

# A study on electrospray mass spectrometry of fullereneol C<sub>60</sub>(OH)<sub>24</sub>

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## Full Research Paper

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## Abstract

Full characterization of fullereneol C<sub>60</sub>(OH)<sub>24</sub> 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 fullereneol C<sub>60</sub>(OH)<sub>24</sub> in both negative and positive modes. While the predominant base peak observed for C<sub>60</sub>(OH)<sub>24</sub> in the negative ionization mode was [M – H]<sup>–</sup> at *m/z* 1127, those observed in the positive mode were multiply charged [M – H<sub>2</sub>O + 4H]<sup>4+</sup> at *m/z* 279 and [M – 12H<sub>2</sub>O + 2NH<sub>3</sub> + 6H]<sup>6+</sup> 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 anti-cancer agents [8-13], polyhydroxylated [C<sub>60</sub>]fullerenes, C<sub>60</sub>(OH)<sub>x</sub>, have received much attention in recent years. However, to the best of our knowledge, except for the compositionally and structurally well characterized C<sub>60</sub>(OH)<sub>24</sub>, prepared by alkaline hydrolysis of C<sub>60</sub>Br<sub>24</sub> [14,15], most of these fullereneols are not pure C<sub>60</sub>(OH)<sub>x</sub>, but a complex mixture of

products with an average composition of C<sub>60</sub>(OH)<sub>x-y</sub>, C<sub>60</sub>O<sub>x</sub>(OH)<sub>y</sub> [16-19] or C<sub>60</sub>(OH)<sub>x</sub>(ONa)<sub>y</sub> [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 fullereneol research. Fullereneols C<sub>60</sub>(OH)<sub>18-44</sub> are very small neutral molecules with the highest density of hydroxy groups on a given particle surface (up to 10.7 OH/nm<sup>2</sup>)