“Biomics” –

Systems chemical analysis in the borderline between petroleomics and metabolomics

EU FT-ICR MS End User School
University of Lille, France
12–16.12.2022

Prof. Janne Jänis
University of Eastern Finland
Department of Chemistry

UNIVERSITY OF EASTERN FINLAND

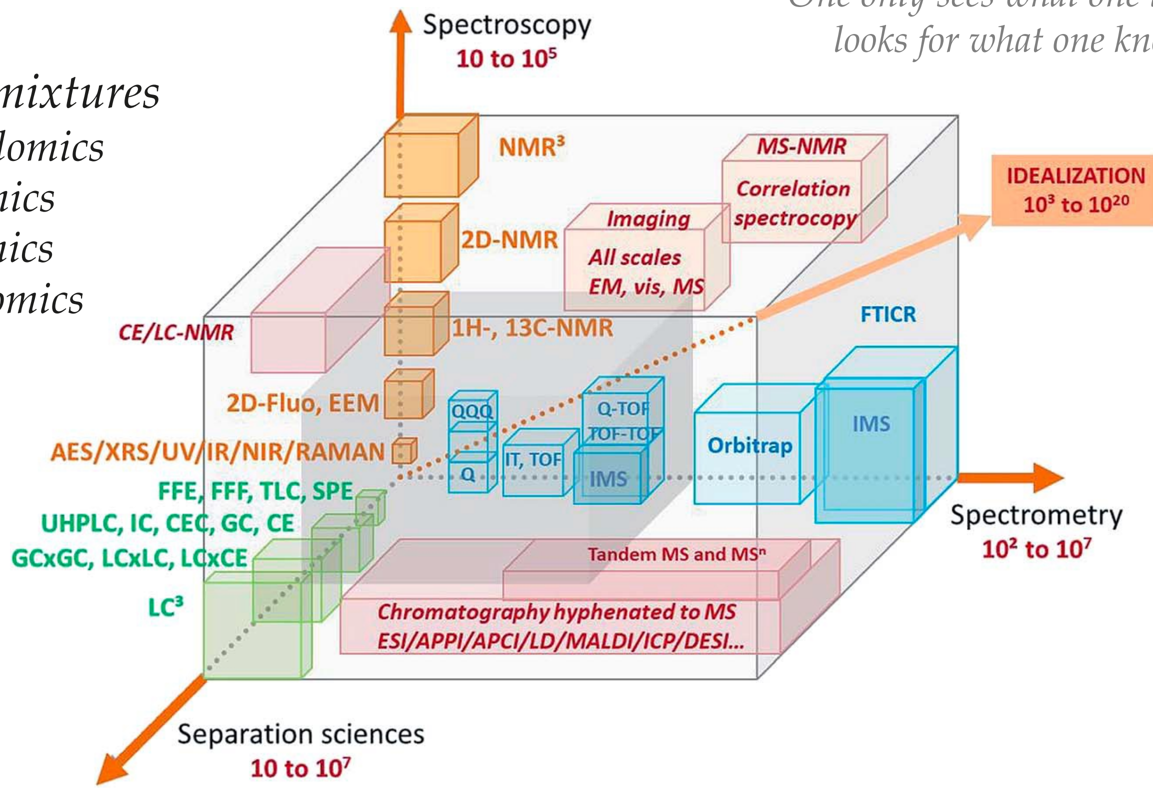
EU FT-ICR MS

Systems chemical analysis requires *orthogonal* analytical approaches

"One only sees what one looks for. One only looks for what one knows" (Goethe)

Complex mixtures

- *Metabolomics*
- *Proteomics*
- *Lipidomics*
- *Petroleomics*



Schmitt-Kopplin P, *et al. Faraday Discussions* **2019**, 218. doi: 10.1039/C9FD00078J.

Pushing the analytical limits with FT-ICR

Chemical Science

ROYAL SOCIETY OF CHEMISTRY

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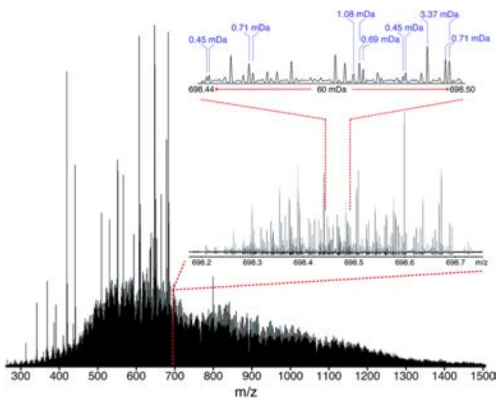
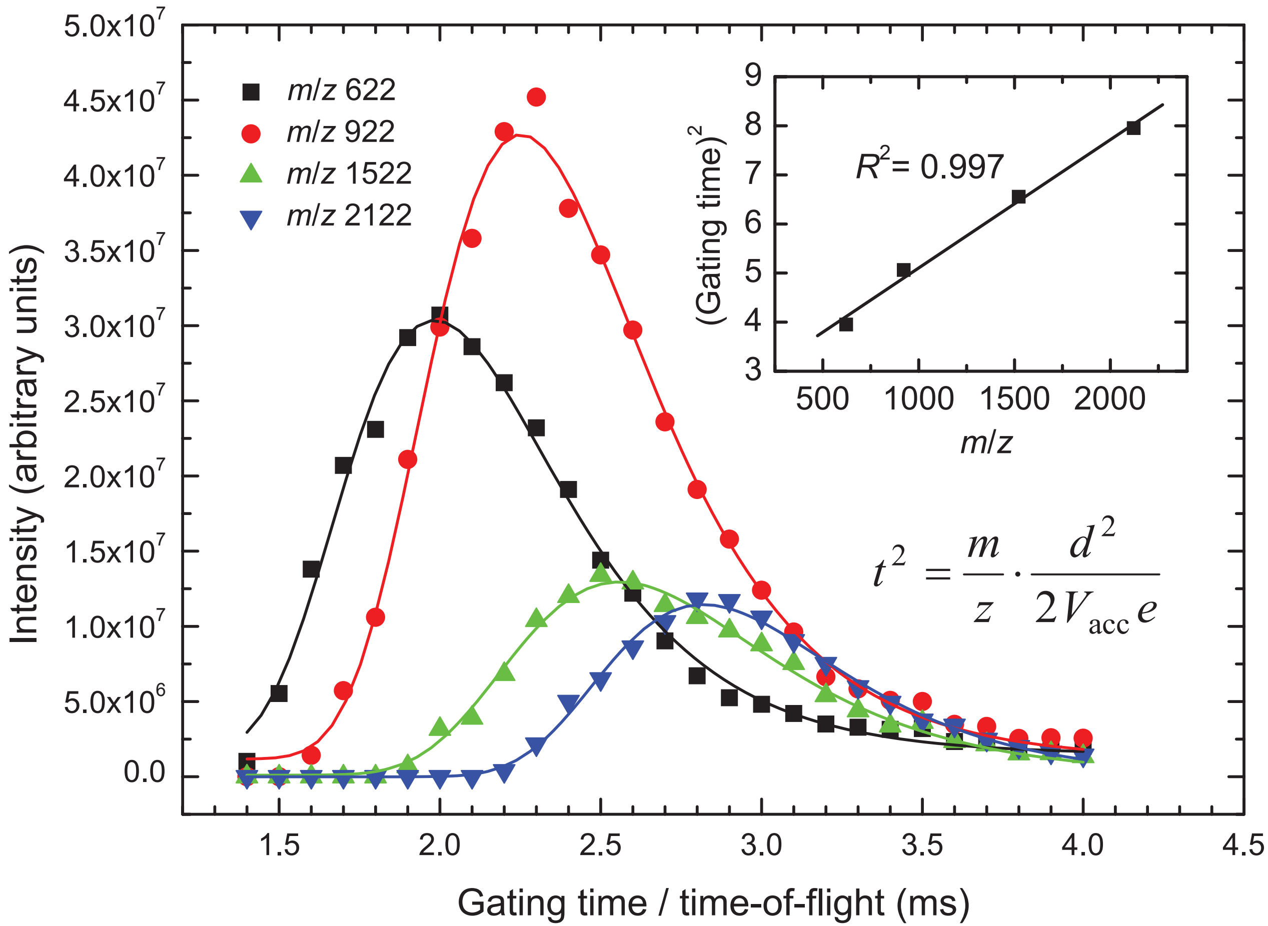
Pushing the analytical limits: new insights into complex mixtures using mass spectra segments of constant ultrahigh resolving power†

Diana Catalina Palacio Lozano,[ab] Remy Gavard,[c] Juan P. Arenas-Diaz,[b] Mary J. Thomas,[ac] David D. Stranz,[d] Enrique Mejía-Ospino,[b] Alexander Guzman,[e] Simon E. F. Spencer,[f] David Rossell[g] and Mark P. Barrow*[a]

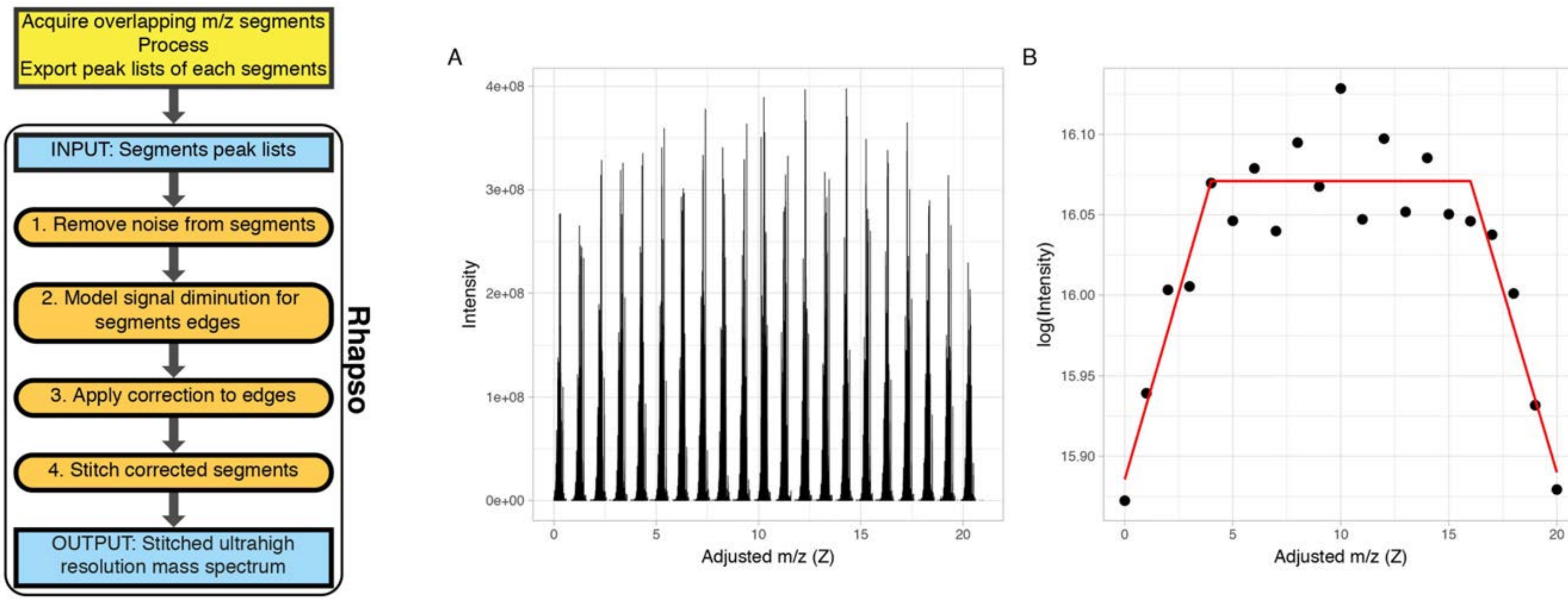


Average resolving power (*m*/*z* 260–1505)	3.12×10^6
Resolving power at *m*/*z* 400	3.07×10^6
Monoisotopic peaks assigned	106 871
Total peaks assigned	244 779
% Assigned	88.44%
RMS mass error for assigned peaks	0.11 ppm
Mean molecular weight	890.3 Da
Peaks with mass error ≤1 ppb	2305
Peaks with mass error ≤20 ppb	66 814
Peaks with mass error ≤50 ppb	122 911
Max. number of peaks assigned per Da	307

Time-of-flight effect in FT-ICR MS

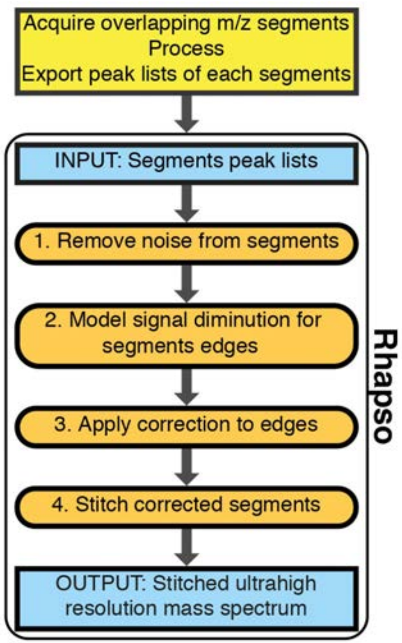


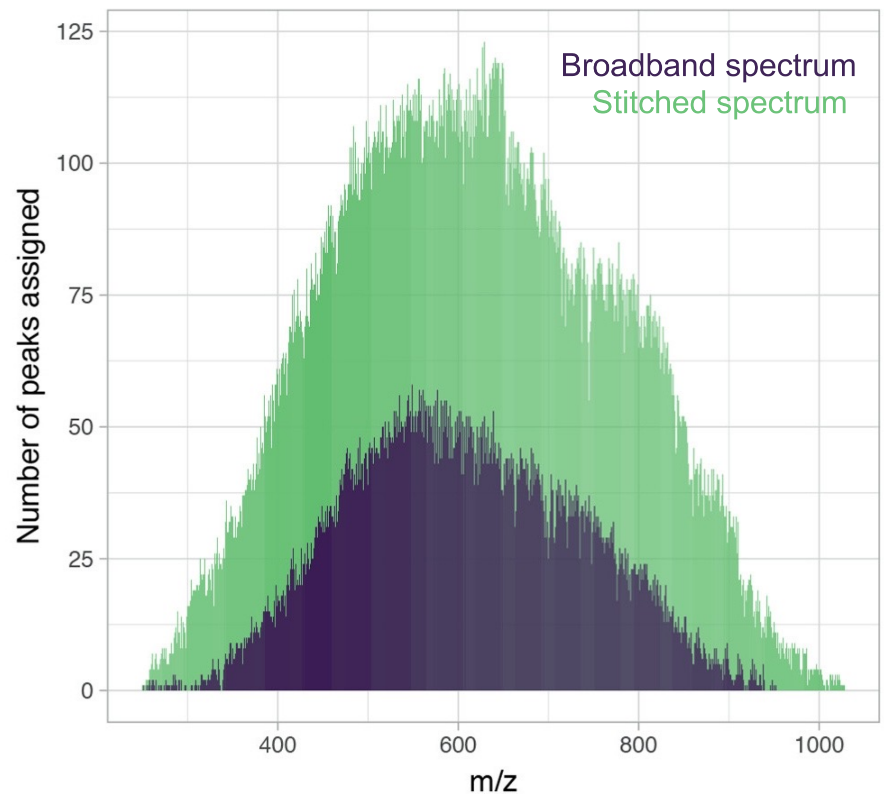
"Stitching" FT-ICR mass spectra to improve dynamic range, resolving power and mass range



Gavard R *et al. Anal. Chem.* **2019**, 91, 23, 15130–15137

”Stitching” FT-ICR mass spectra to improve dynamic range, resolving power and mass range



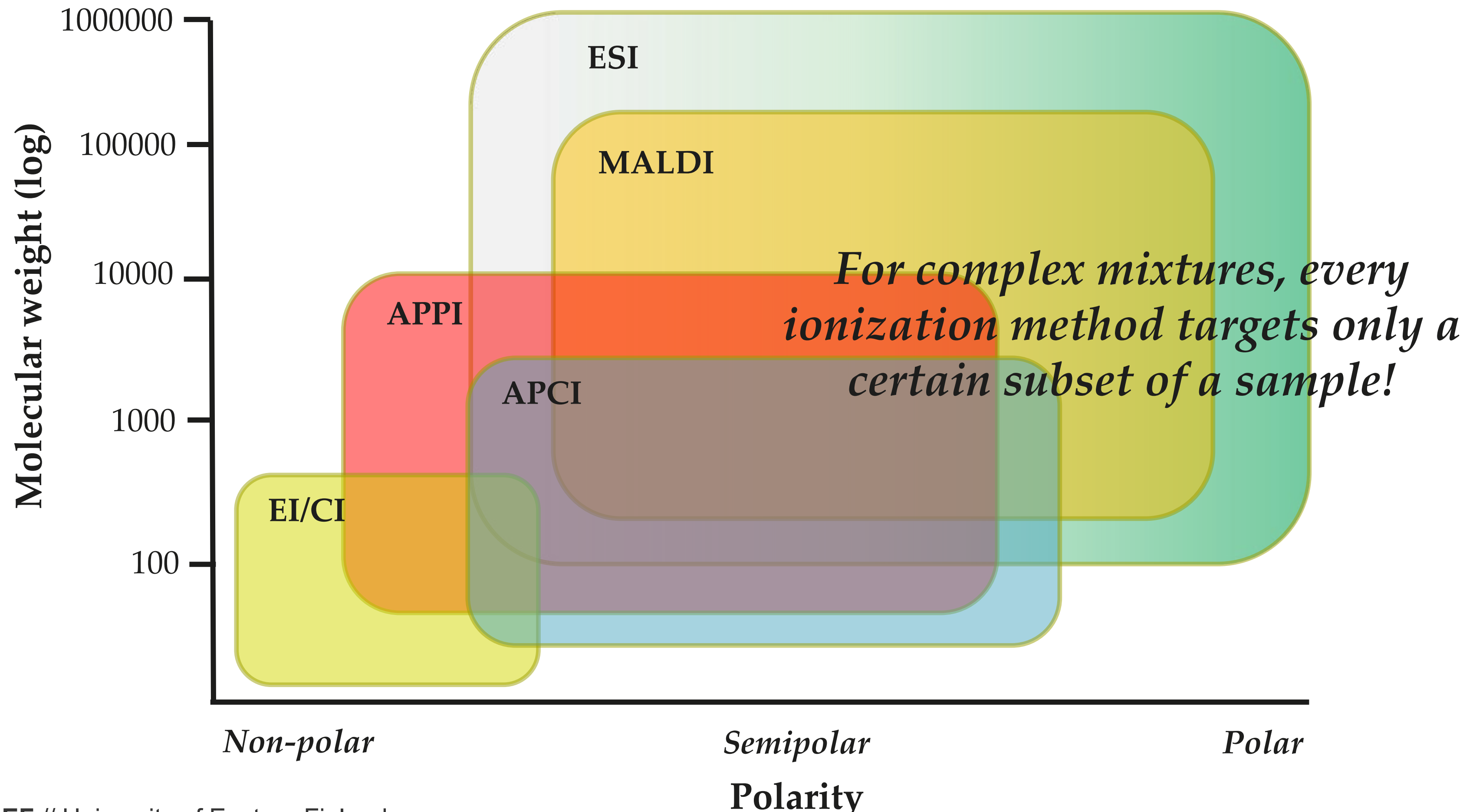


Gavard R *et al. Anal. Chem.* **2019**, 91, 23, 15130–15137

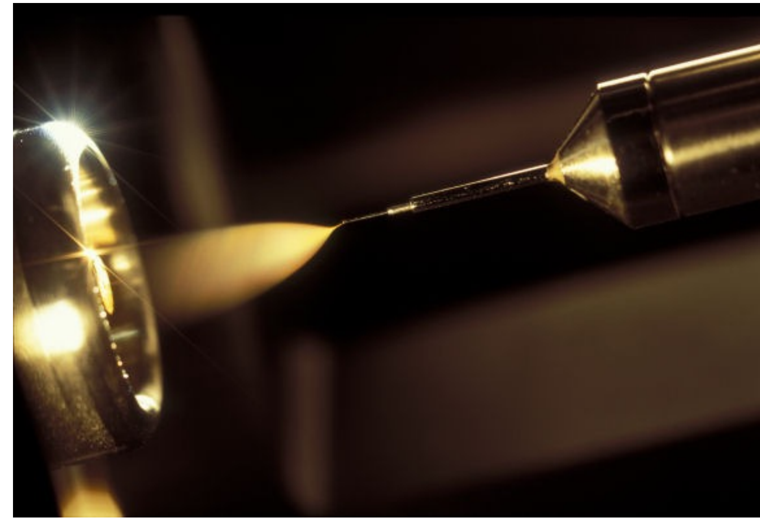
Vacuum and atmospheric pressure ionization

