

Kit for Direct Probe Ionization Mass Spectrometer





Quick and Easy Measurement Without Sample Preparation — Direct Probe Ionization-MS —

The PESI (Probe Electro Spray Ionization) TQ unit can easily replace an ESI unit for use in combination with LCMS*.

Features of PESI (Probe Electro Spray Ionization)

- Perform MS analysis directly on the sample.
- Suitable for thermally labile compounds, no direct heat applied.
- Highly resistant to MS contamination, even with complex matrices.

Simple Workflow



Applications

Field	Chemical	products/Synthesis	Biologic	al/Food samples
Simple pretreatment	ł	Measuring mixture ratio of raw materials Monitoring presence of impurities		Rapid screening directly on the biomaterial sample
Monitoring changes over time		Real-time tracking of synthesis reactions	-0	Oxidation reaction and UV degradation of supplements

DPiMS[™] Can Be Used in Diverse Fields

Measures a Wide Variety of Samples

- Body fluids, such as blood or urine
- Tissue sections, such as from laboratory animals or foods
- Plant materials, such as vegetables and fruits

Applicable for a Wide Variety of Objectives

- Detecting biological components
- Detecting materials for chemical products
- Detecting drugs, poisons, etc.

Measure a Variety of Samples with Only Simple Pretreatment

Rapid and Easy Drug Detection in Forensic Samples

- \bullet Place a piece of each organ on a biological sample plate and add 50 % ethanol (35 $\mu L).$
- Detection is possible by on-plate MRM / Product Ion Scan analysis.





Biological Sample Plate



PESI-MS Measurement Collision Energy: 25 V Mass range: m/z 50 to 450 Scan speed: 405 u/sec Event time: 1 sec Desolvation line: 250°C Heat block: 50°C Polarity: Positive Acquisition time: 0.5 min / event

This data was obtained from joint research with Mr. Kiyotaka Usui from Tohoku University Graduate School of Medicine.

Switch Easily Between PESI-MS and LCMS

The PESI TQ unit can be removed easily. The ability to exchange it with an ESI unit means measurements can be performed using the same theory of ionization and standard substance, which allows comparing data. The DPiMS-8060 was used for quantitative analysis of a forensic sample from a person that took the drug MT-45. As a result, we were able to obtain measurement data consistent with LCMS results in an extremely short time.





Tissue Section	PESI-MS/MS	LC-MS/MS
Tissue Section	(µg/mL)	(µg/mL)
Liver	4.1	3.9
Brain	1.6	1.5
Heart	1.8	2.0
Lung	8.7	10.9
Kidney	1.7	1.5
Measurement Time	0.5 min	20 min

Quantitative Results of MT-45 in Forensic Sample

This data was obtained from joint research with Mr. Kiyotaka Usui from Tohoku University Graduate School of Medicine.

Metabolomic Analysis Performed Easily by Transferring LCMS Analytical Conditions to DPiMS Unit

In this example, transition information for metabolites (26 components) such as amino acids, organic acids, and sugars were used for metabolomic analysis of mouse livers. Metabolomes can be analyzed easily by customizing some of the analytical conditions in the LCMS primary metabolite method package. The DPiMS-8060 system was used to measure the principal components in the model mouse group with acute liver damage induced by carbon tetrachloride and the control group. A significant difference was observed between model and control groups (given p < 0.001 for Welch's t-test), based on the significant contribution of taurine to the separation of groups in the PCA loading plot. The difference was verified with a box-whisker plot.

3-hydroxybutyrate	citric acid	D-glucose
Isocitric acid	G6P	glycine
L-asparagine	L-aspartic acid	L-glutamic acid
L-lactic acid	L-malic acid	L-serine
pyruvic acid	succinic acid	taurine
2-aminobutyricacid	L-glutamine	L-histidine
L-leucine/L-isoleucine	L-methionine	L-ornithine
L-phenylalanine	L-proline	L-threonine
L-tryptophan	L-tyrosine	





This data was obtained from joint research with Associate Professor Kei Zaitsu from Nagoya University Graduate School of Medicine.

Box-whisker Plot of Taurine

DPIMS-8060 t Probe Ionization Mass Spectrometer

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PESI MS Solution Software

PESI MS Solution software is used to control the probe, edit MS method files, and start measurements.

Scan range and SIM settings are specified via the method editing window in LabSolutions[™] LCMS software. Analysis can be started easily by selecting the probe control mode and MS method in PESI MS Solution. During analysis, the status can be confirmed in the LabSolutions LCMS window.

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PESI MS Solution

Probe control method file



Enables Use of LC/MS/MS Method Package

The DPiMS-8060 system uses a direct analysis method that does not involve liquid chromatography using probe electrospray ionization. MRM parameters can be specified based on transition information included in the LC/MS/MS method package. Consequently, methods can be created easily using an Excel template. A key feature of PESI is the easy process flow from pretreatment to measurement.

No.	Compound	Retention Time (min)	Polarity	Quantitation Ion	Reference lon	Compound Type
1	Lysine	0.795	(-)	145.20>145.20		Amino acid
2	Arginine	0.831	(-)	173.10>131.20		Amino acid
3	Histidine	0.842	(-)	154.10>93.10	154.10>137.05	Amino acid
4	Glycine	1.097	(-)	74.10>74.10		Amino acid
5	Serine	1.106	(-)	104.10>74.10		Amino acid
6	Asparagine	1.114	(-)	131.00>113.15	131.00>70.10	Amino acid
7	Alanine	1.132	(-)	88.10>88.10		Amino acid
8	Glutamine	1.143	(-)	145.00>127.10	145.00>109.10	Amino acid
9	Threonine	1.156	(-)	118.00>74.10		Amino acid
10	Cysteine	1.232	(-)	120.00>33.10		Amino acid
11	Methionine sulfone	1.288	(-)	180.10>79.15	180.10>64.10	Standard substance
12	Methionine	2.000	(-)	148.10>47.10	148.10>100.10	Amino acid
13	Tyrosine	3.272	(-)	180.00>119.10	180.00>163.10	Amino acid
14	2-Morpholinoethanesulfonic acid	3.278	(-)	194.10>80.15	194.10>107.10	Standard substance
15	Glutamic acid	3.919	(-)	146.00>102.10	146.00>128.10	Amino acid
16	Aspartic acid	4.084	(-)	132.10>88.20	132.10>115.00	Amino acid
17	Phenylalanine	4.948	(-)	164.00>147.10	164.00>103.10	Amino acid
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Data Analyzed Using LabSolutions LCMS

The system can be used for a wide variety of applications, such as for library searches based on mass spectra obtained from product ion scans, for quantitative analysis based on ion chromatograms obtained from MRM, or for multivariate analysis using scan data. Because the postrun analysis functionality in LabSolutions LCMS is used, data can also be easily compared to LC/MS/MS data.



Analysis System with No Carryover

Only a tiny amount of sample attaches to the probe during each sampling, reducing the risk of contamination inside the mass spectrometer to near zero.

Carryover can even be prevented by changing probes.

Even concentrated samples or samples of unknown concentration can be measured directly without pretreatment.



Mass Spectra After Repeatedly Switching Between Measuring PPGT and Blank Samples (PPGT 10 mg/mL)

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