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# Identification, distribution and geochemical significance of benzo[b]naphthofurans and benzo[b]naphthothiophenes in source rocks from the Beibuwan Basin, South China Sea

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The distribution of benzo[b]naphthofurans (BNFs) and benzo[b]naphthothiophenes (BNTs) and their geochemical significance have been investigated for a set of delta-lacustrine mudstone samples from the Beibuwan Basin, South China Sea. BNF and BNT isomers in source rock extracts are identified in the m/z 218 and m/z 234 mass chromatograms of the aromatic fractions, respectively. The relative content of BN12F and BN21T increases as the increasing of burial depth and maturity, which is corresponding to relative higher calculated thermostability among the BNF and BNT isomers, respectively. Two maturity parameters, BNFR (abundance of BN12F relative to BN21F) and BNTR (abundance of BN21T relative to BN12T), both correlate well with vitrinite reflectance (Ro%), suggesting that these parameters are potential indicators for assessment of source rock maturity (Ro  0.5%) [1]. BNTR is more suitable for the mature stage (Ro  1.0%), as errors in measurement increase in overmaturity due to the low abundance of BN12T. The significant correlation between BNFs and DBF indicates their similar origin, likely an oxic environment with higher plant input. The thermal instability of BNFs at the overmature stage suggests that they may be converted to other compounds at high thermal maturity. The absolute concentrations of BNTs show a growing trend as maturity increases, indicating a thermal origin. Based on geological observation and molecular simulation caculations, BNTs may be generated from phenylnaphthalene isomers by incorporating a sulfur atom into biphenyl during catagenesis. This study achieves a better understanding of the occurrence and significance of BNFs and BNTs in sedimentary organic matter.

[1] Wang, Huang & Zheng (2021), Fuel 288, 119626.