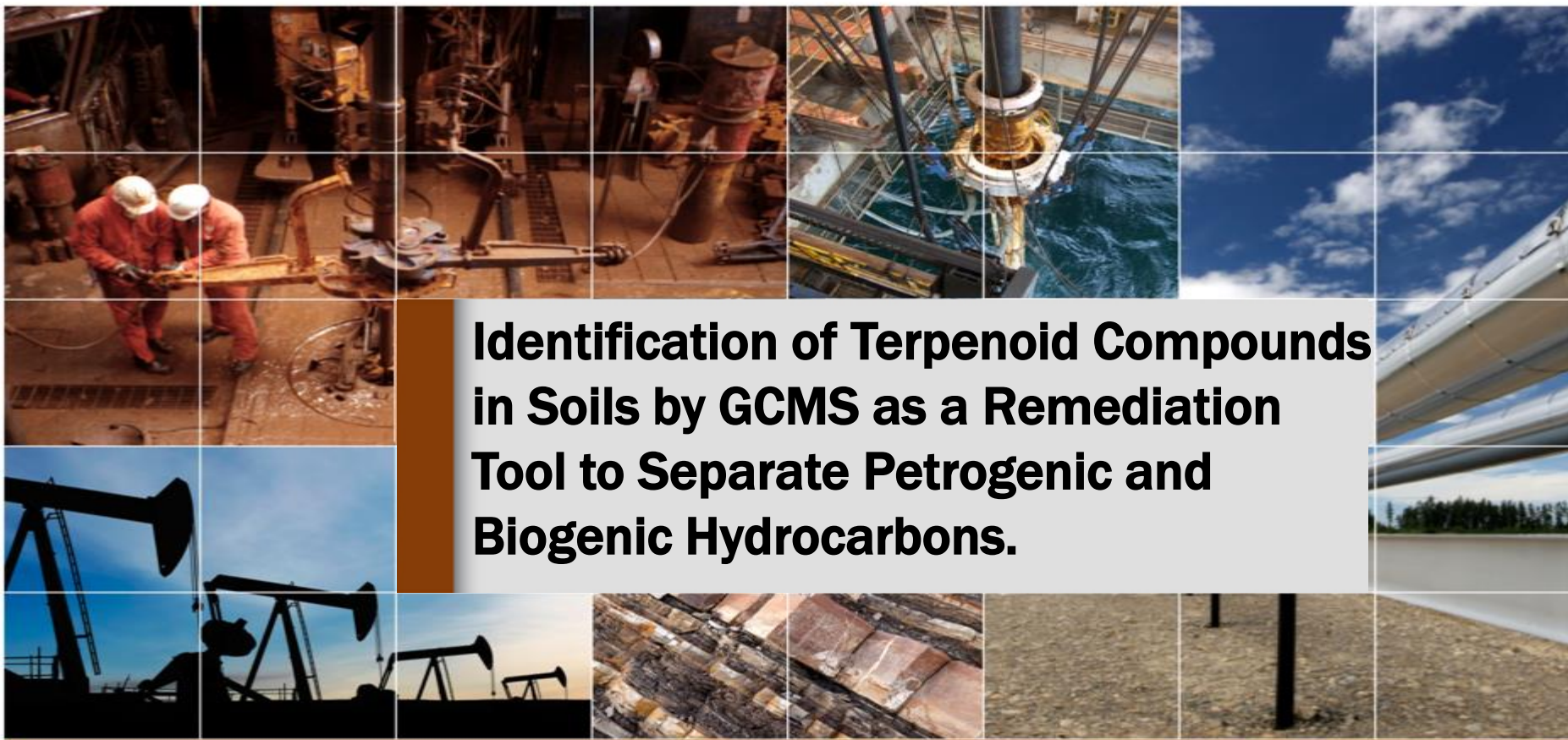




**Identification of Terpenoid Compounds
in Soils by GCMS as a Remediation
Tool to Separate Petrogenic and
Biogenic Hydrocarbons.**

AGAT Laboratories



Canadian Science and Technology
in Action  Coast to Coast

Authors

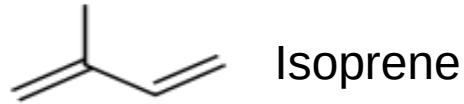
Presented by: Nathan Scott, P. Chem, AGAT Laboratories

Co-Authored by: Ron Brockbank, PhD, AGAT Laboratories

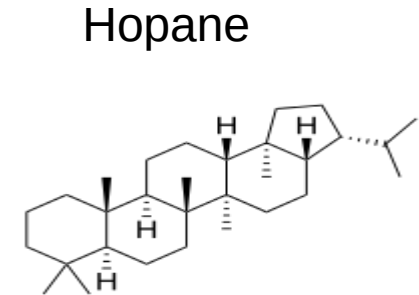
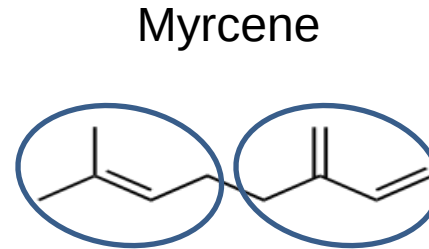
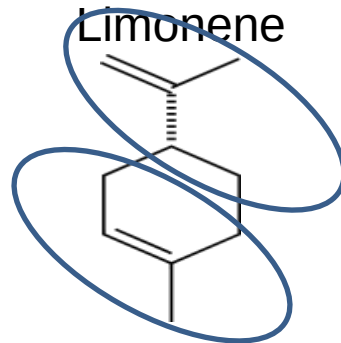
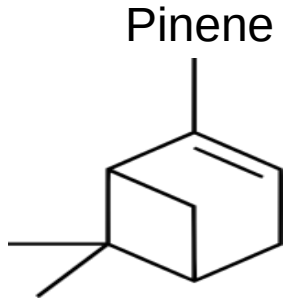
Acknowledgement: Court Sandau, PhD, Chemistry Matters

Terpenes and Terpenoids

- **Terpenes** are naturally occurring compounds formed from linked *isoprene* units.



Typical examples of common terpenes include:

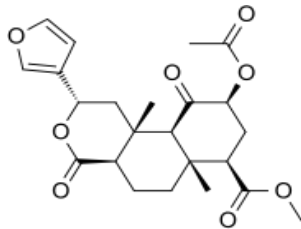


Terpenes and Terpenoids

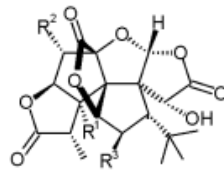
- **Terpenoids** are naturally occurring compounds formed from linked *isoprenoid* units. Isoprenoids are modified isoprenes.

