Supplementary Material

**Supplementary Table 2**. Full biomarker datasets of methane-derived carbonate CarC-05

|  |  |  |  |
| --- | --- | --- | --- |
| Compound | d13C (‰) | Concentration  ng/g rock |  |
| *hydrocarbons* |  |  |  |
| n-C15 | -28 | 28.8 |  |
| n-C16 | -30 | 45.0 |  |
| n-C17 | -31 | 47.8 |  |
| pristane | -30 | 38.4 |  |
| n-C18 | -30 | 44.9 |  |
| crocetane/phytane | -111 | 292.1 |  |
| n-C19 | -29 | 42.7 |  |
| n-C20 | -27 | 38.4 |  |
| n-C21 | -28 | 38.5 |  |
| n-C22 | -29 | 32.9 |  |
| PMI | -109 | 87.4 |  |
| n-C23 | -34 | 32.5 |  |
| PMI:2 & PMI:3 | -107 | 21.7 |  |
| PMI:4 | -104 | 28.3 |  |
| n-C24 | -29 | 28.4 |  |
| n-C25 | -30 | 31.7 |  |
| n-C26 | -30 | 28.5 |  |
| n-C27 | -29 | 36.0 |  |
| n-C28 | -28 | 33.1 |  |
| n-C29 | -28 | 39.3 |  |
| n-C30 | -28 | 27.1 |  |
| n-C31 | -29 | 27.1 |  |
| n-C32 | -30 | 14.8 |  |
| n-C33 | -30 | 10.7 |  |
| n-C15 | -28 | 28.8 |  |
| n-C16 | -30 | 45.0 |  |
| n-C17 | -31 | 47.8 |  |
| pristane | -30 | 38.4 |  |
| n-C18 | -30 | 44.9 |  |
| crocetane/phytane | -111 | 292.1 |  |
| n-C19 | -29 | 42.7 |  |
| n-C20 | -27 | 38.4 |  |
| n-C21 | -28 | 38.5 |  |
| n-C22 | -29 | 32.9 |  |
| PMI | -109 | 87.4 |  |
| n-C23 | -34 | 32.5 |  |
| PMI:2 & PMI:3 | -107 | 21.7 |  |
| PMI:4 | -104 | 28.3 |  |
| n-C24 | -29 | 28.4 |  |
| n-C25 | -30 | 31.7 |  |
| n-C26 | -30 | 28.5 |  |
| n-C27 | -29 | 36.0 |  |
| n-C28 | -28 | 33.1 |  |
| n-C29 | -28 | 39.3 |  |
| n-C30 | -28 | 27.1 |  |
| n-C31 | -29 | 27.1 |  |
| n-C32 | -30 | 14.8 |  |
| n-C33 | -30 | 10.7 |  |
| S hydrocarbons |  | 1096.2 |  |
| *alchools* |  |  |  |
| n-C14-ol | -95 | 10.7 |  |
| iso-C15-ol | n.m. | 7.6 |  |
| anteiso-C15-ol | -108 | 12.4 |  |
| n-C15-ol | -72 | 9.2 |  |
| n-C16:1-ol | n.m. | 6.7 |  |
| n-C16:1-ol | -95 | 14.5 |  |
| n-C16-ol | -85 | 29.8 |  |
| iso-C17-ol | n.m. | 5.4 |  |
| anteiso-C17-ol | -115 | 8.1 |  |
| cyC17:0w5,6-ol | -113 | 11.2 |  |
| n-C17-ol | -51 | 27.2 |  |
| phytanol | -123 | 109.2 |  |
| n-C18-ol | -45 | 17.5 |  |
| phytol | -114 | 15.7 |  |
| sn2-ph-monoether | -122 | 17.6 |  |
| sn3-ph-monoether | -120 | 22.3 |  |
| coprostanol | -37 | 42.3 |  |
| cholest-en-5-ol | -36 | 53.2 |  |
| cholestanol | -34 | 75.4 |  |
| DAGE 30 (iso-C15/iso-C15) | -109 | 53.4 |  |
| DAGE 30 (iso-C15/anteiso-C15) | -103 | 69.0 |  |
| DAGE 30 (anteiso-C15/anteiso-C15) | -113 | 199.2 |  |
| Tetrahymanol | -73 | 109.0 |  |
| DAGE 31:1 (cpC16/anteiso-C15) | -105 | 154.6 |  |
| DAGE 31:1 (cpC17/anteiso-C15) | co-elution | 97.1 |  |
| DAGE 31:2 (C16:1/C16:1) | co-elution | 43.9 |  |
| DAGE 31:1 (C16/cpC17) | -119 | 94.0 |  |
| DAGE 32:2 (C17:1/C16:1) | co-elution | 98.6 |  |
| DAGE 32:2 (cpC16/cpC17) | -98 | 174.3 |  |
| DAGE 32:2 (C17:1/cpC17) | -121 | 137.5 |  |
| archaeol | -122 | 1431.5 |  |
| sn2-hydroxy-archaeol | -121 | 2895.6 |  |
| S alcohols |  | 5385.3 |  |
| *Fatty acids* |  |  |  |
| n-C12-FA | -63 | 11.8 |  |
| iso-C13-FA | n.m. | 7.2 |  |
| anteiso-C13-FA | -95 | 11.4 |  |
| n-C13-FA | n.m. | 3.6 |  |
| iso-C14-FA | -104 | 22.4 |  |
| n-C14:1-FA | -63 | 12.8 |  |
| n-C14:1-FA | -117 | 11.6 |  |
| n-C14-FA | -69 | 71.8 |  |
| iso-C15:1-FA | n.m. | 5.8 |  |
| anteiso-C15:1-FA | n.m. | 4.3 |  |
| iso-C15-FA | -102 | 82.3 |  |
| anteiso-C15-FA | -102 | 143.2 |  |
| n-C15-FA | -75 | 22.1 |  |
| iso-C16-FA | -110 | 43.9 |  |
| n-C16:1(n-7c)-FA | -69 | 109.0 |  |
| n-C16:1 (n-5)-FA | -77 | 24.4 |  |
| n-C16:1(n-7 trans)-FA | -82 | 49.9 |  |
| n-C16-FA | -54 | 204.6 |  |
| iso-C17:1-FA | -93 | 15.5 |  |
| anteiso-C17:1-FA | -103 | 16.2 |  |
| iso-C17-FA | -93 | 16.3 |  |
| anteiso-C17-FA | -105 | 48.8 |  |
| cyC17:0w5,6 FA | -105 | 12.2 |  |
| n-C17-FA | -60 | 11.7 |  |
| phytanoic acid | -107 | 50.1 |  |
| n-C18:2-FA | -95 | 36.2 |  |
| n-C18:2-FA | -77 | 90.0 |  |
| n-C18:2-FA | -86 | 29.6 |  |
| n-C18-FA | -49 | 61.6 |  |
| S fatty acids |  | 1234.6 |  |
|  |  |  |  |

Concentration (ng/g rock) of lipid biomarkers in carbonate sample CarC-05 and their compound-specific isotopic composition (‰VPDB). PMI =pentamethylicosane, DAGE = Dialkyl glycerol diether; n.m.=not measured.