- Electron ionization (EI)
- Chemical ionization (CI)
- Field desorption/field ionization (FD/FI)
- (Direct) photoionization (PI)
- Atmospheric pressure chemical ionization (APCI)
- **Atmospheric pressure photoionization (APPI)**
- Atmospheric pressure laser ionization (APLI)
- **Electrospray ionization (ESI)**
- Desorption electrospray ionization (DESI)
- Laser ablation ionization (LA-ESI, LA-APPI)
- Laser desorption ionization (LDI)
- Matrix-assisted laser desorption ionization (MALDI)

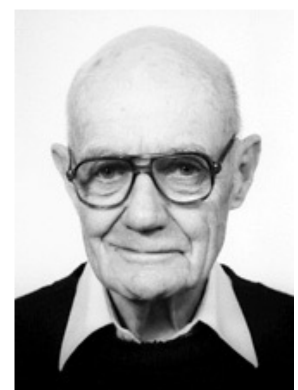
Which ionization method for my complex mixture?



Electrospray ionization (ESI)

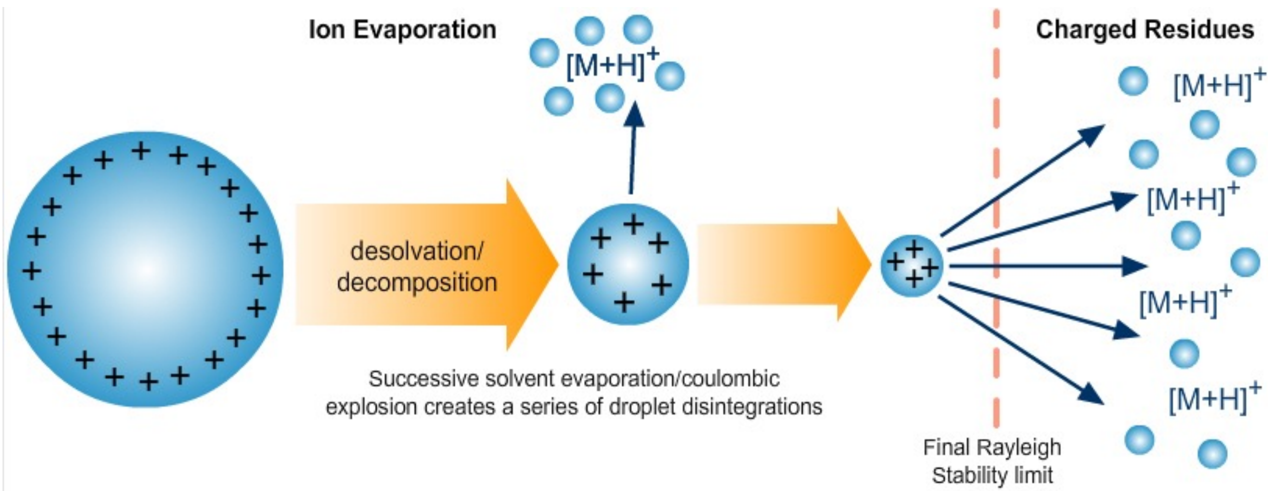


- Ions directly from solution (ambient ionization)
  - Polar or semipolar molecules
  - Nonpolar molecules in some cases (PAHs, fullerenes…)
  - ”Soft” ionization technique; no fragmentation
  - Multiply-charged ions
  - Weak and thermolabile analytes
  - Hyphenation with LC or CE
  - John. B. Fenn – *2002 Chemistry Nobel*



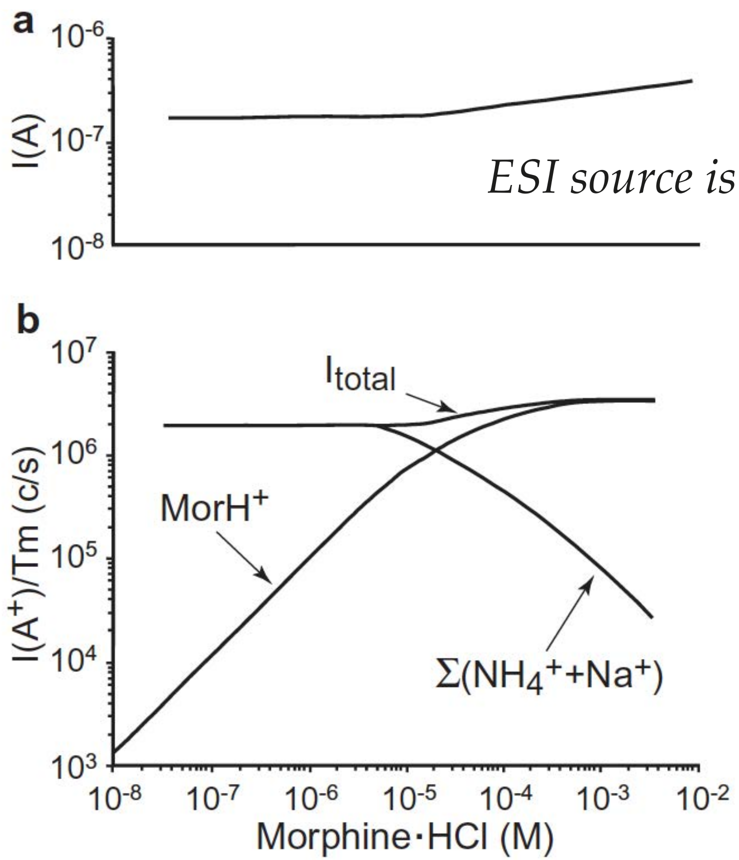
Electrospray ionization (ESI)

- Complicated, multi-phased process
  - A droplet srinkage by evaporation, until the electric field exceeds surface tension (a *Rayleigh limit*); $q^2 \leq 8\pi^2 \varepsilon_0 \gamma R^3$, q = droplet charge, ε_0 = solvent permittivity, γ = surface tension, R = droplet radius



Kebarle P & Verkerk UH, *Mass Spectrom. Rev.* **2009**, 28: 898–917.

Electrospray ionization (ESI)



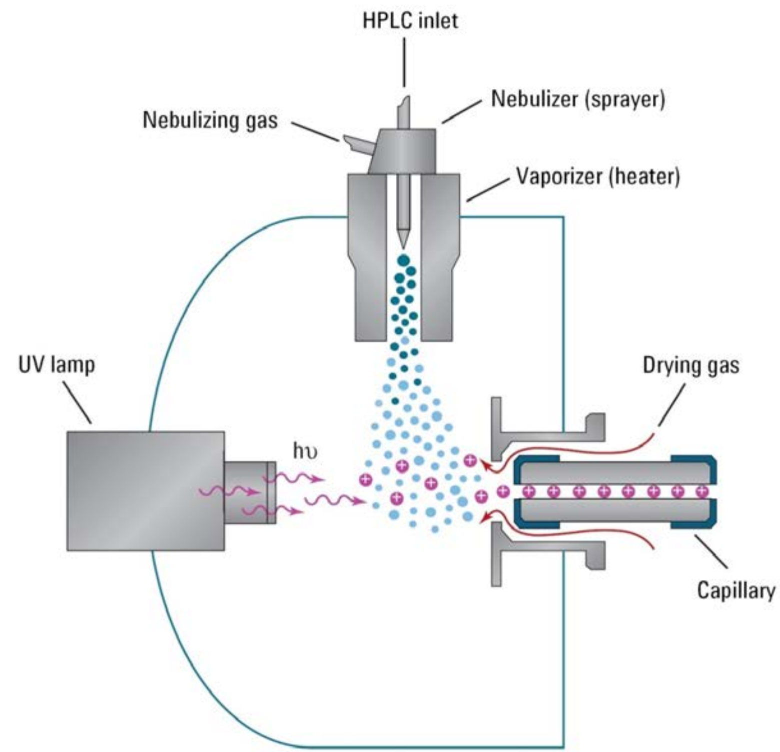
ESI source is a controlled current device!

Total ion current for morphine $[M + H]^+$ ion in the presence of 10 μM salt impurities (Na^+, NH_4^+)

Kebarle P & Verkerk UH, *Mass Spectrom. Rev.* **2009**, 28: 898–917.

Atmospheric pressure photoionization (APPI)

- Ambient pressure ionization technique
  - Ionzation by interaction of photons (*hv*) and molecules
  - Addition of volatile organic compound (dopant) to the eluent (e.g., toluene) to enhance ionization
  - Typical ions: $M^{+\bullet}$, $M^{-\bullet}$ $[M + H]^{+}$ or $[M - H]^{-}$, depending on the compound's *IE*- and *PA*-values
  - Less matrix/ion suppression effects than with ESI; more "quantitative"
  - For ionization of nonpolar, small to medium MW compounds – LC & GC!



Atmospheric pressure photoionization (APPI)

- Typical ionization reactions in positive-ion APPI are:

$$D + h\nu\ (10\ \text{eV}) \rightarrow D^{+\bullet} + e^{-}$$

$$D^{+\bullet} + S \rightarrow [D - H]^{\bullet} + [S + H]^{+},\ \text{if } PA(S) > PA([D - H]^{\bullet})$$

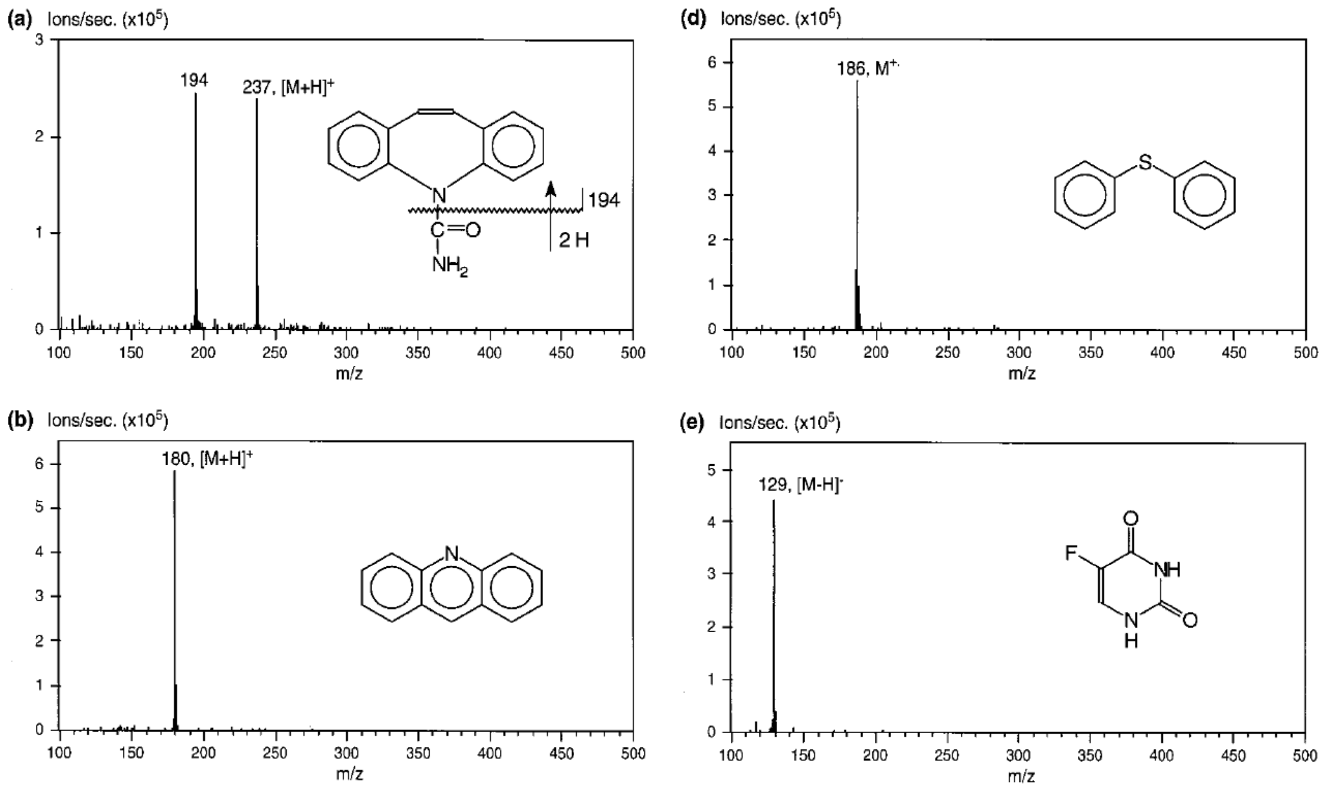
$$\text{Proton transfer: } M + [S + H]^{+} \rightarrow [M + H]^{+} + S,\ \text{if } PA(M) > PA(S),$$

$$\text{Charge exchange: } M + D^{+\bullet} \rightarrow M^{+\bullet} + D,\ \text{if } IE(M) > IE(D)$$

where D = dopand molecule, S = solvent molecule and M = analyte molecule

- In case of negative-ion APPI, ionization by oxygen radical anion ($O^{2-\bullet}$)

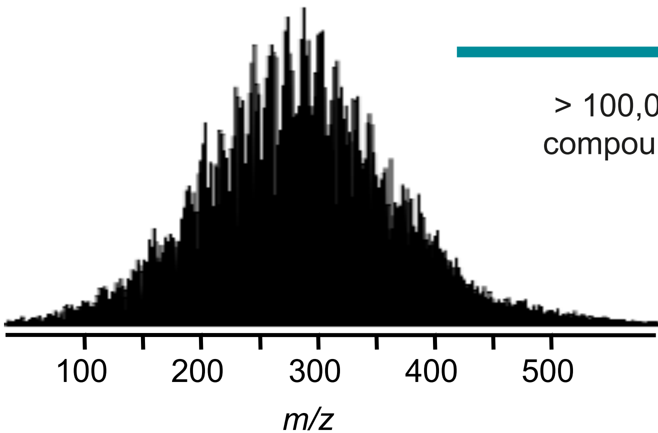
Atmospheric pressure photoionization (APPI)



Carbamazepine, diphenylsulphide, acridine, 5-fluorouracil

Workflow for complex mixture analysis with DI-HRMS

Resolution (FWHM) > 1,000,000



> 100,000 compounds

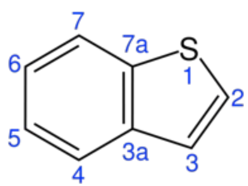
134.019022 Da

Mass measurement accuracy: 10-100 ppb

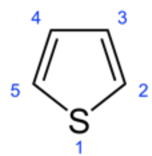
Compass. BRUKER

PETRO ORG

$[C_8H_6S_1 + H]^+$



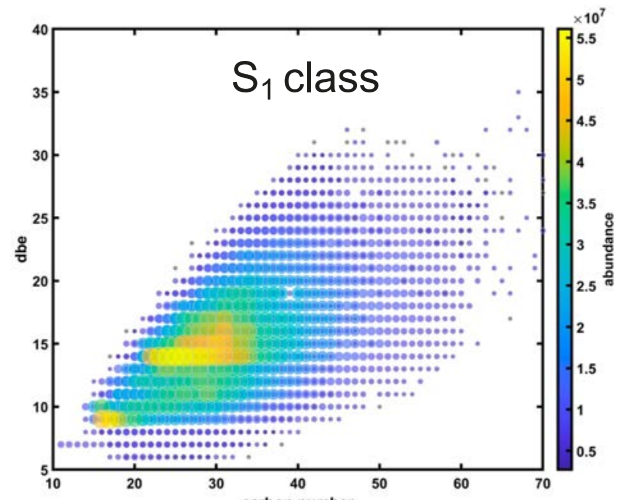
$C_8H_6S_1$, DBE = 6
134.019022 Da



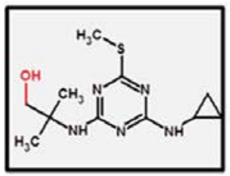
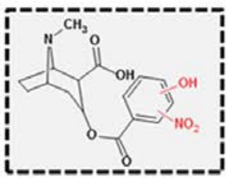
$C_4H_4S_1$, DBE = 3
84.003372 Da

Database search, e.g.

