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Supporting Information

An Amidato Divalent Ytterbium Cluster: Synthesis and molecular Structure, Its Reactivity to Carbodiimides and the Application in the Guanylation Reaction

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Table 1 Crystallographic Data for Complexes **1–4**

	1	**2**	**3**	**4**
Formula	$C_{128}H_{148}N_6O_6Yb_3$	$C_{151}H_{183}N_9O_8Yb_3$	$C_{128}H_{148}N_6O_6Yb_2$	$C_{104}H_{126}N_6O_4Yb_2$
Fw	2385.65	2771.17	2212.60	1870.18
T (K)	223(2)	293(2)	293(2)	293(2)
Cryst syst	Triclinic	Monoclinic	Triclinic	Triclinic
Space group	*P -1*	*P* $2_1/n$	*P -1*	*P -1*
Crystal size (mm^3)	0.20×0.20×0.20	0.30×0.25×0.22	0.70×0.65×0.30	0.32×0.20×0.10
a (Å)	13.9951(4)	29.2664(3)	13.8319(4)	14.2348(4)
b Å)	21.5347(7)	14.09698(13)	14.3956(4)	16.1058(5)
c (Å)	23.3361(8)	33.5205(4)	16.1575(5)	23.8596(9)
α(°)	70.496(3)	90	68.116(3)	103.924(3)
β (°)	80.596(3)	98.7237(10)	67.267(3)	96.231(3)
γ(°)	79.095(3)	90	85.184(2)	108.738(3)
V ($Å^3$)	6471.5(4)	13669.5(2)	2746.7(1)	4924.1(3)
Z	1	4	1	2
D_{calc}(g/cm^3)	1.224	1.347	1.338	1.261
μ (mm^{-1})	2.200	4.117	1.750	1.938
F (000)	2432	5704	1146	1928
ϑ range (°)	2.79 - 25.00	3.06-76.48	3.30-26.37	2.79-26.37
Collected	78070	92525	28571	62644
Unique reflns	22765	27335	11189	20109
R	0.0370	0.0326	0.0357	0.0643
wR	0.0915	0.0795	0.0791	0.1337
R_{int}	0.0407	0.0377	0.0612	0.0782
GOF	1.064	1.014	1.0692	1.096
peak/hole ($e/Å^3$)	1.391, -1.113	1.090, -1.010	2.149, -1.076	1.320, -1.180

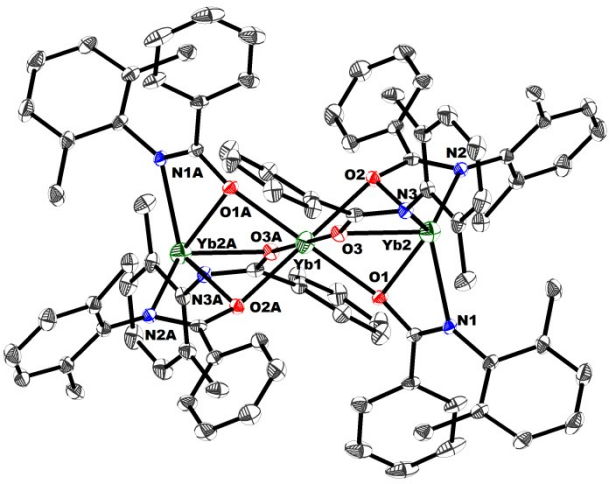


Figure 1 ORTEP diagram of complex **1** with the probability ellipsoids drawn at the 20 % level, carbon atoms on the isopropyl of **HL** and hydrogen atoms are omitted for clarity.

Table 2 Selected bond lengths (Å) and bond angles (°) for complex **1**

Yb(1)-O(1)	2.333(4)	Yb(1)-O(2)	2.354(3)
Yb(1)-O(3)	2.383(2)	Yb(2)-O(1)	2.486(3)
Yb(2)-N(1)	2.445(5)	Yb(2)-O(2)	2.426(4)
Yb(2)-N(2)	2.493(4)	Yb(2)-O(3)	2.454(3)
Yb(2)-N(3)	2.443(4)	C(1)-N(1)	1.297(6)
C(1)-O(1)	1.302(7)	C(20)-O(2)	1.294(5)
C(20)-N(2)	1.311(7)	C(39)-N(3)	1.289(7)
C(39)-O(3)	1.300(4)		
O(1)-Yb(1)-O(2)	79.18(10)	O(1)-Yb(1)-O(3)	79.16(10)
O(2)-Yb(1)-O(3)	75.06(10)	O(1)-Yb(2)-N(1)	53.73(12)
O(2)-Yb(2)-N(2)	53.94(12)	O(3)-Yb(2)-N(3)	54.10(12)
O(1)-C(1)-N(1)	118.03(43)	O(2)-C(20)-N(2)	117.92(41)
O(3)-C(39)-N(3)	118.64(41)	N(1)-Yb(2)-N(3)	110.25(15)
N(2)-Yb(2)-N(3)	127.82(14)	N(1)-Yb(2)-N(2)	119.01(14)
O(2)-Yb(1)-O(2A)	180(0)	Yb(1)-O(2)-Yb(2)	90.16(14)
Yb(1)-O(1)-Yb(2)	89.19(14)	Yb(1)-O(3)-Yb(2)	88.82(7)

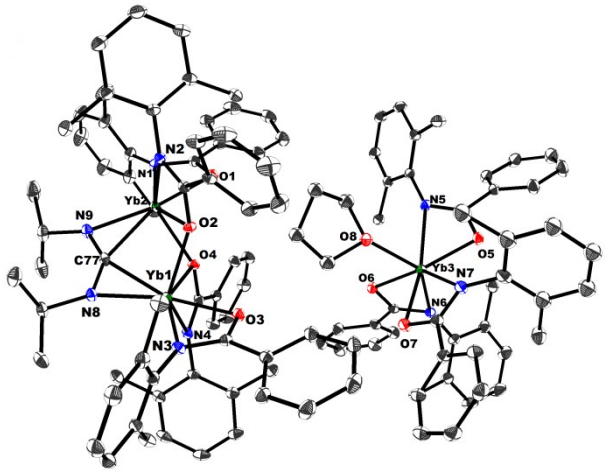


Figure 2 ORTEP diagram of complex **2** with the probability ellipsoids drawn at the 20 % level, carbon atoms on the isopropyl of **HL** and hydrogen atoms are omitted for clarity.

Table 3 Selected bond lengths (Å) and bond angles (°) for complex **2**

Yb(1)-N(8)	2.237(3)	Yb(1)-O(2)	2.244(2)
Yb(1)-O(3)	2.283(2)	Yb(1)-N(3)	2.364(2)
Yb(1)-C(77)	2.369(3)	Yb(1)-N(4)	2.386(3)
Yb(1)-O(4)	2.409(2)	Yb(2)-N(9)	2.235(3)
Yb(2)-O(4)	2.251(2)	Yb(2)-O(1)	1.318(4)
Yb(2)-C(77)	2.365(3)	Yb(2)-N(1)	2.372(3)
Yb(2)-O(2)	2.392(2)	Yb(2)-N(2)	2.401(3)
Yb(3)-O(5)	2.202(2)	Yb(3)-O(6)	2.236(2)
Yb(3)-O(7)	2.308(2)	Yb(3)-O(8)	2.317(2)
Yb(3)-N(7)	2.340(3)	Yb(3)-N(6)	2.381(3)
Yb(3)-N(5)	2.524(3)	O(1)-C(1)	1.289(4)
O(2)-C(20)	1.310(3)	O(3)-C(39)	1.293(4)
O(4)-C(58)	1.307(4)	O(5)-C(84)	1.298(4)
O(6)-C(103)	1.292(4)	O(7)-C(122)	1.286(4)
N(1)-C(1)	1.316(4)	N(2)-C(20)	1.300(4)
N(3)-C(39)	1.327(4)	N(4)-C(58)	1.302(4)
N(5)-C(84)	1.313(4)	N(6)-C(103)	1.321(4)

N(7)-C(122)	1.306(4)	N(8)-C(77)	1.332(4)
N(8)-C(78)	1.478(4)	N(9)-C(77)	1.326(4)
N(9)-C(81)	1.478(4)		
N(8)-Yb(1)-C(77)	33.47(10)	N(9)-Yb(2)-C(77)	33.34(10)
N(9)-C(77)-N(8)	138.1(3)	N(9)-C(77)-Yb(2)	67.92(17)
N(8)-C(77)-Yb(2)	153.6(2)	N(9)-C(77)-Yb(1)	153.4(2)
N(8)-C(77)-Yb(1)	67.82(17)	Yb(2)-C(77)-Yb(1)	86.98(10)

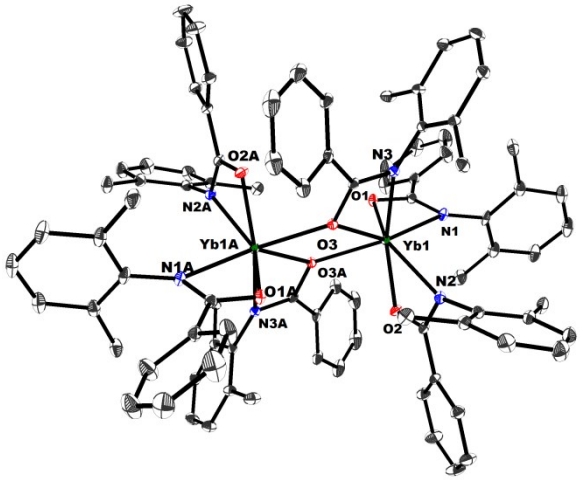


Figure 3 ORTEP diagram of complex **3** with the probability ellipsoids drawn at the 20 % level, carbon atoms on the isopropyl of **HL** and hydrogen atoms are omitted for clarity.

Table 4 Selected bond lengths (Å) and bond angles (°) for complex **3**

Yb(1)-O(2)	2.175(2)	Yb(1)-O(1)	2.223(2)
Yb(1)-O(3)	2.310(2)	Yb(1)-O(3A)	2.358(2)
Yb(1)-N(3)	2.474(3)	Yb(1)-N(1)	2.482(3)
Yb(1)-N(2)	2.521(3)	O(1)-C(1)	1.302(4)
O(2)-C(20)	1.292(4)	O(3)-C(39)	1.318(4)
N(1)-C(1)	1.303(5)	N(2)-C(20)	1.318(4)
N(3)-C(39)	1.293(4)		
O(2)-Yb(1)-O(1)	111.46(9)	O(2)-Yb(1)-O(3)	113.37(10)
O(1)-Yb(1)-O(3)	113.09(8)	O(2)-Yb(1)-O(3A)	78.60(8)

O(1)-Yb(1)-O(3A)	80.69(8)	O(3)-Yb(1)-O(3A)	66.59(8)
O(2)-Yb(1)-N(3)	150.85(9)	O(1)-Yb(1)-N(3)	96.67(9)
O(3)-Yb(1)-N(3)	54.89(8)	O(3A)-Yb(1)-N(3)	114.75(8)
O(2)-Yb(1)-N(1)	93.46(10)	O(1)-Yb(1)-N(1)	55.80(9)
O(3)-Yb(1)-N(1)	149.65(9)	O(3A)-Yb(1)-N(1)	129.46(9)
N(3)-Yb(1)-N(1)	96.25(10)	O(2)-Yb(1)-N(2)	55.47(9)
O(1)-Yb(1)-N(2)	149.97(9)	O(3)-Yb(1)-N(2)	96.47(9)
O(3A)-Yb(1)-N(2)	117.77(9)	N(3)-Yb(1)-N(2)	96.13(9)
N(1)-Yb(1)-N(2)	95.84(9)	C(1)-O(1)-Yb(1)	99.8(2)
C(20)-O(2)-Yb(1)	102.8(2)	C(39)-O(3)-Yb(1)	98.18(18)
C(39)-O(3)-Yb(1A)	136.4(2)	Yb(1)-O(3)-Yb(1A)	113.41(8)
O(1)-C(1)-N(1)	116.4(3)	O(2)-C(20)-N(2)	115.5(3)
N(3)-C(39)-O(3)	115.6(3)		

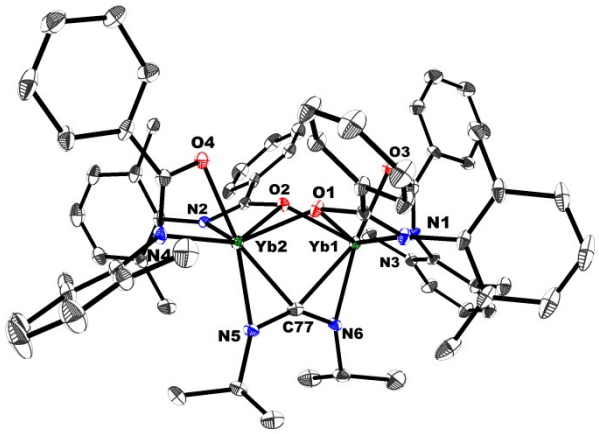


Figure 4 ORTEP diagram of complex **4** with the probability ellipsoids drawn at the 20 % level, carbon atoms on the isopropyl of **HL** and hydrogen atoms are omitted for clarity.

