Supplementary Data

*2.2.1. 2,2'-(4,4'-Ethylenebiphenyl) bis(3-methyl-2-imino-4-phenyl-3H-thiazole) (**4a**)*

Yield 73%; yellow solid; mp 214-216 °C; FT-IR (KBr) (ν_{max}/cm^{-1}): 3062, 2991, 2932, 2856, 2830, 1618, 1595, 1512, 1419, 1366, 1240, 1028, 838, 702. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 2.93 (s, 4H), 3.39 (s, 6H), 5.81 (s, 2H), 7.05 (d, 4H, *J* = 8.0 Hz), 7.16 (d, 4H, *J* = 8.0 Hz), 7.41 (t, 4H, *J* = 4.8 Hz), 7.46 (d, 6H, *J* = 4.8 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 33.5, 37.6, 95.5, 1214, 128.6, 128.7, 129.0, 129.2, 131.5, 136.7, 140.5, 149.2, 160.7 ppm; Anal.Calcd for $C_{34}H_{30}N_4S_2$ (558.76) C, 73.08; H, 5.41; N, 10.02. Found: C, 73.05; H, 5.45; N, 10.05%.

*2.2.2. 2,2'-(4,4'-Ethylenebiphenyl) bis(3-ethyl-2-imino-4-phenyl-3H-thiazole) (**4b**)*

Yield 89%; yellow solid; mp 169-171 °C; FT-IR (KBr) (ν_{max}/cm^{-1}): 3058, 3029, 3003, 2922, 2851, 1616, 1520, 1448, 1319, 1223, 1001, 819, 686. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 1.22 (t, 6H, *J* = 7.2 Hz), 3.90 (q, 4H, *J* = 7.2 Hz), 4.64 (s, 4H), 5.68 (s, 2H), 7.03(d, 4H, *J* = 8.0 Hz), 7.17 (d, 4H, *J* = 8.0 Hz), 7.40-7.48 (m, 10H); ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 13.5, 37.7, 40.3, 95.6, 121.3, 128.6, 129.0, 129.5, 132.0, 136.5, 140.1, 149.6, 159.4 ppm; Anal.Calcd for $C_{36}H_{34}N_4S_2$ (586.82) C, 73.68; H, 5.84; N, 9.54. Found: C, 73.64; H, 5.87; N, 9.58%.

*2.2.3. 2,2'-(4,4'-biphenylsolfone) bis(3-methyl-2-imino-4-phenyl-3H-thiazole) (**5a**)*

Yield 65%; yellow solid; mp 193-195 °C; FT-IR (KBr) ($\nu_{max/cm-1}$): 3100, 2910, 1619, 1591, 1577, 1500, 1420, 1360, 1292, 1140, 1100, 980, 815, 760, 698. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 3.38 (s, 6H), 5.89 (s, 2H), 7.20 (d, 4H, *J* = 7.6 Hz), 7.38 (t, 4H, *J* = 3.2 Hz), 7.48 (d, 6H, *J* = 3.2 Hz), 7.85 (d, 4H, *J* = 7.6 Hz); ^{13}C-NMR ($CDCl_3$, 100

MHz): δ_c: 33.5, 95.9, 114.1, 119.1, 121.8, 128.8, 128.9, 129.6, 131.1, 140.6, 150.6 ppm; Anal.Calcd for $C_{32}H_{26}N_4S_3O_2$ (594.77) C, 64.62; H, 4.40; N, 9.41. Found: C, 64.59; H, 4.37; N, 9.45%.

*2.2.4. 2,2'-(4,4'-biphenylsolfone) bis (3-ethyl-2-imino-4-phenyl-3H-thiazole) (**5b**)*

Yield 69%; yellow solid; mp 182-183 °C; FT-IR (KBr) ($\nu_{max/cm-1}$): 3096, 3059, 2960, 2926, 2856, 1627, 1593, 1500, 1437, 1382, 1280, 1142, 1103, 1071, 1004, 830, 694. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 1.20 (t, 6H, *J* = 6.8 Hz), 3.88 (q, 4H, *J* = 6.8 Hz), 5.83 (s, 2H), 7.19 (d, 4H, *J* = 7.8 Hz), 7.38-7.48 (m, 10H), 7.85 (d, 4H, *J* = 7.8 Hz) ppm; Anal.Calcd for $C_{34}H_{30}N_4S_3O_2$ (622.82) C, 65.56; H, 4.85; N, 8.99. Found: C, 65.59; H, 4.87; N, 8.95%.

*2.2.5. 2,2'-(4,4'-biphenylsolfone) bis(3-allyl-2-imino-4-phenyl-3H-thiazole) (**5c**)*

Yield 64%; yellow solid; mp 119-121 °C; FT-IR (KBr) ($\nu_{max/cm-1}$): 3068, 2960, 2918, 1619, 1595, 1439, 1382, 1280, 1147, 1098, 1075, 833, 698. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 4.44 (m,4H), 5.01 (d, 2H, *J* = 17.2 Hz), 5.16 (d, 2H, *J* = 10.4 Hz), 5.86 (s, 2H), 5.90-5.98 (m, 2H), 7.18 (d, 4H, *J* = 10.8 Hz), 7.54-7.70 (m, 10H), 7.86 (d, 4H, *J* = 10.8 Hz) ppm; Anal.Calcd for $C_{36}H_{30}N_4S_3O_2$ (646.85) C, 66.84; H, 4.67; N, 8.66. Found: C, 66.80; H, 4.72; N, 8.63%.

*2.2.6. 2,2'-(4,4'-methylenebiphenyl) bis(3-methyl-2-imino-4-phenyl-3H-thiazole) (**6a**)*

Yield 62%; yellow solid; mp 158-159 °C; FT-IR (KBr) (ν_{max}/cm^{-1}): 3057, 2918, 1685, 1616, 1577, 1560, 1521, 1446, 1355, 1002, 752, 686. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 3.82 (s, 6H), 4.61 (s, 4H), 5.36 (s, 2H), 6.67 (d, 4H, *J* = 7.6 Hz), 7.06 (d, 4H, *J* = 7.6 Hz), 7.50-7.61 (m, 10H); ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 20.6,, 40.1, 96.5, 113.2, 126.0, 128.5, 128.9, 129.7, 131.3, 133.8, 134.9, 145.2, 158.0 ppm; Anal.Calcd for

$C_{33}H_{28}N_4S_2$ (544.73) C, 72.76; H, 5.18; N, 10.28. Found: C, 72.73; H, 5.21; N, 10.30%.

*2.2.7. 2,2'-(4,4'-methylenebiphenyl) bis(3-ethyl-2-imino-4-phenyl-3H-thiazole) (**6b**)*

Yield 71%; yellow solid; mp 169-171 °C; FT-IR (KBr) (ν_{max}/cm^{-1}): 3057, 2920, 1685, 1616, 1521, 1560, 1521, 1446, 1355, 1002, 752, 686. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 1.51 (t, 6H, *J* = 7.4 Hz), 3.82 (q, 4H, *J* = 7.4 Hz), 4.62 (s, 4H), 5.36 (s, 2H), 6.68 (d, 4H, *J* = 6.8 Hz), 7.06 (d, 4H, *J* = 6.8 Hz), 7.51-7.61 (m, 10H) ppm; Anal.Calcd for $C_{35}H_{32}N_4S_2$ (572.79) C, 73.39; H, 5.63; N, 9.78. Found: C, 73.42; H, 5.59; N, 9.80%.