ChemSpider



Confidence levels for compound identification in metabolomics

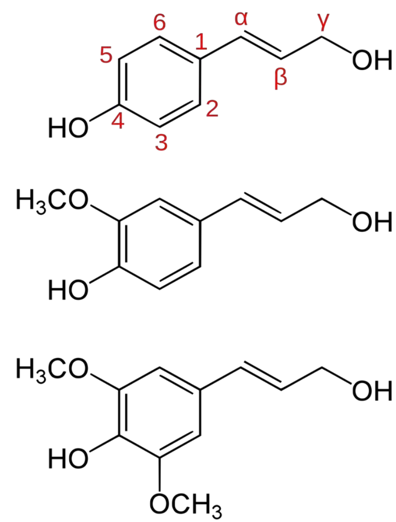
Example	*Identification confidence*	*Minimum data requirements*
	***Level 1: Confirmed structure*** by reference standard	MS, MS^2, RT, Reference Std.
	Level 2: Probable structure a) by library spectrum match; b) by diagnostic evidence	MS, MS^2, Library MS^2; MS, MS^2, Exp. data
	***Level 3: Tentative candidate(s)*** structure, substituent, class	MS, MS^2, Exp. data
$C_6H_5N_3O_4$	***Level 4: Unequivocal molecular formula***	MS isotope/adduct
192.0757	***Level 5: Exact mass*** of interest	MS

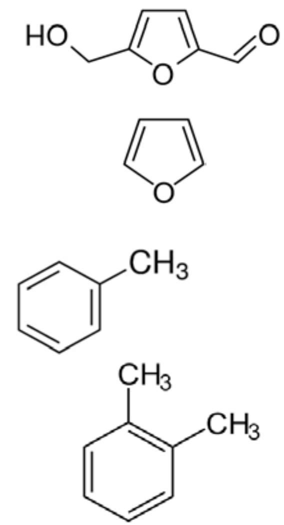
Schymanski *et al. Environ. Sci. Technol.* **2014**, 48, 4, 2097–2098

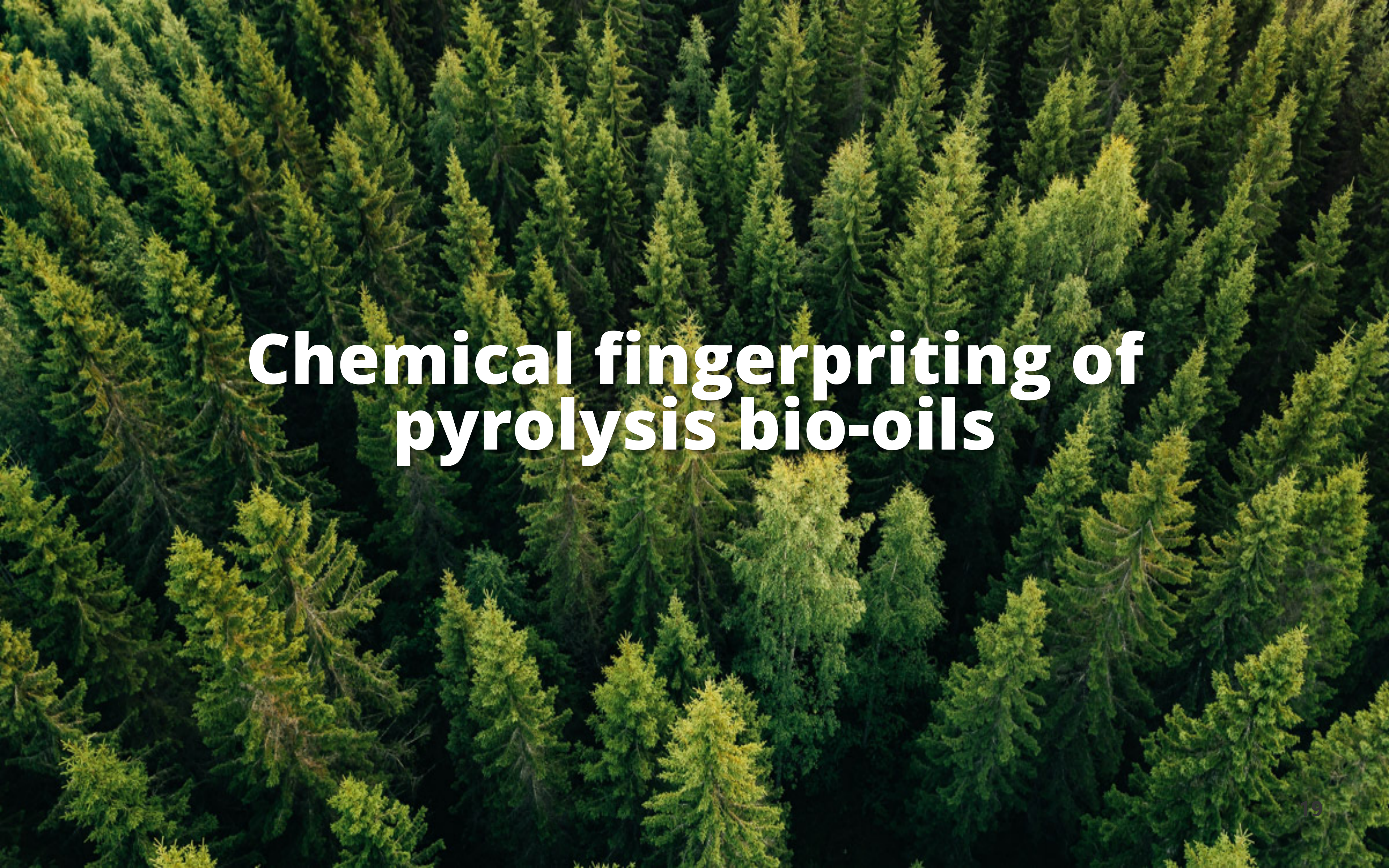
Green transition in industry – get rid of fossils!

- Better utilization of waste and side streams
- Finding substitutes for fossil resources
- Green transition in industry
- Novel materials – new openings

1
2
3

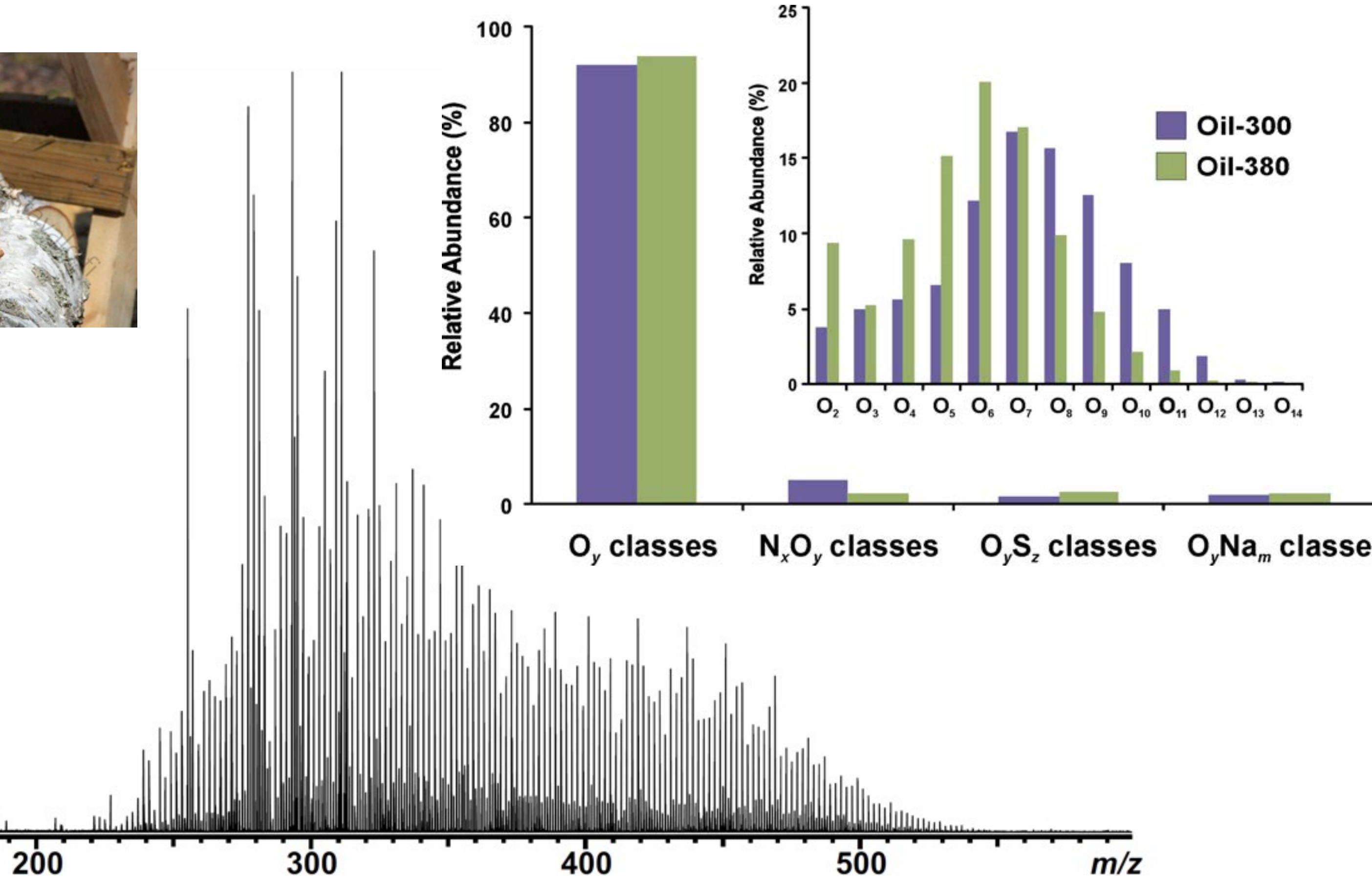






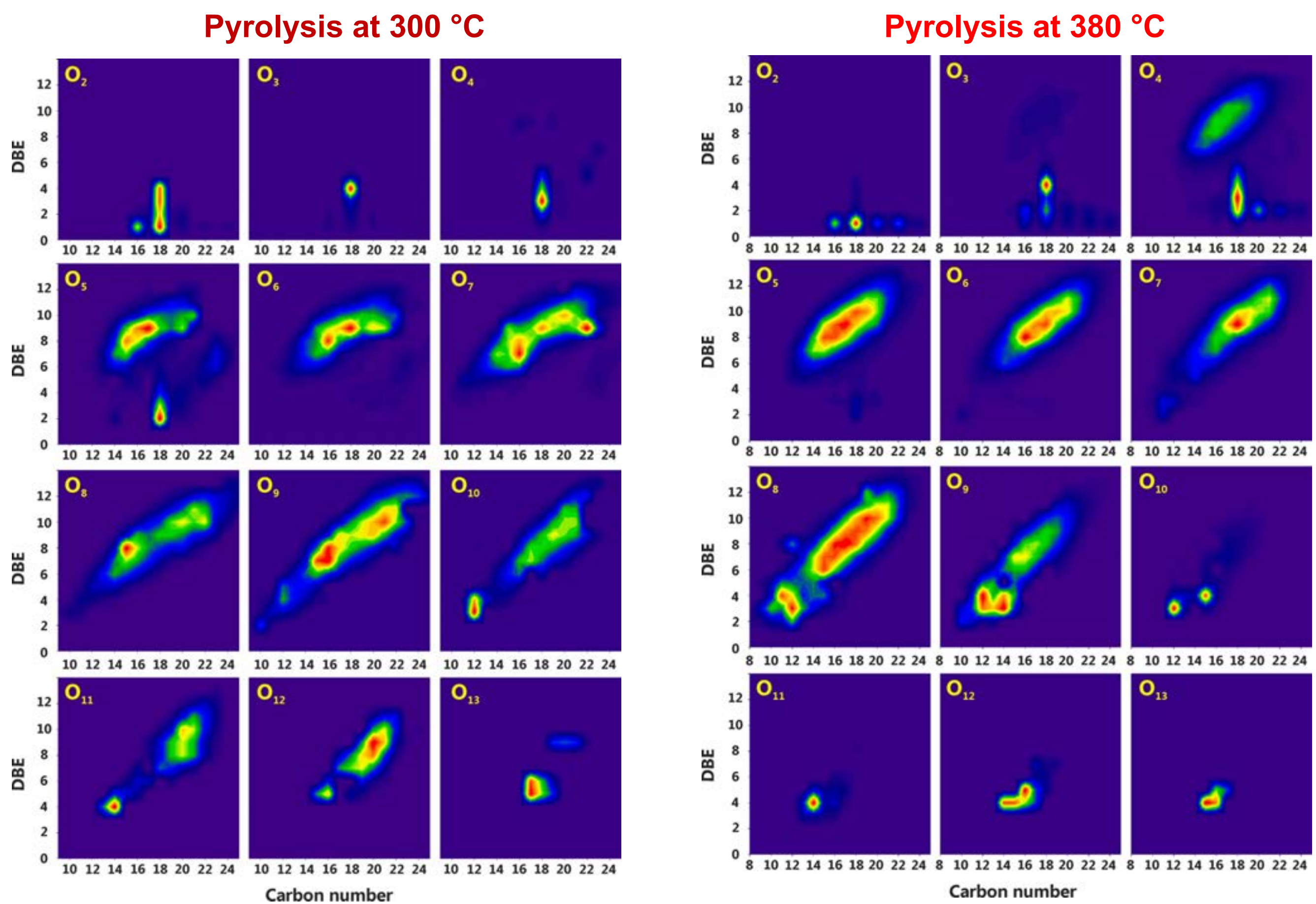
Chemical fingerpriting of pyrolysis bio-oils

HRMS analysis of birch wood fast pyrolysis oil



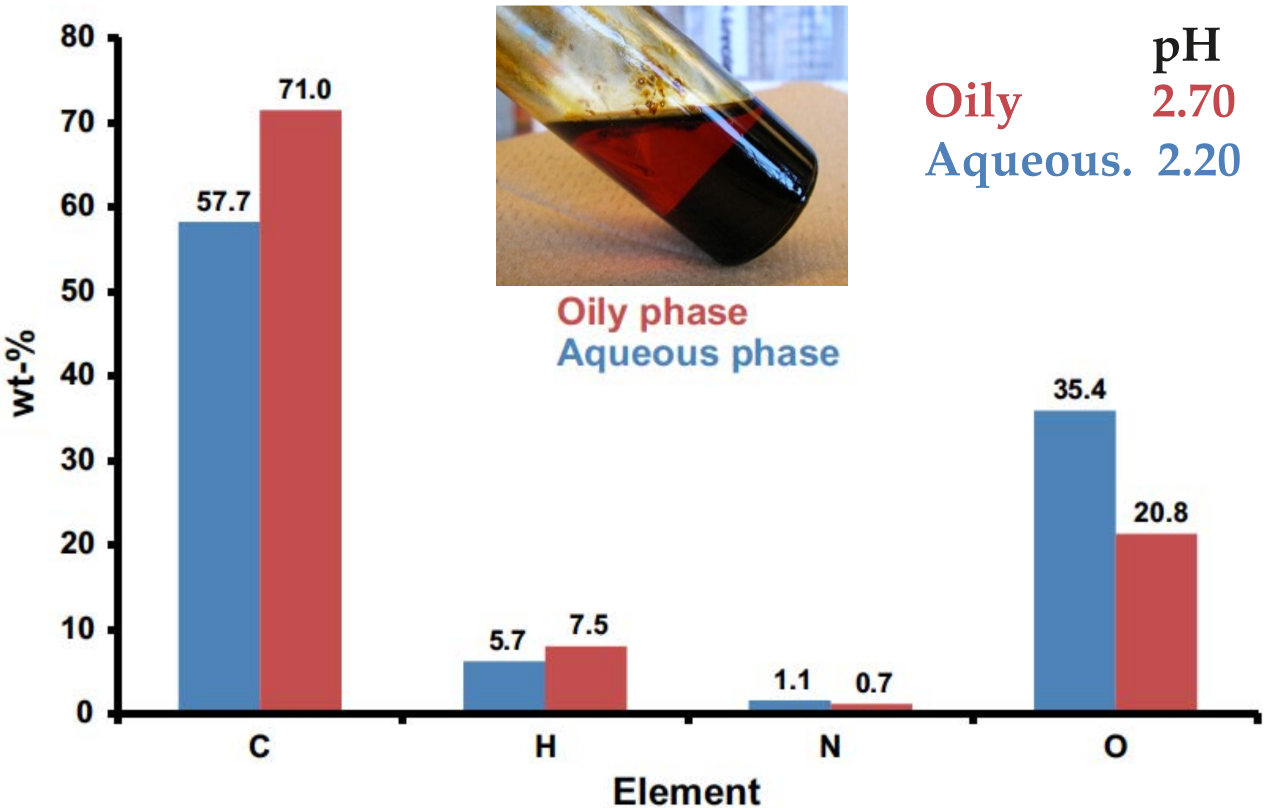
Kekäläinen, T.; Venäläinen, T.; Jänis, J. *ACS Energy & Fuels*, **2014**, 28, 4596.

HRMS analysis of birch wood fast pyrolysis oil



Kekäläinen, T.; Venäläinen, T.; Jänis, J. *ACS Energy & Fuels*, **2014**, 28, 4596.

