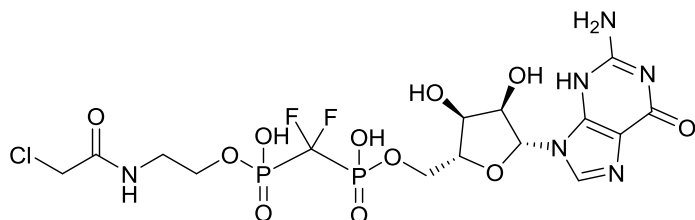


XY-02-082



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	<i>ACS Med. Chem. Lett.</i> , <b>2017</b> , 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)CC1)[C@@H](O)[C@H]1O
	Chemical name	[[[(2R,3S,4R,5R)-5-(2-amino-6-oxo-9,9-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	<a href="https://www.ncbi.nlm.nih.gov/pubmed/28105276">https://www.ncbi.nlm.nih.gov/pubmed/28105276</a>
<i>In vitro</i> profiling	Target (potency)	KRas ( $K_i = 0.38 \mu\text{M}$ , $k_{\text{inact}}/K_i = 0.9 \text{ min}^{-1} \cdot \mu\text{M}^{-1}$ )
	Selectivity	
	Potential reactivity	Cysteine reactive
	SAR	See <a href="#">Covalent Guanosine Mimetic Inhibitors of G12C KRAS</a>
	Mechanism of inhibition	Irreversible
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics		
Synthetic scheme		