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Theoretical investigation of the fragmentation mechanism of singly positively charged 5-methoxyflavone

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ABSTRACT In this study, density functional theory calculations were employed to investigate the dissociation of the molecular ion $[\mathbf{L}]^{+\bullet}$ (**L** = 5-methoxyflavone). Using the Gibbs free energies of the optimized stationary points, $[\mathbf{L}]^{+\bullet}$ dissociation potential energy profiles were constructed, and the dissociation mechanism, including the detailed fragmentation pathways to $[\mathbf{L}-(2H,O)]^{+\bullet}$, $[\mathbf{L}-(H,C,O)]^{+}$ and $[\mathbf{L}-(2H,C,2O)]^{+\bullet}$; fragment configurations; and product distribution, was further explored. Finally, the similarities and differences between the theoretical and available experimental results were discussed in detail. This study provides new insight into the dissociation of flavonoids and their analogues in mass spectrometry.

Keywords 5-Methoxyflavone; Fragmentation; Theoretical computation; Dissociation; Potential energy profile

1. Introduction

Flavonoids, often called “bioflavonoids” [1], are secondary metabolites in various vegetables and fruits [2,3] and exhibit important physiological and medical effects [2,4–12]. Structurally, flavonoids are polyphenol compounds [2,5] that generally consist of two phenyl rings (**A** and **B** rings, see Fig. 1a) linked by a three-carbon-atom chain [13]. These three carbon atoms can be part of an oxygen-containing six- (Fig.