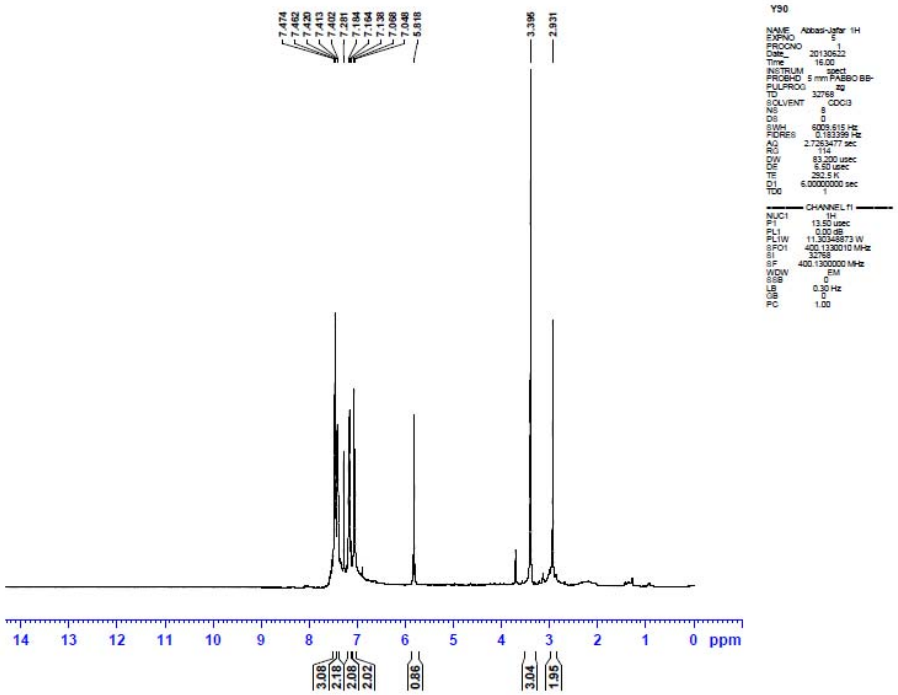
*2.2.8. 2,2'-(1,4-Phenylene) bis (3-methyl-2-imino-4-phenyl-3H-thiazole) (**7a**)*

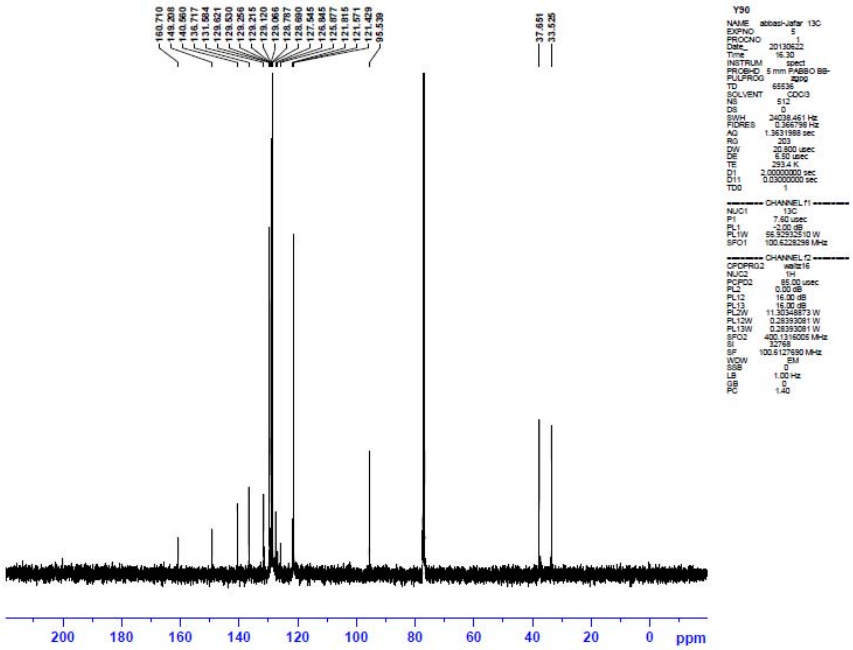
Yield 85%; yellow solid; mp 267-269 °C; FT-IR (KBr) ($\nu_{max/cm-1}$): 3068, 2924, 1608, 1574, 1566, 1496, 1417, 1365, 1240, 1056, 981, 883, 700, 495. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 3.39 (s, 6H), 5.81 (s, 2H), 7.13 (s, 4H), 7.40-7.48 (m, 10H) ppm; Anal.Calcd for $C_{26}H_{22}N_4S_2$ (454.61) C, 68.69; H, 4.87; N, 12.32. Found: C, 68.74; H, 4.90; N, 12.27%.

*2.2.9. 2,2'-(1,4-Phenylene) bis (3-ethyl-2-imino-4-phenyl-3H-thiazole) (**7b**)*

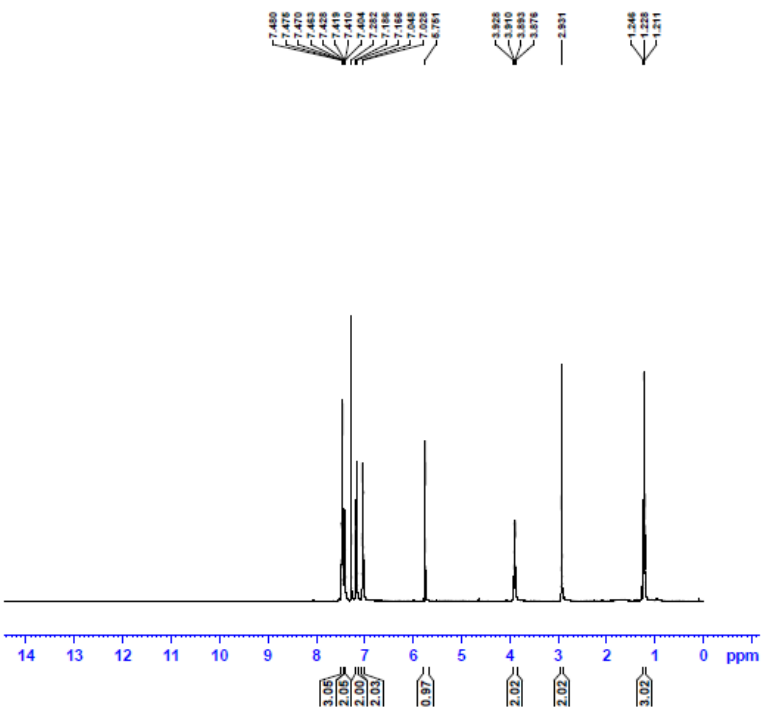
Yield 92%; yellowish solid; mp 254-256 °C; FT-IR (KBr) ($\nu_{max/cm-1}$): 3072, 2931, 1615, 1577, 1560, 1498, 1382, 1321 1236, 1076, 1004, 881, 763, 698. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 1.24 (t, 6H, *J* = 7.2 Hz), 3.91 (q, 4H, *J* = 7.2 Hz), 5.76 (s, 2H), 7.12 (s, 4H), 7.41-7.49 (m, 10H); ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 13.6, 40.4, 95.7, 122.5, 128.7, 128.9, 129,0, 132.1, 140.1, 147.2, 159.4 ppm; Anal.Calcd for $C_{28}H_{26}N_4S_2$ (482.66) C, 69.67; H, 5.42; N, 11.60. Found: C, 69.64; H, 5.44; N, 11.63%.

