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APPI II

**Direct Insertion Probe** 

GC-APCI II

ionBooster

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#### **Ion Sources**

In mass spectrometry, the performance of the MS system in terms of mass resolution, mass accuracy and principally sensitivity, is highly dependent on the method of ion generation. There is no single ion source for all applications; polar and non-polar, small and large molecules require specific ionization techniques.

Numerous ion sources have been developed especially for LC/MS systems to meet the diverse requirements of every potential application. Bruker Daltonics offers the widest variety of ion sources; each with special features and some of them truly unique.

### CaptiveSpray Ion Source

#### The key to performance and reliability for nano flow MS

**The Bruker CaptiveSpray principle:** Stable and robust nanoflow LC/MS is still a challenge in proteomics analysis. The Bruker CaptiveSpray Ion Source is a revolutionary source with a patented design that provides easy operation just as simple as the normal flow electrospray.

CaptiveSpray delivers nanospray sensitivity, resists plugging, and provides reproducible, uninterrupted flow for even the most complex proteomics samples.

#### Plug-and-Play

The CaptiveSpray source mounts directly onto all current Bruker API mass spectrometers. The Ion Transfer Interface connects directly to the front of the capillary, eliminating the need for complex XYZ adjustable stages.

# Bruker's revolutionary CaptiveSpray source is now available with a smart dopant addition option—the nanoBooster

CaptiveSpray nanoBooster brings your MS to the next performance level and provides even higher flexibility.

- · Boosts nanoflow sensitivity
- Pushes up ID rates
- Enables Glycoanalysis











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#### Lechnical Details

#### Ease of Use

CaptiveSpray provides a vortex gas that sweeps around the emitter spray tip to desolvate and focus the Taylor cone into the MS inlet capillary. The vacuum seal to the MS ion guide draws all of the sample ions into the MS increasing the efficiency of sample transfer from the spray tip into the mass spectrometer. The direct connection to the inlet capillary eliminates the need for any source adjustment making the CaptiveSpray source truly Plug-and-Play.

#### **Smart Ionization Support by Dopant-enriched Gas Supply**

The nanoBooster option allows the modification and vapor enrichment of gas that flows around the emitter. Dependent on the used dopant, either charge stripping or charge enhancement of peptides and proteins can be achieved during the ionization process. Charge enhancement is advantageous for the analysis of large biomolecules due to the reduction of the mass-to-charge (m/z) ratio. Furthermore, higher charge stages increase efficiency of electron transfer dissociation (ETD) MS/MS.

#### **Applications**

#### **Glycoanalysis**

The enrichment of the nanoBooster sheath gas with acetonitrile results in improvement of glycopeptide analyzation. The charge state increase provides higher quality ETD spectra and enables highly improved glycopeptide characterization by assignment and identification of the glycosylation sites.

#### Supercharging in Gas Phase

The gas supply is software-controlled. The user can define the dopant enrichment and charge effect. CaptiveSpray nanoBooster provides the capability of post-column charging of peptides without the need to add buffers to the HPLC solvents and thus without influencing the chromatographic performance.

#### **ID Rates**

CaptiveSpray nanoBooster increases the ionization efficiency of peptides significantly, leading to a much higher sensitivity than even conventional nanospray.

This results in a highly improved number of identified proteins in complex mixtures.

#### **VIP-HESI**

The sensitivity of the system is extremely important in most MS analytical tasks. Heated electrospray helps to increase ion yield. Compared to standard electrospray, the VIP-HESI offers a solid gain in sensitivity for many compounds of interest in the fields of metabolomics and pharmaceutical analysis, environmental analysis, food testing and forensic drug investigations. VIP-HESI has proven to be a robust workhorse ion source on Bruker's TQ product range for almost a decade now.

The latest version of VIP-HESI can be used with all timsTOF, and QTOF series instruments, and is quickly and easily installed. For a wide range of compounds, the



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VIP-HESI is a dual source and includes VIP Heated Electrospray and Atmospheric Pressure Chemical Ionization (APCI) probes standard.



