PetroOrg© Software

A chemically intelligent, state of the art software developed specifically for petroleum data analysis acquired by mass spectrometry.

PetroOrg provides a platform for automated, unequivocal elemental composition assignment, automated generation of classic Petroleomic diagrams, automated report construction, and much more.
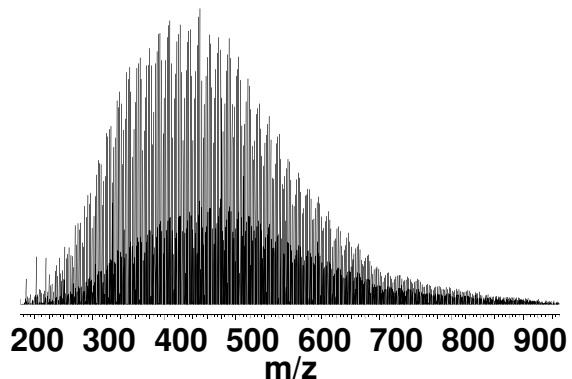
http://www.petroorg.com

The PetroOrg Petroleomic Workflow

FT-ICR MS

~8000 peaks > 6σ
$m/\Delta m_{50\%} = 600{,}000$ at m/z 500

200 300 400 500 600 700 800 900
m/z

1. **Recalibration**
2. **Elemental Composition Assignment**

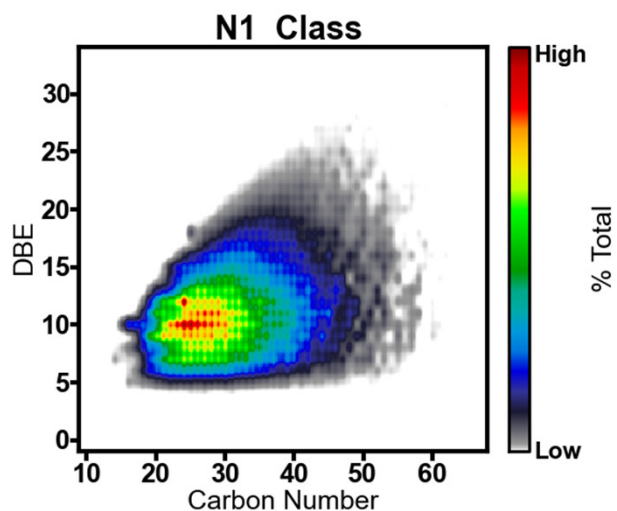| Elemental Composition	Measured Mass	Calculated Mass	ppm error
$C_{29}H_{42}N_1$	404.3323	404.33227	0.16
$C_{30}H_{44}N_1$	418.348	418.34792	0.18
$C_{31}H_{46}N_1$	432.3638	432.36357	0.48
$C_{32}H_{50}N_1$	446.3793	446.37922	0.15
$C_{27}H_{47}O_2$	403.3582	403.35815	0.09
$C_{28}H_{49}O_2$	417.3738	417.37380	-0.13
$C_{29}H_{51}O_2$	431.3895	431.38945	0.18
$C_{30}H_{53}O_2$	445.4052	445.40510	0.12
$C_{31}H_{55}O_2$	459.421	459.42075	0.49
$C_{32}H_{57}O_2$	473.4364	473.43640	-0.07

3. Classification

Carbon Number

Heteroatom Composition
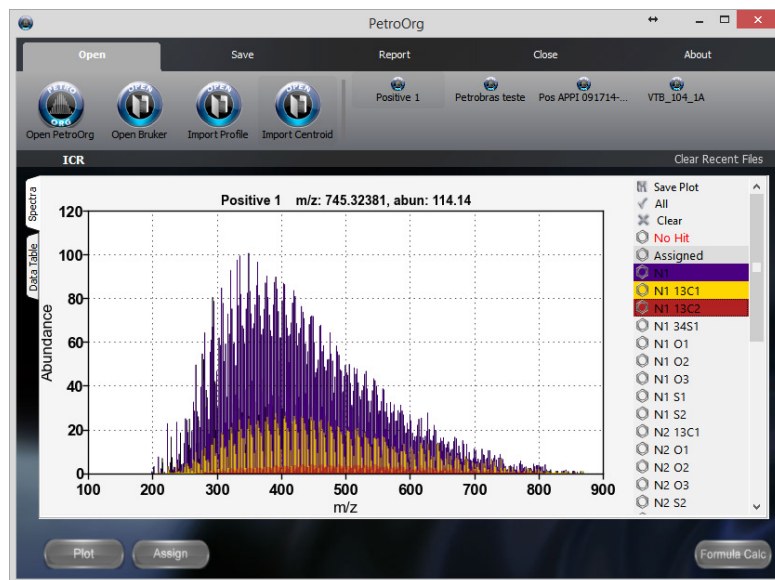
Double Bond Equivalent (DBE)
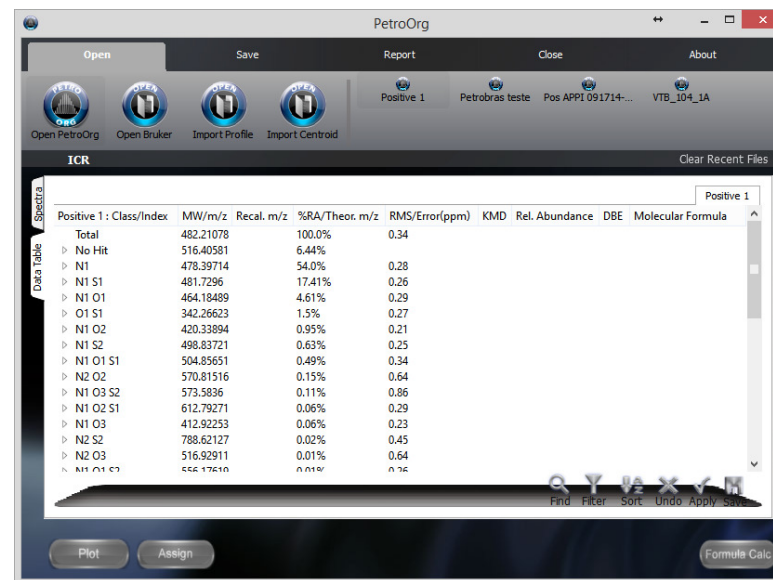
$$DBE = C - \frac{H}{2} + \frac{N}{2} + 1$$

