Article

Discovery of Novel Natural Inhibitors of H5N1 Neuraminidase Using Integrated Molecular Modeling and ADMET Prediction

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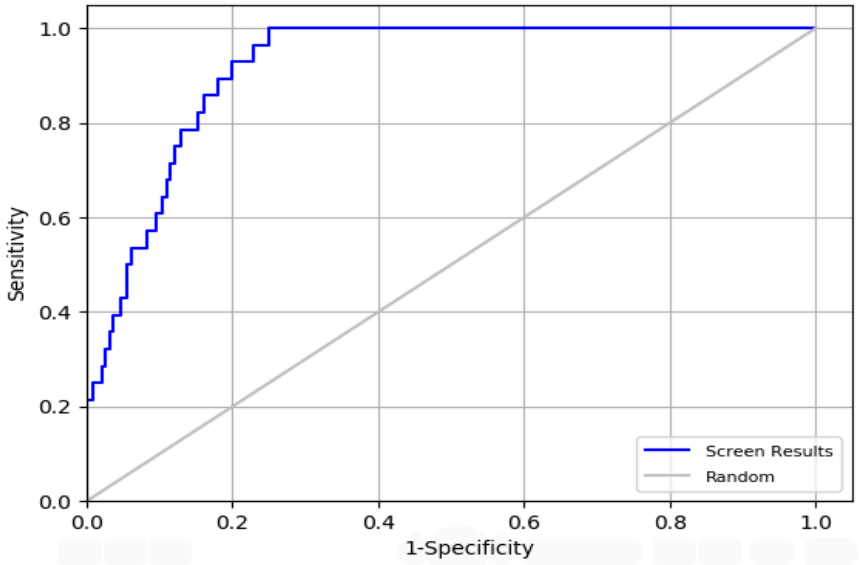


Figure S1. ROC curve after SP docking process.

Table S1. Synonyms, IUPAC names, natural sources, chemical families, and bibliographic references of the three identified natural compounds.

Comp.	Synonym	IUPAC Name	Natural source	Family
C1	Nagstatin	2-[(5R,6R,7S,8S)-8-acetamido 6,7-dihydroxy-5-(hydroxymethyl)-5,6,7,8-tetrahydroimidazo[1,2-a]pyridin-2-yl]acetic acid	Streptomyces amakusaensis MG846-fF3.	Imidazopyridine

C2	Dikojiacid B	3-hydroxy-2-[1-[3-hydroxy-6-(hydroxymethyl)-4-oxopyran-2-yl]ethyl]-6-(hydroxymethyl)pyran-4-one	Aspergillus flavus from the fruit of Garcinia. multiflora	Kojic acid dimer
C3	Dapdiamide E	(2S)-2-[[(2S)-3-amino-2-[(3-carbamoyloxirane-2-carbonyl)amino]propanoyl]amino]-3-methylbutanoic acid	Pantoea agglomerans	Dapdiamide

Table S2. Physicochemical and medicinal properties predictions using ADMETLab 3.

Comp.	**C1**	**C2**	**C3**	**Zanamivir**
MW	299.11	310.07	316.14	332.13
Volume	274.181	288.09	293.734	302.525
nHA	9.0	8.0	10.0	11.0
nHD	5.0	4.0	7.0	9.0
TPSA	144.91	141.34	177.14	198.22
logS	-0.612	-1.135	-1.573	-1.429
logP	-1.56	-0.405	-0.421	-2.316
SAscore	4.0	3.0	3.0	4.0
Lipinski Rule	0	0	0	1.0
Pfizer Rule	0	0	0	0
GSK Rule	0	0	0	0
Golden Triangle	0	0	0	0
PAINS	0	0	0	0
BMS	0	0	0	0