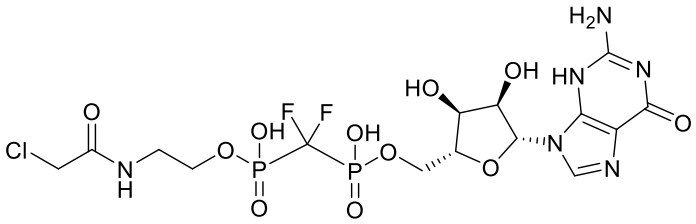
XY-02-082



Chemical Formula: $C_{15}H_{21}ClF_2N_6O_{11}P_2$
Molecular Weight: 596.76

Category	Parameter	Description
Compound	Name	XY-02-082
	Citation	*ACS Med. Chem. Lett.*, **2017**, *8*, 61–66.
	Chemical descriptors	NC1=NC(=O)C2=C(N1)N(C=N2)[C@@H]1O[C@H](COP(O)(=O)C(F)(F)P(O)(=O)OCCNC(=O)CCl)[C@@H](O)[C@H]1O
	Chemical name	[({[(2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy}(hydroxy)phosphoryl)difluoromethyl][2-(2-chloroacetamido)ethoxy]phosphinic acid
	Entries in chemical databases	
	Availability	
	Papers that use the compounds	https://www.ncbi.nlm.nih.gov/pubmed/28105276
In vitro profiling	Target (potency)	KRas (K_i = 0.38 μM, k_{inact}/K_i = 0.9 $min^{-1} \bullet \mu M^{-1}$)
	Selectivity	
	Potential reactivity	Cyeteine reactive
	SAR	See Covalent Guanosine Mimetic Inhibitors of G12C KRAS
	Mechanism of inhibition	Irreversible
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics		
Synthetic scheme