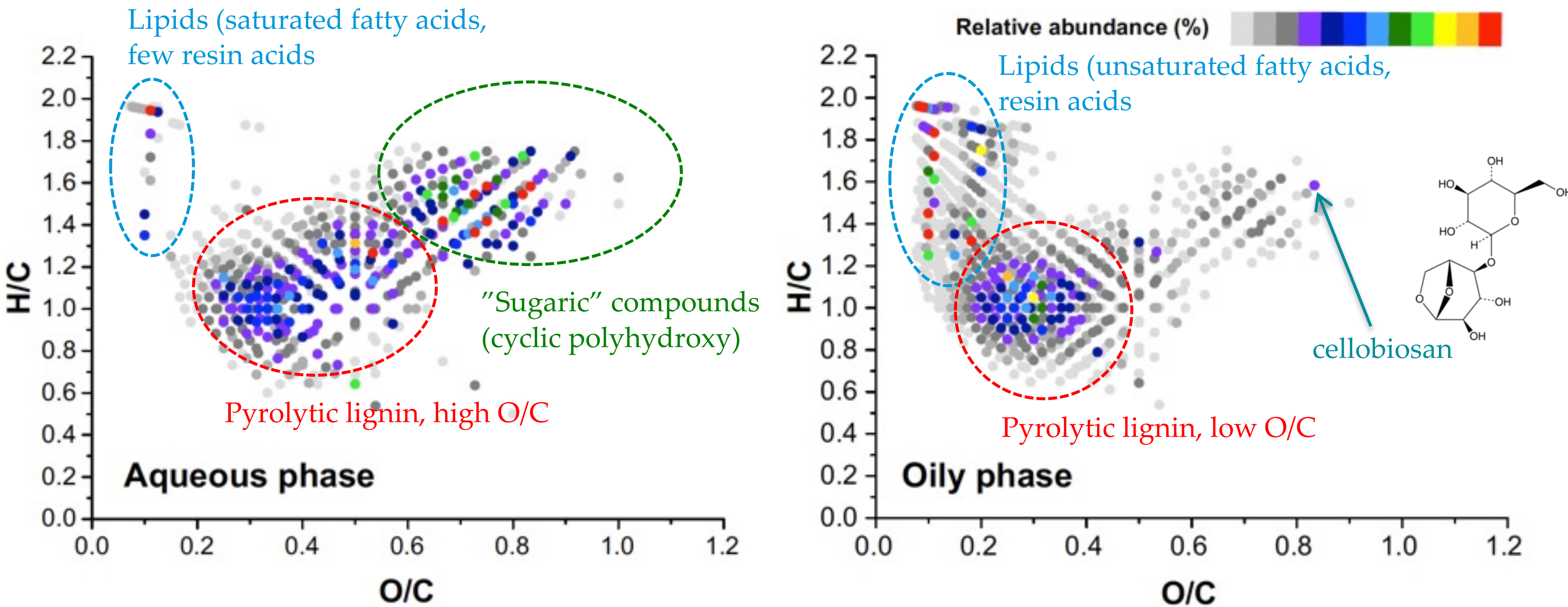
Analysis of phase-separated pine wood SPBO (275 °C)



	pH	TAN	Water-%
Oily	2.70	79	8.1 ± 0.3
Aqueous.	2.20	107	60.4 ± 0.2

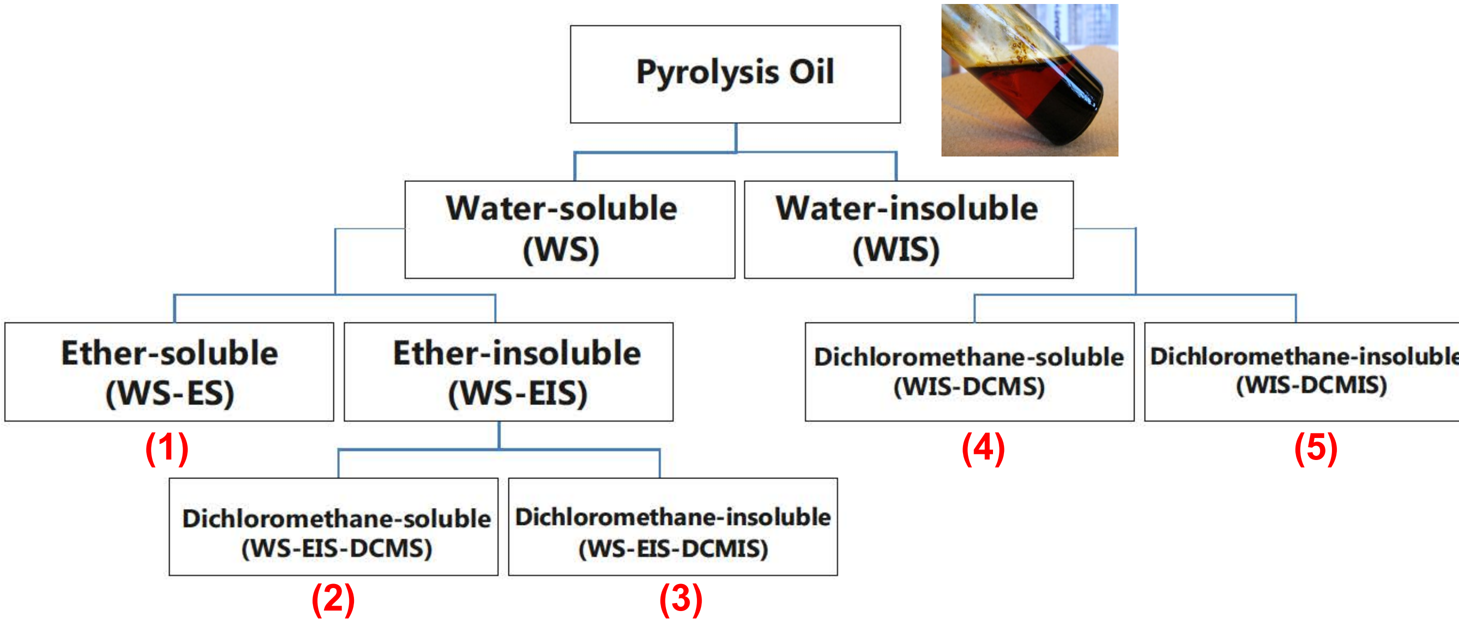
Miettinen I, Mäkinen M, Vilppo T & Jänis J: *Energy Fuels*, **2015**, *29:* 1758

Analysis of phase-separated pine wood SPBO (275 °C)



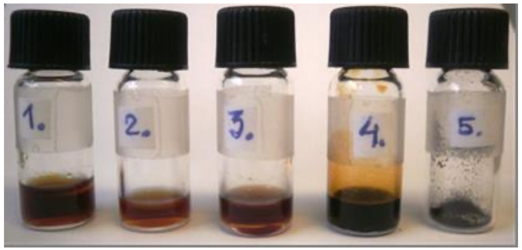
Miettinen I, Mäkinen M, Vilppo T & Jänis J: *Energy Fuels*, **2015**, *29:* 1758

Solvent fractionation of pine wood SPO (275 °C)

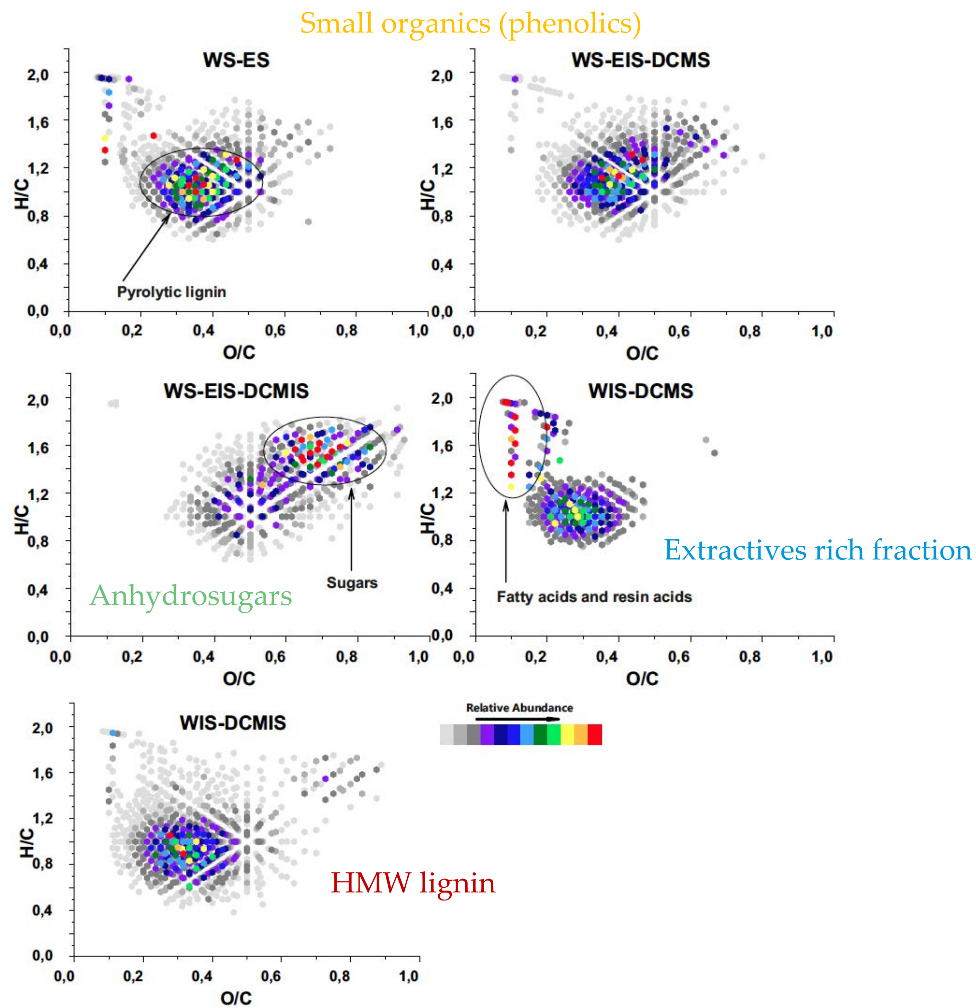


Oasmaa & Peacocke, Properties and use of FPO, VTT guide, 2010:

Solvent fractionation of pine wood SPO (275 °C)



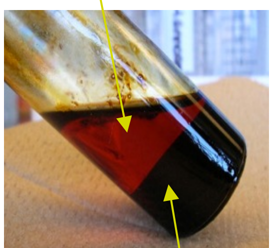
1. WS-ES: ether soluble
2. WS-EIS-DCMS: DCM soluble
3. WS-EIS-DCMIS: water soluble
4. WIS-DCMS: water insoluble
5. WIS-DCMIS: solid residue



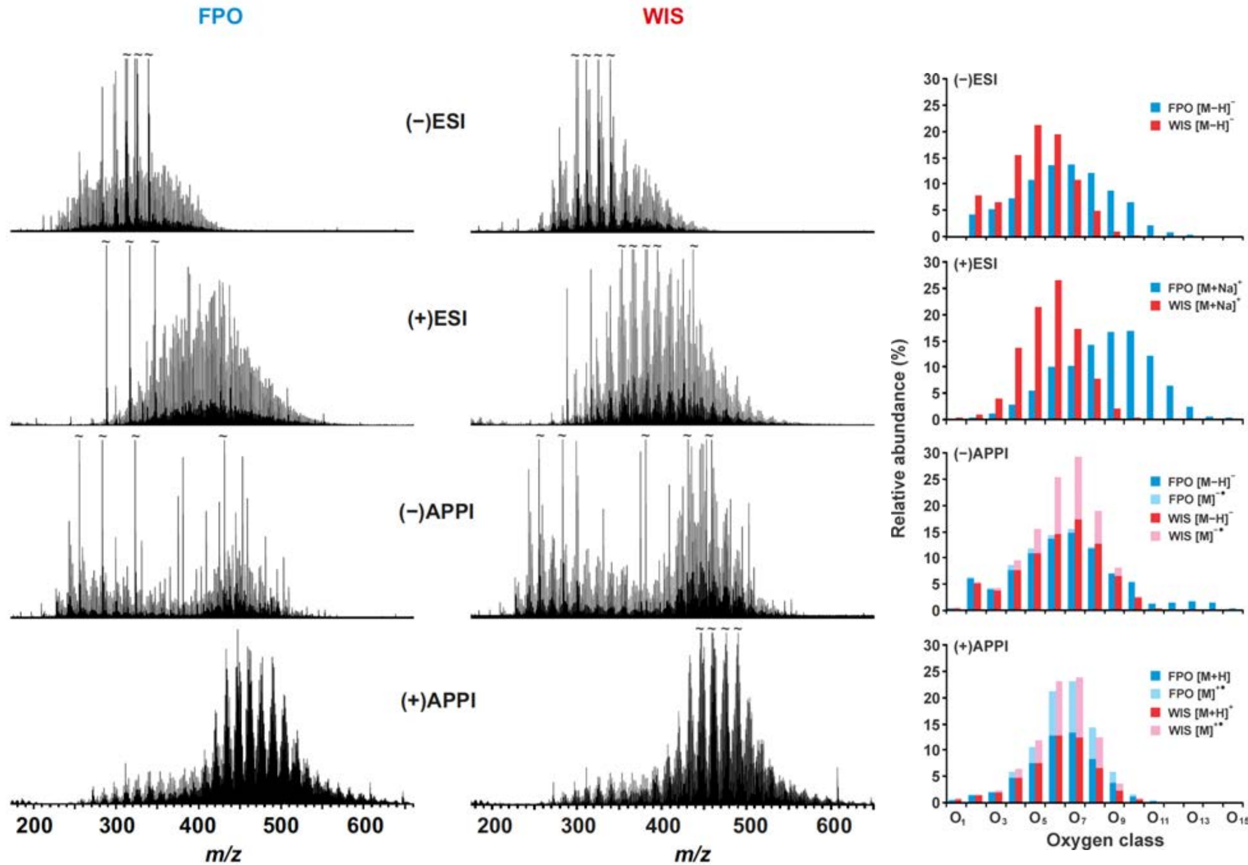
Analysis of wood-based bio-oil fractions with (+)ESI, (–)ESI, (+)APPI & (–)APPI

Pinewood fast pyrolysis oil (FPO)

Water soluble fraction



Water insoluble fraction (WIS)



Sajida *et al.*, unpublished

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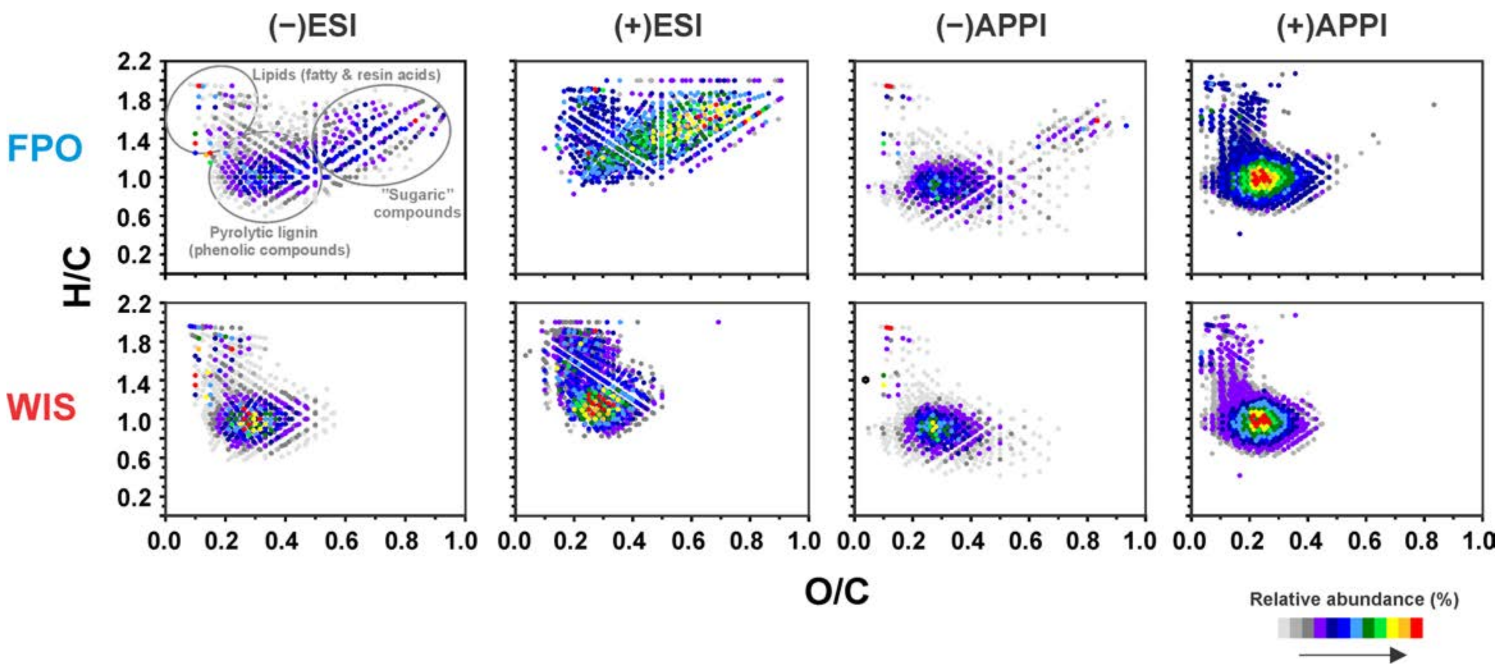

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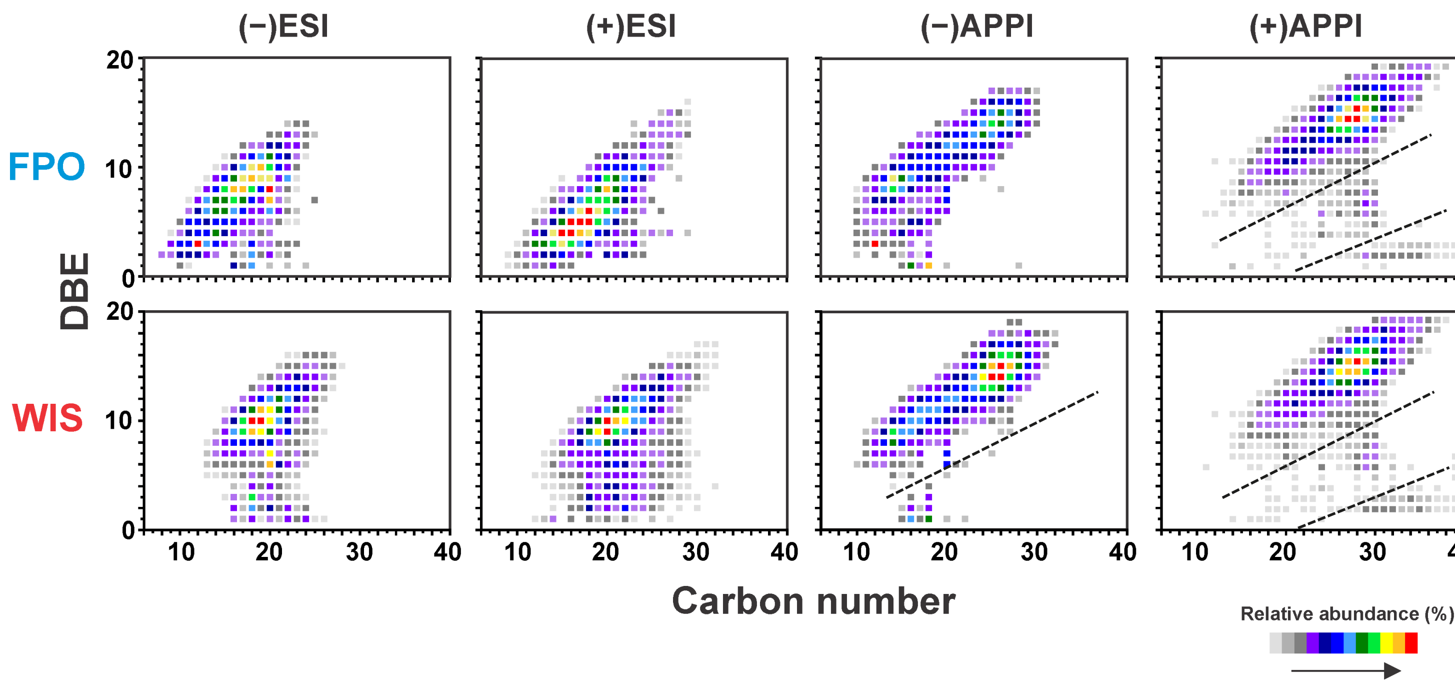

