Certificate of Analysis

Product Name: **NBOH-2C-CN hydrochloride** **Catalog No.: 5171** **Batch No.: 2**

CAS Number: 1539266-32-4

IUPAC Name: 4-[2-[[(2-Hydroxyphenyl)methyl]amino]ethyl]-2,5-dimethoxybenzonitrile hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{20}N_2O_3.HCl.¼H_2O$

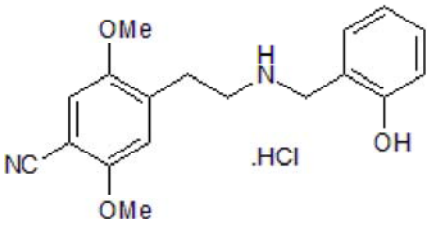
Batch Molecular Weight: 353.32

Physical Appearance: White solid

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

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.32 (Dichloromethane:Methanol [85:15])

HPLC: Shows >99.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.19	6.13	7.93
Found	60.91	6.05	7.87

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Description:

High affinity, selective 5-HT_{2A} agonist (K_i = 1.3 nM). Exhibits 100-fold selectivity for 5-HT_{2A} over 5-HT_{2C}. Elicits head twitch behavior and reduces anxiety-related marble-burying activity in mice.

Physical and Chemical Properties:

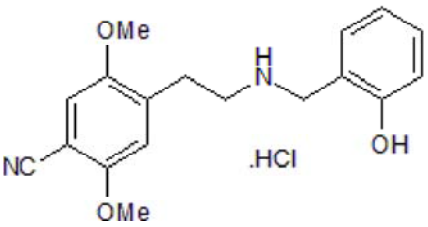
Batch Molecular Formula: $C_{18}H_{20}N_2O_3.HCl.¼H_2O$

Batch Molecular Weight: 353.32

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 10 mM with gentle warming
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. 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.

Other Information:

INFORMATION FOR CUSTOMERS IN THE UK ONLY

This product is a Schedule 1 Home Office controlled substance and customers in the UK are required to hold the relevant licence or be exempt from restrictions in order to purchase and possess this material.

References:

Jensen *et al* (2020) The selective 5-HT_{2A} receptor agonist 25CN-NBOH: Structure-activity relationship, *in vivo* pharmacology, and *in vitro* and *ex vivo* binding characteristics of [^{3}H]25CN-NBOH. Biochem.Pharmacol. ***177*** 113979. PMID: 32298690.

Jensen *et al* (2017) Detailed characterization of the *in vitro* pharmacological and pharmacokinetic properties of *N*-(2-hydroxybenzyl) -2,5-dimethoxy-4-cyanophenylethylamine (25CN-NBOH), a highly selective and brain-penetrant 5-HT_{2A} receptor agonist. J.Pharmacol.Exp.Ther ***361*** 441. PMID: 28360333 .

Fantegrossi *et al* (2014) Hallucinogen-like effects of 2-([2-(4-cyano-2,5-dimethoxyphenyl) ethylamino]methyl)phenol (25CN-NBOH), a novel N-benzylphenethylamine with 100-fold selectivity for 5-HT_{2A} receptors, in mice. Psychopharmacology (Berl.) ***232*** 1039. PMID: 25224567.