

Cite this: DOI: 10.1039/c0xx00000x

www.rsc.org/publishing/journals/mb

supplemental information

Table S1. Computational alanine-scanning mutagenesis: binding free energies of peramivir with the neuraminidase of the 2013 H7N9 influenza A virus

Residue	Inter vdW	Inter Coulomb	Reaction Field	Cavity	Constant	$\Delta G_{\text{Binding}}$ (kcal/mol)
Arg114	-28.51± 2.31	-120.5± 4.20	94.18± 3.07	-8.59± 0.17	-2.89	-9.53 ± 0.23
Arg148	-29.95± 2.31	-123.21± 4.20	95.86± 3.07	-8.82± 0.17	-2.89	-9.81 ± 0.23
Arg367	-28.32± 2.31	-96.58± 4.20	97.61± 3.07	-6.51± 0.17	-2.89	-6.64 ± 0.23
Trp175	-28.13± 2.31	-117.11± 4.20	96.23± 3.07	-8.61± 0.17	-2.89	-8.92 ± 0.23
Asn291	-30.28± 2.31	-120.59± 4.20	94.28± 3.07	-8.61± 0.17	-2.89	-9.72 ± 0.23
Asn342	-29.70± 2.31	-120.22± 4.20	94.35± 3.07	-8.61± 0.17	-2.89	-9.61 ± 0.23
Asp147	-25.98± 2.31	-106.98± 4.20	97.61± 3.07	-6.95± 0.17	-2.89	-7.32 ± 0.23
Glu115	-29.89± 2.31	-121.51± 4.20	94.28± 3.07	-8.63± 0.17	-2.89	-9.77 ± 0.23
Glu224	-28.94± 2.31	-120.19± 4.20	94.36± 3.07	-8.85± 0.17	-2.89	-9.55 ± 0.23
Glu274	-28.11± 2.31	-112.62± 4.20	94.28± 3.07	-8.91± 0.17	-2.89	-8.68 ± 0.23
Gly344	-28.34± 2.31	-119.74± 4.20	95.44± 3.07	-8.22± 0.17	-2.89	-9.26 ± 0.23
Ile145	-29.64± 2.31	-120.65± 4.20	93.38± 3.07	-8.37± 0.17	-2.89	-9.72 ± 0.23
Pro428	-29.69± 2.31	-121.36± 4.20	93.42± 3.07	-8.83± 0.17	-2.89	-9.85 ± 0.23
Ser176	-28.18± 2.31	-112.64± 4.20	92.11± 3.07	-8.81± 0.17	-2.89	-8.91 ± 0.23
Thr436	-29.75± 2.31	-121.21± 4.20	93.79± 3.07	-8.06± 0.17	-2.89	-9.72 ± 0.23
Tyr401	-28.03± 2.31	-122.04± 4.20	95.68± 3.07	-8.01± 0.17	-2.89	-9.42 ± 0.23

Table S2. Computational alanine-scanning mutagenesis: binding free energies of oseltamivir with the neuraminidase of the 2013 H7N9 influenza A virus

