Supplementary Table 1. Detailed sample list

|  |  |
| --- | --- |
| Specimen number | Group identifier for analysis |
| BH1 | BH |
| BH2 | BH |
| BH3 | BH |
| BH4 | BH |
| BH5 | BH |
| BH6 | BH |
| BH7 | BH |
| BH8 | BH |
| BH9 | BH |
| BH10 | BH |
| BH11 | BH |
| BH12 | BH |
| BH13 | BH |
| BH14 | BH |
| NJ1 | NJ |
| NJ2 | NJ |
| NJ3 | NJ |
| NJ4 | NJ |
| NJ5 | NJ |
| NJ6 | NJ |
| NJ7 | NJ |
| NJ8 | NJ |
| NJ9 | NJ |
| NJ10 | NJ |
| NJ11 | NJ |
| NJ12 | NJ |
| NJ13 | NJ |
| NJ14 | NJ |
| NJ15 | NJ |
| NJ16 | NJ |
| TCFR2c | TC |
| TCFR2b | TC |
| TCFR2a | TCFR |
| KujiUG4c | KujiU |
| KujiUG4b | KujiU |
| KujiUG4a | KujiU |
| KujiUG1c | KujiU1 |
| KujiUG1b | KujiU1 |
| KujiUG1a | KujiU1 |
| KujiTAMIII9c | KujiT3 |
| KujiTAMIII9b | KujiT3 |
| KujiTAMIII9a | KujiT3 |
| KujiTAMI1c | KujiT1 |
| KujiTAMI1b | KujiT1 |
| KujiTAMI1a | KujiT1 |
| KujiOK2d | KujiOK |
| KujiOK2c | KujiOK |
| KujiOK2b | KujiOK |
| KujiOK2a | KujiOK |
| KujiKA3b | KujiKA |
| KujiKA3a | KujiKA |
| KujiHO5c | KujiHO |
| KujiHO5b | KujiHO |
| KujiHO5a | KujiHO |
| IoWMS3d | IoWMS |
| IoWMS3c | IoWMS |
| IoWMS3b | IoWMS |
| IoWMS3a | IoWMS |
| IoWMS2d | IoWMS |
| IoWMS2c | IoWMS |
| IoWMS2b | IoWMS |
| IoWMS2a | IoWMS |
| IoWMS1e | IoWMS |
| IoWMS1d | IoWMS |
| IoWMS1c | IoWMS |
| IoWMS1b | IoWMS |
| IoWMS1a | IoWMS |
| IoWHAd | IoWHA |
| IoWHAc | IoWHA |
| IoWHAb | IoWHA |
| IoWHAa | IoWHA |
| FourasFR1c | FR |
| FourasFR1b | FR |
| FourasFR1a | FR |
| Dom6 | Dom |
| Dom5 | Dom |
| Dom4b | Dom |
| Dom4a | Dom |
| Dom3 | Dom |
| Dom2 | Dom |
| Dom1 | Dom |
| BuzFR3c | Buz |
| BuzFR3b | Buz |
| BuzFR3a | Buz |
| Bal11 | Bal |
| Bal10 | Bal |
| Bal9 | Bal |
| Bal8 | Bal |
| Bal7 | Bal |
| Bal6 | Bal |
| Bal5 | Bal |
| Bal4 | Bal |
| Bal3 | Bal |
| Bal2 | Bal |
| Bal1 | Bal |
| ArchFR4c | Arch |
| ArchFR4b | Arch |
| ArchFR4a | Arch |
| TCFR2d | TC |
| TCFR2c | TC |
| TCFR2b | TC |
| TCFR2a | TC |
| Leb1 | Leb |
| Leb2 | Leb |
| Leb3 | Leb |
| Leb4 | Leb |
| CB1a | CB |
| CB1b | CB |
| CB1c | CB |

Figure S1. Combined FTIR-ATR raw spectra (110 spectra) in the 400 – 7000 cm-1 range.

Supplementary Figure S1.

