Supporting Information

Ruthenium-Catalyzed *ortho*-Selective C–H Alkenylation of Aromatic Compounds with Alkenyl Esters and Ethers

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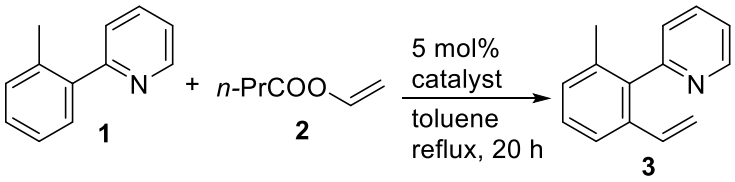
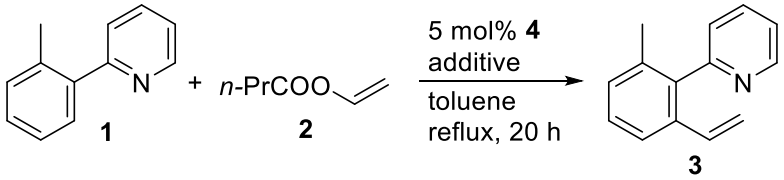
Table S1. Screening of catalysts.[a]



entry	catalyst	yield of **3**[b]
1	$RuH_2(CO)(PPh_3)_3$	0%
2	$RuHCl(CO)(PPh_3)_3$	0%
3	$RuH(OAc)(CO)(PPh_3)_2$	0%
4	$[RuCl_2(C_6H_6)]_2/PPh_3$[c]	0%
5	Ru(cod)(cot) (**4**)	34%
6	$Ru_3(CO)_{12}$	21%
7	$Ru(CO)_3(PPh_3)_2$	0%
8	$RhCl(PPh_3)_3$	0%
9	$[RhCl(coe)_2]_2$	9%
10	$[RhCl(coe)_2]_2/PCy_3$[d]	5%

[a]Reaction conditions: **1** (1 mmol), vinyl *n*-butylate (**2**) (2 mmol), catalyst (0.05 mmol), toluene 1 mL, reflux, 20 h. [b]GC yield. [c]10 mol % of PPh_3. [d]10 mol % of PCy_3.

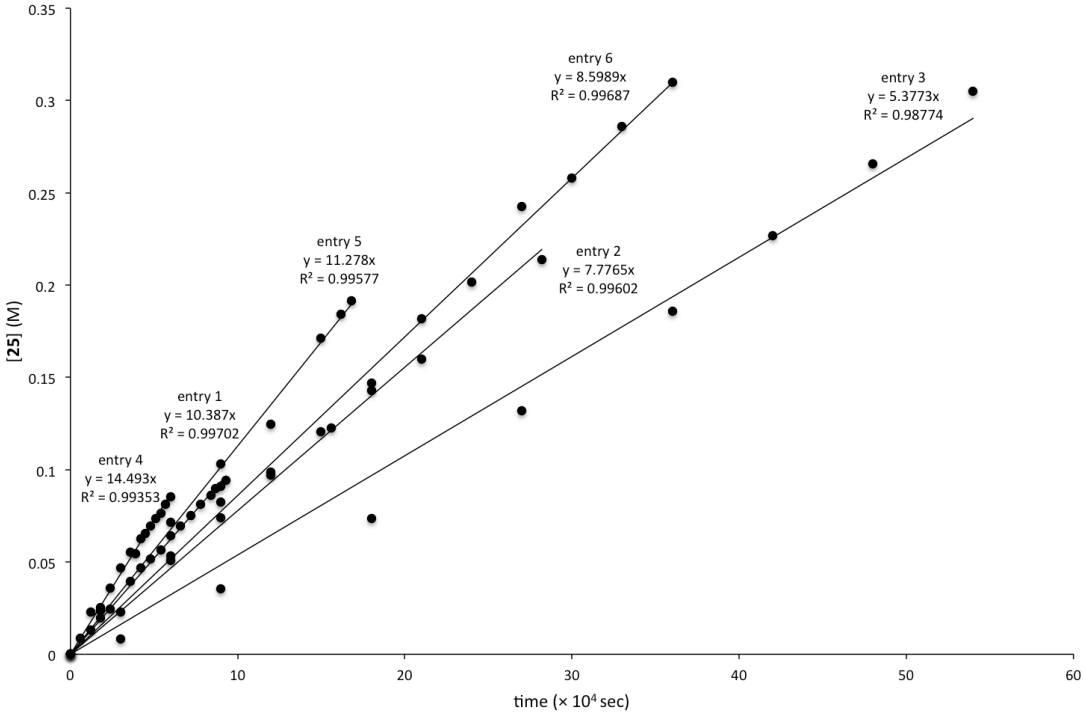
Table S2. Screening of additives.[a]



entry	additive	additive/Ru	yield of **3**[b]
1[c]	none	0	34%
2[d]	none	0	37%[e]
3	PEt_3	1	9%
4	PEt_3	2	8%
5	PPh_3	1	20%
6	PPh_3	2	20%
7[d]	$P(fur)_3$	2	10%[e]
8	dppp	1	12%
9	$P(OPh)_3$	3	0%
10	$P(OEt)_3$	3	0%
11	^{t}BuNC	3	trace

[a]Reaction conditions: **1** (1 mmol), **2** (2 mmol), **4** (0.05 mmol), additive (5-15 mol %), toluene 1 mL, reflux, 20 h. [b]GC yield. [c]The result described in Table 1, entry 5. [d]Performed with 5 mmol of **2** and 0.10 mmol of **4** in 1.5 mL of toluene. [e]Yields were determined based on ^{1}H NMR spectra of **3** isolated as mixtures with starting material **1**.

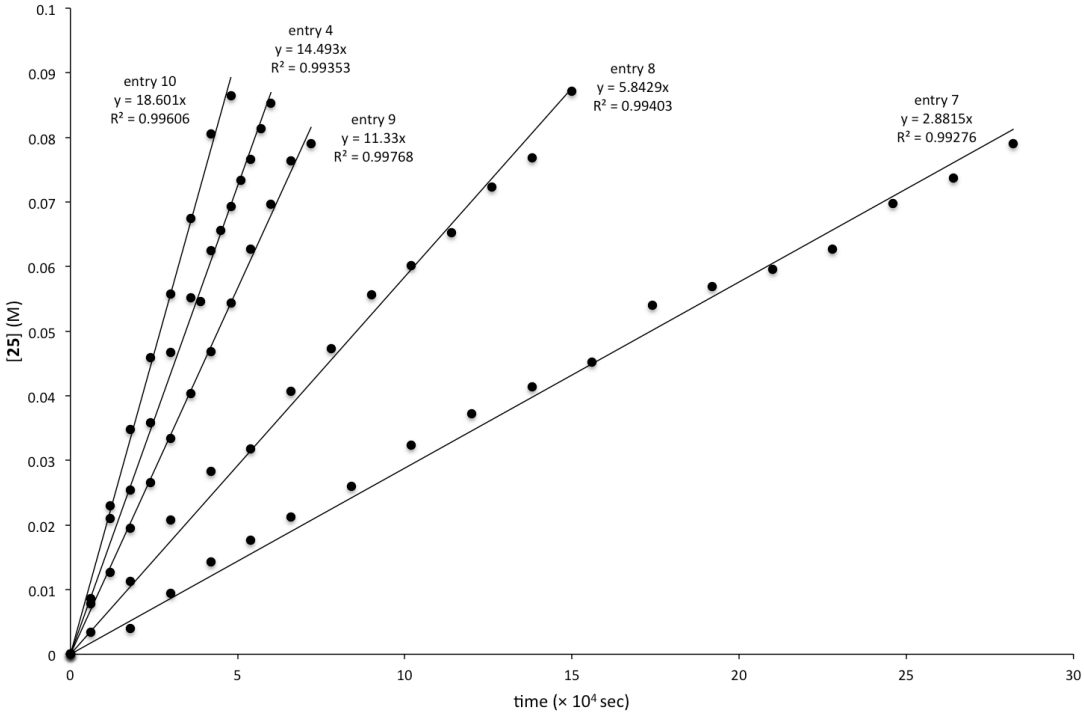
Determination of the Order of the Reaction in Aromatic Compound 24 (Table 8, entries 1-6). In a glove box, 1,3,5-trimethoxybenzene (16.8 mg, 0.1 mmol) as an internal standard and Ru(cod)(cot) (**4**) (3.2 mg, 10 μmol, or 6.3 mg, 20 μmol) were placed in a NMR tube, and then toluene-d_8, 3-methyl-2-phenylpyridine (**24**), and β-styryl acetate (**6d**) (309 μL, 2.0 mmol, *E/Z* = 66:34) were added in this order. The tube was sealed and heated in an oil bath at 90 °C. The reaction mixture was monitored by measuring the concentration of the alkenylation product (**25**) by ^{1}H NMR. The concentrations of **24** were as follows; 0.1 M (16 μL, 0.1 mmol, toluene-d_8: 675 μL), 0.2 M (32 μL, 0.2 mmol, toluene-d_8: 659 μL), 0.3 M (48 μL, 0.3 mmol, toluene-d_8: 643 μL).



entry	[**24**]$_0$ (M)	[**6d**]$_0$ (M)	[**4**]$_0$ (mM)	$k_{obs} \times 10^7$ (M·s^{-1})
1	0.1	2.0	10	10.4
2	0.2	2.0	10	7.8
3	0.3	2.0	10	5.4
4	0.1	2.0	20	14.5
5	0.2	2.0	20	11.3
6	0.3	2.0	20	8.6

Figure S1. Time-concentration plots. Reaction conditions: [**24**]$_0$ = 0.1-0.3 M, [**6d**]$_0$ = 2.0 M, [**4**]$_0$ = 10-20 mM in toluene-d_8, at 90 °C.

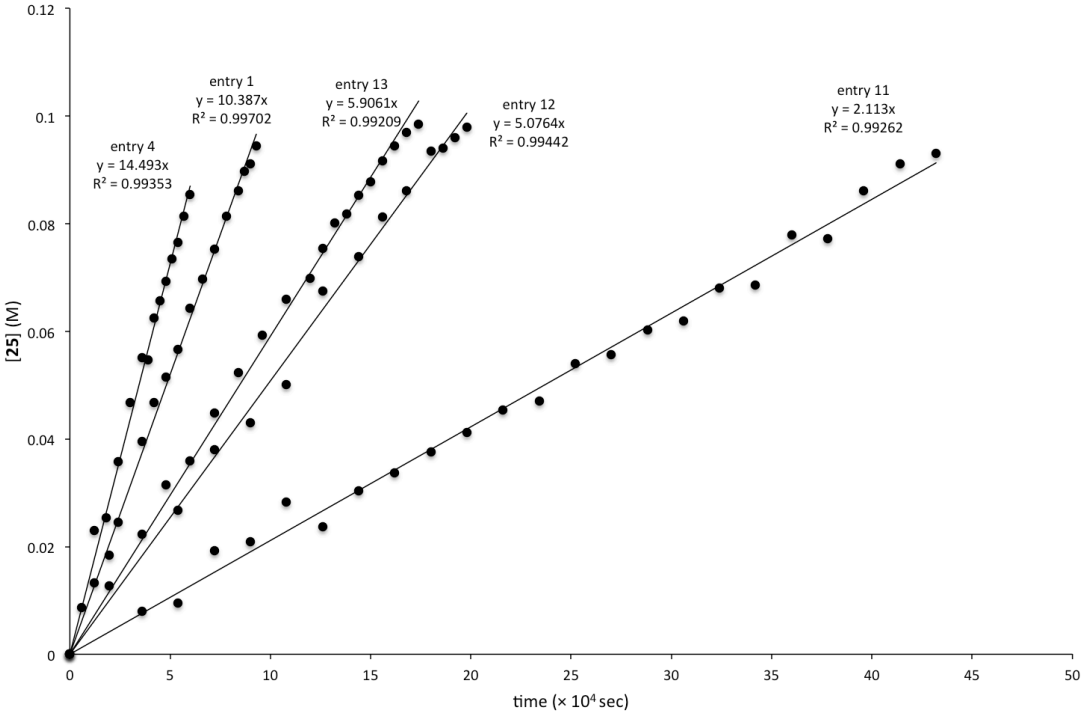
Determination of the Order of the Reaction in Alkenyl Ester 6d (Table 8, entries 4 and 7-10). In a glove box, 1,3,5-trimethoxybenzene (16.8 mg, 0.1 mmol) as an internal standard and Ru(cod)(cot) (**4**) (6.3 mg, 20 μmol) were placed in a NMR tube, and then toluene-d_8, 3-methyl-2-phenylpyridine (**24**) (16 μL, 0.1 mmol), and β-styryl acetate (**6d**) (*E/Z* = 66:34) were added in this order. The tube was sealed and heated in an oil bath at 90 °C. The reaction mixture was monitored by measuring the concentration of the alkenylation product (**25**) by ^{1}H NMR. The concentrations of **6d** were as follows; 0.5 M (78 μL, 0.5 mmol, toluene-d_8: 906 μL), 1.0 M (155 μL, 1.0 mmol, toluene-d_8: 829 μL), 1.5 M (232 μL, 1.5 mmol, toluene-d_8: 752 μL), 2.0 M (309 μL, 2.0 mmol, toluene-d_8: 675 μL), 2.5 M (386 μL, 2.5 mmol, toluene-d_8: 598 μL).



entry	[**24**]$_0$ (M)	[**6d**]$_0$ (M)	[**4**]$_0$ (mM)	$k_{obs} \times 10^7$ (M·s^{-1})
4	0.1	2.0	20	14.5
7	0.1	0.5	20	2.9
8	0.1	1.0	20	5.8
9	0.1	1.5	20	11.3
10	0.1	2.0	20	18.6

Figure S2. Time-concentration plots. Reaction conditions: [**24**]$_0$ = 0.1 M, [**6d**]$_0$ = 0.5-2.5 M, [**4**]$_0$ = 20 mM in toluene-d_8, at 90 °C.