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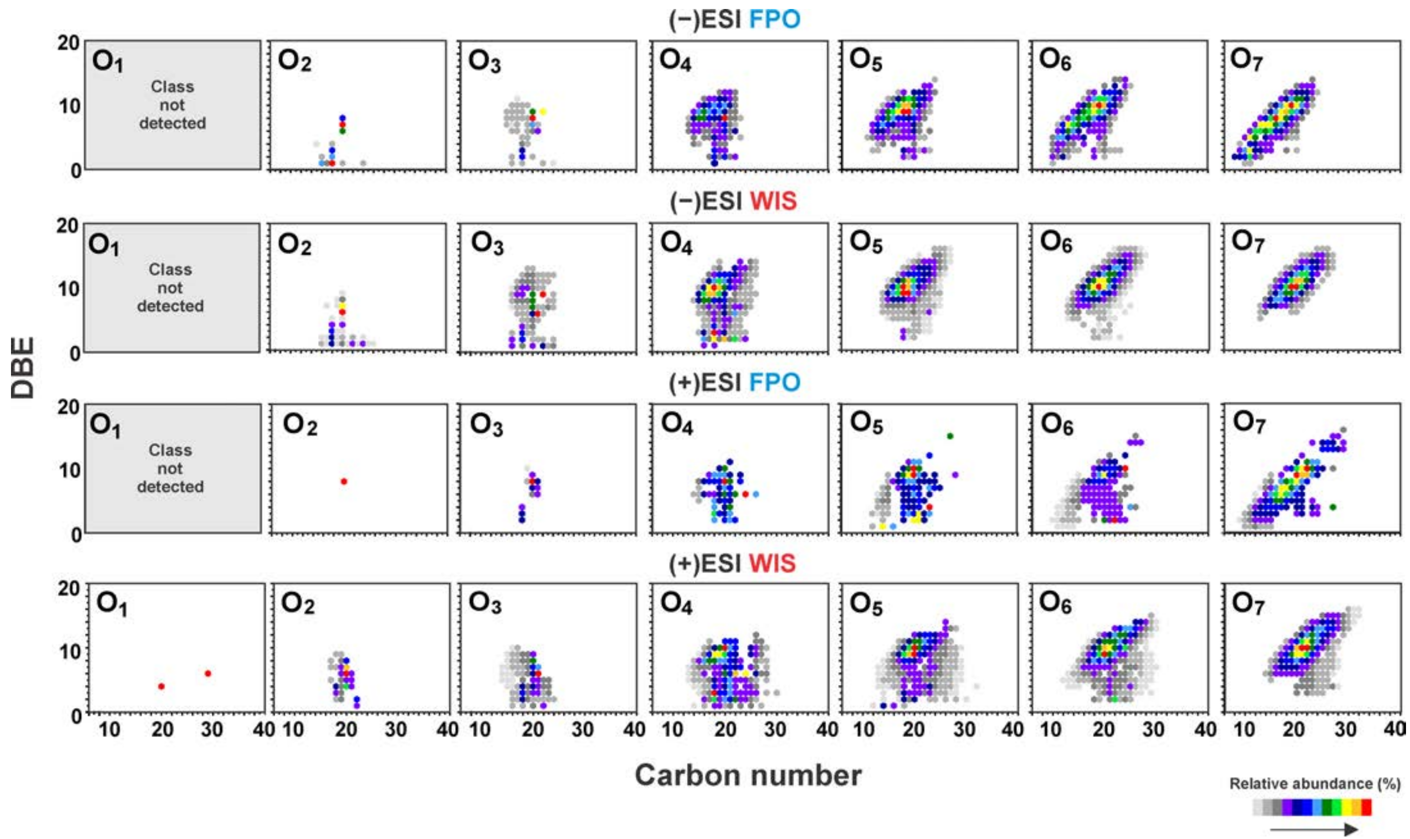

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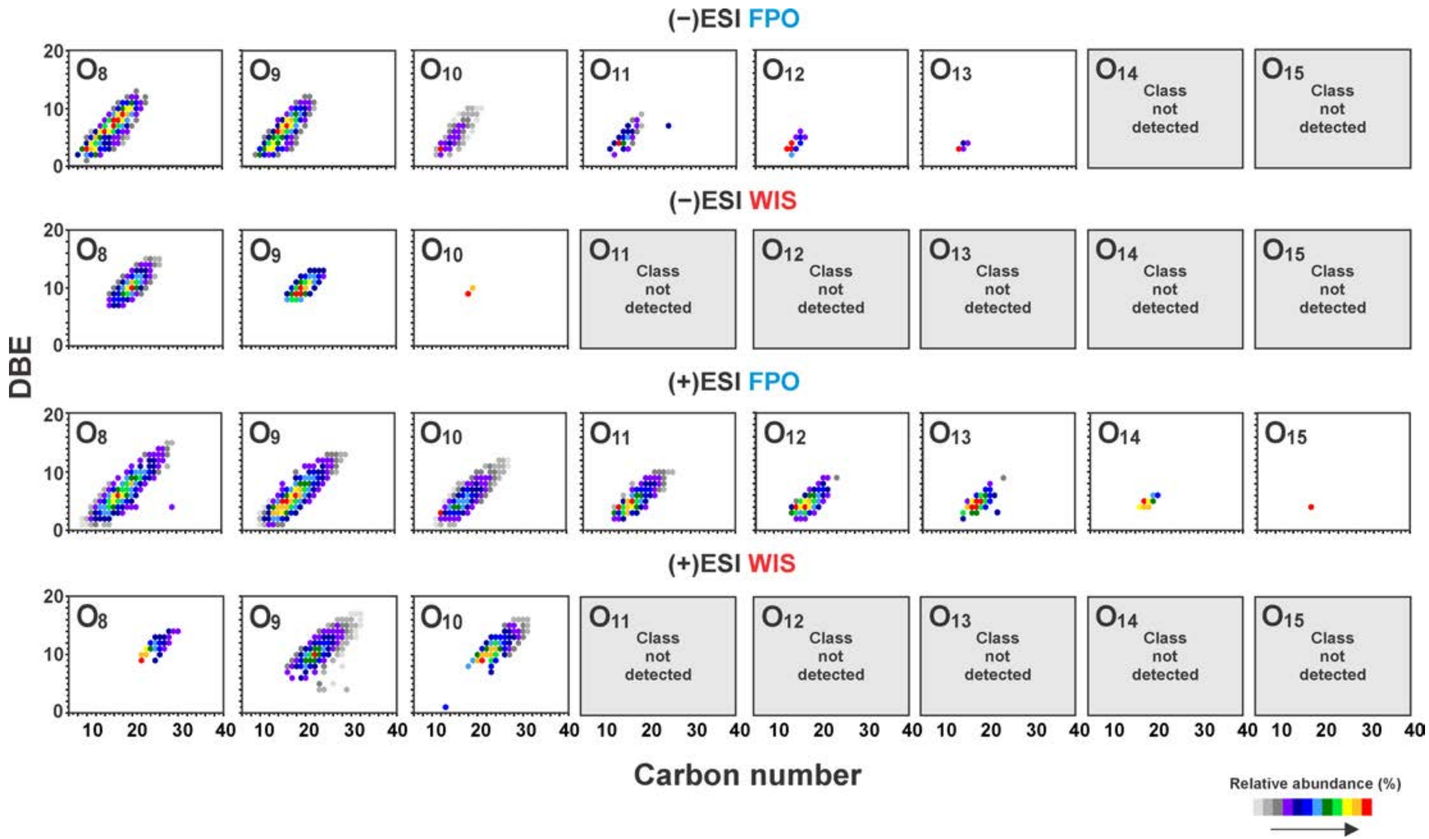

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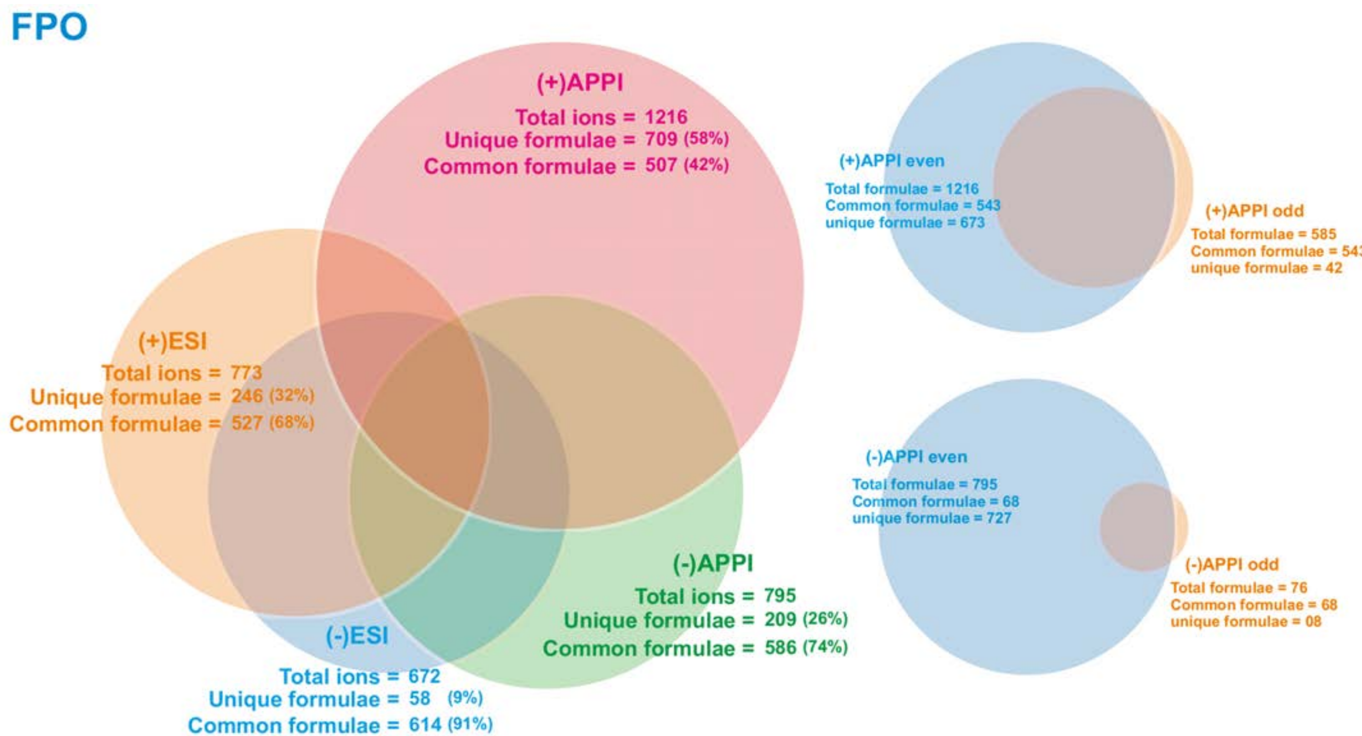
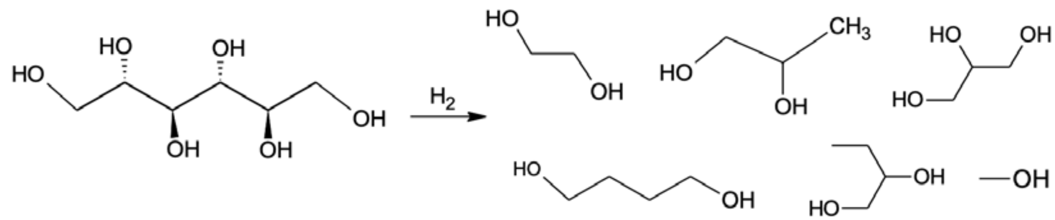
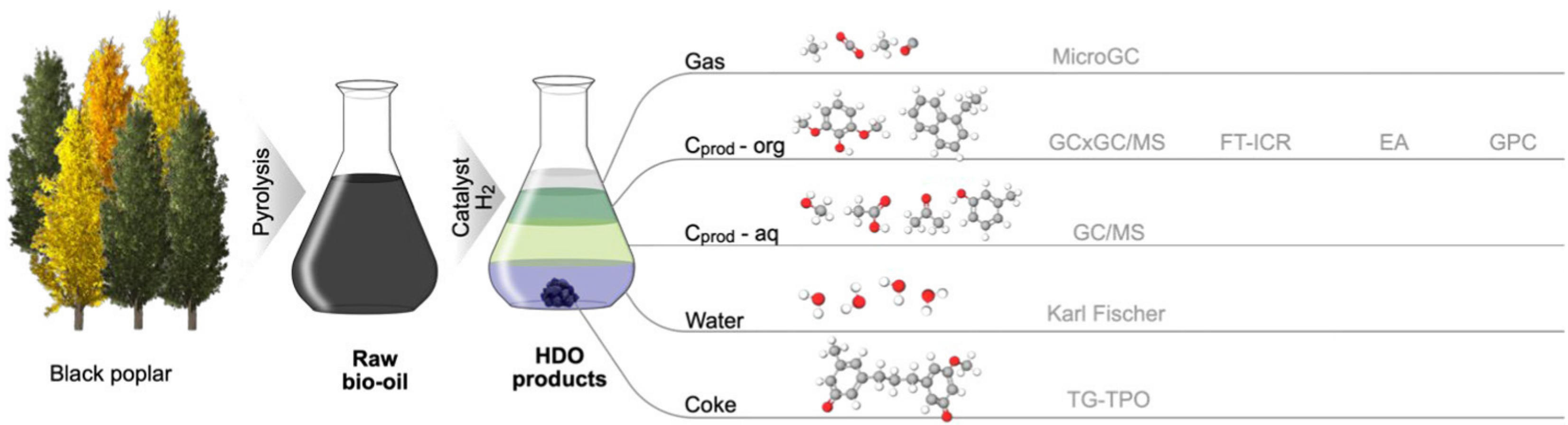


Sajida *et al.*, unpublished

Catalytic upgrading of fast pyrolysis bio-oil





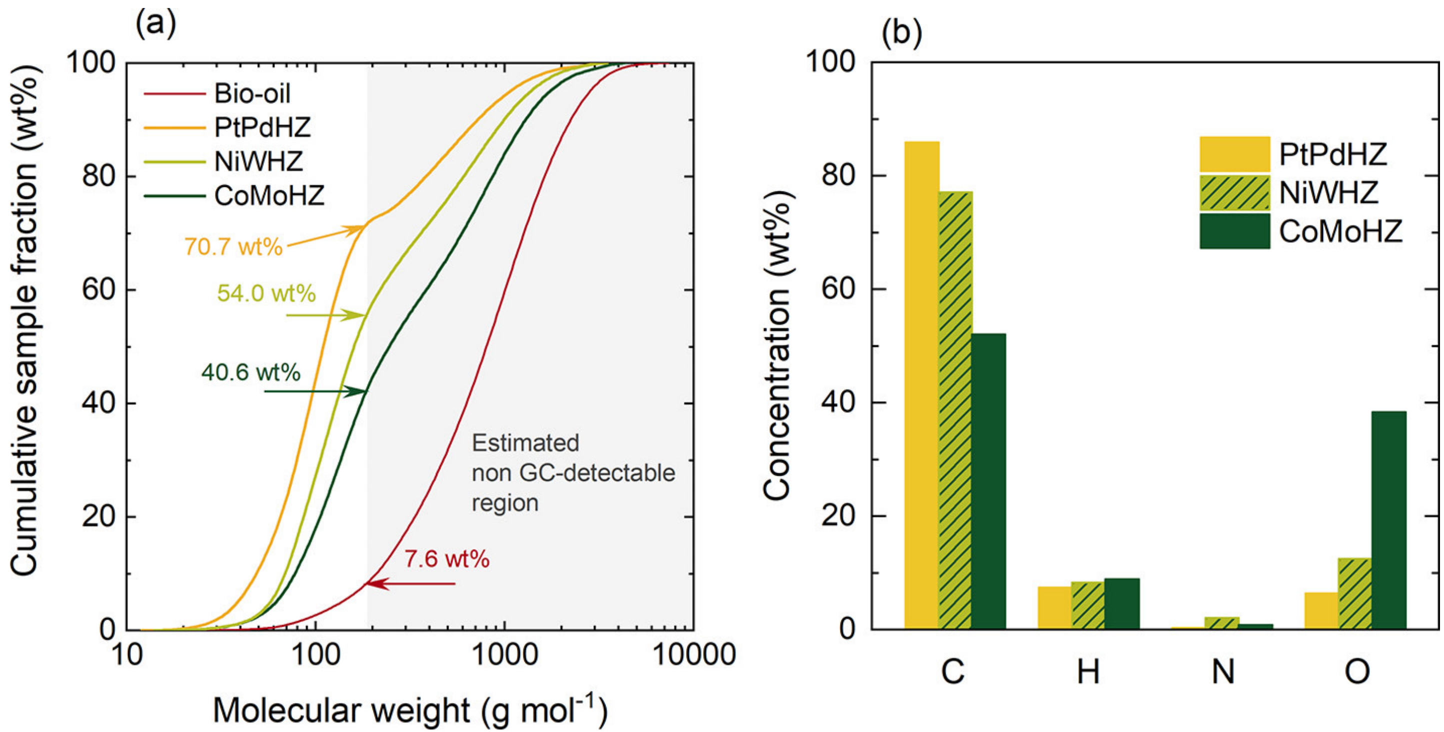
Three zeolite supported catalysts:
- PtPdHZ
- NiWHZ
- CoMoHZ

(–)ESI FT-ICR MS (Acidic O_x)

(+)APPI FT-ICR MS (HCs, neutral O_x and NO_x)

