

Product Name : Birinapant

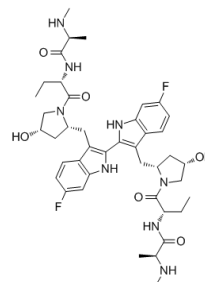
Synonyms : TL-32711

Cat No. : M11075

CAS Number : 1260251-31-7

Molecular Formula : C₄₂H₅₆F₂N₈O₆

Formula Weight : 806.94



Chemical Name : (2S)-N-[(2S)-1-[(2R,4S)-2-[[6-fluoro-2-[6-fluoro-3-[[[(2R,4S)-4-hydroxy-1-[(2S)-2-[(2S)-2-(methylamino)propanoyl]amino]butanoyl]pyrrolidin-2-yl]methyl]-1H-indol-2-yl]-1H-indol-3-yl]methyl]-4-hydroxypyrrolidin-1-yl]-1-oxobutan-2-yl]-2-(methylamino)propanamide

Description : Birinapant is a SMAC mimetic antagonist, mostly to cIAP1 with K_d of <1 nM, less potent to XIAP. Phase 2.

Pathway : Apoptosis

Target : IAP

Receptor : cIAP1; XIAP

Solubility : DMSO:100 mg/mL (123.92 mM); Ethanol:55 mg/mL (68.15 mM); Water: <1 mg/mL (<1 mM)

SMILES : C[C@H](NC)C(N[C@@H](CC)C(N1[C@H](CC2=C(C(N3)=C(C[C@H]4N(C([C@@H](NC([C@@H](NC)C=O)CC)=O)C[C@@H](O)C4)C5=C3C=C(F)C=C5)NC6=C2C=CC(F)=C6)C[C@H](O)C1)=O)=O

Storage : (-20°C)

Stability : ≥ 2 years

Reference :

1.Allensworth JL, et al. Breast Y Res Treat, 2013, 137(2), 359-37