Typical examples of common terpenoids include:

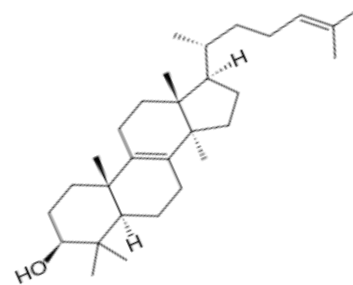
Salvinorin A



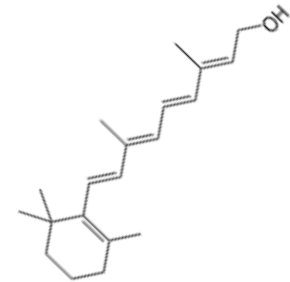
Ginkgolides



Lanosterol



Retinol (Vit. A)



Terpenes and Terpenoids

Common Uses

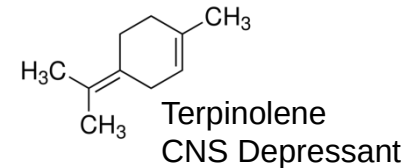
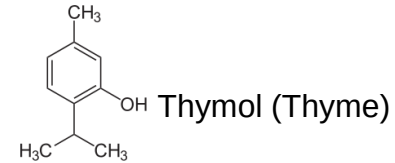
- Commonly found in all organisms, including plants, moss, and fungi in Canadian Forests and Wetlands.

- Commonly used in a number of industries including

- Fragrance/Flavors: citrus, pine, thyme
- Cleaners: Limonene Cleaner, Turpentine (Pinene) Solvents
- Pharmaceuticals and Pharmaceutical Synthesis

- Long term persistence of some terpenoids leads to them being useful biomarkers in Oil Spill Forensics

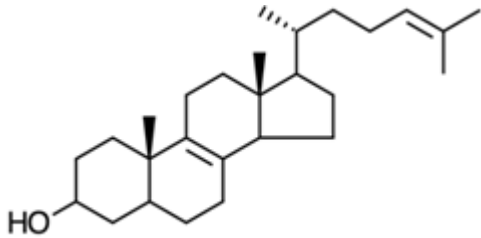
- Hopanes and Steranes



Terpenes and Terpenoids

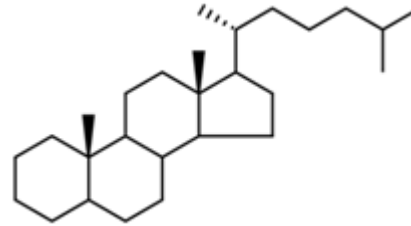
Diagenesis - the physical and chemical changes occurring during the conversion of sediment to sedimentary rock.

