ChemistrySelect

Supporting Information

Structural and Molecular Packing study of Three New Amidophosphoric Acid Esters and Assessment of Their Inhibiting Activity Against SARS-CoV-2 by Molecular Docking

Nafiseh Heidari, Atekeh Tarahhomi,* and Arie van der Lee

Table S1. Selected bond lengths (Å) and angles (°) for compounds **1** – **3**.

1		**1**	
P1—O2	1.5834 (19)	P1—N10	1.603 (2)
P1—O6	1.5843 (19)	P16—N25	1.602 (2)
P1—O9	1.459 (2)	P31—N40	1.603 (2)
P16—O17	1.5811 (19)	C3—O2	1.452 (3)
P16—O21	1.5828 (19)	C18—O17	1.451 (3)
P16—O24	1.460 (2)	C33—O32	1.452 (3)
P31—O32	1.5815 (19)	C11—N10	1.480 (4)
P31—O37	1.582 (2)	C26—N25	1.476 (4)
P31—O39	1.459 (2)	C41—N40	1.469 (4)
O2—P1—O6	102.28 (10)	O17—P16—N25	105.77 (13)
O2—P1—O9	115.00 (11)	O21—P16—N25	105.18 (13)
O6—P1—O9	113.15 (12)	O24—P16—N25	114.54 (12)
O2—P1—N10	105.62 (12)	O32—P31—O37	102.32 (10)
O6—P1—N10	104.80 (13)	O32—P31—O39	114.64 (12)
O9—P1—N10	114.71 (12)	O37—P31—O39	113.13 (12)
O17—P16—O21	102.48 (10)	O32—P31—N40	105.13 (13)
O17—P16—O24	114.70 (12)	O37—P31—N40	105.49 (13)
O21—P16—O24	112.99 (12)	O39—P31—N40	114.89 (12)
2		**3**	
P1—O2	1.4571 (14)	P1—O2	1.4584 (18)
P1—O3	1.5663 (12)	P1—O3	1.5752 (15)
P1—O7	1.5700 (13)	P1—O8	1.5858 (17)
P1—N10	1.6395 (17)	P1—N10	1.599 (2)
C4—O3	1.452 (2)	C7—O8	1.458 (3)
C6—O7	1.449 (2)	C4—O3	1.459 (2)
C11—N10	1.401 (2)	C11—N10	1.474 (3)
C11—N12	1.320 (2)	C14—N10	1.473 (3)
O2—P1—O3	112.01 (8)	O2—P1—O3	114.90 (10)
O2—P1—O7	110.87 (8)	O2—P1—O8	114.12 (10)
O3—P1—O7	105.38 (7)	O3—P1—O8	102.66 (8)
O2—P1—N10	116.10 (9)	O2—P1—N10	113.83 (10)
O3—P1—N10	102.74 (8)	O3—P1—N10	104.96 (10)
O7—P1—N10	108.94 (8)	O8—P1—N10	105.15 (11)

