bio-techne
TOCRIS

Print Date: Dec 2nd 2024

Certificate of Analysis

www.tocris.com

Product Name: **BAY 593** **Catalog No.: 8113** **Batch No.: 1**

CAS Number: 2413020-57-0

IUPAC Name: (2*R*)-3,3,3-Trifluoro-2-methoxy-1-[(7*R*)-7-(2-methoxyphenyl)-3,9-diazaspiro[5.5]undec-3-yl]-2-phenyl-1-propanone hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{31}F_3N_2O_3.HCl.H_2O$

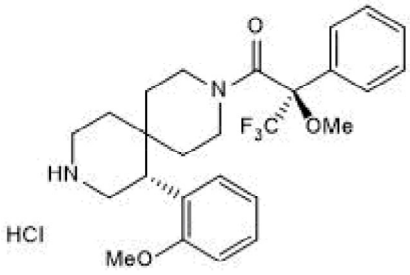
Batch Molecular Weight: 531.02

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100.0% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.81	6.45	5.28
Found	57.9	6.54	5.04

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:

BAY 593 is a geranylgeranyltransferase-I (GGTase-1) inhibitor. Blocks activation of Rho-GTPases to inactivate YAP1/TAZ signaling. Dose-dependently inhibits growth of tumors in xenograft mouse models (IC_{50} values are 38.4 nM and 564 nM in MT-1080 and MDA-MB-231 cells respectively) and PXF 541 xenografts. Orally bioavailable and suitable for use in vivo.

Physical and Chemical Properties:

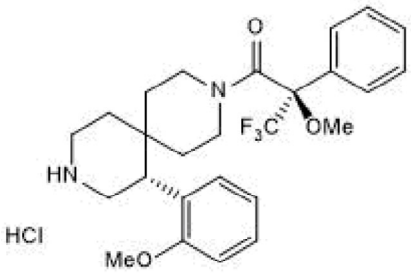
Batch Molecular Formula: $C_{26}H_{31}F_3N_2O_3.HCl.H_2O$

Batch Molecular Weight: 531.02

Physical Appearance: White solid

Minimum Purity: ≥98%

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.

References:

Graham *et al* (2024) Discovery of YAP1/TAZ pathway inhibitors through phenotypic screening with potent anti-tumor activity via blockade of Rho-GTPase signaling. Cell.Chem.Biol. ***31*** 1247. PMID: 38537632.