Sterols to Steranes



Cholestadienol

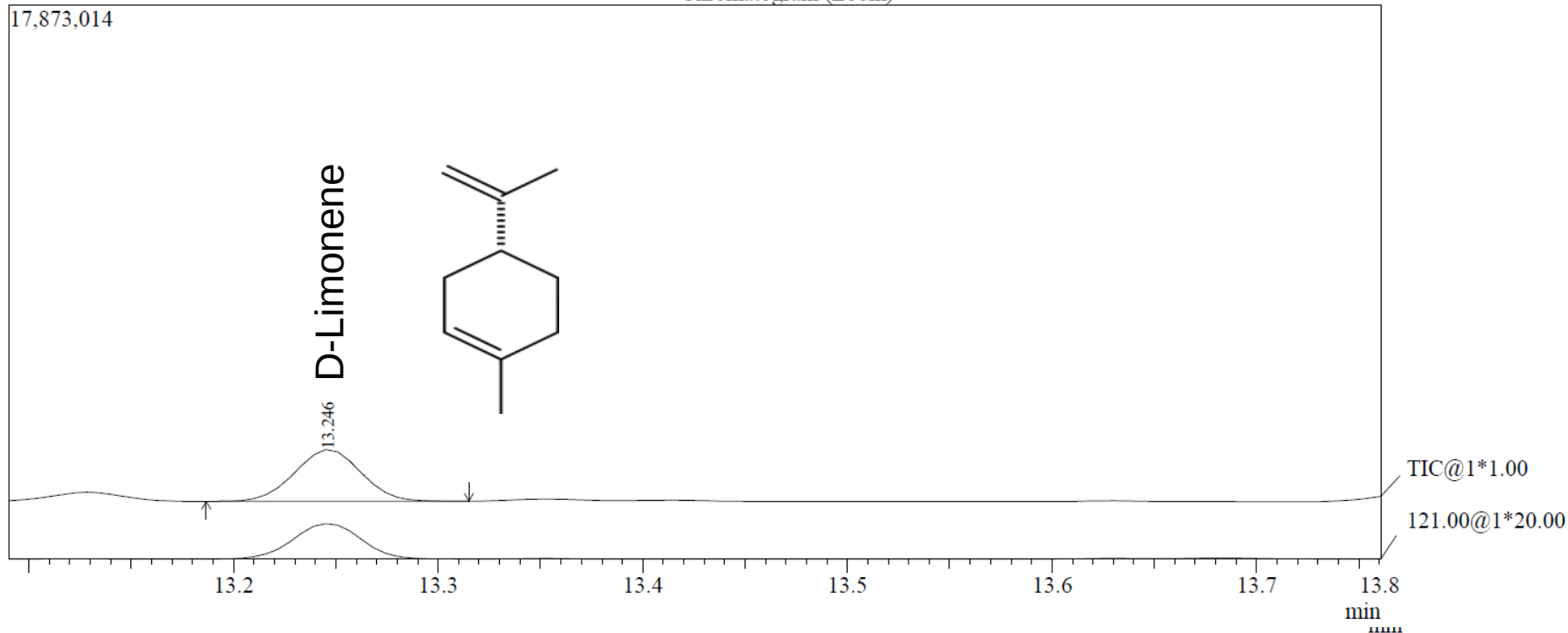
Diagenesis



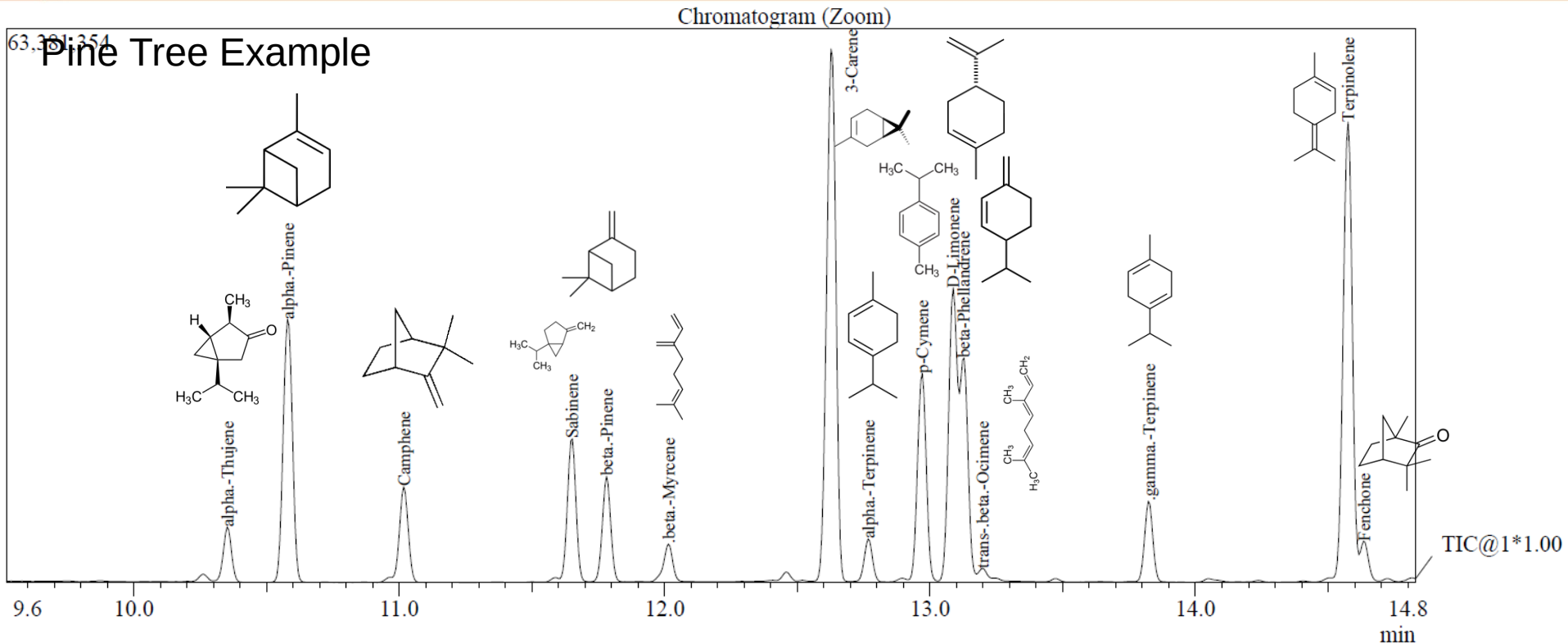
Cholestane

Terpenes and Terpenoids

Chromatogram (Zoom)

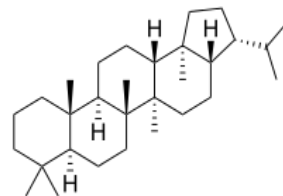


Terpenes and Terpenoids

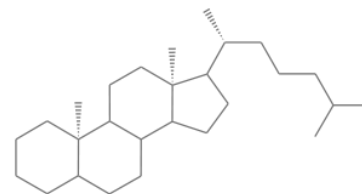


Where do they come from?

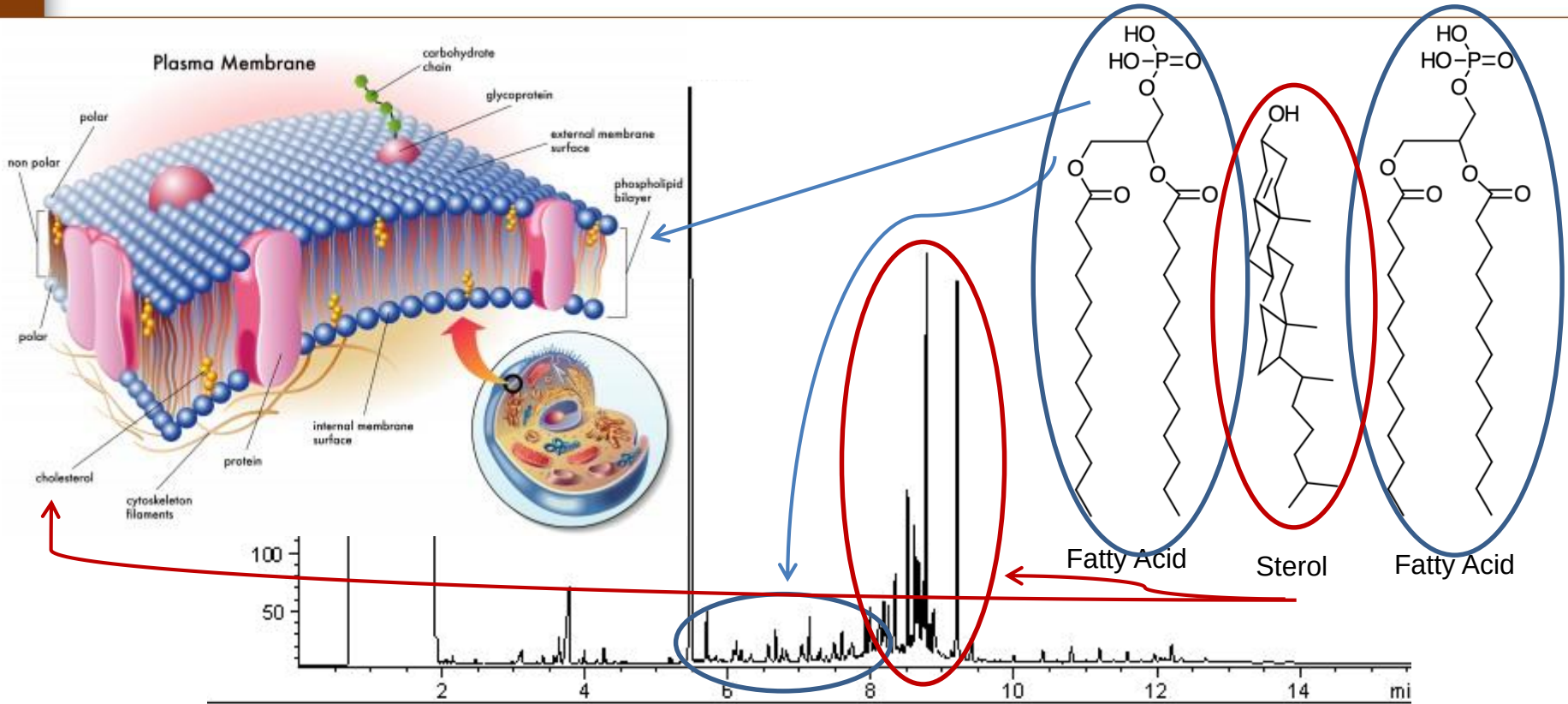
Terpanes – Originate from Prokaryotes (Archaea and Bacteria)



Steranes – Originate from Eukaryotes (Plants and Animals)



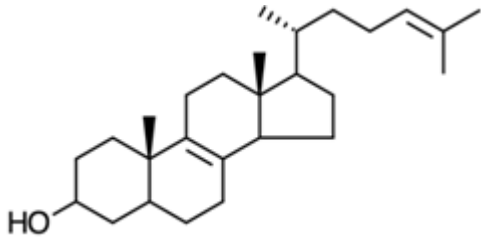
Where do they come from?



Where do they come from?

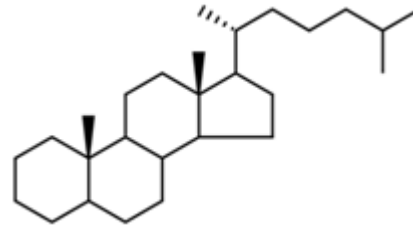
Diagenesis - the physical and chemical changes occurring during the conversion of sediment to sedimentary rock.