Hita I *et al.*, *ACS Sustainable Chem. Eng.* **2020**, 8, 50, 18433–18445

Catalytic upgrading of fast pyrolysis bio-oil



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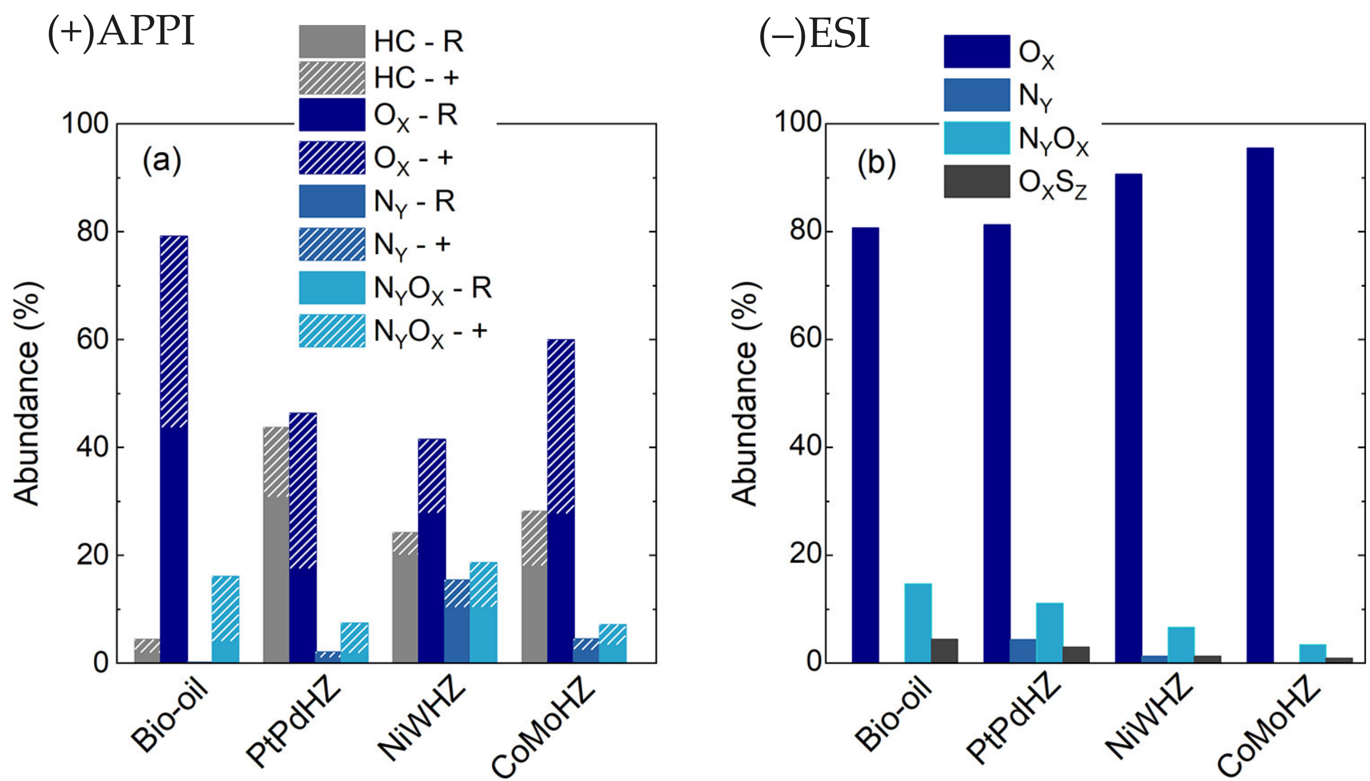

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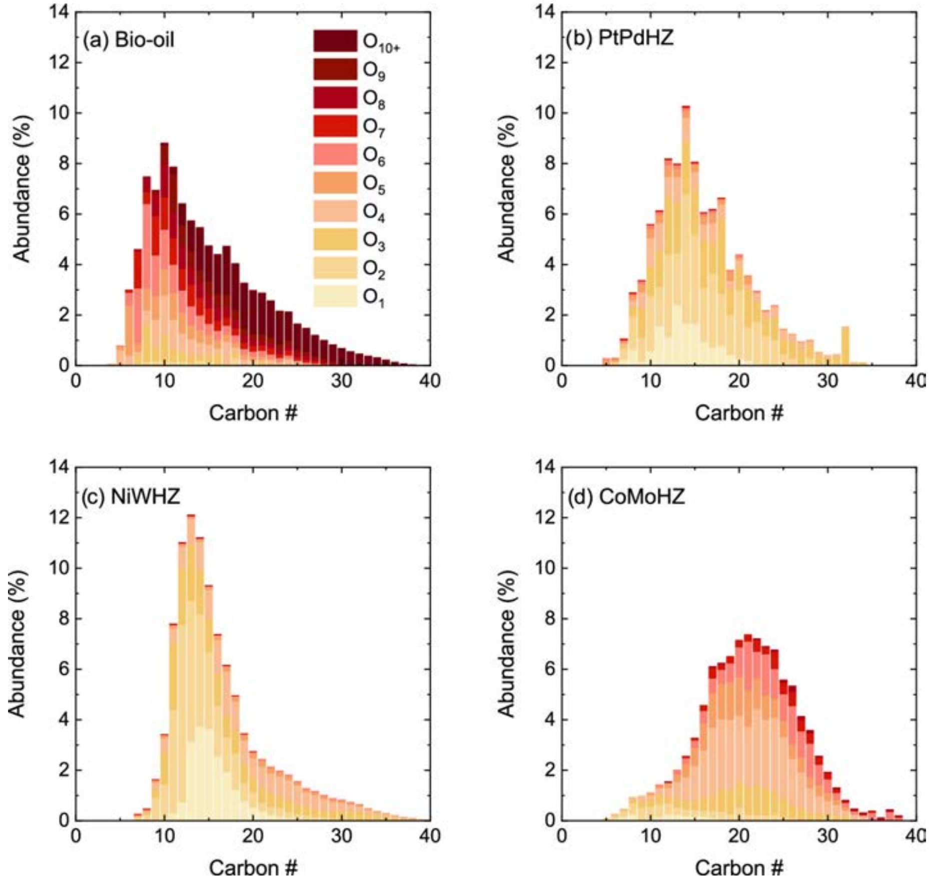
Catalytic upgrading of fast pyrolysis bio-oil

Original bio-oil

PtPdHZ

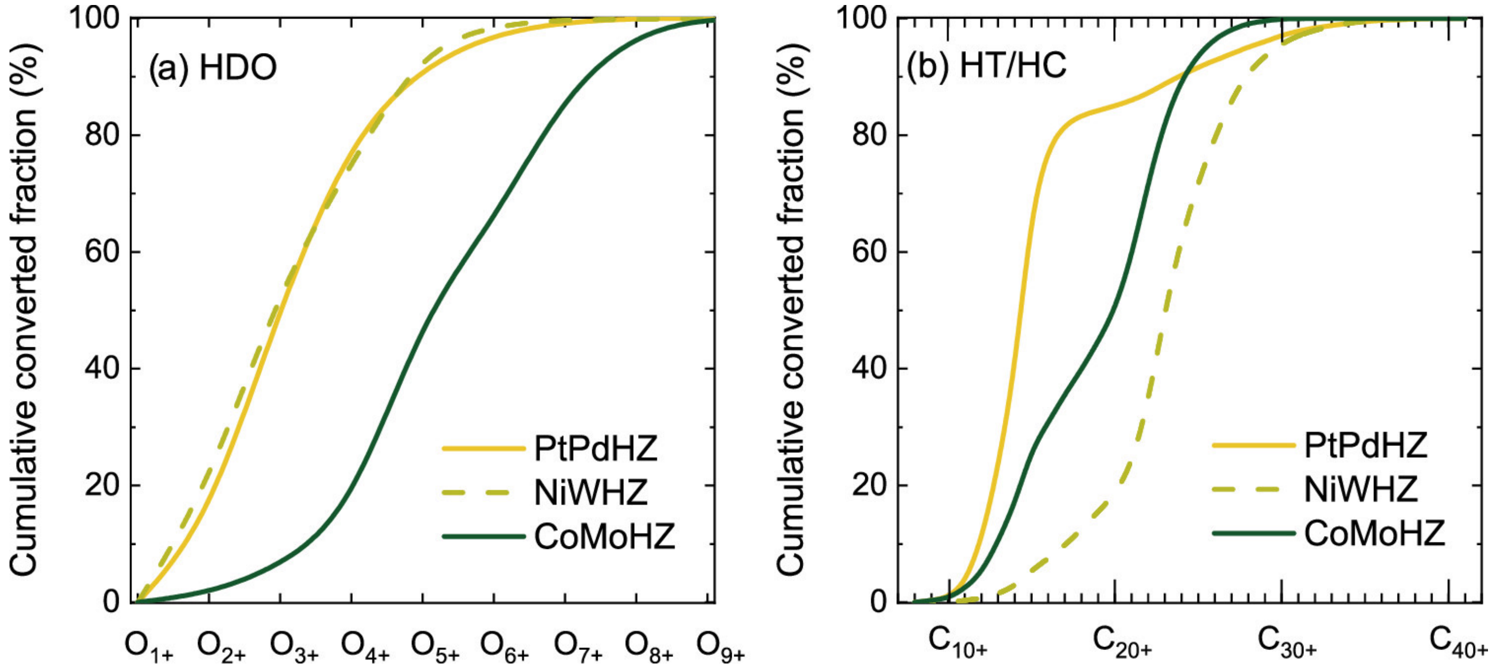


NiWHZ

CoMoHZ

Hita I *et al.*, *ACS Sustainable Chem. Eng.* **2020**, 8, 50, 18433–18445

Catalytic upgrading of fast pyrolysis bio-oil



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Phytochemical screening of conifer needles

Conifer needle chemistry

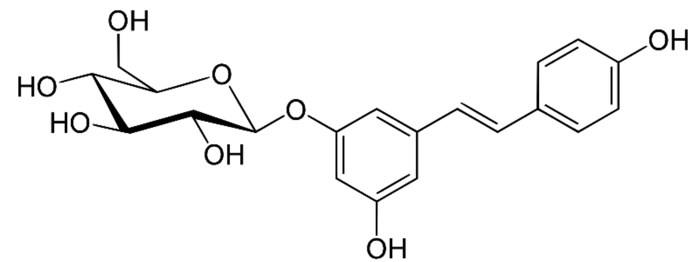
Wide bioactivity spectrum: antioxidant, antimicrobial, antifungal, anti-inflammatory, antitumour activity…

Scots pine

	Cellulose	Hemicelluloses	Lignin	Extractives
Stem wood [1-7, 11, 12, 27]	40.7 (0.7)	26.9 (0.6)	27.0 (0.0)	5.0 (1.0)
Bark [7-12, 27]	22.2 (3.2)	8.1 (0.4)	13.1 (5.4)	25.2 (5.2)
Branches [11-14, 27]	32.0	32.0	21.5 (5.9)	16.6 (7.1)
Needles [3, 11, 12, 27]	29.1	24.9	6.9 (0.8)	39.6 (1.3)
Stump [12]	36.4	28.2	19.5	18.7
Roots [12]	28.6	18.9	29.8	13.3

Norway spruce

	Cellulose	Hemicelluloses	Lignin	Extractives
Stem wood [3-6, 15-18, 27]	42.0 (1.2)	27.3 (1.6)	27.4 (0.7)	2.0 (0.6)
Bark [9-12, 17, 19, 20, 27]	26.6 (1.3)	9.2 (1.1)	11.8 (0.9)	32.1 (3.8)
Branches [11, 12, 14, 17, 27]	29.0	30.0	22.8 (1.7)	16.4 (2.6)
Needles [3, 11, 12, 27]	28.2	25.4	8.4 (2.1)	43.3 (2.3)
Stump [12, 21]	42.9	27.9	29.4 (1.8)	3.8 (0.2)
Roots [12]	29.5	19.2	25.5	15.7



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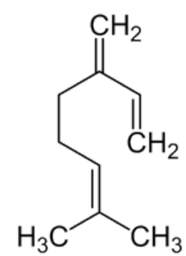
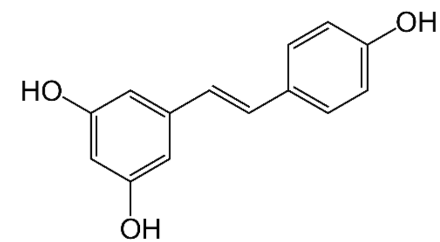


myrcene



Resveratrol (stilbene)

Products from conifer extractives

Pine ice cream (pine needle extract)

Spruce sprout syrup (sprout extract)

Norway spruce resin salve for wound healing
(clinically tested, ISO certified)

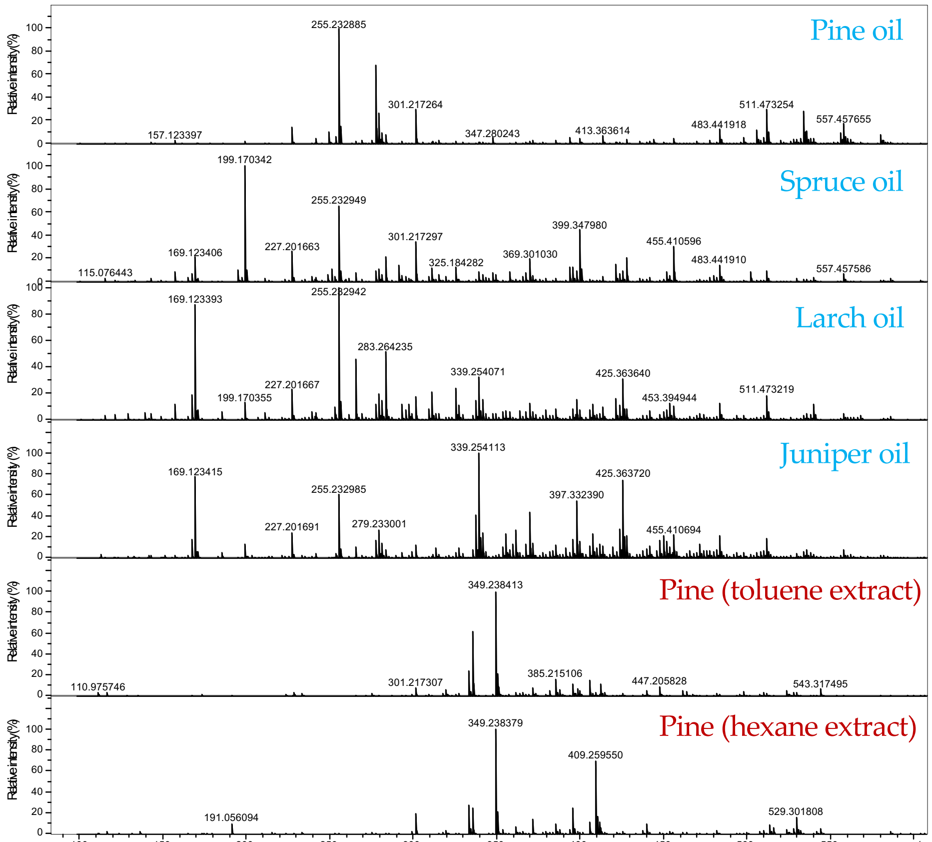
Phytochemicals extraction

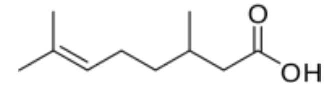
- Needles of four conifer tree species
  - Pine (*Pinus sylvestris*), spruce (*Picea abies*), larch (*Larix decidua*) and juniper (*Juniperus communis*)
  - Collected from Ylä-Valtimo region (North Carelia)
  - Stored at 4 °C until used (to avoid loss of volatile constituents)
- Compound extraction
  - Hydrodistillation (Clevenger apparatus)
  - Solvent extraction (Continuous Soxhlet extraction): toluene, hexane
  - Supercritical hydrothermal extraction (HTE)
- DI-(+)APPI/(-)ESI FT-ICR MS
  - 12-T Bruker solarix-XR with ParaCell



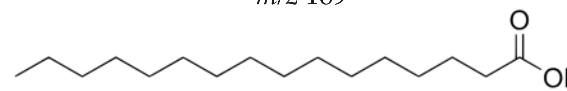


Conifer needle extracts: (-)ESI

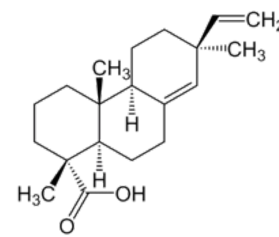




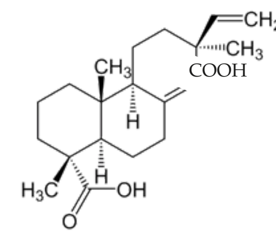
Citronellic acid $C_{10}H_{18}O_2$
m/z 169



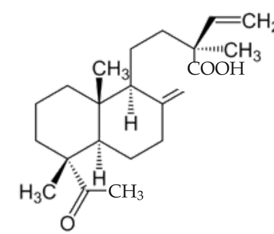
Palmitic acid $C_{16}H_{32}O_2$
m/z 255



Pimaric acid $C_{20}H_{30}O_2$
m/z 301



Pinifolic acid $C_{20}H_{32}O_4$
***m/z* 335**



Methyl pinifolate $C_{21}H_{34}O_4$
***m/z* 349**

ACTA CHEMICA SCANDINAVICA 16 (1962) 607–614

The Constituents of Conifer Needles

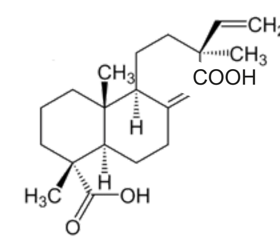
II *. Pinifolic Acid, a new Diterpene Acid Isolated from *Pinus silvestris* L.

