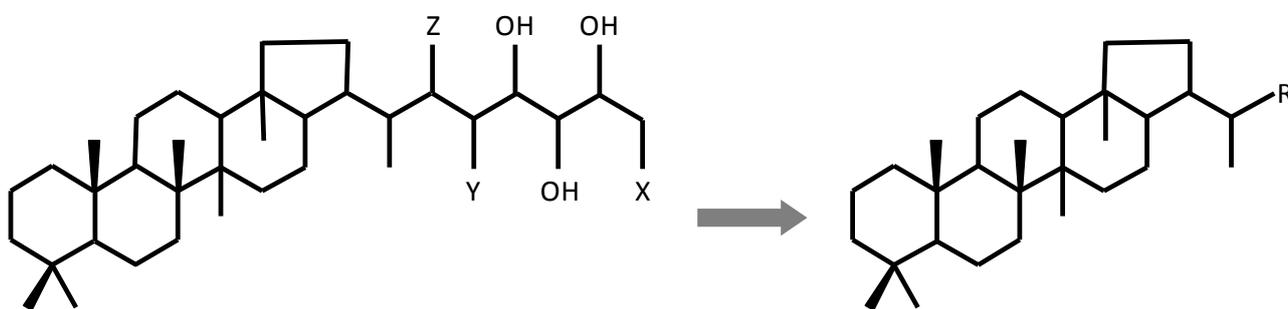


## Source-characteristic information preserved in hopane carbon number composition

by Paul Farrimond

The hopane and sterane biomarkers are among the most extensively used compounds in petroleum geochemistry. Whilst the various diagenetic reactions that convert biologically-derived sterol lipids to sterane biomarkers during sediment burial were well established back in the 1980's (Mackenzie *et al.*, 1982), the diagenetic pathways to hopane biomarkers are very poorly understood. This is perhaps not surprising, as (unlike for sterols and steranes) the biological precursors of hopanes were not identified until many years after the discovery of the hopanes themselves (Ourisson *et al.*, 1979). Furthermore, these biohopanoids are complex functionalized lipids that are difficult to analyze; only relatively recently have methods been devised to allow their compositions to be determined in bacteria and modern sedimentary environments (Talbot & Farrimond, 2007; Talbot *et al.*, 2007).



**Figure 1: Generalized structures of the hopane biomarkers and their biological precursors, the bacteriohopanepolyols. (X, Y & Z represent the sites of various functional groups, often –OH; R represents a hydrocarbon chain of variable length).**

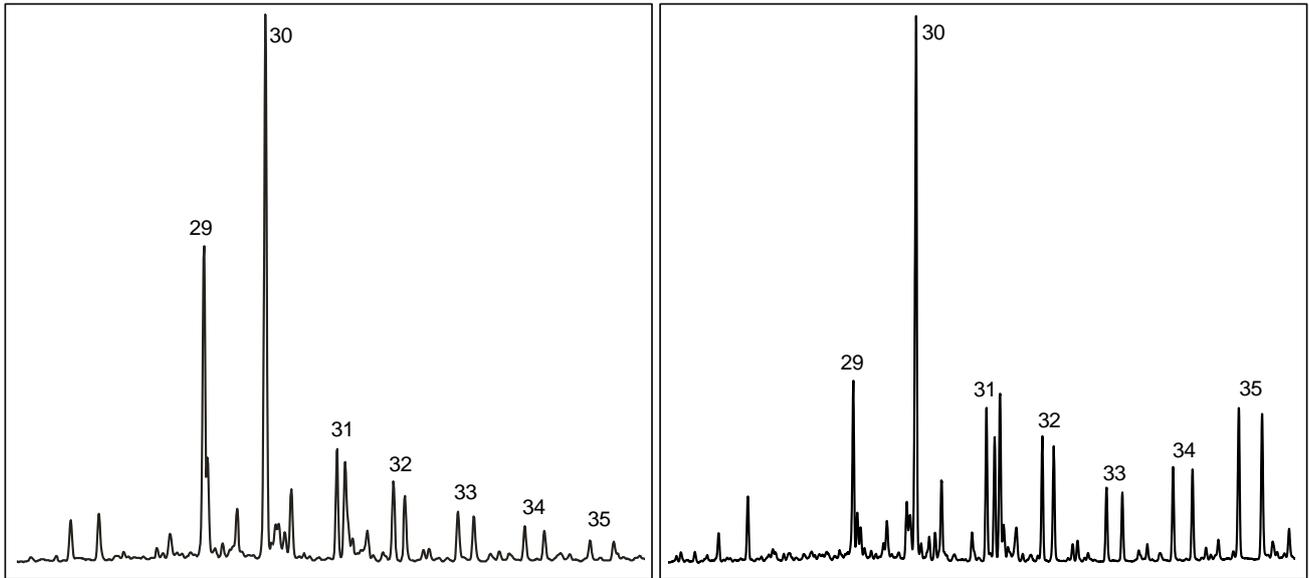
The highly functionalized side chains are extensively altered during sediment burial, resulting in the formation of hopane biomarkers with a range of carbon numbers (mainly C<sub>27</sub> to C<sub>35</sub>) depending on how much of the side chain is preserved. The carbon number distribution of the resulting hopanes is likely to be influenced strongly by both the composition of the original biohopanoid precursors and the environmental and diagenetic conditions.