Sterols to Steranes



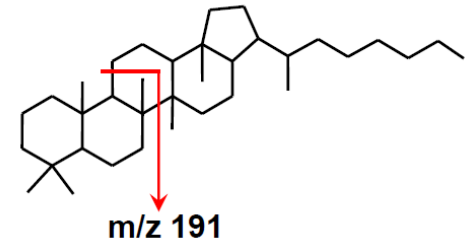
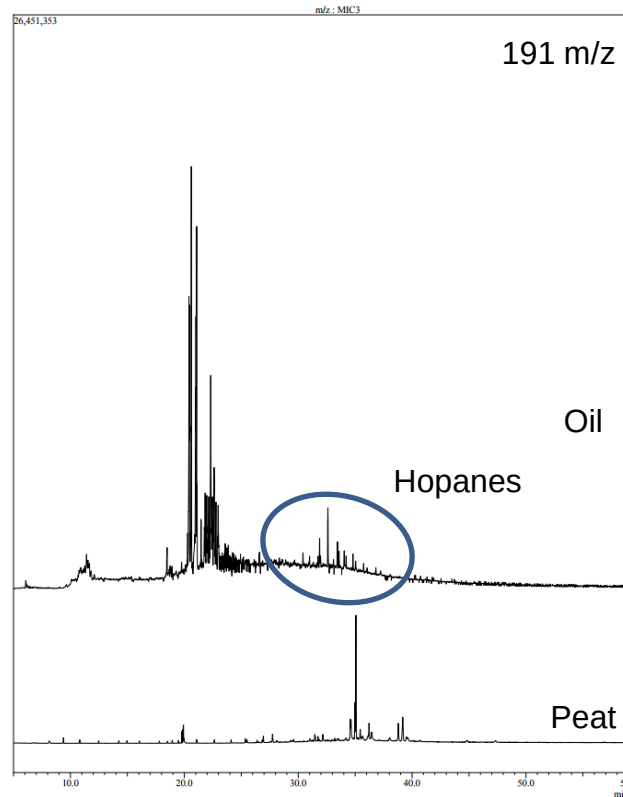
Cholestadienol

Diagenesis

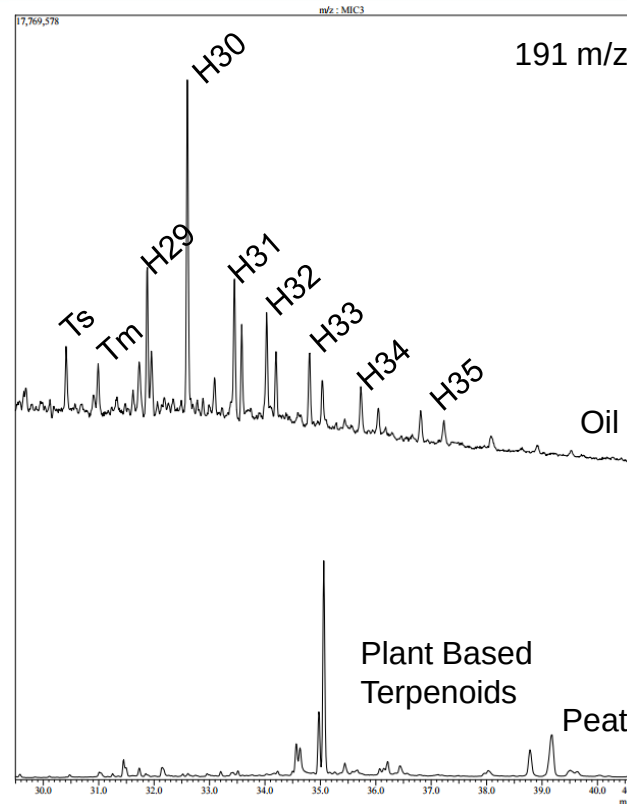


Cholestane

Oil Biomarkers - Hopanes



Oil Biomarkers - Hopanes



Ts = 18 α (H),21 β (H)-22,29,30-trisnorhopane

Tm = 17 α (H),21 β (H)-22,29,30-trisnorhopane

H29 = 17 α (H),21 β (H)-30-norhopane

H30 = 17 α (H),21 β (H)-hopane

H31 = 22S-17 α (H),21 β (H)-30-homohopane

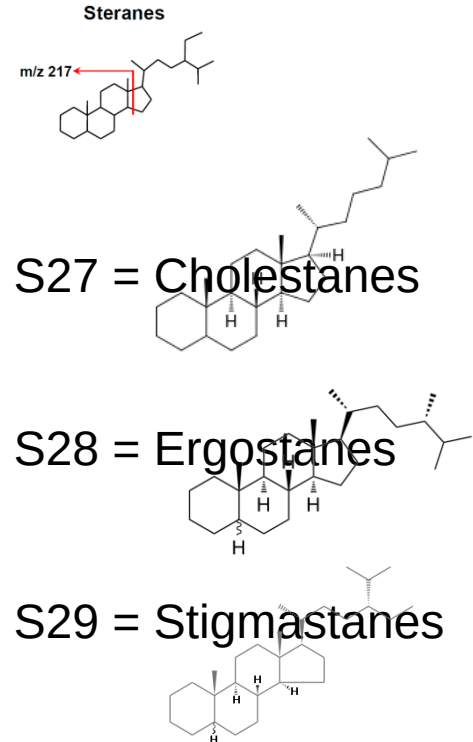
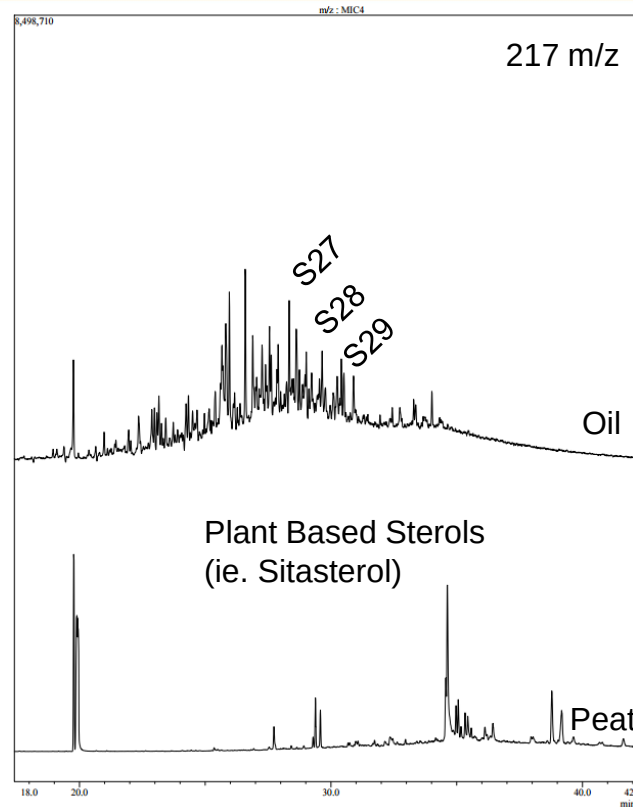
H32 = 22S-17 α (H),21 β (H)-30,31-dihomohopane

H33 = 22S-17 α (H),21 β (H)-30,31,32-trihomohopane

H34 = 22S-17 α (H),21 β (H)-30,31,32,33-tetrakishomohopane

H35 = 22S-17 α (H),21 β (H)-30,31,32,33,34-pentakishomohopane

Oil Biomarkers - Steranes



Case Study Example

- Petroleum release in a peat wetlands.
- Medium to heavy crude oil cleanup.