CURT ENZELL and OLOF THEANDER

Organisk-kemiska Institutionen, Kungl. Tekniska Högskolan and Träkemiska Avdelningen, Svenska Träforskningsinstitutet, Stockholm, Sweden

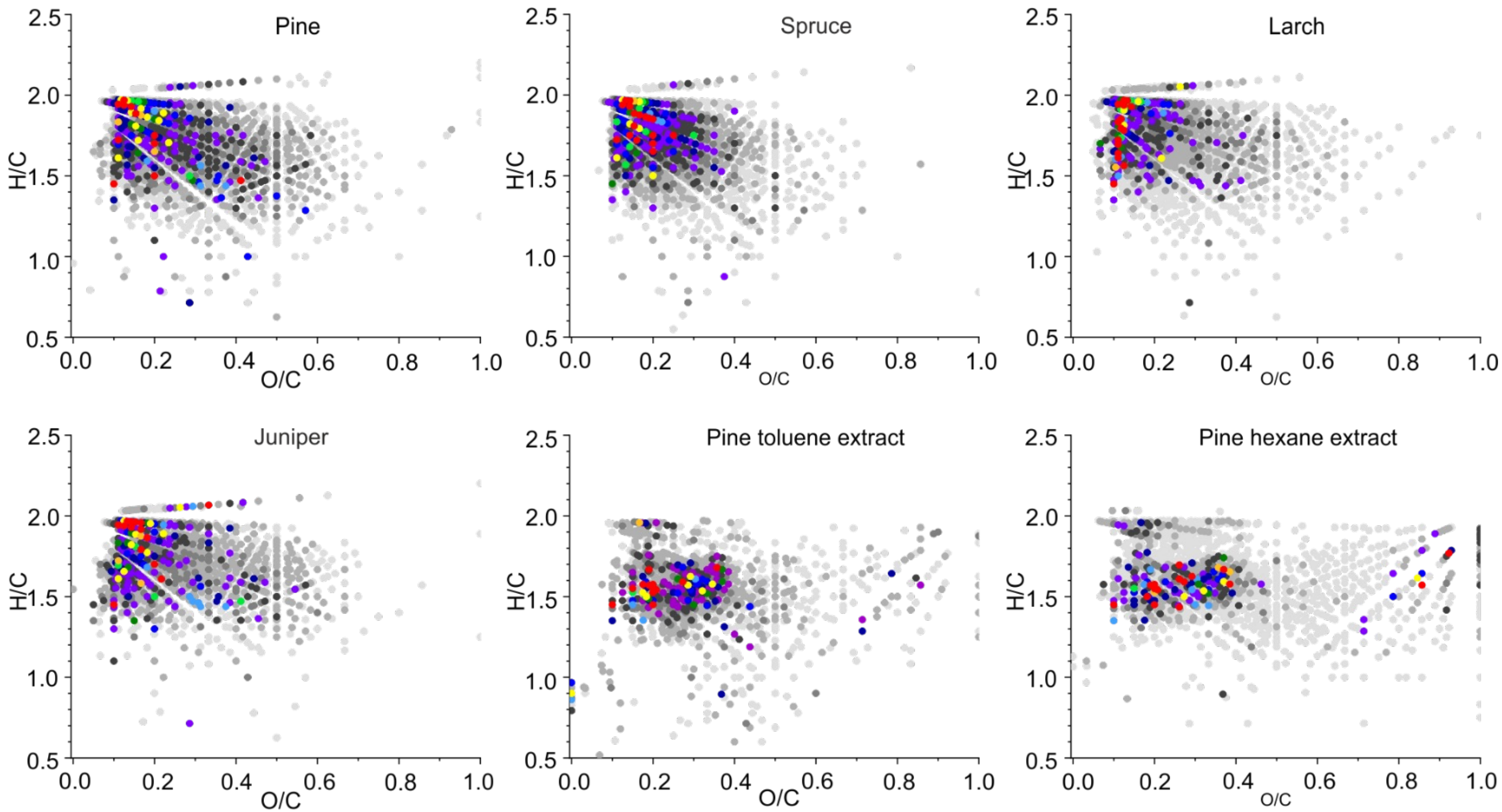
Dedicated to Professor *Holger Erdtman* on his 60th birthday

A diterpene acid, pinifolic acid, has been isolated from the needles of *Pinus silvestris* L. and shown to have structure (1 a).

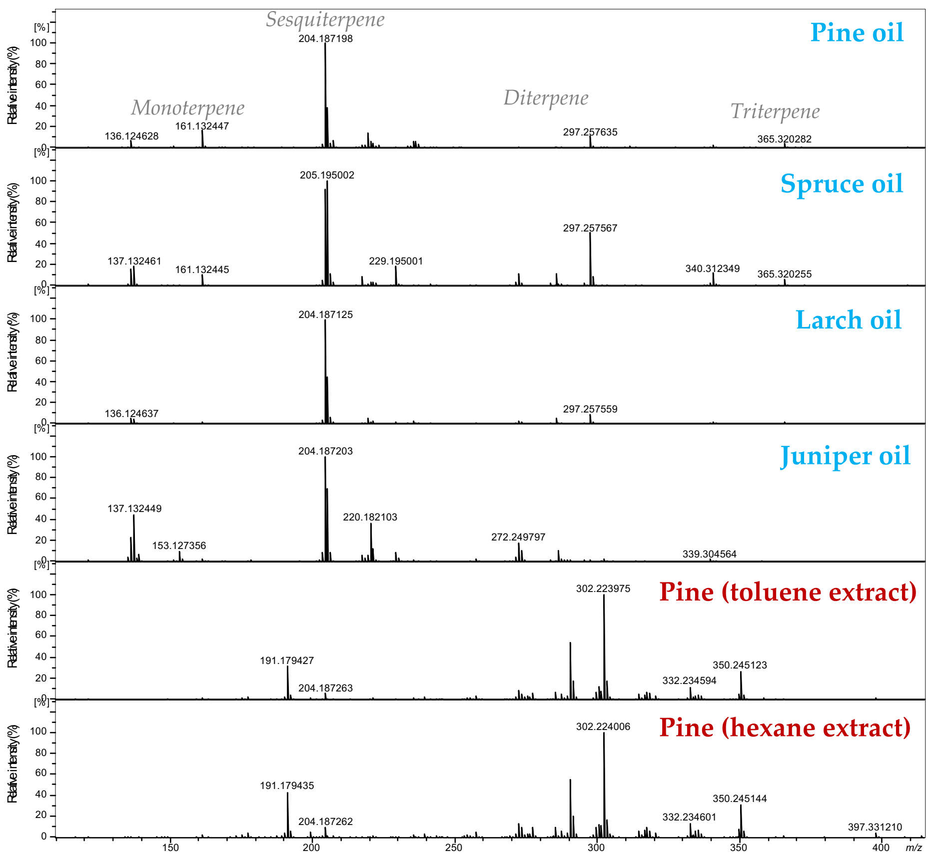


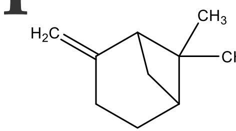
Pinifolic acid $C_{20}H_{32}O_4$
m/z 335

Conifer needle extracts: (-)ESI

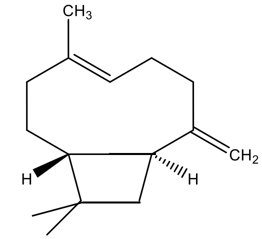


Conifer needle extracts: (+)APPI

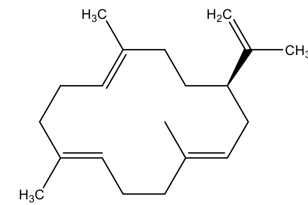




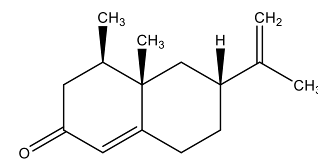
Pinene $C_{10}H_{16}$



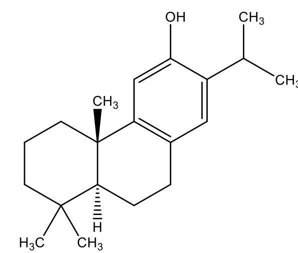
Caryophyllene $C_{15}H_{24}$



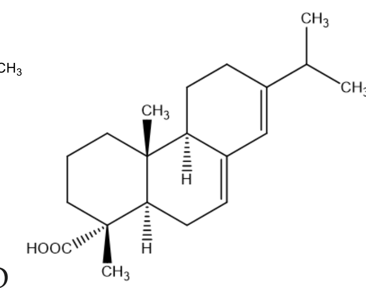
Cembrene $C_{20}H_{32}$



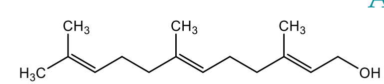
Nootkatone $C_{15}H_{22}O$



Ferruginol $C_{20}H_{30}O$



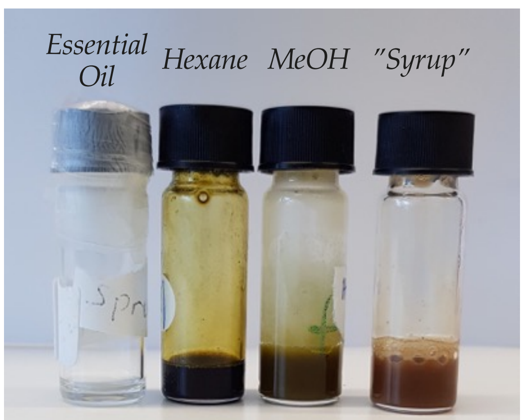
Abietic acid $C_{20}H_{30}O_2$



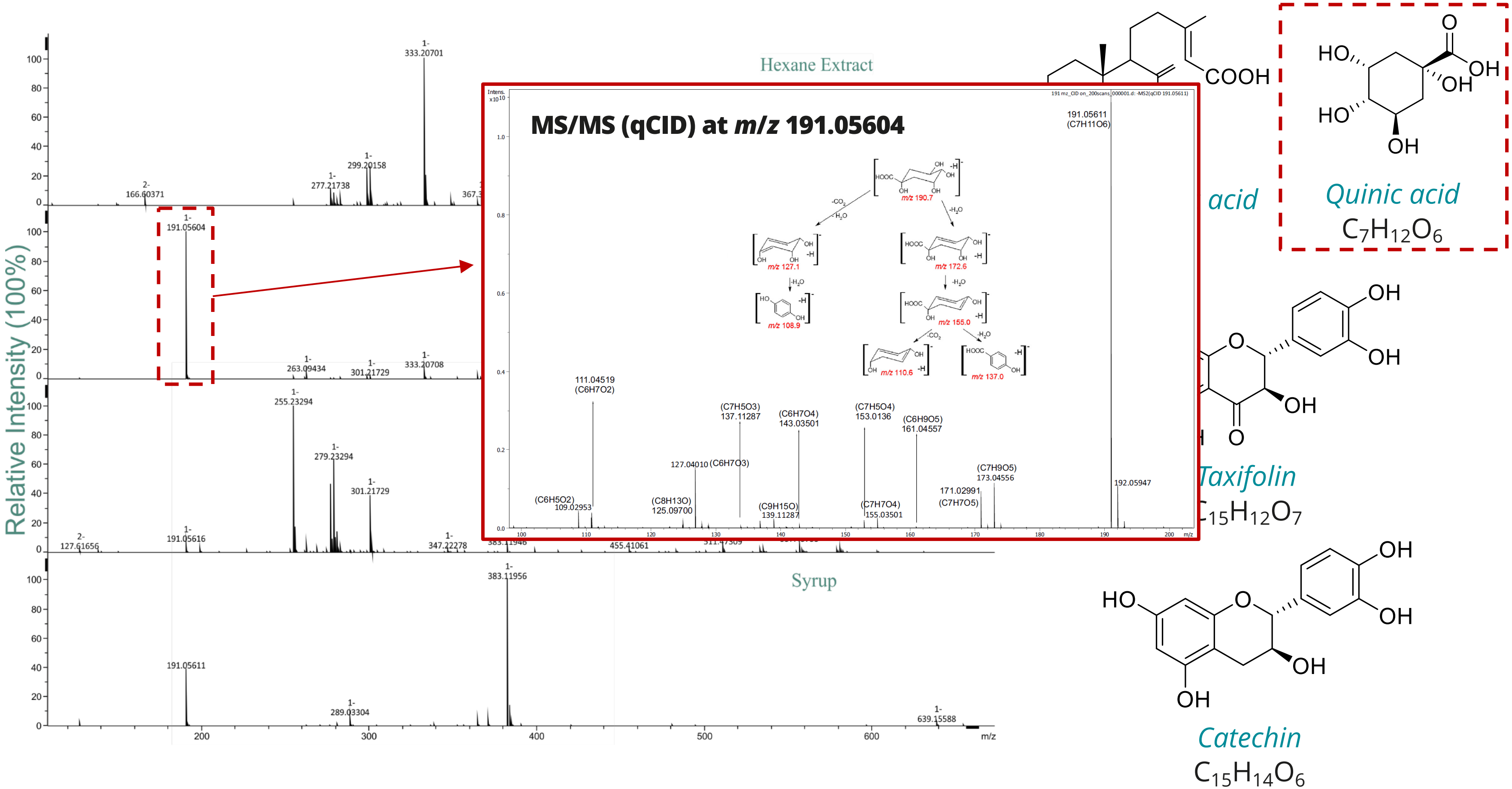
Farnesol $C_{15}H_{26}O$

Norway spruce sprout (buds)

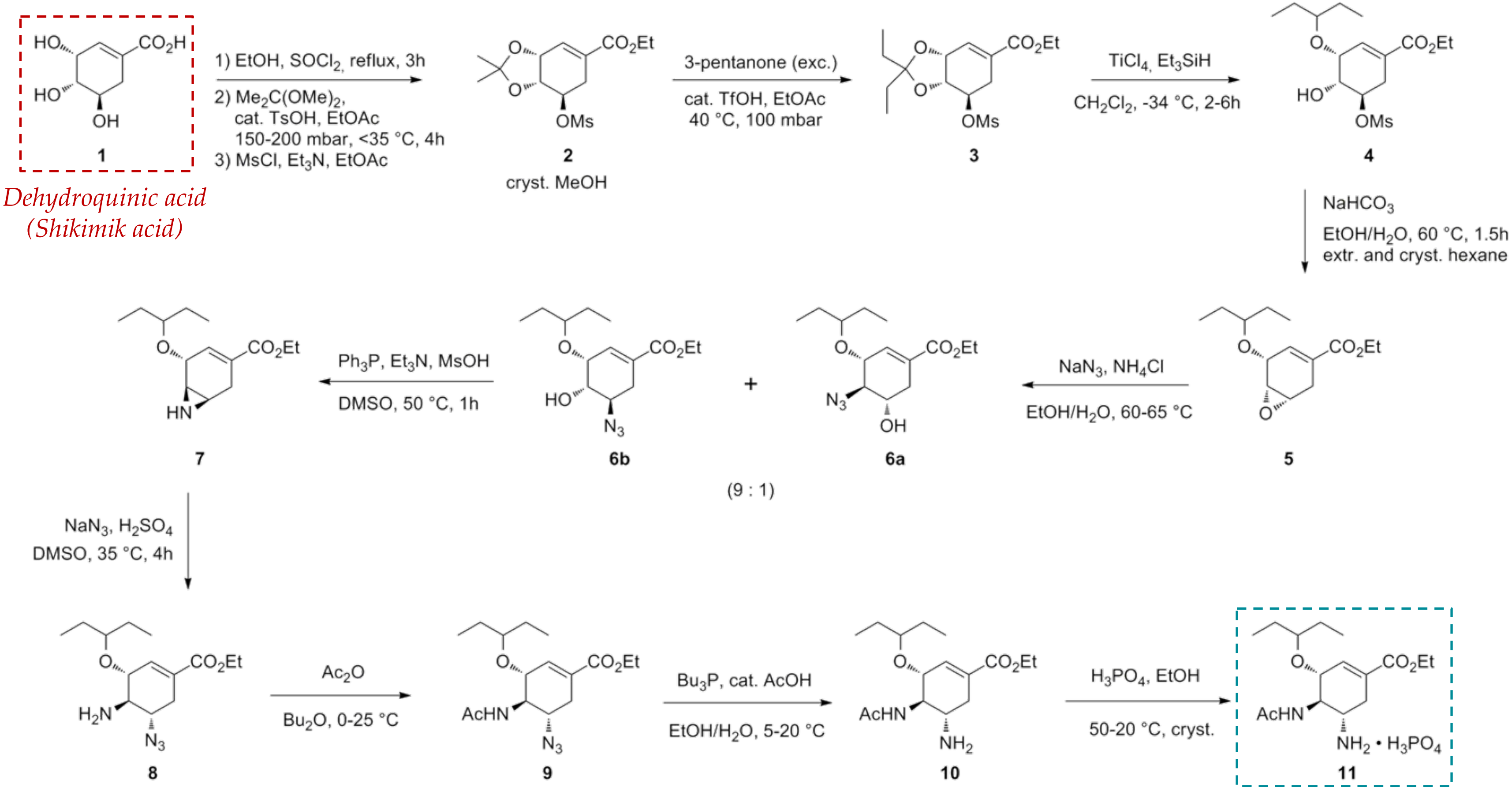
- Traditional sprout syrup – superfood!
- Other nutritional or medicinal uses – forest antivirals
  - Antioxidants (phenolics)
  - A/C vitamin
  - Terpenes & terpenoids



Results: Spruce sprout (buds)



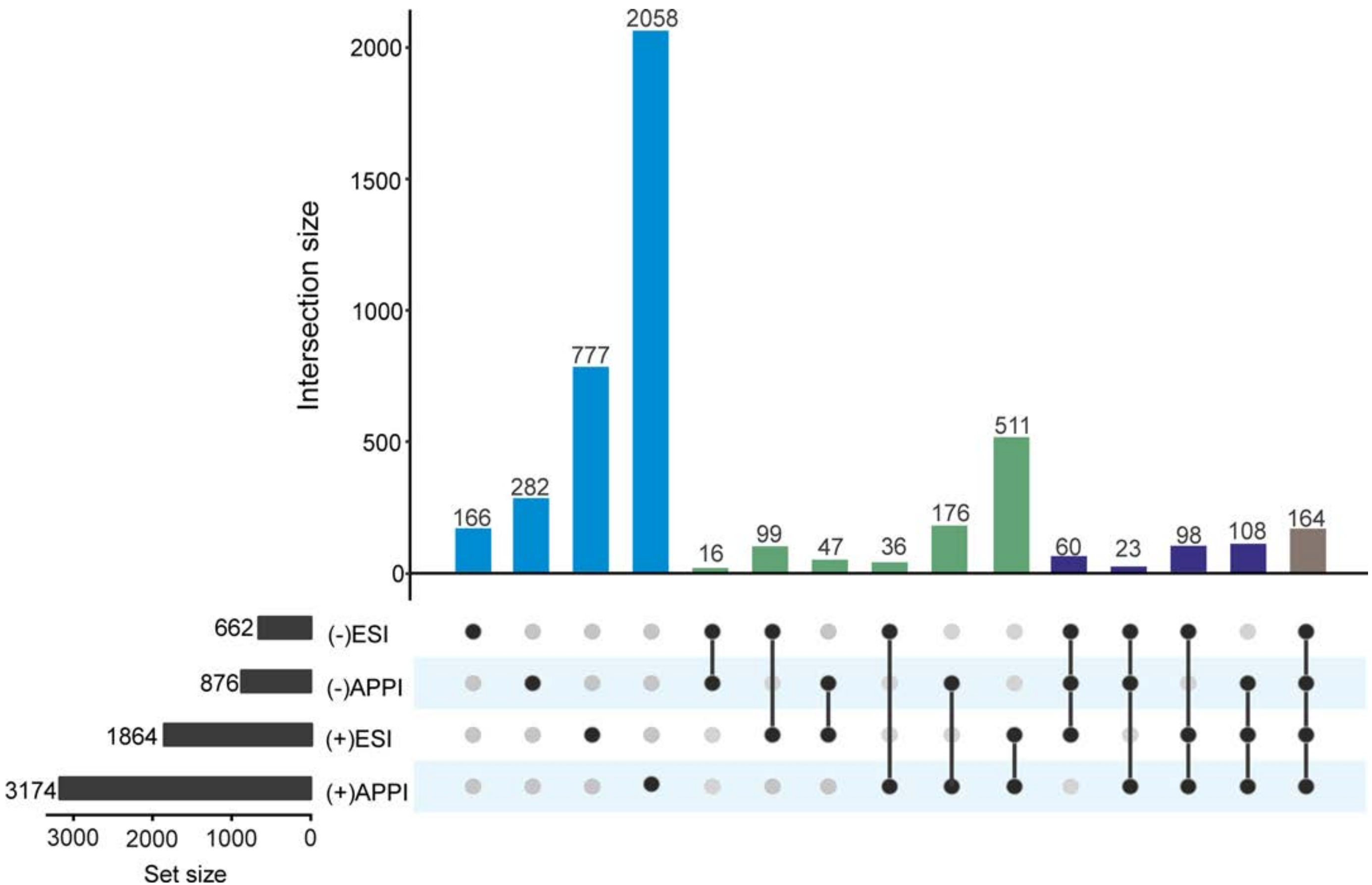
Results: Spruce sprout (buds)



