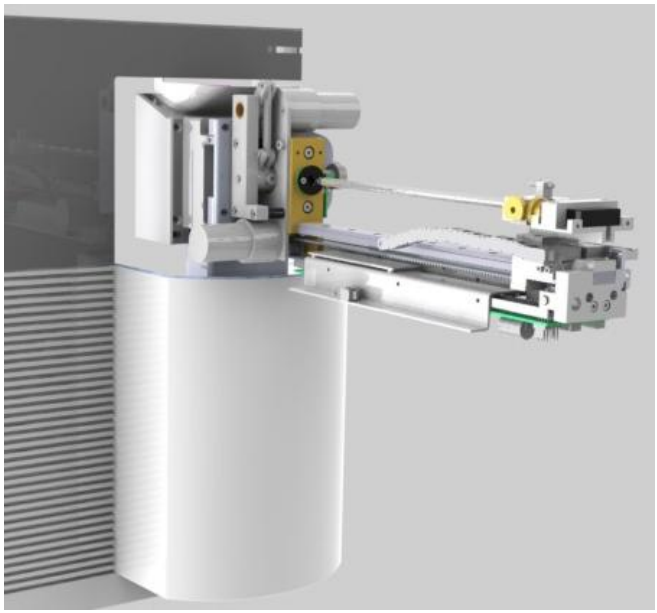
New: Agilent 7200 Series Q-TOF with DIP



➔ combines the advantage of the
Q-TOF System (highly accurate mass assignments)
with the benefit of the
DIP (fast screening method)

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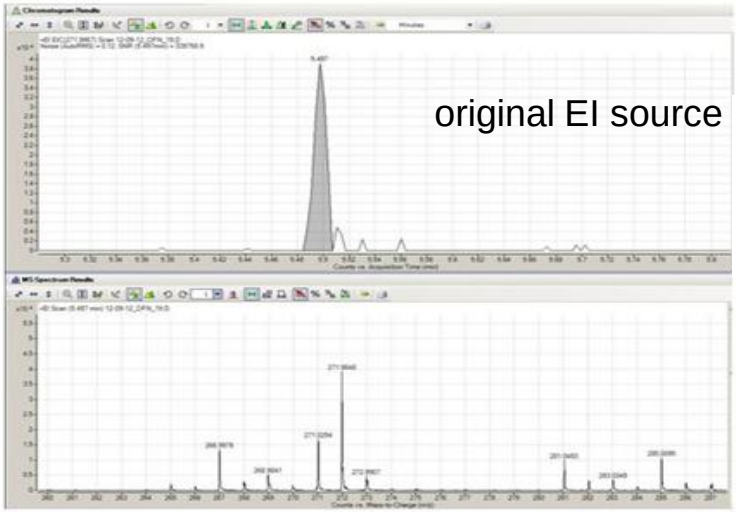
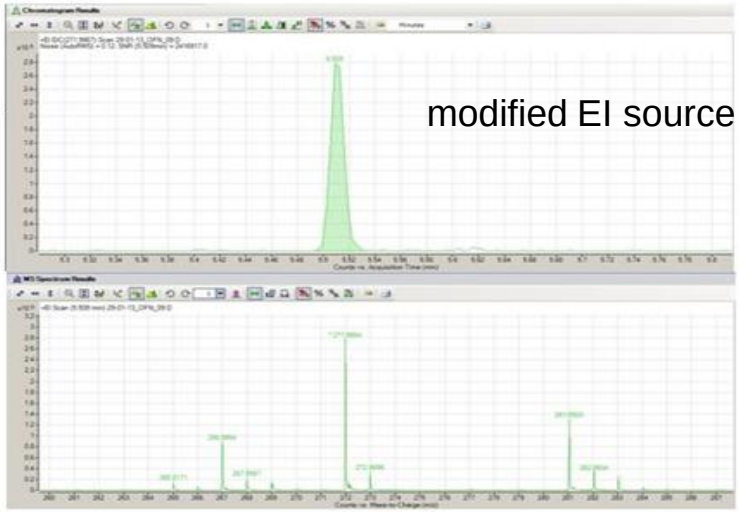
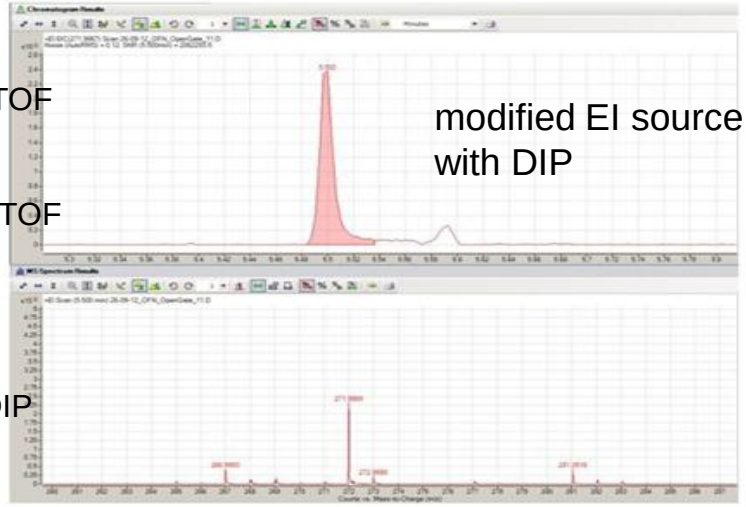
EI Specification:
Original EI Source vs. Modified EI Source







