Supporting Information

Isolation, characterization and X-ray structure determination of Schiff base ligand: 5-Methyl-2-phenyl-4-[phenyl-(4-phenyl-thiazol-2-ylamino)-methylene]-2,4-dihydro-pyrazol-3-one

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1. Experimental

1.1 Materials

The compound 5-methyl-2-phenyl-2,4-dihydro-pyrazol-3-one **1** was obtained from Prima chemicals, Ahmedabad, India. Methanol, dioxane, was obtained from SD's fine chemical Ltd., India. Absolute alcohol was obtained from Baroda Chem. Industry Ltd. and was used after distillation. Calcium hydroxide and benzoyl chloride were obtained from Samir Tech. Chem. Pvt. Ltd. All the chemicals used were of AR grade. Solvents used in this study were purified following the standard procedures.

1.2 Physical measurements

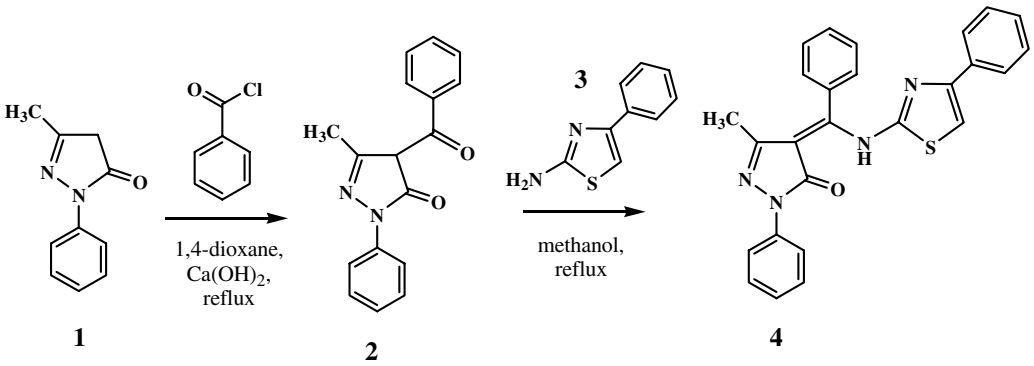
The elemental analysis was obtained from Flash Elemental Analyzer-1112. Infrared spectra (IR) were measured using a Perkin Elmer Precisely Spectrometer100 FT-IR spectrometer. 1H and 13C NMR spectra were measured at 400.22 and 100.63 MHz, respectively, with a Bruker Avance III 400 MHz spectrophotometer by using TMS (tetramethylsilane) as the internal reference. Melting point is recorded on an Ernst Leitz Wetzlar hot stage melting point apparatus. Reactions were monitored by thin layer chromatography (TLC) on aluminum-backed plates coated with Merck Kieselgel 60 F254 silica gel. TLC plates were visualized by UV radiation at a wavelength of 254 nm.

1.3 Synthesis of Schiff base ligand

5-Methyl-2-phenyl-2,4-dihydro-pyrazol-3-one **1** (2 g, 11.5 mmol) was dissolved in hot dioxane (20 mL) in a flask equipped with a stirrer, separating funnel and reflux condenser. Calcium hydroxide (1.7 g, 23 mmol) was added to this solution, followed by benzoyl chloride (3.23 g, 11.5 mmol) added drop wise with precaution, as this reaction was exothermic. During this addition the whole mass was converted into a thick paste. After the complete addition, the reaction mixture was refluxed for half an hour and then it was poured into dilute hydrochloric acid (50 mL, 2 M). The colored crystals of 4-benzoyl-5-methyl-2-phenyl-2,4-dihydro-pyrazol-3-

one **2** thus obtained were separated by filtration and recrystallized from n-hexane to give a bright yellow crystalline solid (2.5 g, 80%).

A solution of 4-benzoyl-5-methyl-2-phenyl-2,4-dihydro-pyrazol-3-one **2** (1 g, 3.6 mmol) in methanol (30 mL) was added to a another solution of 4-phenyl-thiazol-2-ylamine **3** (0.63 g, 3.6 mmol) in methanol (20 mL) under an inert atmosphere. The reaction mixture was refluxed for three hours. Completion of the reaction was monitored by TLC using hexane/ethyl acetate (8:2). The reaction was allowed to cool to room temperature and stirred overnight. A yellow precipitate formed which was then filtered and washed with methanol (10 mL). The crude product, purified by crystallization from ethanol to give brown crystals of the desired product 5-Methyl-2-phenyl-4-[phenyl-(4-phenyl-thiazol-2-ylamino)-methylene]-2,4-dihydro-pyrazol-3-one **4** (1.2 g, 77% yield).