#### **Technical Details**

The ion source enhances sensitivity and lowers detection limits by delivering more efficient ionization across a wide range of applications. Inside the VIP-HESI, an electrospray is maintained at a controlled vaporizing temperature to enable enhanced desolvation of the analyte ions, even at high eluent flow rates in UHPLC separations with sharp chromatographic peaks.

Within the Vacuum Insulated Probe (VIP) the eluent stream including the compounds of interested are shielded against heat by a vacuum barrier just like in a dewar. Combination of heating and eluent stream into the probe make it a simple and easy to maintain design. The powerful active exhaust prevents re-circulation by utilizing Venturi-effect show smart implementation of long known physical principles into modern instrumentation.

## **Applications**

#### **VIP-HESI in Forensics**

Ethyl-Glucuronids (EtG and EtS) are markers for alcohol misuse. The VIP-HESI source yields great sensitivity for determination of EtG from blood. For details, please refer to application note LCMS-122.

#### **VIP-HESI in Food Safety**

Extremely sensitive analytical methods are required for accurate low-level identification, and quantitation of zero-tolerance compounds in food.

Bruker's TargetScreener application is boosted more than 10fold for a representative subset of analytes when used with VIP-HESI instead of regular ESI source. The VIP-HESI achieves a Limit of Quantitation (LOQ) more than 100 times lower than the minimum required performance level (MRPL).

#### **VIP HESI in Glycopeptide Determination**

Glycosylation is a common critical quality attribute (CQA) of therapeutic proteins and needs to be characterized during product development. Typically, this analysis is conducted after enzymatic release and tagging of the glycans followed by fluorescence and MS detection. A more modern workflow is to identify glycan compositions directly from tryptic peptide maps acquired with the timsTOF Pro and PASEF® in combination with analytical LC and the new VIP-HESI ion source. It employs a glycan search method from peptide mapping data and uses previously identified aglycons as mass tags.



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evaporation of the solvent is done by heating the sample in the nebulizer needle. APCI is often used for metabolomics as well as for drug or pesticide screening.

The new Bruker APCI II source is of course compatible to Bruker's unique DirectProbe option DIP. The direct injection probe is a novel smart solid sample introduction technique allowing a rapid analysis of solids. Sample preparation is as simple as dipping a disposable glass capillary into the solid sample.



#### **Technical Details**

#### Unambiguos identification synthetic compound

This example shows the unambiguos identification of a synthetic compound using the autoMSn capability of an amaZon SL ion trap system. During the vaporization of solid (refer to TIC insert) data-dependent MS2 and MS3 spectra are taken. Note that after a simple neutral loss in MS2, MS3 provides rich structural information. Samples were kindly provided by SiChem GmbH, Bremen, Germany.

#### **APPI II**

Atmospheric pressure photo ionization (APPI) is used for less polar or non-polar molecules that can not be ionized in either ESI or APCI.

APPI delivers a wide dynamic range and low chemical noise. With an operational flow range of  $2\mu$ l/min –  $1500\mu$ L/min it is compatible with cap- to analytical chromatography.

APPI II by Bruker Daltonics is the only APPI source with DirectProbe option for direct analysis of solid samples. The direct injection probe is a novel smart solid sample introduction technique allowing a rapid analysis of solids.

Sample preparation is as simple as dipping a disposable glass capillary into the solid sample.



### **Applications**









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#### **Direct Insertion Probe**

The DirectProbe (DIP) add-on for the Bruker APCI II and APPI II ion sources allows direct analysis of liquid and solid samples without tedious sample preparation. In routine organic synthesis analyses, it simplifies identification and characterization of chemical reaction products without compromising sensitivity.