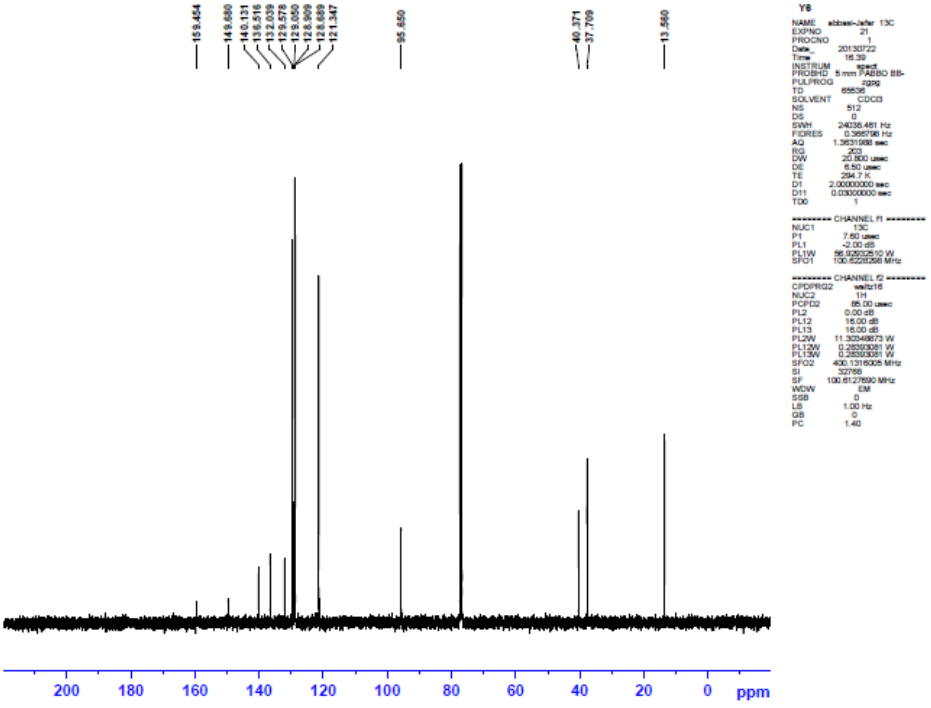
2,2'-(4,4'-Ethylenebiphenyl) bis (3-methyl-2-imino-4-phenyl-3H-thiazole)



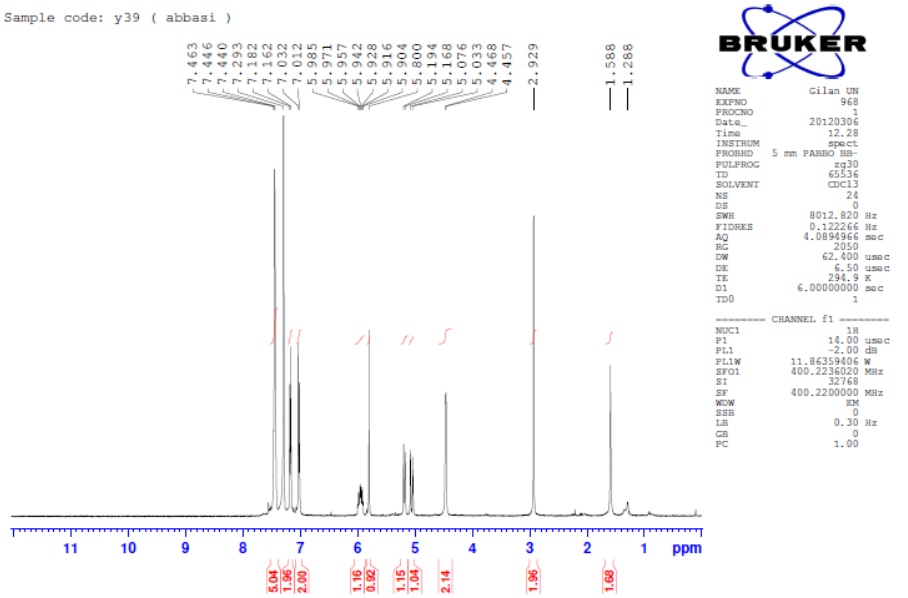


2,2'-(4,4'-Ethylenebiphenyl) bis (3-ethyl-2-imino-4-phenyl-3H-thiazole)