Scheme S1. Synthetic pathway of the Schiff base ligand

Fig. 1 ^{1}H NMR spectra of Schiff base ligand

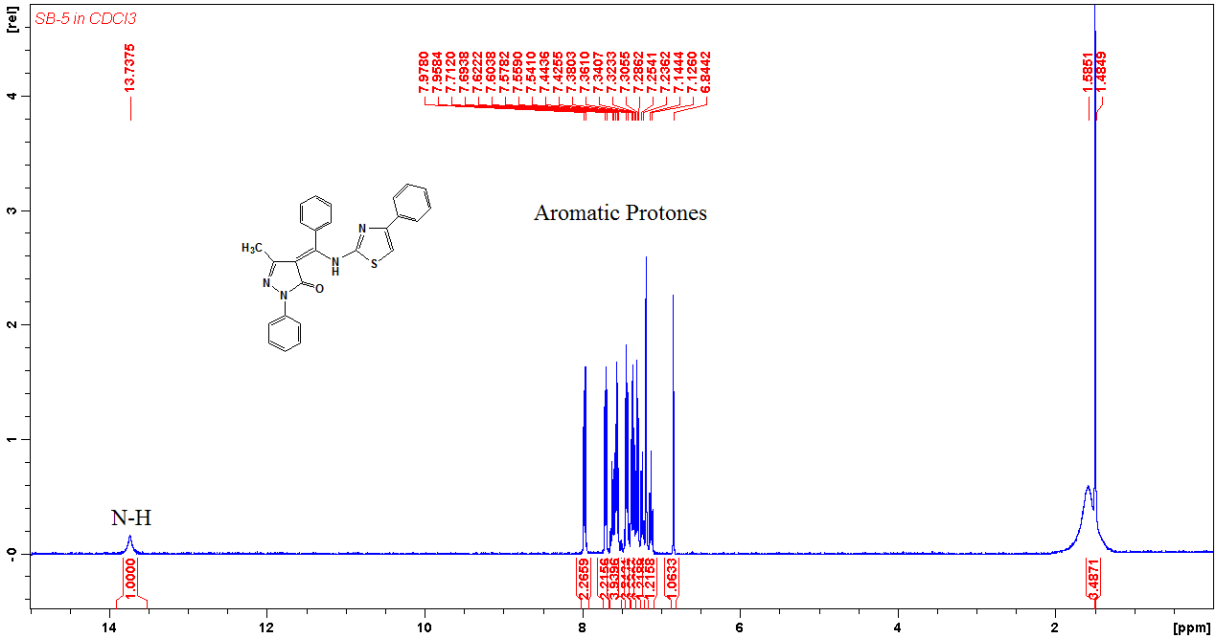


Fig. S2 ^{13}C NMR spectra of Schiff base ligand

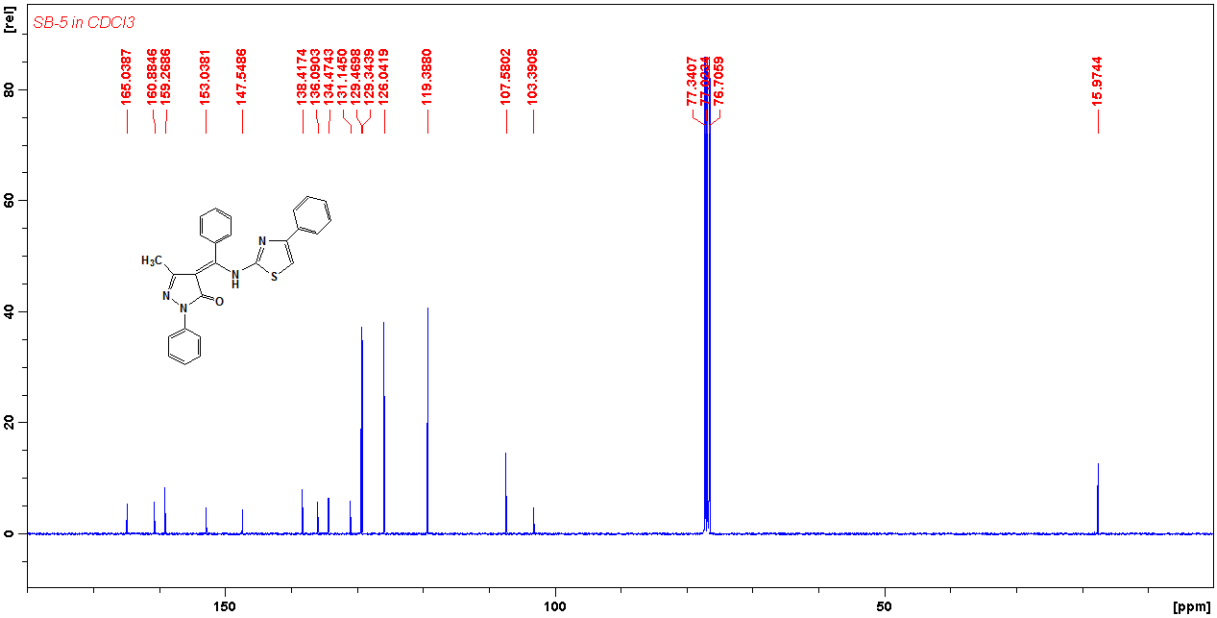