→Specification with original GC-Q-TOF
(1 pg OFN[1)], m/z 271.9867)

→ Specification with original GC-Q-TOF
and modified source
(1 pg OFN[1)], m/z 271.9867)

→Specification with GC-Q-TOF,
modified source ,open gate and DIP
(1 pg OFN[1)], m/z 271.9867)

[1)]OFN = Octofluornaphthalene

EI Specification Report with Modified EI Source and DIP

EI Installation Specification Report

Agilent Technologies

Integration Peak List

RT	Height	Area	SN
5.499	97200.74	71519.71	841783.1
5.499	84877.99	70742.04	735065
5.497	95908.27	70369.23	830590
5.498	100321.8	71062.79	868812.3
5.496	96396.2	75623.58	834815.5
5.496	89940.91	69772.4	778911.2
5.499	89469.49	71820.37	774828.5
5.496	93774.22	71970.23	812108.6
5.498	**93486**	**71610**	**868812.3**

Peak List

Name	m/z	Abund	Formula	Ion	Resolution	Mass Accura
	271.9873	96396.2			12971	2.21
	271.9866	95908.27			12790	0.37
	271.9869	100321.81			12851	0.74
	271.9857	89691.01			13053	3.68
	271.9862	97200.74			12635	1.84
					13053	**3.68**

Specifications	Results	Overall Status
Height RSD < 8%	5.39	PASSED
Area RSD < 8%	2.49	
MAX SN(AutoRMS) > 2000	868812	
Avg ABS Mass Accuracy(ppm) < 5@271.9867	3.68	
Mass Resolution > 12.5k@271.9867	13053	

t(p,N-1)	2.99800
Amount fg	1000.00
N	8.00
Confidence	0.99
IDL < 250 fg	74.66

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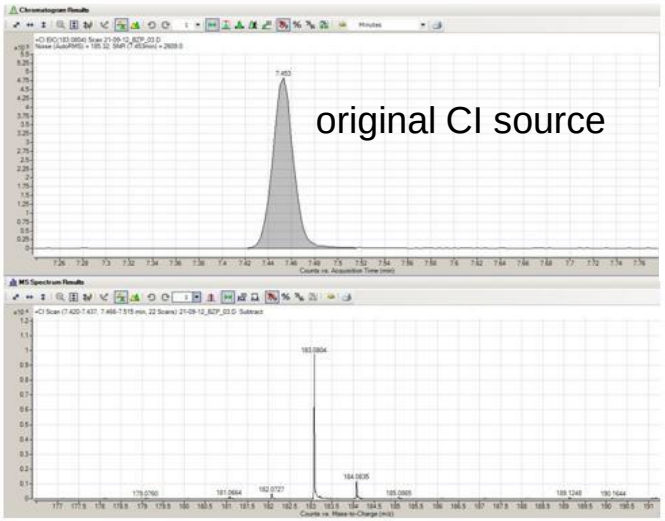
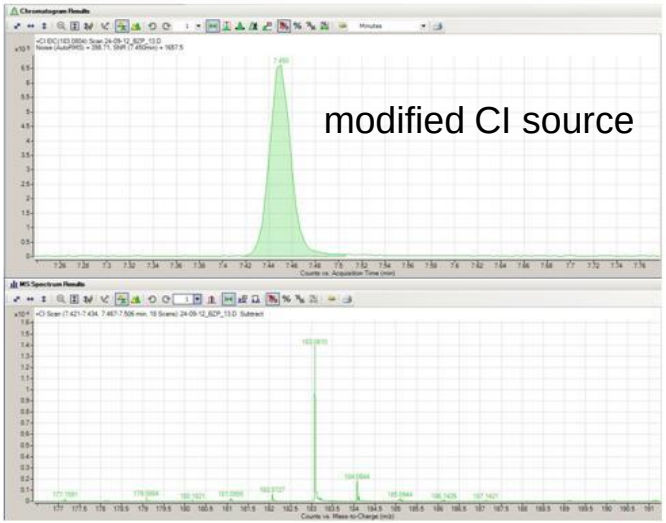
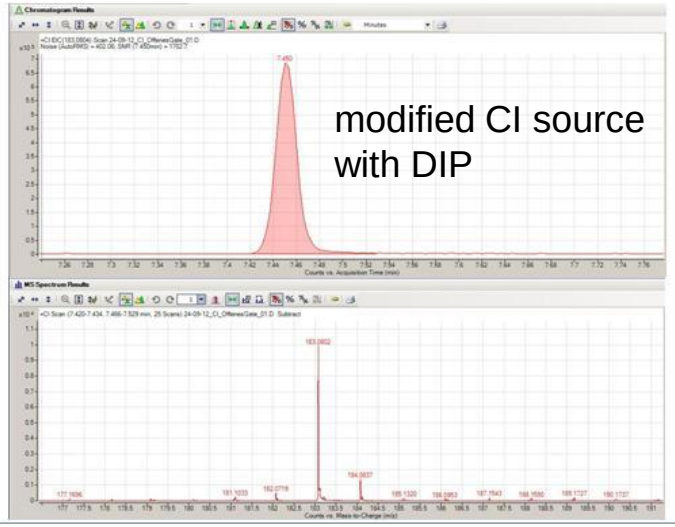
7200 Q-TOF: CI Specification: original CI source vs. modified CI source