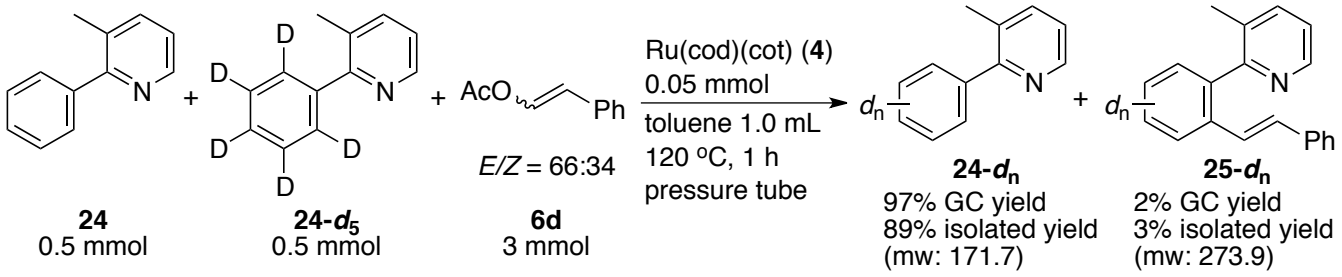
Determination of the Order of the Reaction in Catalyst 4 (Table 8, entries 1, 4 and 11-13). In a glove box, 1,3,5-trimethoxybenzene (16.8 mg, 0.1 mmol) as an internal standard and Ru(cod)(cot) (**4**) were placed in a NMR tube, and then toluene-d_8 (675 μL), 3-methyl-2-phenylpyridine (**24**) (16 μL, 0.1 mmol), and β-styryl acetate (**6d**) (309 μL, 2.0 mmol, *E/Z* = 66:34) were added in this order. The tube was sealed and heated in an oil bath at 90 °C. The reaction mixture was monitored by measuring the concentration of the alkenylation product (**25**) by ^{1}H NMR. The concentrations of **4** were as follows; 1 mM (0.3 mg, 1 μmol), 3 mM (1.0 mg, 3 μmol), 5 mM (1.6 mg, 5 μmol), 10 mM (3.2 mg, 10 μmol), 20 mM (6.3 mg, 20 μmol).

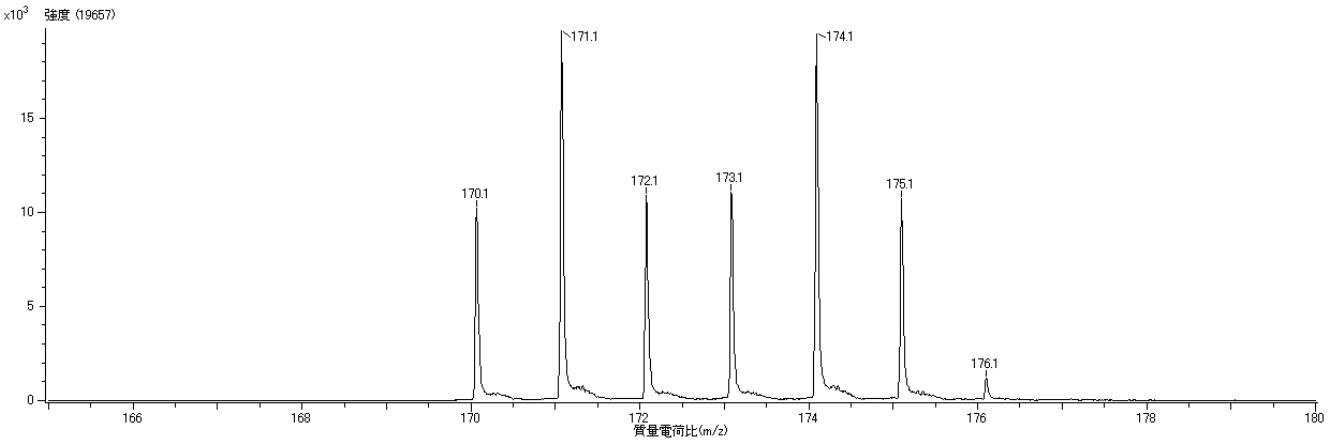


entry	[**24**]$_0$ (M)	[**6d**]$_0$ (M)	[**4**]$_0$ (mM)	$k_{obs} \times 10^7$ (M·s^{-1})
1	0.1	2.0	10	10.4
4	0.1	2.0	20	14.5
11	0.1	2.0	1	2.1
12	0.1	2.0	2	5.1
13	0.1	2.0	3	5.9

Figure S3. Time-concentration plots. Reaction conditions: [**24**]$_0$ = 0.1 M, [**6d**]$_0$ = 2.0 M, [**4**]$_0$ = 1-20 mM in toluene-d_8, at 90 °C.

Observation of Intermolecular H-D Scrambling at the Ortho Positions of 24 and 24-d_5 with 6d Catalyzed by 4 (Table 10, entry 1).

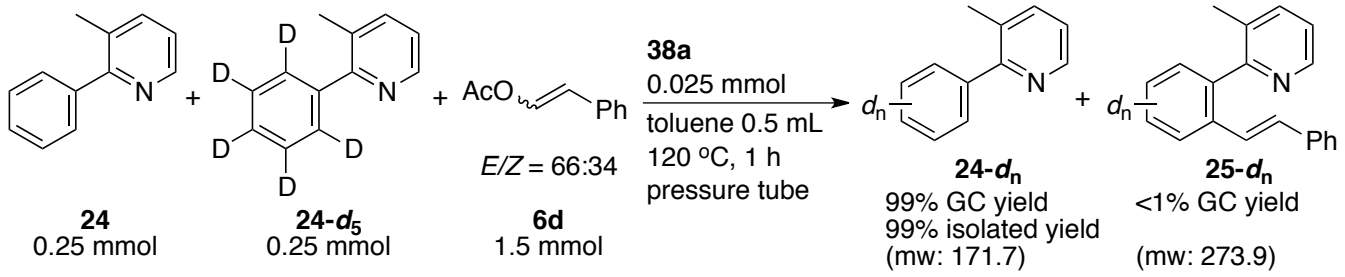


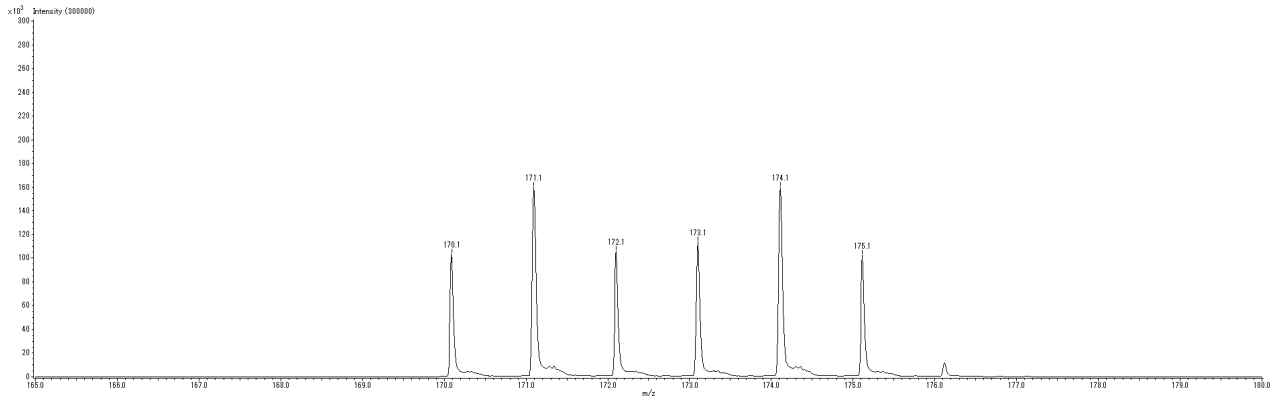


m/z	170.1	171.1	172.1	173.1	174.1	175.1	176.1
integral	31548.80	60333.25	32883.30	33456.60	59302.05	33251.95	3840.90

Figure S4. APCI MS spectrum of **24-d_n**. Exact mass: 170.1 ([**24-d_0+H**]$^+$), 171.1 ([**24-d_1+H**]$^+$), 172.1 ([**24-d_2+H**]$^+$), 173.1 ([**24-d_3+H**]$^+$), 174.1 ([**24-d_4+H**]$^+$), 175.1 ([**24-d_5+H**]$^+$).

Observation of Intermolecular H-D Scrambling at the Ortho Positions of 24 and 24-d_5 with 6d Catalyzed by 38a (Table 10, entry 2).

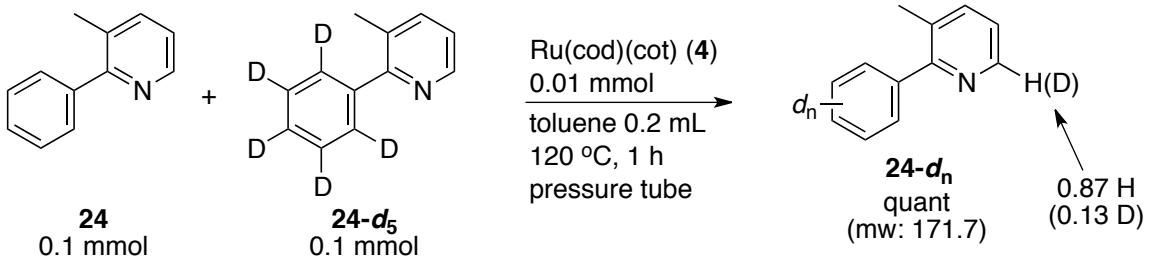




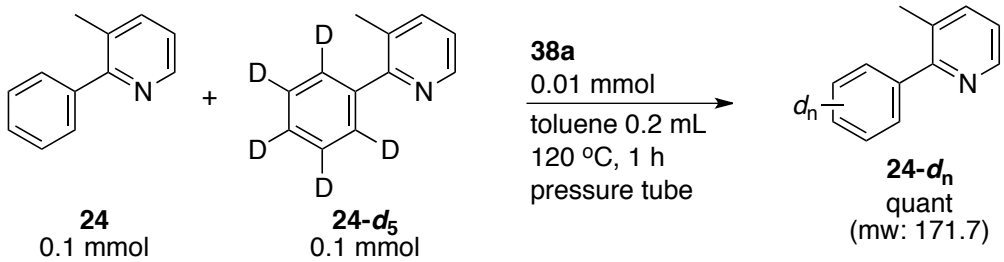
m/z	170.1	171.1	172.1	173.1	174.1	175.1	176.1
integral	427985.53	697028.80	433627.88	458138.33	708246.45	412350.63	42319.96

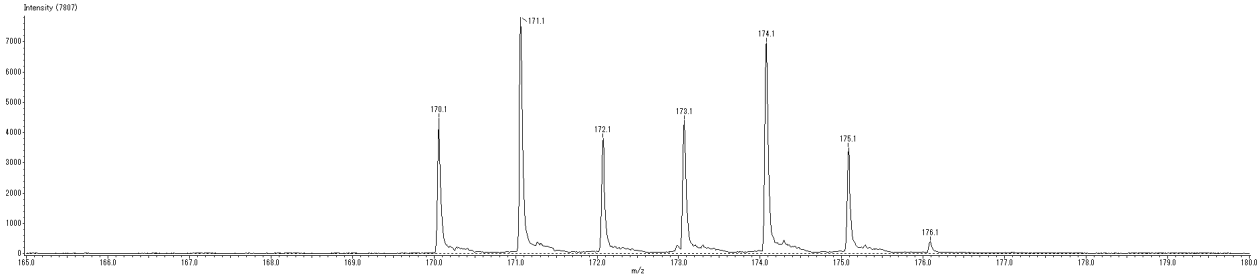
Figure S5. APCI MS spectrum of **24-d_n**. Exact mass: 170.1 ([**24-d_0+H**]$^+$), 171.1 ([**24-d_1+H**]$^+$), 172.1 ([**24-d_2+H**]$^+$), 173.1 ([**24-d_3+H**]$^+$), 174.1 ([**24-d_4+H**]$^+$), 175.1 ([**24-d_5+H**]$^+$).

Observation of Intermolecular H-D Scrambling of 24 and 24-d_5 Catalyzed by 4 (Table 10, entry 3).



Observation of Intermolecular H-D Scrambling at the Ortho Positions of 24 and 24-d_5 Catalyzed by 38a (Table 10, entry 4).