Fig. S3 ^{1}H-^{13}C HSQC spectra of Schiff base ligand

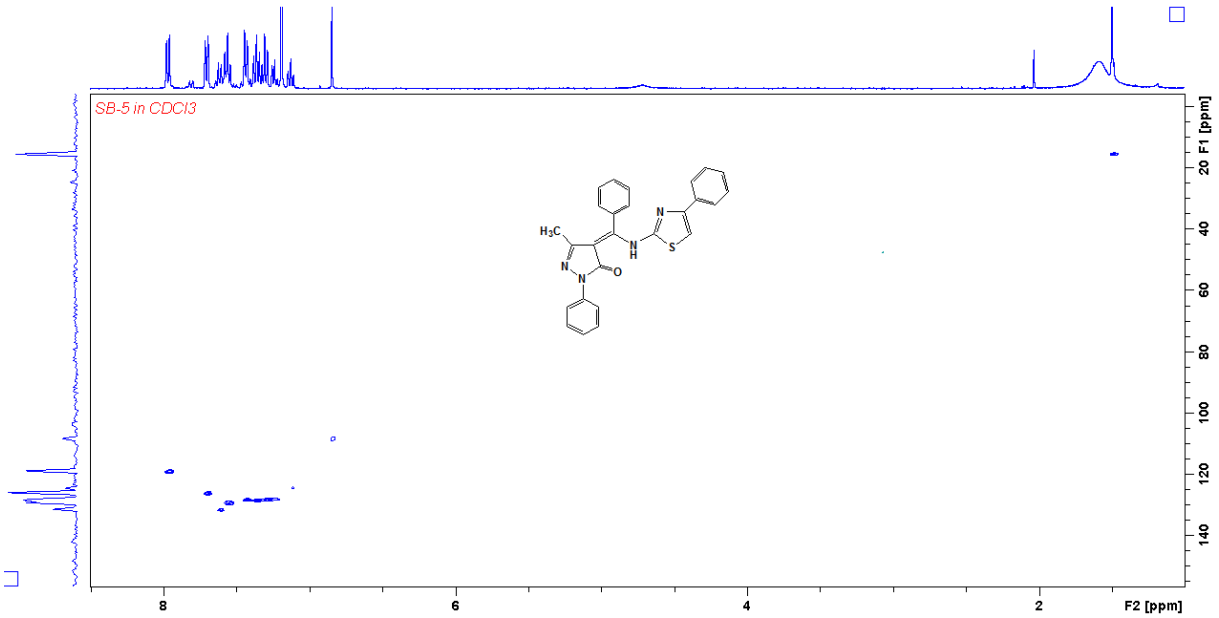


Fig. S4 ^{1}H-^{13}C HMBC spectra of Schiff base ligand

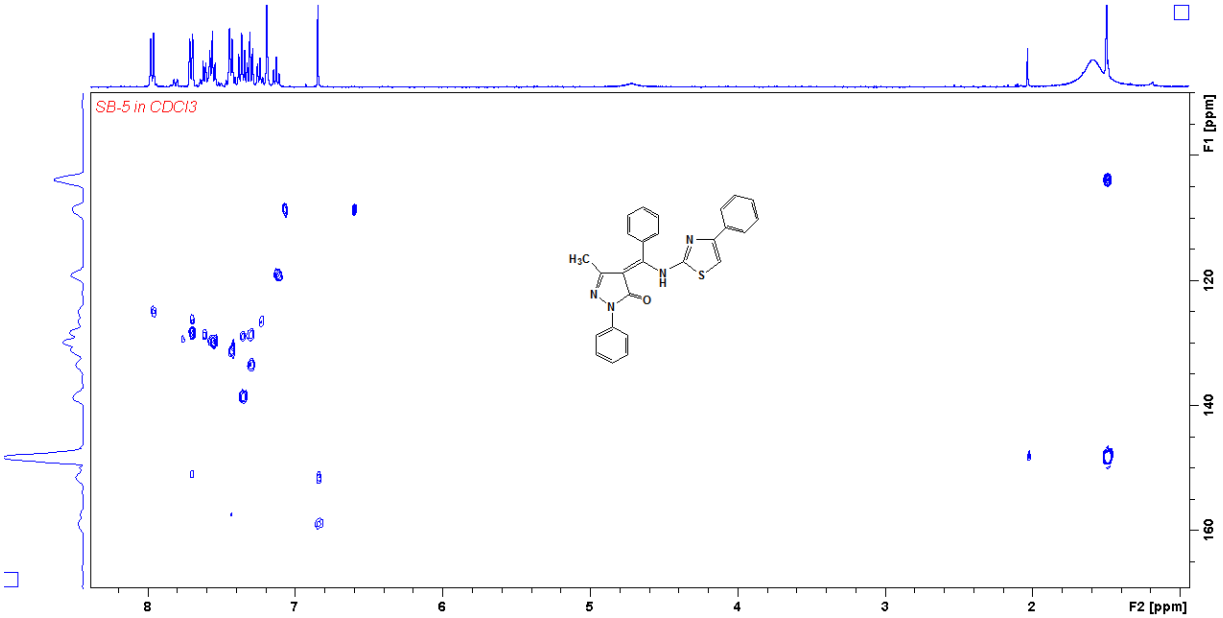


Fig. S5 COSY spectra of Schiff base ligand

