Electronic Supplementary Material for CrystEngComm

	A1	**A2**	**A3**	**B5**	**C6**	**D7**
Formula moiety	$(C_8H_5BrN_2O)$ (C_6H_6BrNO)	$(C_8H_5BrN_2O)$ $(C_{15}H_{13}BrN_2)$	$(C_8H_5BrN_2O)$ $(C_{14}H_{11}BrN_2)$	$(C_8H_5N_2OF)_2$ $(C_{12}H_{10}N_2)$	$(C_{22}H_{18}N_4)$ $(C_8H_5N_2OCl)_2$	$(C_{15}H_{15}N_3)$ $(C_8H_5N_2OF)$
Empirical formula	$C_{14}H_{11}Br_2N_3O_2$	$C_{23}H_{18}Br_2N_4O$	$C_{22}H_{16}Br_2N_4O$	$C_{28}H_{20}F_2N_6O_2$	$C_{38}H_{28}Cl_2N_8O_2$	$C_{23}H_{20}FN_5O$
Molecular weight	413.08	526.23	512.21	510.50	699.58	401.44
Color, Habit	colorless prism	colorless needle	colorless block	colorless plate	colourless plate	colourless plate
Crystal size, mm	0.35 x 0.30 x 0.15	0.40 x 0.12 x 0.66	0.48 x 0.30 x 0.18	0.40 x 0.20 x 0.08	0.30 x 0.30 x 0.15	0.30 x 0.15 x 0.05
Crystal system	Triclinic	Monoclinic	Triclinic	Triclinic	Monoclinic	Monoclinic
Space group, Z	P-1, 2	$P2_1/c$, 4	P-1, 2	P-1, 1	$P2_1/n$, 2	$P2_1/n$, 4
a, Å	6.9907(6)	4.9374(6)	5.3033(6)	3.8189(6)	13.6335(10)	16.1659(12)
b, Å	8.0552(7)	22.597(3)	13.2294(15)	11.2941(18)	4.4402(3)	6.4146(5)
c, Å	15.3027(13)	19.233(2)	15.0601(17)	14.107(2)	27.297(2)	21.0074(16)
α, °	79.305(5)		102.536(2)	98.884(10)		
β, °	89.038(5)	96.869(2)	99.505(2)	93.147(11)	94.084(3)	105.945(5)
γ, °	64.660(5)		94.752(2)	94.624(10)		
Volume, $Å^3$	763.37(11)	2130.5(4)	1009.5(2)	597.79(16)	1648.2(2)	2094.6(3)
Density, g/cm^3	1.797	1.641	1.685	1.418	1.410	1.273
Temperature, K	173(2)	100(2)	100(2)	173(2)	120(2)	120(2)
X-ray wavelength	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
θ_{min}, °	1.4	2.3	2.8	1.5	1.6	1.4
θ_{max}, °	27.9	30.0	30.1	27.5	31.0	30.5
Reflections						
collected	5513	24200	11582	4295	40395	20522
independent	3350	6170	5763	2606	5259	6367
observed	2663	4792	4972	1734	3883	2616
Abs. correction	multi-scan	multi-scan	multi-scan	none	none	none
μ, mm^{-1}	5.316	3.828	4.036	0.104	0.247	0.088
Threshold expression	$>2\sigma(I)$	$>2\sigma(I)$	$>2\sigma(I)$	$>2\sigma(I)$	$>2\sigma(I)$	$>2\sigma(I)$
R_1 (observed)	0.058	0.034	0.027	0.060	0.042	0.053
wR_2 (all)	0.170	0.089	0.074	0.175	0.112	0.132

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X-ray experimental information

X-ray data were collected on a Bruker SMART 1000 four-circle CCD diffractometer at 173 K (**A1**, **B4**), SMART APEX CCD diffractometer at 100 K (**A2** and **A3**), or Kappa APEXII CCD diffractometer at 120 K (**C5** and **D6**) using, in each case, a fine-focus molybdenum Kα tube. Data were collected using SMART (**A1**, **B5**)[(a)] or APEX2 (**A2**, **A3**, **C6** and **D7**) [(b)] software. Initial cell constants were found by small widely separated "matrix" runs. Generally, an entire hemisphere of reciprocal space was collected regardless of Laué symmetry. Scan speed and scan width were chosen based on scattering power and peak rocking curves.

Unit cell constants and orientation matrix were improved by least-squares refinement of reflections thresholded from the entire dataset. Integration was performed with SAINT,[(c)] using this improved unit cell as a starting point. Precise unit cell constants were calculated in SAINT from the final merged dataset. Lorenz and polarization corrections were applied. Laué symmetry, space group, and unit cell contents were found with XPREP.

Data were reduced with SHELXTL.[(d)] The structures were solved in all cases by direct methods without incident. None of the crystals contained solvent or water of hydration, and the only structure showing disorder was **B5**, whose 2-fluoro substituent was disordered over both ortho sites. Except for the oxime hydrogen atoms, whose coordinates were allowed to refine, hydrogen atoms were assigned to idealized positions and were allowed to ride. Where possible, the coordinates of the amide hydrogen atoms were allowed to refine. Heavy atoms were refined with anisotropic displacement parameters. Datasets for the samples containing bromine (**A1**, **A2** and **A3**) were corrected for absorption.

(a) SMART v5.060, © 1997 - 1999, Bruker Analytical X-ray Systems, Madison, WI.
(b) APEX2 v2.2.0 © 2005 - 2007, Bruker AXS, Madison, WI.
(c) SAINT v7.46a, © 1997 - 2007, Bruker AXS, Madison, WI.
(d) SHELXTL v6.10, © 2001 , Bruker AXS, Madison, WI.