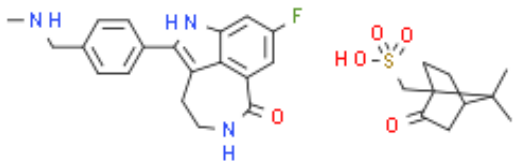
Product Data Sheet

Cas No.:	1859053-21-6	Cat. No:	PL08922
Product Name:	Rucaparib monocamsylate		
Product synonym:	瑞卡帕布樟脑磺酸盐;(1S,4R)-7,7-二甲基-2-氧代-双环[2.2.1]庚烷-1-甲烷磺酸与8-氟-1,3,4,5-四氢-2-[4-[(甲基氨基)甲基]苯基]-6H-吡咯并[4,3,2-ef][2]苯并氮杂卓-6-酮的化合物		
Chemical name:	Rucaparib monocamsylate		
MF:	C29H34FN3O5S	FW:	555.6608
Purity:	≥99%	Batch No.:	-
Storage:			
Structural formula:			
λmax:	-	Formulation:	-
Solubility :			
SMILES :	S(C([H])([H])[C@@]12C(C([H])([H])[C@@]([H])(C([H])([H])C1([H])[H])C2(C([H])([H])[H])C([H])([H])[H])=O)(=O)(=O)O[H].FC1=C([H])C2C(N([H])C([H])([H])C([H])([H])C3=C(C4C([H])=C([H])C(C([H])([H])N([H])C([H])([H])[H])=C([H])C=4[H])N([H])C(=C1[H])C3=2)=O		
InChI Code:	-		
InChI Key:			
WARNING This product is not for human or veterinary use.			

Product Description

Rucaparib (AG014699) monocamsylate 是一种口服有效的 PARP 蛋白 (PARP-1, PARP-2 and PARP-3) 抑制剂，对 PARP-1 的 K_i 为 1.4 nM。Rucaparib monocamsylate 是六磷酸己糖脱氢酶 (H6PD) 抑制剂。Rucaparib monocamsylate 具有用于去势抵抗性前列腺癌 (CRPC) 研究的潜力。

生物活性	Rucaparib (AG014699) monocamsylate is an orally active, potent inhibitor of PARP proteins (PARP-1, PARP-2 and PARP-3) with a K i of 1.4 nM for PARP1. Rucaparib monocamsylate is a modest hexose-6-phosphate dehydrogenase (H6PD) inhibitor. Rucaparib monocamsylate has the potential for castration-resistant prostate cancer (CRPC) research.
IC50 & Target[1][2]	PARP-1 1.4 nM (Ki) PARP-2

体外研究(In Vitro)	Rucaparib (AG014699) monocamsylate is a possible N-demethylation metabolite of AG14644. Rucaparib (0.1, 1, 10, 100 μM; 24 hours) monocamsylate is cytotoxic and has the LC50 being 5?μM in Capan-1 (BRCA2 mutant) cells and only 100?nM in MX-1 (BRCA1 mutant) cells. The radio-sensitization by Rucaparib monocamsylate is due to downstream inhibition of activation of NF-κB, and is independent of SSB repair inhibition. Rucaparib monocamsylate can target NF-κB activated by DNA damage and overcome toxicity observed with classical NF-κB inhibitors without compromising other vital inflammatory functions. Rucaparib monocamsylate inhibits PARP-1 activity by 97.1% at a concentration of 1 μM in permeabilised D283Med cells. has not independently confirmed the accuracy of these methods. They are for reference
体内研究(In Vivo)	Rucaparib (AG014699) monocamsylate and AG14584 significantly increase Temozolomide toxicity. Rucaparib (1 mg/kg) monocamsylate significantly increases Temozolomide-induced body weight loss. Rucaparib (0.1 mg/kg) monocamsylate results in a 50% increase in the temozolomide-induced tumor growth delay. Rucaparib (10?mg/kg for i.p. or 50, 150 mg/kg for p.o.; daily for 5 days per week for 6 weeks) monocamsylate significantly inhibits the growth of the tumor, and there is one complete tumor regression and two persistent partial regressions. Rucaparib (150?mg/kg; p.o.; once per week for 6 weeks or three times per week for 6 weeks) monocamsylate has greatest antitumor effect with three complete regressions. Rucaparib monocamsylate enhances the antitumor activity of temozolomide and indicates complete and sustained tumor regression in NB1691 and SHSY5Y xenografts.
包装储存	4°C, sealed storage, away from moistur In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)
溶解度数据	In Vitro: DMSO : 83.33 mg/mL (149.97 mM; Need ultrasonic)配制储备液