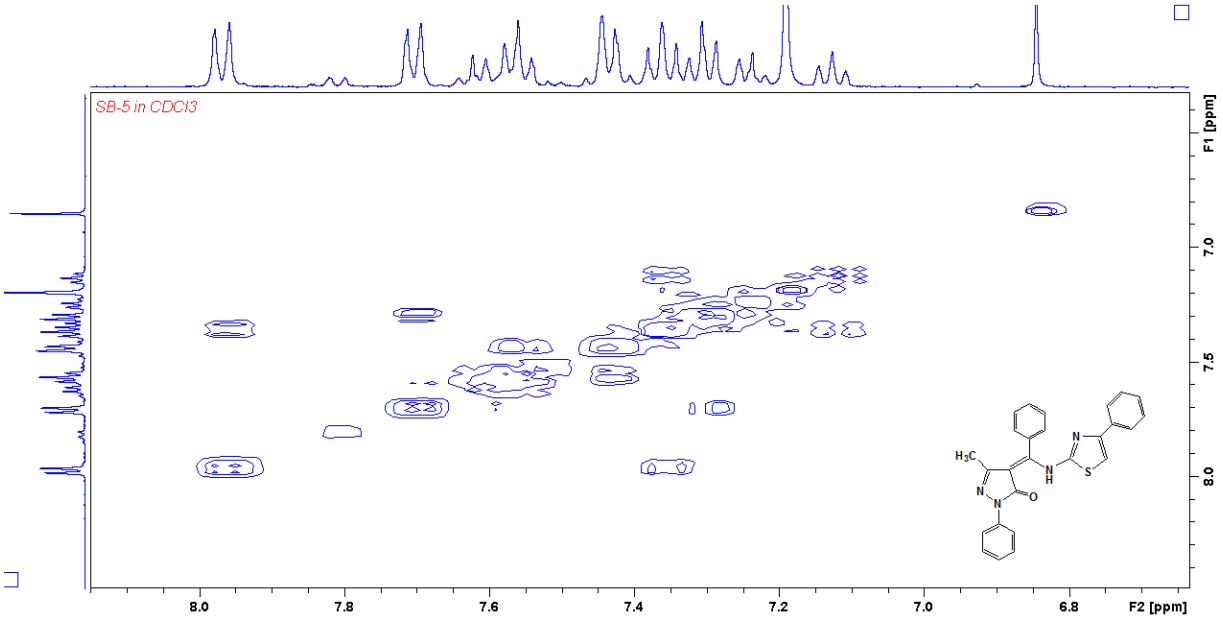
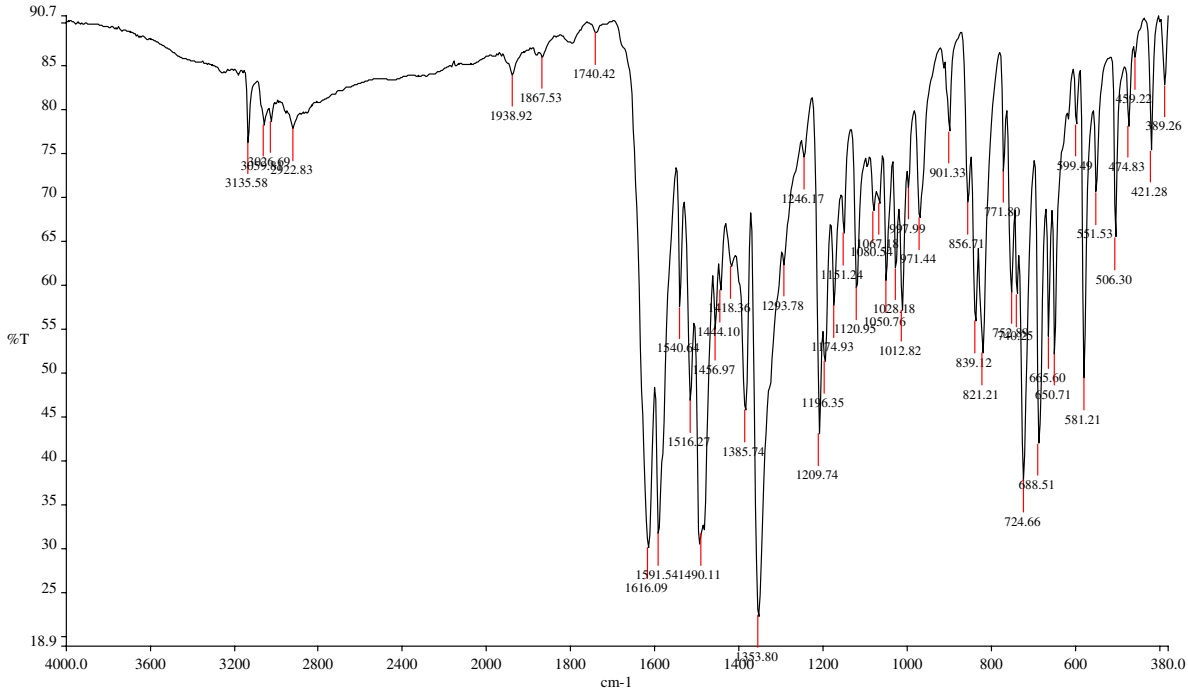


Fig. S6 IR spectra of Schiff base ligand



9. X-ray crystallography data of Schiff base ligand

Fig. S7 ORTEP diagram showing atom numbering scheme.

