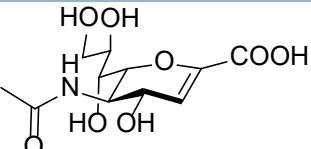
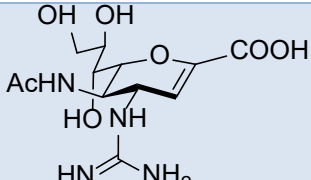
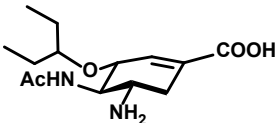
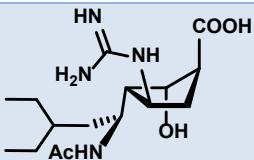
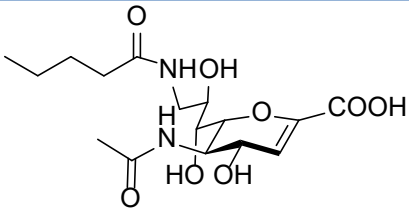
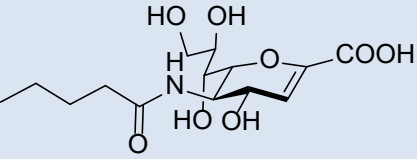
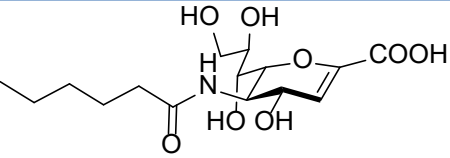
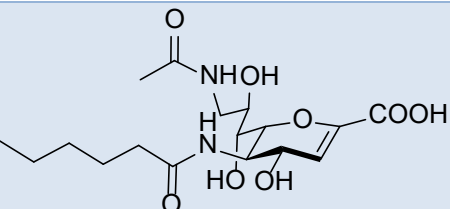
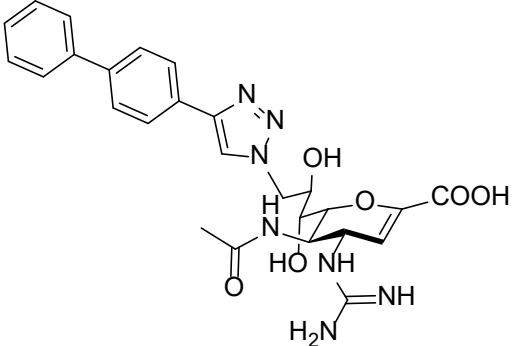
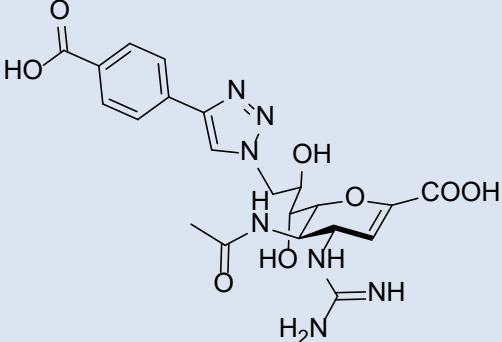
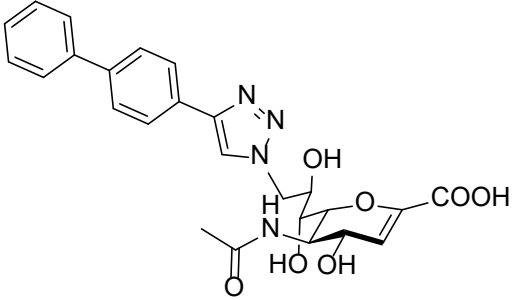
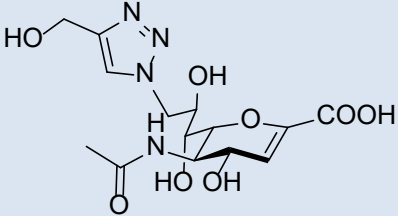


Human neuraminidase inhibitors – References and unique identifiers

Unique identifier (alternative ident) PubChem ID	Structure	Selectivity (IC_{50} [μM])	References (<i>cmpd</i>) [‡]
DANA* (Neu5Ac2en) 65309		NEU3,4 5X (8)	1
zanamivir* 60855		NEU2,3 6X (8)	1, 2
oseltamivir* 449381		N/A (>500)	1, 2
peramivir* 154234		NEU2 (70)	1
C9-BA-DANA* 7159107		NEU1 32X (3)	3, 4 (10h)
CG14600 145979480		NEU1 33X (1)	4 (11c)
CG25900 142476532		NEU1 35X (0.4)	4 (11d)
CG33300 145989099		NEU1 330X (0.14)	4 (17f)

