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Supplementary Information

A new building block, bis(thiophene vinyl)-pyrimidine, for constructing excellent two-photon absorption materials: synthesis, crystal structure and properties

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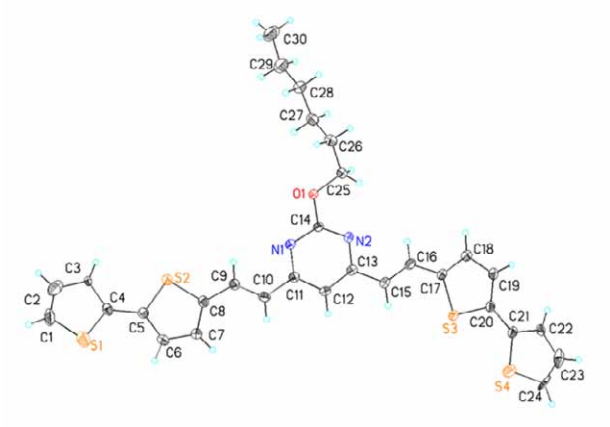
The details of the crystal data for Py1



Single crystal structure plot of **Py1**

CCDC number: 843125.

Table 1 Crystal data and structure refinement.

Empirical formula	$C_{30}H_{28}N_2OS_4$	
Formula weight	560.82	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.9129(8) Å	α= 90°
	b = 31.483(2) Å	β= 105.132(2)°
	c = 18.6483(14) Å	γ = 90°
Volume	5618.1(8) $Å^3$	
Z	8	
Density (calculated)	1.326 Mg/m^3	
Absorption coefficient	0.365 mm^{-1}	
F(000)	2352	
Crystal size	0.16 x 0.12 x 0.10 mm^3	
Theta range for data collection	2.22 to 25.02°	
Index ranges	$-11 \le h \le 11, -36 \le k \le 37, -22 \le l \le 14$	
Reflections collected	29669	
Independent reflections	9906 [R(int) = 0.0958]	
Completeness to θ = 25.02	99.8 %	
Absorption correction	None	
Max. and min. transmission	0.9644 and 0.9439	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9906 / 0 / 761
Goodness-of-fit on F^2	1.043
Final R indices [I>2σ (I)]	R1 = 0.0734, wR2 = 0.1810
Largest diff. peak and hole	0.443 and -0.401 e.Å^{-3}

Table 2 Some main torsion angles.

S(1)-C(4)-C(5)-C(6)	8.1(6)
S(1)-C(4)-C(5)-S(2)	-169.7(2)
C(7)-C(8)-C(9)-C(10)	3.0(8)
C(8)-C(9)-C(10)-C(11)	-174.5(4)
C(9)-C(10)-C(11)-N(1)	16.1(6)
N(2)-C(13)-C(15)-C(16)	-7.7(7)
C(12)-C(13)-C(15)-C(16)	170.0(4)
C(13)-C(15)-C(16)-C(17)	-173.1(4)
C(15)-C(16)-C(17)-C(18)	167.7(5)
C(15)-C(16)-C(17)-S(3)	-8.3(7)
C(19)-C(20)-C(21)-C(22)	-5(20)
S(3)-C(20)-C(21)-C(22)	172(11)