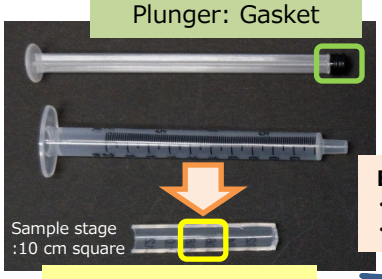
HR-MS of solvent extracts at 1mmϕ spatial resolution ～Elution Profile based on Solvent Polarity, Analyte Region～

LESA(Liquid Extract Surface Analysis) nano ESI-MS systems capable of surface analysis under atmospheric pressure can solvent-extract surfaces at 1mmϕ spatial resolution to assign the structure of eluted molecules from materials by HR(High Resolution)-MS.
Extraction and direct analysis can rapidly provide information on various solvents in each area.

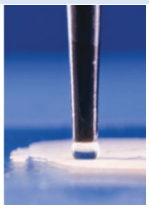
LESA(Liquid Extract Surface Analysis) nano ESI-MS Analysis Flow-Examples of Medical Materials



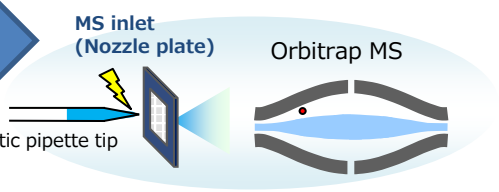
-Before acid treatment
-After acid treatment

LESA (solvent-extraction at spatial 1 mmφ resolution)
※almost all the solvent can be selected

Extraction solvent
・10% ethanol aq.
・Isopropanol (IPA)



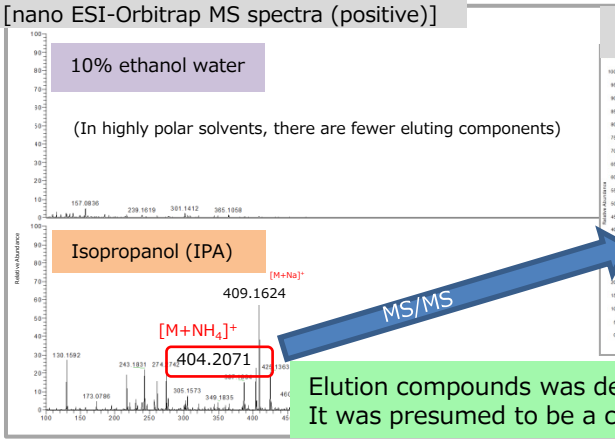
Nano ESI-MS (High Resolution MS)



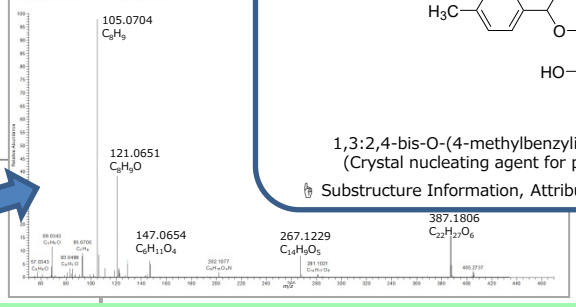
LESA can extract and analyze areas using various solvents even in irregular samples!

Comparison of eluates between 2 solvents (syringe: inner wall, before acid treatment)

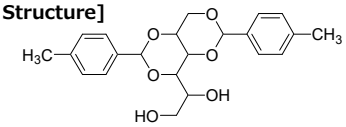
[nano ESI-Orbitrap MS spectra (positive)]



MS/MS spectrum



[Estimated Structure]



$C_{22}H_{26}O_6$
Exact Mass: 386.1729

1,3:2,4-bis-O-(4-methylbenzylidene)-D-sorbitol
(Crystal nucleating agent for polyolefin resin)

Substructure Information, Attributed from our Database

Elution compounds was detected with isopropanol, a lower polarity solvent.
It was presumed to be a crystal nucleating agent for resin by detailed structural analysis.

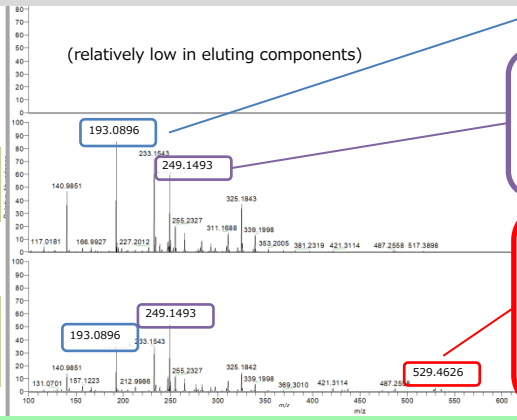
Comparison of eluates between 2 areas (extraction solvent: IPA)

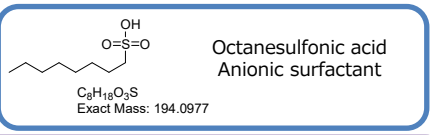
[nano ESI-Orbitrap MS spectrum (detected as negative ion, [M-H]⁻)]

Syringe: Inner wall
(before acid treatment)

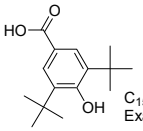
Plunger: Gasket
(before acid treatment)

Plunger: Gasket
(After acid treatment)





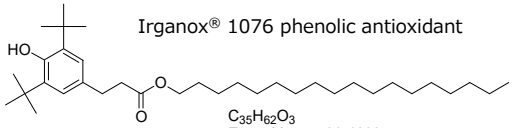
Octanesulfonic acid
Anionic surfactant
$C_8H_{18}O_3S$
Exact Mass: 194.0977



Di-butyl tert-hydroxybenzoate
(Estimated as a decomposition product of phenolic antioxidants)
$C_{15}H_{22}O_3$
Exact Mass: 250.1569

[Characteristic components after acid treatment]

Irganox® 1076 phenolic antioxidant



$C_{35}H_{62}O_3$
Exact Mass: 530.4699

✓ Characteristically anionic surfactant and phenolic antioxidant decomposition products were detected in the gasket.
✓ After acid treatment, phenolic antioxidants of high molecular weight components were further extracted.

LESA nano ESI-MS can be used to rapidly characterize differences in solvent species, respective analyte regions, and eluted components with degradation.

Toray Research Center, Inc.