Reference:



chemistry
matters

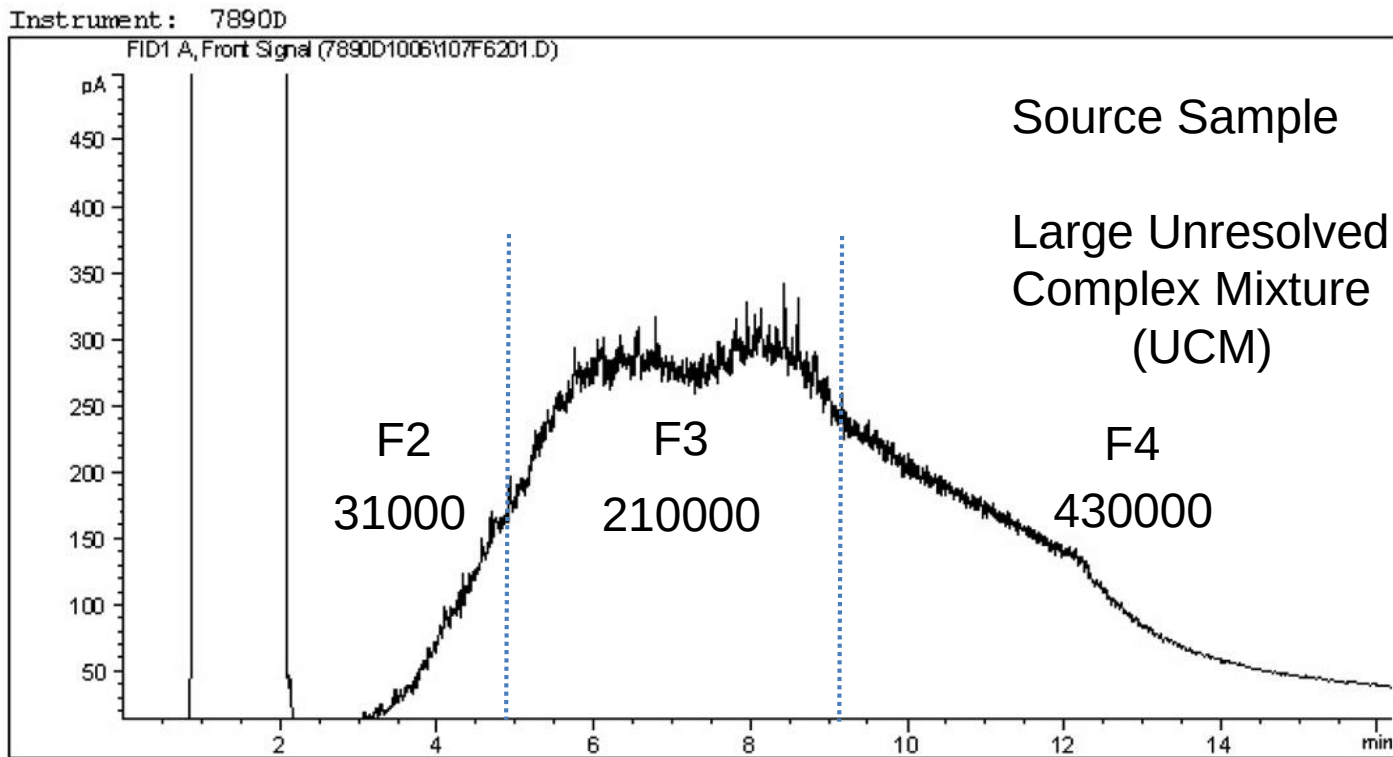
Case Study Example

Petroleum Hydrocarbons (PHC's)

F3 Fraction Above Guideline

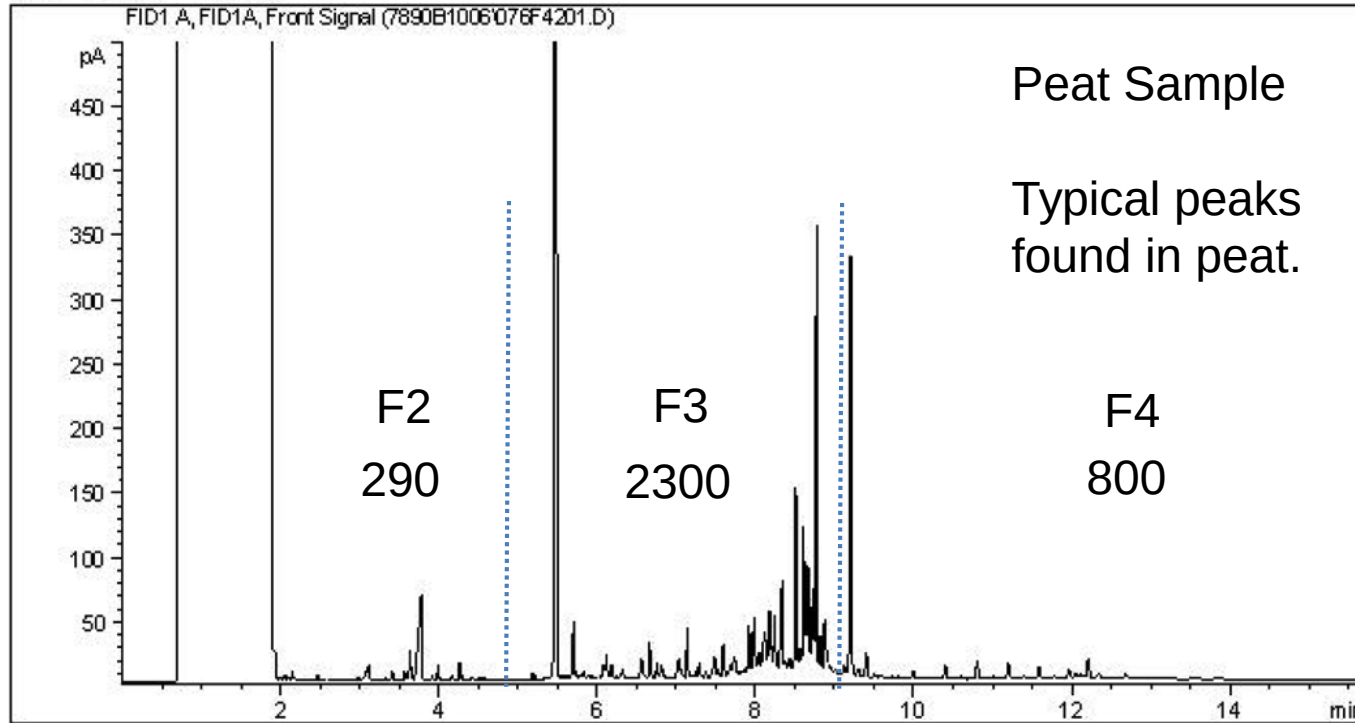
Sample	BTEX/F1 (C6 - C10)	F2 (C>10-C16)	F3 (C>16-C34)	F4 (C>34)
Sample 1	<53	<94	1300	<470
Sample 2	<51	<91	980	<460
Sample 3	<59	<110	780	<530
Sample 4	<35	82	1100	<310
Sample 5	<47	<85	1300	<420
Sample 6	<41	290	2300	800
Sample 7	<44	<79	760	<400
Sample 8	<52	<93	750	<460
Sample 9	<44	<79	1400	<400
Sample 10	<45	81	870	<400
Sample 11	<61	150	1600	<540
Sample 12	<80	<140	1000	<710
Source 1	49	31000	210000	430000
Beneath Source 1	<23	<42	700	210
AB T1 - Coarse, Surface, Natural Areas	210	150	300	2800

