

Supporting Information

Maturity-driven Generation and Transformation of Acidic Compounds in the Organic-rich Posidonia Shale as revealed by Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

Stefanie Poetz*, Brian Horsfield and Heinz Wilkes

GFZ German Research Centre for Geosciences, Telegrafenberg, D-14473 Potsdam

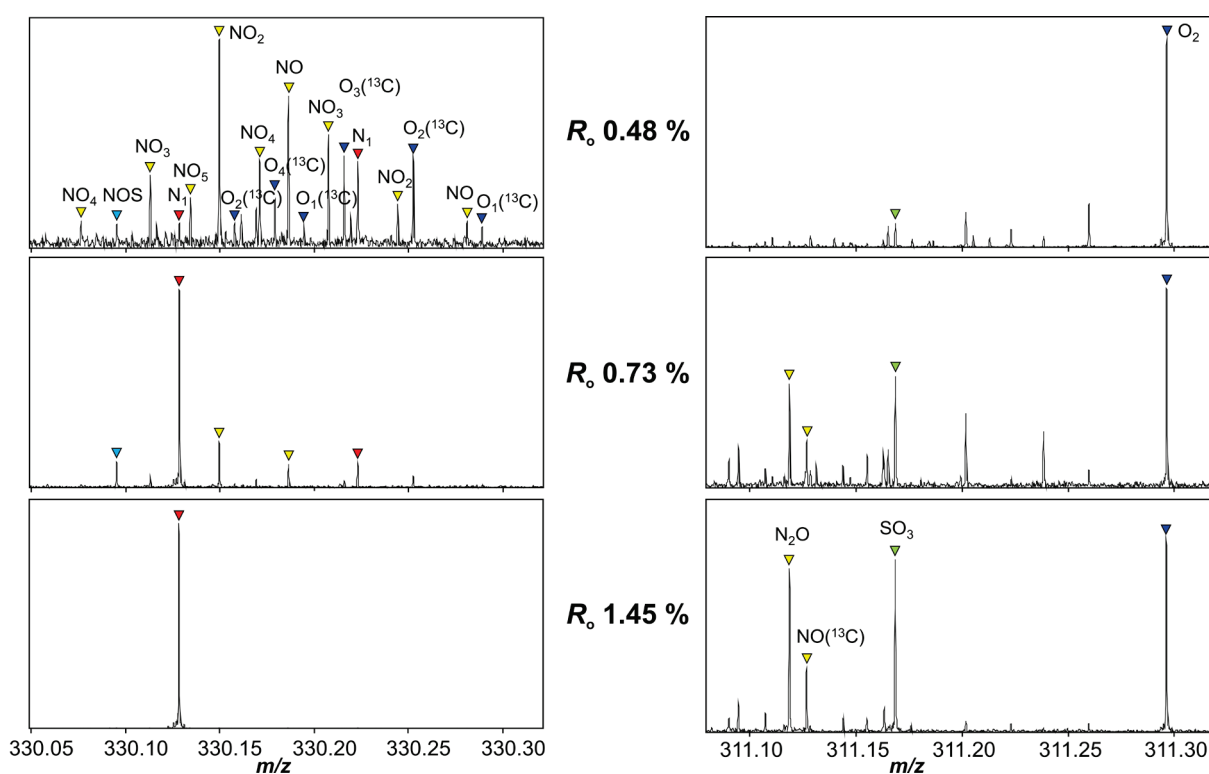


Figure SI 1: A more detailed view into the enlarged mass segments of two nominal masses m/z 330 (contains the most abundant peak in the most mature sample HAD) and m/z 311 (contains the most abundant peak in the least mature sample WE) of the WE, DO and HAD samples. The spectrum of the immature WE sample contains a number of peaks with an even nominal mass m/z 330 in low abundance representing a variety of compound types, e.g. different N1O_x compounds with 1 to 5 oxygen atoms. Almost all these compounds decrease with increasing maturity (DO sample) until there is only the signal of the N1 compounds left

at Ro 1.45 % (sample HAD). For the odd nominal mass m/z 311, the opposite is observed: for low maturities, there is only one signal of an O2 compound in the spectrum, while at Ro 1.45 %, additional signals of other compounds like N2O1 or S1O3 arise.