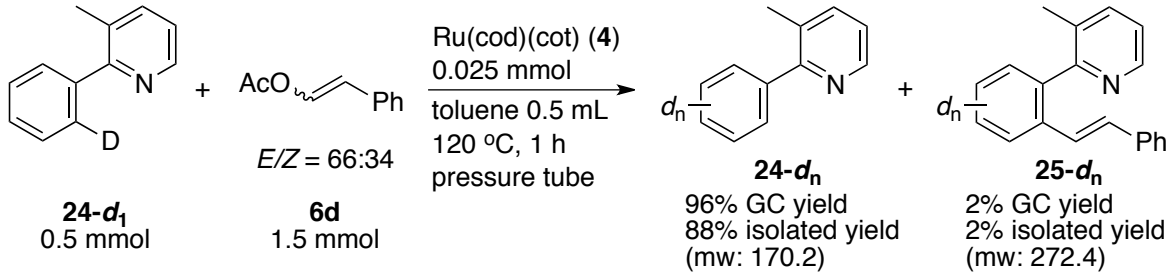


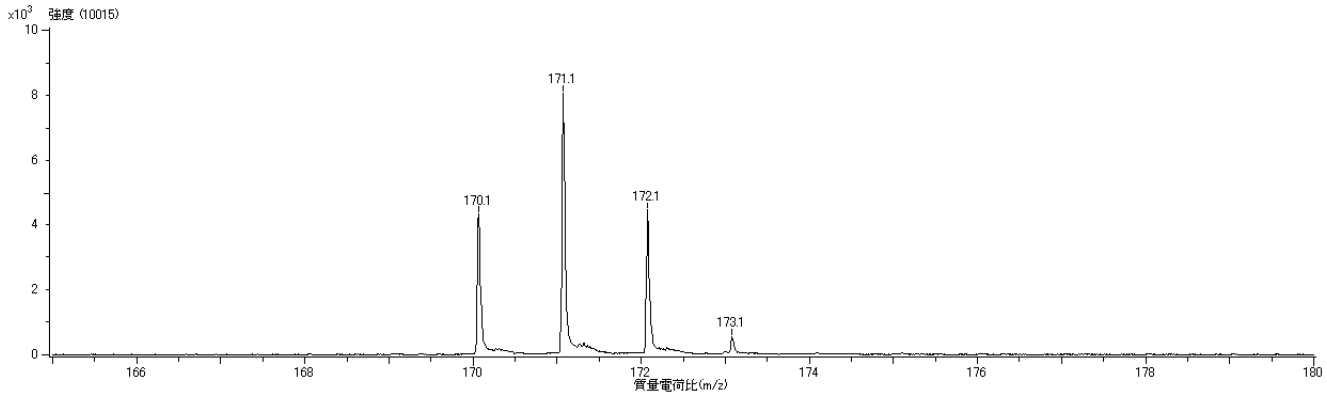


m/z	170.1	171.1	172.1	173.1	174.1	175.1	176.1
integral	28789.75	47142.33	24296.65	27901.04	43439.50	22163.65	2709.02

Figure S6. APCI MS spectrum of **24-d_n**. Exact mass: 170.1 ([**24-d_0+H**]$^+$), 171.1 ([**24-d_1+H**]$^+$), 172.1 ([**24-d_2+H**]$^+$), 173.1 ([**24-d_3+H**]$^+$), 174.1 ([**24-d_4+H**]$^+$), 175.1 ([**24-d_5+H**]$^+$).

Observation of Intramolecular H-D Scrambling at the Ortho Positions of 24-d_1 with 6d Catalyzed by 4.





m/z	170.1	171.1	172.1	173.1
integral	11940.06	22831.27	12353.33	1474.50

Figure S7. APCI MS spectrum of **24-d_n**. Exact mass: 170.1 ([**24-d_0+H**]$^+$), 171.1 ([**24-d_1+H**]$^+$), 172.1 ([**24-d_2+H**]$^+$).

X-ray Crystallographic Data

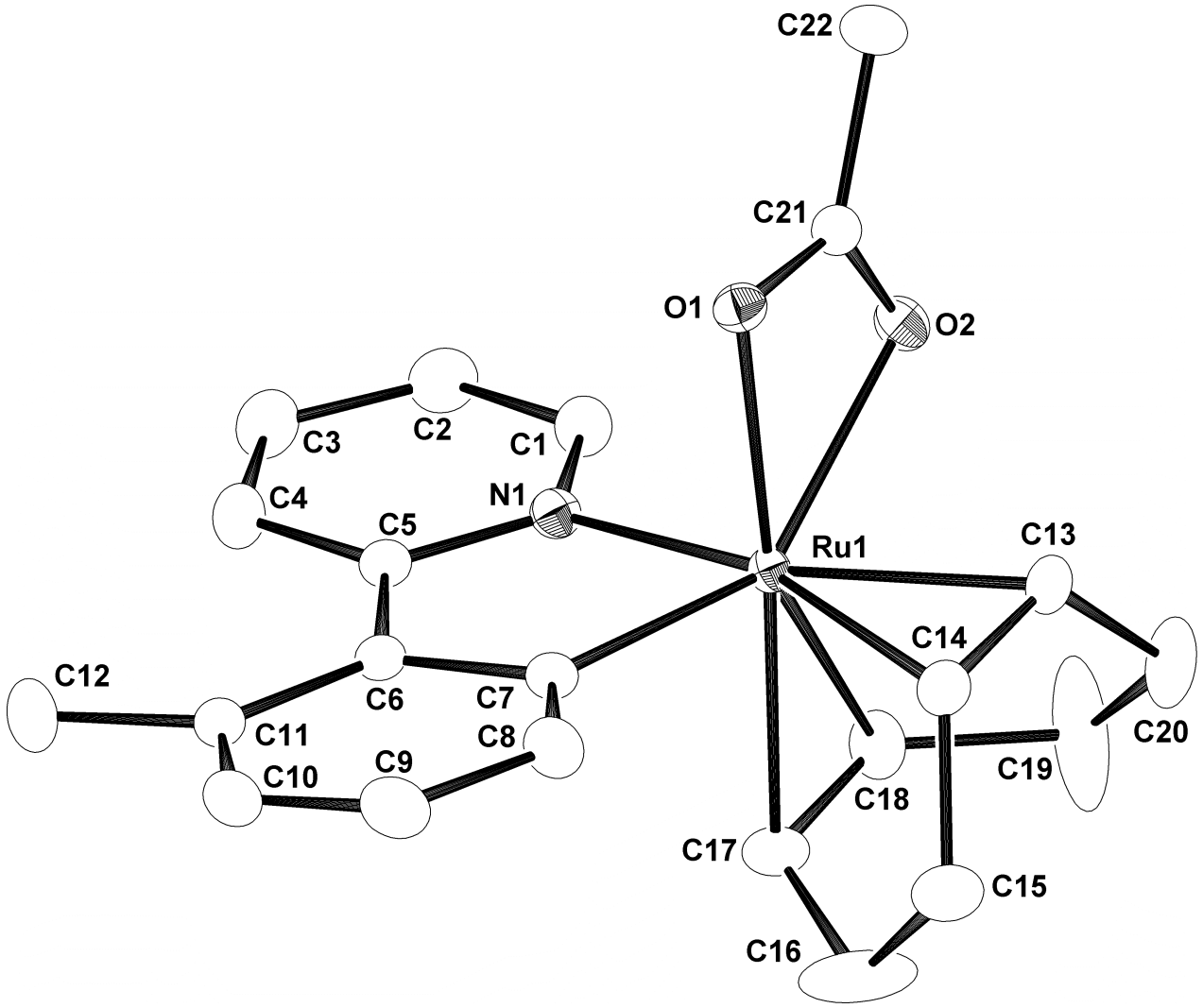


Figure S8. An ORTEP drawing of complex **38b**. Hydrogen atoms are omitted for clarity.

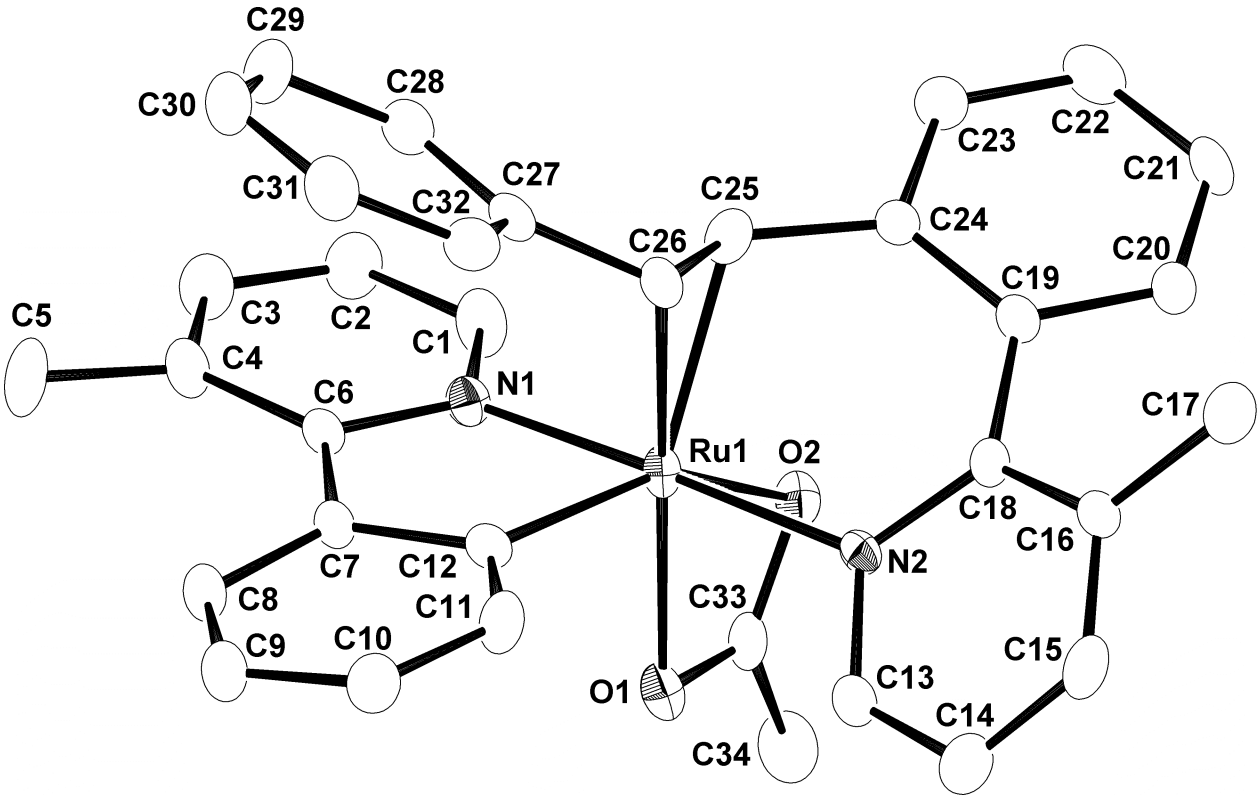


Figure S9. An ORTEP drawing of complex **39a**. Hydrogen atoms and a toluene molecule contained in the unit cell are omitted for clarity.

Table S3. Crystal data and structure refinement for **38b** and **39a**.

	38b	**39a**
Empirical formula	$C_{22}H_{25}NO_2Ru$	$C_{34}H_{30}N_2O_2Ru{\cdot}0.5C_7H_8$
Formula weight	436.50	645.74
Temperature	93(2) K	123(2) K
Crystal color, habit	Yellow, Block	Red, Platelet
Crystal dimensions	0.50 x 0.40 x 0.20 mm	0.30 x 0.20 x 0.10 mm
Crystal system	Triclinic	Triclinic
Space group	*P*-1	*P*-1
a (Å)	9.3192(12)	9.3382(9)
b (Å)	10.6453(14)	10.7006(11)
c (Å)	10.8679(14)	16.4644(15)
α (°)	108.651(4)	74.606(2)
β (°)	111.833(3)	74.799(3)
γ (°)	99.462(4)	71.863(3)
V ($Å^3$)	897.7(2)	1478.1(2)
Z	2	2
Density (calculated)	1.615 mg/mm^3	1.451 mg/mm^3
F(000)	448	666
Absorption coefficient	0.890 mm^{-1}	0.568 mm^{-1}
Theta range for data collection	3.18 to 27.49°	3.08 to 25.00°
Reflections collected	8614	10726
Independent reflections	4045 [R(int) = 0.0211]	4995 [R(int) = 0.0450]
Number of parameters	237	372
Goodness-of-fit on F^2	1.260	1.118
Final R indices [I>2sigma(I)]	R1 = 0.0306	R1 = 0.0419
	wR2 = 0.0837	wR2 = 0.0871
R indices (all data)	R1 = 0.0327	R1 = 0.0582
	wR2 = 0.0906	wR2 = 0.1010

[a] Goodness of Fit = $\{\Sigma[w\,(|F_o| - |F_c|)^2] / (N_{obs} - N_{parameters})\}^{1/2}$
[b] $R = \Sigma\,||F_o| - |F_c|| / \Sigma\,|F_o|$, $R_w = \{\Sigma[w\,(|F_o| - |F_c|)^2] / \Sigma[wF_o^2]\}^{1/2}$

Table S4. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **38b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	8926(1)	7341(1)	7357(1)	11(1)
N(1)	8785(3)	5341(2)	7233(3)	15(1)
C(1)	7425(4)	4235(3)	6227(3)	18(1)
C(2)	7264(4)	2894(3)	6146(3)	22(1)
C(3)	8544(4)	2687(3)	7151(4)	25(1)
C(4)	9941(4)	3800(3)	8155(4)	23(1)
C(5)	10073(3)	5147(3)	8188(3)	15(1)
C(6)	11452(3)	6462(3)	9200(3)	15(1)
C(7)	11176(3)	7684(3)	9016(3)	15(1)
C(8)	12368(3)	8978(3)	10034(3)	20(1)
C(9)	13811(4)	9067(3)	11144(3)	23(1)
C(10)	14095(3)	7871(4)	11253(3)	22(1)
C(11)	12940(4)	6555(3)	10315(3)	20(1)
C(12)	13385(4)	5333(4)	10583(4)	30(1)
C(13)	8202(4)	9028(3)	6809(3)	16(1)
C(14)	9842(4)	9606(3)	7836(3)	17(1)
C(15)	11191(4)	9925(3)	7411(4)	25(1)
C(16)	11506(6)	8692(4)	6596(6)	46(1)
C(17)	10454(4)	7266(3)	6256(3)	20(1)
C(18)	8804(4)	6661(3)	5240(3)	22(1)
C(19)	7819(8)	7343(6)	4377(4)	71(2)
C(20)	7592(5)	8612(4)	5180(4)	31(1)
O(1)	7811(2)	7669(2)	8821(2)	15(1)
C(21)	6372(3)	7083(3)	7761(3)	15(1)
O(2)	6189(2)	6611(2)	6464(2)	17(1)
C(22)	4909(4)	6970(3)	8058(4)	24(1)

Table S5. Bond lengths [Å] and angles [°] for **38b**.

