Table S3 NMR data 1H and 13C for compound AF53611

|  |  |  |
| --- | --- | --- |
| **Atom C** | **AF53611 (1H, δ, MeOD)** | **AF53611(13C, δ, MeOD)** |
| C1 (C) | - | 126.22 |
| C2 (CH) | 8.47, dd, *J*= 8.64, 1.5 | 133.68 |
| C3 (CH) | 8.08, m | 129.83 |
| C4 (CH) | 8.86, dd, *J*= 7.08, 1.5 | 134.94 |
| C4a (C) | - | 142.50 |
| C5a (C) | - | 143.06 |
| C6 (C) | - | 129.02 |
| C7 (CH) | 8.03, m | 131.51 |
| C8 (CH) | 8.06, m | 131.96 |
| C9 (CH) | 8.38, m | 128.91 |
| C9a (C) | - | 140.49 |
| C10a (C) | - | 140.18 |
| C1’ (C=OOH) | 15.61, s | 163.90 |
| C2’ (C=OO) | - | 161.80 |
| C3’ (C) | - | 138.36 |
| C4’ (C-OH) | 7.14, m | 123.61 |
| C5’ (CH) | 7.40, m | 118.84 |
| C6’ (C-O) | - | 147.29 |
| C7’ (CH) | 7.22, m | 123.61 |
| C8’(CH) | 7.45, m | 124.52 |
| C9’ (CH3) | 1.34, m | 29.36 |

\* δH, ppm, 600 MHz; δC, ppm, 150 MHz; *J* couplings, *J*, Hz