

# **Acidic and Neutral Polar NSO Compounds in Heavily Biodegraded Oils Characterized by Negative-Ion ESI FT-ICR MS**

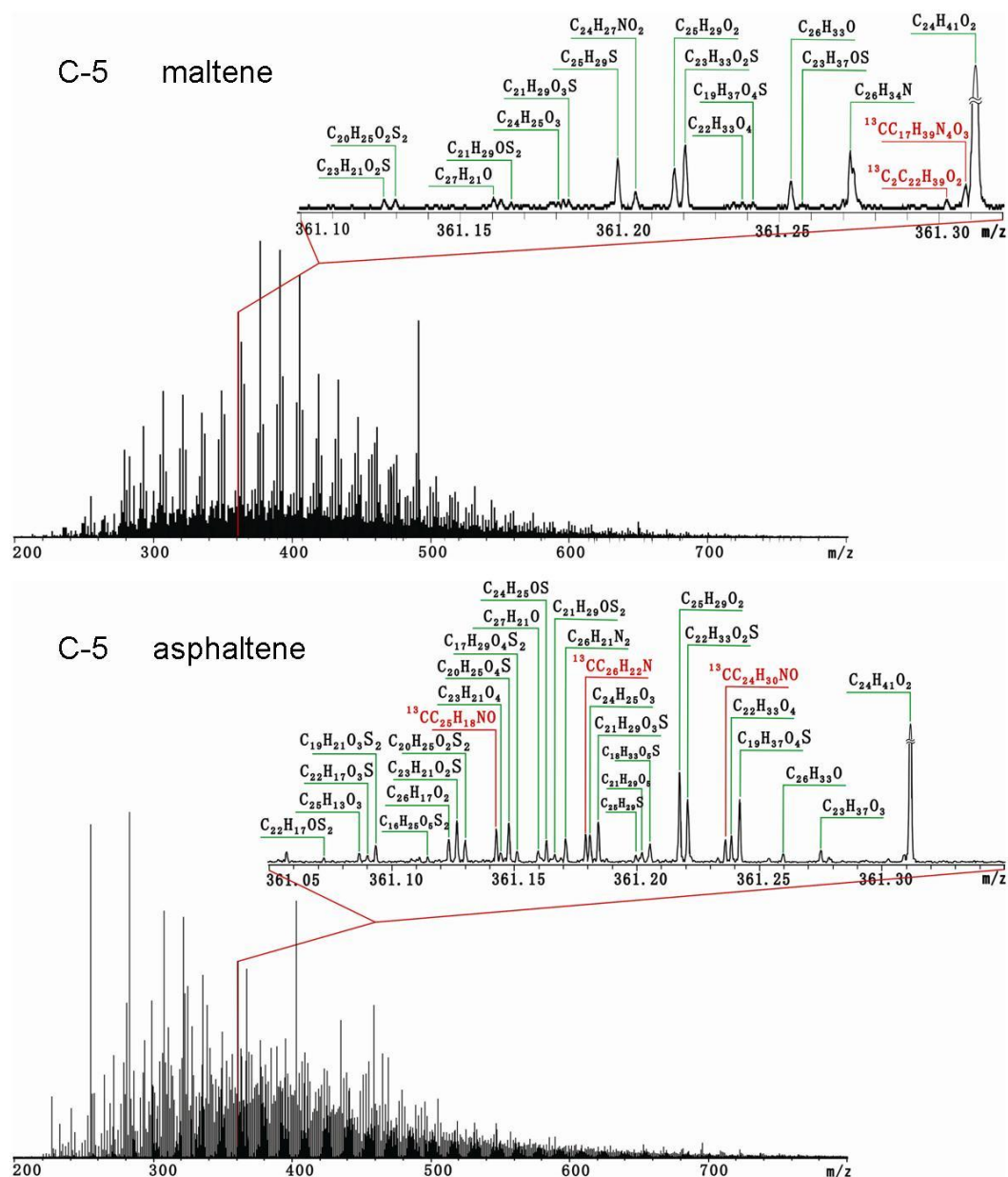
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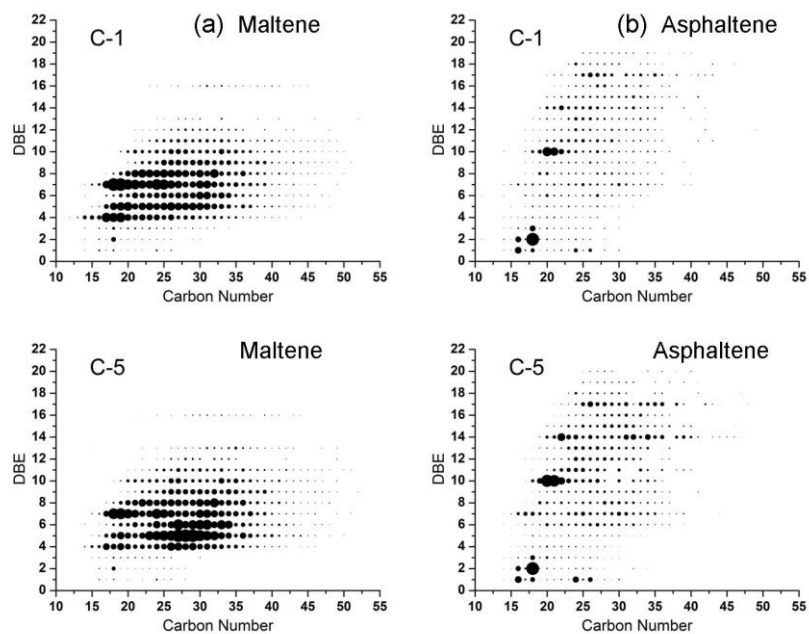
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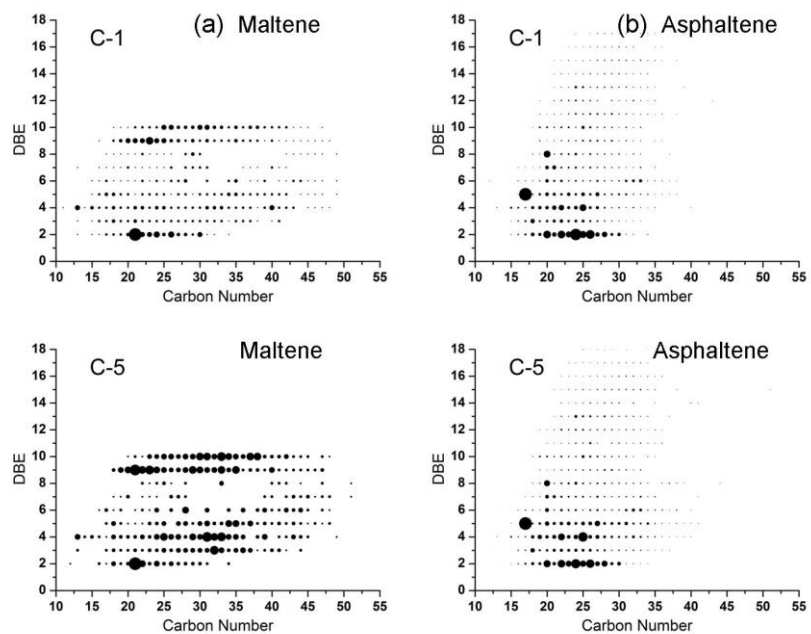
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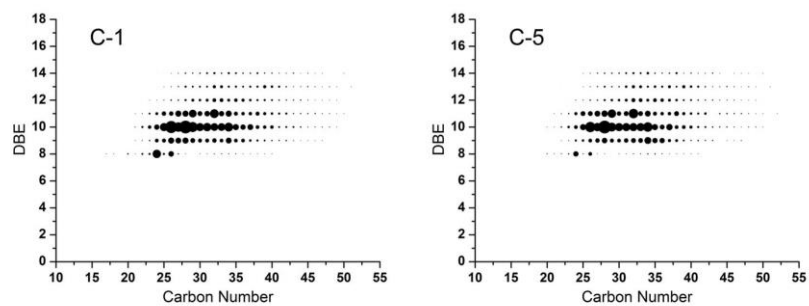
**Figure S-1. Negative-ion electrospray FT-ICR mass spectra of maltene and asphaltene fractions separated from tar sand bitumen sample C-5. The inset shows the expanded 300 mDa mass scale at  $m/z$  361, indicating the complexity of the polar NSO compound composition. The asphaltene fraction exhibits more peaks than the maltene fraction.**