Ru(1)-N(1)	2.069(2)	C(6)-C(7)	1.427(4)
Ru(1)-C(7)	2.073(3)	C(7)-C(8)	1.402(4)
Ru(1)-C(18)	2.131(3)	C(8)-C(9)	1.397(4)
Ru(1)-C(17)	2.170(3)	C(9)-C(10)	1.374(5)
Ru(1)-O(1)	2.1745(19)	C(10)-C(11)	1.391(5)
Ru(1)-C(13)	2.196(3)	C(11)-C(12)	1.509(4)
Ru(1)-C(14)	2.237(3)	C(13)-C(14)	1.393(4)
Ru(1)-O(2)	2.2533(19)	C(13)-C(20)	1.523(4)
Ru(1)-C(21)	2.565(3)	C(14)-C(15)	1.517(4)
N(1)-C(1)	1.357(4)	C(15)-C(16)	1.474(5)
N(1)-C(5)	1.361(4)	C(16)-C(17)	1.511(5)
C(1)-C(2)	1.382(4)	C(17)-C(18)	1.399(4)
C(2)-C(3)	1.391(5)	C(18)-C(19)	1.504(5)
C(3)-C(4)	1.378(5)	C(19)-C(20)	1.452(5)
C(4)-C(5)	1.407(4)	O(1)-C(21)	1.277(3)
C(5)-C(6)	1.481(4)	C(21)-O(2)	1.268(3)
C(6)-C(11)	1.425(4)	C(21)-C(22)	1.508(4)
N(1)-Ru(1)-C(7)	78.13(10)	C(4)-C(3)-C(2)	119.6(3)
N(1)-Ru(1)-C(18)	88.79(11)	C(3)-C(4)-C(5)	120.6(3)
C(7)-Ru(1)-C(18)	114.63(11)	N(1)-C(5)-C(4)	119.0(3)
N(1)-Ru(1)-C(17)	92.13(10)	N(1)-C(5)-C(6)	112.9(2)
C(7)-Ru(1)-C(17)	78.41(11)	C(4)-C(5)-C(6)	128.1(3)
C(18)-Ru(1)-C(17)	37.95(12)	C(11)-C(6)-C(7)	120.8(3)
N(1)-Ru(1)-O(1)	90.67(8)	C(11)-C(6)-C(5)	124.3(3)
C(7)-Ru(1)-O(1)	92.16(9)	C(7)-C(6)-C(5)	114.8(2)
C(18)-Ru(1)-O(1)	152.44(10)	C(8)-C(7)-C(6)	117.5(3)
C(17)-Ru(1)-O(1)	169.38(10)	C(8)-C(7)-Ru(1)	127.1(2)
N(1)-Ru(1)-C(13)	159.13(11)	C(6)-C(7)-Ru(1)	115.1(2)
C(7)-Ru(1)-C(13)	122.73(11)	C(9)-C(8)-C(7)	121.4(3)
C(18)-Ru(1)-C(13)	81.62(11)	C(10)-C(9)-C(8)	120.2(3)
C(17)-Ru(1)-C(13)	91.60(11)	C(9)-C(10)-C(11)	121.6(3)
O(1)-Ru(1)-C(13)	89.41(9)	C(10)-C(11)-C(6)	118.4(3)

N(1)-Ru(1)-C(14)	163.60(10)	C(10)-C(11)-C(12)	116.2(3)
C(7)-Ru(1)-C(14)	86.34(11)	C(6)-C(11)-C(12)	125.4(3)
C(18)-Ru(1)-C(14)	92.97(12)	C(14)-C(13)-C(20)	124.4(3)
C(17)-Ru(1)-C(14)	79.48(11)	C(14)-C(13)-Ru(1)	73.32(16)
O(1)-Ru(1)-C(14)	95.20(9)	C(20)-C(13)-Ru(1)	109.61(19)
C(13)-Ru(1)-C(14)	36.63(10)	C(13)-C(14)-C(15)	121.7(3)
N(1)-Ru(1)-O(2)	85.78(8)	C(13)-C(14)-Ru(1)	70.06(16)
C(7)-Ru(1)-O(2)	147.31(9)	C(15)-C(14)-Ru(1)	112.68(19)
C(18)-Ru(1)-O(2)	93.02(10)	C(16)-C(15)-C(14)	115.3(3)
C(17)-Ru(1)-O(2)	130.97(10)	C(15)-C(16)-C(17)	117.4(3)
O(1)-Ru(1)-O(2)	59.47(7)	C(18)-C(17)-C(16)	123.9(3)
C(13)-Ru(1)-O(2)	76.32(9)	C(18)-C(17)-Ru(1)	69.53(16)
C(14)-Ru(1)-O(2)	110.39(9)	C(16)-C(17)-Ru(1)	113.8(2)
N(1)-Ru(1)-C(21)	87.94(9)	C(17)-C(18)-C(19)	125.3(4)
C(7)-Ru(1)-C(21)	120.51(10)	C(17)-C(18)-Ru(1)	72.53(16)
C(18)-Ru(1)-C(21)	122.64(11)	C(19)-C(18)-Ru(1)	110.7(2)
C(17)-Ru(1)-C(21)	160.54(11)	C(20)-C(19)-C(18)	117.6(3)
O(1)-Ru(1)-C(21)	29.84(8)	C(19)-C(20)-C(13)	116.3(3)
C(13)-Ru(1)-C(21)	81.82(10)	C(21)-O(1)-Ru(1)	92.25(16)
C(14)-Ru(1)-C(21)	104.68(9)	O(2)-C(21)-O(1)	119.4(2)
O(2)-Ru(1)-C(21)	29.63(8)	O(2)-C(21)-C(22)	120.6(3)
C(1)-N(1)-C(5)	120.2(2)	O(1)-C(21)-C(22)	120.0(3)
C(1)-N(1)-Ru(1)	120.81(19)	O(2)-C(21)-Ru(1)	61.45(14)
C(5)-N(1)-Ru(1)	119.01(19)	O(1)-C(21)-Ru(1)	57.91(13)
N(1)-C(1)-C(2)	122.4(3)	C(22)-C(21)-Ru(1)	177.8(2)
C(1)-C(2)-C(3)	118.1(3)	C(21)-O(2)-Ru(1)	88.91(16)

Table S6. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **38b**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	11(1)	11(1)	10(1)	4(1)	4(1)	3(1)
N(1)	16(1)	13(1)	16(1)	6(1)	8(1)	6(1)
C(1)	19(1)	16(1)	15(1)	5(1)	6(1)	4(1)
C(2)	26(2)	15(1)	21(1)	3(1)	11(1)	3(1)
C(3)	32(2)	16(1)	32(2)	12(1)	17(1)	10(1)
C(4)	27(2)	22(2)	29(2)	16(1)	14(1)	13(1)
C(5)	18(1)	17(1)	15(1)	7(1)	10(1)	7(1)
C(6)	14(1)	20(1)	13(1)	8(1)	7(1)	5(1)
C(7)	13(1)	20(1)	12(1)	6(1)	6(1)	5(1)
C(8)	17(1)	19(1)	17(1)	4(1)	5(1)	4(1)
C(9)	15(1)	27(2)	16(1)	3(1)	3(1)	1(1)
C(10)	13(1)	35(2)	13(1)	11(1)	3(1)	7(1)
C(11)	17(1)	31(2)	21(1)	17(1)	11(1)	11(1)
C(12)	21(2)	38(2)	35(2)	25(2)	7(1)	13(1)
C(13)	21(1)	14(1)	16(1)	8(1)	8(1)	7(1)
C(14)	20(1)	12(1)	21(1)	7(1)	11(1)	6(1)
C(15)	24(2)	22(2)	33(2)	12(1)	17(1)	5(1)
C(16)	56(3)	24(2)	73(3)	11(2)	55(3)	5(2)
C(17)	24(1)	21(1)	21(1)	7(1)	16(1)	8(1)
C(18)	30(2)	27(2)	12(1)	7(1)	11(1)	17(1)
C(19)	122(5)	90(4)	14(2)	21(2)	21(2)	88(4)
C(20)	46(2)	32(2)	18(2)	14(1)	11(1)	21(2)
O(1)	16(1)	15(1)	14(1)	6(1)	7(1)	4(1)
C(21)	15(1)	13(1)	19(1)	8(1)	8(1)	4(1)
O(2)	13(1)	17(1)	16(1)	5(1)	5(1)	4(1)
C(22)	18(1)	28(2)	30(2)	14(1)	15(1)	8(1)

Table S7. Torsion angles [°] for **38b**.

C(7)-Ru(1)-N(1)-C(1)	179.8(2)	C(17)-Ru(1)-C(14)-C(15)	-9.7(2)
C(18)-Ru(1)-N(1)-C(1)	-64.8(2)	O(1)-Ru(1)-C(14)-C(15)	161.0(2)
C(17)-Ru(1)-N(1)-C(1)	-102.6(2)	C(13)-Ru(1)-C(14)-C(15)	-117.0(3)
O(1)-Ru(1)-N(1)-C(1)	87.7(2)	O(2)-Ru(1)-C(14)-C(15)	-139.7(2)
C(13)-Ru(1)-N(1)-C(1)	-2.4(4)	C(21)-Ru(1)-C(14)-C(15)	-170.2(2)
C(14)-Ru(1)-N(1)-C(1)	-161.2(3)	C(13)-C(14)-C(15)-C(16)	-72.1(4)
O(2)-Ru(1)-N(1)-C(1)	28.4(2)	Ru(1)-C(14)-C(15)-C(16)	7.7(4)
C(21)-Ru(1)-N(1)-C(1)	58.0(2)	C(14)-C(15)-C(16)-C(17)	0.9(6)
C(7)-Ru(1)-N(1)-C(5)	0.33(19)	C(15)-C(16)-C(17)-C(18)	71.1(5)
C(18)-Ru(1)-N(1)-C(5)	115.8(2)	C(15)-C(16)-C(17)-Ru(1)	-9.4(5)
C(17)-Ru(1)-N(1)-C(5)	78.0(2)	N(1)-Ru(1)-C(17)-C(18)	85.30(19)
O(1)-Ru(1)-N(1)-C(5)	-91.7(2)	C(7)-Ru(1)-C(17)-C(18)	162.7(2)
C(13)-Ru(1)-N(1)-C(5)	178.2(2)	O(1)-Ru(1)-C(17)-C(18)	-169.5(4)
C(14)-Ru(1)-N(1)-C(5)	19.4(4)	C(13)-Ru(1)-C(17)-C(18)	-74.15(19)
O(2)-Ru(1)-N(1)-C(5)	-151.1(2)	C(14)-Ru(1)-C(17)-C(18)	-108.9(2)
C(21)-Ru(1)-N(1)-C(5)	-121.5(2)	O(2)-Ru(1)-C(17)-C(18)	-0.9(2)
C(5)-N(1)-C(1)-C(2)	1.8(4)	C(21)-Ru(1)-C(17)-C(18)	-4.5(4)
Ru(1)-N(1)-C(1)-C(2)	-177.6(2)	N(1)-Ru(1)-C(17)-C(16)	-155.6(3)
N(1)-C(1)-C(2)-C(3)	0.8(4)	C(7)-Ru(1)-C(17)-C(16)	-78.2(3)
C(1)-C(2)-C(3)-C(4)	-2.2(5)	C(18)-Ru(1)-C(17)-C(16)	119.1(4)
C(2)-C(3)-C(4)-C(5)	1.1(5)	O(1)-Ru(1)-C(17)-C(16)	-50.5(7)
C(1)-N(1)-C(5)-C(4)	-2.9(4)	C(13)-Ru(1)-C(17)-C(16)	44.9(3)
Ru(1)-N(1)-C(5)-C(4)	176.6(2)	C(14)-Ru(1)-C(17)-C(16)	10.2(3)
C(1)-N(1)-C(5)-C(6)	179.7(2)	O(2)-Ru(1)-C(17)-C(16)	118.1(3)
Ru(1)-N(1)-C(5)-C(6)	-0.9(3)	C(21)-Ru(1)-C(17)-C(16)	114.6(4)
C(3)-C(4)-C(5)-N(1)	1.4(4)	C(16)-C(17)-C(18)-C(19)	-2.1(5)
C(3)-C(4)-C(5)-C(6)	178.5(3)	Ru(1)-C(17)-C(18)-C(19)	103.4(3)
N(1)-C(5)-C(6)-C(11)	179.3(2)	C(16)-C(17)-C(18)-Ru(1)	-105.5(3)
C(4)-C(5)-C(6)-C(11)	2.1(4)	N(1)-Ru(1)-C(18)-C(17)	-95.01(19)
N(1)-C(5)-C(6)-C(7)	1.1(3)	C(7)-Ru(1)-C(18)-C(17)	-18.7(2)
C(4)-C(5)-C(6)-C(7)	-176.0(3)	O(1)-Ru(1)-C(18)-C(17)	175.85(18)
C(11)-C(6)-C(7)-C(8)	-4.4(4)	C(13)-Ru(1)-C(18)-C(17)	103.59(19)
C(5)-C(6)-C(7)-C(8)	173.8(2)	C(14)-Ru(1)-C(18)-C(17)	68.67(19)