→Specification with original GC-Q-TOF (100 pg BZP[2)], m/z 183.0804)

→ Specification with original GC-Q-TOF and modified source (100 pg BZP[2)], m/z 183.0804)

→Specification with GC-Q-TOF, modified source and open gate (100 pg BZP[2)], m/z 183.0804)

[2)] BZP = Benzophenone

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PCI Specification Report with modified CI source and DIP

PCI Installation Specification Report

Agilent Technologies

Integration Peak List

RT	Height	Area	SN
7.449	677905.38	873776.78	1551.4
7.447	653219.08	853866.23	1639.1
7.45	660845.69	856612.23	1657.5
7.448	645686.96	851918.78	1603
7.45	646338.92	846005.92	1546.3
7.449	**656799**	**856436**	**1657.5**

Peak List

Name	m/z	Abund	Formula	Ion	Resolution	Mass Accura
	183.0811	9970.59			11896	3.82
	183.081	10593.36			11486	3.28
	183.0809	7875.33			11596	2.73
	183.081	7935.55			11388	3.28
	183.081	13971.67			11796	3.28
					11896	2.73

Specifications	Overall Results
MAX SN(AutoRMS) > 1500	1658

New: LIFDI Liquid Injection Field Desorption ionisation

SOFT IONISATION FOR 7200 GC Q-TOF

Field Ionisation:
removal of electrons from any species by interaction with a high electrical field

➔ very soft ionisation technique

different sample supplies

	FI Field Ionisation	**FD** Field Desorption	**LIFDI** Liquid Injection FD ionisation
analyte	gaseous	dissolved solid	gaseous, liquid or dissolved solid
supplied to emitter	continuously via gas inlet/GC/DIP	discontinuously outside of the vacuum	discont. / continuously inside of the vacuum

SIM Scientific Instruments Manufacturer GmbH

Source:
Linden ChroMasSpec GmbH, Germany

ADVANTAGES OF LIFDI

Liquid Injection Field Desorption ionisation

- combines all feature of FI and FD but with higher sensitivity
- ionizes non-polar and polar as well as volatile – non volatile samples
- analyzes gaseous, liquid or dissolved solid analytes

➔ convenient, universal soft ionisation for difficult samples (e.g. metal complexes)

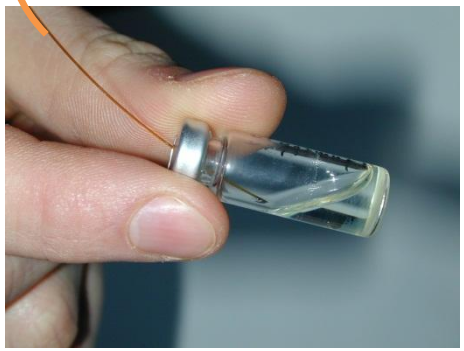
➔ main difference to FI/FD: sample supply under vacuum

SIM Scientific Instruments Manufacturer GmbH

Source:
Linden ChroMasSpec GmbH, Germany

LIFDI Sample Supply

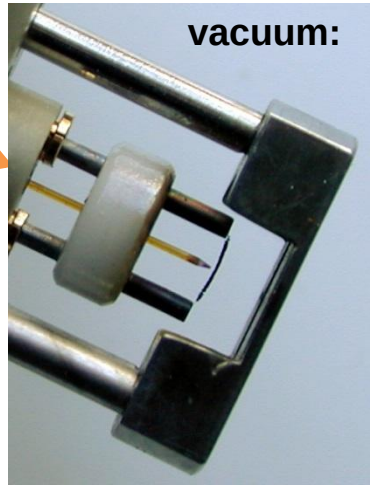
ambient pressure:



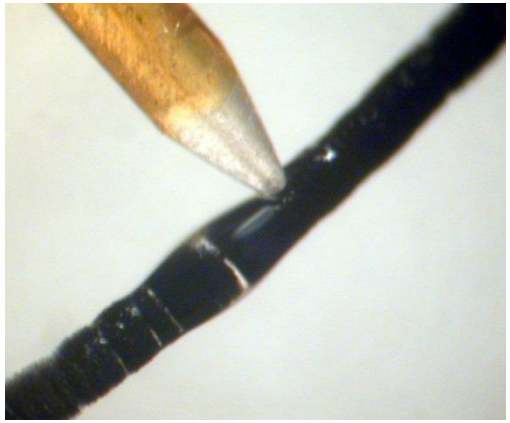
LIFDI
supplies analyte from the vial directly to the emitter in the ion source without breaking vacuum.

➔ sample has no contact with air
➔ convenient and fast
➔ analysis of air sensitive samples without experimental effort.