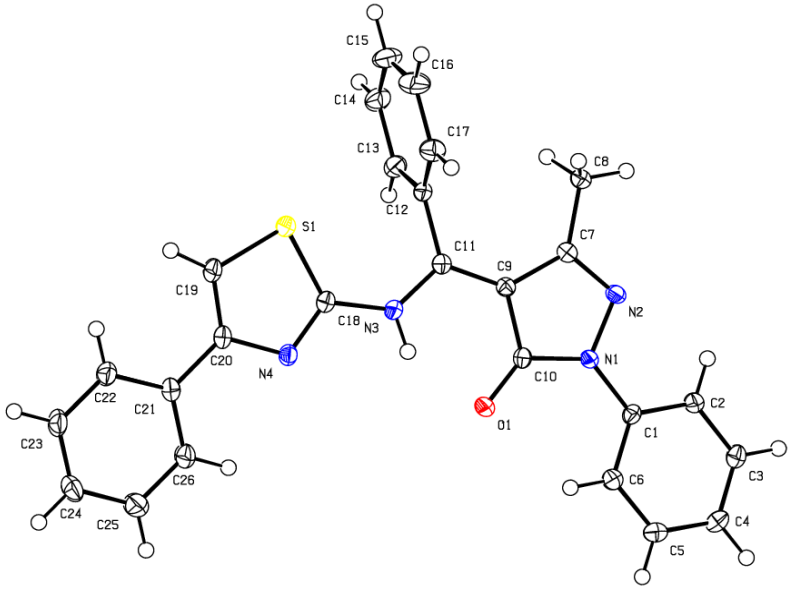


Table S1 Crystal data and structure refinement

Identification code	13bo_hbf_at3_0ma	
Empirical formula	C26 H20 N4 O S	
Formula weight	436.52	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 13.9867(3) Å	= 90°.
b = 21.2378(4) Å	= 95.7990(10)°.	
c = 7.22470(10) Å	= 90°.	
Volume	2135.09(7) Å^3	
Z	4	
Density (calculated)	1.358 Mg/m^3	

Absorption coefficient	0.179 mm^{-1}
F(000)	912
Crystal size	0.46 x 0.25 x 0.23 mm^3
Theta range for data collection	1.75 to 28.41°.
Index ranges	-17<=h<=18, -28<=k<=27, -9<=l<=9
Reflections collected	58780
Independent reflections	5358 [R(int) = 0.0260]
Completeness to theta = 28.41°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9600 and 0.9223
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5358 / 0 / 294
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.0913
R indices (all data)	R1 = 0.0476, wR2 = 0.0978
Largest diff. peak and hole	0.572 and -0.285 e.$Å^{-3}$

Table S2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	376(1)	6621(1)	2484(2)	15(1)
C(2)	-459(1)	6706(1)	3370(2)	18(1)
C(3)	-1022(1)	6188(1)	3708(2)	22(1)
C(4)	-769(1)	5587(1)	3187(2)	24(1)
C(5)	62(1)	5507(1)	2312(2)	23(1)
C(6)	637(1)	6018(1)	1950(2)	19(1)
C(7)	1232(1)	8163(1)	2131(2)	15(1)
C(8)	1029(1)	8851(1)	2265(2)	19(1)
C(9)	2077(1)	7856(1)	1590(2)	15(1)
C(10)	1861(1)	7184(1)	1623(2)	15(1)

C(11)	2955(1)	8089(1)	1200(2)	15(1)
C(12)	3212(1)	8770(1)	1367(2)	17(1)
C(13)	3678(1)	8985(1)	3045(2)	21(1)
C(14)	3920(1)	9616(1)	3238(2)	27(1)
C(15)	3704(1)	10030(1)	1773(2)	31(1)
C(16)	3240(1)	9817(1)	107(2)	31(1)
C(17)	2993(1)	9185(1)	-107(2)	24(1)
C(18)	4552(1)	7766(1)	276(2)	17(1)
C(19)	6097(1)	8094(1)	-555(2)	22(1)
C(20)	5977(1)	7461(1)	-442(2)	17(1)
C(21)	6703(1)	6979(1)	-743(2)	18(1)
C(22)	7573(1)	7149(1)	-1409(2)	23(1)
C(23)	8260(1)	6699(1)	-1700(2)	26(1)
C(24)	8087(1)	6071(1)	-1342(2)	28(1)
C(25)	7226(1)	5894(1)	-686(2)	29(1)
C(26)	6538(1)	6345(1)	-390(2)	23(1)
N(1)	947(1)	7154(1)	2167(1)	15(1)
N(2)	573(1)	7757(1)	2469(1)	16(1)
N(3)	3621(1)	7672(1)	745(2)	18(1)
N(4)	5083(1)	7275(1)	28(2)	17(1)
O(1)	2388(1)	6734(1)	1290(1)	19(1)
S(1)	5081(1)	8489(1)	-58(1)	23(1)

Table S3 Bond lengths [Å] and angles [°]