C(11)-C(6)-C(7)-Ru(1)	-179.1(2)	O(2)-Ru(1)-C(18)-C(17)	179.28(18)
C(5)-C(6)-C(7)-Ru(1)	-0.9(3)	C(21)-Ru(1)-C(18)-C(17)	178.21(16)
N(1)-Ru(1)-C(7)-C(8)	-173.8(3)	N(1)-Ru(1)-C(18)-C(19)	143.1(4)
C(18)-Ru(1)-C(7)-C(8)	103.1(3)	C(7)-Ru(1)-C(18)-C(19)	-140.6(4)
C(17)-Ru(1)-C(7)-C(8)	91.5(3)	C(17)-Ru(1)-C(18)-C(19)	-121.9(4)
O(1)-Ru(1)-C(7)-C(8)	-83.5(2)	O(1)-Ru(1)-C(18)-C(19)	53.9(5)
C(13)-Ru(1)-C(7)-C(8)	7.2(3)	C(13)-Ru(1)-C(18)-C(19)	-18.3(4)
C(14)-Ru(1)-C(7)-C(8)	11.5(3)	C(14)-Ru(1)-C(18)-C(19)	-53.2(4)
O(2)-Ru(1)-C(7)-C(8)	-111.6(3)	O(2)-Ru(1)-C(18)-C(19)	57.4(4)
C(21)-Ru(1)-C(7)-C(8)	-93.4(3)	C(21)-Ru(1)-C(18)-C(19)	56.3(4)
N(1)-Ru(1)-C(7)-C(6)	0.34(19)	C(17)-C(18)-C(19)-C(20)	-63.1(7)
C(18)-Ru(1)-C(7)-C(6)	-82.8(2)	Ru(1)-C(18)-C(19)-C(20)	19.7(7)
C(17)-Ru(1)-C(7)-C(6)	-94.4(2)	C(18)-C(19)-C(20)-C(13)	-7.2(8)
O(1)-Ru(1)-C(7)-C(6)	90.57(19)	C(14)-C(13)-C(20)-C(19)	74.4(5)
C(13)-Ru(1)-C(7)-C(6)	-178.74(18)	Ru(1)-C(13)-C(20)-C(19)	-8.4(5)
C(14)-Ru(1)-C(7)-C(6)	-174.4(2)	N(1)-Ru(1)-O(1)-C(21)	-84.67(17)
O(2)-Ru(1)-C(7)-C(6)	62.5(3)	C(7)-Ru(1)-O(1)-C(21)	-162.82(17)
C(21)-Ru(1)-C(7)-C(6)	80.7(2)	C(18)-Ru(1)-O(1)-C(21)	4.0(3)
C(6)-C(7)-C(8)-C(9)	3.2(4)	C(17)-Ru(1)-O(1)-C(21)	170.0(5)
Ru(1)-C(7)-C(8)-C(9)	177.1(2)	C(13)-Ru(1)-O(1)-C(21)	74.45(17)
C(7)-C(8)-C(9)-C(10)	0.4(5)	C(14)-Ru(1)-O(1)-C(21)	110.66(17)
C(8)-C(9)-C(10)-C(11)	-2.8(5)	O(2)-Ru(1)-O(1)-C(21)	0.03(15)
C(9)-C(10)-C(11)-C(6)	1.5(4)	Ru(1)-O(1)-C(21)-O(2)	0.0(3)
C(9)-C(10)-C(11)-C(12)	-178.2(3)	Ru(1)-O(1)-C(21)-C(22)	-179.4(2)
C(7)-C(6)-C(11)-C(10)	2.2(4)	N(1)-Ru(1)-C(21)-O(2)	-85.09(16)
C(5)-C(6)-C(11)-C(10)	-175.9(3)	C(7)-Ru(1)-C(21)-O(2)	-160.00(16)
C(7)-C(6)-C(11)-C(12)	-178.1(3)	C(18)-Ru(1)-C(21)-O(2)	2.2(2)
C(5)-C(6)-C(11)-C(12)	3.8(4)	C(17)-Ru(1)-C(21)-O(2)	5.5(4)
N(1)-Ru(1)-C(13)-C(14)	-170.1(2)	O(1)-Ru(1)-C(21)-O(2)	180.0(3)
C(7)-Ru(1)-C(13)-C(14)	7.3(2)	C(13)-Ru(1)-C(21)-O(2)	76.67(17)
C(18)-Ru(1)-C(13)-C(14)	-106.61(18)	C(14)-Ru(1)-C(21)-O(2)	105.53(17)
C(17)-Ru(1)-C(13)-C(14)	-69.89(18)	N(1)-Ru(1)-C(21)-O(1)	94.96(16)
O(1)-Ru(1)-C(13)-C(14)	99.53(17)	C(7)-Ru(1)-C(21)-O(1)	20.0(2)
O(2)-Ru(1)-C(13)-C(14)	158.18(18)	C(18)-Ru(1)-C(21)-O(1)	-177.80(16)
C(21)-Ru(1)-C(13)-C(14)	128.50(17)	C(17)-Ru(1)-C(21)-O(1)	-174.5(3)

N(1)-Ru(1)-C(13)-C(20)	-48.8(4)	C(13)-Ru(1)-C(21)-O(1)	-103.28(17)
C(7)-Ru(1)-C(13)-C(20)	128.7(2)	C(14)-Ru(1)-C(21)-O(1)	-74.43(17)
C(18)-Ru(1)-C(13)-C(20)	14.7(2)	O(2)-Ru(1)-C(21)-O(1)	-180.0(3)
C(17)-Ru(1)-C(13)-C(20)	51.4(2)	N(1)-Ru(1)-C(21)-C(22)	109(6)
O(1)-Ru(1)-C(13)-C(20)	-139.2(2)	C(7)-Ru(1)-C(21)-C(22)	34(6)
C(14)-Ru(1)-C(13)-C(20)	121.3(3)	C(18)-Ru(1)-C(21)-C(22)	-163(6)
O(2)-Ru(1)-C(13)-C(20)	-80.5(2)	C(17)-Ru(1)-C(21)-C(22)	-160(5)
C(21)-Ru(1)-C(13)-C(20)	-110.2(2)	O(1)-Ru(1)-C(21)-C(22)	14(5)
C(20)-C(13)-C(14)-C(15)	2.3(4)	C(13)-Ru(1)-C(21)-C(22)	-89(6)
Ru(1)-C(13)-C(14)-C(15)	104.9(3)	C(14)-Ru(1)-C(21)-C(22)	-60(6)
C(20)-C(13)-C(14)-Ru(1)	-102.7(3)	O(2)-Ru(1)-C(21)-C(22)	-166(6)
N(1)-Ru(1)-C(14)-C(13)	167.5(3)	O(1)-C(21)-O(2)-Ru(1)	0.0(3)
C(7)-Ru(1)-C(14)-C(13)	-173.82(18)	C(22)-C(21)-O(2)-Ru(1)	179.4(2)
C(18)-Ru(1)-C(14)-C(13)	71.67(18)	N(1)-Ru(1)-O(2)-C(21)	93.25(17)
C(17)-Ru(1)-C(14)-C(13)	107.31(18)	C(7)-Ru(1)-O(2)-C(21)	33.1(3)
O(1)-Ru(1)-C(14)-C(13)	-81.98(17)	C(18)-Ru(1)-O(2)-C(21)	-178.18(17)
O(2)-Ru(1)-C(14)-C(13)	-22.66(18)	C(17)-Ru(1)-O(2)-C(21)	-177.60(17)
C(21)-Ru(1)-C(14)-C(13)	-53.21(18)	O(1)-Ru(1)-O(2)-C(21)	-0.03(15)
N(1)-Ru(1)-C(14)-C(15)	50.4(4)	C(13)-Ru(1)-O(2)-C(21)	-97.57(17)
C(7)-Ru(1)-C(14)-C(15)	69.1(2)	C(14)-Ru(1)-O(2)-C(21)	-83.89(17)
C(18)-Ru(1)-C(14)-C(15)	-45.4(2)		

Table S8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **39a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	5478(1)	3942(1)	2453(1)	15(1)
N(1)	4047(4)	3409(3)	1938(2)	17(1)
C(1)	2660(5)	3266(5)	2394(3)	23(1)
C(2)	1719(5)	2827(5)	2084(3)	26(1)
C(3)	2245(5)	2494(5)	1280(3)	27(1)
C(4)	3645(5)	2641(4)	787(3)	22(1)
C(5)	4177(6)	2176(6)	-51(3)	39(1)
C(6)	4540(5)	3165(4)	1123(2)	16(1)
C(7)	6042(5)	3437(4)	726(2)	16(1)
C(8)	6726(5)	3467(4)	-148(3)	20(1)
C(9)	8179(5)	3663(4)	-461(3)	23(1)
C(10)	8978(5)	3835(4)	90(3)	24(1)
C(11)	8279(5)	3866(4)	938(3)	20(1)
C(12)	6812(5)	3709(4)	1277(3)	18(1)
N(2)	6935(4)	4558(3)	2959(2)	15(1)
C(13)	7591(5)	5516(4)	2438(3)	18(1)
C(14)	8715(5)	5905(5)	2634(3)	22(1)
C(15)	9237(5)	5232(4)	3384(3)	21(1)
C(16)	8569(5)	4258(4)	3950(3)	18(1)
C(17)	9249(5)	3522(5)	4745(3)	24(1)
C(18)	7306(5)	4011(4)	3754(2)	15(1)
C(19)	6269(5)	3265(4)	4413(2)	16(1)
C(20)	5947(5)	3477(4)	5257(3)	18(1)
C(21)	4896(5)	2929(4)	5902(3)	22(1)
C(22)	4094(5)	2198(5)	5718(3)	28(1)
C(23)	4349(5)	1997(4)	4901(3)	23(1)
C(24)	5433(5)	2496(4)	4230(3)	17(1)
C(25)	5610(5)	2168(4)	3391(3)	21(1)
C(26)	6990(5)	1934(4)	2775(3)	19(1)
C(27)	7374(5)	947(4)	2218(3)	20(1)
C(28)	6303(5)	341(4)	2122(3)	23(1)

C(29)	6728(6)	-559(5)	1576(3)	28(1)
C(30)	8235(6)	-885(5)	1111(3)	28(1)
C(31)	9290(6)	-319(5)	1217(3)	27(1)
C(32)	8871(5)	581(4)	1763(3)	23(1)
O(1)	4466(3)	6035(3)	1983(2)	21(1)
C(33)	3429(5)	6163(4)	2648(3)	19(1)
O(2)	3380(3)	5158(3)	3274(2)	21(1)
C(34)	2250(6)	7485(5)	2695(3)	31(1)
C(35)	-2390(14)	-180(13)	6166(8)	52(3)
C(36)	-992(6)	-63(8)	5480(4)	37(2)
C(37)	319(8)	-112(8)	5749(4)	36(3)
C(38)	1665(6)	-28(8)	5151(6)	50(3)
C(39)	1700(7)	104(9)	4284(5)	59(4)
C(40)	388(9)	152(8)	4014(3)	47(3)
C(41)	-958(7)	69(7)	4613(4)	20(2)

Table S9. Bond lengths [Å] and angles [°] for **39a**.

Ru(1)-N(1)	2.039(3)	C(13)-C(14)	1.379(6)
Ru(1)-C(12)	2.040(4)	C(14)-C(15)	1.380(6)
Ru(1)-C(25)	2.098(4)	C(15)-C(16)	1.389(6)
Ru(1)-N(2)	2.103(3)	C(16)-C(18)	1.416(6)
Ru(1)-O(1)	2.157(3)	C(16)-C(17)	1.521(6)
Ru(1)-C(26)	2.188(4)	C(18)-C(19)	1.491(6)
Ru(1)-O(2)	2.306(3)	C(19)-C(20)	1.406(6)
Ru(1)-C(33)	2.581(4)	C(19)-C(24)	1.425(6)
N(1)-C(1)	1.348(5)	C(20)-C(21)	1.384(6)
N(1)-C(6)	1.366(5)	C(21)-C(22)	1.370(6)
C(1)-C(2)	1.368(6)	C(22)-C(23)	1.366(6)
C(2)-C(3)	1.387(6)	C(23)-C(24)	1.403(6)
C(3)-C(4)	1.377(6)	C(24)-C(25)	1.470(6)
C(4)-C(6)	1.420(6)	C(25)-C(26)	1.415(6)
C(4)-C(5)	1.500(6)	C(26)-C(27)	1.481(6)
C(6)-C(7)	1.467(6)	C(27)-C(32)	1.390(6)
C(7)-C(8)	1.409(6)	C(27)-C(28)	1.409(6)
C(7)-C(12)	1.428(6)	C(28)-C(29)	1.388(6)
C(8)-C(9)	1.380(6)	C(29)-C(30)	1.400(7)
C(9)-C(10)	1.394(6)	C(30)-C(31)	1.374(7)
C(10)-C(11)	1.382(6)	C(31)-C(32)	1.389(6)
C(11)-C(12)	1.381(6)	O(1)-C(33)	1.264(5)
N(2)-C(13)	1.346(5)	C(33)-O(2)	1.280(5)
N(2)-C(18)	1.370(5)	C(33)-C(34)	1.505(6)
N(1)-Ru(1)-C(12)	79.58(15)	C(11)-C(12)-C(7)	117.4(4)
N(1)-Ru(1)-C(25)	89.97(15)	C(11)-C(12)-Ru(1)	129.1(3)
C(12)-Ru(1)-C(25)	114.78(16)	C(7)-C(12)-Ru(1)	113.4(3)
N(1)-Ru(1)-N(2)	178.06(14)	C(13)-N(2)-C(18)	118.9(3)
C(12)-Ru(1)-N(2)	100.01(15)	C(13)-N(2)-Ru(1)	116.4(3)
C(25)-Ru(1)-N(2)	91.92(15)	C(18)-N(2)-Ru(1)	124.7(3)
N(1)-Ru(1)-O(1)	90.33(12)	N(2)-C(13)-C(14)	123.2(4)
C(12)-Ru(1)-O(1)	92.16(13)	C(13)-C(14)-C(15)	118.0(4)

