Agilent 500 Ion Trap LC/MS With SelecTemp

Technical Overview

Introduction

SelecTemp is a temperature-programmable atmospheric pressure ionization (API) drying gas control and is a unique feature of the Agilent 500 Ion Trap LC/MS. Positive and negative temperature programming ensures the optimum drying gas temperature for all mobile phase compositions in gradient separations resulting in greater sensitivity and productivity.

Experimental Conditions

The drying gas temperature is specified based on the mobile phase composition during the run, as shown in Figure 1. Generally gradient LC analysis increases the percent of organic phase and decreases the percent of aqueous phase during the run. Therefore, the optimum drying gas temperature should also decrease during the run. Constant temperatures result in excess heating of the electrospray droplets and may cause destruction of the thermally labile compounds. However, at the end of a gradient run when the column is being regenerated and the aqueous composition of the mobile phase is high, it is advantageous to have a high drying gas temperature to ensure complete desolvation of droplets to reduce contamination of the API interface.

Agilent Technologies

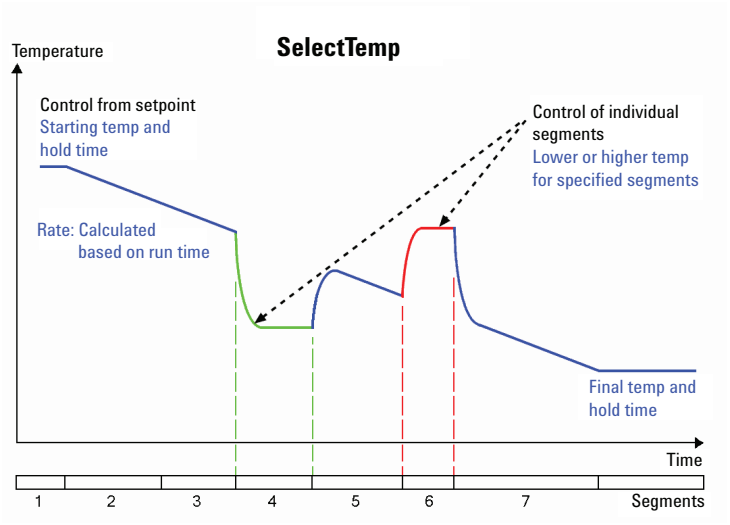

Figure 1. Schematic of SelecTemp.

Using SelecTemp, start and end temperatures are specified with their hold time, and the rate is calculated based on the full run time. The temperature profile created by these specifications can be overwritten by lower or higher values specified for the individual time segments as shown in Figure 2. Setpoint specifications apply to the whole run, while segment specification applies only for the duration of the specified time segment (Figure 3).

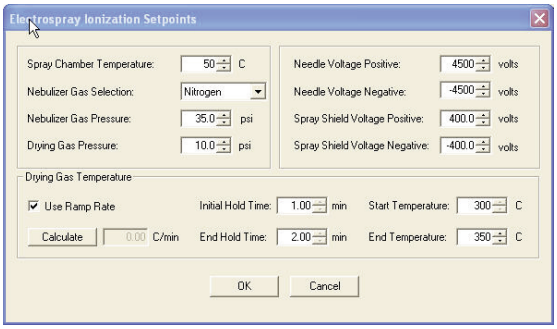

Figure 2. ESI and SelecTemp setpoints for total analysis run.

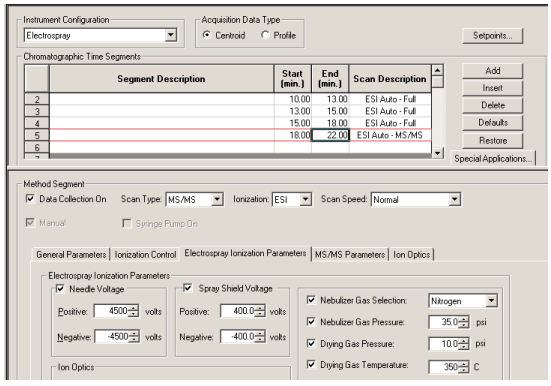

Figure 3. ESI and SelecTemp setpoints for chromatographic segment time.