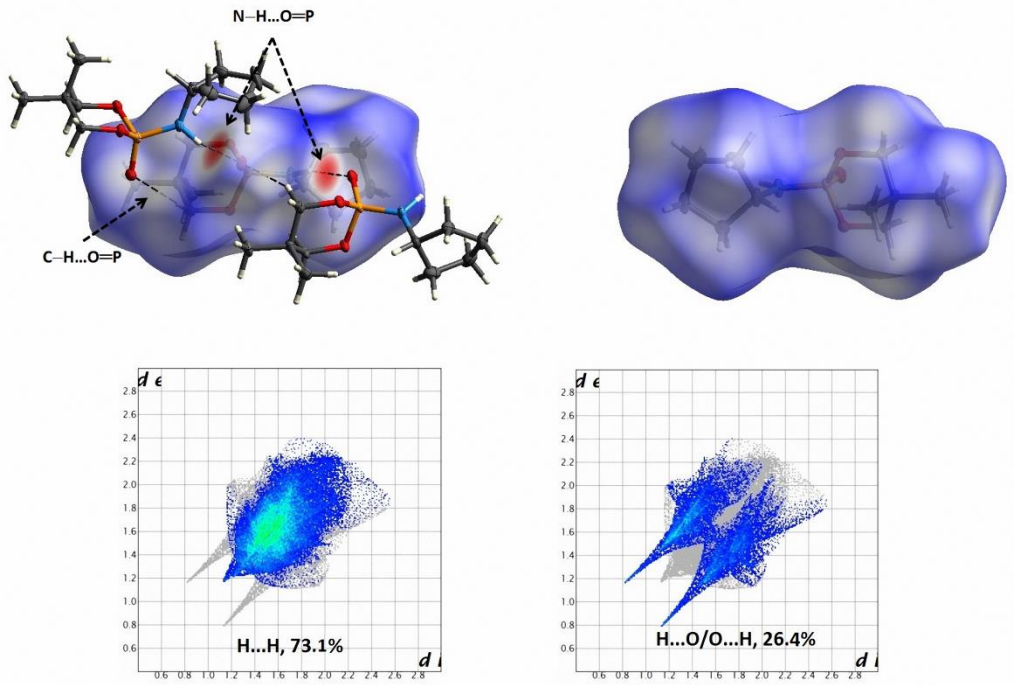

Figure S1. Views of the d_{norm} Hirshfeld surface maps (up) plotted on the molecule P16 of **1** in two orientations, introducing close contacts, along with the H…H and H…O/O…H fingerprint plots (down).

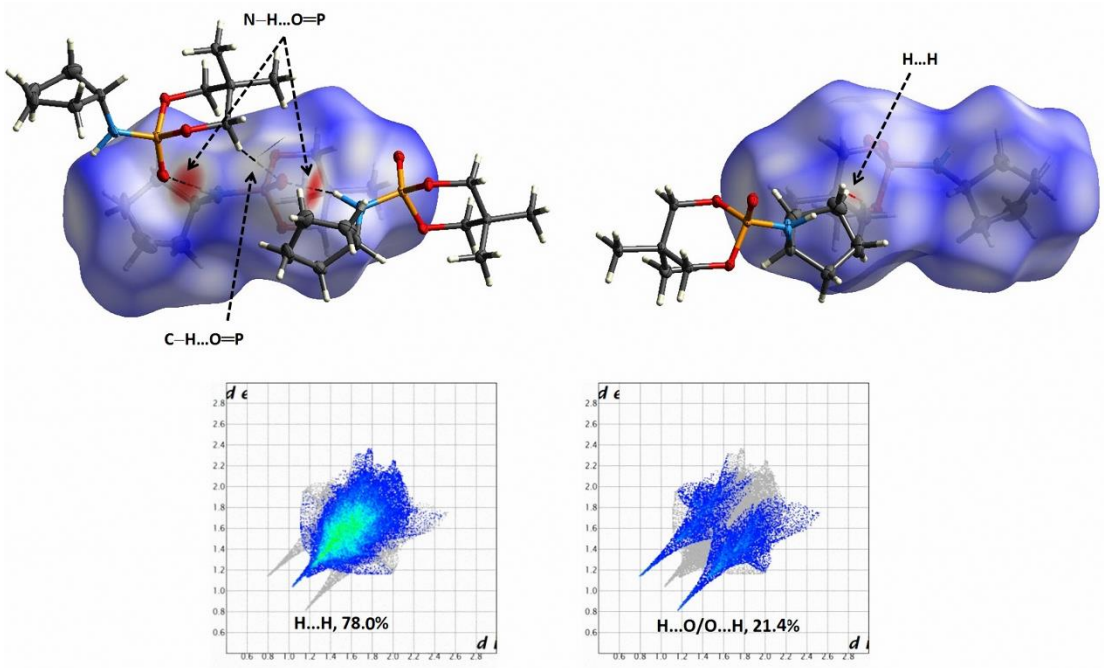

Figure S2. Views of the d_{norm} Hirshfeld surface maps (up) plotted on the molecule P31 of **1** in two orientations, introducing close contacts, along with the H…H and H…O/O…H fingerprint plots (down).

