**Supporting Information**

**for**

**In silico approach: Anthocyanin derivatives as potential inhibitors of the COVID-19 main protease**

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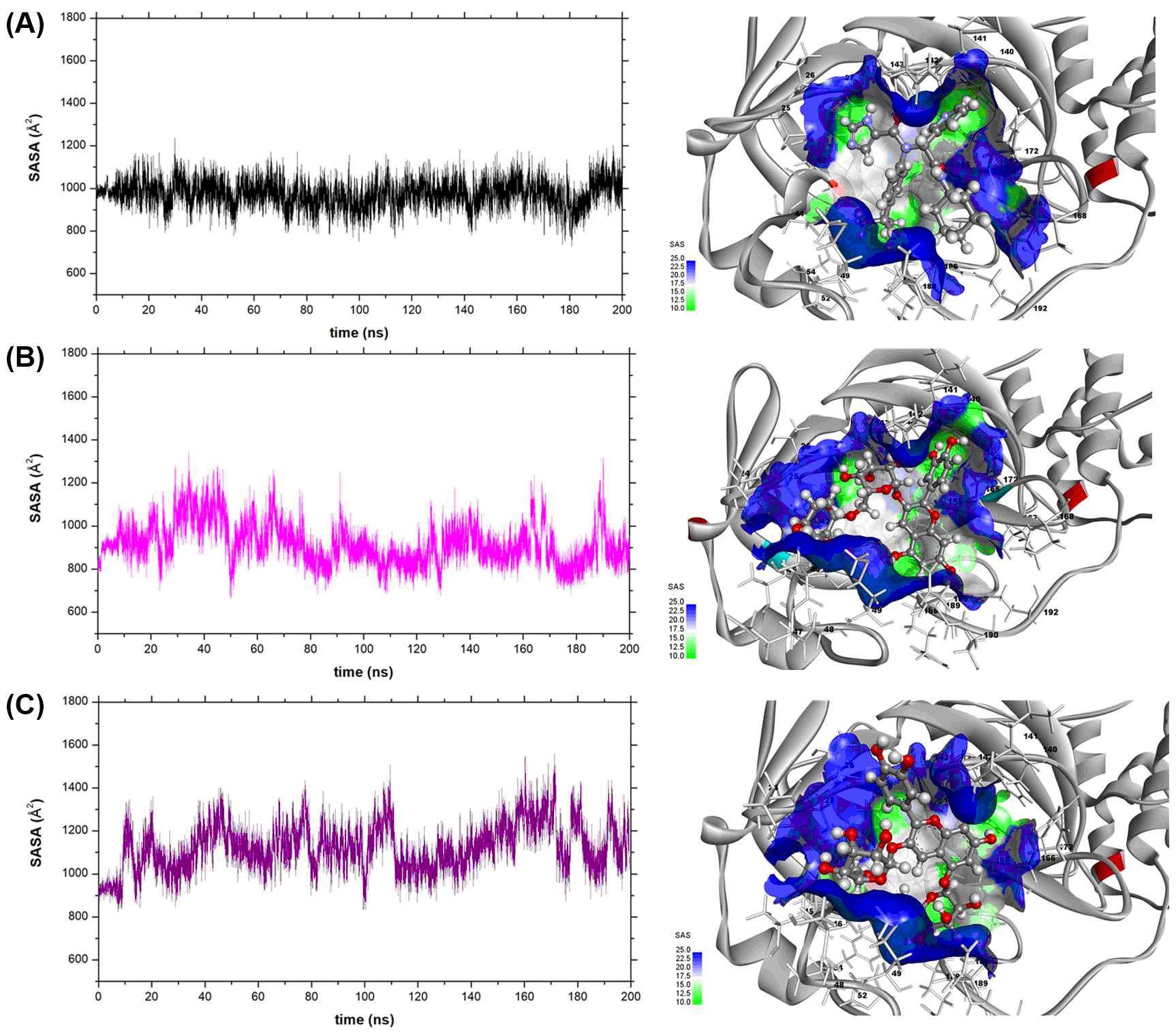
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**Additional data**

**Solvent Accessibility Surface Area**



**Figure S1:** Solvent accessibility surface area of COVID-19 main protease active site plot along the simulation time (200 ns) of each complex: (A) X77, (B) C5, and (C) C6.

**Bioavailability and Drug-Likeness Screening**

**Table S1:** Prediction of ADMET properties used admetSAR service website.

|  |  |  |
| --- | --- | --- |
| Parameters | Code C5 | Code C6 |
| Blood-brain barrier | BBB- | BBB- |
| Human intestinal absorption | HIA+ | HIA+ |
| P-glycoprotein substrate | Substrate | Substrate |
| P-glycoprotein inhibitor | Non-inhibitor | Non-inhibitor |
| Renal organic cation transporter | Non-inhibitor | Non-inhibitor |
| Aqueous solubility (LogS) | -2.63 | -2.10 |
| Subcellular localization | Mitochondria | Mitochondria |
| CYP450 2C9 subtrate | Non-substrate | Non-substrate |
| CYP450 2C9 inhibitor | Non-inhibitor | Non-inhibitor |
| CYP450 2D6 subtrate | Non-substrate | Non-substrate |
| CYP450 2D6 inhibitor | Non-inhibitor | Non-inhibitor |
| CYP450 3A4 subtrate | Non-substrate | Non-substrate |
| CYP450 3A4 inhibitor | Non-inhibitor | Non-inhibitor |
| CYP450 1A2 inhibitor | Non-inhibitor | Non-inhibitor |
| CYP450 2C19 inhibitor | Non-inhibitor | Non-inhibitor |
| Human ether-a-go-go-related-gene-inhibition | Weak inhibitor | Weak inhibitor |
| AMES toxicity | Non-AMES toxic | Non-AMES toxic |
| carcinoges | Non-Carcinogens | Non-Carcinogens |
| biodegradation | Not-ready-biodegradable | Not-ready-Biodegradable |
| Acute oral toxicity | III | IV |
| Carcinogenicity (three-class) | Non-required | Non-required |
| Rat acute toxicity (LD50, mol/kg) | 2.27 | 2.16 |