

Product Name: ABT 639

Catalog No.: 6770

Batch No.: 1

CAS Number: 1235560-28-7

IUPAC Name: 4-Chloro-2-fluoro-N-(2-fluorophenyl)-5-[[*(8aR)*-hexahydropyrrolo[1,2-*a*]pyrazin-2(1*H*)-yl]carbonyl]benzenesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₀ClF₂N₃O₃S

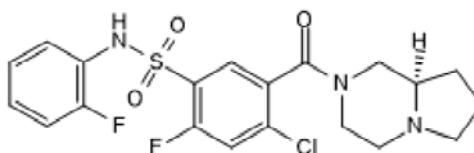
Batch Molecular Weight: 455.91

Physical Appearance: Off White solid

Solubility: DMSO to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.69	4.42	9.22
Found	52.5	4.32	9.23

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Ca_v3.2 channel blocker (IC₅₀ = 2.3 μM). Also blocks low voltage-activated (Ca_v3.1) currents in native rat DRG neurons (IC₅₀ = 7.6 μM). Exhibits little or no activity at other ion channels and receptors. Displays antinociceptive effects in a mechanical hyperalgesia model in vivo. Orally bioavailable.

Physical and Chemical Properties:

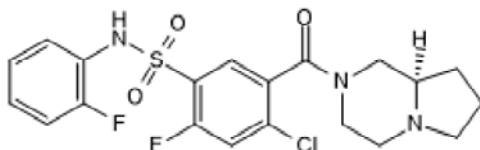
Batch Molecular Formula: C₂₀H₂₀ClF₂N₃O₃S

Batch Molecular Weight: 455.91

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Zhang *et al* (2015) Optimization of ADME properties for sulfonamides leading to the discovery of a T-type calcium channel blocker, ABT-639. ACS Med.Chem.Lett. **6** 641. PMID: 26101566.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 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. Our standard recommendations are:

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.

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