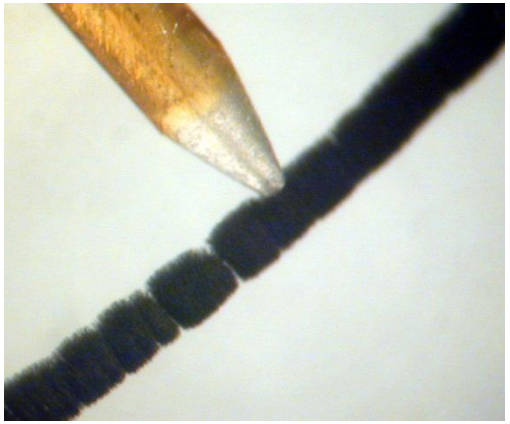
vacuum:



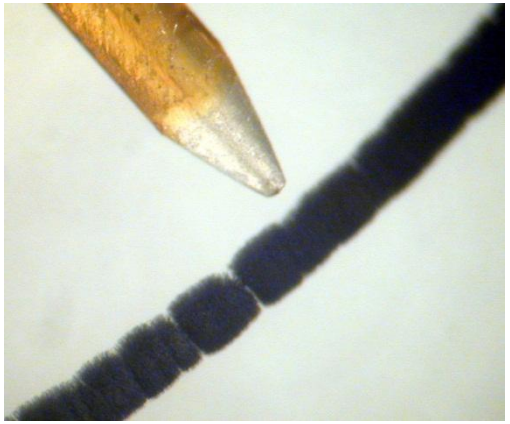
vacuum:



emitter wetted with sample solution



solvent evaporated

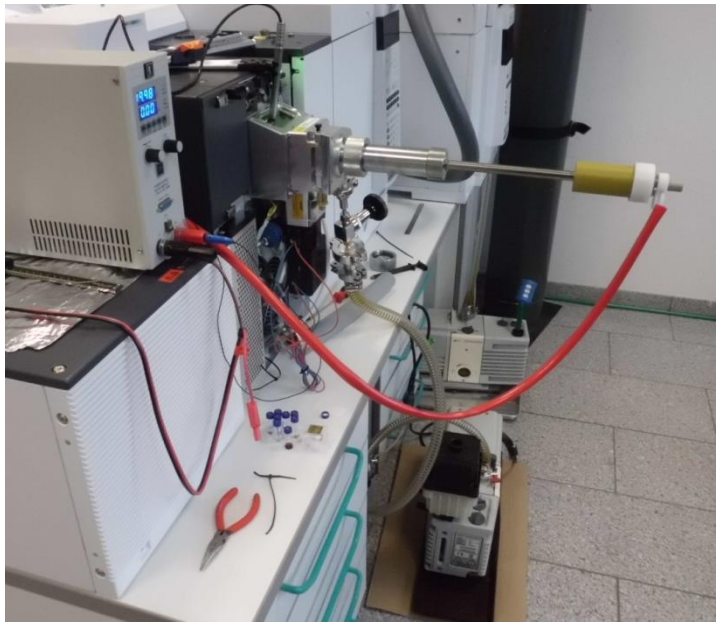


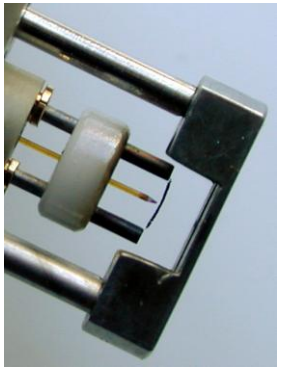
high voltage switched on

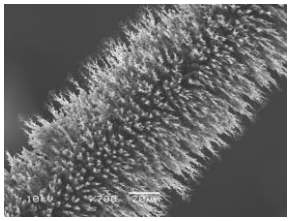
SIM Scientific Instruments Manufacturer GmbH

Source:
Linden ChroMasSpec GmbH, Germany

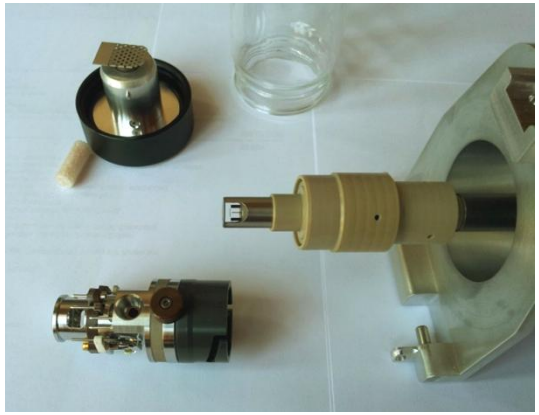
SIM Prototype: LIFD at Agilent GC-Q-TOF







LIFDI emitter:
tungsten wire with thousands of micro graphite dendrites
➔ large surface for adsorption of sample molecules



1. capillary aspirates sample solution (1-3 s)
2. 40 – 60 nL sample reach the emitter (10 s)
3. solvent evaporates (5 – 10 s)
4. high voltage on, emitter wire heated (to support diffusion to the wisker tips):
   emission of sample ions at the whisker tips
5. high voltage off:
   ready for the next sample