C(1)-C(6)	1.3957(17)
C(1)-C(2)	1.3982(17)
C(1)-N(1)	1.4165(15)
C(2)-C(3)	1.3892(17)
C(2)-H(2)	0.9500
C(3)-C(4)	1.3865(19)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3879(19)
C(4)-H(4)	0.9500
C(5)-C(6)	1.3918(18)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-N(2)	1.3038(16)
C(7)-C(9)	1.4390(16)
C(7)-C(8)	1.4940(16)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800

C(8)-H(8C)	0.9800
C(9)-C(11)	1.3799(16)
C(9)-C(10)	1.4596(16)
C(10)-O(1)	1.2441(15)
C(10)-N(1)	1.3762(15)
C(11)-N(3)	1.3499(15)
C(11)-C(12)	1.4928(17)
C(12)-C(17)	1.3917(18)
C(12)-C(13)	1.3933(18)
C(13)-C(14)	1.3875(18)
C(13)-H(13)	0.9500
C(14)-C(15)	1.385(2)
C(14)-H(14)	0.9500
C(15)-C(16)	1.384(2)
C(15)-H(15)	0.9500
C(16)-C(17)	1.391(2)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-N(4)	1.3047(16)
C(18)-N(3)	1.3919(15)
C(18)-S(1)	1.7316(13)
C(19)-C(20)	1.3593(18)
C(19)-S(1)	1.7191(13)
C(19)-H(19)	0.9500
C(20)-N(4)	1.3864(15)
C(20)-C(21)	1.4726(17)
C(21)-C(26)	1.3930(18)
C(21)-C(22)	1.3998(17)
C(22)-C(23)	1.3858(19)
C(22)-H(22)	0.9500
C(23)-C(24)	1.384(2)
C(23)-H(23)	0.9500
C(24)-C(25)	1.3897(19)
C(24)-H(24)	0.9500
C(25)-C(26)	1.3888(19)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
N(1)-N(2)	1.4086(14)
N(3)-H(3A)	0.883(19)

C(6)-C(1)-C(2)	119.87(11)
C(6)-C(1)-N(1)	121.35(11)
C(2)-C(1)-N(1)	118.78(11)
C(3)-C(2)-C(1)	119.56(12)
C(3)-C(2)-H(2)	120.2
C(1)-C(2)-H(2)	120.2

C(4)-C(3)-C(2)	121.02(12)
C(4)-C(3)-H(3)	119.5
C(2)-C(3)-H(3)	119.5
C(3)-C(4)-C(5)	119.07(12)
C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
C(4)-C(5)-C(6)	121.01(12)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(5)-C(6)-C(1)	119.48(12)
C(5)-C(6)-H(6)	120.3
C(1)-C(6)-H(6)	120.3
N(2)-C(7)-C(9)	111.46(10)
N(2)-C(7)-C(8)	119.56(10)
C(9)-C(7)-C(8)	128.94(11)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(11)-C(9)-C(7)	131.68(11)
C(11)-C(9)-C(10)	123.04(11)
C(7)-C(9)-C(10)	105.19(10)
O(1)-C(10)-N(1)	127.27(11)
O(1)-C(10)-C(9)	128.22(11)
N(1)-C(10)-C(9)	104.48(10)
N(3)-C(11)-C(9)	117.68(11)
N(3)-C(11)-C(12)	119.26(10)
C(9)-C(11)-C(12)	122.96(11)
C(17)-C(12)-C(13)	120.46(12)
C(17)-C(12)-C(11)	121.20(11)
C(13)-C(12)-C(11)	118.34(11)
C(14)-C(13)-C(12)	119.39(12)
C(14)-C(13)-H(13)	120.3
C(12)-C(13)-H(13)	120.3
C(15)-C(14)-C(13)	120.33(13)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(16)-C(15)-C(14)	120.21(13)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(15)-C(16)-C(17)	120.12(13)
C(15)-C(16)-H(16)	119.9
C(17)-C(16)-H(16)	119.9
C(16)-C(17)-C(12)	119.48(13)

C(16)-C(17)-H(17)	120.3
C(12)-C(17)-H(17)	120.3
N(4)-C(18)-N(3)	118.55(11)
N(4)-C(18)-S(1)	115.67(9)
N(3)-C(18)-S(1)	125.77(9)
C(20)-C(19)-S(1)	111.16(9)
C(20)-C(19)-H(19)	124.4
S(1)-C(19)-H(19)	124.4
C(19)-C(20)-N(4)	114.61(11)
C(19)-C(20)-C(21)	126.01(11)
N(4)-C(20)-C(21)	119.37(11)
C(26)-C(21)-C(22)	118.50(12)
C(26)-C(21)-C(20)	120.98(11)
C(22)-C(21)-C(20)	120.52(12)
C(23)-C(22)-C(21)	120.96(13)
C(23)-C(22)-H(22)	119.5
C(21)-C(22)-H(22)	119.5
C(24)-C(23)-C(22)	119.93(12)
C(24)-C(23)-H(23)	120.0
C(22)-C(23)-H(23)	120.0
C(23)-C(24)-C(25)	119.82(13)
C(23)-C(24)-H(24)	120.1
C(25)-C(24)-H(24)	120.1
C(26)-C(25)-C(24)	120.24(13)
C(26)-C(25)-H(25)	119.9
C(24)-C(25)-H(25)	119.9
C(25)-C(26)-C(21)	120.54(12)
C(25)-C(26)-H(26)	119.7
C(21)-C(26)-H(26)	119.7
C(10)-N(1)-N(2)	111.85(9)
C(10)-N(1)-C(1)	129.65(10)
N(2)-N(1)-C(1)	118.48(9)
C(7)-N(2)-N(1)	107.02(9)
C(11)-N(3)-C(18)	130.59(11)
C(11)-N(3)-H(3A)	113.7(12)
C(18)-N(3)-H(3A)	115.7(12)
C(18)-N(4)-C(20)	110.24(11)
C(19)-S(1)-C(18)	88.32(6)