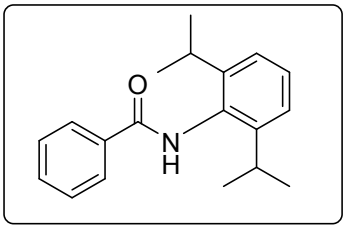
Table 5 Selected bond lengths (Å) and bond angles (°) for complex **4**

Yb(1)-O(1)	2.385(5)	Yb(1)-O(2)	2.250(5)
Yb(1)-O(3)	2.280(6)	Yb(1)-N(1)	2.369(6)
Yb(1)-N(3)	2.380(7)	Yb(2)-N(5)	2.227(7)
Yb(1)-N(6)	2.220(7)	Yb(1)-C(77)	2.365(9)

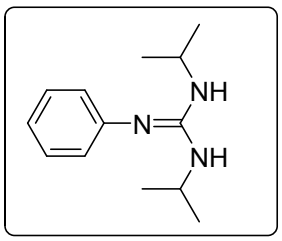
Yb(2)-C(77)	2.369(8)	Yb(2)-O(1)	2.253(5)
Yb(2)-O(2)	2.394(5)	Yb(2)-O(4)	2.266(5)
Yb(2)-N(2)	2.414(6)	Yb(2)-N(4)	2.383(6)
O(1)-C(1)	1.313(9)	O(2)-C(20)	1.318(9)
O(3)-C(39)	1.293(9)	O(4)-C(58)	1.288(10)
N(1)-C(1)	1.300(9)	N(2)-C(20)	1.284(10)
N(3)-C(39)	1.311(11)	N(4)-C(58)	1.320(11)
N(5)-C(77)	1.339(11)	N(6)-C(77)	1.317(10)
N(6)-Yb(1)-O(2)	102.9(2)	N(6)-Yb(1)-O(3)	158.6(2)
O(2)-Yb(1)-O(3)	83.26(19)	N(6)-Yb(1)-C(77)	33.2(2)
O(2)-Yb(1)-C(77)	80.1(2)	O(3)-Yb(1)-C(77)	163.0(2)
N(6)-Yb(1)-N(1)	104.1(2)	O(2)-Yb(1)-N(1)	125.3(2)
O(3)-Yb(1)-N(1)	88.1(2)	C(77)-Yb(1)-N(1)	98.6(3)
N(6)-Yb(1)-N(3)	102.9(2)	O(2)-Yb(1)-N(3)	112.5(2)
O(3)-Yb(1)-N(3),	56.3(2)	C(77)-Yb(1)-N(3)	134.6(3)
N(3)-Yb(1)-N(1)	106.4(2)	N(6)-Yb(1)-O(1)	55.47(9)
O(2)-Yb(1)-O(1)	72.00(17)	O(3)-Yb(1)-O(1)	93.89(19)
C(77)-Yb(1)-O(1)	77.7(2)	N(1)-Yb(1)-O(1)	54.85(18)
N(3)-Yb(1)-O(1)	147.4(2)	N(5)-Yb(2)-O(1)	104.2(2)
N(5)-Yb(2)-O(4)	160.0(2)	O(1)-Yb(2)-O(4)	83.47(19)
N(5)-Yb(2)-C(77)	33.7(3)	O(1)-Yb(2)-C(77)	80.2(2)
O(4)-Yb(2)-C(77)	162.9(3)	N(5)-Yb(2)-N(4)	103.5(3)
O(1)-Yb(2)-N(4)	110.9(2)	O(4)-Yb(2)-N(4)	56.6(2)
C(77)-Yb(2)-N(4)	135.0(3)	N(5)-Yb(2)-O(2)	107.0(2)
O(1)-Yb(2)-O(2)	71.79(18)	O(4)-Yb(2)-O(2)	92.99(19)
C(77)-Yb(2)-O(2)	77.2(2)	N(4)-Yb(2)-O(2)	147.7(2)
N(5)-Yb(2)-N(2)	103.0(2)	O(1)-Yb(2)-N(2)	124.8(2)
O(4)-Yb(2)-N(2)	86.8(2)	C(77)-Yb(2)-N(2)	98.4(2)
N(4)-Yb(2)-N(2)	108.0(2)	O(2)-Yb(2)-N(2)	54.6(2)

C(1)-O(1)-Yb(2)	149.7(5)	C(1)-O(1)-Yb(1)	95.0(4)
Yb(2)-O(1)-Yb(1)	89.44(18)	C(20)-O(2)-Yb(1)	150.2(5)
C(20)-O(2)-Yb(2)	94.6(4)	Yb(1)-O(2)-Yb(2)	89.28(17)
C(39)-O(3)-Yb(1)	96.5(5)	C(58)-O(4)-Yb(2)	97.0(5)
C(1)-N(1)-Yb(1)	96.1(5)	C(20)-N(2)-Yb(2)	94.6(5)
C(39)-N(3)-Yb(1)	91.4(5)	C(58)-N(4)-Yb(2)	90.8(5)
C(77)-N(5)-C(78)	126.0(7)	C(77)-N(5)-Yb(2)	79.0(5)
C(77)-N(6)-C(81)	125.9(8)	C(77)-N(6)-Yb(1)	79.5(5)
N(1)-C(1)-O(1)	113.8(7)	N(2)-C(20)-O(2)	116.1(7)
O(3)-C(39)-N(3)	115.3(8)	O(4)-C(58)-N(4)	115.5(7)
N(6)-C(77)-N(5)	139.0(8)	N(6)-C(77)-Yb(1)	67.3(5)
N(5)-C(77)-Yb(1)	153.5(6)	N(6)-C(77)-Yb(2)	153.0(7)
N(5)-C(77)-Yb(2)	67.3(4)	Yb(1)-C(77)-Yb(2)	87.2(3)

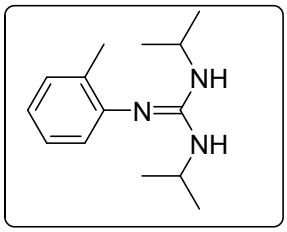
Characteristic data：



$C_6H_5CONH(2,6\text{-}^iPr_2\text{-}C_6H_3)$ (HL). ($C_{19}H_{23}NO$), White solid. Mp. 265.4-265.6 °C. ^{1}H NMR (400 MHz, DMSO-d_6)：δ 9.75 (br. s, 1H, NH)，8.00 (d, *J* = 8 Hz, 2H, aryl H)，7.60 (t, *J* = 8 Hz, 1H, aryl H)，7.54 (t, *J* = 8 Hz, 2H, aryl H)，7.30 (t, *J* = 8 Hz, 1H, aryl H)，7.20 (d, *J* = 8 Hz, 2H, aryl H)，3.08 (septet, *J* = 8 Hz, 2H, $CH(CH_3)_2$)，1.16 (d, *J* = 8 Hz, 6H, $CH(CH_3)_2$)，1.10 (d, *J* = 8 Hz, 6H, $CH(CH_3)_2$) ppm. ^{13}C NMR (400 MHz, DMSO-d_6): δ 166.2, 146.2, 134.4, 132.8, 131.4, 128.4, 127.6, 127.5, 122.9, 28.2, 23.5 ppm.

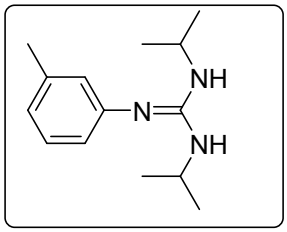


1,3-diisopropyl-2-phenylguanidine(5a). Colorless solid, Yield: 99%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24 (m, 2H, C_6H_5); 6.93 (m, 1H, C_6H_5); 6.86 (d, *J* = 7.6Hz, 2H, C_6H_5); 3.77 (s, 2H, NH); 3.59 (s, 2H, $CH(CH_3)_2$); 1.17 (d, *J* = 6.4Hz, 12H, $CH(CH_3)_2$) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.5, 150.4, 129.3, 123.6, 121.4, 43.3, 23.4 ppm.

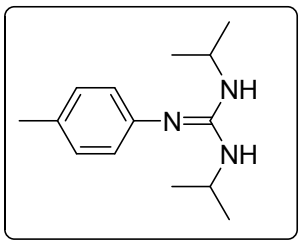


1,3-diisopropyl-2-*o*-tolylguanidine(5b). Colorless solid, Yield: 99%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.14 (d, *J* = 7.4 Hz, 1H, C_6H_4); 7.09 (t, *J* = 7.5 Hz, 1H, C_6H_4); 6.87 (t, *J*

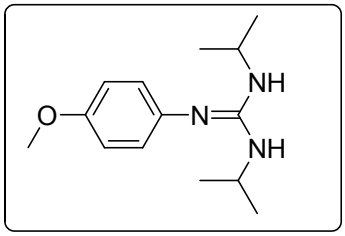
= 7.3 Hz, 1H, C_6H_4); 6.76 (d, *J* = 7.7 Hz, 1H, C_6H_4); 3.76 (s, 2H, NH); 3.43 (s, 1H, CH); 2.14 (s, 3H, $ArCH_3$); 1.16 (d, *J* = 6.4 Hz, 12H, $CH(CH_3)_2$) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.9, 148.4, 130.5, 130.4, 126.6, 123.2, 121.8, 43.2, 23.5, 18.1 ppm.



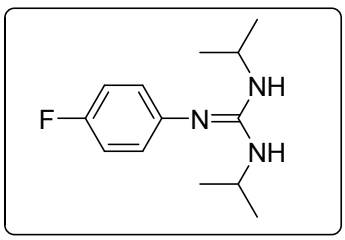
1,3-diisopropyl-2-*m*-tolylguanidine(5c). Colorless solid, Yield: 98%; ^1H NMR (400 MHz, $CDCl_3$): δ 7.11 (t, *J* = 7.6 Hz, 1H, C_6H_4), 6.76 – 6.59 (m, 3H, C_6H_4), 3.75-3.74 (m, 2H, NH), 3.55 (s, 2H, CH), 2.26 (s, 3H, $ArCH_3$), 1.14 (d, *J* = 6.3 Hz, 12H, $CH(CH_3)_2$) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.3, 150.3, 129.1, 124.5, 122.3, 120.4, 43.4, 23.5, 21.6 ppm.



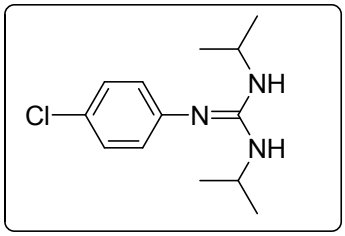
1,3-diisopropyl-2-p-tolylguanidine(5d). Colorless solid, Yield: 99%; ^1H NMR (400 MHz, $CDCl_3$): δ 7.05 (d, *J* = 7.6 Hz, 2 H, C_6H_4); 6.74 (d, *J* = 7.7 Hz, 2 H, C_6H_4); 3.76 (br, 2 H, NH); 3.56 (m, 2 H, CH); 2.28 (s, 3 H, $ArCH_3$); 1.16 (d, *J* = 6.1 Hz, 12 H, $CH(CH_3)_2$) ppm.^{13}C NMR (100 MHz, $CDCl_3$): δ = 150.6, 147.6, 130.5, 129.9, 123.3, 43.2, 23.4, 20.8 ppm.



1,3-diisopropyl-2-(4-methoxyphenyl)guanidine(5e). Colorless solid, Yield: 97%; ^1H NMR (400 MHz, $CDCl_3$): δ 6.83–6.76 (m, 4H, C_6H_4); 3.77 (m, 5H, OCH_3, NH); 3.57 (br, 2H, CH); 1.15 (d, *J* = 6.1 Hz, 12H, $CH(CH_3)_2$) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.7, 150.9, 143.4, 124.5, 114.8, 55.6, 43.4, 23.6 ppm.

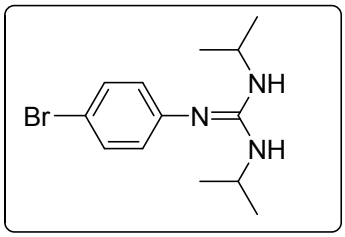


2-(4-fluorophenyl)-1,3-diisopropylguanidine(5f). Colorless solid, Yield: 98%; ^1H NMR (400 MHz, $CDCl_3$): δ 6.94 (t, *J* = 8.7 Hz, 2H, C_6H_4); 6.78 (m, 2H, C_6H_4); 3.76 (s, 2H, NH); 3.52 (s, 2H, CH); 1.16 (d, *J* = 6.3 Hz, 12H, $CH(CH_3)_2$) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.5, 146.0, 141.8, 124.7, 115.7, 43.2, 23.4 ppm.

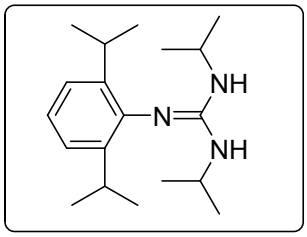


2-(4-chlorophenyl)-1,3-diisopropylguanidine(5g). Colorless solid, Yield:

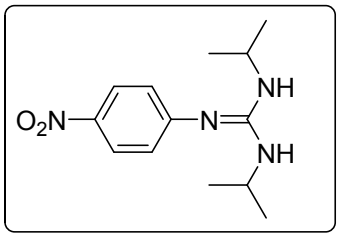
95%; ^{1}H NMR (400 MHz, $CDCl_3$): δ7.19 (d, *J* = 8.5 Hz, 2H, C_6H_4); 6.77 (d, *J* = 8.5 Hz, 2H, C_6H_4); 3.75 (br, 2H, NH); 3.60 (br, 2H, CH); 1.16 (d, *J* = 6.3 Hz, 12H, $CH(CH_3)_2$) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.5, 148.9, 129.4, 126.3, 124.7, 43.2, 23.4 ppm



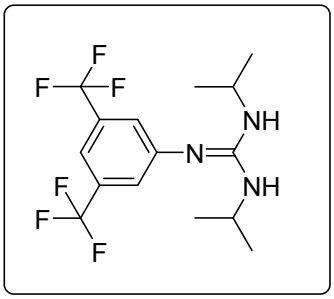
2-(4-bromophenyl)-1,3-diisopropylguanidine(5h). Colorless solid, Yield: 96%; ^{1}H NMR (400 MHz , $CDCl_3$): δ7.33 (d, *J* = 8.4 Hz, 2H, C_6H_4); 6.73 (d, *J* = 8.4 Hz, 2H, C_6H_4); 3.76 (m, 2 H, NH); 3.55 (s, 2H, CH); 1.16 (d, *J* = 6.3 Hz, 12H, $CH(CH_3)_2$) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.2, 149.6, 132.2, 125.4, 113.9, 43.2, 23.4 ppm.



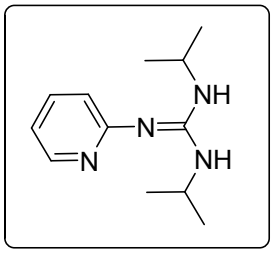
2-(2,6-diisopropylphenyl)-1,3-diisopropylguanidine(5i). Colorless solid, Yield: 50%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.07-7.03(m, 2H, C_6H_3); 6.96-6.90 (m, 1H, C_6H_3); 4.13 (s, 2H, NH); 3.44-3.10 (m, 2H, ArCH); 3.10-3.05 (m, 2H, CH); 1.25-1.04 (m, 24H, $CH(CH_3)_2$) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.7, 143.8, 141.7, 123.0, 122.4, 43.5, 42.3, 28.1, 22.9 ppm.