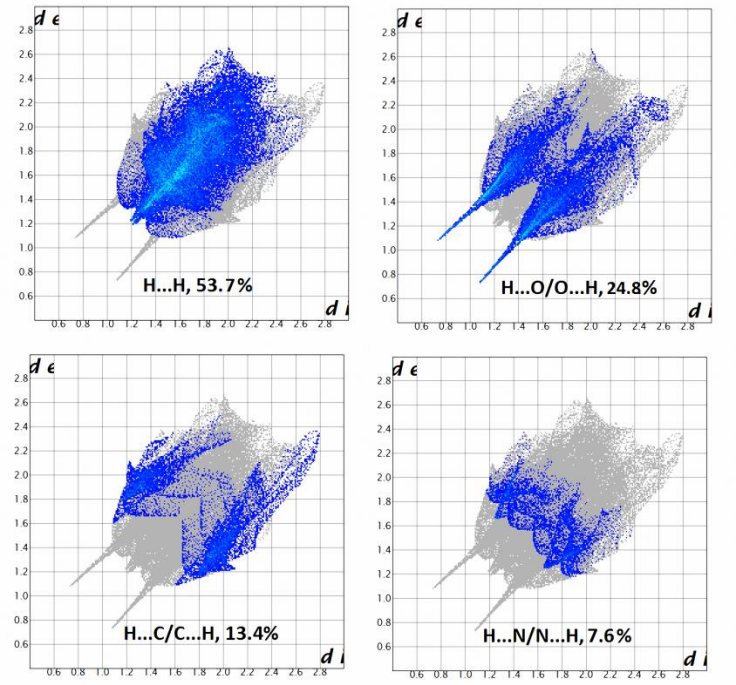

Figure S3. The decomposed fingerprint plots for the compound **2** have been presented.

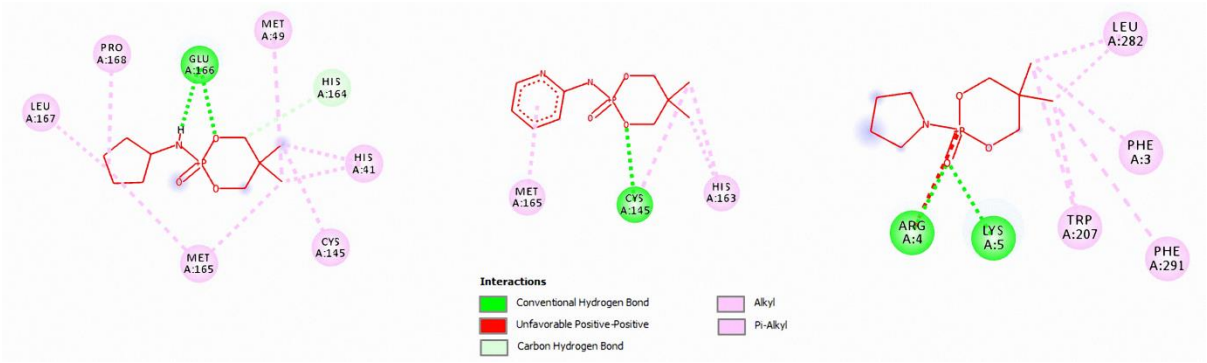

Figure S4. The 2D ligand maps of the compounds **1** – **3** with amino acid sites inside of the active pocket of 6M03.