- Extremely sensitive down to the sub-ng range of pure substance amount not visible at all!
- Minimum sample preparation
- · Direct analysis of liquid & solid samples
- Short analysis time
- No memory due to single-use glass tubes



# **Applications**

#### Fields of applications are

- General Chemistry → Synthesis control
- Manual quality control of solids (Pharma, oil, explosives)
- Customs → Drugs of abuse, explosives
- · Homeland security
- Environmental
- Thermal degradation processes (plastic production)
- Classical routine analysis (e.g. confirmation of sum formula)

#### Direct injection Probe with APCI for ID synthetic compounds

This example shows the unambiguos identification of a synthetic compound using the autoMSn capability of an amaZon SL ion trap system. During the vaporization of solid (refer to TIC insert) data-dependent MS2 and MS3 spectra are taken. Note that after a simple neutral loss in MS2, MS3 provides rich structural information. Samples were kindly provided by SiChem GmbH, Bremen, Germany.

#### Direct injection Probe with APPI for QC in Production

The example shows the results of a quick manual QC and Comparison of petroleum cuts with an amaZon SL. The three candidates gas oil vacuum gas oil and vacuum residue are clearly distinguishable without any sample preparation and no memory-effect due to single use sample tubes.









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LC or GC use.

With its second generation GC-APCI source, Bruker offers the greatest flexibility and highest performance with a combined GC frontend and high-resolution MS system for confident ID of unknown compounds using complementary MS technology. The GC-APCI II interface can be coupled to any Bruker MS system with the common Apollo II source design.

GC-APCI II is designed to connect to state-of-the-art GC systems including Bruker's 436-GC and 456-GC but can also be used with third party GC systems. The flexible, heated transfer line, automatic MS calibration and outstanding sensitivity make GC-APCI II the best solution for unknown ID in metabolomics and small molecule research.



#### **Technical Details**

Making a dedicated and expensive GC-TOF-MS used infrequently for just a few samples a thing of the past.

The GC-APCI II source enables GC coupling to any Bruker TOF or QTOF, trap or FTMS system originally designed for LC coupling.

Switching of the sources without venting the vacuum

The system has the capability to be easily switched from GC to LC and vice versa without tools and within minutes. There is no need to vent the MS vacuum.

#### **Greater Flexibility**

The design of the flexible heated transfer line means that the GC and MS must no longer be precisely aligned. Interfacing the GC and MS is simpler, giving more options in positioning the MS and GC while preserving the obtained GC separation.

#### **Automatic MS Calibration**

The unique calibrant reservoir of the GC-APCI II interface enables software-controlled calibrant delivery.

#### **Improved LLOQ**

The optimized ionization chamber provides improved GC-MS performance including lower background and higher sensitivity.

# **Applications**

#### **Unknown ID in Metabolomics**

GC-MS is one of the few standard techniques in metabolomic analysis. In recent years the combination of gas chromatography and Atmospheric Pressure Chemical Ionization (APCI) with high resolution mass spectrometry techniques has proven to be an important additional tool for the analysis of highly complex mixtures of natural products from plants and body fluids. While standard GC-EI-MS is

Atmospheric Pressure Chemical Ionization (APCI) in combination with high resolution mass spectrometry techniques opens a new dimension in terms of sensitivity. APCI can be used in combination with GC and LC separation to cover the whole range of PAHs.

#### **Dibenzodioxins and -furans**

Dioxins are banned since the 1970s due to their ability to









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samples.

#### Polycyclic Aromatic Hydrocarbons (PAH)

Polycyclic Aromatic Hydrocarbons (PAH) are ubiquitous in the environment and many of them are considered to be carcinogenic. The analysis of these compounds at low concentrations is therefore an important task in environmental and food analysis.

mixtures of a few hundred congeners difficult to chromatographically resolve. GC-APCI can be ideally combined with hydrogen as carrier gas for highest chromatographic resolving power amongst all carrier gases.

Both environmental and food analysis can benefit not only for dioxin- and furan analysis but also other POPs like polychlorinated Biphenyls or brominated compounds.

#### ionBooster

The sensitivity of the system is extremely important in most MS analytical tasks. Compared to standard electrospray, the ionBooster offers a 5–100x gain in sensitivity for many compounds of interest in the fields of environmental analysis, food testing and therapeutic drug monitoring. The ionBooster enhances sensitivity and lowers detection limits by increasing ionization efficiency in a wide range of applications.