1,3-diisopropyl-2-(4-nitrophenyl)guanidine(5j). Colorless solid, Yield: 93%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 8.9 Hz, 1H, C_6H_4); 6.89 (d, *J* = 8.9 Hz, 2H, C_6H_4); 3.79 (br, 4H, NH, CH); 1.19 (d, *J* = 5.6 Hz, 12H, $CH(CH_3)_2$) ppm.^{13}C NMR (100 MHz, $CDCl_3$): δ 158.3, 150.4, 140.9, 125.6, 122.8, 43.3, 23.2 ppm.

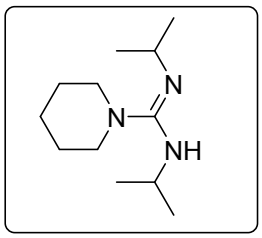


2-(3,5-bis(trifluoromethyl)phenyl)-1,3-diisopropylguanidine(5k). Colorless solid, Yield: 98%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 (s, 1H, C_6H_3), 7.28 (s, 2H, C_6H_3), 3.78 (dq, *J* = 12.8, 6.5 Hz, 2H, NH), 3.61 (d, *J* = 7.4 Hz, 2H, CH), 1.19 (d, *J* = 6.4 Hz, 12H, $CH(CH_3)_2$) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.2, 150.6, 132.7, 132.4, 132.1, 131.7, 127.6, 124.9, 123.4, 122.2, 119.5, 113.9, 43.3, 23.2 ppm.

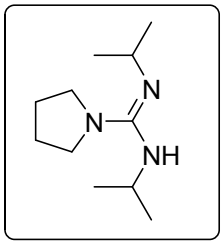


1,3-diisopropyl-2-(pyridin-2-yl)guanidine(5l). Colorless solid, Yield: 97%; ^{1}H NMR

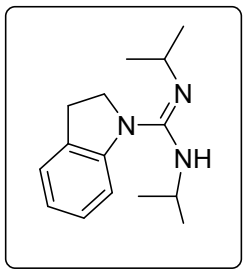
(400 MHz, $CDCl_3$): δ 8.07 (dd, *J* = 5.1, 1.4 Hz, 1H, PyH); 7.42 (ddd, *J* = 8.4, 7.1, 2.1 Hz, 1H, PyH); 6.83 (d, *J* = 8.3 Hz, 1H, PyH); 6.61 (ddd, *J* = 7.0, 5.1, 1.0 Hz, 1H, PyH); 3.93 (d, *J* = 4.5 Hz, 2H, CH); 1.25 (d, *J* = 6.4 Hz, 12H, $CH(CH_3)_2$) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.6, 153.8, 136.7, 120.3, 114.0, 42.6, 23.5 ppm.



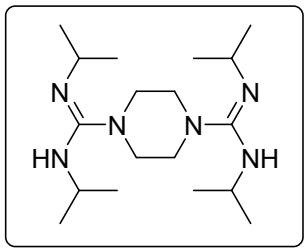
N,N'-bis(1-methylethyl)-1-piperidinecarboximidamide(5m). Colorless solid, Yield: 90%; ^1H NMR (400 MHz, $CDCl_3$): δ 3.36 (m, 2H, CH), 3.04 (br, 4H, CH_2), 1.52 (br, 6H, CH_2), 1.09 (m, 12H, $CH(CH_3)_2$) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.0, 49.1, 46.6, 26.0, 24.9, 24.0 ppm.



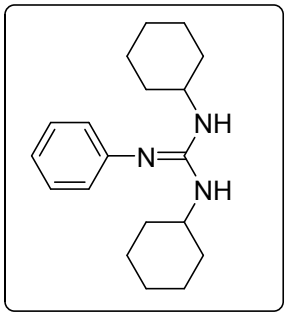
N,N'-diisopropylpyrrolidine-1-carboximidamide(5n). Colorless solid, Yield: 86%; ^1H NMR (400 MHz, $CDCl_3$): δ 3.39(m, 2H, CH); 3.76(m, 4H, CH_2); 1.80 (m, 4H, CH_2); 1.11 (d, *J* = 6.4 Hz, 12H, CH_3) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.6, 47.9, 46.6, 25.1, 24.6 ppm.



N,N'-diisopropylindoline-1-carboximidamide(5o). Colorless solid, Yield: 93%; ^1H NMR (400 MHz, $CDCl_3$): δ 7.19-6.73 (m, 4H, ArH), 3.88-3.78 (m, 4H, CH_2), 3.45-3.44 (m, 2H, CH), 2.99-2.95 (m, 2H, CH_2), 1.15-1.13 (m, 12H, CH_3) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.3, 146.1, 131.0, 126.6, 124.0, 119.0, 111.0, 50.1, 46.7, 45.2, 27.3, 24.4, 23.4 ppm.

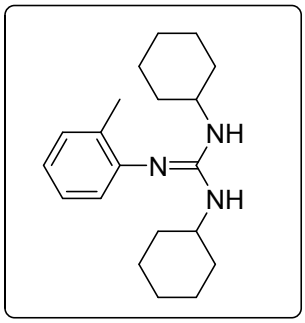


N1,N'1,N4,N'4-tetraisopropylpiperazine-1,4-bis(carboximidamide)(5p). Colorless solid, Yield: 88%; ^1H NMR (400 MHz, $CDCl_3$): δ 3.51-3.34 (m, 2H, CH), 3.31-3.17 (m, 2H, CH), 3.01 (s, 8H, CH_2), 1.03 (d, *J* = 5.5Hz, 24H, CH_3) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.2, 47.8, 46.6, 45.6, 24.3, 23.2 ppm.

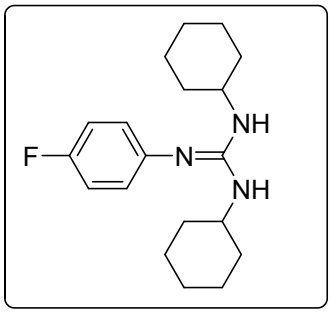


1,3-dicyclohexyl-2-phenylguanidine(5q). Colorless solid, Yield: 99%; ^1H NMR (400 MHz, $CDCl_3$): δ 7.25 – 7.21 (m, 2H, C_6H_5); 6.95 – 6.95 – 6.89 (m, 1H, C_6H_5); 6.88 – 6.86 (m, 2H, C_6H_5); 3.65 (s, 2H, NH); 3.42 (s, 2H, CH); 2.01 – 1.12 (m, 20H, CH_2) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.7, 150.7, 129.5, 123.9, 121.6, 50.5, 34.1,

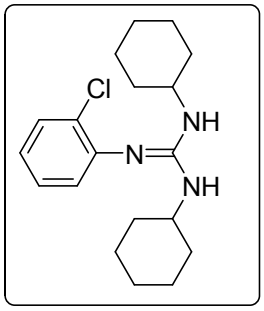
26.0, 25.2 ppm.



1,3-dicyclohexyl-2-o-tolylguanidine(5r). Colorless solid, Yield: 97%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.93 (m, 2H, C_6H_4); 6.78 (m, 2H, C_6H_4); 3.62 (br, 2H, NH); 3.40 (br, 2H, CH); 2.00(s, 3H, CH_3); 1.97-1.03 (m, 20H, CH_2) ppm. ^{13}CNMR (100 MHz , $CDCl_3$): δ 148.94, 148.70, 131.86, 130.60, 126.84, 123.48, 121.88, 50.40, 34.18, 25.94, 25.22, 18.41 ppm.

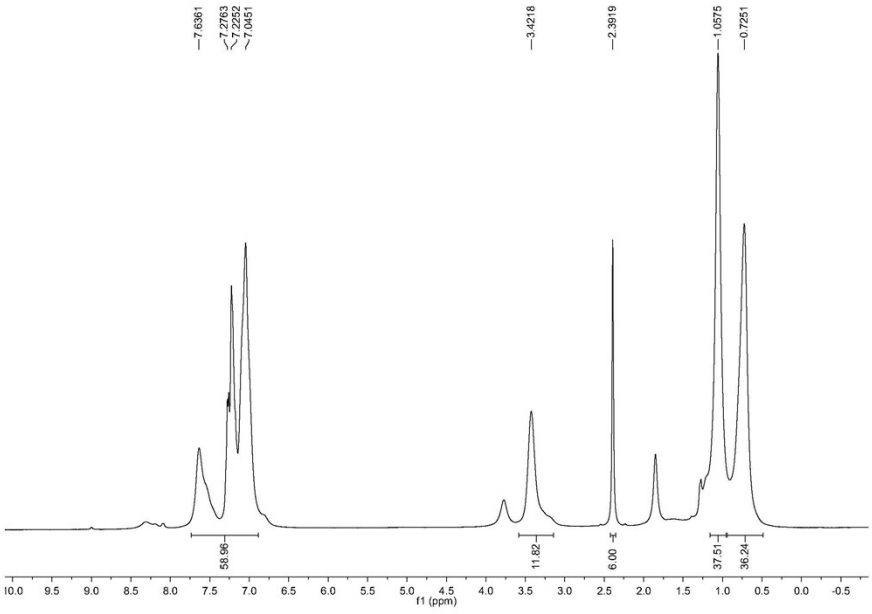


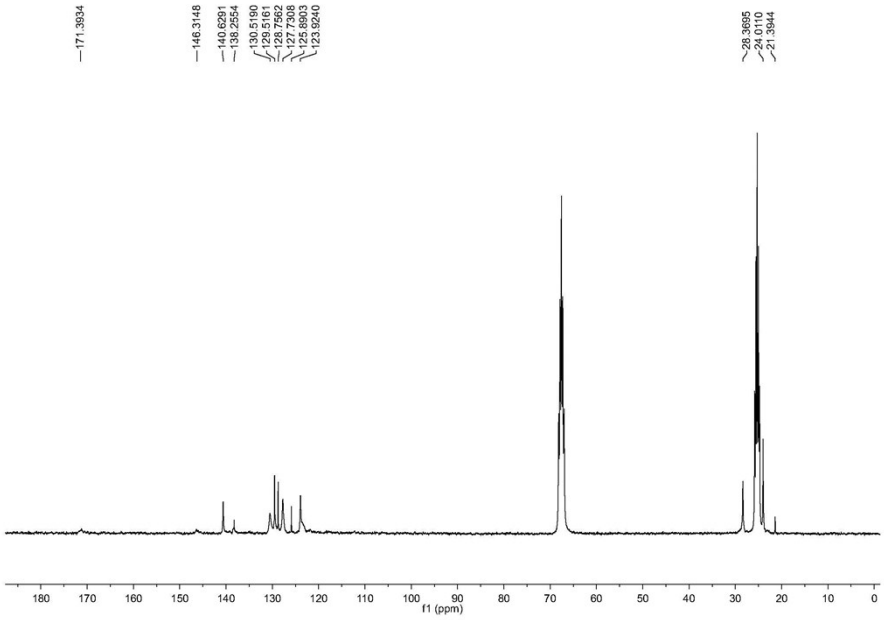
1,3-dicyclohexyl-2-(4-fluorophenyl)guanidine(5s). Colorless solid, Yield: 99%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.94 – 6.90 (m, 2 H, C_6H_4); 6.77 – 6.73 (m, 2 H, C_6H_4); 3.59 (s, 2 H, NH); 3.38 – 3.36 (m, 2 H, CH); 1.99 – 1.03 (m, 20 H, CH_2) ppm.^{13}C NMR (100 MHz, $CDCl_3$): δ 150.6, 124.9, 124.8, 116.1, 115.9, 50.4, 34.1, 25.9, 25.2 ppm.



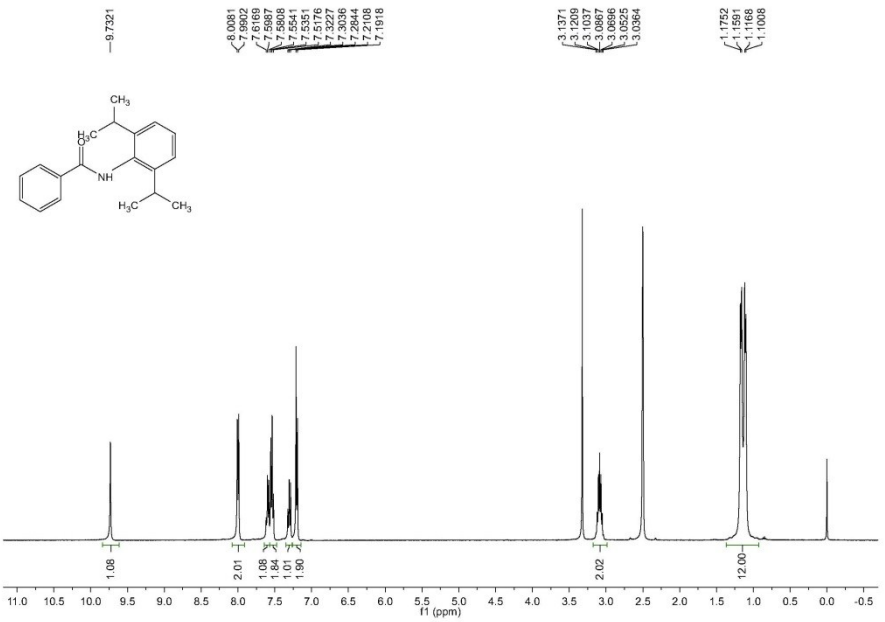
2-(2-chlorophenyl)-1,3-dicyclohexylguanidine(5t). Colorless solid, Yield: 98%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 – 7.33 (m, 1H, C_6H_4), 7.15 – 7.11(m, 1H, C_6H_4); 6.92 – 6.85 (m, 2H, C_6H_4); 3.56 (s, 2H, NH); 3.42 (s, 2H, CH); 2.05 – 1.06(m, 20H, CH_2) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.1, 147.6, 130.1, 128.7, 127.8, 125.6, 122.6, 50.5, 34.1, 26.0, 25.2 ppm.

