Exploration of binding mechanism of a potential Streptococcus pneumoniae neuraminidase inhibitor from herbaceous plants by molecular simulation

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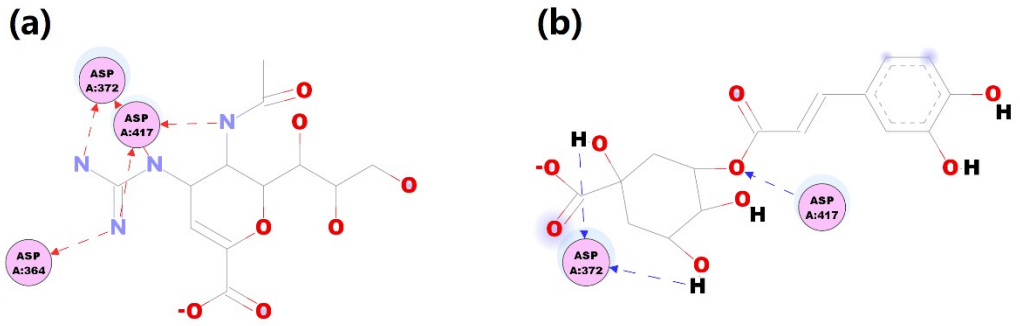

Fig. S1 The detail difference of binding mode between (a) zanamivir and (b) chlorogenic acid

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    320       330       340       350       360       370       380       390
....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|.
LPEGAALTEKTDIFESGRNGKPNKDGIKSYRIPALLKTDKGTLIAGADERRLHSSDWGDIGMVIRRSEDNGKTWGDRVTI

    400       410       420       430       440       450       460       470
...|....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|.
TNLRDNPKASDPSIGSPVNIDMVLVQDPETKRIFSIYDMFPEGKGIFGMSSQKEEAYKKIDGKTYQILYREGEKGAYTIR

    480       490       500       510       520       530       540       550
...|....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|.
ENGTVYTPDGKATDYRVVVDPVKPAYSDKGDLYKGNQLLGNIYFTTNKTSPFRIAKDSYLWMSYSDDDGKTWSAPQDITP

    560       570       580       590       600       610       620       630
...|....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|.
MVKADWMKFLGVGPGTGIVLRNGPHKGRILIPVYTTNNVSHLNGSQSSRIIYSDDHGKTWHAGEAVNDNRQVDGQKIHSS

    640       650       660       670       680       690       700       710
...|....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|.
TMNNRRAQNTESTVVQLNNGDVKLFMRGLTGDLQVATSKDGGVTWEKDIKRYPQVKDVYVQMSAIHTMHEGKEYIILSNA

    720       730       740       750       760       770       780       790
...|....|....|....|....|....|....|....|....|....|....|....|....|....|....|...
GGPKRENGMVHLARVEENGELTWLKHNPIQKGEFAYNSLQELGNGEYGILYEHTEKGQNAYTLSFRKFNWDFLSKDL
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Fig. S2 The sequence of NanA

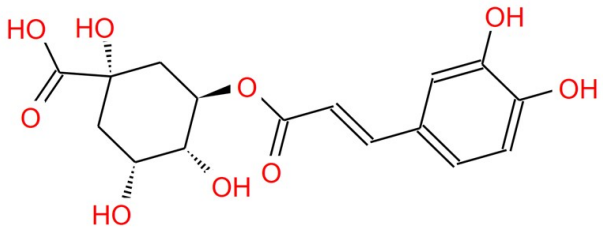

Fig. S3 The structure of Chlorogenic acid

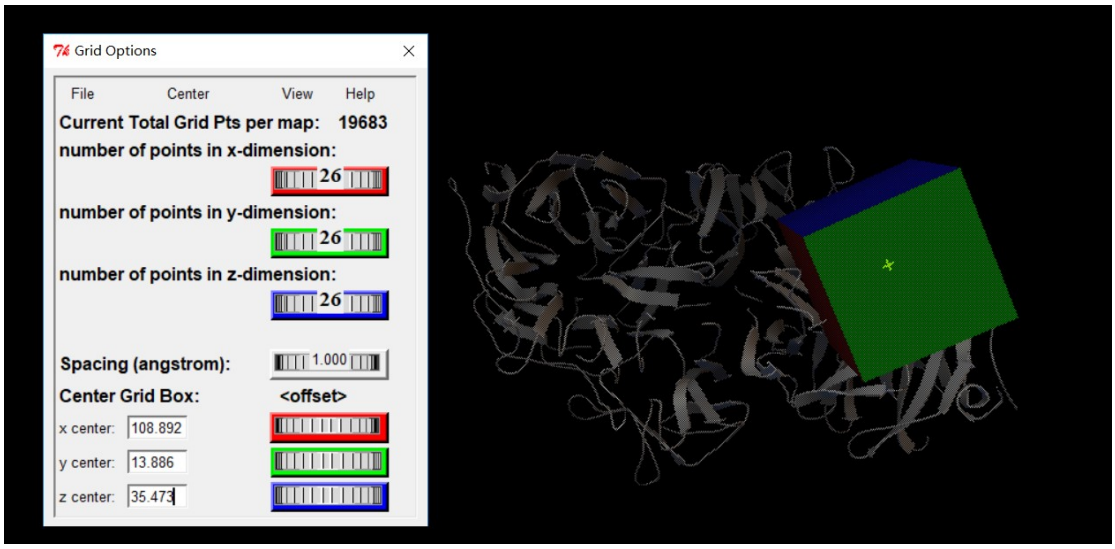

Fig. S4 The grid detail used in the docking simulation

Tab. S1 Protonation states for titratable residues of NanA

Protonated residues in complex	
ChainA	ChainB
all Arg, all Lys; Asp417, Asp434, Glu620, His612, His 634	all Arg, all Lys; Asp364 Asp417, Asp434, His612, His634