Surface Induced Dissociation (SID) with Quadrupole Mass Filters: MS/MS without Collision Gas

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Abstract

Surface Induced Dissociation (SID) is well recognized to provide analytical information about chemical species, via MS/MS. Compared with Collision Induced Dissociation (CID), SID promises more reproducible energy resolved breakdown curves, and access to higher energy fragmentation pathways, which can increase selectivity for MS/MS experiments.

CID generally has much better conversion efficiency of parent to progeny ions (approaching 100% in some cases involving ion traps), which in turn increases ultimate sensitivity. For the chemical species that we analyzed, we found typical SID conversion efficiency to be $^{\sim}20\%$, not as efficient as ion traps claim, but still analytically useful.

A major disadvantage to CID for MS/MS, at least for quadrupole instruments, is the requirement for bottled pure collision gas, with its associated plumbing, regulators and flow control and pressure measurement, as well as the additional pumping required to get rid of the collision gas after you leak it into the chamber.

MS/MS using a tandem quadrupole configuration promises less ambiguous results than in an ion trap configuration due to the ion trap's potential complications of space charge and ion molecule reactions.

This work explores the analytical utility of SID for tandem quadrupole MS/MS, both in selectivity and sensitivity.

A component electrospray quadrupole mass spectrometer was configured with a 9.25mm round rod resolving quadrupole, followed by an in-line SID collision cell, followed by a collision-free RF-only rectilinear quadrupole ion guide, leading into a second 9.25 mm resolving quadrupole mass filter and electron multiplier detector.

The SID collision assembly consisted of an entrance lens, an exit lens, with a split pair of SID surfaces in between, for a total ion path length of 0.6 inches.

A novel self-assembled monolayer of 2-perfluorohexyl ethyl thiol was deposited onto a polished copper surface, and SID performance using this surface was compared to untreated polished stainless steel, with the two surfaces being mirrored halves of the center split lens pair.

The collision-free ion guide was included in these experiments to evaluate the timeline of progeny ion formation. Ions born immediately upon interacting with the surface would be expected to have an effective birth potential of the surface, whereas ions born inside the ion guide would be expected to have an effective birth potential matching the ion guide centerline potential. The final instrument does not require this ion guide.

Ion fragmentation energetics were studied for various species to better understand the advantages and trade-offs of SID versus CID for MS/MS.

Finally, we will present a proposed size and cost reduced quadrupole SID MS/MS system suitable for non-traditional installations where access to bottled gases is inconvenient.

Biography - Randall E. Pedder

Randall Pedder, Ph.D. is founder and President of Ardara Technologies L.P., a designer and manufacturer of quadrupole, TOF, and ion trap mass spectrometers and related components. Randy graduated from the University of Florida in 1992, under the guidance of Richard Yost, with a Ph.D thesis entitled "Fundamental Studies in Quadrupole Ion Trap Mass Spectrometry". Randy has spent the last 35 years working at instrument companies doing research, product development, and collaborating with researchers worldwide, with a specific interest in providing enabling technologies for research and development of portable mass spectrometers. Past employers included Finnigan MAT, Inficon, Extrel, and Waters.

Keywords

SID, MS/MS, Quadrupole mass filters, Fundamentals