Though more fragment ions are obtained in EPI scans, the QTRAP system also offers the ability to perform MSMS fragmentation inside the linear ion trap via frequency excitation of the intact precursor ion. This mode of operation, generates fragmentation patterns that are similar to the traditional 3D trap MSMS. However, since fragment ions are produced in a linear trap, the CID process in the linear trap is performed via a high pressure collision. MS3 is performed in the linear ion trap portion of the QTRAP system (Q3). First generation of fragment ions is produced via a high pressure collision. MS3 is performed in the linear ion trap of the mass spectrometer via single frequency excitation. Dextromethorphan (Figure 1) was dissolved into water/methanol (3:7) with 0.1% formic acid to yield a concentration of 2ng/µL. The compound was infused via a Harvard syringe pump at a flow rate of 10µL/min.

The ions labeled with red and blue arrows were also found in the fragmentation of 215 and 213, respectively. Proposed genealogy of dextromethorphan obtained at 60% of activation energy. The key features of the mass spectrum are: (1) lower intensities over even masses of active ions (<10e3) and (2) significant differences in the fragment ions. Therefore, the QTRAP can be used to either acquire ‘quad-like’ or ‘trap-like’ mass spectra on the same instrument.

CONCLUSIONS

The efficiency of the CID process in the QTRAP enables the user to obtain in a single experiment, sufficient fragmentation information to get maximum structural coverage. Combining efficient generation of fragment ions with MS capabilities makes the QTRAP a powerful tool for structural elucidation. Further more, the QTRAP offers two modes of fragmentation on the same instrument, enabling the user to gain orthogonal information on the fragmentation pathway with the same set-up. This information can be obtained by operating the QTRAP to provide either ‘quad-like’ or ‘trap-like’ fragmentation—a unique feature that can translate into improved throughput as well as automation of structural elucidation.

REFERENCES


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