C(25)-Ru(1)-O(1)	152.63(14)	C(14)-C(15)-C(16)	120.7(4)
N(2)-Ru(1)-O(1)	87.80(12)	C(15)-C(16)-C(18)	118.3(4)
N(1)-Ru(1)-C(26)	97.27(15)	C(15)-C(16)-C(17)	117.5(4)
C(12)-Ru(1)-C(26)	79.01(15)	C(18)-C(16)-C(17)	124.2(4)
C(25)-Ru(1)-C(26)	38.47(16)	N(2)-C(18)-C(16)	119.8(3)
N(2)-Ru(1)-C(26)	84.49(15)	N(2)-C(18)-C(19)	118.1(3)
O(1)-Ru(1)-C(26)	167.06(13)	C(16)-C(18)-C(19)	121.8(3)
N(1)-Ru(1)-O(2)	89.97(12)	C(20)-C(19)-C(24)	117.7(4)
C(12)-Ru(1)-O(2)	149.36(13)	C(20)-C(19)-C(18)	117.2(4)
C(25)-Ru(1)-O(2)	93.74(14)	C(24)-C(19)-C(18)	124.6(4)
N(2)-Ru(1)-O(2)	89.47(12)	C(21)-C(20)-C(19)	122.0(4)
O(1)-Ru(1)-O(2)	58.90(10)	C(22)-C(21)-C(20)	119.8(4)
C(26)-Ru(1)-O(2)	131.21(13)	C(23)-C(22)-C(21)	119.9(4)
N(1)-Ru(1)-C(33)	89.86(13)	C(22)-C(23)-C(24)	122.5(4)
C(12)-Ru(1)-C(33)	120.75(15)	C(23)-C(24)-C(19)	118.1(4)
C(25)-Ru(1)-C(33)	123.42(15)	C(23)-C(24)-C(25)	116.3(4)
N(2)-Ru(1)-C(33)	88.74(13)	C(19)-C(24)-C(25)	125.6(4)
O(1)-Ru(1)-C(33)	29.22(12)	C(26)-C(25)-C(24)	126.0(4)
C(26)-Ru(1)-C(33)	160.03(14)	C(26)-C(25)-Ru(1)	74.2(2)
O(2)-Ru(1)-C(33)	29.69(11)	C(24)-C(25)-Ru(1)	108.6(3)
C(1)-N(1)-C(6)	120.4(4)	C(25)-C(26)-C(27)	123.1(4)
C(1)-N(1)-Ru(1)	121.1(3)	C(25)-C(26)-Ru(1)	67.3(2)
C(6)-N(1)-Ru(1)	118.4(3)	C(27)-C(26)-Ru(1)	121.0(3)
N(1)-C(1)-C(2)	122.3(4)	C(32)-C(27)-C(28)	117.4(4)
C(1)-C(2)-C(3)	117.9(4)	C(32)-C(27)-C(26)	118.9(4)
C(4)-C(3)-C(2)	121.7(4)	C(28)-C(27)-C(26)	123.6(4)
C(3)-C(4)-C(6)	117.9(4)	C(29)-C(28)-C(27)	120.8(4)
C(3)-C(4)-C(5)	118.4(4)	C(28)-C(29)-C(30)	120.5(4)
C(6)-C(4)-C(5)	123.6(4)	C(31)-C(30)-C(29)	118.8(4)
N(1)-C(6)-C(4)	119.5(4)	C(30)-C(31)-C(32)	120.9(5)
N(1)-C(6)-C(7)	111.8(3)	C(31)-C(32)-C(27)	121.5(4)
C(4)-C(6)-C(7)	128.6(4)	C(33)-O(1)-Ru(1)	94.4(2)
C(8)-C(7)-C(12)	119.7(4)	O(1)-C(33)-O(2)	119.6(4)
C(8)-C(7)-C(6)	124.2(4)	O(1)-C(33)-C(34)	120.0(4)
C(12)-C(7)-C(6)	116.1(3)	O(2)-C(33)-C(34)	120.4(4)

C(9)-C(8)-C(7)	120.5(4)	O(1)-C(33)-Ru(1)	56.4(2)
C(8)-C(9)-C(10)	119.9(4)	O(2)-C(33)-Ru(1)	63.2(2)
C(11)-C(10)-C(9)	119.5(4)	C(34)-C(33)-Ru(1)	176.1(3)
C(12)-C(11)-C(10)	122.8(4)	C(33)-O(2)-Ru(1)	87.1(2)

Table S10. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **39a**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	13(1)	21(1)	13(1)	-7(1)	-2(1)	-4(1)
N(1)	16(2)	20(2)	15(2)	-4(2)	-3(1)	-4(2)
C(1)	12(2)	39(3)	18(2)	-11(2)	4(2)	-8(2)
C(2)	17(3)	37(3)	29(3)	-9(2)	-4(2)	-10(2)
C(3)	21(3)	37(3)	29(3)	-6(2)	-11(2)	-12(2)
C(4)	22(3)	29(2)	18(2)	-4(2)	-9(2)	-7(2)
C(5)	49(4)	63(4)	27(3)	-17(3)	-4(2)	-39(3)
C(6)	19(2)	17(2)	13(2)	-2(2)	-4(2)	-4(2)
C(7)	16(2)	18(2)	12(2)	-4(2)	-3(2)	-3(2)
C(8)	20(2)	26(2)	17(2)	-6(2)	-5(2)	-6(2)
C(9)	24(3)	30(3)	17(2)	-9(2)	-1(2)	-8(2)
C(10)	24(3)	27(3)	22(2)	-9(2)	1(2)	-7(2)
C(11)	12(2)	27(2)	23(2)	-12(2)	-4(2)	-4(2)
C(12)	21(2)	15(2)	16(2)	-1(2)	-7(2)	-3(2)
N(2)	17(2)	18(2)	10(2)	-2(1)	0(1)	-6(2)
C(13)	20(2)	20(2)	14(2)	-5(2)	-2(2)	-3(2)
C(14)	15(2)	28(2)	26(2)	-11(2)	0(2)	-7(2)
C(15)	13(2)	27(2)	27(2)	-13(2)	-7(2)	-4(2)
C(16)	23(3)	16(2)	14(2)	-3(2)	-5(2)	-2(2)
C(17)	21(3)	27(2)	28(2)	-7(2)	-10(2)	-6(2)
C(18)	15(2)	16(2)	14(2)	-6(2)	-2(2)	-2(2)
C(19)	16(2)	15(2)	14(2)	-3(2)	-5(2)	1(2)
C(20)	18(2)	16(2)	19(2)	-5(2)	-9(2)	2(2)
C(21)	28(3)	25(2)	11(2)	-5(2)	-3(2)	-1(2)
C(22)	25(3)	35(3)	19(2)	-1(2)	2(2)	-12(2)
C(23)	24(3)	27(2)	21(2)	-3(2)	-4(2)	-12(2)
C(24)	21(2)	14(2)	16(2)	-2(2)	-7(2)	-2(2)
C(25)	21(3)	23(2)	24(2)	-8(2)	-6(2)	-8(2)
C(26)	20(2)	23(2)	14(2)	-2(2)	-6(2)	-8(2)
C(27)	24(3)	20(2)	13(2)	1(2)	-6(2)	-5(2)
C(28)	26(3)	22(2)	19(2)	-5(2)	-4(2)	-3(2)

C(29)	33(3)	28(3)	29(3)	-11(2)	-12(2)	-7(2)
C(30)	40(3)	23(2)	21(2)	-10(2)	-10(2)	0(2)
C(31)	27(3)	27(3)	22(2)	-9(2)	-4(2)	2(2)
C(32)	23(3)	21(2)	23(2)	-3(2)	-5(2)	-4(2)
O(1)	22(2)	27(2)	14(2)	-5(1)	-4(1)	-6(1)
C(33)	19(2)	24(2)	18(2)	-7(2)	-9(2)	-5(2)
O(2)	23(2)	24(2)	18(2)	-7(1)	-5(1)	-5(1)
C(34)	28(3)	32(3)	30(3)	-10(2)	-9(2)	3(2)

Table S11. Torsion angles [°] for **39a**.

C(12)-Ru(1)-N(1)-C(1)	178.0(4)	C(18)-C(19)-C(20)-C(21)	174.3(4)
C(25)-Ru(1)-N(1)-C(1)	62.7(3)	C(19)-C(20)-C(21)-C(22)	-2.5(6)
N(2)-Ru(1)-N(1)-C(1)	-104(4)	C(20)-C(21)-C(22)-C(23)	0.9(7)
O(1)-Ru(1)-N(1)-C(1)	-89.9(3)	C(21)-C(22)-C(23)-C(24)	1.1(7)
C(26)-Ru(1)-N(1)-C(1)	100.6(3)	C(22)-C(23)-C(24)-C(19)	-1.4(7)
O(2)-Ru(1)-N(1)-C(1)	-31.0(3)	C(22)-C(23)-C(24)-C(25)	178.4(4)
C(33)-Ru(1)-N(1)-C(1)	-60.7(3)	C(20)-C(19)-C(24)-C(23)	-0.2(6)
C(12)-Ru(1)-N(1)-C(6)	-0.4(3)	C(18)-C(19)-C(24)-C(23)	-171.7(4)
C(25)-Ru(1)-N(1)-C(6)	-115.6(3)	C(20)-C(19)-C(24)-C(25)	-179.9(4)
N(2)-Ru(1)-N(1)-C(6)	77(4)	C(18)-C(19)-C(24)-C(25)	8.6(7)
O(1)-Ru(1)-N(1)-C(6)	91.8(3)	C(23)-C(24)-C(25)-C(26)	-146.3(4)
C(26)-Ru(1)-N(1)-C(6)	-77.7(3)	C(19)-C(24)-C(25)-C(26)	33.4(7)
O(2)-Ru(1)-N(1)-C(6)	150.7(3)	C(23)-C(24)-C(25)-Ru(1)	130.0(3)
C(33)-Ru(1)-N(1)-C(6)	121.0(3)	C(19)-C(24)-C(25)-Ru(1)	-50.3(5)
C(6)-N(1)-C(1)-C(2)	2.6(7)	N(1)-Ru(1)-C(25)-C(26)	101.8(3)
Ru(1)-N(1)-C(1)-C(2)	-175.7(3)	C(12)-Ru(1)-C(25)-C(26)	23.3(3)
N(1)-C(1)-C(2)-C(3)	1.5(7)	N(2)-Ru(1)-C(25)-C(26)	-78.7(3)
C(1)-C(2)-C(3)-C(4)	-2.3(7)	O(1)-Ru(1)-C(25)-C(26)	-167.6(3)
C(2)-C(3)-C(4)-C(6)	-0.8(7)	O(2)-Ru(1)-C(25)-C(26)	-168.3(2)
C(2)-C(3)-C(4)-C(5)	176.2(5)	C(33)-Ru(1)-C(25)-C(26)	-168.4(2)
C(1)-N(1)-C(6)-C(4)	-5.7(6)	N(1)-Ru(1)-C(25)-C(24)	-134.9(3)
Ru(1)-N(1)-C(6)-C(4)	172.6(3)	C(12)-Ru(1)-C(25)-C(24)	146.7(3)
C(1)-N(1)-C(6)-C(7)	177.4(4)	N(2)-Ru(1)-C(25)-C(24)	44.7(3)
Ru(1)-N(1)-C(6)-C(7)	-4.2(4)	O(1)-Ru(1)-C(25)-C(24)	-44.2(5)
C(3)-C(4)-C(6)-N(1)	4.8(6)	C(26)-Ru(1)-C(25)-C(24)	123.4(4)
C(5)-C(4)-C(6)-N(1)	-172.0(4)	O(2)-Ru(1)-C(25)-C(24)	-44.9(3)
C(3)-C(4)-C(6)-C(7)	-178.9(4)	C(33)-Ru(1)-C(25)-C(24)	-45.0(4)
C(5)-C(4)-C(6)-C(7)	4.3(7)	C(24)-C(25)-C(26)-C(27)	145.0(4)
N(1)-C(6)-C(7)-C(8)	-170.2(4)	Ru(1)-C(25)-C(26)-C(27)	-113.2(4)
C(4)-C(6)-C(7)-C(8)	13.4(7)	C(24)-C(25)-C(26)-Ru(1)	-101.8(4)
N(1)-C(6)-C(7)-C(12)	8.6(5)	N(1)-Ru(1)-C(26)-C(25)	-80.7(3)
C(4)-C(6)-C(7)-C(12)	-167.9(4)	C(12)-Ru(1)-C(26)-C(25)	-158.6(3)
C(12)-C(7)-C(8)-C(9)	4.6(6)	N(2)-Ru(1)-C(26)-C(25)	100.1(3)