CG33100 145980895		NEU1 220X (0.40)	4 (17g)
CZ28100 (Neu5AcN ₃ 2en) 52948463		NEU3,4 4X (5)	4 (12)
CG18800 145982311		NEU2 30X (4)	4 (13c)
CG32100 145984892		NEU2 7X (2)	4 (22)
CZ82100 71606077		NEU2 12X (90)	5 (8b)
CG18400 145979690		NEU2 30X (3)	4 (13d)
CG11500 137638962		NEU3,4 37X (1)	6 (7h)
CZ53100 71606073		NEU3 40X (24)	5 (5c)

CG22600 137660481		NEU3 10X (0.6)	6 (8b)
CG19900 137635553		NEU3 40X (0.6)	6 (8a)
CG17700 137652080		NEU3,4 46X (0.7)	6 (7i)
CY16600 (C9-4HMT-DANA) 52948862		NEU4 500X (0.16)	7, 8 (6, 6f)

*, compounds first reported by others; ‡, where applicable the compound number used in the original reference is included.

References

- (1) Richards, M. R., Guo, T., Hunter, C. D., and Cairo, C. W. (2018) Molecular dynamics simulations of viral neuraminidase inhibitors with the human neuraminidase enzymes: Insights into isoenzyme selectivity. *Bioorg. Med. Chem.* 26, 5349-5358. <http://dx.doi.org/10.1016/j.bmc.2018.05.035>
- (2) Hata, K., Koseki, K., Yamaguchi, K., Moriya, S., Suzuki, Y., Yingsakmongkon, S., Hirai, G., Sodeoka, M., von Itzstein, M., and Miyagi, T. (2008) Limited inhibitory effects of oseltamivir and zanamivir on human sialidases. *Antimicrob. Agents Chemother.* 52, 3484-91. <http://dx.doi.org/10.1128/AAC.00344-08>
- (3) Magesh, S., Moriya, S., Suzuki, T., Miyagi, T., Ishida, H., and Kiso, M. (2008) Design, synthesis, and biological evaluation of human sialidase inhibitors. Part 1: Selective inhibitors of lysosomal sialidase (NEU1). *Bioorg. Med. Chem. Lett.* 18, 532-537. <http://dx.doi.org/10.1016/j.bmcl.2007.11.084>
- (4) Guo, T., Heon-Roberts, R., Zou, C., Zheng, R., Pshezhetsky, A. V., and Cairo, C. W. (2018) Selective Inhibitors of Human Neuraminidase 1 (NEU1). *J. Med. Chem.* 61, 11261-11279. <http://dx.doi.org/10.1021/acs.jmedchem.8b01411>
- (5) Zhang, Y., Albohy, A., Zou, Y., Smutova, V., Pshezhetsky, A., and Cairo, C. W. (2013) Identification of selective inhibitors of human sialidase isoenzymes using C4, C7-modified 2-deoxy-2,3-didehydro-*N*-acetylneuraminic acid (DANA) analogs. *J. Med. Chem.* 56, 2948-2958. <http://dx.doi.org/https://doi.org/10.1021/jm301892f>
- (6) Guo, T., Datwyler, P., Demina, E., Richards, M. R., Ge, P., Zou, C., Zheng, R., Fougerat, A., Pshezhetsky, A. V., Ernst, B., and Cairo, C. W. (2018) Selective Inhibitors of Human Neuraminidase 3. *J. Med. Chem.* 61, 1990-2008. <http://dx.doi.org/10.1021/acs.jmedchem.7b01574>
- (7) Albohy, A., Zhang, Y., Smutova, V., Pshezhetsky, A. V., and Cairo, C. W. (2013) Identification of Selective Nanomolar Inhibitors of the Human Neuraminidase, NEU4. *ACS Med Chem Lett* 4, 532-7. <http://dx.doi.org/10.1021/ml400080t>
- (8) Zou, Y., Albohy, A., Sandbhor, M., and Cairo, C. W. (2010) Inhibition of human neuraminidase 3 (NEU3) by C9-triazole derivatives of 2,3-didehydro-*N*-acetyl-neuraminic acid. *Bioorg. Med. Chem. Lett.* 20, 7529-7533. <http://dx.doi.org/10.1016/j.bmcl.2010.09.111>