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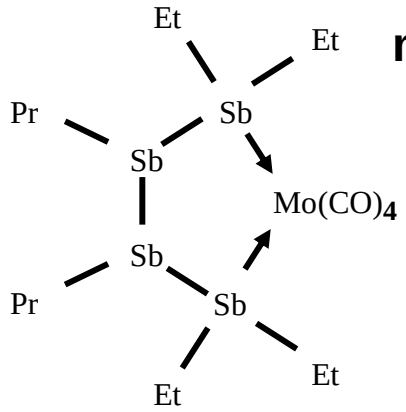
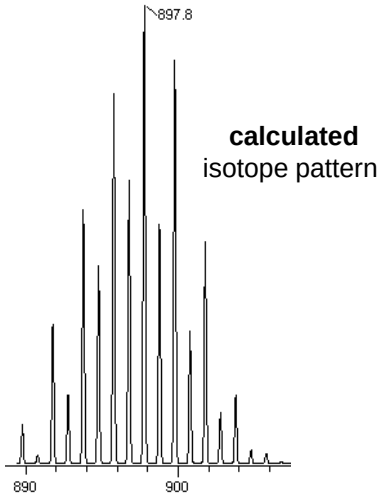
LIFDI: when all other techniques fail

$Mo(CO)_4(Sb_4Et_4Pr_2)$

formula and structure assumed by H.J. Breunig, University Bremen, Germany



m/z = 897,8



calculated isotope pattern

oily, very air sensitive sample:

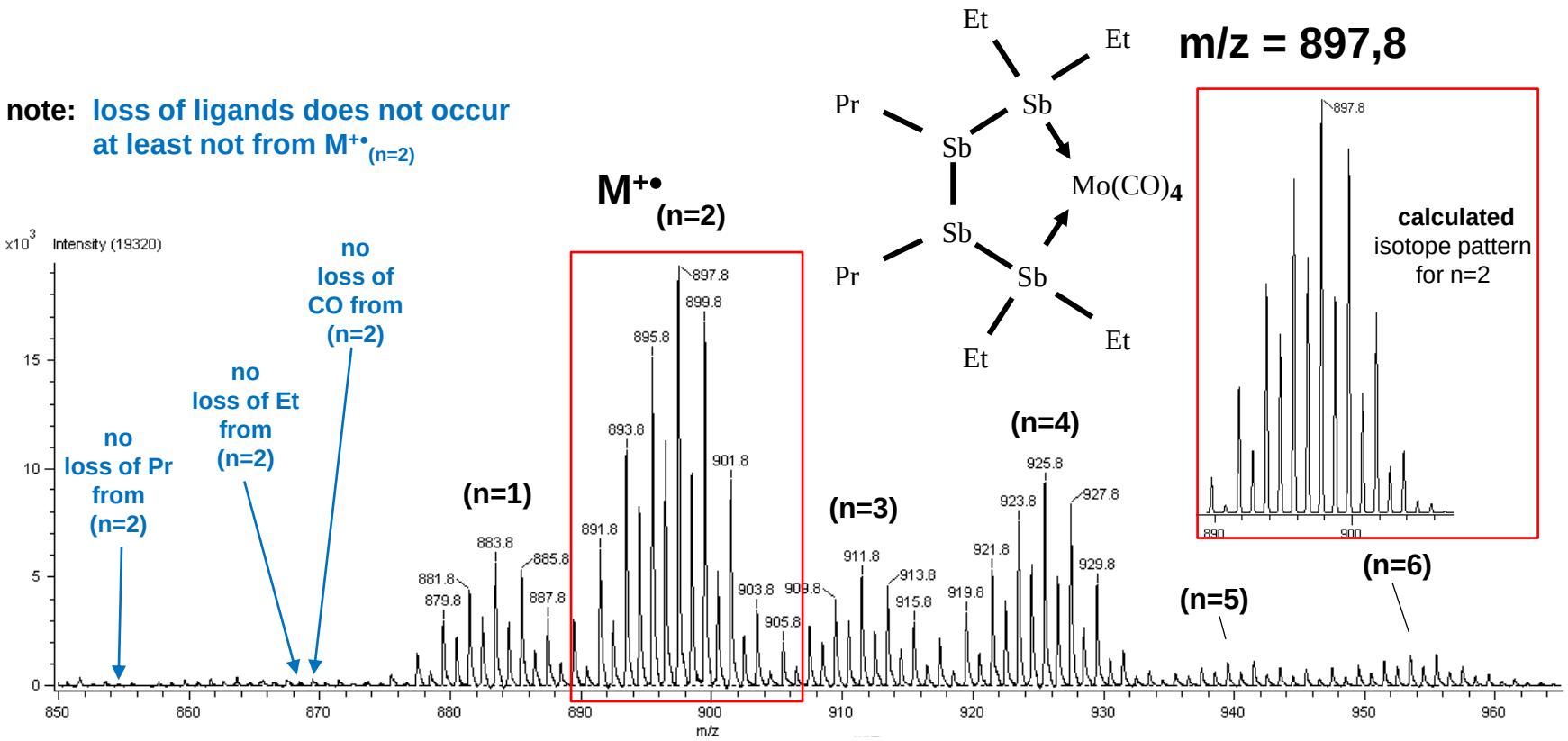
- decomposition upon **chromatography**
- no crystals for **X-ray** characterization
- ambiguous **NMR** data
- **elemental analysis** not confirming the MW
- **ESI** - ineffectual due to dry toluene as solvent
- **MALDI** - rather impossible under inert conditions

