K16 The Electroanalytical Identification of 25I-NBOH and 2C-I Via Differential Pulse Voltammetry: A Rapid and Sensitive Screening Method to Avoid Misidentification

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The goal of this presentation is to present a new electrochemical method to identify 25I-NBOH, a new, potent serotonin 5-HT2A receptor agonist usually identified in blotter paper.

This presentation will impact the forensic science community by introducing a new, selective, and sensitive method for the identification of 25I-NBOH, a compound that is usually misidentified by routine Gas Chromatography/Mass Spectrometry (GC/MS) methods.

Recently, a new potent serotonin 5-HT2A receptor agonist was identified in blotter paper seizures in Brazil.[1] This compound, named 25I-NBOH, is a label molecule that undergoes degradation when examined under routine GC/MS conditions, leading to misidentification as it degrades into 2C-I, an amphetamine-type stimulant.[2] The prevalence of this substance on the Novel Psychoactive Substances (NPS) market can be underestimated under GC/MS conditions, the most widely and routinely utilized analytical technique for drug sample analyses, as it can misidentify 25I-NBOH because of its degradation into 2C-I (and corresponding 2C for the other members of the series).[2] Despite many attempts in adjusting GC/MS conditions and even changing the extraction solvent, Coelho Neto et al. stated that degradation could not be avoided.[2] The degradation takes place inside the GC/MS injector and appears to be caused by the high temperature inside the injector with the degradation products reacting with the alcohol used in the extraction procedure.[2] Another recent study described the analytical determination of phenethylamines derivatives; compounds of the NBOMe group via cyclic and differential pulse voltammetry.[3] Noting that 25I-NBOH has only a single modification regarding 25I-NBOMe, a substitution of a metoxy group for a hydroxy group in the position 3 of the secondary aromatic ring, a very sensitive and specific method to identify 25X-NBOH avoiding misidentification as 2C-X of this class of compounds was developed.

The voltammetric behavior of 25I-NBOH and 2C-I were investigated and their electroanalytical characteristics determined. The investigation of the electrochemical behavior by Cyclic Voltammetry (CV) using a carbon Screen-Printed Electrode (SCPE) showed two oxidative waves observed at +0.74 V and +1.09 V for 25I-NBOH and one single oxidative wave at +1.20 V for 2C-I. The first oxidative peak is a result of the electrochemical oxidation of the secondary amine present in the NBOH compound and the second oxidative wave is due to the halogen oxidation to a hydroxyl group and subsequent oxidation to a ketone (quinone/catechol equilibrium). The effect of scan rate (v) on the peak current (ip) and the peak potential (Ep) upon the electrochemical oxidation of both drugs were also examined. The slope values observed were close enough to the theoretically expected value of 0.5 for a purely diffusion-controlled current. The pH analyses revealed a linear dependence in the order of magnitude to that expected for a monoelectronic/monoprotonic reaction. To achieve unmistakable identification, differential pulse voltammetry was also used. The method uses the electrochemical oxidation of these molecules to produce an analytical signal that can be related to each compound concentration with an average lower limit of quantitation of 0.01mg/mL. The analytical identification for 25I-NBOH, 25I-NBOMe, and 2C-I was performed using the second oxidation wave, although the first oxidation wave was used in the quantification analysis.

A novel, fast, and sensitive electrochemical method for detection of 25I-NBOH using SCPE was achieved and all method characteristics demonstrated the method to be analytically valuable. The method is selective enough to identify the three compounds individually, even given the great similarity in their structure. The method is selective and achieved full differentiation between 25I-NBOH, 2C-I, and 25I-NBOMe.

Reference(s):

1. Arantes L.C., Ferrari Junior E., Souza L.F., Cardoso A.C., Alcantara T.L.F., Liao L.M., Machado Y., Araujo L.R., Coelho Neto J., Andrade A.F.B. 25I-NBOH: A New Potent Serotonin 5-HT 2A Receptor Agonist Identified in Blotter Paper Seizures in Brazil. *Forensic Toxicology.* 2017. doi:10.1007/s11419-017-0357-x.
2. Coelho Neto J., Andrade A.F.B., Lordeiro R.A., Machado Y., Elie M., Ferrari Junior E., Arantes L.C. Preventing Misidentification of 25I-NBOH as 2C-I on Routine GC-MS Analyses. *Forensic Toxicology.* 2017. doi:10.1007/s11419-017-0362-0.
3. Andrade A.F.B., Mamo S.K., Gonzalez-Rodriguez J. Rapid Screening Method for New Psychoactive Substances of Forensic Interest: Electrochemistry and Analytical Determination of Phenethylamines Derivatives (NBOMe) via Cyclic and Differential Pulse Voltammetry. *Analytical Chemistry.* 2017:89(3):1445–52. doi:10.1021/acs.analchem.6b02426.

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