# Drug similarity and structure-based screening of medicinal compounds to target Macrodomain-I from SARS-CoV-2 to rescue the host immune system: A molecular dynamics study

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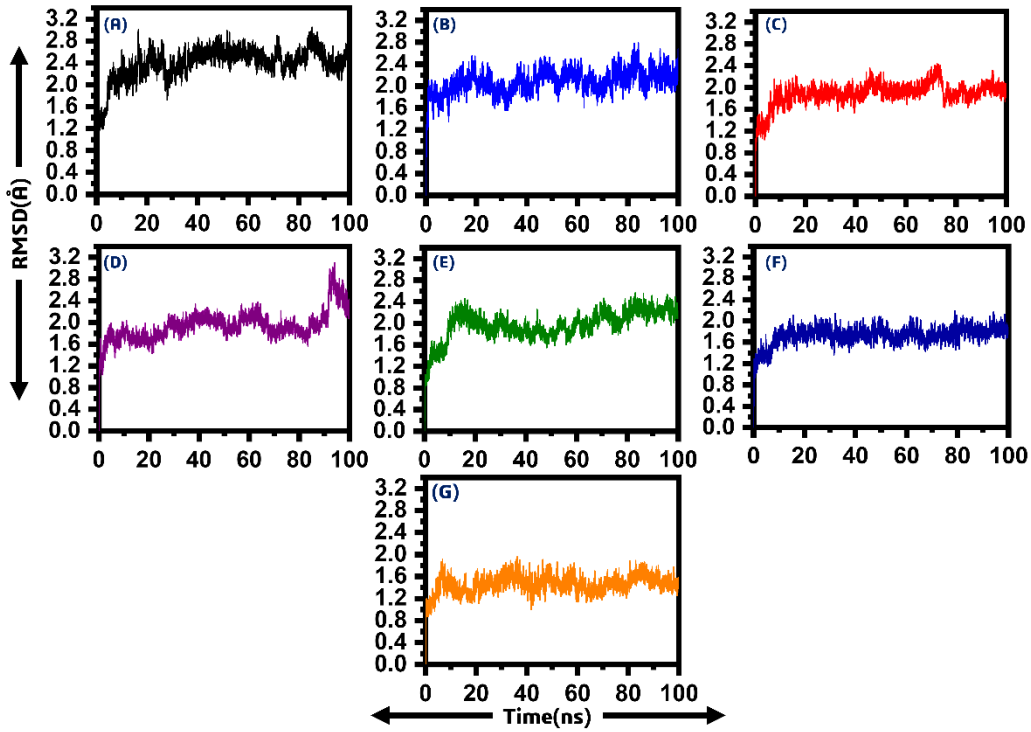
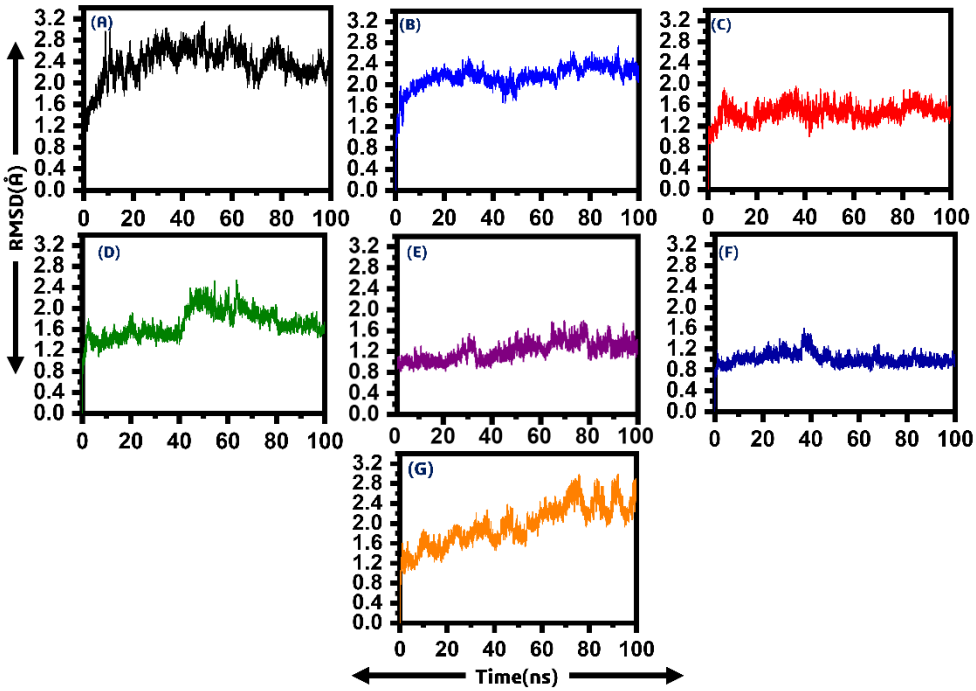
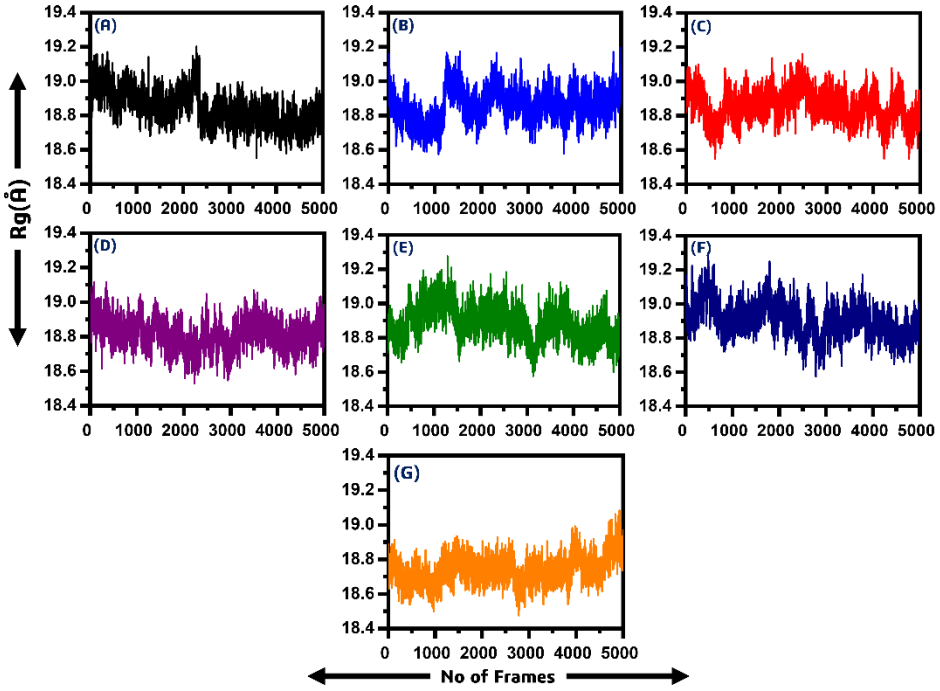