SIM Scientific Instruments Manufacturer GmbH

Source:
Linden ChroMasSpec GmbH, Germany

LIFDI revealed intact $Mo(CO)_4[(Sb_4Et_{(6-n)}Pr_n)]^{+\bullet}$ with scrambling alkyl ligands ($1 \leq n \leq 6$)

note: loss of ligands does not occur at least not from $M^{+\bullet}_{(n=2)}$

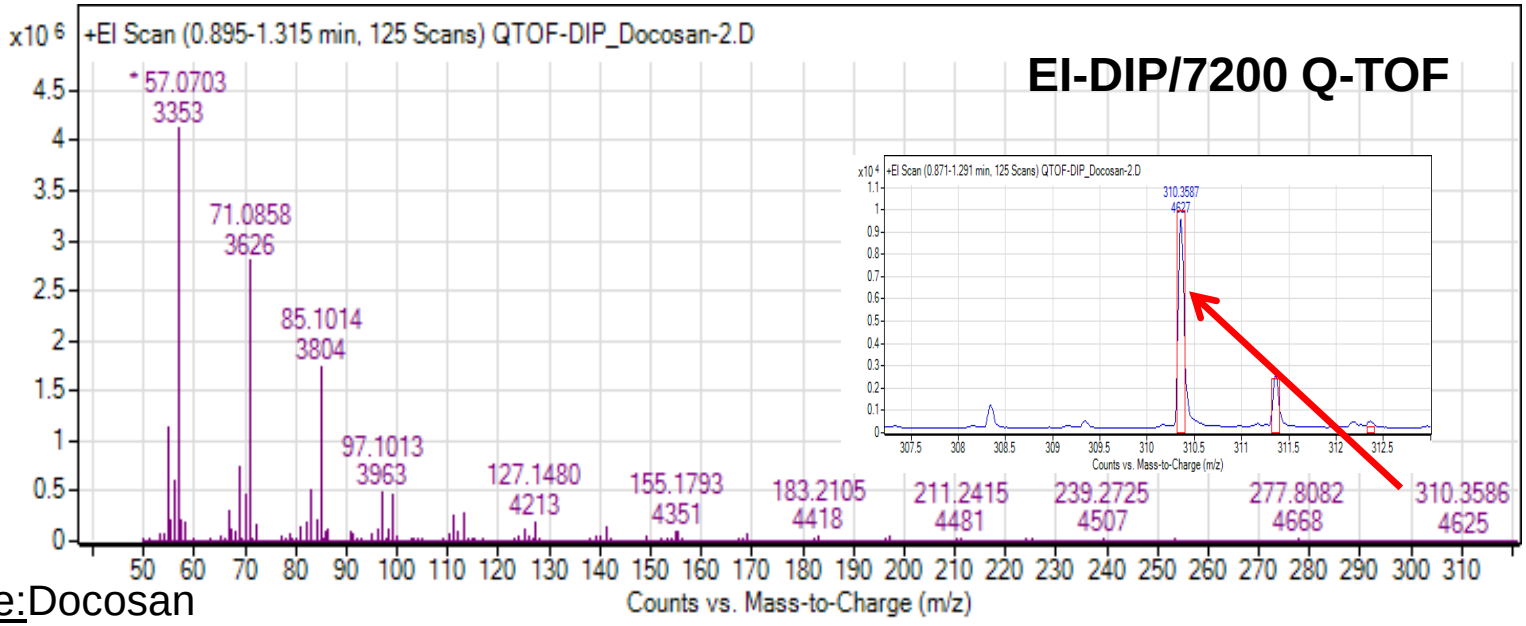


Liquid Injection Field Desorption Ionization Mass Spectrometry of Cyclic Metal Carbonyl Complexes with Tetra-Antimony Ligands, H. J. Breunig, H. B. Linden, O. Moldovan, *J. Am. Soc. Mass Spectrom.*, **2013**, 24, 164-166

SIM Scientific Instruments Manufacturer GmbH

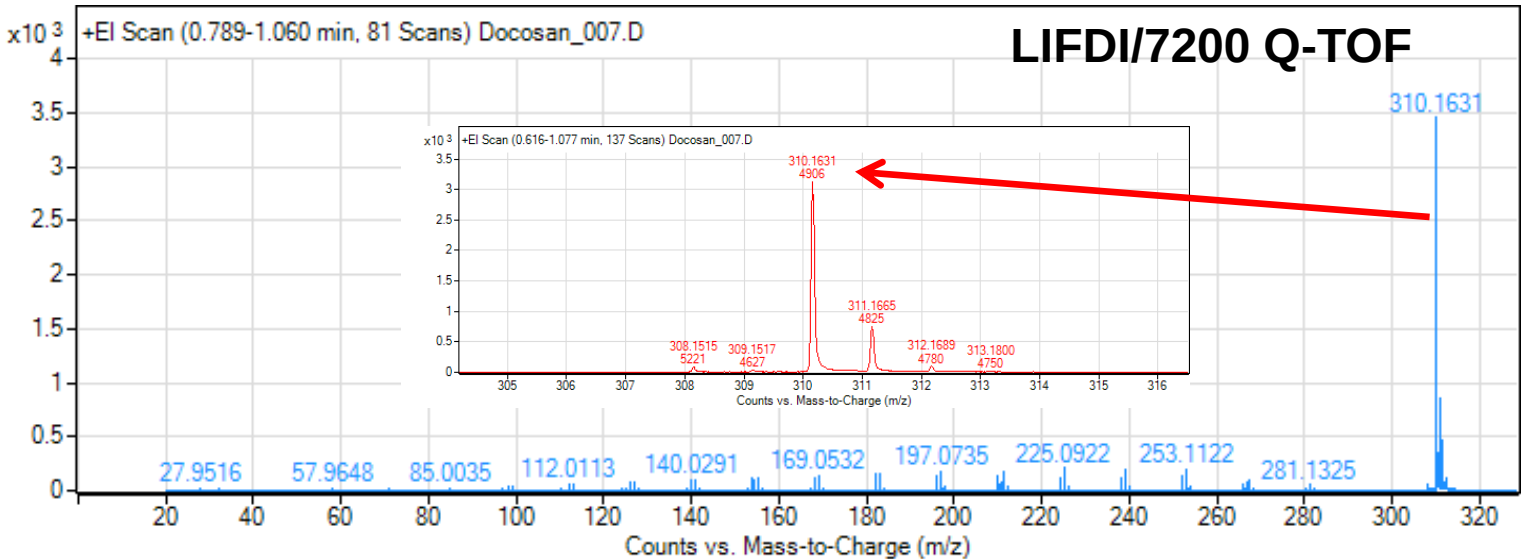
Source:
Linden ChroMasSpec GmbH, Germany