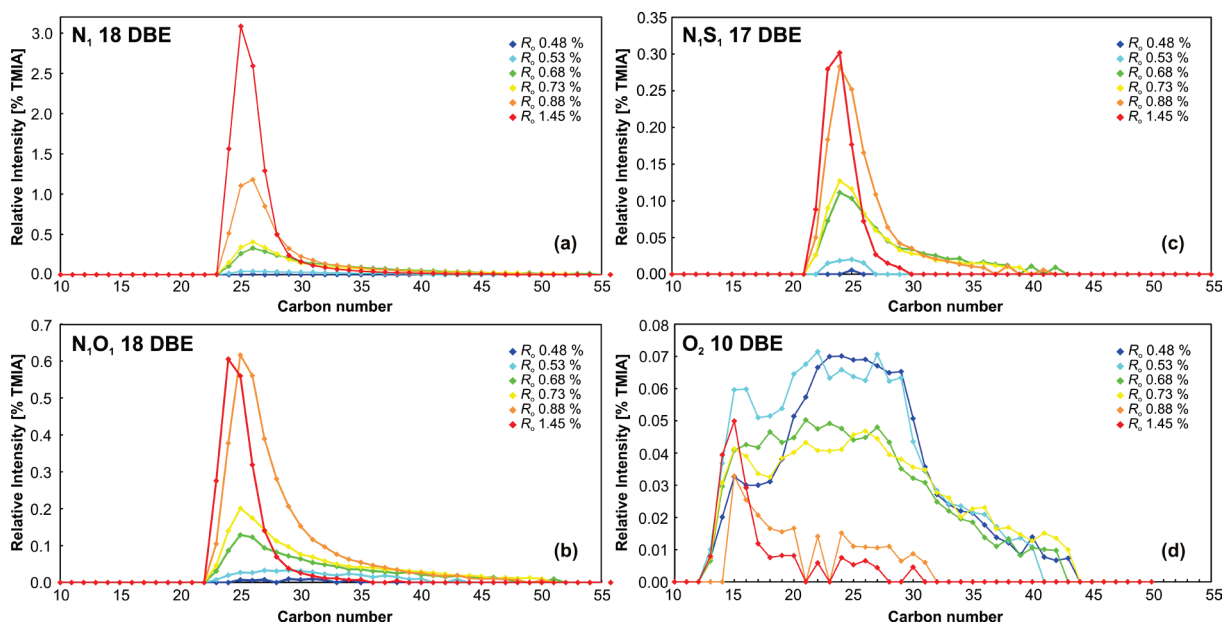


Figure SI 2: Carbon number distributions of the N₁ 18 DBE class (a), N₁O₁ 18 DBE class (b), N₁S₁ 17 DBE class (c) and O₂ 10 DBE class (d) of the six Posidonia Shale samples.

