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Positive Chemical Ionization (PCI) Operating Parameters for the 5973N PCI Standard Turbo MSD

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Introduction

The Standard Turbo (ST) MSD system (Product Nos. G2588A and G1788A) is designed for high sensitivity in positive chemical ionization (PCI) with lower cost than that of the Performance Turbo (PT) MSD system (Product Nos. G2589A and G1789A). Despite the difference in pumping capacities, the ST system can achieve sensitivities equivalent to those of the PT system for the primary protonated species for most compounds, within the column flow constraints.[1] This is especially important in confirming compound molecular weights or in doing sensitive analyses to detect the presence of compounds in complicated extracts by detection of the protonated molecular ions. However, the difference in pumping speeds between the PT and ST does impose some differences in the performance of PCI on the ST beyond those of sensitivity and carrier-gas flow restrictions. The primary differences are found in the CI reagent gas flow to the source, and they are reflected in the generation of adduct ion ratios; these differences are described in this document.

Suggested Tuning and Reagent-Gas Flow Parameters

PCI performance is influenced by several factors, most importantly, by the characteristics of the compound to be analyzed for, by the CI reagent gas, and by the source parameters of temperature and reagent-gas pressure. Typically the source temperature is 250°C in PCI on the 5973N. Once a PCI reagent gas is selected, the most important parameter becomes the reagent-gas source pressure. In the autotuning process, the software suggests particular ranges of ratios for the CI reagent ions, based on PCI reagent-source pressure for the three most common PCI gases (methane, isobutane, and ammonia). These ranges are intended as initial parameters for optimizing PCI sensitivity for the particular compound of interest. Beginning with these ion ratios, which are manipulated by adjusting CI reagent flow into the source via the Mass Flow Controller (MFC) module on the CI unit, the sensitivity for a given compound is optimized by serially injecting a standard under different CI flow settings. The suggested reagent ion ratios and initial flow setting for the CI reagent MFC for the most common CI gases are given in Table 1.

Table 1. Suggested initial PCI tuning parameters for the ST system.

Reagent Gas	Reagent Ion Masses and Composition	Ion Ratio Range Percent of Total Flow	Initial Mass Flow Controller Setting as
Methane	28 / 27 ($C_2H_4^+$ / $C_2H_3^+$)	0.5 – 3.0	10
Isobutane	57 /43 ($C_4H_9^+$ / $C_3H_7^+$)	1.0 – 5.0	10
Ammonia	35 / 18 ($N_2H_7^+$ / NH_4^+)	0.02 – 0.2	10

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The flow setting changes necessary to achieve a given ion ratio—and, consequently, the signal for the protonated molecular ion of the compound of interest—are smaller for the ST system than they are for the PT system. That is, the lower pumping speed of the ST allows larger changes in ion ratios to be achieved with smaller changes in reagent-gas flow to the source.

Optimizing Sensitivity

The suggested approach to maximizing PCI sensitivity is the same on both the ST and PT systems, and it is as follows. After selection of CI reagent gas and source temperature, start at the lowest MFC setting of reagent gas that provides the lowest ion ratio cited in Table 1. Inject a standard and examine the ion abundance for the compound, then increase the pressure and re-inject. As explained above, the user will find that small increases in the MFC setting will increase the reagent ion ratio on the ST system. This means that the optimal range of source pressures is narrower on the ST than on the PT system. Regardless, comparable sensitivity and reproducibility for a compound's most abundant positive ion can be obtained on the ST system as on the PT system at a comparable or slightly lower MFC setting.

Adduct Ion Ratios

The protonated molecular species, $(M+H)^+$, is usually the most common species formed in PCI, and as the reagent pressure increases from low source pressures or flows, there is an increase in this species abundance. At some point the pressure becomes optimal and there is a maximum in the M+1 signal beyond which increases in source pressure result in a decrease in signal. Concomitant with the increase in source pressure is the increase in condensation reactions which result in adducts $(M+R)^+$. This is most pronounced for ammonia reagent gas, which readily forms $(M+NH_4)^+$ and results in adduct ions at M+18 *m/z,* as well as the usual M+1 *m/z.* Because higher source pressures and lower analyzer pressures can be produced in the PT system, higher percentages of adducts can be generated with the PT system than with the ST system. Therefore if the user is interested in using adducts as confirmation ions in SIM or scan for trace-level analysis and wishes to have the largest possible latitude in manipulating the adduct ratios, the PT system is recommended. However, if adduct ratios are not an issue, then sensitivity for the M+1 ion by the ST and PT systems will be comparable (all else being equal) and the ST should be suitable for the application.

Summary

The sensitivity of the Standard Turbo PCI system is essentially equivalent to that obtained by the Performance Turbo system for the most abundant species generated in PCI, that is, the protonated molecular ion. The difference between the two platforms appears in the capability to generate high relative percentages of adduct ions. If the user is interested in adduct-ion information, the Performance Turbo system is a more appropriate platform. However, if sensitive detection of the protonated molecular species is the most important information, then the Standard Turbo system is a cost-effective alternative within the other constraints imposed by the 70-L turbomolecular pumping system.[1]

References

1. Prest, H; 5973N*etwork* Series MSDs: GC Column Selection and Pumping Considerations for Electron and Chemical Ionization MSD operation. Technical Note (23) 5968-7958E.

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