Symmetry transformations used to generate equivalent atoms:

Table S4 Anisotropic displacement parameters ($Å^2 x\ 10^3$)

The anisotropic displacement factor exponent takes the form: $-2\ ^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	14(1)	16(1)	15(1)	2(1)	1(1)	-2(1)
C(2)	17(1)	17(1)	21(1)	1(1)	4(1)	1(1)
C(3)	17(1)	23(1)	28(1)	2(1)	7(1)	-2(1)
C(4)	22(1)	19(1)	31(1)	2(1)	5(1)	-6(1)
C(5)	24(1)	16(1)	29(1)	-2(1)	4(1)	-1(1)
C(6)	18(1)	18(1)	21(1)	-1(1)	4(1)	0(1)
C(7)	17(1)	16(1)	14(1)	0(1)	2(1)	1(1)
C(8)	18(1)	15(1)	24(1)	-1(1)	5(1)	1(1)
C(9)	15(1)	15(1)	15(1)	0(1)	2(1)	1(1)
C(10)	14(1)	18(1)	13(1)	1(1)	2(1)	-1(1)
C(11)	15(1)	16(1)	14(1)	0(1)	1(1)	0(1)
C(12)	14(1)	15(1)	22(1)	-2(1)	5(1)	-1(1)
C(13)	21(1)	20(1)	22(1)	-1(1)	2(1)	-3(1)
C(14)	27(1)	24(1)	31(1)	-8(1)	2(1)	-5(1)
C(15)	37(1)	16(1)	42(1)	-3(1)	9(1)	-5(1)
C(16)	41(1)	20(1)	33(1)	6(1)	5(1)	2(1)
C(17)	27(1)	21(1)	23(1)	1(1)	1(1)	1(1)
C(18)	14(1)	19(1)	17(1)	0(1)	3(1)	-2(1)
C(19)	15(1)	24(1)	28(1)	2(1)	7(1)	-2(1)
C(20)	13(1)	22(1)	16(1)	0(1)	2(1)	-1(1)
C(21)	14(1)	23(1)	16(1)	-1(1)	1(1)	1(1)
C(22)	17(1)	24(1)	28(1)	-3(1)	6(1)	-2(1)
C(23)	16(1)	32(1)	33(1)	-6(1)	8(1)	-1(1)
C(24)	20(1)	30(1)	34(1)	-4(1)	7(1)	6(1)
C(25)	27(1)	23(1)	37(1)	3(1)	11(1)	3(1)
C(26)	19(1)	25(1)	27(1)	2(1)	9(1)	0(1)
N(1)	14(1)	13(1)	18(1)	0(1)	4(1)	1(1)
N(2)	16(1)	14(1)	18(1)	0(1)	3(1)	2(1)
N(3)	14(1)	16(1)	24(1)	-1(1)	5(1)	-2(1)
N(4)	14(1)	19(1)	19(1)	-1(1)	3(1)	-1(1)
O(1)	17(1)	16(1)	24(1)	-1(1)	6(1)	2(1)
S(1)	17(1)	17(1)	36(1)	3(1)	9(1)	-1(1)

Table S5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3)

	x	y	z	U(eq)
H(2)	-639	7115	3739	22
H(3)	-1591	6246	4306	27
H(4)	-1158	5236	3425	29
H(5)	241	5096	1954	28
H(6)	1202	5958	1345	23
H(8A)	996	9041	1023	28
H(8B)	1543	9053	3078	28
H(8C)	414	8912	2783	28
H(13)	3829	8701	4048	25
H(14)	4235	9766	4380	33
H(15)	3875	10462	1912	38
H(16)	3090	10103	-891	38
H(17)	2676	9037	-1250	28
H(19)	6668	8293	-868	26
H(22)	7694	7578	-1664	28
H(23)	8849	6821	-2144	32
H(24)	8555	5761	-1544	33
H(25)	7106	5464	-439	34
H(26)	5951	6221	57	28
H(3A)	3433(13)	7276(9)	780(20)	35(5)

Table S6 Torsion angles [°]