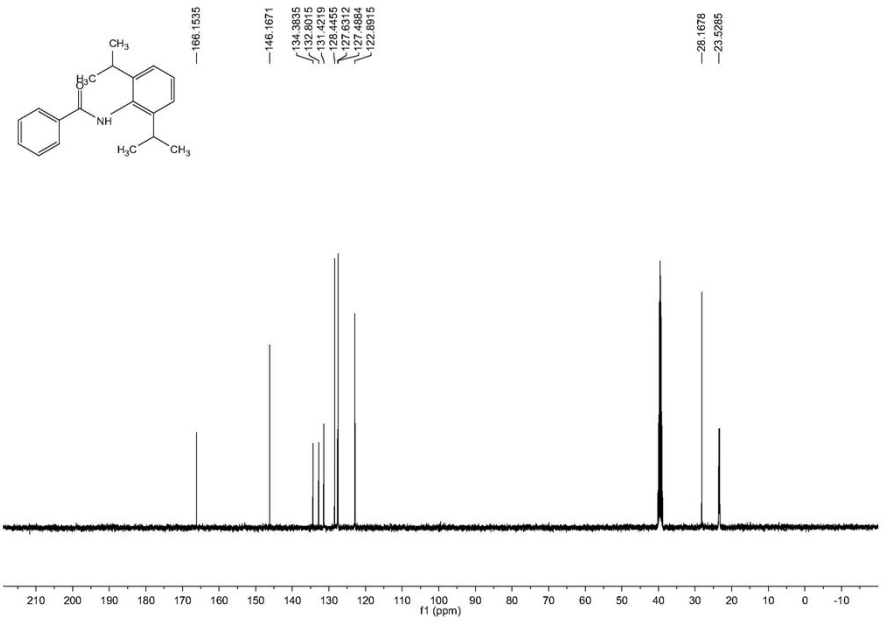
^{1}H NMR and ^{13}C NMR spectra of complex **1**



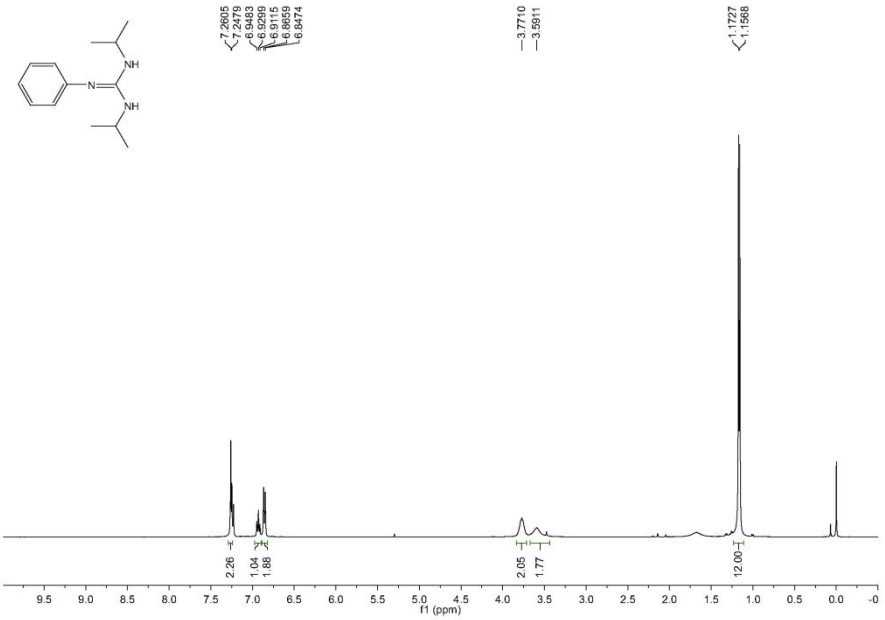


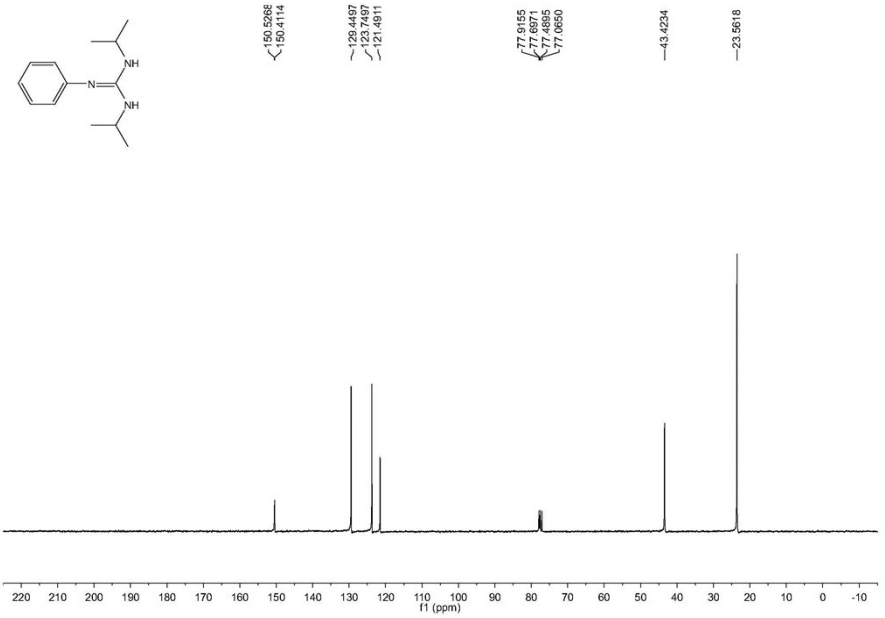
^{1}H NMR and ^{13}C NMR spectra of **HL**



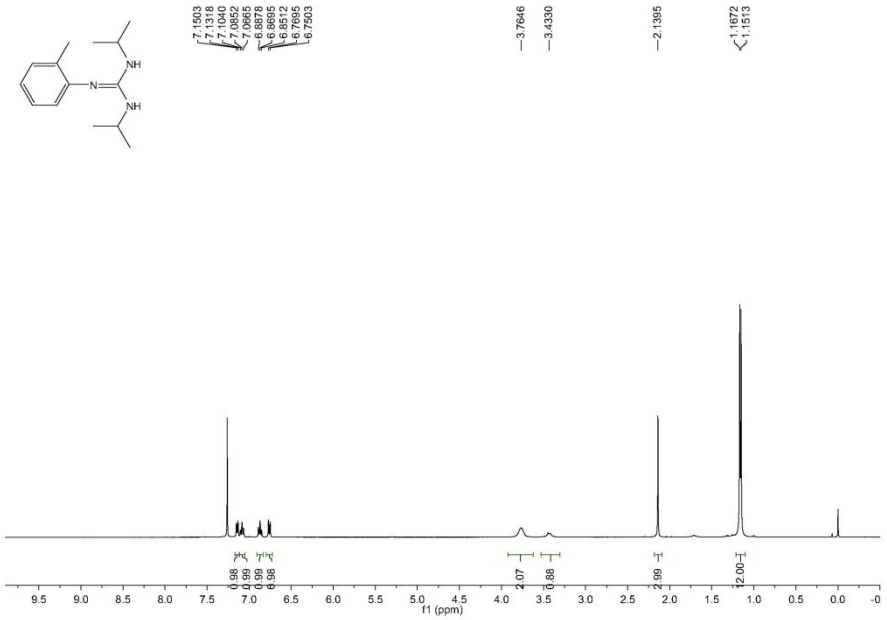


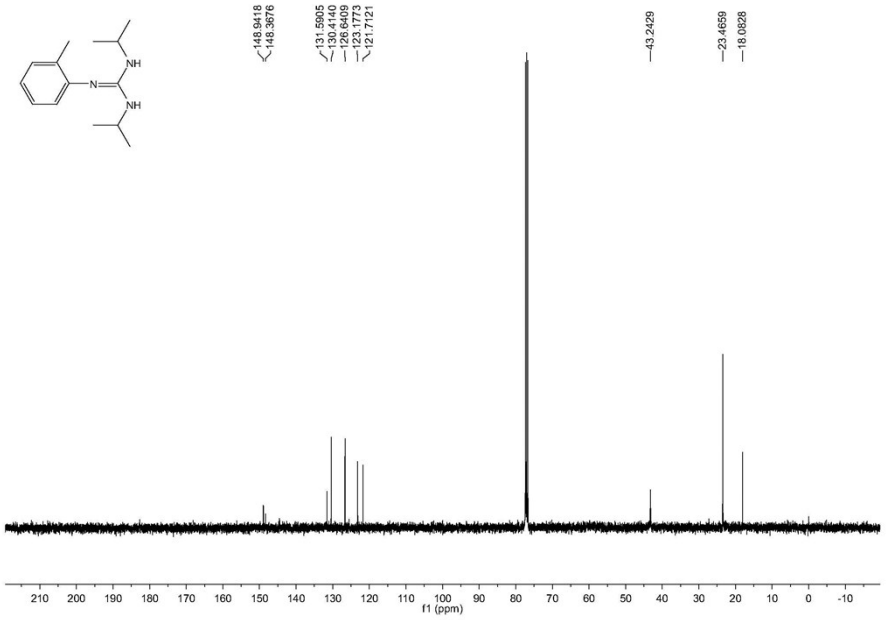
^{1}H NMR and ^{13}C NMR spectra of **5a**