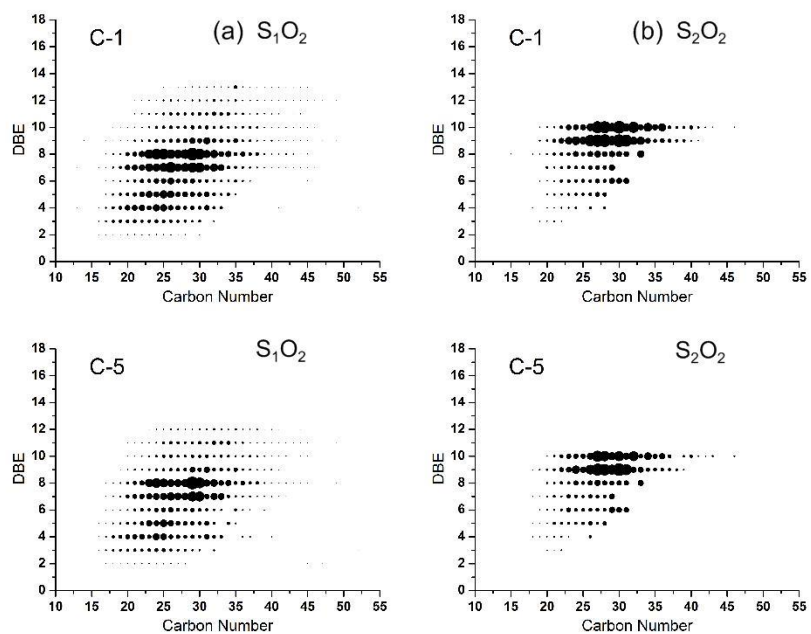
**Figure S-2. Iso-abundance plots of DBE versus carbon number of  $O_3$  class in maltene fractions of bitumen samples C-1 and C-5.**



**Figure S-3. Iso-abundance plots of DBE versus carbon number of O<sub>4</sub> class in maltene fractions of bitumen samples C-1 and C-5.**



**Figure S-4. Iso-abundance plots of DBE versus carbon number of  $S_1$  class in maltene fractions of bitumen samples C-1 and C-5.**



**Figure S-5. Iso-abundance plots of DBE versus carbon number of (a) S<sub>1</sub>O<sub>2</sub> class and (b) S<sub>2</sub>O<sub>2</sub> class in maltene fractions.**

**Table 1 Selected properties of tar sand bitumen samples**

| Sample No. | PM index | $\delta^{13}\text{C}(\text{‰})$ | %N   | %S   | %O   | %Mal | %Asph |
|------------|----------|---------------------------------|------|------|------|------|-------|
| C-1        | 6        | -30.3                           | 0.47 | 4.88 | 3.15 | 94.5 | 5.5   |
| C-2        | 6-7      | -30.3                           | 0.48 | 5.14 | 2.49 | 89.1 | 10.9  |
| C-3        | 6-7      | -30.4                           | 0.51 | 5.21 | 2.45 | 87.4 | 12.6  |
| C-4        | 6-7      | -30.4                           | 0.50 | 4.93 | 2.13 | 85.1 | 14.9  |
| C-5        | 7        | -30.3                           | 0.49 | 4.99 | 1.89 | 83.9 | 16.1  |

**PM index, Biodegradation index described in Peters et al.<sup>77</sup>;  $\delta^{13}\text{C}(\text{‰})$ , bulk carbon isotope value; %NSO, wt% polar compounds; %Mal, wt% maltene fraction; %Asph, wt% asphaltene fraction.**