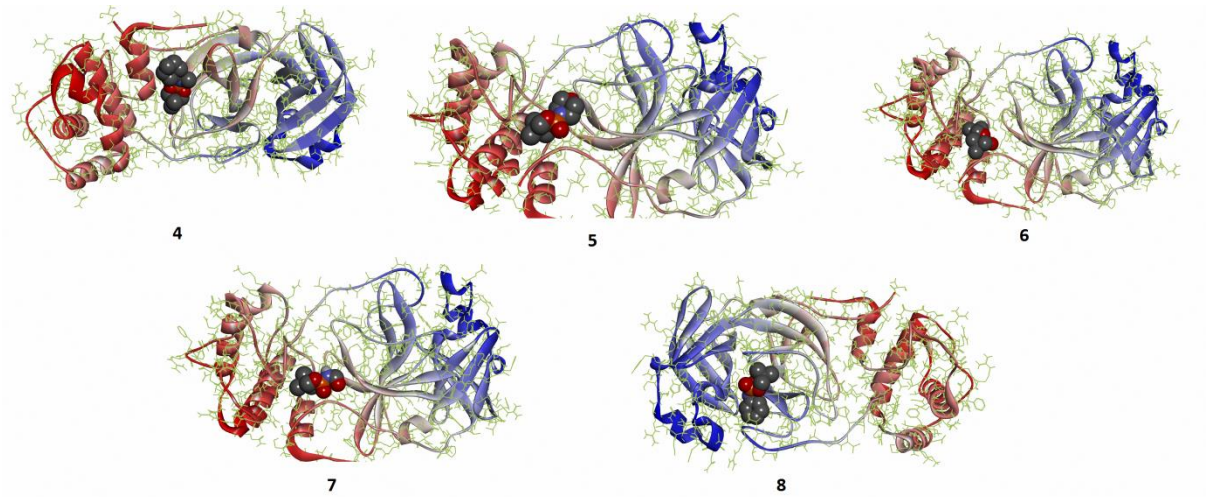

Figure S5. The best poses of the 3D compounds **4** – **8** in the binding pocket of 6M03.

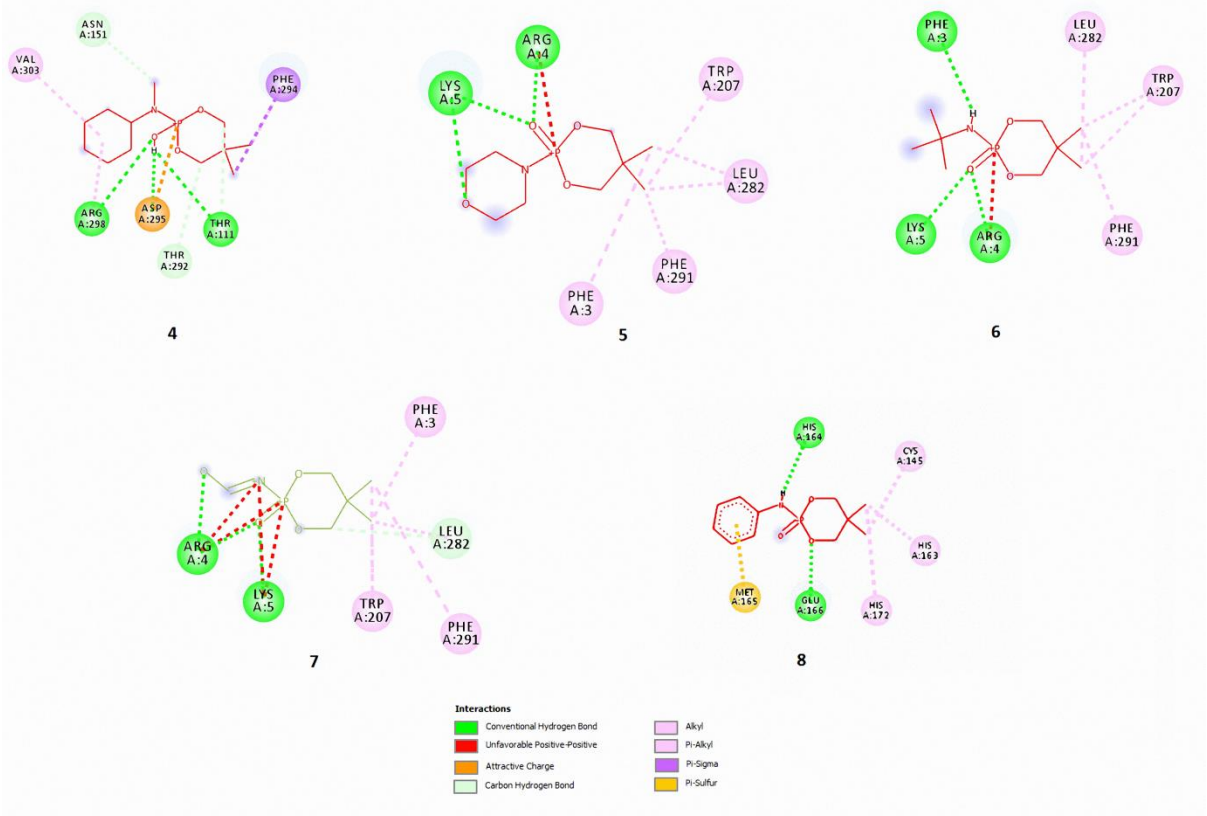

Figure S6. The 2D ligand maps of the compounds **4** – **8** with amino acid sites inside of the active pocket of 6M03.