Residue	Inter vdW	Inter Coulomb	Reaction Field	Cavity	Constant	$\Delta G_{\text{Binding}}$ (kcal/mol)
Arg114	-26.03± 1.41	-108.02± 3.81	96.59± 3.62	-7.79± 0.09	-2.89	-7.63± 0.28
Arg148	-27.23± 1.41	-105.16± 3.81	94.18± 3.62	-7.81± 0.09	-2.89	-7.71± 0.28
Arg367	-25.01± 1.41	-87.19± 3.81	96.59± 3.62	-7.04± 0.09	-2.89	-5.26± 0.28
Trp175	-26.27± 1.41	-105.57± 3.81	96.24± 3.62	-7.62± 0.09	-2.89	-7.41± 0.28
Asn291	-26.32± 1.41	-105.04± 3.81	96.58± 3.62	-7.72± 0.09	-2.89	-7.34± 0.28
Asn342	-25.01± 1.41	-106.07± 3.81	96.98± 3.62	-7.61± 0.09	-2.89	-7.25± 0.28
Asp147	-25.04± 1.41	-81.19± 3.81	96.59± 3.62	-7.03± 0.09	-2.89	-4.63± 0.28
Glu115	-26.71± 1.41	-105.75± 3.81	96.06± 3.62	-7.91± 0.09	-2.89	-7.53± 0.28
Glu224	-27.34± 1.41	-106.61± 3.81	96.29± 3.62	-7.97± 0.09	-2.89	-7.67± 0.28
Glu274	-28.63± 1.41	-106.35± 3.81	94.18± 3.62	-7.81± 0.09	-2.89	-7.98± 0.28
Gly344	-25.03± 1.41	-104.19± 3.81	96.59± 3.62	-7.67± 0.09	-2.89	-7.11± 0.28
Ile145	-19.75± 1.41	-103.03± 3.81	98.97± 3.62	-7.01± 0.09	-2.89	-6.11± 0.28
Pro428	-26.02± 1.41	-105.12± 3.81	96.54± 3.62	-7.75± 0.09	-2.89	-7.32± 0.28
Ser176	-25.78± 1.41	-105.01± 3.81	96.76± 3.62	-7.54± 0.09	-2.89	-7.24± 0.28
Thr436	-25.67± 1.41	-104.07± 3.81	96.37± 3.62	-7.61± 0.09	-2.89	-7.18± 0.28
Tyr401	-27.89± 1.41	-106.94± 3.81	96.03± 3.62	-7.98± 0.09	-2.89	-7.79± 0.28

Table S3. Computational alanine-scanning mutagenesis: binding free energies of zanamivir with the neuraminidase of the 2013 H7N9 influenza A virus

Residue	Inter vdW	Inter Coulomb	Reaction Field	Cavity	Constant	$\Delta G_{\text{Binding}}$ (kcal/mol)
Arg114	-26.01± 1.02	-88.52± 2.47	79.81± 1.98	-6.05± 0.08	-2.89	-7.16± 0.13
Arg148	-28.04± 1.02	-89.11± 2.47	79.84± 1.98	-6.04± 0.08	-2.89	-7.43± 0.13
Arg367	-26.01± 1.02	-81.24± 2.47	79.97± 1.98	-6.47± 0.08	-2.89	-6.42± 0.13
Trp175	-28.95± 1.02	-89.91± 2.47	79.91± 1.98	-6.89± 0.08	-2.89	-7.69± 0.13
Asn291	-28.91± 1.02	-90.89± 2.47	79.34± 1.98	-6.71± 0.08	-2.89	-7.83± 0.13
Asn342	-29.19± 1.02	-90.69± 2.47	79.01± 1.98	-7.15± 0.08	-2.89	-7.92± 0.13
Asp147	-27.02± 1.02	-78.67± 2.47	80.95± 1.98	-6.01± 0.08	-2.89	-6.11± 0.13
Glu115	-28.03± 1.02	-89.01± 2.47	79.97± 1.98	-6.17± 0.08	-2.89	-7.41± 0.13
Glu224	-27.13± 1.02	-89.08± 2.47	79.94± 1.98	-6.06± 0.08	-2.89	-7.32± 0.13
Glu274	-27.01± 1.02	-85.18± 2.47	79.96± 1.98	-6.21± 0.08	-2.89	-6.91± 0.13
Gly344	-29.94± 1.02	-89.98± 2.47	78.15± 1.98	-6.96± 0.08	-2.89	-7.99± 0.13
Ile145	-28.01± 1.02	-88.37± 2.47	79.87± 1.98	-6.39± 0.08	-2.89	-7.38± 0.13
Pro428	-27.72± 1.02	-89.82± 2.47	79.82± 1.98	-6.01± 0.08	-2.89	-7.47± 0.13
Ser176	-28.73± 1.02	-89.83± 2.47	79.85± 1.98	-6.85± 0.08	-2.89	-7.66± 0.13
Thr436	-27.54± 1.02	-85.01± 2.47	79.95± 1.98	-6.18± 0.08	-2.89	-6.95± 0.13
Tyr401	-28.73± 1.02	-90.78± 2.47	79.31± 1.98	-6.77± 0.08	-2.89	-7.81± 0.13