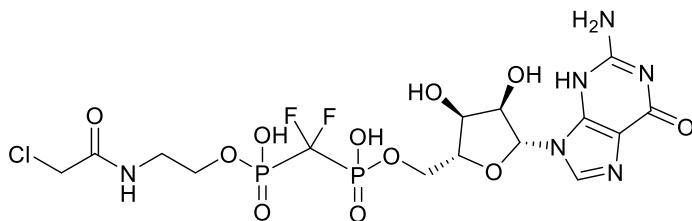


XY-02-082



Chemical Formula: C₁₅H₂₁ClF₂N₆O₁₁P₂
Molecular Weight: 596.76

Category	Parameter	Description
Compound	Name	XY-02-082
	Citation	<i>ACS Med. Chem. Lett.</i> , 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-ylmethoxy](hydroxyphosphoryl)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 ($K_i = 0.38 \mu\text{M}$, $k_{inact}/K_i = 0.9 \text{ min}^{-1} \cdot \mu\text{M}^{-1}$)
	Selectivity	
	Potential reactivity	Cysteine 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		<p>The synthetic scheme for XY-02-082 begins with a purine nucleoside derivative. It reacts with PO(OEt)₃ at 0°C to form a phosphite intermediate. This intermediate then reacts with HO-CH₂-NH-Boc to yield a phosphinic acid intermediate. Subsequent steps involve TFA/DCM treatment to remove the Boc group and reaction with a cyclic anhydride to complete the synthesis of XY-02-082.</p>