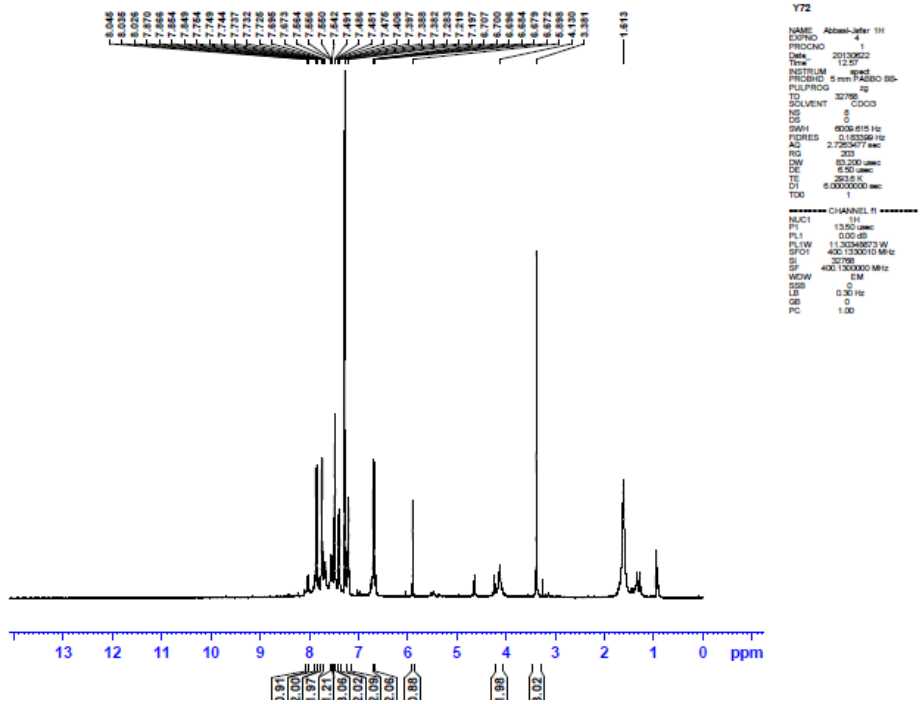


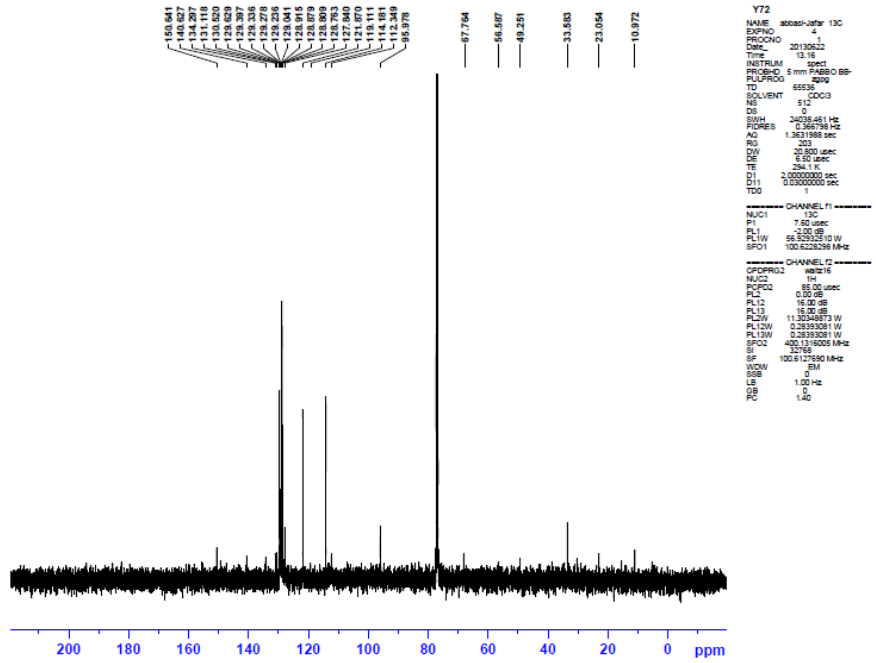


2,2'-(4,4'-Ethylenebiphenyl) bis (3-allyl-2-imino-4-phenyl-3H-thiazole)

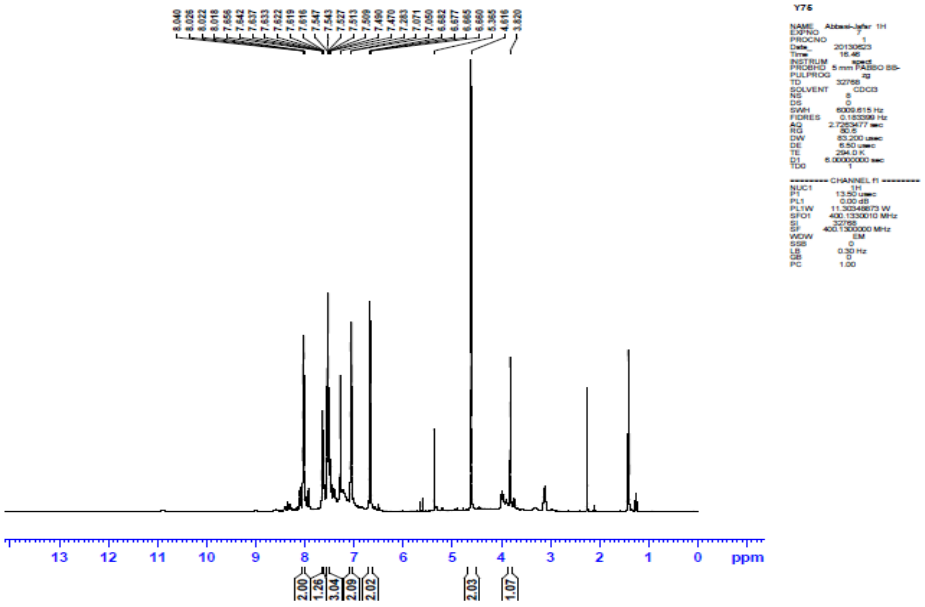


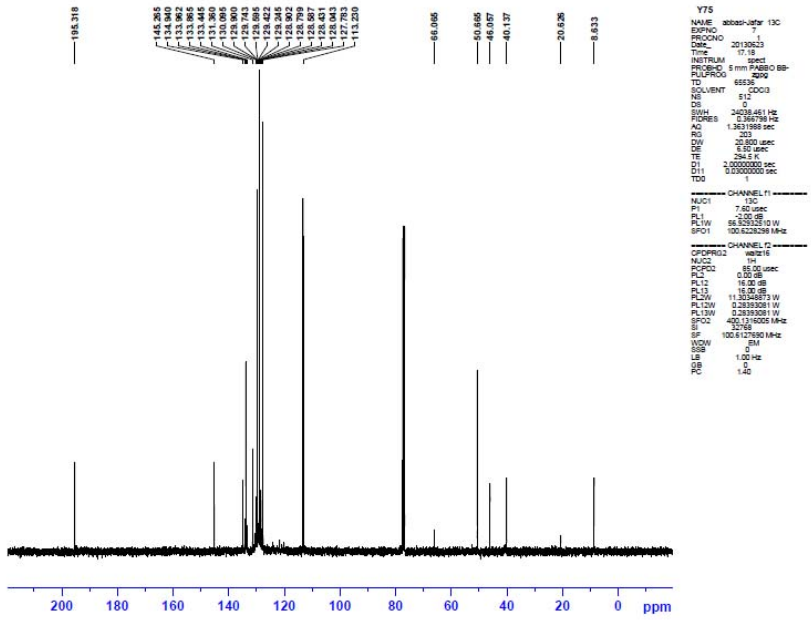
2,2'-(4,4'-biphenylsolfone)bis(3-methyl-2-imino-4-phenyl-3H-thiazole)



