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A study on electrospray mass spectrometry of fullerenol $C_{60}(OH)_{24}$

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Abstract

Full characterization of fullerenol $C_{60}(OH)_{24}$ by HPLC ESI-MS in negative and positive ionization modes was achieved. Fragmentor voltage and capillary voltage were optimized in order to obtain a good signal stability and the best peak intensity distribution for the fullerenol $C_{60}(OH)_{24}$ in both negative and positive modes. While the predominant base peak observed for $C_{60}(OH)_{24}$ in the negative ionization mode was $[M - H]^-$ at *m/z* 1127, those observed in the positive mode were multiply charged $[M - H_2O + 4H]^{4+}$ at *m/z* 279 and $[M - 12H_2O + 2NH_3 + 6H]^{6+}$ at *m/z* 158.

Introduction

Because of their potential for chemical tunability and exciting range of biological activities as glutamate-receptor antagonists [1] and antiproliferative [2,3], neuroprotective [4-7], and anticancer agents [8-13], polyhydroxylated [C_{60}]fullerenes, $C_{60}(OH)_x$, have received much attention in recent years. However, to the best of our knowledge, except for the compositionally and structurally well characterized $C_{60}(OH)_{24}$, prepared by alkaline hydrolysis of $C_{60}Br_{24}$ [14,15], most of these fullerenols are not pure $C_{60}(OH)_x$, but a complex mixture of products with an average composition of $C_{60}(OH)_{x-y}$, $C_{60}O_x(OH)_y$ [16-19] or $C_{60}(OH)_x(ONa)_y$ [20].

Therefore, the HPLC separation and accurate measurement of the molecular weight for structure characterization by electrospray ionization mass spectrometry (ESI-MS) have become essential for fullerenol research. Fullerenols $C_{60}(OH)_{18-44}$ are very small neutral molecules with the highest density of hydroxy groups on a given particle surface (up to 10.7 OH/nm^2)