Supporting Information

for

COSMO-RS-based Descriptors for the Machine Learning-Enabled Screening of Nucleotide Analog Drugs against SARS-CoV-2

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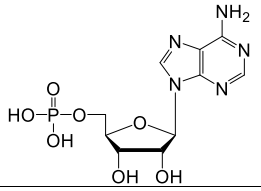
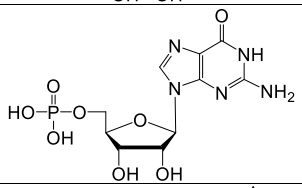
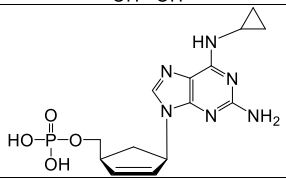
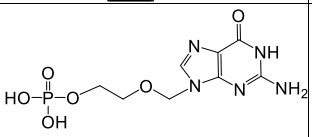
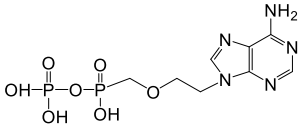
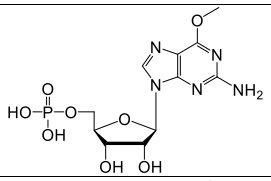
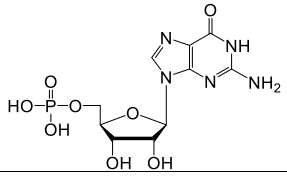
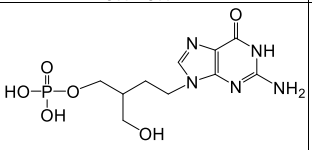
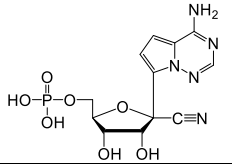
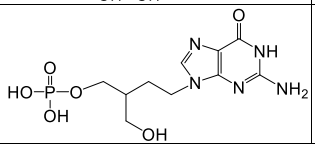
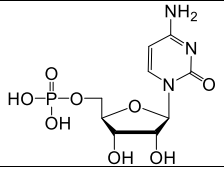
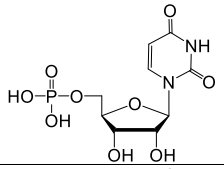
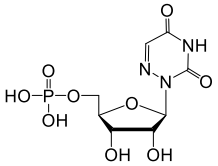
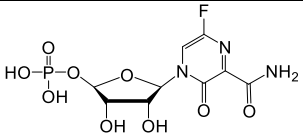
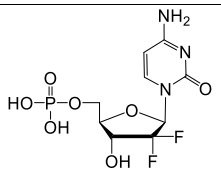
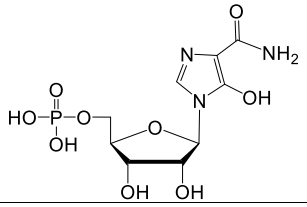
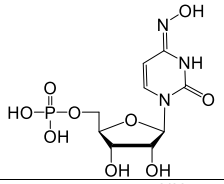
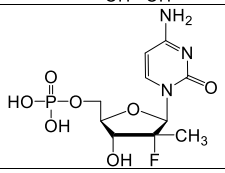
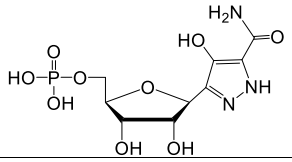
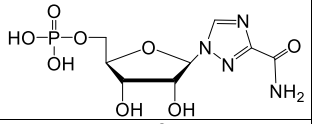
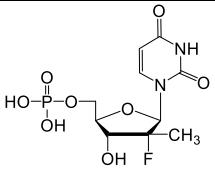
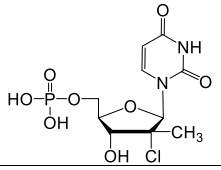
Table S1. Structure, number of conformers included in the study, status in term of COVID-19 treatment, and references on clinical research related to COVID-19 for the 4 nucleoside monophosphates and 18 nucleoside drug analogs in active monophosphate forms included in the study. The Status column lists the most advanced status in terms of COVID-19 treatment and is not intended to be comprehensive.

Drug	Number of conformers	Structure	Status	References
Pyrimidine bases and pyrimidine analog drugs				
Adenosine monophosphate	3		Physiological counterpart	-
Guanosine monophosphate	4		Physiological counterpart	-
Abacavir monophosphate	4		FDA-approved nucleoside RT inhibitor for HIV/AIDS treatment	1,2
Acyclovir monophosphate	4		Extends the life of patients with ventilator-associated pneumonia; Inhibits viral DNA polymerase; Incorporates into and terminates the growing viral DNA chain; Inactivates viral DNA polymerase	2,3
Adefovir monophosphate	3		Anti-hepatitis B virus; Blocks the enzyme crucial for virus reproduction	2,4

BMS-986094 monophosphate	3		Anti-hepatitis C virus; Applied alone or in combination with ribavirin	5,6
IDX-184 monophosphate	4		Nucleotide polymerase inhibitor of hepatitis C virus	2
Penciclovir monophosphate	4		Reduces COVID-19 infection at high concentrations; Anti-herpesvirus	7,2,8
Remdesivir monophosphate	3		COVID-19 clinical trials	9,10
Tenofovir monophosphate	3		COVID-19 prevention clinical trials	11,12,13
Purine bases and purine analog drugs				
Cytidine monophosphate	3		Physiological counterpart	-
Uridine monophosphate	3		Physiological counterpart	-
6-Azauridine monophosphate	3		Broad-spectrum antimetabolite; Inhibits both DNA and RNA virus multiplication; Active against flaviviruses	14,15
Favipinavir monophosphate	1		COVID-19 clinical studies; Inhibits viral RNA polymerase, thus interfering with viral replication	16,17,2

Gemcitabine monophosphate	3		Planned COVID-19 trials as an adjuvant in combination with other drugs; Pancreatic cancer drug	18,19
Mizoribine monophosphate	2		Inhibits the replication of SARS-CoV and herpesvirus	20,21
EIDD-2081 (N(4)-Hydro-xycytidine) monophosphate	3		COVID-19 clinical trials in UK	-
PSI-6130 monophosphate	3		Anti-hepatitis C	22
Pyrazofurin monophosphate	1		Inhibits in vitro replication of a number of RNA viruses	23
Ribavirin monophosphate	1		Reduces COVID-19 infection at high concentrations	19,20
Sofosbuvir monophosphate	3		Reduces recovery time of COVID-19 patients in combination with other drugs; Anti-hepatitis C virus	24
Uprifosbuvir monophosphate	3		Anti-hepatitis C virus	25

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