### Abundance of C<sub>30</sub> hopane

It has long been recognized that lacustrine-sourced oils often contain a high proportion of C<sub>30</sub> hopane compared to the C<sub>31</sub>-C<sub>35</sub> homologues (Fig.2). Development of techniques to determine the precursor biohopanoids in modern sediments has shown that lake sediments are relatively enriched in compounds with six functional groups on the side chain (Farrimond *et al.*, 2000), and it is likely that this leads to preferential cleavage of the chain between the Y and Z groups (Fig.1), giving increased proportions of C<sub>30</sub> hopane.

### Abundance of C<sub>35</sub> hopanes

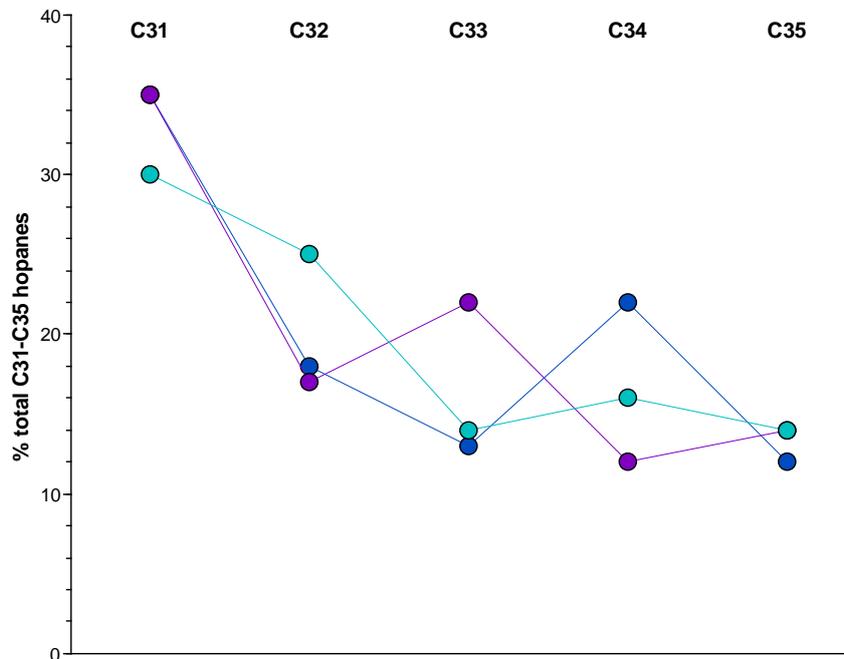
Source rocks with a high proportion of organic sulphur tend to produce oils with prominent C<sub>35</sub> hopanes; such source rocks are typically deposited in marine anoxic (sulphidic) and/or carbonate settings. It seems that binding of precursor biohopanoids into the kerogen by relatively weak carbon-sulphur (and sulphur-sulphur) bonds favours the preservation of the intact side chain, resulting in preferred liberation of C<sub>35</sub> hopanes (Fig.2).



**Figure 2: M/z 191 mass chromatograms showing a lacustrine-sourced oil (left) with a high relative abundance of C<sub>30</sub> hopane compared with the extended (C<sub>31</sub>-C<sub>35</sub>) homologues, and (right) a sulphur-rich sample with abundant C<sub>35</sub> hopanes.**

### Abundance of C<sub>32</sub>, C<sub>33</sub> or C<sub>34</sub> hopanes

Some oils and source rocks have hopane distributions with enhanced relative amounts of the C<sub>32</sub>, C<sub>33</sub> or C<sub>34</sub> homologue (e.g. Moldowan *et al.*, 1992). Although useful in correlations, and often shown on carbon number “profile” plots (Fig.3), the origin and significance of these unusual distributions are not known. Specific precursor biohopanoids contributing to the source rock are the most likely cause.



**Figure 3: Example hopane carbon number “profile” plot comparing the hopane fingerprints of three oils (produced using IGI’s p:IGI software).**

Further information on the origin of hopane biomarkers and their use in petroleum geochemistry can be found in IGI's ig.NET software, together with details of many other biomarker applications.

#### References:

- Farrimond P., Head I.M. & Innes H.E. (2000). Environmental influence on the biohopanoid composition of recent sediments. *Geochimica et Cosmochimica Acta* **64**, 2985-2992.
- Mackenzie A.S., Brassell S.C., Eglinton G. & Maxwell J.R. (1982). Chemical fossils: The geological fate of steroids. *Science* **217**, 491-505.
- Moldowan J. M., Lee C.Y., Sundararaman P., Salvatori T., Alajbeg A., Gjukić B., Demaison G.J., Slougui N.-E. & Watt D.S. (1992). Source correlation and maturity assessment of select oils and rocks from the Central Adriatic Basin (Italy and Yugoslavia). In: *Biological Markers in Sediments and Petroleum* (J. M. Moldowan, P. Albrecht and R. P. Philp, eds.), New Jersey, Prentice Hall, 370-471.
- Ourisson G., Albrecht P. & Rohmer M. (1979). The hopanoids: Palaeochemistry and biochemistry of a group of natural products. *Pure & Applied Chemistry* **51**, 709-729.
- Talbot H.M. & Farrimond P. (2007). Bacterial populations recorded in diverse sedimentary biohopanoid distributions. *Org. Geochem.* **38**, 1212-1225.
- Talbot H.M., Rohmer M. & Farrimond P. (2007). Rapid structural elucidation of composite bacterial hopanoids by atmospheric pressure chemical ionisation liquid chromatography/ion trap mass spectrometry. *Rapid Communications in Mass Spectrometry* **21**, 880-892.