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Enantioseparation and racemization of MDPV by liquid chromatography

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Resumo

Introduction: Synthetic cathinones are a vast group of new psychoactive substances, similar to amphetamines and widely abused due to their psychostimulant effects [1]. Although they are chiral, few studies report the influence of the stereochemistry in their biological/toxicological properties [2, 3]. To study the enantiomers, the development of enantiomeric resolution methods is crucial, being liquid chromatography the technique of choice [4] Furthermore, under certain conditions such as high temperature and acidic/basic environments, pure enantiomers in solution can undergo racemization. Thus, racemization studies are of great importance [5]. **Objectives:** The aims of this work were the semi-preparative enantiomeric resolution of the synthetic cathinone MDPV along with a racemization study with the collected enantiomers. The potential enantioselectivity of MDPV in neurotoxicity will be further evaluated. **Material and methods:** The semi-preparative enantiomeric resolution and racemization study were performed by liquid chromatography using polysaccharide-based chiral stationary phases (CSPs). For the racemization study, the enantiomers were exposed to different temperatures (room temperature, 37ºC and 70ºC) in the presence/absence of diisopropylethylamine for 48 h. **Results:** The enantiomers of MDPV were separated with a resolution factor (Rs) of 1.7 and selectivity factor (α) of 1.4. The enantiomeric ratio values for the collected enantiomers were >99% for the first enantiomer and 90% for the second with recovery rates of 96% found for both enantiomers. While no racemization occurred after 3 hours for all tested conditions, signs of racemization started to appear for both enantiomers after 48 h at 37ºC and after 24 h at 70ºC. **Conclusions:** The enantiomers of MDPV were successfully separated with a good resolution and enantioselectivity and collected with high enantiomeric ratio and recovery rates. Racemization starts to occur after 48 h at 37ºC and 24 h at 70ºC.

Keywords: synthetic cathinones; enantioselectivity; liquid chromatography; racemization

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