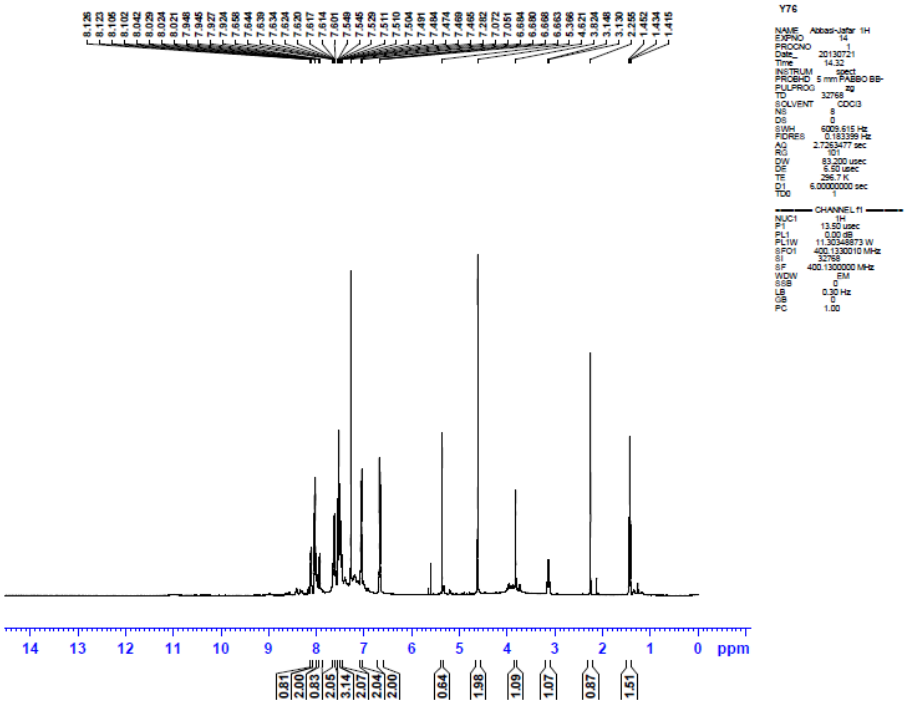


2,2'-(4,4'-methylenebiphenyl) bis (3-methyl-2-imino-4-phenyl-3H-thiazole)

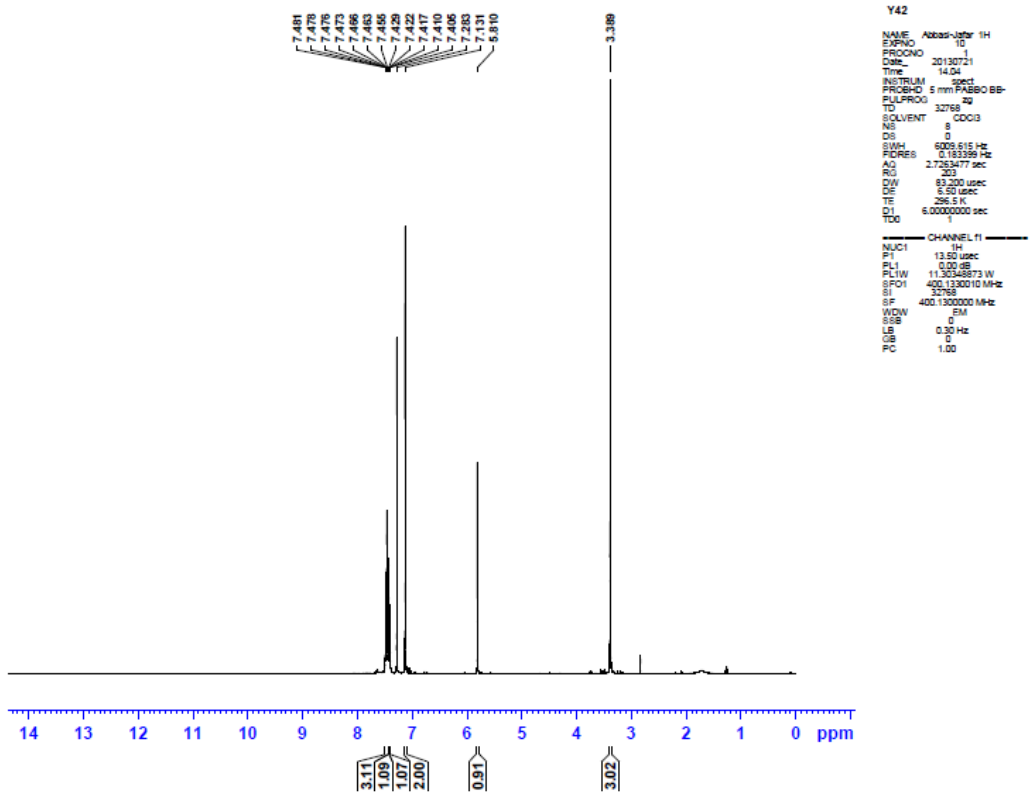




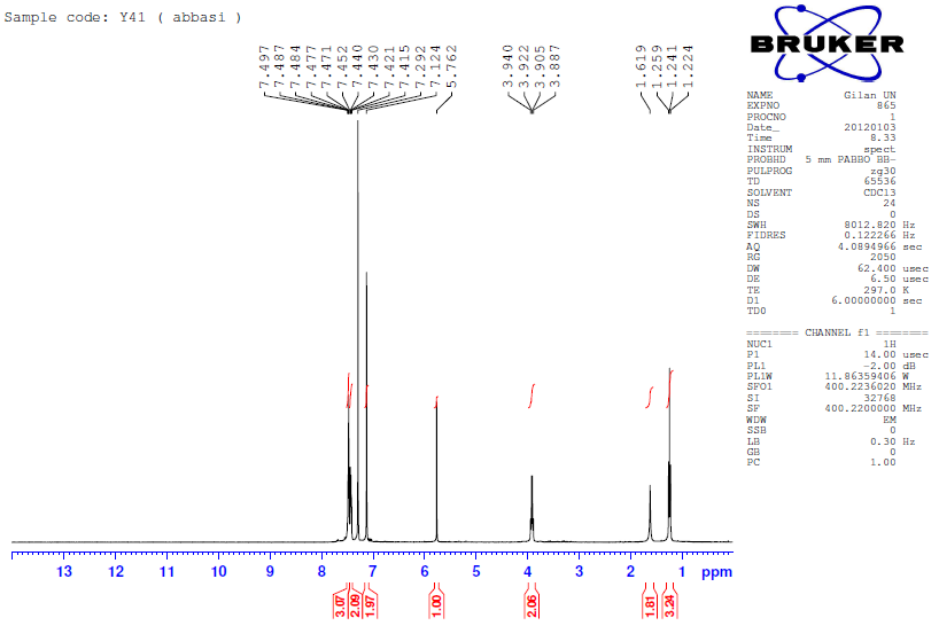
2,2'-(4,4'-methylenebiphenyl) bis (3-ethyl-2-imino-4-phenyl-3H-thiazole)



2,2'-(1,4-Phenylene) bis (3-methyl-2-imino-4-phenyl-3H-thiazole)



2,2'-(1,4-Phenylene) bis (3-ethyl-2-imino-4-phenyl-3H-thiazole)