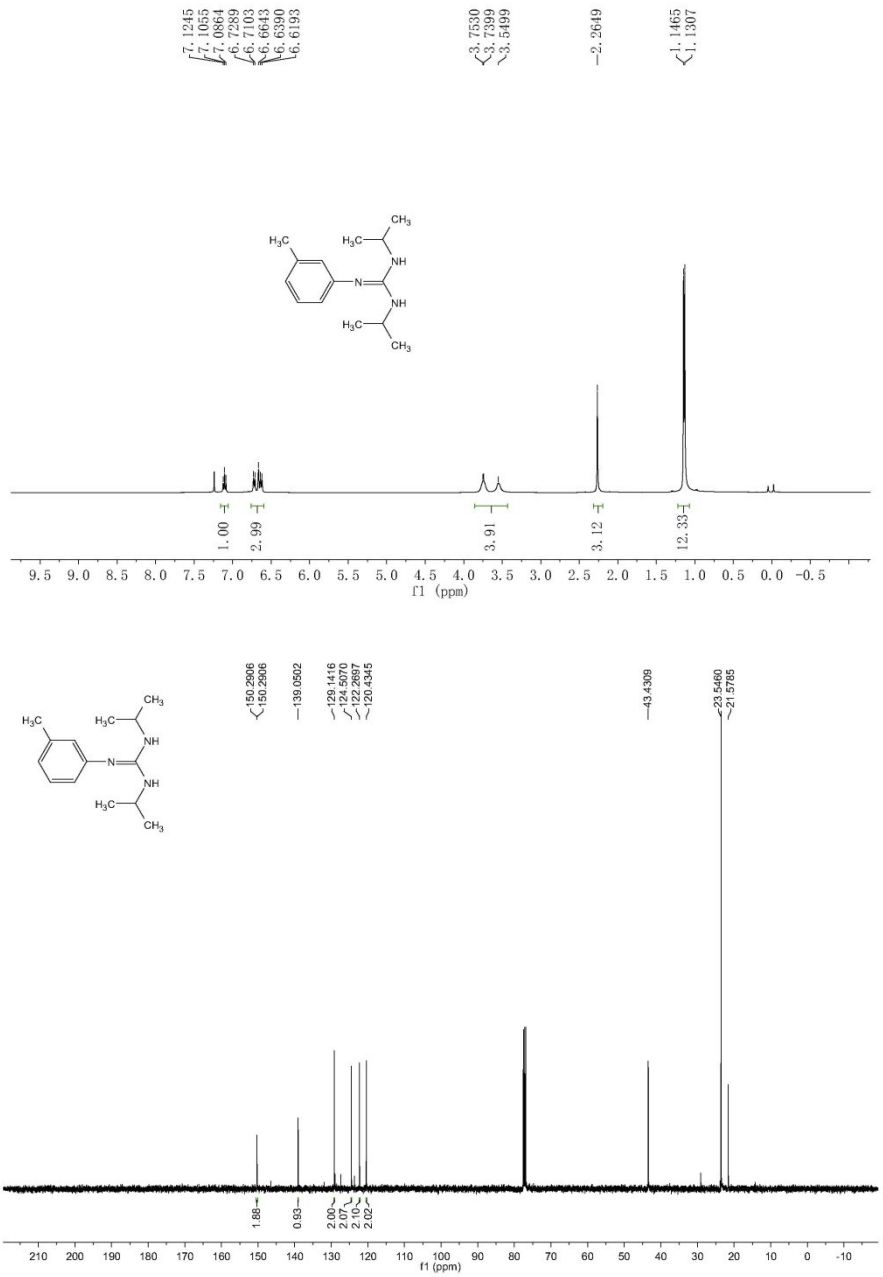


^{1}H NMR and ^{13}C NMR spectra of **5b**

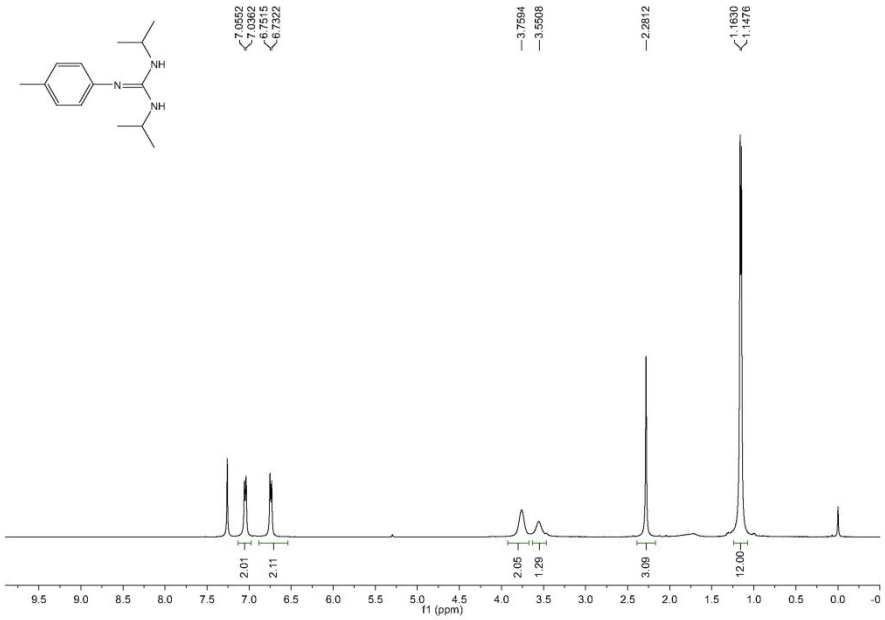


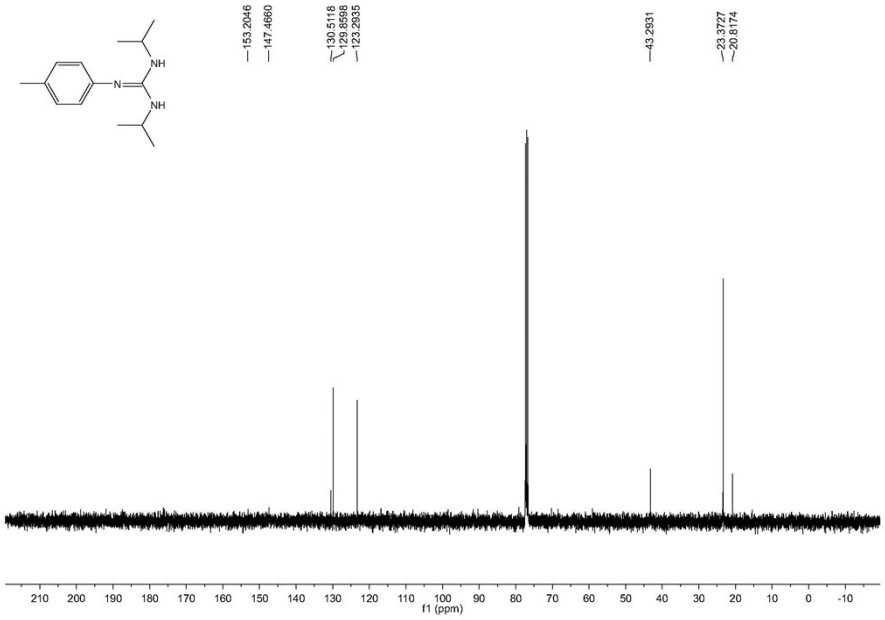


^{1}H NMR and ^{13}C NMR spectra of **5c**

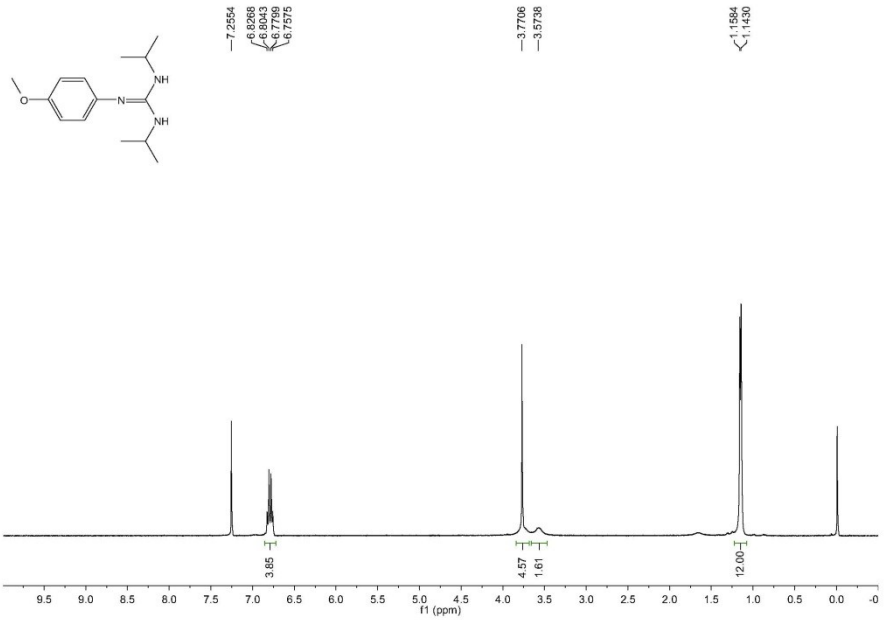


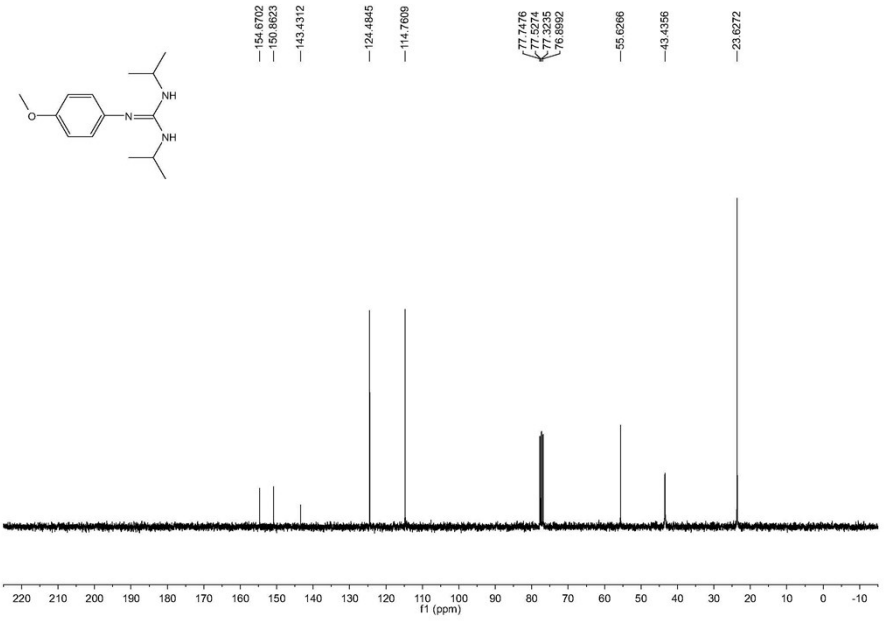
^{1}H NMR and ^{13}C NMR spectra of **5d**



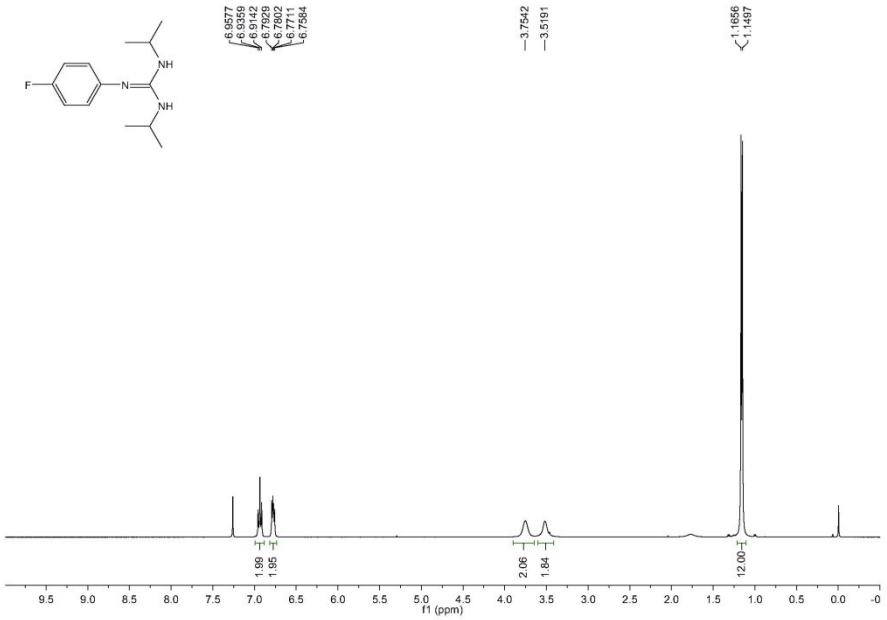


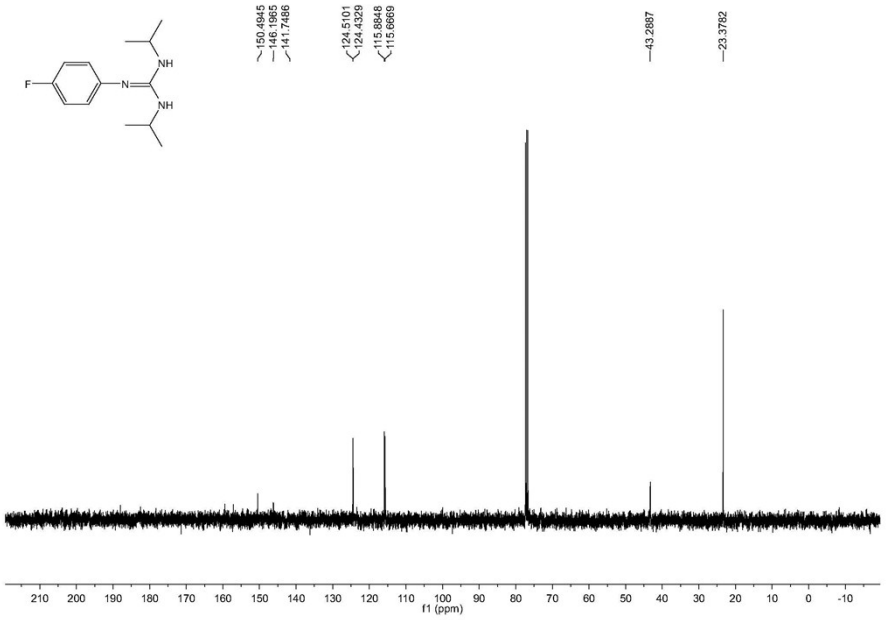
^{1}H NMR and ^{13}C NMR spectra of **5e**



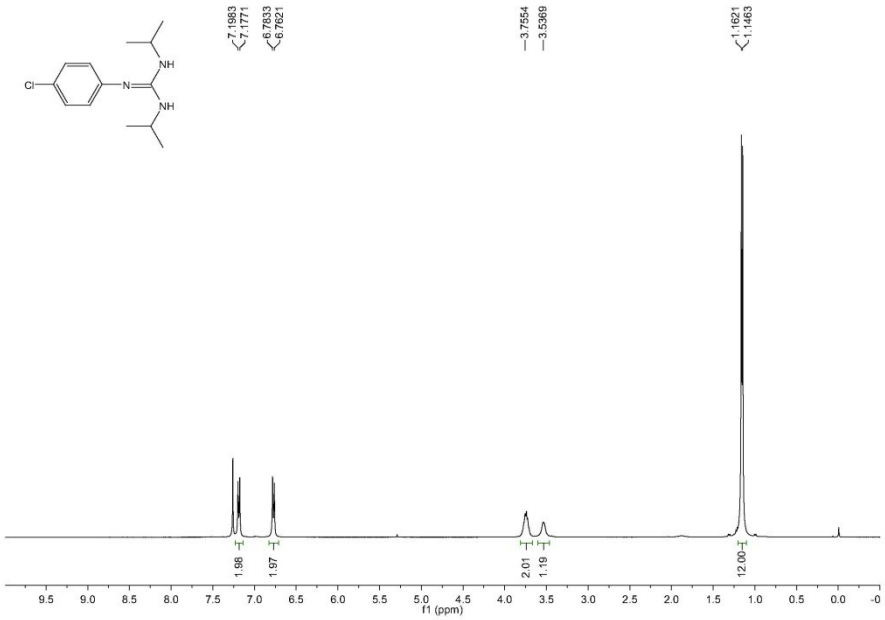


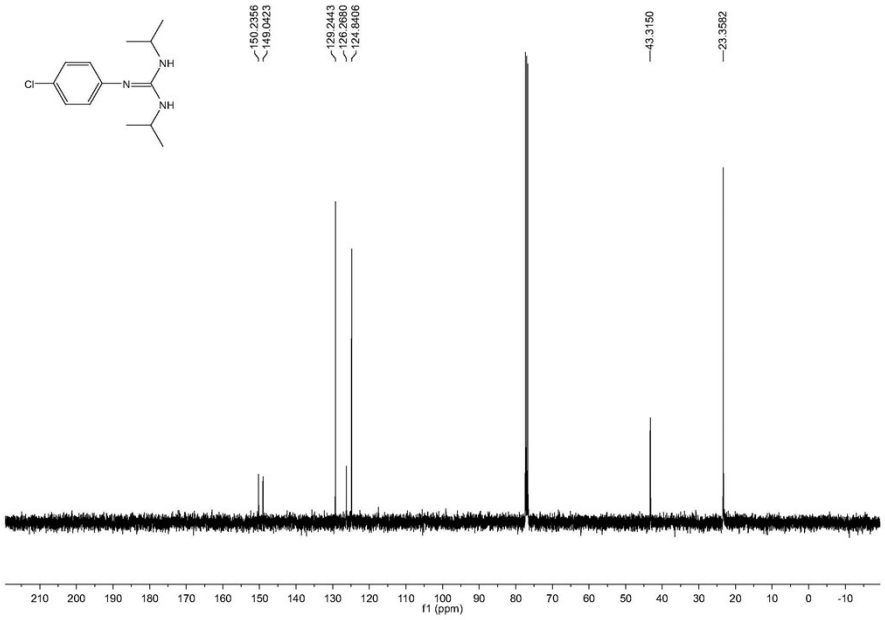
^{1}H NMR and ^{13}C NMR spectra of **5f**