Case Study Example



Case Study Example

Instrument: 7890B



Case Study Example

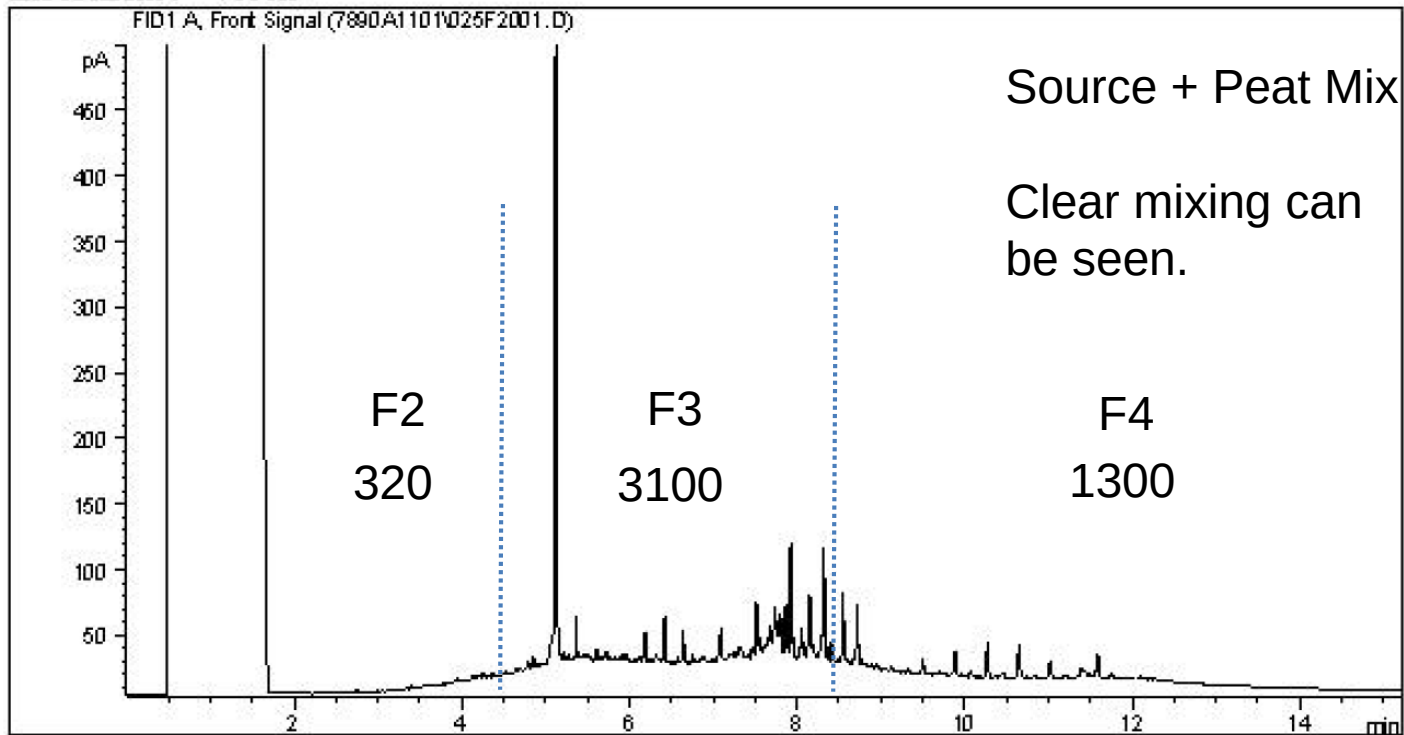
Petroleum Hydrocarbons (PHC's)

F3 Fraction Above Guideline

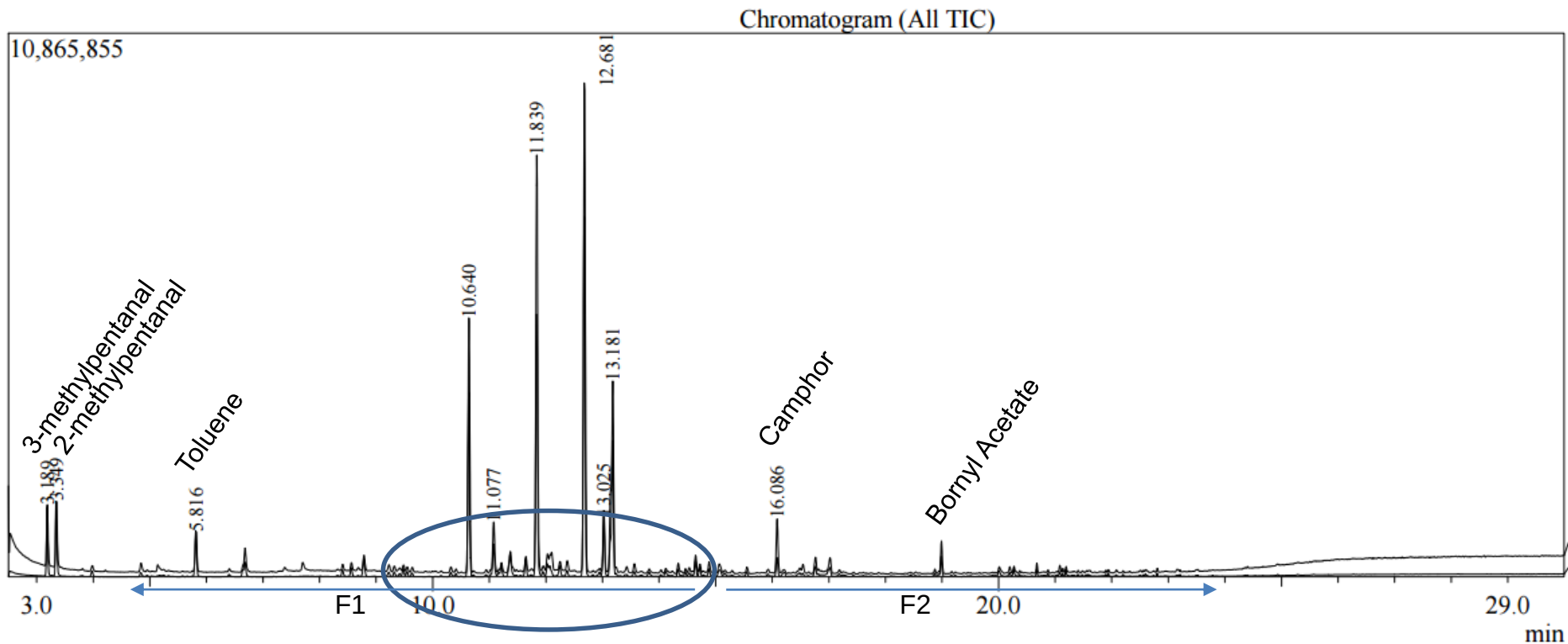
Sample	BTEX/F1 (C6 - C10)	F2 (C>10-C16)	F3 (C>16-C34)	F4 (C>34)
Sample 1	<53	<94	1300	<470
Sample 2	<51	<91	980	<460
Sample 3	<59	<110	780	<530
Sample 4	<35	82	1100	<310
Sample 5	<47	<85	1300	<420
Sample 6	<41	290	2300	800
Sample 7	<44	<79	760	<400
Sample 8	<52	<93	750	<460
Sample 9	<44	<79	1400	<400
Sample 10	<45	81	870	<400
Sample 11	<61	150	1600	<540
Sample 12	<80	<140	1000	<710
Source 1	49	31000	210000	430000
Beneath Source 1	<23	<42	700	210
AB T1 - Coarse, Surface, Natural Areas	210	150	300	2800