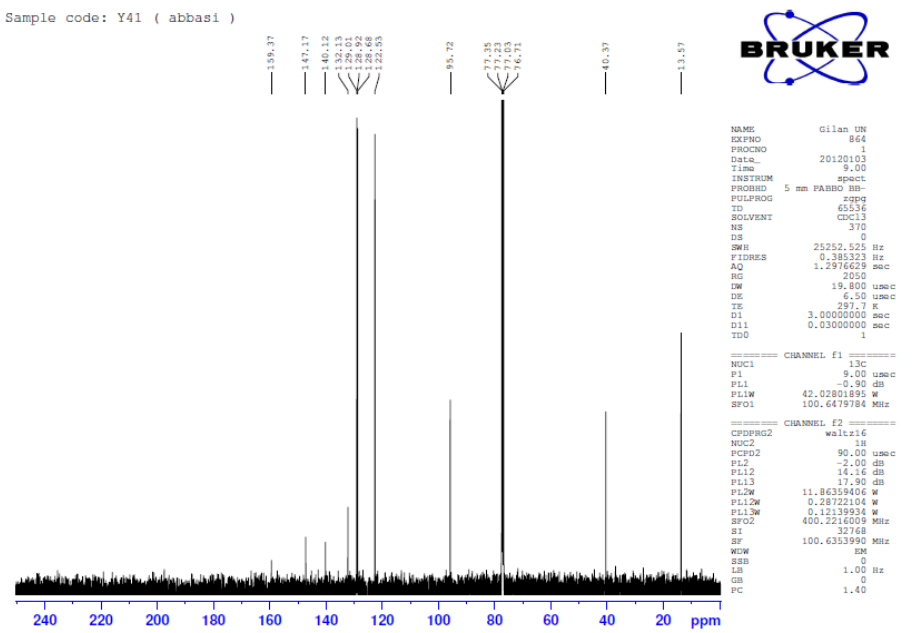


Table 1. Crystal data and structure refinement for test1.

Identification code	test1	
Empirical formula	C28 H26 N4 S2	
Formula weight	482.65	
Temperature	302(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 18.3241(15) Å	α= 90°.
	b = 17.7525(15) Å	β= 92.331(3)°.
	c = 7.3532(5) Å	γ = 90°.
Volume	2390.0(3) $Å^3$	
Z	4	
Density (calculated)	1.341 Mg/m^3	
Absorption coefficient	0.248 mm^{-1}	
F(000)	1016	
Crystal size	0.490 x 0.160 x 0.100 mm^3	
Theta range for data collection	3.001 to 26.000°.	
Index ranges	-22<=h<=22, -21<=k<=21, -9<=l<=8	

Reflections collected	88745
Independent reflections	4681 [R(int) = 0.3018]
Completeness to theta = 25.242°	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4681 / 0 / 309
Goodness-of-fit on F^2	1.151
Final R indices [I>2sigma(I)]	R1 = 0.0949, wR2 = 0.1267
R indices (all data)	R1 = 0.1658, wR2 = 0.1454
Extinction coefficient	n/a
Largest diff. peak and hole	0.300 and -0.286 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for test1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	6077(1)	4875(1)	212(1)	40(1)
S(2)	8785(1)	6579(1)	6662(1)	36(1)
N(1)	7151(2)	5696(2)	-1395(4)	31(1)
N(2)	6462(2)	4833(2)	-3110(4)	26(1)
N(3)	8994(2)	6460(2)	2956(4)	32(1)
N(4)	9991(2)	6530(2)	5003(4)	28(1)
C(1)	8026(2)	6094(2)	912(5)	26(1)
C(2)	8244(2)	6490(2)	2475(5)	26(1)
C(3)	7722(2)	6918(2)	3327(5)	33(1)
C(4)	7008(2)	6921(2)	2656(5)	34(1)
C(5)	6796(2)	6507(2)	1141(5)	32(1)
C(6)	7308(2)	6088(2)	240(5)	27(1)
C(7)	6641(2)	5205(2)	-1504(5)	26(1)
C(8)	5643(2)	4265(2)	-1322(5)	38(1)
C(9)	5899(2)	4311(2)	-2984(5)	27(1)
C(10)	6831(2)	5038(2)	-4760(5)	34(1)
C(11)	7593(2)	4717(3)	-4819(6)	55(1)
C(12)	5609(2)	3874(2)	-4572(5)	28(1)
C(13)	4863(2)	3876(3)	-4967(6)	43(1)
C(14)	4564(3)	3443(3)	-6367(6)	51(1)
C(15)	5007(3)	3000(3)	-7378(6)	52(1)
C(16)	5746(3)	2987(3)	-6994(6)	52(1)
C(17)	6049(2)	3420(2)	-5602(6)	43(1)
C(18)	9241(2)	6531(2)	4593(5)	26(1)
C(19)	9609(2)	6555(2)	7916(5)	36(1)
C(20)	10184(2)	6532(2)	6854(5)	27(1)
C(21)	10482(2)	6319(2)	3573(5)	33(1)
C(22)	10499(2)	5482(3)	3256(6)	49(1)
C(23)	10959(2)	6541(2)	7532(5)	28(1)
C(24)	11439(2)	7093(2)	7000(5)	30(1)
C(25)	12146(2)	7110(3)	7727(6)	38(1)
C(26)	12377(2)	6578(3)	8975(6)	41(1)
C(27)	11908(2)	6025(3)	9500(6)	43(1)

C(28)	11197(2)	6003(2)	8770(5)	38(1)

Table 3. Bond lengths [Å] and angles [°] for test1.

S(1)-C(8)	1.732(4)
S(1)-C(7)	1.763(4)
S(2)-C(19)	1.736(4)
S(2)-C(18)	1.768(4)
N(1)-C(7)	1.278(4)
N(1)-C(6)	1.408(4)
N(2)-C(7)	1.380(4)
N(2)-C(9)	1.394(5)
N(2)-C(10)	1.458(5)
N(3)-C(18)	1.275(4)
N(3)-C(2)	1.405(5)
N(4)-C(20)	1.392(4)
N(4)-C(18)	1.395(4)
N(4)-C(21)	1.460(5)
C(1)-C(6)	1.386(5)
C(1)-C(2)	1.391(5)
C(1)-H(1)	0.9300
C(2)-C(3)	1.391(5)
C(3)-C(4)	1.380(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.377(5)
C(4)-H(4)	0.9300
C(5)-C(6)	1.387(5)
C(5)-H(5)	0.9300
C(8)-C(9)	1.329(5)
C(8)-H(8)	0.9300
C(9)-C(12)	1.482(5)
C(10)-C(11)	1.511(5)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-C(13)	1.386(5)
C(12)-C(17)	1.386(5)
C(13)-C(14)	1.380(6)

C(13)-H(13)	0.9300
C(14)-C(15)	1.371(6)
C(14)-H(14)	0.9300
C(15)-C(16)	1.371(6)
C(15)-H(15)	0.9300
C(16)-C(17)	1.378(6)
C(16)-H(16)	0.9300
C(17)-H(17)	0.9300
C(19)-C(20)	1.338(5)
C(19)-H(19)	0.9300
C(20)-C(23)	1.486(5)
C(21)-C(22)	1.504(6)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-C(28)	1.377(5)
C(23)-C(24)	1.384(5)
C(24)-C(25)	1.382(5)
C(24)-H(24)	0.9300
C(25)-C(26)	1.372(6)
C(25)-H(25)	0.9300
C(26)-C(27)	1.372(6)
C(26)-H(26)	0.9300
C(27)-C(28)	1.388(5)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300

C(8)-S(1)-C(7)	90.49(19)
C(19)-S(2)-C(18)	91.43(19)
C(7)-N(1)-C(6)	120.9(3)
C(7)-N(2)-C(9)	114.3(3)
C(7)-N(2)-C(10)	119.4(3)
C(9)-N(2)-C(10)	126.2(3)
C(18)-N(3)-C(2)	122.7(3)
C(20)-N(4)-C(18)	114.8(3)
C(20)-N(4)-C(21)	124.4(3)

