

Electronic Supplementary Information

Exploring the Permeability of Covid-19 Drugs within the Cellular Membrane: A Molecular Dynamics Simulation Study

Tahereh Ghaed-Sharaf,^a Akbar Omidvar^{a*}

^a Faculty of Chemistry, Department of Physical Chemistry, University of Isfahan, 81746-73441 Isfahan, Iran

***Corresponding Author**

Akbar Omidvar

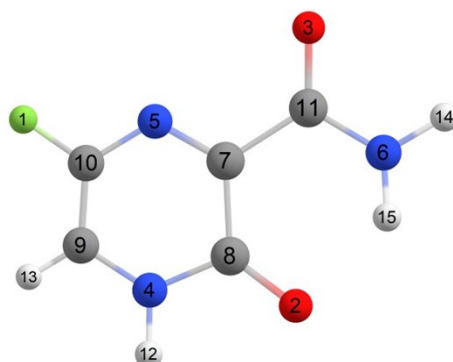
ORCID: 0000-0003-4691-4564

E-mail: a.omidvar@chem.ui.ac.ir

Phone: +98-3137934924

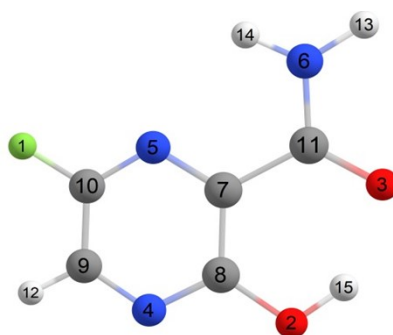
Fax: +98-3136689732

Table S1. Atomic charges of FAV-Keto.



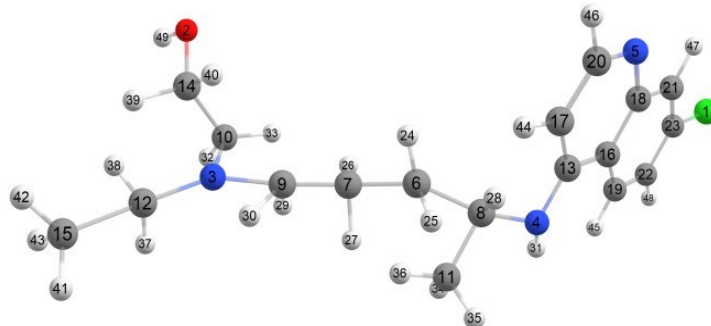
Atoms	Atomic Number	Atomic Charge
F	1	-0.33827000
O	2	-0.57101000
O	3	-0.57192000
N	4	-0.54480000
N	5	-0.44040000
N	6	-0.79722000
C	7	0.10433000
C	8	0.59767000
C	9	-0.01327000
C	10	0.50740000
C	11	0.62477000
H	12	0.41640000
H	13	0.22589000
H	14	0.39643000
H	15	0.40401000

Table S2. Atomic charges of FAV- Enol.



Atoms	Atomic Number	Atomic Charge
F	1	-0.33719000
O	2	-0.64678000
O	3	-0.65867000
N	4	-0.42363000
N	5	-0.44815000
N	6	-0.76980000
C	7	0.01505000
C	8	0.52983000
C	9	0.01074000
C	10	0.55168000
C	11	0.63837000
H	12	0.20939000
H	13	0.40401000
H	14	0.41654000
H	15	0.50861000

Table S3. Atomic charges of Hydroxychloroquine.



Atoms	Atomic Number	Atomic Charge
Cl	1	-0.00360000
O	2	-0.73023000
N	3	-0.58615000
N	4	-0.61507000
N	5	-0.52322000
C	6	-0.40076000
C	7	-0.39499000
C	8	-0.01196000
C	9	-0.15595000
C	10	-0.18633000
C	11	-0.57783000
C	12	-0.16200000
C	13	0.23821000
C	14	-0.03039000
C	15	-0.57731000
C	16	-0.16743000
C	17	-0.32892000
C	18	0.31838000
C	19	-0.17272000
C	20	0.08573000
C	21	-0.22986000
C	22	-0.21621000
C	23	-0.02464000
H	24	0.22251000
H	25	0.19463000
H	26	0.18828000
H	27	0.19660000
H	28	0.19211000
H	29	0.17027000
H	30	0.19004000
H	31	0.37474000
H	32	0.15762000
H	33	0.19695000
H	34	0.19412000
H	35	0.21104000
H	36	0.20929000
H	37	0.16159000
H	38	0.18830000
H	39	0.14672000
H	40	0.18693000
H	41	0.19100000

H	42	0.20222000
H	43	0.19977000
H	44	0.21057000
H	45	0.18948000
H	46	0.18184000
H	47	0.23200000
H	48	0.21843000
H	49	0.44620000