4. Data Visualization

N1 Class
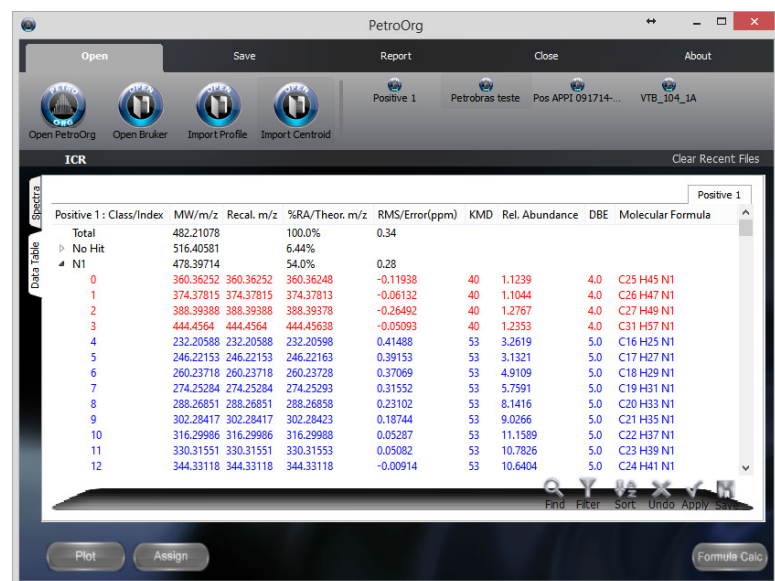
DBE vs Carbon Number

% Total (High / Low)

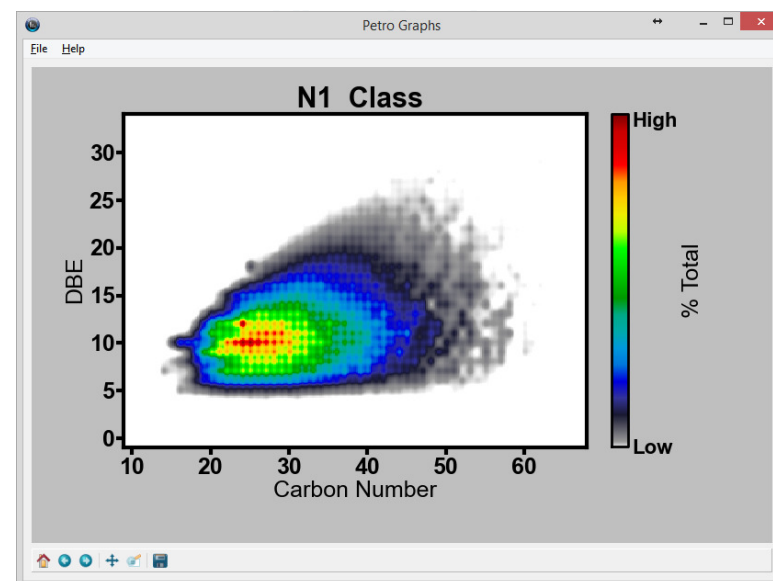## Dynamic and Flexible Class Visualization

Data Organization by Heteroatomic Class

Complete Molecular Characterization and Detail for Each Class

Comprehensive, Customizable, and Batch Data Visualization

Integration with the Bruker solariX

solariX® XR data

m/z

m/z
**Carbon Number
Heteroatom Class
DBE**

1. **Recalibration**

2. **Elemental Composition Assignments**

3. **Classification**

4. **DATA VISUALIZATION**

5. **REPORT GENERATION**

BATCH PROCESSING & DATA VISUALIZATION