajectories

| System | D53-Q63 | F350-V378 |
|---|---|---|
| Ligand-free protein(run-1) | 18.82% | 3.08% |
| Ligand-free protein(run-2) | 20.46% | 5.47% |
| Ligand-free protein(run-3) | 17.38% | 3.72% |
| Ligand-free protein(Average) | 18.89% | 4.09% |
| Catechin-bounded protein(run-1) | 36.51% | 12.82% |
| Catechin-bounded protein(run-2) | 37.75% | 11.76% |
| Catechin-bounded protein(run-3) | 29.48% | 17.16% |
| Catechin-bounded protein(Average) | 34.58% | 13.91% |
| Epicatechin-bounded protein(run-1) | 65.88% | 19.71% |
| Epicatechin-bounded protein(run-2) | 57.79% | 16.34% |
| Epicatechin-bounded protein(run-3) | 60.43% | 20.18% |
| Epicatechin-bounded protein(Average) | 61.37% | 18.74% |
| Chlorogenic acid-bounded protein(run-1) | 24.99% | 4.79% |
| Chlorogenic acid-bounded protein(run-2) | 27.31% | 4.35% |
| Chlorogenic acid-bounded protein(run-3) | 21.07% | 6.14% |
| Chlorogenic acid-bounded protein(Average) | 24.46% | 5.09% |
| Oxalic acid-bounded protein(run-1) | 22.42% | 2.71% |
| Oxalic acid-bounded protein(run-2) | 25.61% | 4.48% |
| Oxalic acid-bounded protein(run-3) | 20.87% | 2.59% |
| Oxalic acid-bounded protein(Average) | 22.97% | 4.16% |

**Figure S9** Implied Timescales (ITS) analysis results

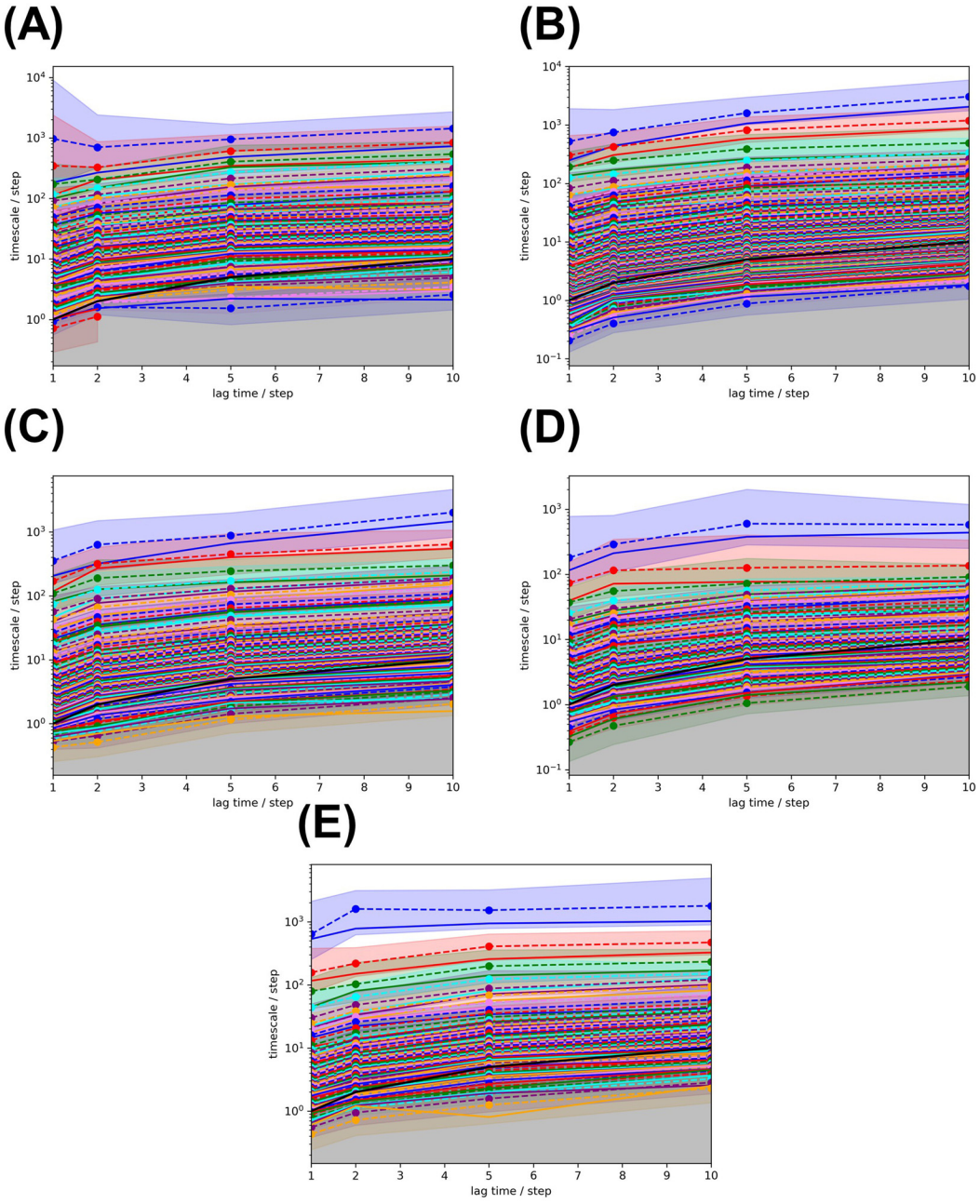


**Figure S10** Chapman-Kolmogorov test results

