TOCRIS
a bio-techne brand

Print Date: Jan 15th 2016

Certificate of Analysis

www.tocris.com

Product Name: **ZK 93423 hydrochloride** **Catalog No.: 1994** **Batch No.: 1**

CAS Number: 1216574-52-5

IUPAC Name: 4-(Methoxymethyl)-6-(phenylmethoxy)-9*H*-pyrido[3,4-*b*]indole-3-carboxylic acid ethyl ester hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{22}N_2O_4.HCl.¼H_2O$

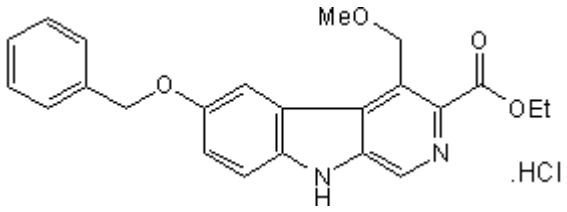
Batch Molecular Weight: 431.4

Physical Appearance: Yellow solid

Solubility: DMSO to 30 mM
ethanol to 5 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Ethyl acetate)

HPLC: Shows >98% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.04	5.49	6.49
Found	64.04	5.39	6.54

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

Product Name: **ZK 93423 hydrochloride** **Catalog No.: 1994** **Batch No.: 1**

CAS Number: 1216574-52-5

IUPAC Name: 4-(Methoxymethyl)-6-(phenylmethoxy)-9*H*-pyrido[3,4-*b*]indole-3-carboxylic acid ethyl ester hydrochloride

Description:

Potent benzodiazepine receptor agonist (IC_{50} = 1 nM). Non-selective between α1-, α2-, α3- and α5-subunit containing $GABA_A$ receptors (K_i values are 4.1, 4.2, 6 and 4.5 nM for inhibition of [^{3}H]Ro15-1788 binding to human recombinant α1β3γ2, α2β3γ2, α3β3γ2 and α5β3γ2 receptors respectively). Anxiolytic following systemic administration in vivo.

Physical and Chemical Properties:

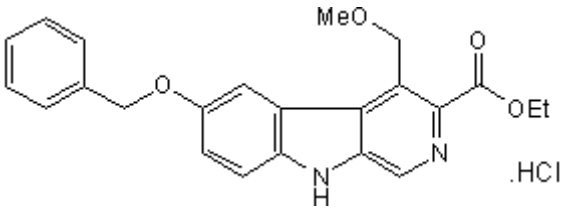
Batch Molecular Formula: $C_{23}H_{22}N_2O_4.HCl.¼H_2O$

Batch Molecular Weight: 431.4

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 30 mM
ethanol to 5 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.

References:

Stephens *et al* (1984) Discriminative stimulus properties of β-carbolines characterized as agonists and inverse agonists at central benzodiazepine receptors. Psychopharmacology ***83*** 233. PMID: 6089245.

File and Baldwin (1987) Effects of β-carbolines in animal models of anxiety. Brain Res.Bull. ***19*** 293. PMID: 3315125.

Cox *et al* (1998) Synthesis and evaluation of analogues of the partial agonist 6-(propyloxy)-4-(methoxymethyl)-β-carboline-3-carboxylic acid ethyl ester (6-PBC) and the full agonist 6-(benzyloxy)-4-(methoxymethyl)-β-carboline-3-carboxylic acid ethyl ester (ZK 93423) at wild type and recombinant $GABA_A$ receptors. J.Med.Chem. ***41*** 2537. PMID: 9651158.