25B-NBOH

<table>
<thead>
<tr>
<th>Preferred Name</th>
<th>25B-NBOH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Synonyms</td>
<td>2C-B-NBOH, NBOH-2C-B</td>
</tr>
<tr>
<td>Formal Name</td>
<td>2-[[2-(4-bromo-2,5-dimethoxy-phenyl)ethylamino]methyl]phenol</td>
</tr>
<tr>
<td>InChI Key</td>
<td>RSUNJYKZRKIBNB-UHFFFAOYSA-N</td>
</tr>
<tr>
<td>CAS Number</td>
<td>1539266-16-4</td>
</tr>
<tr>
<td>Chemical Formula</td>
<td>C_{17}H_{20}BrNO_{3}</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>366.25</td>
</tr>
<tr>
<td>Molecular Ion [M^+]</td>
<td>365</td>
</tr>
<tr>
<td>Exact Mass [M+H]^*</td>
<td>366.0699</td>
</tr>
</tbody>
</table>
25B-NBOH

Characterization & Intelligence

The following information was compiled in June 2023 and is subject to change as new research is conducted and as new information becomes available:

Description: 25B-NBOH is a novel synthetic hallucinogen bearing structural similarity to 25B-NBOMe and other “NBOH” and “NBOMe” analogues. In November 2022, 25B-NBOH was detected by our laboratory for the first time in the United States; however, this drug first emerged as early as June 2016 in Europe.

Sample Source: Los Angeles (LA) County Medical Examiner – Coroner.

Sample Appearance: Toxicology specimen – blood.

Pharmacology: Several pharmacological characterization studies involving 25B-NBOH have been published. 25B-NBOH is reported to be a potent serotonin receptor agonist, similar to 25B-NBOMe. Based on structural similarity, 25B-NBOH is expected to exhibit similar adverse effects to related “NBOH” and “NBOMe” analogues. A case report documenting hospitalizations after 25B-NBOH ingestion reported hallucinations, mydriasis, tachycardia, hypertension, and agitation, among other symptoms and effects.

Toxicology: 25B-NBOH has been detected in one toxicology case at the CFSRE.

Drug Materials: 25B-NBOH has not been identified in drug materials at the CFSRE.

Demographics / Geographics: The toxicology case originated from the state of California.

Legal Status: 25B-NBOH is not explicitly scheduled in the United States.

References:
▶ Cayman Chemical: 25B-NBOH
▶ National Forensic Laboratory (Slovenia): 25B-NBOH (test purchase) & 25B-NBOH (reference material)
▶ Ivory et al. A cluster of 25B-NBOH poisonings following exposure to powder sold as lysergic acid diethylamide (LSD). Clinical Toxicology, 2022, 60 (8), 966-969.

About: In collaboration with medical examiner and coroner offices, crime laboratories, clinical partners, and other stakeholders, the Center for Forensic Science Research and Education (CFSRE) is documenting first confirmations of NPS through analysis of drug materials and/or toxicology samples. These reports are generated using comprehensive analytical techniques (e.g., GC-MS, LC-QTOF-MS, NMR) and include available information about the new substances identified at the time of reporting, as well as the analytical data generated during testing. Our new drug monographs are intended to assist with the rapid identification of NPS in forensic casework and related disciplines, and should not be used for confirmatory purposes alone.

Analytical Notes: All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material. A GC-MS mass spectrum for the reference material is not included herein due to analytical breakdown of 25B-NBOH to 2C-B, which is a common phenomenon for these drugs. The linked references included GC-MS data for derivatized 25B-NBOH.

Acknowledgements: This report was prepared by Alex J. Krotulski, Sarah Buxton de Quintana, Sara E. Walton, Melissa F. Fogarty, and Barry K. Logan at the Center for Forensic Science Research and Education (CFSRE) at the Fredric Rieders Family Foundation. The authors acknowledge colleagues for their involvements and contributions. For more information, contact npsdiscovery@cfsre.org or visit www.npsdiscovery.org.

Funding: CFSRE’s NPS Discovery is supported by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 15PNIJ-22-GG-04434-MUMU, “Implementation of NPS Discovery – An Early Warning System for Novel Drug Intelligence, Surveillance, Monitoring, Response, and Forecasting using Drug Materials and Toxicology Populations in the US”). The opinions, findings, conclusions and/or recommendations expressed in this publication are those of the author(s) and do not necessarily represent the official position or policies of the U.S. Department of Justice.

Suggested Citation: Krotulski, AJ; de Quintana, SB; Walton, SE; Fogarty, MF; Logan, BK. (2023) 25B-NBOH — NPS Discovery New Drug Monograph, Center for Forensic Science Research and Education, United States.
Liquid Chromatography Quadrupole Time-of-Flight Mass Spectrometry (LC-QTOF-MS)

**Laboratory:** Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

**Sample Preparation:** Liquid-liquid extraction

**Instrument:** Sciex X500R LC-QTOF-MS

**Methods:** [www.cfsre.org/nps-discovery/monographs](http://www.cfsre.org/nps-discovery/monographs)

**LC-QTOF-MS:** TOF-MS Precursor Ion Mass Spectrum

**LC-QTOF-MS:** TOF-MS/MS Product Ion Mass Spectrum

**Confirmation Using Drug Standard:** Reference material (Batch: 0475709-54) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be 25B-NBOH based on retention time (sample: 6.79 min vs. standard: 6.67 min) and mass spectral data comparisons.