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## Fragmentation pathway of harmful chemicals in soft ionization mode and its application in novel analogue screening

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The MS/MS fragmentation pathway of the cinnamic esters additives was illustrated. There were four analytes (butyl heptanoate, ethyl cinnamate, n-propyl cinnamate and benzyl cinnamate) had m/z ratio 131 with higher abundance. By analyzing the structure of compound ethyl cinnamate, n-propyl cinnamate and benzyl cinnamate, these similar fragments were due to consecutive losses of the cinnamoyl moiety (m/z 131). The mechanisms show the common fragmentation behavior of the cinnamic esters. The fragmentation mechanism of mass spectra of these  $\beta$ -agonists shows that dehydration reactions occurred in the pathway of each compound. A common characteristic was observed that there was neutral loss of a water molecule for all  $\beta$ -agonists and for 7  $\beta$ -agonists, loss of an alkyl group from the secondary amine was demonstrated. Moreover, m/z at 74 and 60 were for the butyl and propyl derivatives respectively. The fragmentation pathway of crocin, crocetin and geniposide were studied. The DP and CE values of crocin were higher than those of crocetin which may be because of the stable gentiobiosyl bond and large molecular weight of crocin. The precursor ion [M-H] – (m/z 975) of crocin had potential to loss gentiobiosyl (m/z 324) for [M-H-gen] – (m/z 651) and to loss two gentiobiosyl (m/z 648) for crocetin (m/z 327).

### Biography

Fengming CHEN, was born in 1984 in Fujian province, China, Dr. Fengming CHEN obtained the doctor degree in Tokyo Metropolitan University. And as postdoctoral in Department of Chemistry, Tsinghua University during 2014-2017, Entering Chinese Academy of Inspection and Quarantine in 2017 and focused his attention on the application of chromatography/mass spectrometry in food and sing-cell analysis, measurement and standard material development and other fields.

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