Certificate of Analysis

Product Name: **BRD 0539** **Catalog No.: 7153** **Batch No.: 1**

CAS Number: 1403838-79-8

IUPAC Name: (3a*R*,4*R*,9b*R*)-8-(2-Fluorophenyl)-2,3,3a,4,5,9b-hexahydro-1-[(4-methylphenyl)sulfonyl]-1*H*-pyrrolo[3,2-*c*]quinoline-4-methanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{25}FN_2O_3S$.

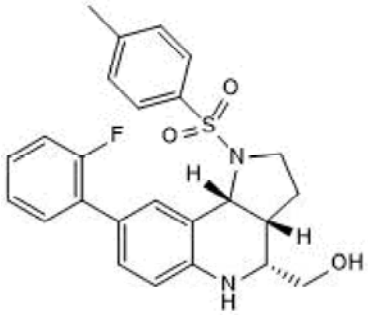
Batch Molecular Weight: 452.54

Physical Appearance: Pale pink to beige solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.35	5.57	6.19
Found	66.32	5.56	6.21

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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Description:

BRD 0539 is a cell-permeable and reversible SpCas9 (Streptococcus pyogenes Cas9) inhibitor. BRD 0539 shows dose-dependent SpCas9 inhibition in an in vitro DNA cleavage assay (apparent IC_{50} = 22 µM) and in an eGFP disruption assay (apparent EC_{50} = 11 µM). Allows dose and temporal control of SpCas9-based systems.

Physical and Chemical Properties:

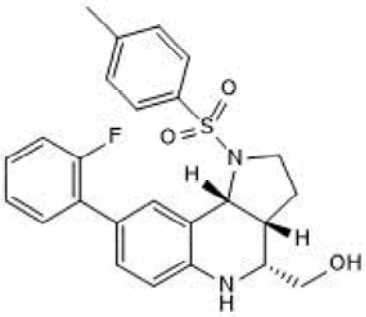
Batch Molecular Formula: $C_{25}H_{25}FN_2O_3S$.

Batch Molecular Weight: 452.54

Physical Appearance: Pale pink to beige solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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. 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.

Licensing Information:

Sold under licence from the Broad Institute

References:

Maji *et al* (2019) A high-throughput platform to identify small-molecule inhibitors of CRISPR-Cas9. Cell ***177*** 1067. PMID: 31051099.