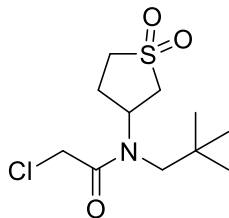


Pin1-3/Sulfopin



Chemical Formula: C₁₁H₂₀ClNO₃S
Molecular Weight: 281.80

Category	Parameter	Description
Compound	Name	Pin1-3 / Sulfopin
	Citation	<i>Nature Chemical Biology</i> 2021 , <i>17</i> , 954-63
	Chemical descriptors	CC(C)(C)CN(C1CCS(=O)=O)C(=O)CCl
	Chemical name	2-chloro-N-(1,1-dioxidotetrahydrothiophen-3-yl)-N-neopentylacetamide
	Entries in chemical databases	CID 155804394
	Availability	Enamine Catalog ID: EN300-6495949
<i>In vitro</i> profiling	Target (potency)	Pin1 with a second-order constant (K_{inact}/K_i) of 84 M ⁻¹ s ⁻¹ .
	Target (potency)	
	Selectivity	
	Potential reactivity	Cysteine reactive (C113)
	SAR	
	Mechanism of inhibition	Irreversible
Cellular profiling	Structure of target-probe complex	6VAJ
	Validation of cellular target	Pin1-3 reduces cell viability after 6 to 8 days of drug treatment in PATU-8988T cells, while it has no effect on proliferation in corresponding Pin1 knockout cells.
	Validation of cellular specificity	
Pharmacodynamics		Pin1-3 displays effective Pin1 engagement in mice spleen with 20 and 40 mg kg ⁻¹ treatment of drug.
Pharmacokinetics		T _{1/2} = 49 min CL = 18.2 ml/min/Kg F = 30%

Synthetic scheme