Dehydroquinic acid (Shikimik acid)

Oseltamivir (Tamiflu®)

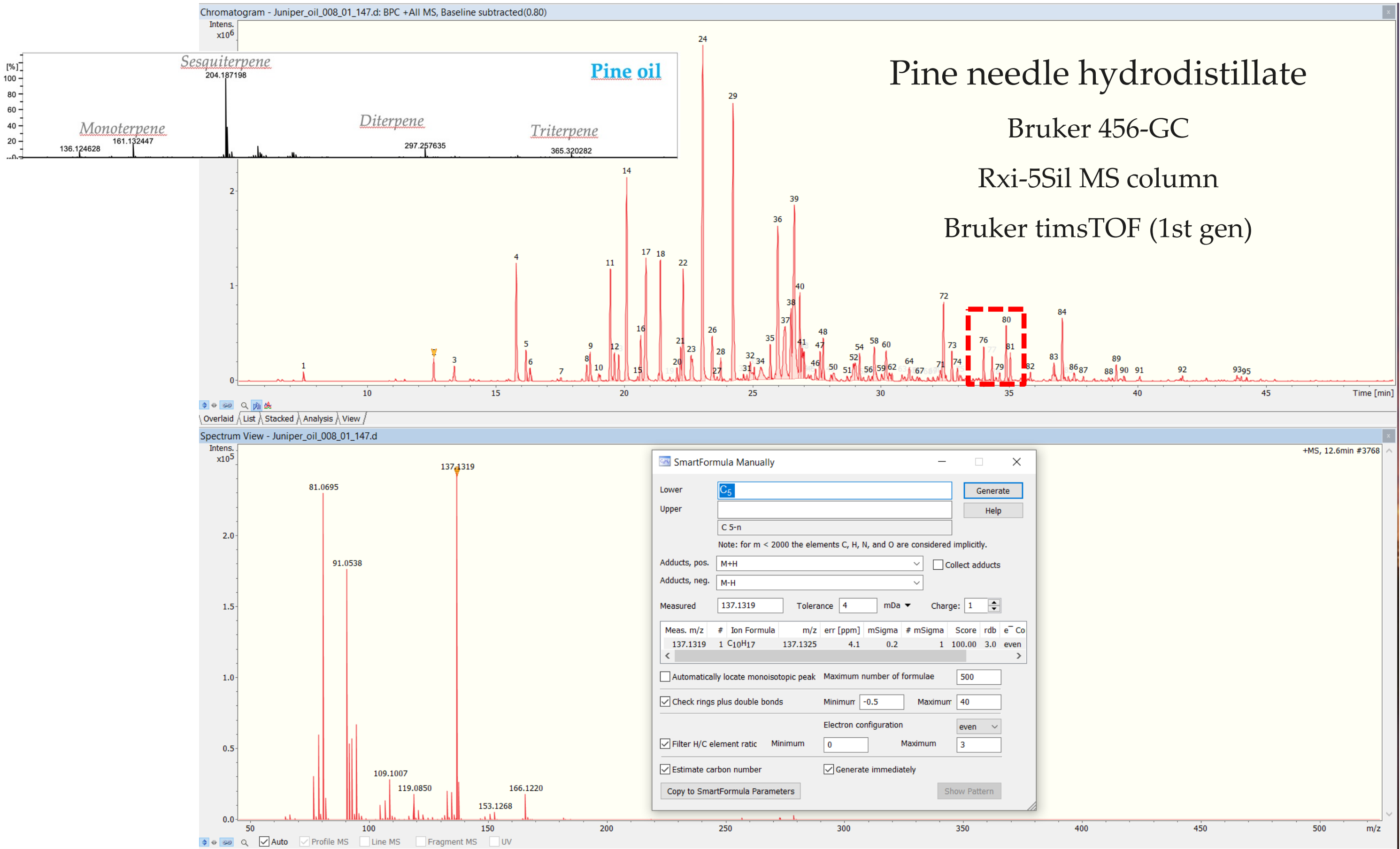
Results: Spruce sprout (buds)



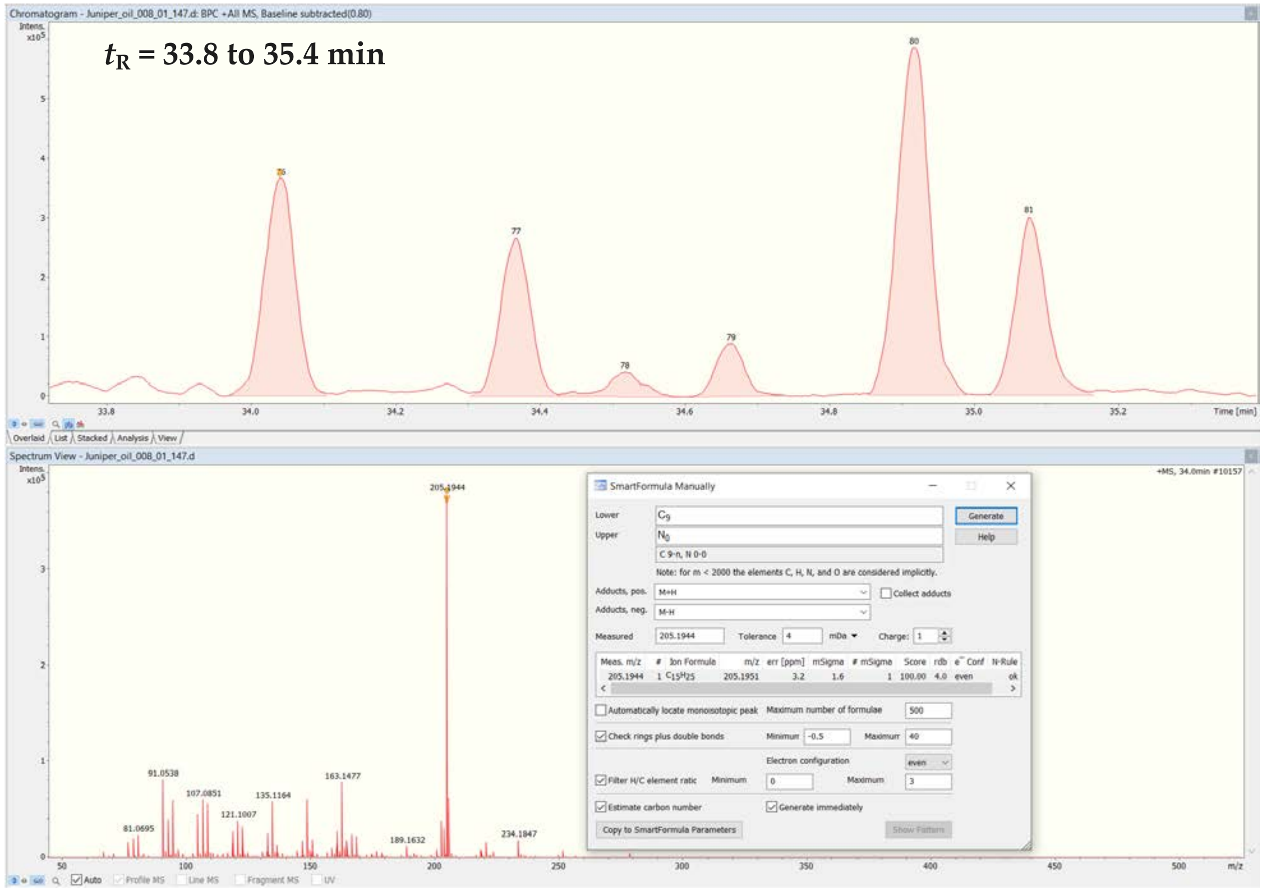
Results: Spruce sprout (buds)

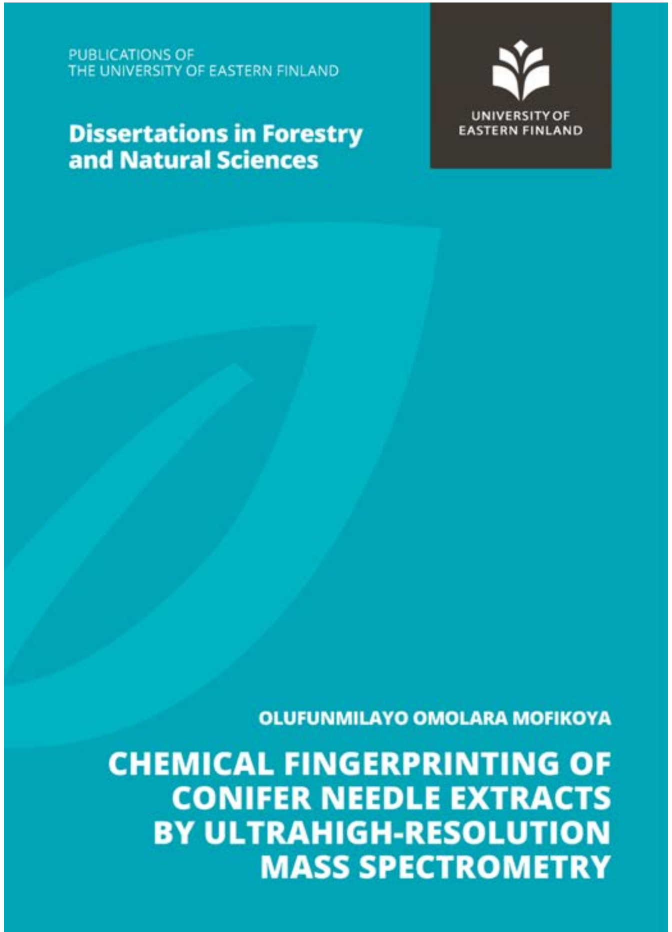
Calculated *m/z*	Observed m/z	DBE	Elemental Formula	Error (ppm)	Relative Intensity (%)								Putative compound(s)
					Methanol	Ethanol	Water	Acetone	DCM	Hexane	Toluene	Essential oil	
104.070605	104.070607	1	$C_4H_9NO_2$	-0.021	N.D	N.D	0.0277	N.D	N.D	N.D	N.D	N.D	Aminobutyric acid[35]
107.049141	107.049131	5	C_7H_8O	0.096	0.5882	0.1179	0.2404	0.1385	N.D	N.D	N.D	N.D	Benzaldehyde
116.070605	116.070586	2	$C_5H_9NO_2$	0.165	0.1056	0.0184	0.1373	0.0791	0.0886	0.0735	0.0061	N.D	Proline[35]
120.065520	120.065542	1	$C_4H_9NO_3$	-0.182	N.D	0.0041	0.0341	0.0196	N.D	N.D	N.D	N.D	Threonine[35]
123.044056	123.044043	5	$C_7H_6O_2$	0.102	0.1666	0.0417	0.1716	0.0988	0.1008	0.0826	0.0256	N.D	Benzoic acid[35]
125.059706	125.059699	4	$C_7H_8O_2$	0.057	0.1457	N.D	N.D	N.D	N.D	N.D	N.D	N.D	4-Methylcatechol
135.080441	135.080434	5	$C_9H_{10}O$	0.056	0.0332	0.0081	0.0209	0.0121	0.0333	0.0289	0.0356	0.0078	Cinnamyl alcohol
135.116827	135.116827	4	$C_{10}H_{14}$	-0.003	0.0303	0.0186	0.0681	0.0392	N.D	N.D	N.D	0.2224	Verbenene[22]
137.059706	137.059696	5	$C_8H_8O_2$	0.074	0.0988	0.0315	0.2402	0.1383	0.0781	0.0512	0.1148	N.D	Piceol
137.132477	137.132464	3	$C_{10}H_{16}$	0.096	0.0169	0.0100	0.0383	0.0221	0.0355	0.0293	0.1114	0.3873	Monoterpene[22]
138.127726	138.127737	3	$C_9H_{15}N$	-0.078	0.4128	0.4128	2.0280	1.5703	N.D	0.0121	N.D	N.D	1,6-hydropinidine[25, 26]
139.038971	139.038968	5	$C_7H_6O_3$	0.018	0.3042	0.1932	1.6518	0.9515	0.0483	0.0314	0.0112	N.D	4-Hydroxybenzoic acid[35]
139.075356	139.075341	4	$C_8H_{10}O_2$	0.111	4.4783	0.7722	0.9191	0.5294	3.6526	2.7714	0.8562	0.0180	Tyrosol
140.143376	140.143378	2	$C_9H_{17}N$	-0.013	0.0103	N.D	0.0297	0.0297	N.D	N.D	N.D	N.D	Pinidine[25, 26]
145.122306	145.122275	1	$C_8H_{16}O_2$	0.218	0.0062	N.D	N.D	N.D	N.D	N.D	0.0057	N.D	Hexyl acetate
147.044056	147.044058	7	$C_9H_6O_2$	-0.013	0.0407	N.D	N.D	N.D	N.D	N.D	N.D	N.D	Coumarin
149.059706	149.059707	6	$C_9H_8O_2$	-0.009	0.0369	0.0120	0.0616	0.0355	0.0264	0.0177	0.0327	N.D	Cinnamic acid
151.111742	151.111744	4	$C_{10}H_{14}O$	-0.016	N.D	N.D	0.0803	0.0463	0.0434	N.D	0.0963	N.D	Thymol, Carvacrol, verbenone, Ca
153.054621	153.054638	5	$C_8H_8O_3$	-0.114	0.4061	0.1953	1.7088	0.9843	0.0556	0.0279	0.0154	N.D	Vanillin
153.127392	153.127397	3	$C_{10}H_{16}O$	-0.036	0.0502	0.0248	0.1356	0.0781	0.0453	0.0430	0.1017	0.0720	Methyl thymol, Thujone, Piperito
154.122641	154.122660	3	$C_9H_{15}NO$	-0.128	1.0294	0.3355	2.8221	2.0197	0.1252	0.01425	N.D	N.D	Dehydropinidinone[25, 26]
155.033885	155.033887	5	$C_7H_6O_4$	-0.011	0.0447	0.0233	0.0827	0.0476	0.0206	0.0144	0.0081	N.D	Protocatechuic acid
155.070271	155.070269	4	$C_8H_{10}O_3$	0.011	0.0848	0.0246	0.0908	0.0523	0.0542	0.0337	0.0168	N.D	Hydroxytyrosol
155.143042	155.143045	2	$C_{10}H_{18}O$	-0.022	0.0268	0.0044	0.0092	0.0053	0.0124	0.0108	0.0183	N.D	Terpinen-4-ol[22]
156.138291	156.138295	2	$C_9H_{17}NO$	-0.029	0.1129	0.1607	3.1644	0.7777	0.0234	N.D	N.D	N.D	Pinidinone[25, 26]
158.153941	158.153955	1	$C_9H_{19}NO$	-0.090	0.1177	0.0995	0.6927	0.4511	0.0249	0.0106	N.D	N.D	Pinidinol[25, 26]
159.137956	159.137949	1	$C_9H_{18}O_2$	0.045	0.0071	N.D	N.D	N.D	0.0047	0.0040	0.0071	N.D	Nonanoic acid
165.054621	165.054632	6	$C_9H_8O_3$	-0.071	0.0259	0.0170	0.1558	0.0898	0.0092	0.0056	0.0126	N.D	P-coumaric acid[35]
165.075750	165.075756	1	$C_6H_{12}O_5$	-0.036	N.D	N.D	0.0513	0.0295	N.D	N.D	N.D	N.D	Rhamnose
165.091006	165.091019	5	$C_{10}H_{12}O_2$	-0.076	0.0394	0.0154	0.0630	0.0363	0.0293	0.0197	0.0488	0.0145	2-phenyl ethyl acetate, Eugeno
165.127392	165.127397	4	$C_{11}H_{16}O$	-0.031	0.0171	0.0113	0.0199	0.0115	0.0174	0.0175	0.0555	0.0281	Thymol methyl ether[22]
167.106656	167.106669	4	$C_{10}H_{14}O_2$	-0.077	0.0695	N.D	0.2036	0.1173	N.D	N.D	0.1159	0.0187	Perillic acid
169.049535	169.049531	5	$C_8H_8O_4$	0.025	0.0330	0.0243	0.1400	0.0807	0.0112	0.0066	N.D	N.D	Vanillic acid
169.122306	169.122319	3	$C_{10}H_{16}O_2$	-0.075	0.0357	0.0235	0.1323	0.0762	0.0245	0.0142	0.0579	0.0109	Ascaridole
171.028800	171.028803	5	$C_7H_6O_5$	-0.019	0.0065	N.D	0.0077	0.0045	N.D	N.D	N.D	N.D	Gallic acid[35]
173.044450	173.044454	4	$C_7H_8O_5$	-0.027	0.0126	0.0075	0.0509	0.0293	0.0050	N.D	N.D	N.D	Dehydroshikimic acid
175.060100	175.060121	3	$C_7H_{10}O_5$	-0.122	0.0114	0.0418	N.D	N.D	0.0135	0.0094	0.0076	N.D	Shikimic acid[35,34,41]
176.070605	176.070592	7	$C_{10}H_9NO_2$	0.073	0.0030	N.D	N.D	N.D	N.D	N.D	N.D	N.D	Indole-3-acetic acid
178.086255	178.086262	6	$C_{10}H_{11}NO_2$	-0.038	0.0085	N.D	N.D	N.D	N.D	N.D	N.D	N.D	Indole-3-ethanol
179.033885	179.033885	7	$C_9H_6O_4$	0.002	0.0192	0.0185	0.1560	0.0899	0.0040	N.D	N.D	N.D	Aesculetin

Complementary analysis by GC-APCI-timsTOF



Complementary analysis by GC-APCI-timsTOF





Doctoral defence of Omolara Mofikoya:

"Chemical fingerprinting of conifer needle extracts by ultrahigh-resolution mass spectrometry"

December 19, 2022 UEF Chemistry @ Joensuu


Thank you!
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EASTERN FINLAND
EU FT-ICR MS
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