C(18)-N(4)-C(21)	118.4(3)
C(6)-C(1)-C(2)	122.3(4)
C(6)-C(1)-H(1)	118.8
C(2)-C(1)-H(1)	118.8
C(3)-C(2)-C(1)	118.0(3)
C(3)-C(2)-N(3)	126.1(3)
C(1)-C(2)-N(3)	115.7(3)
C(4)-C(3)-C(2)	120.0(4)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	121.3(4)
C(5)-C(4)-H(4)	119.4
C(3)-C(4)-H(4)	119.4
C(4)-C(5)-C(6)	119.9(3)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(1)-C(6)-C(5)	118.4(3)
C(1)-C(6)-N(1)	117.9(3)
C(5)-C(6)-N(1)	123.6(3)
N(1)-C(7)-N(2)	121.8(3)
N(1)-C(7)-S(1)	129.0(3)
N(2)-C(7)-S(1)	109.2(3)
C(9)-C(8)-S(1)	113.0(3)
C(9)-C(8)-H(8)	123.5
S(1)-C(8)-H(8)	123.5
C(8)-C(9)-N(2)	113.1(3)
C(8)-C(9)-C(12)	124.3(4)
N(2)-C(9)-C(12)	122.6(3)
N(2)-C(10)-C(11)	112.9(3)
N(2)-C(10)-H(10A)	109.0
C(11)-C(10)-H(10A)	109.0
N(2)-C(10)-H(10B)	109.0
C(11)-C(10)-H(10B)	109.0
H(10A)-C(10)-H(10B)	107.8
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5

H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(13)-C(12)-C(17)	118.5(4)
C(13)-C(12)-C(9)	118.8(4)
C(17)-C(12)-C(9)	122.5(3)
C(14)-C(13)-C(12)	120.9(4)
C(14)-C(13)-H(13)	119.6
C(12)-C(13)-H(13)	119.6
C(15)-C(14)-C(13)	119.9(4)
C(15)-C(14)-H(14)	120.1
C(13)-C(14)-H(14)	120.1
C(16)-C(15)-C(14)	119.9(4)
C(16)-C(15)-H(15)	120.0
C(14)-C(15)-H(15)	120.0
C(15)-C(16)-C(17)	120.6(5)
C(15)-C(16)-H(16)	119.7
C(17)-C(16)-H(16)	119.7
C(16)-C(17)-C(12)	120.3(4)
C(16)-C(17)-H(17)	119.9
C(12)-C(17)-H(17)	119.9
N(3)-C(18)-N(4)	120.9(3)
N(3)-C(18)-S(2)	130.9(3)
N(4)-C(18)-S(2)	108.1(3)
C(20)-C(19)-S(2)	112.3(3)
C(20)-C(19)-H(19)	123.9
S(2)-C(19)-H(19)	123.9
C(19)-C(20)-N(4)	113.4(3)
C(19)-C(20)-C(23)	124.7(3)
N(4)-C(20)-C(23)	121.9(3)
N(4)-C(21)-C(22)	112.4(3)
N(4)-C(21)-H(21A)	109.1
C(22)-C(21)-H(21A)	109.1
N(4)-C(21)-H(21B)	109.1
C(22)-C(21)-H(21B)	109.1
H(21A)-C(21)-H(21B)	107.8
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5

C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(28)-C(23)-C(24)	119.3(4)
C(28)-C(23)-C(20)	119.2(4)
C(24)-C(23)-C(20)	121.4(3)
C(25)-C(24)-C(23)	120.1(4)
C(25)-C(24)-H(24)	119.9
C(23)-C(24)-H(24)	119.9
C(26)-C(25)-C(24)	120.3(4)
C(26)-C(25)-H(25)	119.9
C(24)-C(25)-H(25)	119.9
C(27)-C(26)-C(25)	120.0(4)
C(27)-C(26)-H(26)	120.0
C(25)-C(26)-H(26)	120.0
C(26)-C(27)-C(28)	120.0(4)
C(26)-C(27)-H(27)	120.0
C(28)-C(27)-H(27)	120.0
C(23)-C(28)-C(27)	120.3(4)
C(23)-C(28)-H(28)	119.9
C(27)-C(28)-H(28)	119.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for test1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	43(1)	52(1)	24(1)	-7(1)	6(1)	-10(1)
S(2)	26(1)	50(1)	31(1)	-6(1)	0(1)	3(1)
N(1)	26(2)	45(2)	22(2)	-3(2)	-3(1)	-7(2)
N(2)	22(2)	34(2)	21(2)	0(2)	-2(1)	-3(2)
N(3)	28(2)	39(2)	28(2)	-6(2)	-8(2)	-3(2)
N(4)	24(2)	38(2)	22(2)	-4(2)	-2(1)	-2(2)
C(1)	26(2)	33(2)	20(2)	1(2)	-2(2)	-1(2)
C(2)	28(2)	27(2)	22(2)	3(2)	-3(2)	-4(2)
C(3)	36(3)	33(2)	30(2)	-10(2)	-9(2)	-2(2)
C(4)	30(2)	35(3)	37(3)	-6(2)	0(2)	4(2)
C(5)	23(2)	38(3)	33(2)	-1(2)	-7(2)	0(2)
C(6)	26(2)	33(2)	22(2)	2(2)	-3(2)	-7(2)
C(7)	22(2)	34(2)	21(2)	-1(2)	-4(2)	2(2)
C(8)	36(3)	46(3)	32(3)	-4(2)	4(2)	-15(2)
C(9)	24(2)	31(2)	26(2)	2(2)	0(2)	2(2)
C(10)	41(3)	40(3)	21(2)	-1(2)	-3(2)	-11(2)
C(11)	37(3)	78(4)	49(3)	-18(3)	16(2)	-16(3)
C(12)	31(2)	26(2)	27(2)	-1(2)	-4(2)	-5(2)
C(13)	38(3)	43(3)	49(3)	-6(2)	-8(2)	1(2)
C(14)	46(3)	45(3)	60(3)	-6(3)	-23(2)	-5(3)
C(15)	70(4)	46(3)	39(3)	-6(2)	-20(3)	-18(3)
C(16)	62(4)	48(3)	45(3)	-21(2)	6(3)	-9(3)
C(17)	37(3)	49(3)	43(3)	-8(2)	2(2)	-8(2)
C(18)	23(2)	23(2)	33(2)	-6(2)	0(2)	-4(2)
C(19)	36(3)	49(3)	24(2)	0(2)	-5(2)	1(2)
C(20)	30(2)	27(2)	24(2)	0(2)	-2(2)	-1(2)
C(21)	25(2)	47(3)	26(2)	3(2)	0(2)	-7(2)
C(22)	48(3)	51(3)	48(3)	-7(2)	17(2)	1(2)
C(23)	30(2)	36(2)	17(2)	-4(2)	-3(2)	2(2)
C(24)	29(2)	33(2)	28(2)	-1(2)	-1(2)	0(2)
C(25)	30(2)	44(3)	41(3)	-4(2)	-2(2)	-3(2)
C(26)	26(2)	55(3)	43(3)	-11(2)	-10(2)	6(2)
C(27)	46(3)	48(3)	34(3)	4(2)	-8(2)	10(2)

