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Impact of Thermal Maturity on NSO Compounds in the Qing1 Source Rocks, Songliao Basin: An ESI (+) FT-ICR MS Investigation

DR. FEI XIAO, PHD[1,2], JIANGUO YANG[1,2], YULAI YAO[1,2], SHICHAO LI[1,2] AND YIMING HUANG[1,2]

[1]Shenyang Center of China Geological Survey/Northeast Geological S&T Innovation Center of China Geological Survey
[2]Shale Oil Technology Innovation Center of China Geological Survey

Assessing thermal maturity is vital for oil/gas resource evaluation and exploration. Most studies focus on its effect on saturated/aromatic fractions in source rocks, while NSO compound fractions receive less attention (Xiao et al., 2025). ESI FT-ICR MS enables comprehensive NSO compound detection. Prior research mainly examined acidic/neutral NSO compounds in negative ion mode, with basic NSO compounds in positive ion mode receiving less attention. This study investigated NSO compound distribution/composition in positive ion mode for lacustrine oil-prone source rocks from the first member of the Upper Cretaceous Qingshankou Formation (Qing1, Songliao Basin, NE China) across thermal maturity stages. Samples from four wells (SYY1: Ro 0.53-0.58%; SYY2: 0.82-0.94%; SYY3: 1.26%; SYYD1: 1.35-1.44%) were analyzed. We identified maturity's influence on NSO compounds and proposed two new maturity indicators.

The NSO compounds detected are primarily N_x, N_1O_x, N_2O_1, O_x, and O_xS_1. Their distribution shifts with maturity. N_1 compounds dominate in medium-low maturity samples from the SYY3 and SYYD1 wells, whereas O_x dominates in high maturity samples from the SYY1 and SYY2 wells, followed by N_1 and N_1O_x. With increasing thermal maturity, abundances of N_x, N_2O_1, and O_xS_1 decline, while N_1O_x and O_x increase. The (double bond equivalent) DBE values of N_1 and N_1O_1 compounds show a strong positive correlation with R_o (Figure 1a-b), marked by a rise in high-DBE and fall in low-DBE compounds. Two novel maturity indicators were proposed: DBE_{12+15}/DBE_6-N_1 and DBE_{11+15}/DBE_9-N_1O_1, both correlating positively with R_o (Figure 1c-d). The DBE_{11+15}/DBE_9-N_1O_1 ratio, however, plateaus at medium maturity (Figure 1d), indicating it is best for assessing low-to-medium maturity samples (~0.5-1.0% R_o). The DBE_{12+15}/DBE_6-N_1 index covers a wider maturity range (~0.5-1.5% R_o). Carbon number distributions for N_1 and O_1 compounds broaden with maturity. Overall, thermal maturity strongly governs the relative abundance, DBE, and carbon number distribution of NSO compounds analyzed in positive ion mode.

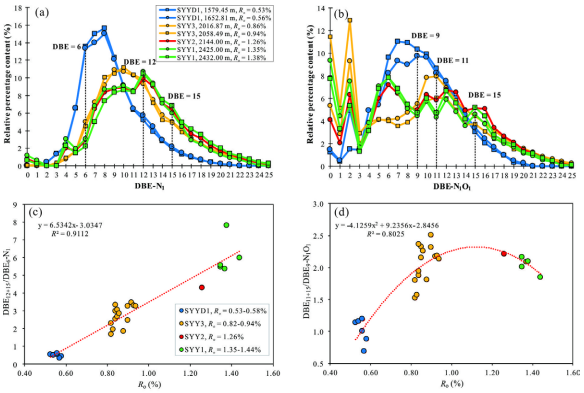


Fig. 1 DBE distribution characteristics of N_1 and N_1O_1 compounds (a-b) and correlation plots of related geochemical parameters with *Ro* (c-d) for the Qing1 source rocks.

References

Xiao, F., Yang, J., Yao, Y., Li, S., Huang, Y., & Gao, X. (2025), Acta Geologica Sinica (English Edition) 99, 840-861.

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