

Product Name: IBG3

Catalog No.: 8129

Batch No.: 1

IUPAC Name: *tert*-Butyl 2-((*S*)-4-(4-((4'-((*S*)-6-(2-(*tert*-butoxy)-2-oxoethyl)-2,3,9-trimethyl-6*H*-thieno[3,2-*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepin-4-yl)-[1,1'-biphenyl]-4-carboxamido)methyl)phenyl)-2,3,9-trimethyl-6*H*-thieno[3,2-*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepin-6-yl)acetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₅₄H₅₇N₉O₅S₂·½H₂O

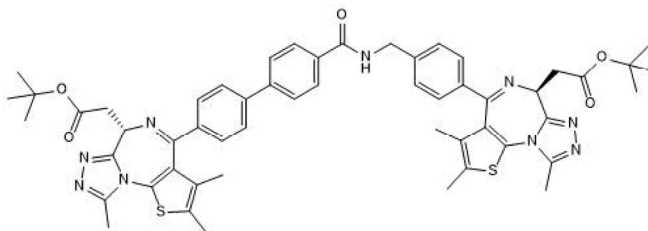
Batch Molecular Weight: 980.73

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	66.13	5.91	12.85
Found	65.08	5.9	12.4

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Description:

IBG3 is a very potent JQ1-containing molecular glue Degradator of BET bromodomains BRD4 and BRD2 (DC₅₀ values are 6.7 pM and 8.6 pM respectively). Induces proximity between BRD4 and DCAF16 to form a ternary complex (EC₅₀ = 32 nM).

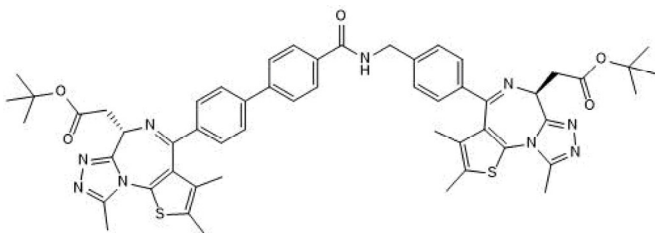
Physical and Chemical Properties:

Batch Molecular Formula: C₅₄H₅₇N₉O₅S₂·¼H₂O

Batch Molecular Weight: 980.73

Physical Appearance: Off White solid

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Other Information:

We certify that this product meets our quality release criteria.

References:

Hsia *et al* (2024) Targeted protein degradation via intramolecular bivalent glues. *Nature* **627** 204. PMID: 38383787.

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