C(28)	37(3)	45(3)	30(2)	6(2)	-7(2)	0(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for test1.

	x	y	z	U(eq)
H(1)	8374	5824	297	32
H(3)	7855	7203	4350	40
H(4)	6663	7209	3237	41
H(5)	6310	6508	724	38
H(8)	5270	3940	-1014	46
H(10A)	6858	5582	-4840	41
H(10B)	6544	4858	-5809	41
H(11A)	7892	4925	-3841	82
H(11B)	7799	4842	-5960	82
H(11C)	7573	4179	-4693	82
H(13)	4560	4173	-4280	52
H(14)	4063	3451	-6623	61
H(15)	4808	2709	-8325	63
H(16)	6044	2684	-7677	62
H(17)	6550	3408	-5353	52
H(19)	9645	6556	9181	44
H(21A)	10972	6492	3907	39
H(21B)	10327	6569	2450	39
H(22A)	10641	5231	4372	73
H(22B)	10845	5369	2349	73
H(22C)	10023	5313	2847	73
H(24)	11285	7454	6151	36
H(25)	12466	7483	7369	46
H(26)	12853	6592	9465	49
H(27)	12065	5664	10345	51
H(28)	10881	5625	9118	45

Table 6. Torsion angles [°] for test1.

C(6)-C(1)-C(2)-C(3)	-3.0(6)
C(6)-C(1)-C(2)-N(3)	-178.2(3)
C(18)-N(3)-C(2)-C(3)	32.4(6)
C(18)-N(3)-C(2)-C(1)	-152.8(4)
C(1)-C(2)-C(3)-C(4)	2.2(6)
N(3)-C(2)-C(3)-C(4)	176.9(4)
C(2)-C(3)-C(4)-C(5)	-0.1(6)
C(3)-C(4)-C(5)-C(6)	-1.3(6)
C(2)-C(1)-C(6)-C(5)	1.6(6)
C(2)-C(1)-C(6)-N(1)	177.3(3)
C(4)-C(5)-C(6)-C(1)	0.6(6)
C(4)-C(5)-C(6)-N(1)	-174.8(4)
C(7)-N(1)-C(6)-C(1)	128.1(4)
C(7)-N(1)-C(6)-C(5)	-56.4(5)
C(6)-N(1)-C(7)-N(2)	177.9(3)
C(6)-N(1)-C(7)-S(1)	-3.2(6)
C(9)-N(2)-C(7)-N(1)	179.5(3)
C(10)-N(2)-C(7)-N(1)	-4.0(5)
C(9)-N(2)-C(7)-S(1)	0.4(4)
C(10)-N(2)-C(7)-S(1)	176.9(3)
C(8)-S(1)-C(7)-N(1)	-179.0(4)
C(8)-S(1)-C(7)-N(2)	0.0(3)
C(7)-S(1)-C(8)-C(9)	-0.4(3)
S(1)-C(8)-C(9)-N(2)	0.6(5)
S(1)-C(8)-C(9)-C(12)	-177.8(3)
C(7)-N(2)-C(9)-C(8)	-0.7(5)
C(10)-N(2)-C(9)-C(8)	-176.9(4)
C(7)-N(2)-C(9)-C(12)	177.8(3)
C(10)-N(2)-C(9)-C(12)	1.6(6)
C(7)-N(2)-C(10)-C(11)	77.5(4)
C(9)-N(2)-C(10)-C(11)	-106.4(4)
C(8)-C(9)-C(12)-C(13)	50.5(6)
N(2)-C(9)-C(12)-C(13)	-127.8(4)
C(8)-C(9)-C(12)-C(17)	-124.9(5)
N(2)-C(9)-C(12)-C(17)	56.8(5)
C(17)-C(12)-C(13)-C(14)	-0.7(6)

C(9)-C(12)-C(13)-C(14)	-176.3(4)
C(12)-C(13)-C(14)-C(15)	0.4(7)
C(13)-C(14)-C(15)-C(16)	0.2(7)
C(14)-C(15)-C(16)-C(17)	-0.4(7)
C(15)-C(16)-C(17)-C(12)	0.1(7)
C(13)-C(12)-C(17)-C(16)	0.5(6)
C(9)-C(12)-C(17)-C(16)	175.9(4)
C(2)-N(3)-C(18)-N(4)	-177.3(3)
C(2)-N(3)-C(18)-S(2)	7.5(6)
C(20)-N(4)-C(18)-N(3)	-173.6(3)
C(21)-N(4)-C(18)-N(3)	-10.2(5)
C(20)-N(4)-C(18)-S(2)	2.6(4)
C(21)-N(4)-C(18)-S(2)	166.0(3)
C(19)-S(2)-C(18)-N(3)	173.4(4)
C(19)-S(2)-C(18)-N(4)	-2.3(3)
C(18)-S(2)-C(19)-C(20)	1.6(3)
S(2)-C(19)-C(20)-N(4)	-0.4(5)
S(2)-C(19)-C(20)-C(23)	177.3(3)
C(18)-N(4)-C(20)-C(19)	-1.5(5)
C(21)-N(4)-C(20)-C(19)	-163.8(4)
C(18)-N(4)-C(20)-C(23)	-179.2(3)
C(21)-N(4)-C(20)-C(23)	18.5(6)
C(20)-N(4)-C(21)-C(22)	85.0(5)
C(18)-N(4)-C(21)-C(22)	-76.7(4)
C(19)-C(20)-C(23)-C(28)	55.5(6)
N(4)-C(20)-C(23)-C(28)	-127.1(4)
C(19)-C(20)-C(23)-C(24)	-122.0(5)
N(4)-C(20)-C(23)-C(24)	55.4(5)
C(28)-C(23)-C(24)-C(25)	-1.0(6)
C(20)-C(23)-C(24)-C(25)	176.6(4)
C(23)-C(24)-C(25)-C(26)	0.2(6)
C(24)-C(25)-C(26)-C(27)	0.3(6)
C(25)-C(26)-C(27)-C(28)	-0.1(6)
C(24)-C(23)-C(28)-C(27)	1.2(6)
C(20)-C(23)-C(28)-C(27)	-176.4(4)
C(26)-C(27)-C(28)-C(23)	-0.7(6)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for test1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(11)-H(11A)...N(1)	0.96	2.67	3.191(5)	114.2
C(10)-H(10B)...S(1)#1	0.97	3.01	3.905(4)	153.2
C(3)-H(3)...S(2)	0.93	2.61	3.128(4)	116.1
C(3)-H(3)...S(2)	0.93	2.61	3.128(4)	116.1
C(10)-H(10B)...S(1)#1	0.97	3.01	3.905(4)	153.2
C(11)-H(11A)...N(1)	0.96	2.67	3.191(5)	114.2

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1