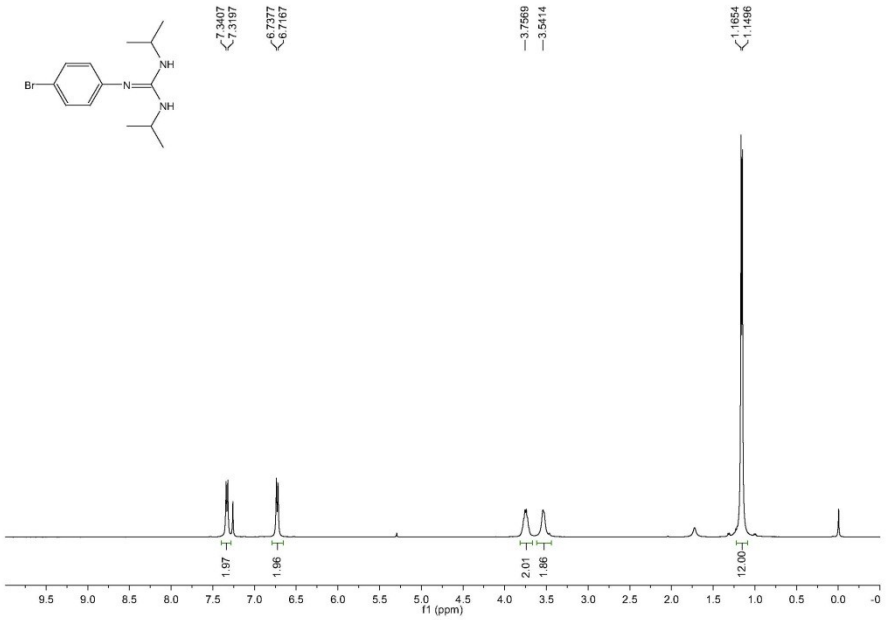


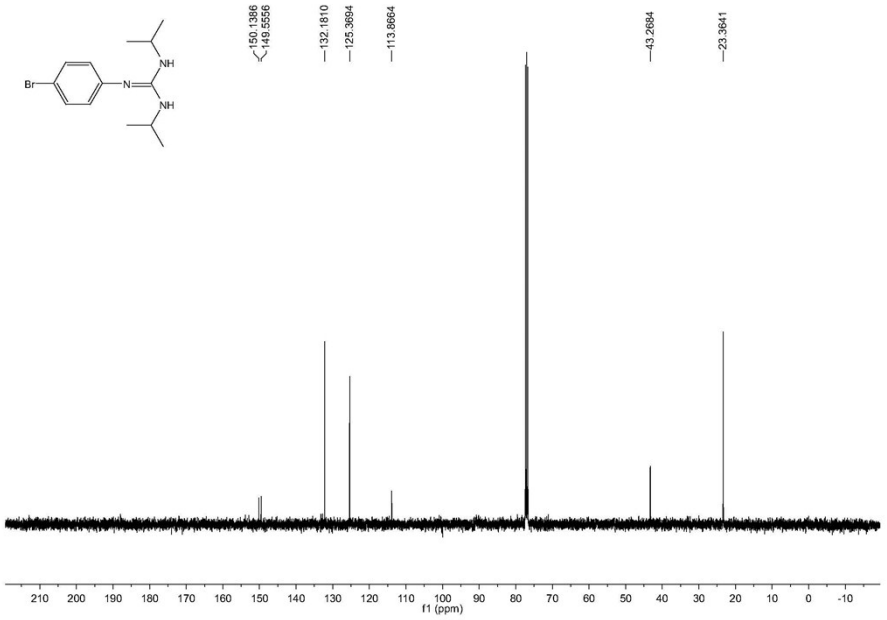
^{1}H NMR and ^{13}C NMR spectra of **5g**



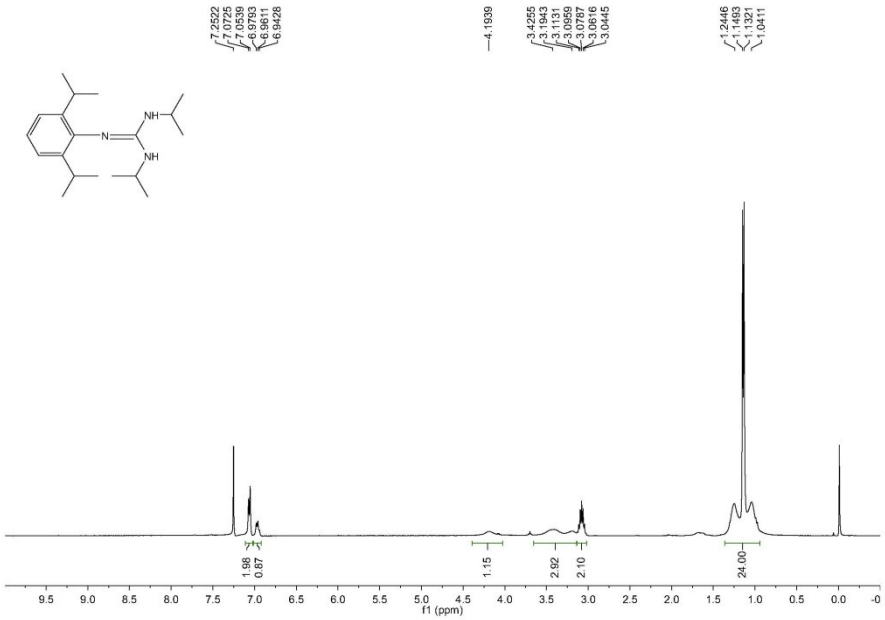


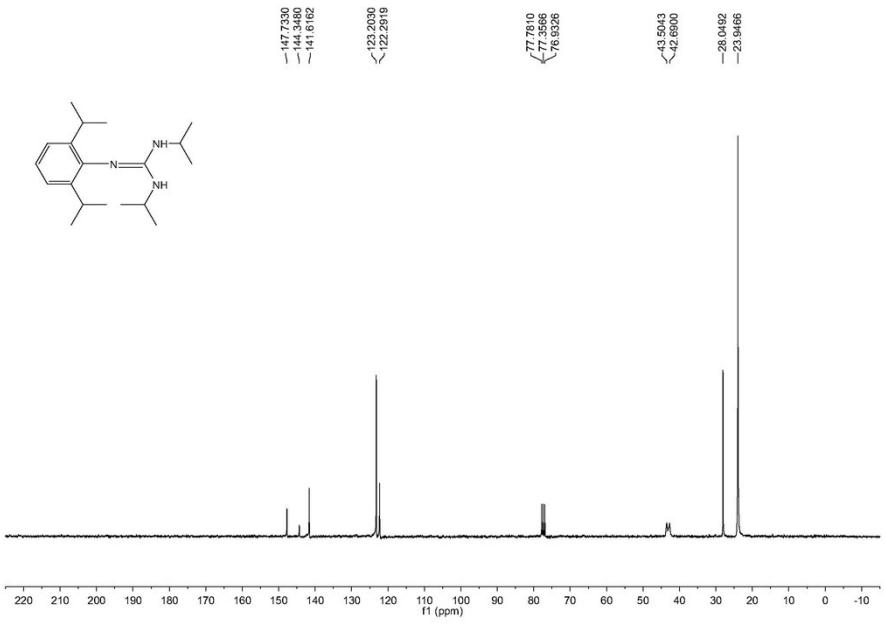
^{1}H NMR and ^{13}C NMR spectra of **5h**



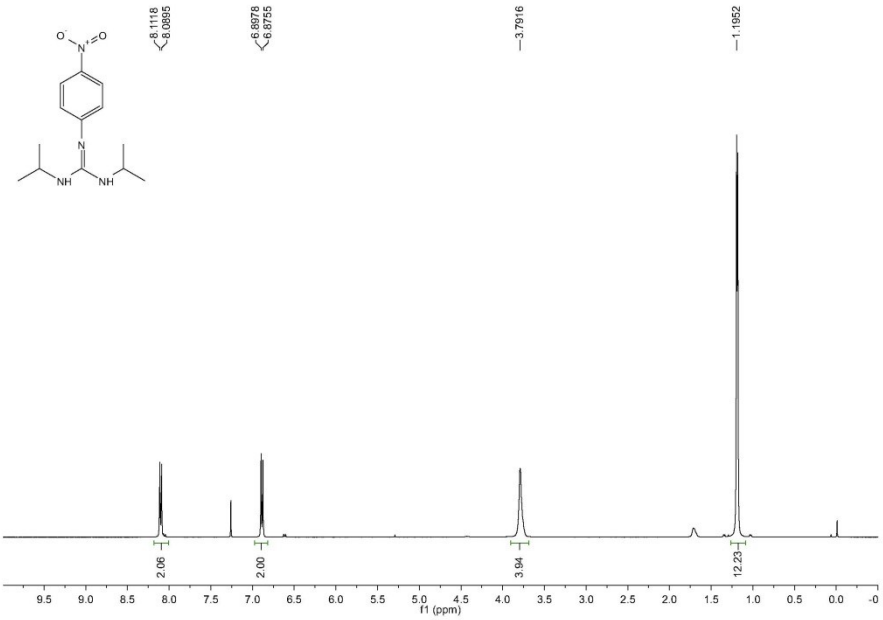


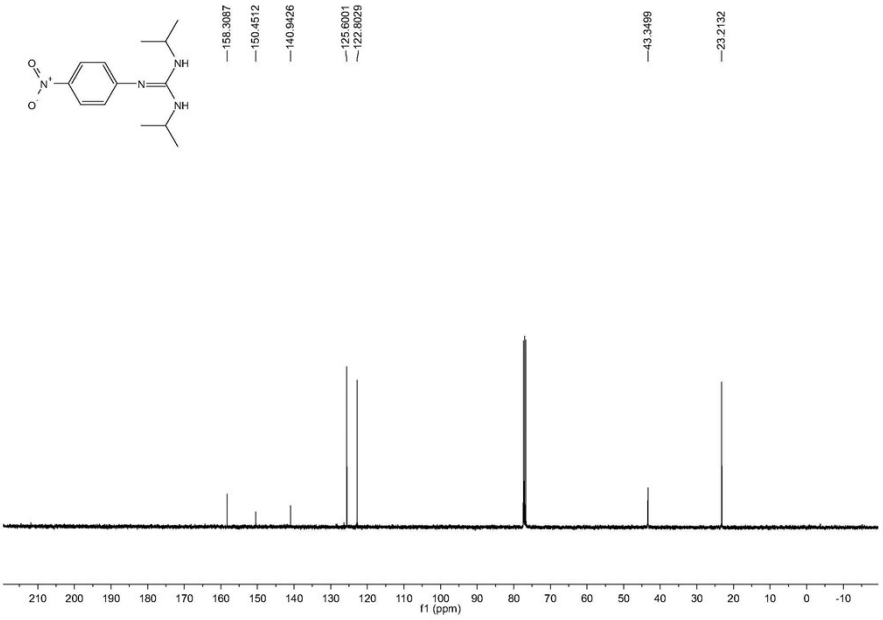
^{1}H NMR and ^{13}C NMR spectra of **5i**



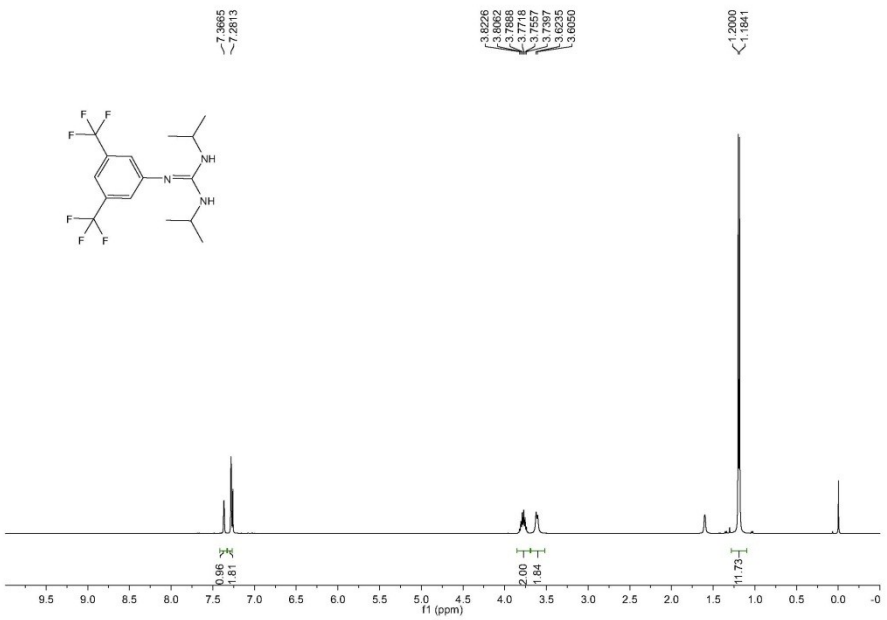


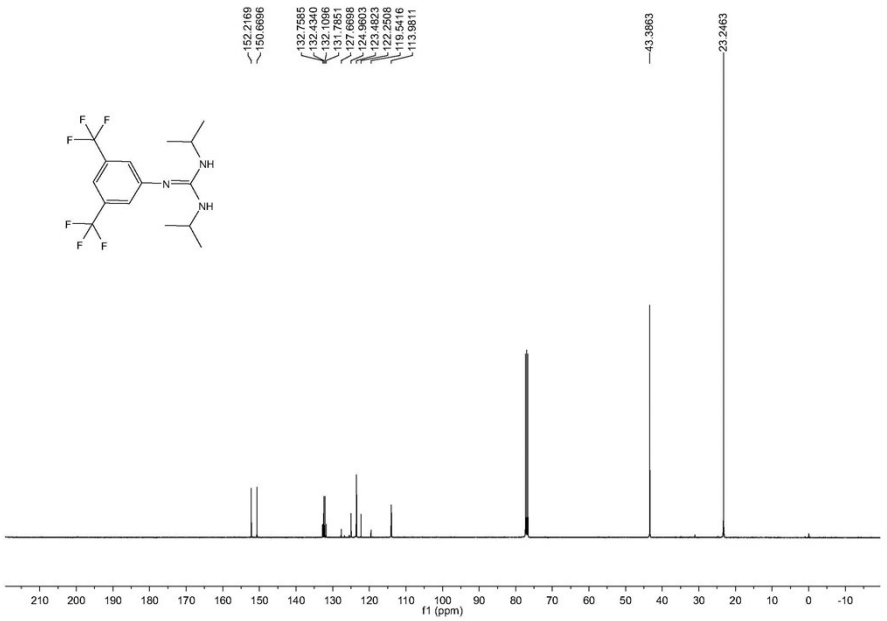
^{1}H NMR and ^{13}C NMR spectra of **5j**