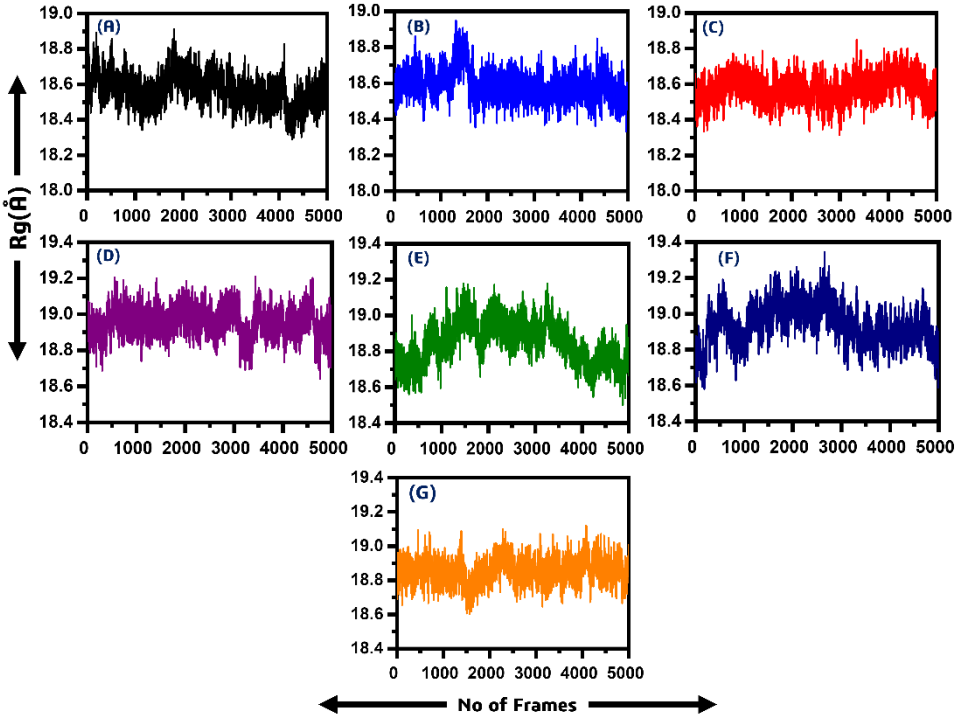

**Supplementary Figure S1:** RMSDs of all the complexes (replicate 2).




**Supplementary Figure S2:** RMSDs of all the complexes (replicate 3).




**Supplementary Figure S3:** Rg of all the complexes (replicate 2).




**Supplementary Figure S4:** Rg of all the complexes (replicate 3).

**Supplementary Table S1:** MMGBSA of all the complexes (replicate 2).

| Complexes | MM-GBSA (kcal/mol) | | | | |
|---|---|---|---|---|---|
| | $\Delta_{vdW}$ | $\Delta_{elec}$ | $\Delta_{ps}$ | $\Delta_{SASA}$ | $\Delta G_{Total}$ |
| ***P1,P5-Di(guanosine-5') pentaphosphate ammonium salt (ChemSpider ID: 4484327)*** | -85.142 | -11.247 | 34.462 | -5.111 | -69.326 |
| ***(R)-RETRO-THIORPHAN (ChemSpider ID: 394363)*** | -78.716 | -22.569 | 32.669 | -4.100 | -67.877 |
| ***P(1),P(6)-bis(5'-adenosyl)hexaphosphate (ChemSpider ID: 110267)*** | -66.324 | -23.426 | 30.185 | -5.212 | -68.587 |
| ***(Rib5)ppA (ChemSpider ID: 30975)*** | -60.011 | -14.178 | 20.211 | -2.287 | -68.010 |
| ***NA7 (ChemSpider ID: 393480)*** | -63.852 | -11.981 | 23.251 | -3.252 | -69.314 |
| ***dephospho-CoA (ChemSpider ID: 24785028)*** | -67.259 | -17.548 | 18.874 | -4.276 | -63.258 |
| ***ADPr*** | -64.147 | -17.326 | 19.253 | -5.158 | -65.923 |

**Supplementary Table S2:** MMGBSA of all the complexes (replicate 3).

| Complexes | MM-GBSA (kcal/mol) | | | | |
|---|---|---|---|---|---|
| | $\Delta_{vdW}$ | $\Delta_{elec}$ | $\Delta_{ps}$ | $\Delta_{SASA}$ | $\Delta G_{Total}$ |
| ***P1,P5-Di(guanosine-5') pentaphosphate ammonium salt (ChemSpider ID: 4484327)*** | -84.385 | -11.475 | 29.221 | -4.278 | -70.531 |
| ***(R)-RETRO-THIORPHAN (ChemSpider ID: 394363)*** | -83.224 | -17.581 | 30.272 | -4.658 | -68.012 |
| ***P(1),P(6)-bis(5'-adenosyl)hexaphosphate (ChemSpider ID: 110267)*** | -62.158 | -21.759 | 32.135 | -4.522 | -65.948 |
| ***(Rib5)ppA (ChemSpider ID: 30975)*** | -63.240 | -13.586 | 23.586 | -2.485 | -68.003 |
| ***NA7 (ChemSpider ID: 393480)*** | -63.369 | -14.485 | 23.254 | -3.758 | -70.699 |
| ***dephospho-CoA (ChemSpider ID: 24785028)*** | -69.582 | -16.125 | 21.485 | -3.478 | -66.741 |
| ***ADPr*** | -61.186 | -13.895 | 22.241 | -5.352 | -64.964 |