The controlled drying gas temperature also increases sensitivity for thermally labile compounds. To demonstrate this, 1 ng of naphthol glucuronide (Figure 4), was injected onto a column at different drying gas temperatures, with otherwise identical conditions. The mobile phase was 0.1% acetic acid in water (solvent A) and 0.1% acetic acid in acetonitrile (solvent B) at 0.2 mL/min. The gradient conditions are given in Table 1.

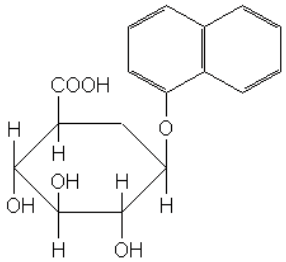

Figure 4. Chemical structure of naphthol-glucuronide.

Table 1. HPLC Conditions Used for the Study

Time min:sec	%A	%B	Flow rate mL/min
0:00	95	5	0.2
1:30	95	5	0.2
2:00	57	43	0.2
3:45	5	95	0.2
4:30	5	95	0.2
4:45	95	5	0.2
5:00	95	5	0.2

The temperature program of the drying gas started at 330 °C with a 2 min hold time, followed by programming the temperature from 330 °C to 300 °C in 3 min.

Discussion and Results

The reconstructed ion chromatogram for m/z = 199 from positive ESI MRM (precursor 343 → product 175–205) is shown in Figure 5. The red trace shows naphthol glucuronide with programmed drying gas (down ramped), the green trace shows it with isothermal drying gas. Note the signal intensity increase and noise decrease using the temperature programming of the drying gas, ultimately resulting in an S/N increase of 146 to 462. Although the temperature of the drying gas was only lowered by 30 °C from the initial value, SelecTemp provided a factor of three improvement in signal-to-noise.

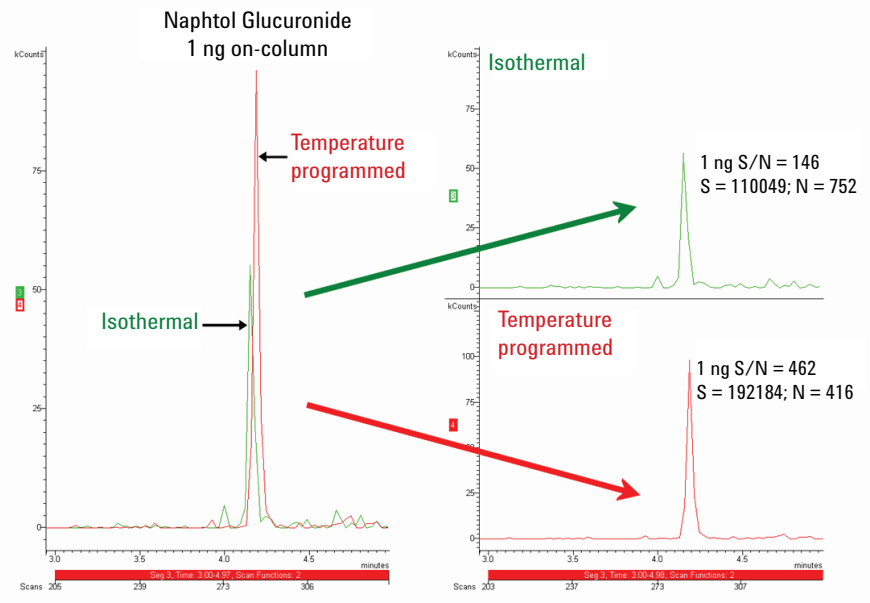

Figure 5. Use of SelecTemp directly translates into improved S/N ratio for naphthol-glucuronide.

Benefits

SelecTemp allows the Agilent 500 Ion Trap LC/MS to deliver increased sensitivity and selectivity for all analytes, including thermally labile compounds. Other benefits include reduced interface contamination, improved throughput, simplified setup, and automatically recorded parameters for GLP purposes.

www.agilent.com/chem

Printed in the USA
February 24, 2011
SI-0243

Agilent Technologies