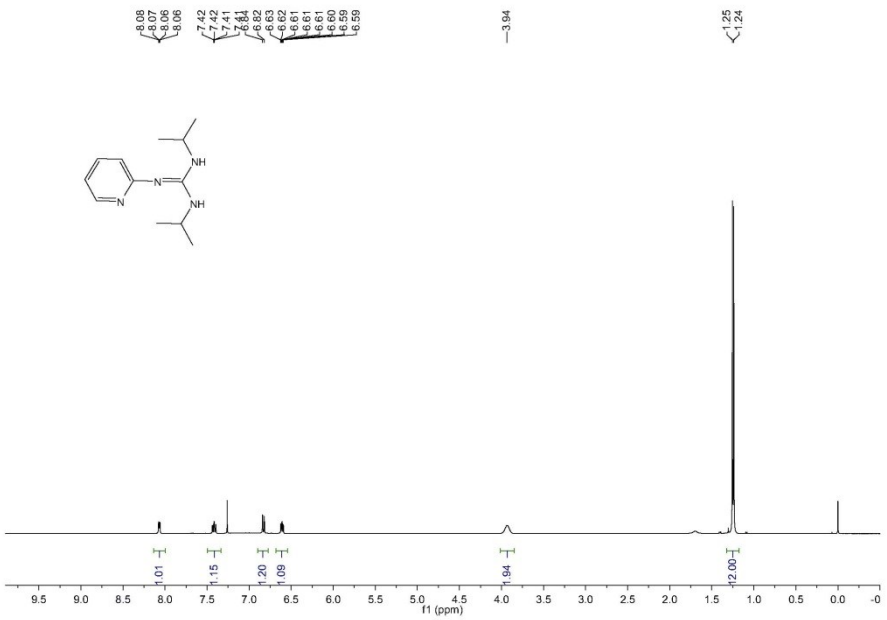


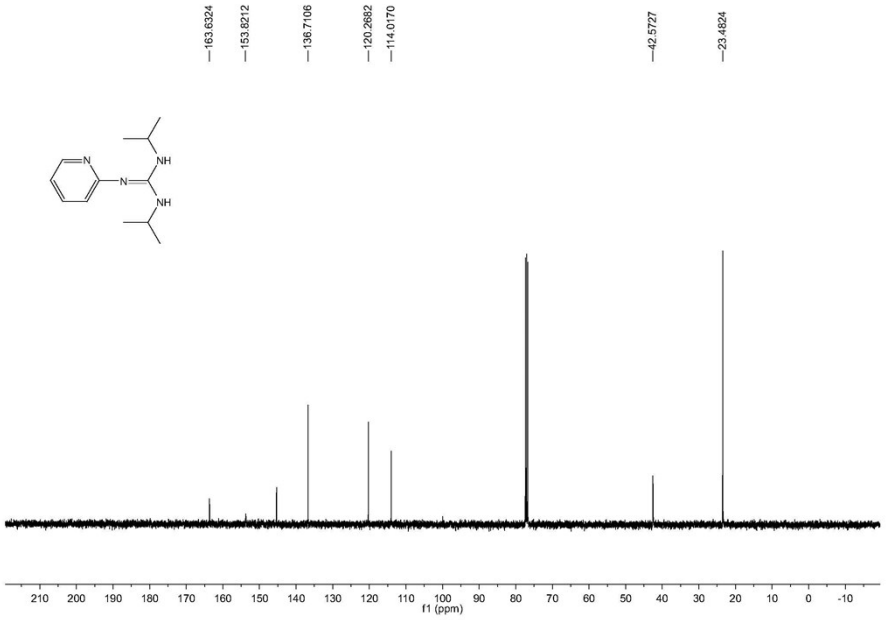
^{1}H NMR and ^{13}C NMR spectra of **5k**



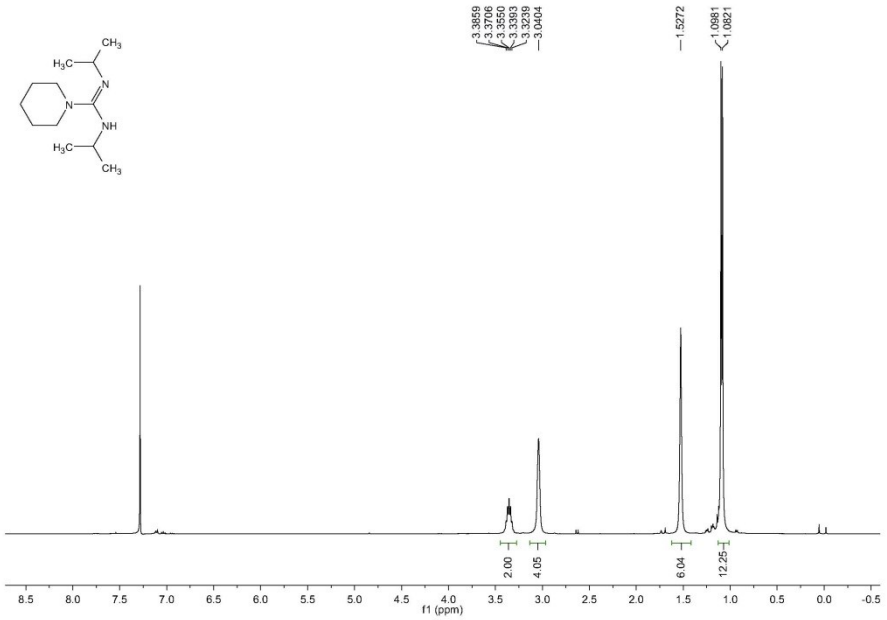


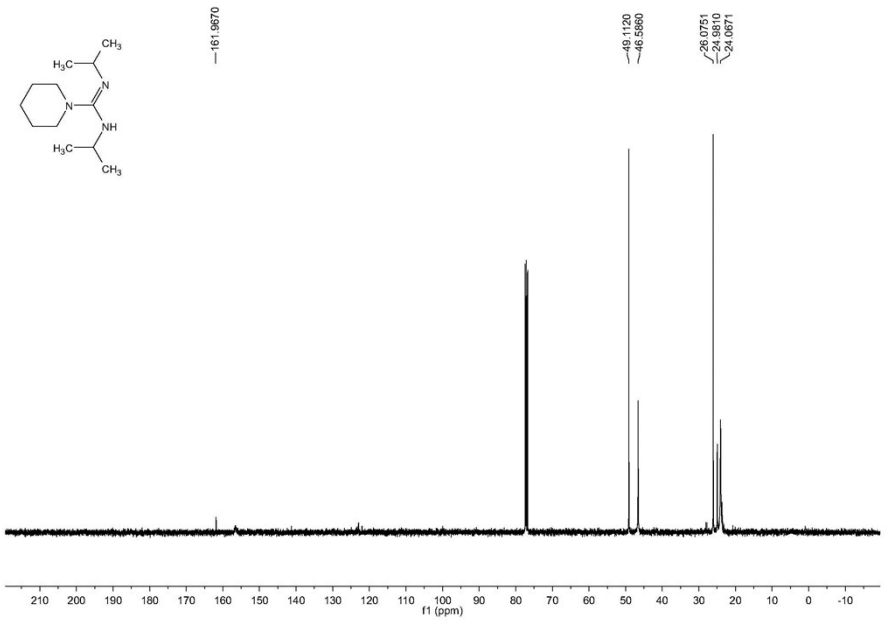
^{1}H NMR and ^{13}C NMR spectra of **5l**



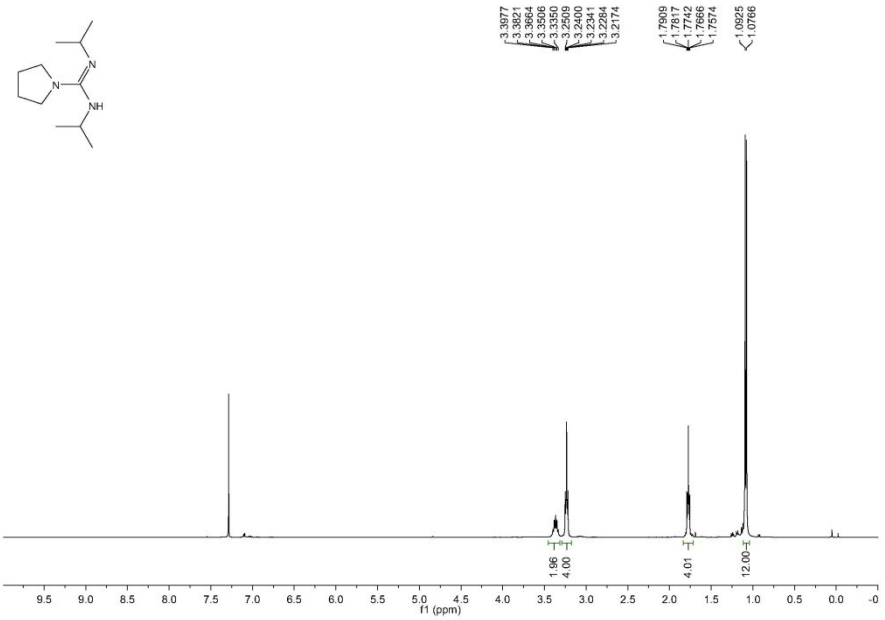


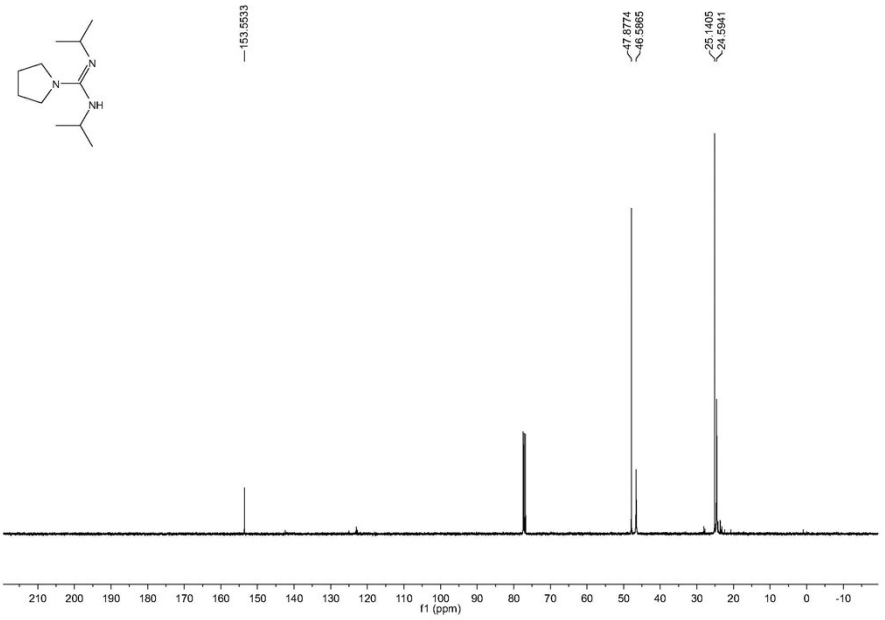
^{1}H NMR and ^{13}C NMR spectra of **5m**



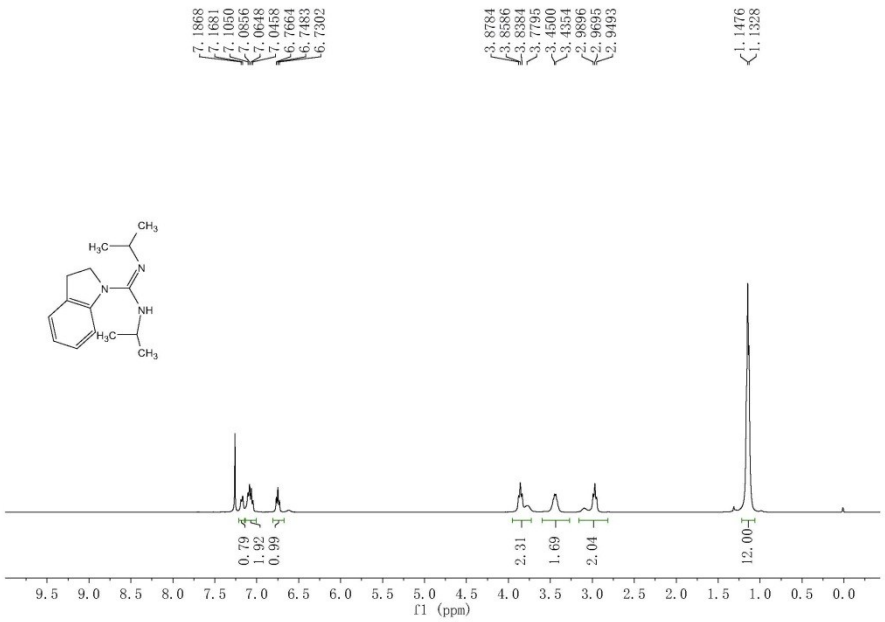


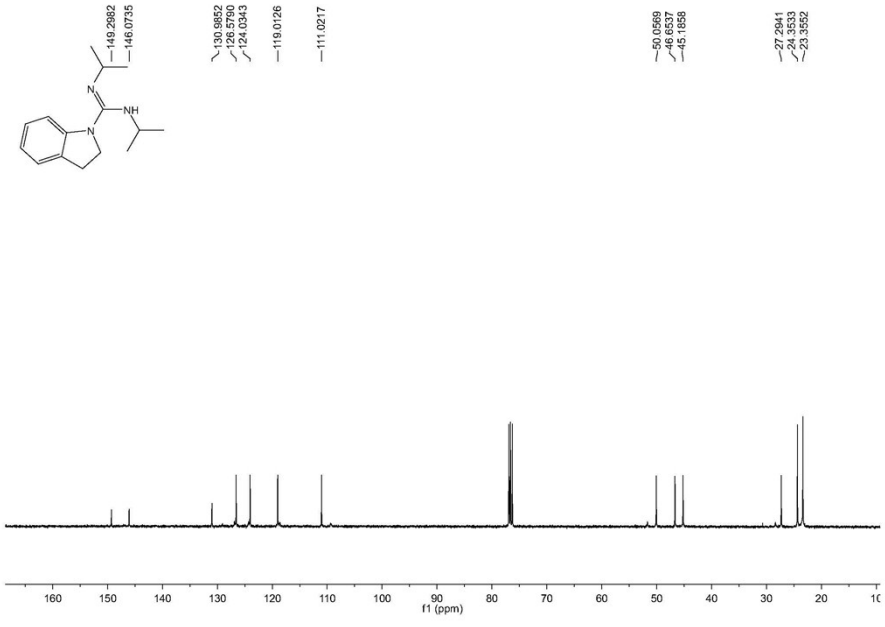
^{1}H NMR and ^{13}C NMR spectra of **5n**