C(6)-C(1)-C(2)-C(3)	-0.13(18)
N(1)-C(1)-C(2)-C(3)	-179.42(11)
C(1)-C(2)-C(3)-C(4)	0.3(2)
C(2)-C(3)-C(4)-C(5)	-0.1(2)
C(3)-C(4)-C(5)-C(6)	-0.2(2)
C(4)-C(5)-C(6)-C(1)	0.3(2)
C(2)-C(1)-C(6)-C(5)	-0.15(18)
N(1)-C(1)-C(6)-C(5)	179.11(11)
N(2)-C(7)-C(9)-C(11)	-176.26(12)
C(8)-C(7)-C(9)-C(11)	6.2(2)
N(2)-C(7)-C(9)-C(10)	0.22(14)
C(8)-C(7)-C(9)-C(10)	-177.33(12)
C(11)-C(9)-C(10)-O(1)	-1.6(2)

C(7)-C(9)-C(10)-O(1)	-178.44(12)
C(11)-C(9)-C(10)-N(1)	176.60(11)
C(7)-C(9)-C(10)-N(1)	-0.26(12)
C(7)-C(9)-C(11)-N(3)	179.17(12)
C(10)-C(9)-C(11)-N(3)	3.22(18)
C(7)-C(9)-C(11)-C(12)	2.8(2)
C(10)-C(9)-C(11)-C(12)	-173.12(11)
N(3)-C(11)-C(12)-C(17)	96.12(15)
C(9)-C(11)-C(12)-C(17)	-87.59(16)
N(3)-C(11)-C(12)-C(13)	-84.03(15)
C(9)-C(11)-C(12)-C(13)	92.26(15)
C(17)-C(12)-C(13)-C(14)	0.17(19)
C(11)-C(12)-C(13)-C(14)	-179.69(12)
C(12)-C(13)-C(14)-C(15)	-0.3(2)
C(13)-C(14)-C(15)-C(16)	0.3(2)
C(14)-C(15)-C(16)-C(17)	-0.3(2)
C(15)-C(16)-C(17)-C(12)	0.2(2)
C(13)-C(12)-C(17)-C(16)	-0.2(2)
C(11)-C(12)-C(17)-C(16)	179.69(12)
S(1)-C(19)-C(20)-N(4)	0.33(15)
S(1)-C(19)-C(20)-C(21)	-178.77(10)
C(19)-C(20)-C(21)-C(26)	172.83(13)
N(4)-C(20)-C(21)-C(26)	-6.23(18)
C(19)-C(20)-C(21)-C(22)	-7.7(2)
N(4)-C(20)-C(21)-C(22)	173.23(11)
C(26)-C(21)-C(22)-C(23)	-0.4(2)
C(20)-C(21)-C(22)-C(23)	-179.90(12)
C(21)-C(22)-C(23)-C(24)	0.4(2)
C(22)-C(23)-C(24)-C(25)	-0.2(2)
C(23)-C(24)-C(25)-C(26)	0.0(2)
C(24)-C(25)-C(26)-C(21)	-0.1(2)
C(22)-C(21)-C(26)-C(25)	0.3(2)
C(20)-C(21)-C(26)-C(25)	179.73(13)
O(1)-C(10)-N(1)-N(2)	178.44(11)
C(9)-C(10)-N(1)-N(2)	0.24(13)
O(1)-C(10)-N(1)-C(1)	0.0(2)
C(9)-C(10)-N(1)-C(1)	-178.21(11)
C(6)-C(1)-N(1)-C(10)	-11.39(19)
C(2)-C(1)-N(1)-C(10)	167.88(12)
C(6)-C(1)-N(1)-N(2)	170.25(11)
C(2)-C(1)-N(1)-N(2)	-10.48(16)
C(9)-C(7)-N(2)-N(1)	-0.07(13)
C(8)-C(7)-N(2)-N(1)	177.73(10)
C(10)-N(1)-N(2)-C(7)	-0.11(13)
C(1)-N(1)-N(2)-C(7)	178.53(10)
C(9)-C(11)-N(3)-C(18)	179.47(12)

C(12)-C(11)-N(3)-C(18)	-4.0(2)
N(4)-C(18)-N(3)-C(11)	174.79(12)
S(1)-C(18)-N(3)-C(11)	-6.4(2)
N(3)-C(18)-N(4)-C(20)	179.52(11)
S(1)-C(18)-N(4)-C(20)	0.57(14)
C(19)-C(20)-N(4)-C(18)	-0.57(15)
C(21)-C(20)-N(4)-C(18)	178.59(11)
C(20)-C(19)-S(1)-C(18)	-0.01(10)
N(4)-C(18)-S(1)-C(19)	-0.33(10)
N(3)-C(18)-S(1)-C(19)	-179.20(12)

Symmetry transformations used to generate equivalent atoms:

Table S7 Hydrogen bonds [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	Symmetry operator
N(3)-H(3A)…O(1)	0.883(19)	1.925(18)	2.6901(13)	144.1(17)	x, y, z
C(2)-H(2)…N(2)	0.95	2.43	2.7706(16)	101	x, y, z
C(6)-H(6)…O(1)	0.95	2.34	2.9626(15)	122	x, y, z
C(17)-H(17)…O(1)	0.95	2.42	3.2954(16)	153	x, ½-y, ½+z
C(23)-H(23)…N(2)	0.95	2.61	3.5437(16)	166	-1+x, ½-y, ½+z
C(26)-H(26)…N(4)	0.95	2.55	2.8728(16)	100	x, y, z