Comparison: EI-DIP and LIFDI with Agilent Q-TOF



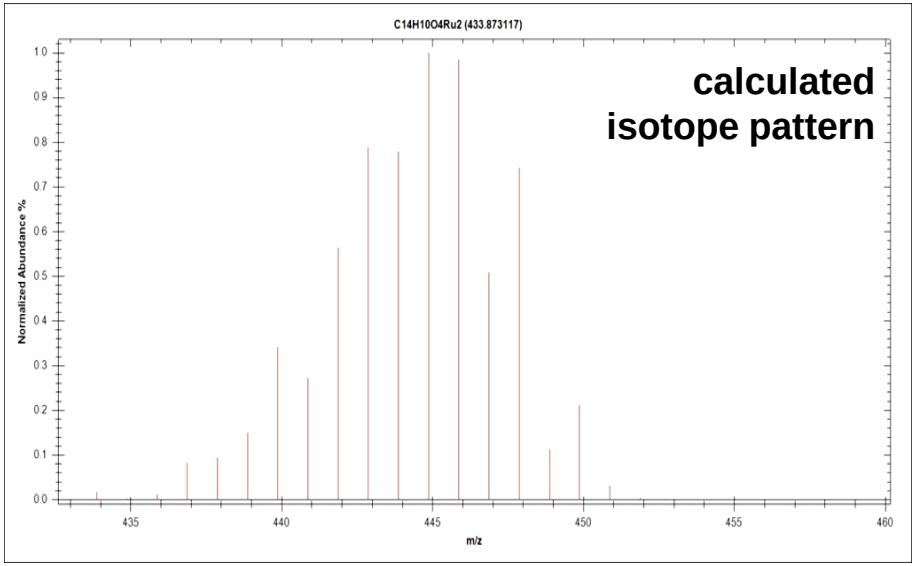
sample:Docosan ($C_{22}H_{46}$)
310.358 m/z
dissolved in hexane

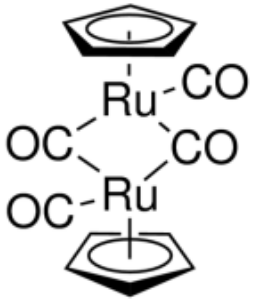
➔ LIFDI very soft ionisation, hardly any fragmentation!



