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Acidity of substituted cathinones studied by capillary electrophoresis using the standard and fast alternative approaches

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Abstract

Cathinone derivatives are notorious but still weakly characterized molecules, known mainly as components of the designer and illicit drugs. The knowledge on their acidity is scarce and incomplete, therefore, we decided to determine the pK_a values for six of them: 2-methylmethcathinone, 3-methylmethcathinone, 4-methylmethcathinone, α -pyrrolidinovalerophenone, methylenedioxypropylamphetamine and ephedrone. For that purpose we employed capillary electrophoresis, which is known for its accurateness in comparison to other analytical techniques. We used and compared two methodologically different approaches. The standard method relied on measuring electrophoretic mobility across the broad pH range and fitting the sigmoidal function. The obtained pK_a values were in the range 8.59 – 9.10, thus these molecules remain mostly protonated and positively ionized in the physiological conditions. The alternative two-values (TVM) and one-value methods (OVM), proposed by us previously, have been used herein for the first time to the cationic molecules. TVM enables estimation of pK_a using only two electrophoretic mobility values, referring to the total and partial ionization. OVM requires only a single measurement because mobility of ion is predicted theoretically. Both TVM and OVM yielded only a small deviation of pK_a from the standard approach, averagely 0.07 – 0.09 pH unit. Two important issues have also been addressed: the potential of a maximally fast calculation method using no repetition at the given pH, and the accuracy of method with regard to pH attributed to partial ionization. As a whole, the analytical potential of the TVM/OVM approach seems to be huge and invaluable for fast pK_a screening/estimation.

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