**JAB1904** – **1**

**Supporting Information — X-Ray Crystallography**

**The X-ray crystal structure of 1**

*Crystal data for* **1**: C19H19NO5, *M* = 341.35, monoclinic, *P*21 (no. 4), *a* = 5.7625(4), *b* = 16.4131(12), *c* = 18.2857(13) Å, β = 96.264(7)°, *V* = 1719.1(2) Å3, *Z* = 4 [2 independent molecules], *D*c = 1.319 g cm–3, μ(Mo-Kα) = 0.096 mm–1, *T* = 173 K, colourless blocks, Agilent Xcalibur 3 E diffractometer; 7419 independent measured reflections (*R*int = 0.0260), *F*2 refinement,[X1,X2] *R*1(obs) = 0.0342, *wR*2(all) = 0.0686, 5765 independent observed absorption-corrected reflections [|*F*o| > 4σ(|*F*o|), completeness to θfull(25.2°) = 99.4%], 463 parameters. The absolute structure of **1** could not be determined [Flack parameter *x*+ = +0.1(7)]. CCDC xxxxxx.

The crystal of **1** that was studied was found to be a two component twin in a *ca*. 58:42 ratio, with the two lattices related by the approximate twin law [–1.00 0.00 0.00 0.00 –1.00 0.00 0.71 0.00 1.00]. The structure was found to contain two crystallographically independent molecules, **1-A** and **1-B**. The O(6)–H hydrogen atom in each molecule was located from a Δ*F* map and refined freely subject to an O–H distance constraint of 0.90 Å.

**References**

[X1] SHELXTL v5.1, Bruker AXS, Madison, WI, 1998.

[X2] SHELX-2013, G.M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3-8.

**Figures**

**Fig. S1** The structure of **1-A**, one of the two independent molecules present in the crystal of **1** (50% probability ellipsoids).

**Fig. S2** The structure of **1-B**, one of the two independent molecules present in the crystal of **1** (50% probability ellipsoids).