

Supplemental material

Detailed description of sample preparation instrumentation and modified atmospheric interface for Sciex API 4000 Q-Trap instrument is given here. Technical details of custom-built instrumentation fall out of the focus of the paper, however this supplemental information is necessary for the proper reproduction of results described in the main text.

Elutor device

The single channel elutor device (Figure S1a.) consists of a stainless steel cartridge holder, a gas heater unit and a fluid delivery unit. SPE cartridges are placed into the female luer connectors of a standard SPE vacuum manifold (Biotage, Uppsala, Sweden). Gas heating is implemented by using standard 1/8" copper tubing equipped with a Ni-Cr resistance heater and a Cu/Constantane thermocouple. The temperature is controlled by a CAL 3300 (CAL Controls Ltd., Brighton, UK) temperature controller device. The fluid delivery unit consists of a dual syringe pump (Harvard Apparatus, Holliston, MA), a 6-port valve (Vici AG International, Schenkon, Switzerland), and a cartridge insert. The latter is designed to fit perfectly into the cartridges in order to minimize dead volume in the systems. A 1 mL glass syringe (Hamilton, Bonaduz, Switzerland) is connected to cartridge.

The 96-channel elutor device (Figure S1b.) employs an 8 x 12 array of individual SPE cartridges inserted into a PPS plate. Device consists of a ventilator/fan, a heater block with 96 (8 x 12) drilled holes, an aluminum frame for a 96 channel SPE plate and a 96 channel gas introduction part. Four stainless steel bolts are utilized to secure perfect alignment of nozzles, cartridges and gas inlets.

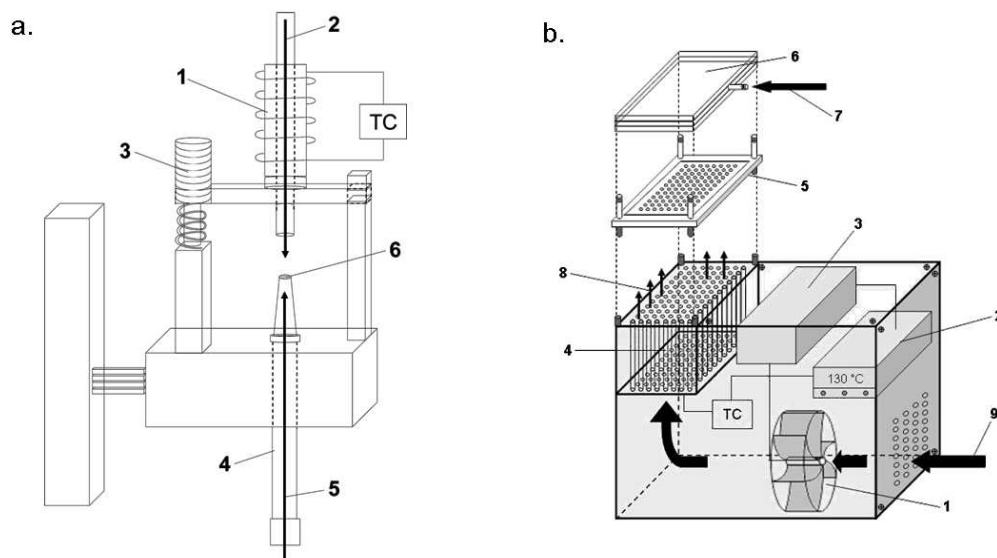


Figure S1. Scheme of elutor devices. a. Single channel elutor device. (1) heated gas jet, (2) nitrogen gas, (3) positioner, (4) SPE cartridge, (5) eluent, (6) sample. b. 96-channel elutor. (1) ventilator, (2) temperature controller, (3) power supply, (4) heated aluminium block, (5) 96 well-plate, (6) cover plate, (7) nitrogen, (8) hot air flow.

The new interface consists of a PEEK housing and a 200 mm long 0.53 mm internal diameter 1/16" outer diameter stainless steel capillary inlet. The capillary is equipped with resistance heating, thermocouple and temperature controller unit (HAGA, Budapest, Hungary). The capillary is bent in 120 degrees in the middle to provide optimal access to the individual SPE cartridges during the analysis of the 96 well SPE plates. The exact position of the heated capillary is set by a manual micrometer screw driven linear stage, built onto the external housing of the mass spectrometer.

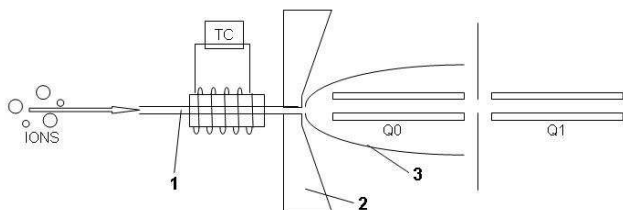


Figure S2. Home built atmospheric interface for the API 4000 QTRAP hybrid triple quadrupole/ion trap mass spectrometer. (1) heated capillary, (2) PEEK housing, (3) skimmer.