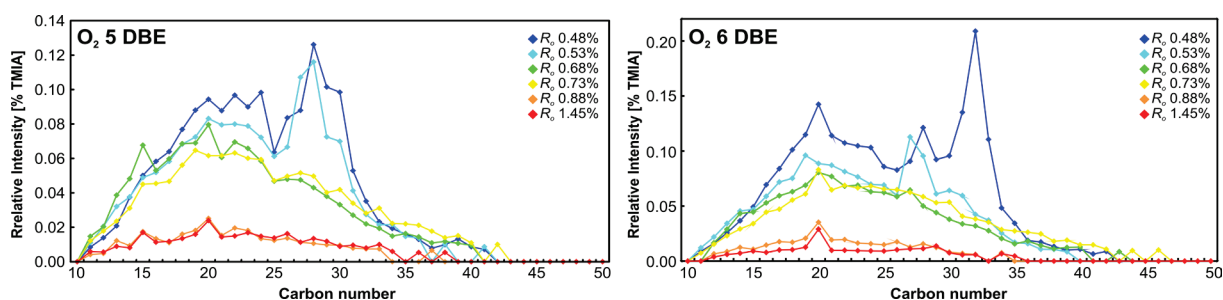


Figure SI 3: Carbon number distributions of the O₂ 5 DBE class containing the steroidal acids (C₂₇₋₂₉) and of the O₂ 6 DBE class containing the hopanoid acids (C₂₈₋₃₆) which both are enriched in the immature samples.

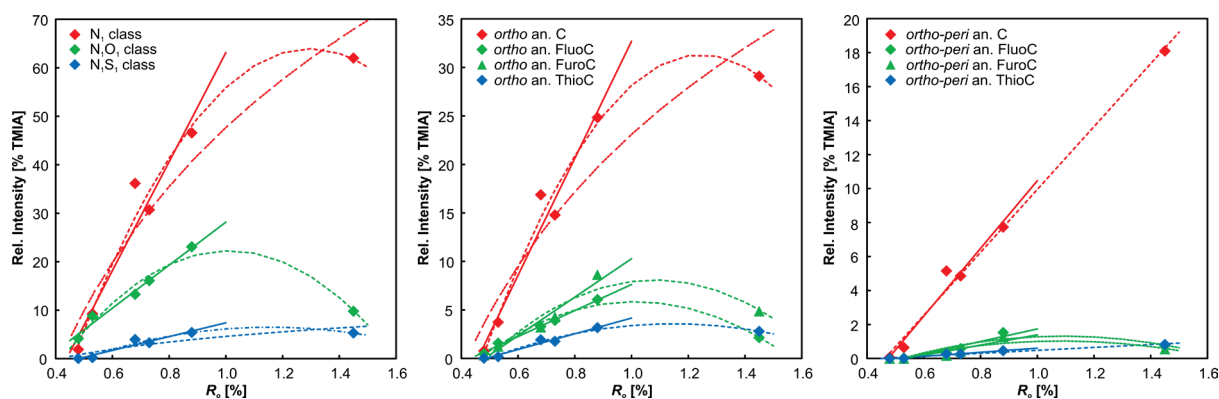


Figure SI 4: Maturity-related changes in relative abundances of a) the N_1 , N_1O_1 and N_1S_1 compound classes, b) the *ortho*-fused carbazoles, fluorenocarbazoles, furanocarbazoles and thiophenocarbazoles and c) the *ortho*- and *peri*-fused carbazoles, fluorenocarbazoles, furanocarbazoles and thiophenocarbazoles.

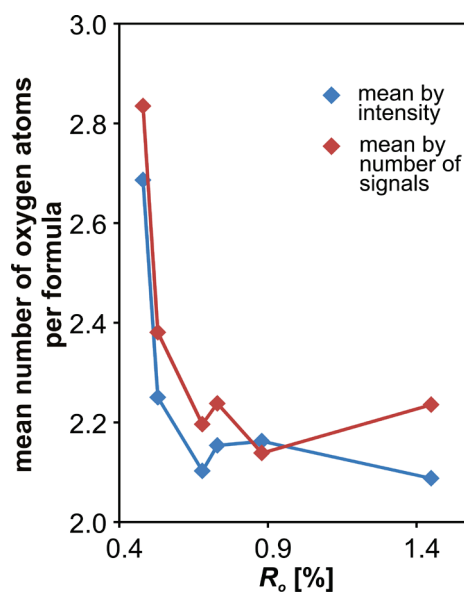


Figure SI 5: The mean number of oxygen atoms (mean by intensity and mean by number of signals) decreases with increasing maturity.