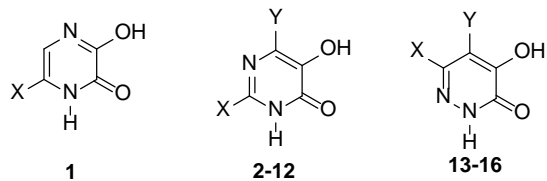


Supporting Information:

Phenyl substituted 4-hydroxypyridazin-3(2H)-ones and 5-hydroxypyrimidin-4(3H)-ones: Inhibitors of influenza A endonuclease

Hye Yeon Sagong, Joseph D. Bauman, Disha Patel, Kalyan Das, Eddy Arnold and Edmond J. LaVoie



- 1**; X = *p*-fluorophenyl; Y = H
2; X = H; Y = *p*-fluorophenyl
3-12; X = *o*-, *m*-, *p*-fluorophenyl; *o*-, *m*-, *p*-biphenyl; *m*- or *p*-cyanophenyl; 3- or 4-(5-tetrazoyl); Y = H
13; X = *p*-fluorophenyl; Y = H
14-16; X = *p*-fluorophenyl; *p*-cyanophenyl, 4-(5-tetrazoyl); Y = H

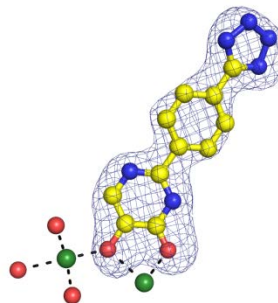


Table 1S: X-ray data and refinement statistics

Protein Data Bank (PDB) accession code	4W9S
Compound	11
X-ray source	CHESS F1
Wavelength (Å)	0.917
Space group	C222 ₁
Cell constants (a, b, c in Å)	87.99, 101.64, 66.51
Resolution range (last shell) (Å)	50.00-1.80 (1.83-1.80)
Completeness (last shell) (%)	99.2 (99.2)
R _{merge} (last shell)	0.051 (0.592)
Average I/σ (I) (last shell)	22.39 (1.83)
Sigma cut-off (I)	I < -3.0σ

Refinement Statistics	
Total no. of atoms (solvent atoms)	3449 (153)
Resolution (Å)	1.80
No. of reflections (R _{free} set)	27,807 (1,395)
Completeness (R _{free} set)	99.31 (5.02)
R _{work}	0.176
R _{free}	0.209
Ramachandran statistics (% of residues in favored/disallowed regions)	97.98/0.00
RMSD bond length (Å)	0.012
RMSD bond angles (°)	1.28