TOCRIS
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Print Date: Jan 14th 2016

Certificate of Analysis

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Product Name: **SCH 51344** **Catalog No.: 5280** **Batch No.: 1**

CAS Number: 171927-40-5

IUPAC Name: 2-[2-[(6-Methoxy-3-methyl-1*H*-pyrazolo[3,4-*b*]quinolin-4-yl)amino]ethoxy]ethanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{20}N_4O_3$

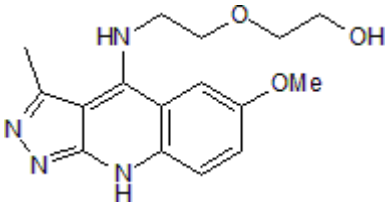
Batch Molecular Weight: 316.35

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 10 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.75	6.37	17.71
Found	60.71	6.3	17.74

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Product Information

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Description:

Potent MTH1 inhibitor (K_d = 49 nM). Inhibits Ras-induced malignant transformation and increases α-actin promoter-driven CAT activity in Ras-transformed cells. Has no effect on Ras-induced ERK and JNK activation. Inhibits Ras-induced membrane ruffling in REF-52 fibroblasts and blocks anchorage-independent growth of Ras-transformed tumor cell lines. Also induces DNA damage in SW480 colon cancer cells.

Physical and Chemical Properties:

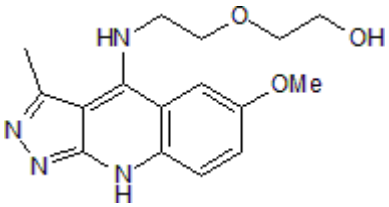
Batch Molecular Formula: $C_{16}H_{20}N_4O_3$

Batch Molecular Weight: 316.35

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 10 mM with gentle warming

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.

References:

Walsh *et al* (1997) SCH 51344-induced reversal of RAS-transformation is accompanied by the specific inhibition of the RAS and RAC-dependent cell morphology pathway. Oncogene ***15*** 2553. PMID: 9399643.

Kumar *et al* (1999) SCH 51344, an inhibitor of RAS/RAC-mediated cell morphology pathway. Ann.N.Y.Acad.Sci. ***886*** 122. PMID: 10667210.

Huber *et al* (2014) Stereospecific targeting of MTH1 by (S)-crizotinib as an anticancer strategy. Nature ***508*** 222. PMID: 24695225.

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