Article 2 Supplementary Material (Galhano, J. *et al.*)

Single monocrystals were obtained for both pyridine derivates using the slow evaporation technique. For BTI-Pyr slow evaporation was performed using a mixture of CH_2Cl_2/CH_3OH at room temperature and in a protected cabinet in the dark, resulting in yellow needles. In the case of DBI-Pyr, slow evaporation was performed using only $CHCl_3$ in the dark, leading to the successful growth of orange prismatic monocrystals.

Supplementary Table

Table S1 | Crystallographic data recorded on both **BTI-Pyr** and **DBI-Pyr**.

Crystal	**BTI-Pyr**	**DBI-Pyr**
Formula	$C_{28}\ H_{22}\ N_2\ O_2\ S$	$C_{32}\ H_{24}\ N_2\ O_2\ S,\ C\ H\ Cl_3$
Molecular weight	450.53	619.96
Temperature (K)	200.0(1)	200.0(1)
Wavelength (Å)	1.54184	1.54184
Crystal system	Monoclinic	Monoclinic
Space group	P 21/c	P 21/c
a (Å)	11.7336(4)	12.1608(4)
b (Å)	26.2645(9)	7.4803(3)
c (Å)	7.1842(3)	32.0649(11)
α (°)	90	90
β (°)	102.004 (4)	99.977 (4)
γ (°)	90	90
Volume ($Å^3$)	2163.56 (14)	2872.72(18)
Z	4	4
D_c ($g.cm^{-3}$)	1.383	1.433
Absorption coefficient (mm^{-1})	1.563	3.847
F(000)	944	1280
Crystal size (mm^3)	0.371 x 0.064 x 0.048	0.244 x 0.108 x 0.088
Crystal color and form	Yellow needle	Orange prism
θ (min/max) (°)	3.365/72.306	3.365/72.306
Limiting indices	$-14 \le h \le 14, -32 \le k \le 32, -8 \le l \le 8$	$-13 \le h \le 14, -8 \le k \le 9, -28 \le l \le 37$
Data collected	7130	13187
Data unique	7130	5490
Completeness to θ = 75.000	98.2	98.5
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Transmission (min/max)	0.37898/1.00000	0.13668/1.00000

Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	7130 / 1 / 330	5495 / 0 / 372
Goodness-on-fit on F^2	0.943	1.041
Final *R* indices [I > 2σ(I)]	R_1 = 0.0543, wR_2 = 0.1412 [5061 Fo]	R_1 = 0.0778, wR_2 = 0.12015 [4710 Fo]
R indices (all data)	R_1 = 0.0699, wR_2 = 0.1437	R_1 = 0.0852, wR_2 = 0.2103
Largest diff. peak and hole ($e.A^{-3}$)	0.363 / -0.457	1.100/ -0.655

Supplementary Figures

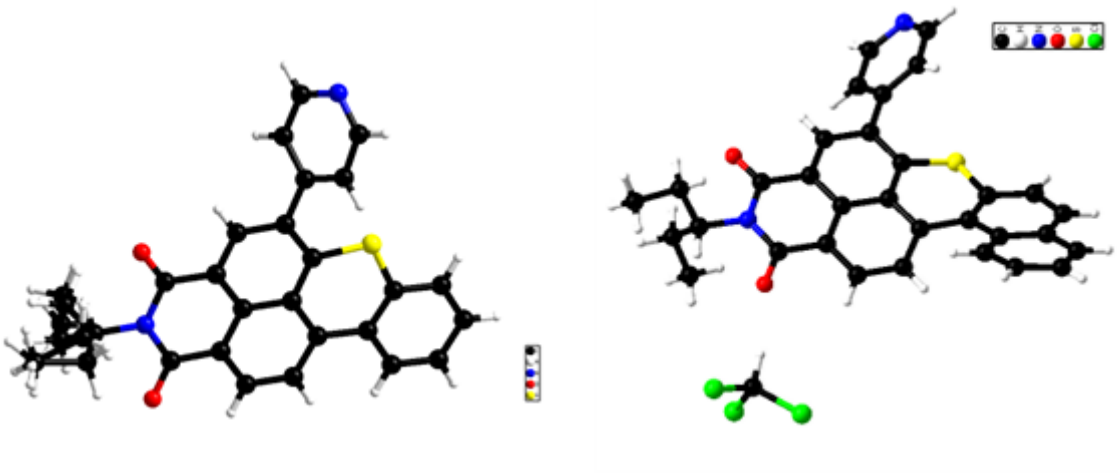

Figure S1 | X-ray structures of both **BTI-Pyr** and **DBI-Pyr** carried out on single crystals obtained by slow evaporation technique.