Case Study Example

Instrument: 7890A

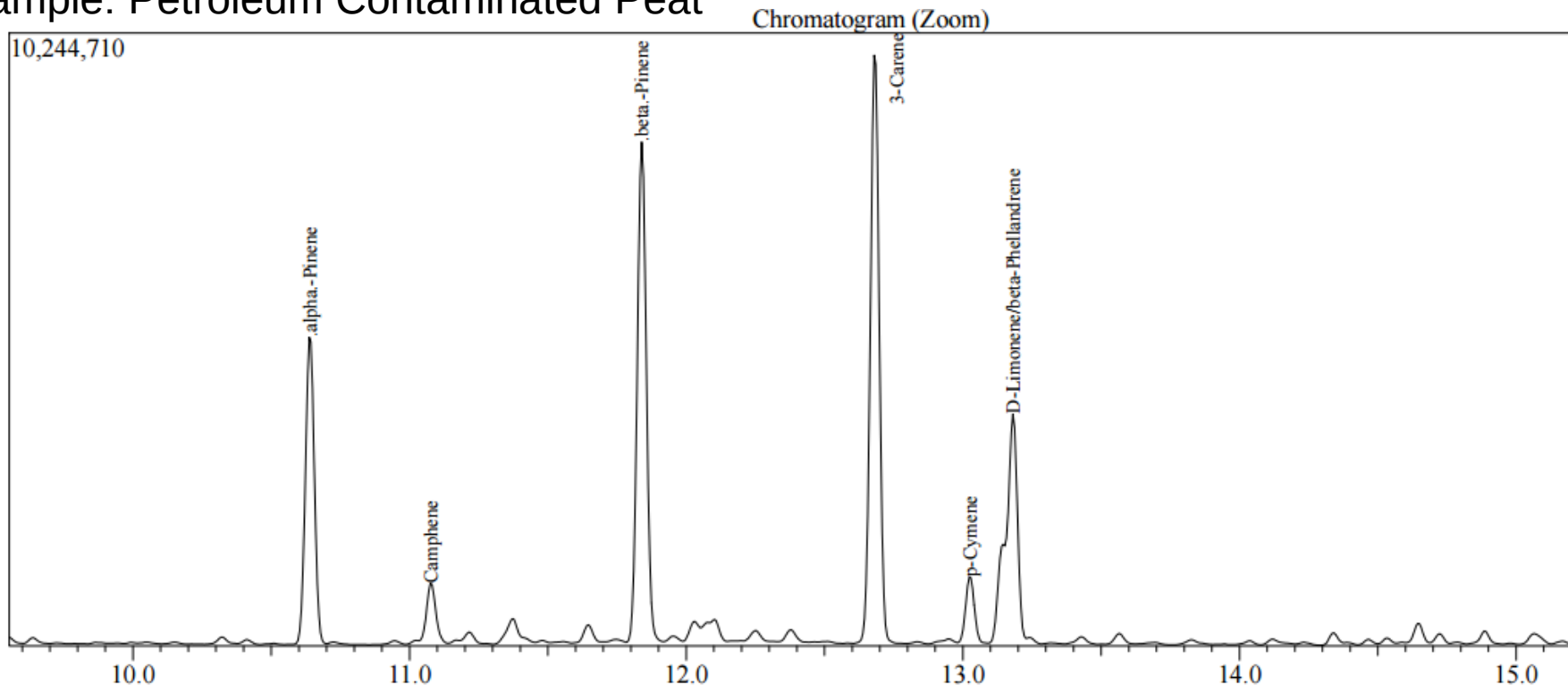


Terpenoids in Peat

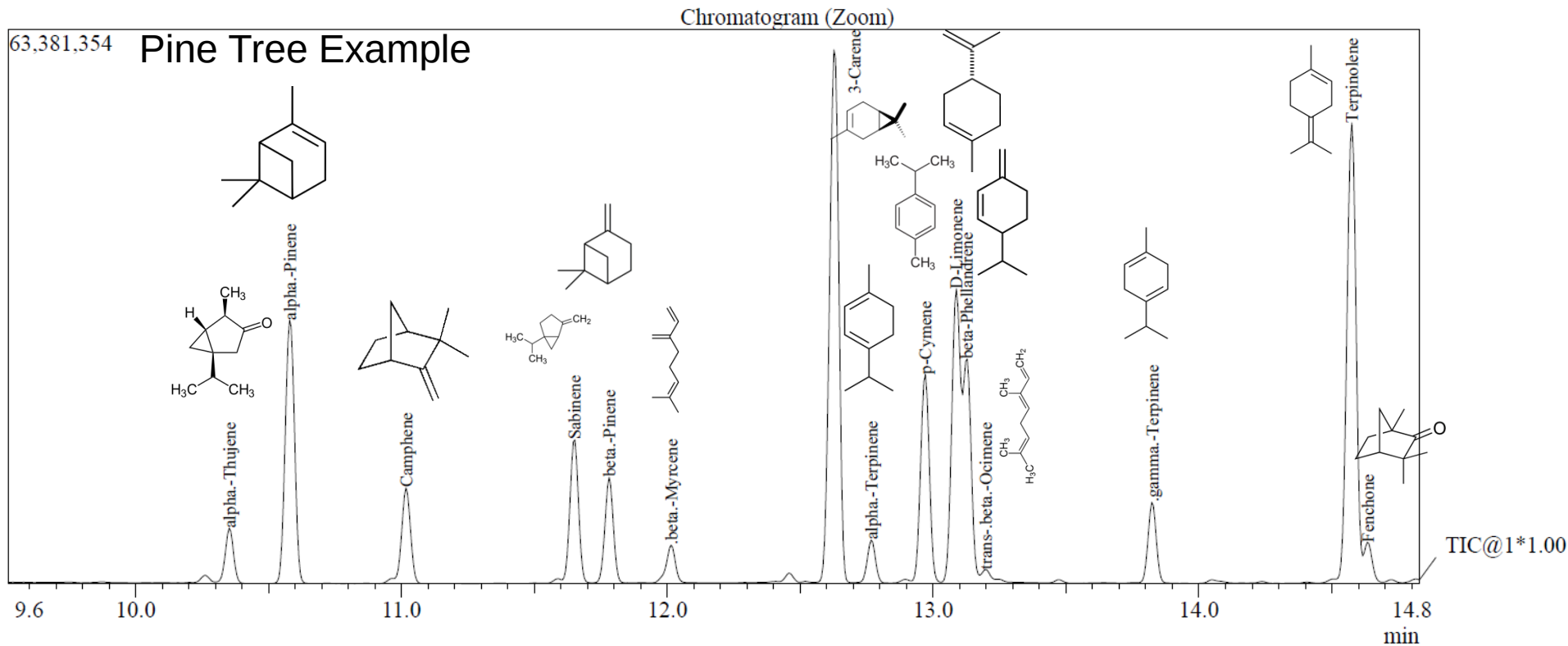


Terpenoids in Peat

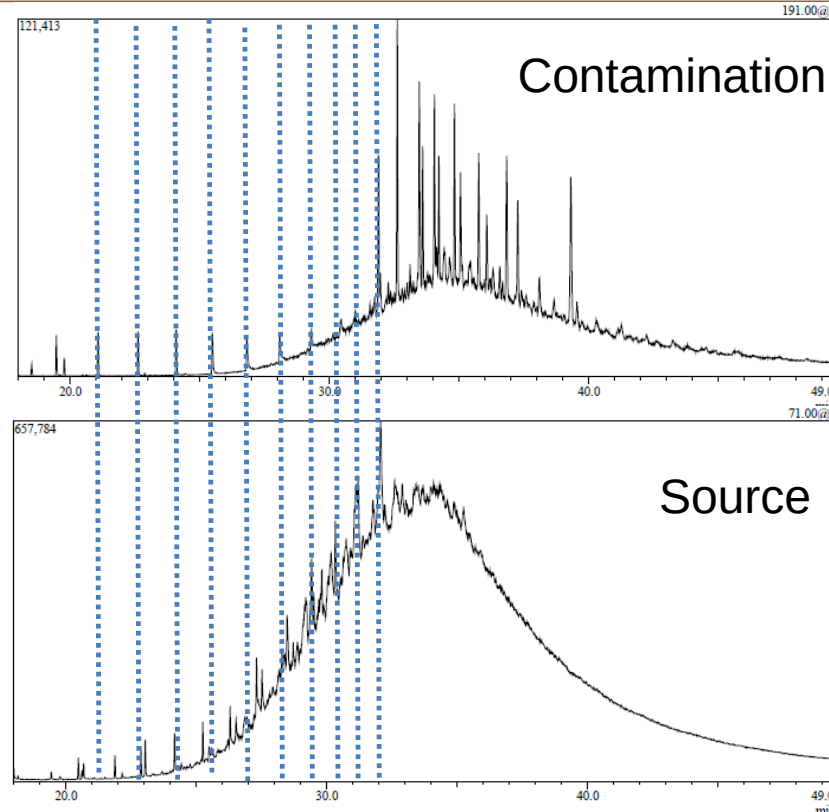
Example: Petroleum Contaminated Peat



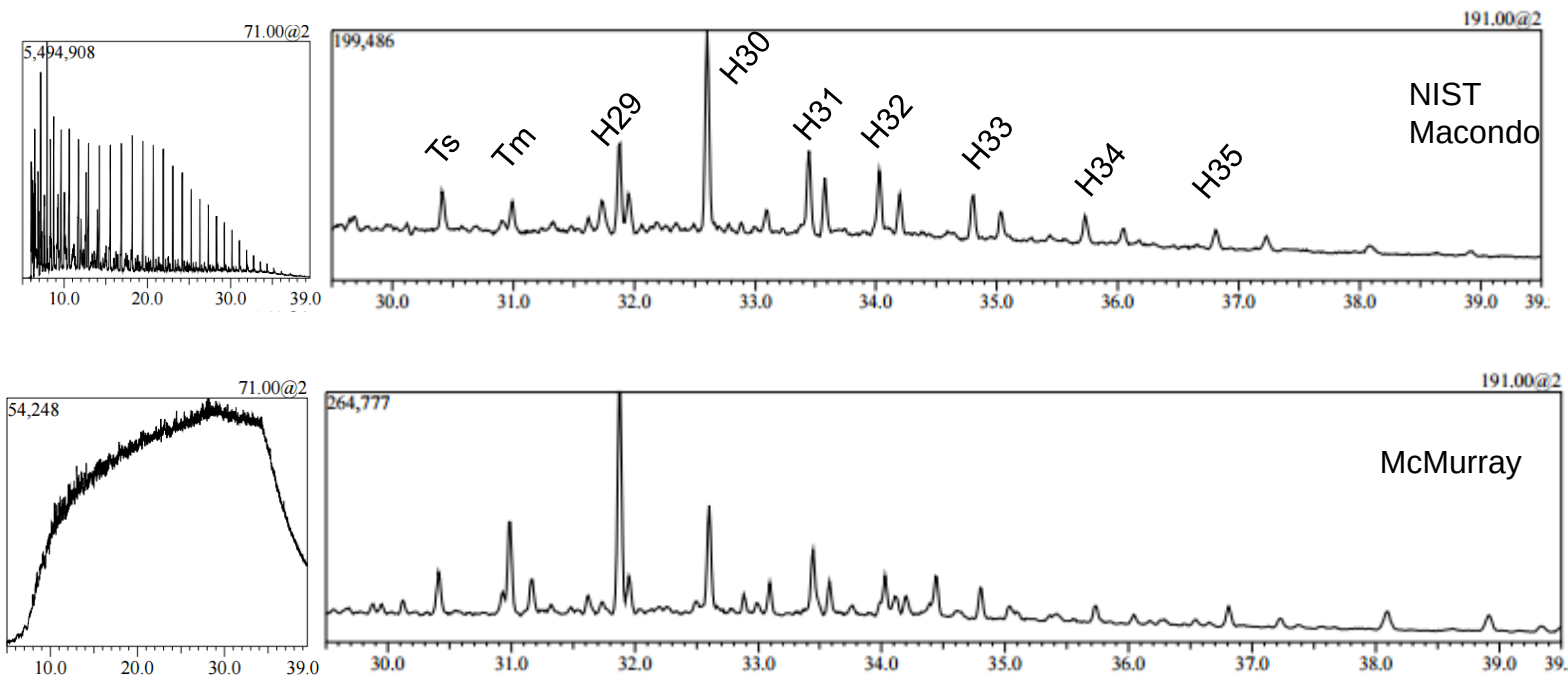
Terpenes and Terpenoids



Hopanes in Gear Oil



Hopanes in WCSB Oils



Hopanes in WCSB Oils

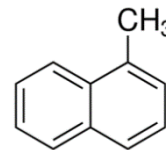
Diagnostic Ratios

	Tm/Ts	H30/H29	H31S/H31R	H32S/H32R	H33S/H33R
NIST Macando	0.83	2.42	1.54	1.47	1.63
Belly River	0.12	2.51	2.08	1.90	1.74
Frobisher Beds	1.00	1.16	1.77	1.63	1.59
Glaucinitic	1.56	1.63	1.58	1.60	1.45
Leduc	0.86	1.97	1.82	1.69	1.46
McMurray	2.15	0.53	2.20	1.66	1.83

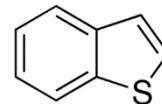
End of the Story?

Biomarkers Continued...

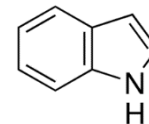
- Polycyclic Aromatic Hydrocarbons (PAHs/Alkyl-PAHs)



- Polycyclic Aromatic Sulfur Heterocycles (PASHs)



- Polycyclic Aromatic Nitrogen Heterocycles (PANHs)



- Isotopes $\delta^{13}\text{C}$



Thank You

Questions and Discussion

Terpenes and Terpenoids