C(6)-C(7)-C(8)-C(9)	-176.7(4)	O(1)-Ru(1)-C(26)-C(25)	153.8(5)
C(7)-C(8)-C(9)-C(10)	-0.1(7)	O(2)-Ru(1)-C(26)-C(25)	15.7(3)
C(8)-C(9)-C(10)-C(11)	-2.8(7)	C(33)-Ru(1)-C(26)-C(25)	29.4(6)
C(9)-C(10)-C(11)-C(12)	1.1(7)	N(1)-Ru(1)-C(26)-C(27)	35.3(3)
C(10)-C(11)-C(12)-C(7)	3.3(6)	C(12)-Ru(1)-C(26)-C(27)	-42.5(3)
C(10)-C(11)-C(12)-Ru(1)	-171.8(3)	C(25)-Ru(1)-C(26)-C(27)	116.1(4)
C(8)-C(7)-C(12)-C(11)	-6.1(6)	N(2)-Ru(1)-C(26)-C(27)	-143.8(3)
C(6)-C(7)-C(12)-C(11)	175.1(4)	O(1)-Ru(1)-C(26)-C(27)	-90.1(7)
C(8)-C(7)-C(12)-Ru(1)	169.8(3)	O(2)-Ru(1)-C(26)-C(27)	131.7(3)
C(6)-C(7)-C(12)-Ru(1)	-9.0(5)	C(33)-Ru(1)-C(26)-C(27)	145.4(4)
N(1)-Ru(1)-C(12)-C(11)	-179.7(4)	C(25)-C(26)-C(27)-C(32)	-166.7(4)
C(25)-Ru(1)-C(12)-C(11)	-94.6(4)	Ru(1)-C(26)-C(27)-C(32)	111.6(4)
N(2)-Ru(1)-C(12)-C(11)	2.3(4)	C(25)-C(26)-C(27)-C(28)	12.9(6)
O(1)-Ru(1)-C(12)-C(11)	90.4(4)	Ru(1)-C(26)-C(27)-C(28)	-68.8(5)
C(26)-Ru(1)-C(12)-C(11)	-80.1(4)	C(32)-C(27)-C(28)-C(29)	-1.7(6)
O(2)-Ru(1)-C(12)-C(11)	108.5(4)	C(26)-C(27)-C(28)-C(29)	178.7(4)
C(33)-Ru(1)-C(12)-C(11)	96.8(4)	C(27)-C(28)-C(29)-C(30)	0.3(7)
N(1)-Ru(1)-C(12)-C(7)	5.1(3)	C(28)-C(29)-C(30)-C(31)	1.2(7)
C(25)-Ru(1)-C(12)-C(7)	90.2(3)	C(29)-C(30)-C(31)-C(32)	-1.2(7)
N(2)-Ru(1)-C(12)-C(7)	-173.0(3)	C(30)-C(31)-C(32)-C(27)	-0.3(7)
O(1)-Ru(1)-C(12)-C(7)	-84.9(3)	C(28)-C(27)-C(32)-C(31)	1.7(6)
C(26)-Ru(1)-C(12)-C(7)	104.7(3)	C(26)-C(27)-C(32)-C(31)	-178.7(4)
O(2)-Ru(1)-C(12)-C(7)	-66.8(4)	N(1)-Ru(1)-O(1)-C(33)	89.1(3)
C(33)-Ru(1)-C(12)-C(7)	-78.5(3)	C(12)-Ru(1)-O(1)-C(33)	168.7(3)
N(1)-Ru(1)-N(2)-C(13)	-31(4)	C(25)-Ru(1)-O(1)-C(33)	-1.4(4)
C(12)-Ru(1)-N(2)-C(13)	46.4(3)	N(2)-Ru(1)-O(1)-C(33)	-91.4(3)
C(25)-Ru(1)-N(2)-C(13)	162.0(3)	C(26)-Ru(1)-O(1)-C(33)	-144.7(6)
O(1)-Ru(1)-N(2)-C(13)	-45.4(3)	O(2)-Ru(1)-O(1)-C(33)	-0.6(2)
C(26)-Ru(1)-N(2)-C(13)	124.2(3)	Ru(1)-O(1)-C(33)-O(2)	1.1(4)
O(2)-Ru(1)-N(2)-C(13)	-104.3(3)	Ru(1)-O(1)-C(33)-C(34)	-178.1(4)
C(33)-Ru(1)-N(2)-C(13)	-74.6(3)	N(1)-Ru(1)-C(33)-O(1)	-90.9(2)
N(1)-Ru(1)-N(2)-C(18)	152(4)	C(12)-Ru(1)-C(33)-O(1)	-13.2(3)
C(12)-Ru(1)-N(2)-C(18)	-130.4(3)	C(25)-Ru(1)-C(33)-O(1)	179.2(2)
C(25)-Ru(1)-N(2)-C(18)	-14.8(3)	N(2)-Ru(1)-C(33)-O(1)	87.7(2)
O(1)-Ru(1)-N(2)-C(18)	137.8(3)	C(26)-Ru(1)-C(33)-O(1)	157.8(4)

C(26)-Ru(1)-N(2)-C(18)	-52.6(3)	O(2)-Ru(1)-C(33)-O(1)	178.9(4)
O(2)-Ru(1)-N(2)-C(18)	78.9(3)	N(1)-Ru(1)-C(33)-O(2)	90.2(2)
C(33)-Ru(1)-N(2)-C(18)	108.6(3)	C(12)-Ru(1)-C(33)-O(2)	167.9(2)
C(18)-N(2)-C(13)-C(14)	5.4(6)	C(25)-Ru(1)-C(33)-O(2)	0.3(3)
Ru(1)-N(2)-C(13)-C(14)	-171.7(3)	N(2)-Ru(1)-C(33)-O(2)	-91.2(2)
N(2)-C(13)-C(14)-C(15)	3.1(7)	O(1)-Ru(1)-C(33)-O(2)	-178.9(4)
C(13)-C(14)-C(15)-C(16)	-4.4(6)	C(26)-Ru(1)-C(33)-O(2)	-21.1(5)
C(14)-C(15)-C(16)-C(18)	-2.3(6)	N(1)-Ru(1)-C(33)-C(34)	-66(5)
C(14)-C(15)-C(16)-C(17)	177.6(4)	C(12)-Ru(1)-C(33)-C(34)	12(5)
C(13)-N(2)-C(18)-C(16)	-12.3(6)	C(25)-Ru(1)-C(33)-C(34)	-156(5)
Ru(1)-N(2)-C(18)-C(16)	164.5(3)	N(2)-Ru(1)-C(33)-C(34)	113(5)
C(13)-N(2)-C(18)-C(19)	162.5(4)	O(1)-Ru(1)-C(33)-C(34)	25(5)
Ru(1)-N(2)-C(18)-C(19)	-20.7(5)	C(26)-Ru(1)-C(33)-C(34)	-177(5)
C(15)-C(16)-C(18)-N(2)	10.8(6)	O(2)-Ru(1)-C(33)-C(34)	-156(5)
C(17)-C(16)-C(18)-N(2)	-169.1(4)	O(1)-C(33)-O(2)-Ru(1)	-1.1(4)
C(15)-C(16)-C(18)-C(19)	-163.8(4)	C(34)-C(33)-O(2)-Ru(1)	178.2(4)
C(17)-C(16)-C(18)-C(19)	16.3(6)	N(1)-Ru(1)-O(2)-C(33)	-89.8(2)
N(2)-C(18)-C(19)-C(20)	-138.4(4)	C(12)-Ru(1)-O(2)-C(33)	-20.6(4)
C(16)-C(18)-C(19)-C(20)	36.3(6)	C(25)-Ru(1)-O(2)-C(33)	-179.7(3)
N(2)-C(18)-C(19)-C(24)	33.1(6)	N(2)-Ru(1)-O(2)-C(33)	88.4(2)
C(16)-C(18)-C(19)-C(24)	-152.2(4)	O(1)-Ru(1)-O(2)-C(33)	0.6(2)
C(24)-C(19)-C(20)-C(21)	2.1(6)	C(26)-Ru(1)-O(2)-C(33)	170.6(2)

X-ray Crystallographic Data

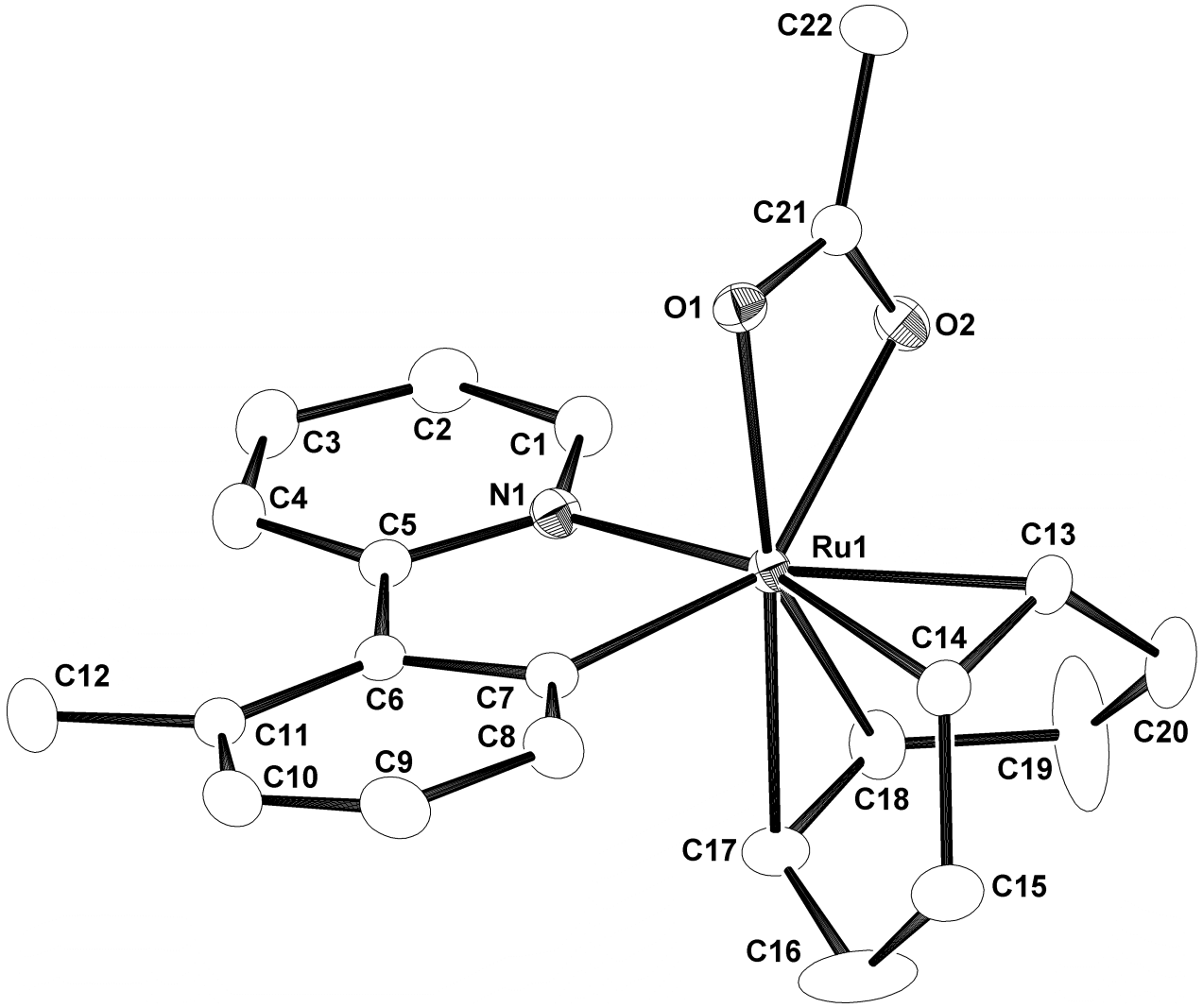


Figure S8. An ORTEP drawing of complex **38b**. Hydrogen atoms are omitted for clarity.

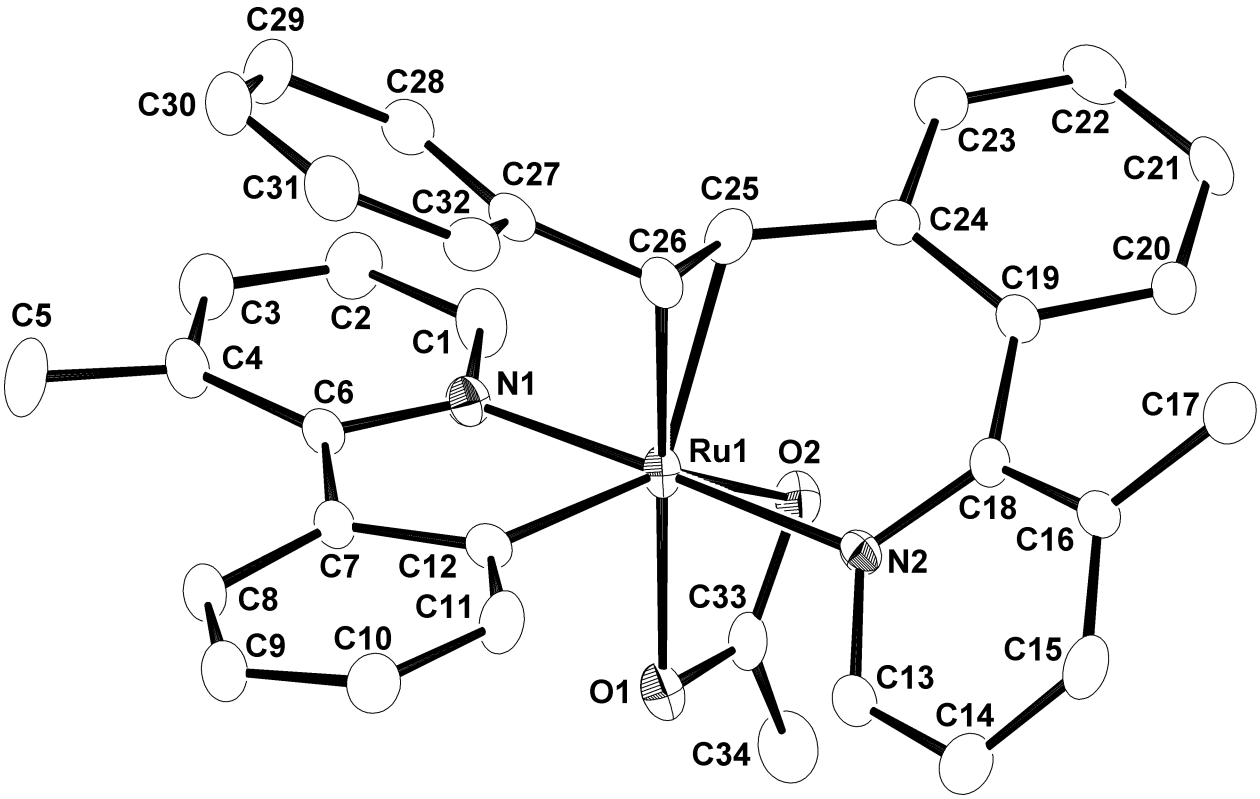


Figure S9. An ORTEP drawing of complex **39a**. Hydrogen atoms and a toluene molecule contained in the unit cell are omitted for clarity.

Table S3. Crystal data and structure refinement for **38b** and **39a**.