SIM Scientific Instruments M

Cyclopentandienylruthenium-dicarbonyl-complex

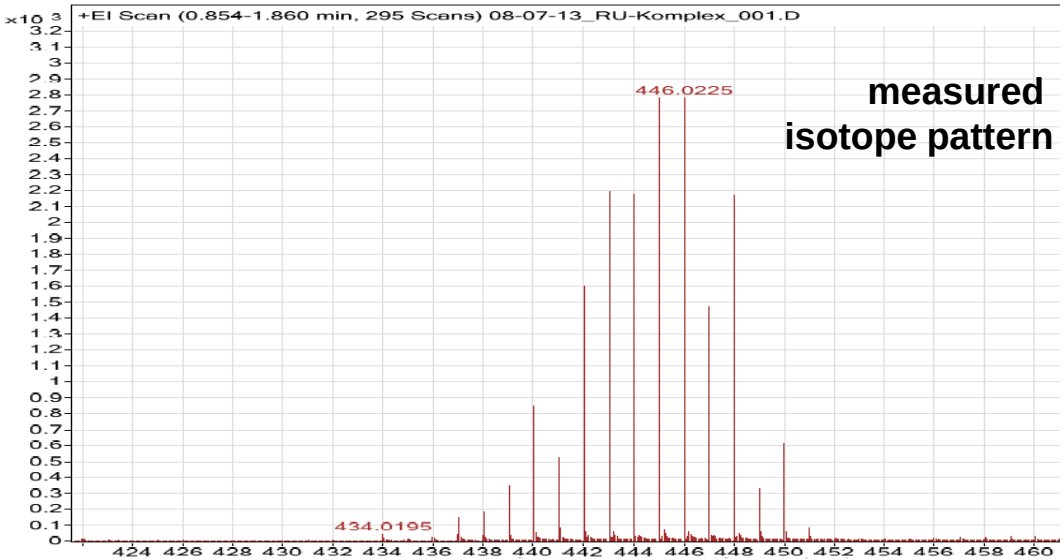




$[C_5H_6Ru(CO_2)]_2$

433.8731 m/z

LIFDI-7200 Q-TOF



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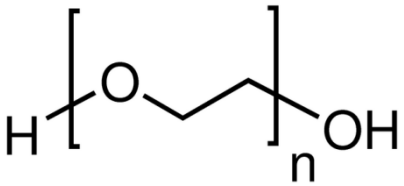
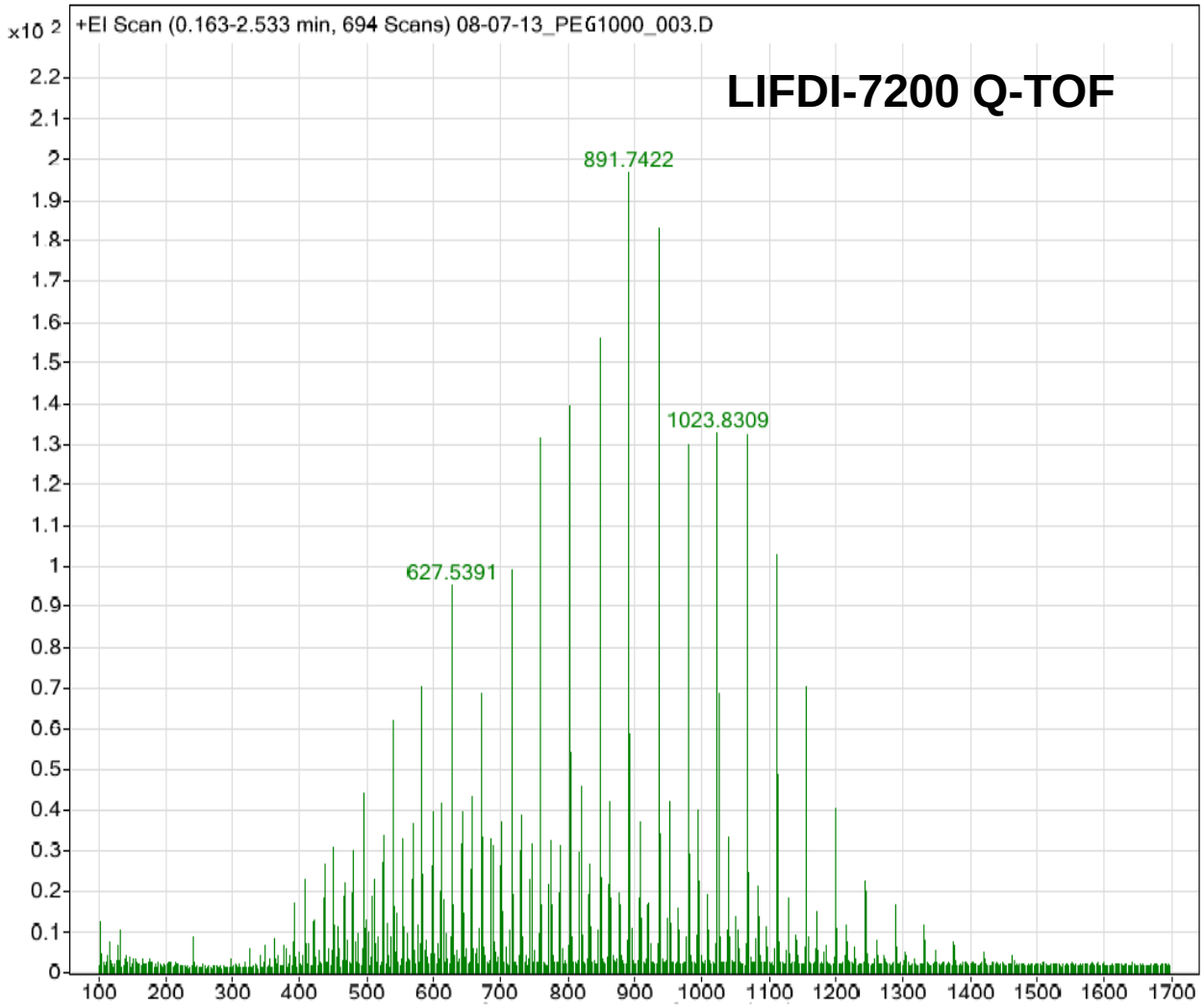
LIFDI – 7200 Q-TOF: PEG 1000

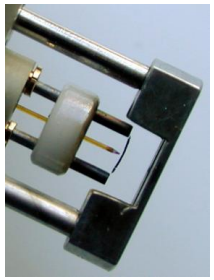


PEG 1000
m/z ~ 950 - 1050



4. SUMMARY




- **enhancement** of the MS application range:
  analysis of low volatile samples (liquid and solid)
  → MS + GC/MS or LC/MS, LIFDI/MS for soft ionisation
- **short analysis time** for mass spectra:
  ideal for high throughput quality control analysis (screening)
- **quick changeover** from GC/MS and LC/MS to DIP-MS:
  it is not necessary to uncouple the GC/MS interface
- **ease of use for DIP technique**:
  controlled sampling minimizes the change of accidental venting the MS
- **extensive data analysis**
  using the tools of MS ChemStation and MassHunter software
- **possibility of automation** and **online analysis** with PAL autosampler