The ionBooster can be used with the latest Bruker amaZon speed, maXis, maXis impact or solariX MS systems, and is quickly and easily installed. For a wide range of compounds, the ionBooster achieves sensitivities that rival those of industry-leading QQQs, while still providing the known benefits of MSn or accurate mass values with  $TIP^{TM}$  (True Isotopic Pattern). The ionBooster has simple operating parameters and nitrogen consumption requirements that are similar to those of conventional sources.

#### **Technical Details**

The ion source enhances sensitivity and lowers detection limits by delivering more efficient ionization across a wide range of applications. Inside the ionBooster, an electrospray is maintained at a controlled vaporizing temperature to enable enhanced desolvation of the analyte ions, even at high eluent flow rates in UHPLC

separations with sharp chromatographic peaks.

The exact response with the ionBooster depends upon the type of compound and its specific chemical characteristics and thermal properties.

# **Applications**

#### ionBooster in Forensics

Ethyl-Glucuronids (EtG and EtS) are markers for alcohol

LC-MS full scan method for lower limit quantification and confirmation on a maXis UHR-TOF system, without









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Extremely sensitive analytical methods are required for accurate low-level identification, and quantitation of zerotolerance compounds in food. The broad-spectrum antibiotic Chloramphenicol (CAP) is such a compound. Determination of CAP is often performed by LC-MS/MS using MRM measurements on traditional triple-quadrupole instruments. Using the ionBooster, CAP can be determined in an

Top: Compare Chloramphenicol signal trace of ionBooster with traditional Electrospray at 0.25 µg/kg in matrix (CAP in beef muscle).

Bottom: Six replicate injections, at 0.0025 µg/kg CAP in matrix meat. Mean Signal: Noise 10:1, Peak width 3.4 sec (FWHM), Peak area RSD 9%. Figures from Application Note ET-27.

#### **Literature Room Mass Spectrometry**

Search for related Ion Sources literature



Results 1 - 7 of 7

Sub-ppm HCP Screening in 15 minutes using dia-PASEF. By taking advantage of the unique capabilities of the timsTOF Pro 2, you can now confidently detect sub-ppm levels of host cell proteins in 15 minutes. Use of dia-PASEF benefits from the correlation between ion mobility and m/z to maximize ion utilization, enabling the measurement of low abundant Host Cell Proteins in therapeutic protein preparations. The workflow utilises a standard UHPLC at analytical flow rates to maximize ease of use and r...

#### , ↓, FN 21 - VIP-HESI HCP

No Compromises: Fast, Sensitive and Robust HCP Analysis with timsTOF Pro 2. The timsTOF Pro 2 enables the discovery of previously unidentified low abundant Host Cell Proteins in therapeutic protein preparations. Samples are analyzed by RP-LC with the Elute UHPLC and VIP-HESI ion source at analytical flow rates, a configuration which can also be adapted for highly sensitive routine QC analysis by using shorter gradients.



#### **■** BROCHURE BRUKER PRODUCT OVERVIEW FOR MASS SPECTROMETRY 2021

, ↓, FN 20 - SUB-PPM HCP SCREENING IN 15 MINUTES USING DIA-PASEF

Life Science Mass Spectrometry Instruments and Solutions



#### LCMS 188 - GLYCOPEPTIDE ANALYSIS IN PEPTIDE MAPPING WORKFLOW

How to Determine Glycan Profiles of Biopharmaceuticals from Peptide Mapping Data. A new and sensitive approach combining BioPharma Compass, PASEF and VIP-HESI.



#### **BROCHURE VIP-HESI DUAL SOURCE - NEXT GENERATION IN MASS SPECTROMETRY** SENSITIVITY

Vacuum Insulated Probe – Heated Electrospray Ionisation (VIP-HESI) has been migrated from the proven EVOQ Elite and coupled to Bruker QTOF and timsTOF systems.



#### **■** BROCHURE WARRANTY EXTENSION

LabScape™Service & Lifecycle Support