Electronic Supplementary Material (ESI) for Analyst.

A computational and experimental study of the fragmentation of L-leucine, L-isoleucine and L-allo-isoleucine under collision-induced dissociation tandem mass spectrometry.

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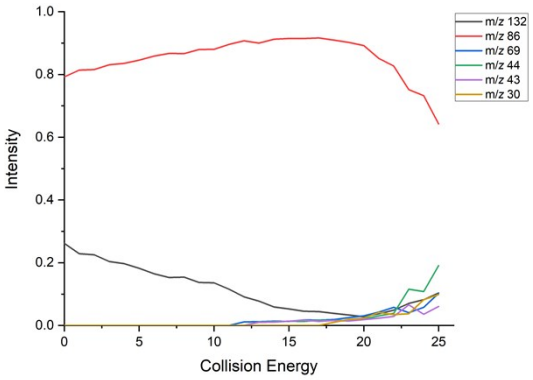
Supplementary information.

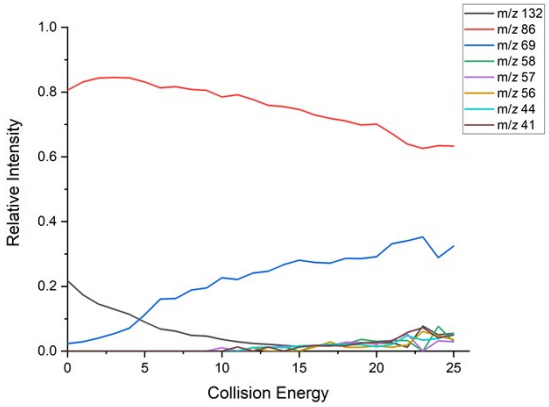
Energy breakdown graphs were constructed from the tandem mass spectra obtained from Synapt G2S. Due to the nature of the collision cell, the CID energy used in this part of the experiment runs from 0 to to 25 eV. The signal/noise/ ratio becomes undesirable when the energy is above 25 eV. Even at 0 eV energy, all three amino acids start to fragment. The results obtained agree with the observation obtained from Orbitrap analysis 9 see figure 2. Peak intensities for product ion *m/z* 69 of the three amino acids follow the trend *I*(69)Ile > *I*(69)L-allo-Ile > *I*(69)Leu. Leu produced very different energy breakdown graph compared to the other two. At the highest collision energy, peak intensity of product ion *m/z* 69 for is almost four times less compared to Ile. This is also evident from the MS/MS spectra in figure 3.

Figure S1.

(a)



(b)



(c)

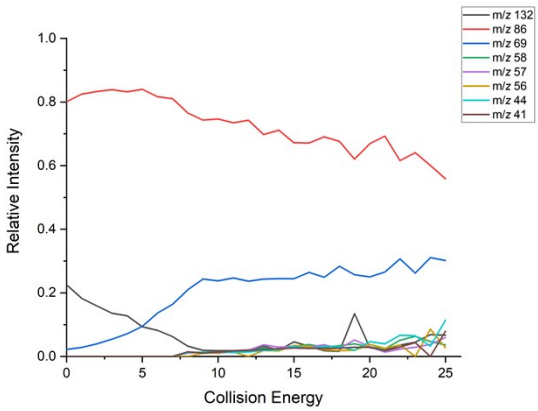


Figure S1. Energy breakdown graphs from the Synapt G2S for the fragmentation of protonated Leu (a), Ile (b) and L-allo-Ile (c) by Synapt. The precursor ion (*m/z* 132) is shown in black; product ion *m/z* 86 in red and product ion *m/z* 69 in blue. Peak intensities are normalised to sum = 1.