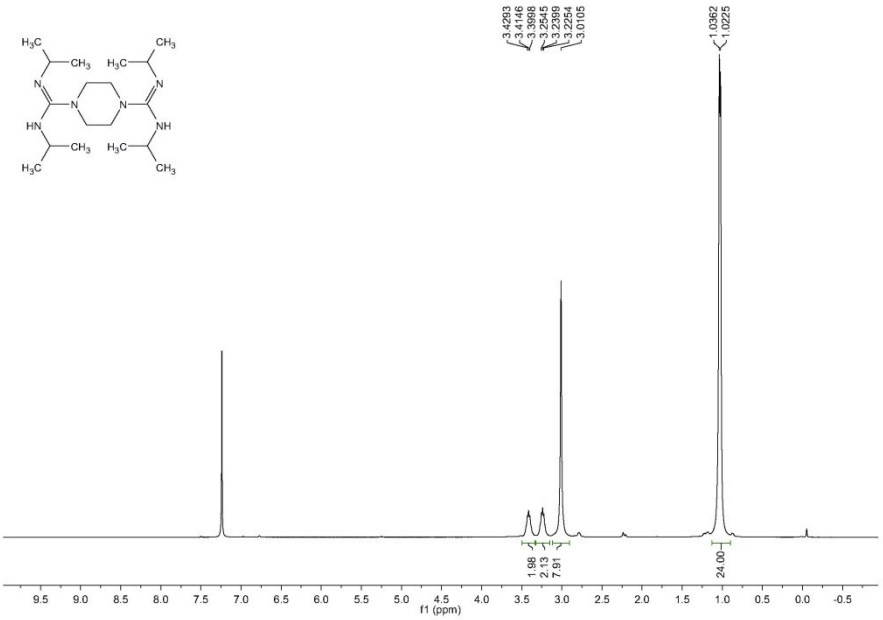


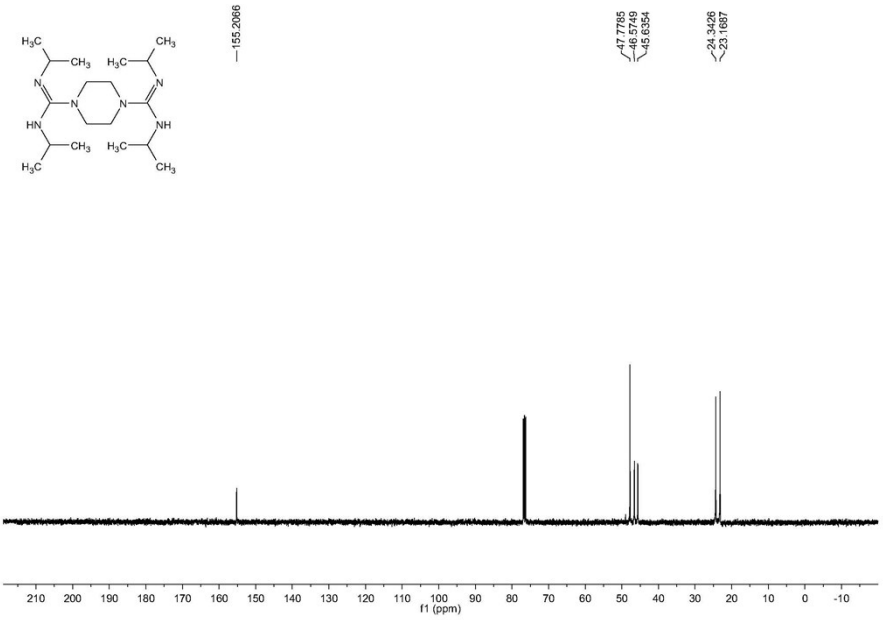
^{1}H NMR and ^{13}C NMR spectra of **5o**



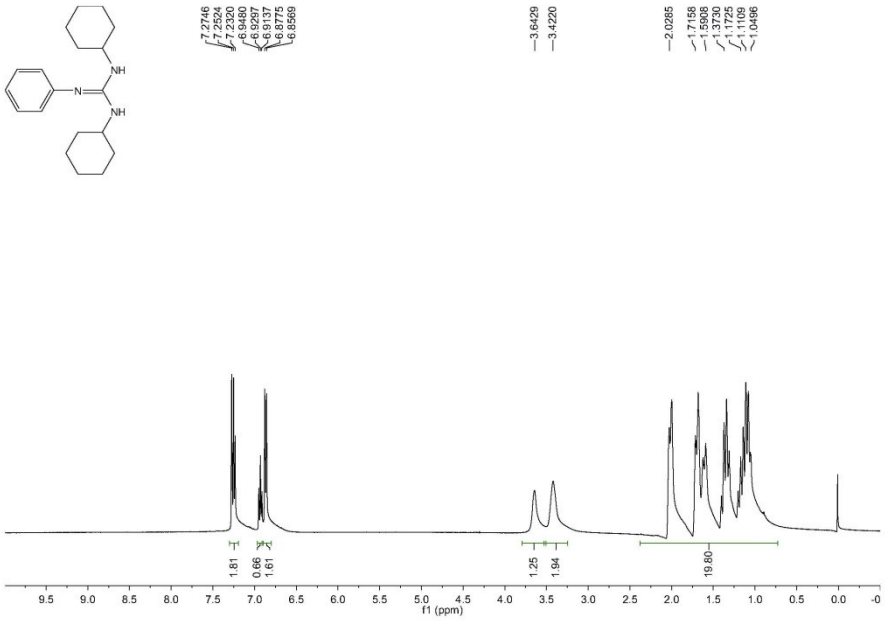


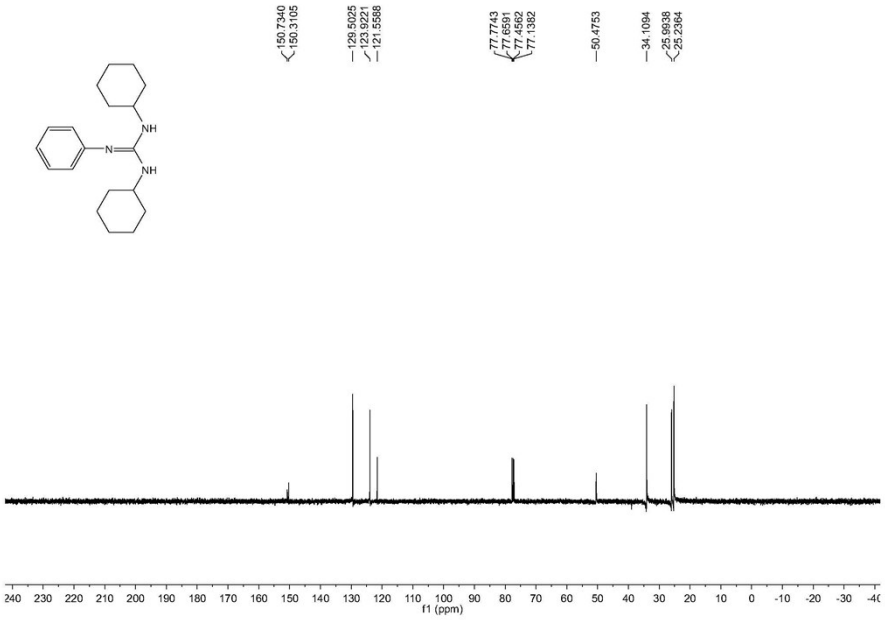
^{1}H NMR and ^{13}C NMR spectra of **5p**



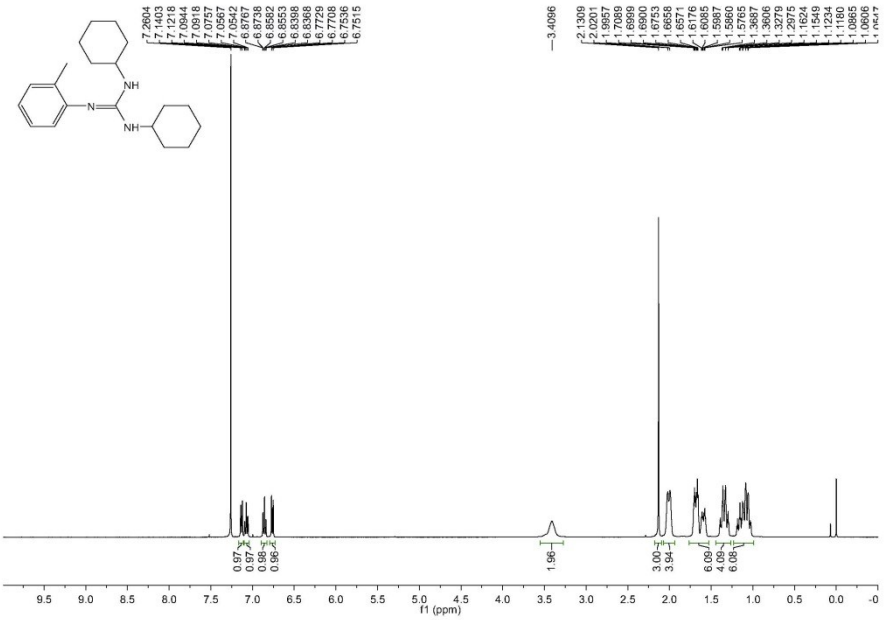


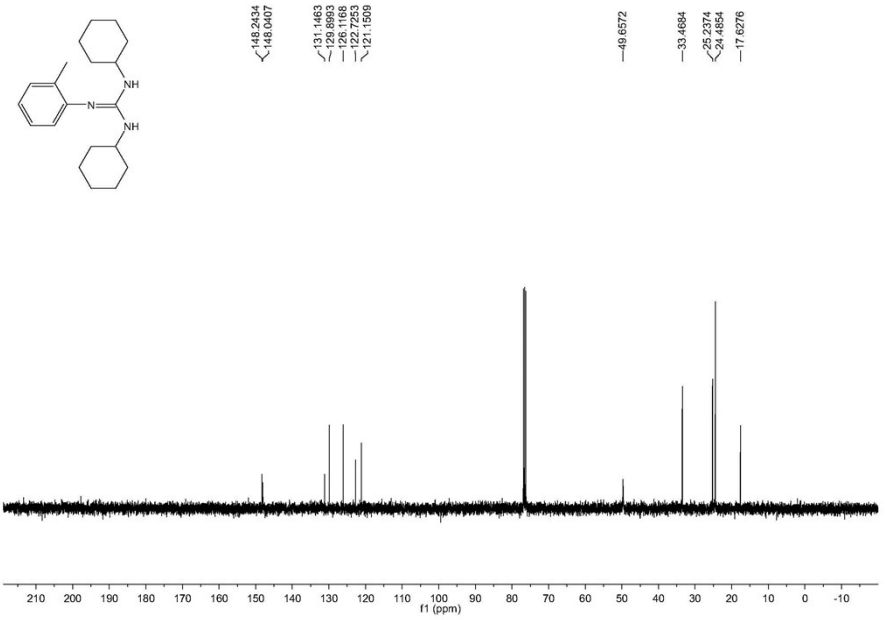
^{1}H NMR and ^{13}C NMR spectra of **5q**



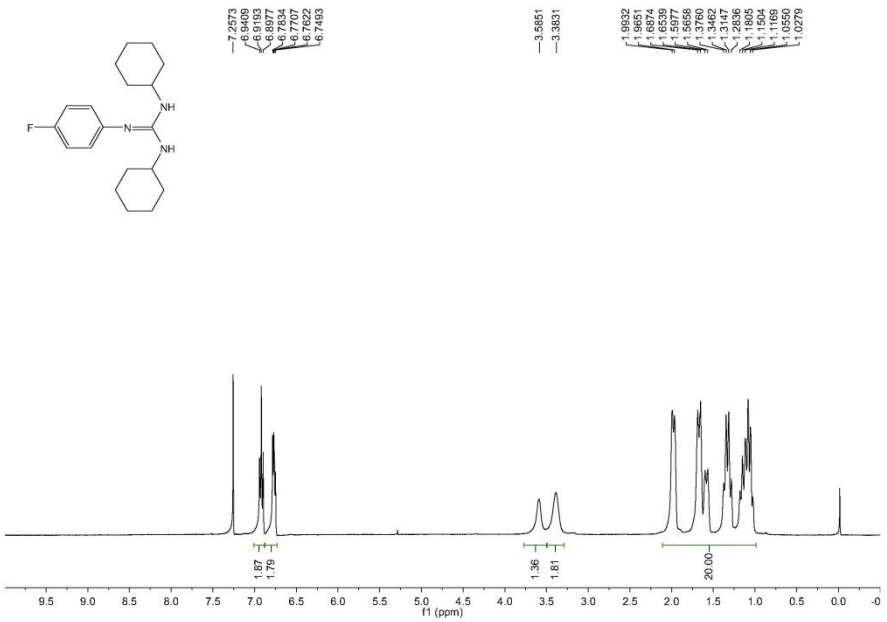


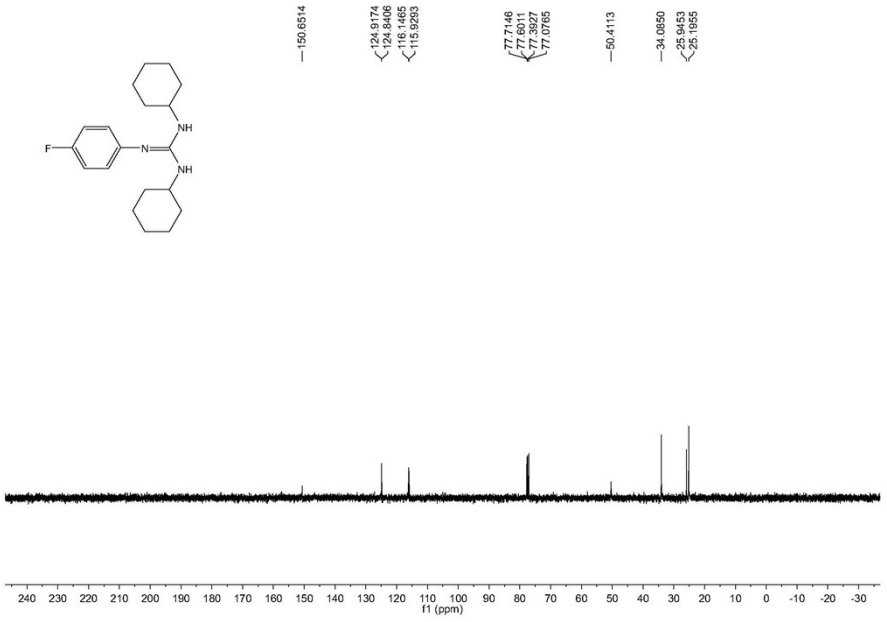
^{1}H NMR and ^{13}C NMR spectra of **5r**





^{1}H NMR and ^{13}C NMR spectra of **5s**





^{1}H NMR and ^{13}C NMR spectra of **5t**