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X-ray Crystallography

Single-crystal X-ray diffraction data of **3i** were collected at 100 K on Rigaku AFC12 goniometer equipped with an enhanced sensitivity (HG) Saturn 724+ detector mounted at the window of an FR-E+ Superbright MoKα rotating anode generator with HF Varimax optics [1].

Unit cell parameters were refined against all data. An empirical absorption correction was carried out using CrystalClear [2] software.

The crystal structure of **3i** was solved by direct methods and refined on Fo^2 by full-matrix least-squares refinements using programs of the SHELX-2013 software [3]. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were added at calculated positions and refined using a riding model with isotropic displacement parameters based on the equivalent isotropic displacement parameter (U_{eq}) of the parent atom.

Crystallographic data (excluding structure factors) for the structures in this paper have been deposited with the Cambridge Crystallographic Data Centre; CCDC deposition number 978247 contains the supplementary crystallographic data for this paper. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal data and structure refinement details for crystal structure of **3i**.

Empirical formula	$C_{20}H_{17}BrN_2O_5$	
Formula weight	445.26	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	*P*–1	
Unit cell dimensions	a = 8.9971(4) Å	α = 70.132(5)°
	b = 10.0949(4) Å	β = 68.095(5)°
	c = 11.5631(8) Å	γ = 80.935(6)°
Volume	915.83(9) $Å^3$	
Z	2	
Density (calculated)	1.615 Mg / m^3	
Absorption coefficient	2.280 mm^{-1}	
F(000)	452	
Crystal	Plate; Colourless	
Crystal size	0.240 × 0.200 × 0.040 mm^3	
θ range for data collection	3.194 – 27.477°	
Index ranges	$-11 \le h \le 11$, $-13 \le k \le 13$, $-14 \le l \le 14$	
Reflections collected	12120	
Independent reflections	4167 [R_{int} = 0.0244]	
Completeness to θ = 25.242°	99.6 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	1.000 and 0.672	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4167 / 0 / 255	
Goodness-of-fit on F^2	1.082	
Final *R* indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0257, *wR2* = 0.0675	
R indices (all data)	*R1* = 0.0273, *wR2* = 0.0684	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.455 and –0.431 e $Å^{-3}$	

1 S.J Coles and P.A. Gale, (2012) Chemical Science, (3), 683-689.
2 CrystalClear-SM Expert 3.1 b26 (Rigaku, 20112).
3 SHELX-2013 - G. Sheldrick, G.M. (2008), Acta Cryst. A64, 112-122.