**Supplementary file**

**Amentoflavone derivatives against SARS-CoV-2 main protease (MPRO): An *in silico* study**

Rajib Hossain,1 Shafi Mahmud,2 Abul Bashar Ripon Khalipha,1 Abu Saim Mohammad Saikat,3 Dipta Dey,4 Rasel Ahmed Khan,4 Abdur Rauf,5\* Abdul Wadood,6 Humaria Rafique,6 Sami Bawazeer,7 Anees Ahmed Khalil,8 Zainab M. Almarhoon9, Yahia N. Mabkhot 10, Khalid J Alzahrani11, Muhammad Torequl Islam1\*, Khalaf F Alsharif12,Haroon Khan 13\*

1Department of Pharmacy, Life Science Faculty, Bangabandhu Sheikh Mujibur Rahman Science and Technology University, Gopalganj-8100 (Dhaka), Bangladesh.

2Microbiology Laboratory, Bioinformatics Division, Department of Genetic Engineering and Biotechnology, Faculty of Life science, University of Rajshahi, Rajshahi, Bangladesh.

3Department of Biochemistry and Molecular Biology, Bangabandhu Sheikh Mujibur Rahman Science and Technology University, Gopalganj-8100 (Dhaka), Bangladesh.

4Pharmacy Discipline, School of Life Science, Khulna University, Khulna, Bangladesh.

5Department of Chemistry University of Swabi, Swabi, Anbar-23430 KPK, Pakistan.

6Department of Biochemistry, Abdul Wali Khan University Mardan, KP, Pakistan

7Department of Pharmacognosy, Faculty of Pharmacy, Umm Al-Qura University, Makkah, P.O. Box 42, Kingdom of Saudi Arabia

8University Institute of Diet and Nutritional Sciences, Faculty of Allied Health Sciences, The University of Lahore, Pakistan

9 Department of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia

10 Department of Pharmaceutical Chemistry, College of Pharmacy, King Khalid University, Abha, Saudi Arabia

11 Department of Clinical Laboratories sciences, College of Applied Medical Sciences, Taif

University, P.O. Box 11099, Taif 21944, Saudi Arabia

12 Department of Clinical Laboratory, College of Applied Medical Science, Taif University, P.O. Box 11099, Taif 21944, Saudi Arabia

13 Department of Pharmacy, Abdul Wali Khan University Mardan 23200, Mardan Pakistan

**Table S1.** The smiles structures of amentofavone derivatives.

|  |  |
| --- | --- |
| **Compound Name** | **Smile Structures** |
| 4',4'''-Dimethylamentoflavone | O=C1C2=C(OC(C(C=C3)=CC=C3OC)C1)C(C(C=C(C4=CC(O)C5=C(O)C=C(O)C=C5O4)C=C6)=C6OC)=C(O)C=C2O |
| 4''',7--Di-O-methylamentoflavone | OC1=C(C2=C(O)C=C(O)C3=C2OC(C(C=C4)=CC=C4OC)CC3=O)C=C(C(OC5=C6C(O)=CC(OC)=C5)=CC6=O)C=C1 |
| 4''''''-methylamenoflavone | OC1=C(C2=C(O)C=C(O)C3=C2OC(C(C=C4)=CC=C4OC)CC3=O)C=C(C(OC5=C6C(O)=CC(O)=C5)=CC6=O)C=C1 |
| 4'-Monomethylamentoflavone | OC1=CC2=C(C(O)=C1)C(C=C(C3=CC(C4=C(O)C=C(O)C5=C4OC(C(C=C6)=CC=C6OC)CC5=O)=C(C=C3)OC)O2)=O |
| 7,4'-Dimethylamenoflavone | OC1=C2C(C=C(C3=CC(C4=C(O)C=C(O)C5=C4OC(C6=CC=C(O)C=C6)CC5=O)=C(C=C3)OC)OC2=CC(OC)=C1)=O |
| 7'-O-Methylamenoflavone | OC1=CC(O)=C2C(C=C(C3=CC(C(C(OC(C4=CC=C(O)C=C4)CC5=O)=C5C(O)=C6)=C6OC)=C(C=C3)OC)OC2=C1)=O |
| 7-O-Methylamentoflavone | OC1=C(C2=C(O)C=C(O)C3=C2OC(C4=CC=C(O)C=C4)CC3=O)C=C(C(OC5=CC(OC)=CC(O)=C65)=CC6=O)C=C1 |
| Heveaflavone | OC1=C(C(C(OC(C(C=C2)=CC=C2OC)CC3=O)=C3C(O)=C4)=C4OC)C=C(C(OC5=CC(OC)=CC(O)=C65)=CC6=O)C=C1 |
| kayaflavone | OC1=CC(O)=C2C(C=C(C3=CC(C(C(OC(C(C=C4)=CC=C4OC)CC5=O)=C5C(O)=C6)=C6OC)=C(C=C3)OC)OC2=C1)=O |
| sciadopitysin | OC1=C2C(C=C(C3=CC(C4=C(O)C=C(O)C5=C4OC(C(C=C6)=CC=C6OC)CC5=O)=C(C=C3)OC)OC2=CC(OC)=C1)=O |