

Enantioselective Study of MDMA and its Phase-1 Metabolites Using Different Separation Methods

Vazha Tkemaladze^{1}, Saba Djorbenadze¹, Giorgi amiranashvili¹ Bezhan Chankvetadze¹*

Email: vajadasergi@gmail.com

1. Chair of Physical and Analytical Chemistry, Faculty of Exact and Natural Sciences, Ivane Javakhishvili Tbilisi State University, I. Chavchavadze Ave. 1, 0179, Tbilisi, Georgia

The frequent use of psychotropic substances leads to the development of dependence in humans and is characterized by a negative impact on both, physical and mental health. Lethal outcome is also frequent. The development of enantioselective methods for the precise identification of these substances represents a highly relevant challenge in forensic and toxicological analysis.

The study employed two different separation methods: supercritical fluid chromatography (SFC) and high-performance liquid chromatography (HPLC), with detection performed using a triple quadrupole mass spectrometer. SFC and HPLC are similar separation methods; both use mobile and stationary phases for separation. Separation is caused by the differential distribution of various substances between these two phases. The main difference lies in the composition of the mobile phase. In SFC, the eluent primarily consists of a supercritical fluid.

Within the framework of this research, an enantioselective method was developed for the identification of MDMA and its Phase-1 metabolites using supercritical fluid chromatography-tandem mass spectrometry (SFC-MS/MS) and high-performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS).

On the method development step various chiral chromatographic columns and mobile phases of different compositions were used. Using SFC, baseline separation of the enantiomers of the studied substance was achieved on a Lux cellulose-4 column. The mobile phase consisted of supercritical fluid and an organic modifier in a 70%-30% ratio. Using HPLC, baseline separation of the enantiomers of the studied substance was achieved on a Lux-Amp column. The mobile phase consisted of acetonitrile and an aqueous ammonium bicarbonate solution with a pH of 11, in a 75%-25% ratio. The analysis of Phase-1 metabolites was conducted under the same chromatographic conditions using both methods. Furthermore, the pharmacokinetics of this substance in various human biological matrices were studied.