	38b	**39a**
Empirical formula	$C_{22}H_{25}NO_2Ru$	$C_{34}H_{30}N_2O_2Ru{\cdot}0.5C_7H_8$
Formula weight	436.50	645.74
Temperature	93(2) K	123(2) K
Crystal color, habit	Yellow, Block	Red, Platelet
Crystal dimensions	0.50 x 0.40 x 0.20 mm	0.30 x 0.20 x 0.10 mm
Crystal system	Triclinic	Triclinic
Space group	*P*-1	*P*-1
a (Å)	9.3192(12)	9.3382(9)
b (Å)	10.6453(14)	10.7006(11)
c (Å)	10.8679(14)	16.4644(15)
α (°)	108.651(4)	74.606(2)
β (°)	111.833(3)	74.799(3)
γ (°)	99.462(4)	71.863(3)
V ($Å^3$)	897.7(2)	1478.1(2)
Z	2	2
Density (calculated)	1.615 mg/mm^3	1.451 mg/mm^3
F(000)	448	666
Absorption coefficient	0.890 mm^{-1}	0.568 mm^{-1}
Theta range for data collection	3.18 to 27.49°	3.08 to 25.00°
Reflections collected	8614	10726
Independent reflections	4045 [R(int) = 0.0211]	4995 [R(int) = 0.0450]
Number of parameters	237	372
Goodness-of-fit on F^2	1.260	1.118
Final R indices [I>2sigma(I)]	R1 = 0.0306	R1 = 0.0419
	wR2 = 0.0837	wR2 = 0.0871
R indices (all data)	R1 = 0.0327	R1 = 0.0582
	wR2 = 0.0906	wR2 = 0.1010

[a] Goodness of Fit = $\{\Sigma[w\,(|F_o| - |F_c|)^2] / (N_{obs} - N_{parameters})\}^{1/2}$
[b] $R = \Sigma\,||F_o| - |F_c|| / \Sigma\,|F_o|$, $R_w = \{\Sigma[w\,(|F_o| - |F_c|)^2] / \Sigma[wF_o^2]\}^{1/2}$

Table S4. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **38b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	8926(1)	7341(1)	7357(1)	11(1)
N(1)	8785(3)	5341(2)	7233(3)	15(1)
C(1)	7425(4)	4235(3)	6227(3)	18(1)
C(2)	7264(4)	2894(3)	6146(3)	22(1)
C(3)	8544(4)	2687(3)	7151(4)	25(1)
C(4)	9941(4)	3800(3)	8155(4)	23(1)
C(5)	10073(3)	5147(3)	8188(3)	15(1)
C(6)	11452(3)	6462(3)	9200(3)	15(1)
C(7)	11176(3)	7684(3)	9016(3)	15(1)
C(8)	12368(3)	8978(3)	10034(3)	20(1)
C(9)	13811(4)	9067(3)	11144(3)	23(1)
C(10)	14095(3)	7871(4)	11253(3)	22(1)
C(11)	12940(4)	6555(3)	10315(3)	20(1)
C(12)	13385(4)	5333(4)	10583(4)	30(1)
C(13)	8202(4)	9028(3)	6809(3)	16(1)
C(14)	9842(4)	9606(3)	7836(3)	17(1)
C(15)	11191(4)	9925(3)	7411(4)	25(1)
C(16)	11506(6)	8692(4)	6596(6)	46(1)
C(17)	10454(4)	7266(3)	6256(3)	20(1)
C(18)	8804(4)	6661(3)	5240(3)	22(1)
C(19)	7819(8)	7343(6)	4377(4)	71(2)
C(20)	7592(5)	8612(4)	5180(4)	31(1)
O(1)	7811(2)	7669(2)	8821(2)	15(1)
C(21)	6372(3)	7083(3)	7761(3)	15(1)
O(2)	6189(2)	6611(2)	6464(2)	17(1)
C(22)	4909(4)	6970(3)	8058(4)	24(1)

Table S5. Bond lengths [Å] and angles [°] for **38b**.

Ru(1)-N(1)	2.069(2)	C(6)-C(7)	1.427(4)
Ru(1)-C(7)	2.073(3)	C(7)-C(8)	1.402(4)
Ru(1)-C(18)	2.131(3)	C(8)-C(9)	1.397(4)
Ru(1)-C(17)	2.170(3)	C(9)-C(10)	1.374(5)
Ru(1)-O(1)	2.1745(19)	C(10)-C(11)	1.391(5)
Ru(1)-C(13)	2.196(3)	C(11)-C(12)	1.509(4)
Ru(1)-C(14)	2.237(3)	C(13)-C(14)	1.393(4)
Ru(1)-O(2)	2.2533(19)	C(13)-C(20)	1.523(4)
Ru(1)-C(21)	2.565(3)	C(14)-C(15)	1.517(4)
N(1)-C(1)	1.357(4)	C(15)-C(16)	1.474(5)
N(1)-C(5)	1.361(4)	C(16)-C(17)	1.511(5)
C(1)-C(2)	1.382(4)	C(17)-C(18)	1.399(4)
C(2)-C(3)	1.391(5)	C(18)-C(19)	1.504(5)
C(3)-C(4)	1.378(5)	C(19)-C(20)	1.452(5)
C(4)-C(5)	1.407(4)	O(1)-C(21)	1.277(3)
C(5)-C(6)	1.481(4)	C(21)-O(2)	1.268(3)
C(6)-C(11)	1.425(4)	C(21)-C(22)	1.508(4)
N(1)-Ru(1)-C(7)	78.13(10)	C(4)-C(3)-C(2)	119.6(3)
N(1)-Ru(1)-C(18)	88.79(11)	C(3)-C(4)-C(5)	120.6(3)
C(7)-Ru(1)-C(18)	114.63(11)	N(1)-C(5)-C(4)	119.0(3)
N(1)-Ru(1)-C(17)	92.13(10)	N(1)-C(5)-C(6)	112.9(2)
C(7)-Ru(1)-C(17)	78.41(11)	C(4)-C(5)-C(6)	128.1(3)
C(18)-Ru(1)-C(17)	37.95(12)	C(11)-C(6)-C(7)	120.8(3)
N(1)-Ru(1)-O(1)	90.67(8)	C(11)-C(6)-C(5)	124.3(3)
C(7)-Ru(1)-O(1)	92.16(9)	C(7)-C(6)-C(5)	114.8(2)
C(18)-Ru(1)-O(1)	152.44(10)	C(8)-C(7)-C(6)	117.5(3)
C(17)-Ru(1)-O(1)	169.38(10)	C(8)-C(7)-Ru(1)	127.1(2)
N(1)-Ru(1)-C(13)	159.13(11)	C(6)-C(7)-Ru(1)	115.1(2)
C(7)-Ru(1)-C(13)	122.73(11)	C(9)-C(8)-C(7)	121.4(3)
C(18)-Ru(1)-C(13)	81.62(11)	C(10)-C(9)-C(8)	120.2(3)
C(17)-Ru(1)-C(13)	91.60(11)	C(9)-C(10)-C(11)	121.6(3)
O(1)-Ru(1)-C(13)	89.41(9)	C(10)-C(11)-C(6)	118.4(3)

N(1)-Ru(1)-C(14)	163.60(10)	C(10)-C(11)-C(12)	116.2(3)
C(7)-Ru(1)-C(14)	86.34(11)	C(6)-C(11)-C(12)	125.4(3)
C(18)-Ru(1)-C(14)	92.97(12)	C(14)-C(13)-C(20)	124.4(3)
C(17)-Ru(1)-C(14)	79.48(11)	C(14)-C(13)-Ru(1)	73.32(16)
O(1)-Ru(1)-C(14)	95.20(9)	C(20)-C(13)-Ru(1)	109.61(19)
C(13)-Ru(1)-C(14)	36.63(10)	C(13)-C(14)-C(15)	121.7(3)
N(1)-Ru(1)-O(2)	85.78(8)	C(13)-C(14)-Ru(1)	70.06(16)
C(7)-Ru(1)-O(2)	147.31(9)	C(15)-C(14)-Ru(1)	112.68(19)
C(18)-Ru(1)-O(2)	93.02(10)	C(16)-C(15)-C(14)	115.3(3)
C(17)-Ru(1)-O(2)	130.97(10)	C(15)-C(16)-C(17)	117.4(3)
O(1)-Ru(1)-O(2)	59.47(7)	C(18)-C(17)-C(16)	123.9(3)
C(13)-Ru(1)-O(2)	76.32(9)	C(18)-C(17)-Ru(1)	69.53(16)
C(14)-Ru(1)-O(2)	110.39(9)	C(16)-C(17)-Ru(1)	113.8(2)
N(1)-Ru(1)-C(21)	87.94(9)	C(17)-C(18)-C(19)	125.3(4)
C(7)-Ru(1)-C(21)	120.51(10)	C(17)-C(18)-Ru(1)	72.53(16)
C(18)-Ru(1)-C(21)	122.64(11)	C(19)-C(18)-Ru(1)	110.7(2)
C(17)-Ru(1)-C(21)	160.54(11)	C(20)-C(19)-C(18)	117.6(3)
O(1)-Ru(1)-C(21)	29.84(8)	C(19)-C(20)-C(13)	116.3(3)
C(13)-Ru(1)-C(21)	81.82(10)	C(21)-O(1)-Ru(1)	92.25(16)
C(14)-Ru(1)-C(21)	104.68(9)	O(2)-C(21)-O(1)	119.4(2)
O(2)-Ru(1)-C(21)	29.63(8)	O(2)-C(21)-C(22)	120.6(3)
C(1)-N(1)-C(5)	120.2(2)	O(1)-C(21)-C(22)	120.0(3)
C(1)-N(1)-Ru(1)	120.81(19)	O(2)-C(21)-Ru(1)	61.45(14)
C(5)-N(1)-Ru(1)	119.01(19)	O(1)-C(21)-Ru(1)	57.91(13)
N(1)-C(1)-C(2)	122.4(3)	C(22)-C(21)-Ru(1)	177.8(2)
C(1)-C(2)-C(3)	118.1(3)	C(21)-O(2)-Ru(1)	88.91(16)

Table S6. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **38b**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	11(1)	11(1)	10(1)	4(1)	4(1)	3(1)
N(1)	16(1)	13(1)	16(1)	6(1)	8(1)	6(1)
C(1)	19(1)	16(1)	15(1)	5(1)	6(1)	4(1)
C(2)	26(2)	15(1)	21(1)	3(1)	11(1)	3(1)
C(3)	32(2)	16(1)	32(2)	12(1)	17(1)	10(1)
C(4)	27(2)	22(2)	29(2)	16(1)	14(1)	13(1)
C(5)	18(1)	17(1)	15(1)	7(1)	10(1)	7(1)
C(6)	14(1)	20(1)	13(1)	8(1)	7(1)	5(1)
C(7)	13(1)	20(1)	12(1)	6(1)	6(1)	5(1)
C(8)	17(1)	19(1)	17(1)	4(1)	5(1)	4(1)
C(9)	15(1)	27(2)	16(1)	3(1)	3(1)	1(1)
C(10)	13(1)	35(2)	13(1)	11(1)	3(1)	7(1)
C(11)	17(1)	31(2)	21(1)	17(1)	11(1)	11(1)
C(12)	21(2)	38(2)	35(2)	25(2)	7(1)	13(1)
C(13)	21(1)	14(1)	16(1)	8(1)	8(1)	7(1)
C(14)	20(1)	12(1)	21(1)	7(1)	11(1)	6(1)
C(15)	24(2)	22(2)	33(2)	12(1)	17(1)	5(1)
C(16)	56(3)	24(2)	73(3)	11(2)	55(3)	5(2)
C(17)	24(1)	21(1)	21(1)	7(1)	16(1)	8(1)
C(18)	30(2)	27(2)	12(1)	7(1)	11(1)	17(1)
C(19)	122(5)	90(4)	14(2)	21(2)	21(2)	88(4)
C(20)	46(2)	32(2)	18(2)	14(1)	11(1)	21(2)
O(1)	16(1)	15(1)	14(1)	6(1)	7(1)	4(1)
C(21)	15(1)	13(1)	19(1)	8(1)	8(1)	4(1)
O(2)	13(1)	17(1)	16(1)	5(1)	5(1)	4(1)
C(22)	18(1)	28(2)	30(2)	14(1)	15(1)	8(1)

Table S7. Torsion angles [°] for **38b**.

C(7)-Ru(1)-N(1)-C(1)	179.8(2)	C(17)-Ru(1)-C(14)-C(15)	-9.7(2)
C(18)-Ru(1)-N(1)-C(1)	-64.8(2)	O(1)-Ru(1)-C(14)-C(15)	161.0(2)
C(17)-Ru(1)-N(1)-C(1)	-102.6(2)	C(13)-Ru(1)-C(14)-C(15)	-117.0(3)
O(1)-Ru(1)-N(1)-C(1)	87.7(2)	O(2)-Ru(1)-C(14)-C(15)	-139.7(2)
C(13)-Ru(1)-N(1)-C(1)	-2.4(4)	C(21)-Ru(1)-C(14)-C(15)	-170.2(2)
C(14)-Ru(1)-N(1)-C(1)	-161.2(3)	C(13)-C(14)-C(15)-C(16)	-72.1(4)
O(2)-Ru(1)-N(1)-C(1)	28.4(2)	Ru(1)-C(14)-C(15)-C(16)	7.7(4)
C(21)-Ru(1)-N(1)-C(1)	58.0(2)	C(14)-C(15)-C(16)-C(17)	0.9(6)
C(7)-Ru(1)-N(1)-C(5)	0.33(19)	C(15)-C(16)-C(17)-C(18)	71.1(5)
C(18)-Ru(1)-N(1)-C(5)	115.8(2)	C(15)-C(16)-C(17)-Ru(1)	-9.4(5)
C(17)-Ru(1)-N(1)-C(5)	78.0(2)	N(1)-Ru(1)-C(17)-C(18)	85.30(19)
O(1)-Ru(1)-N(1)-C(5)	-91.7(2)	C(7)-Ru(1)-C(17)-C(18)	162.7(2)
C(13)-Ru(1)-N(1)-C(5)	178.2(2)	O(1)-Ru(1)-C(17)-C(18)	-169.5(4)
C(14)-Ru(1)-N(1)-C(5)	19.4(4)	C(13)-Ru(1)-C(17)-C(18)	-74.15(19)
O(2)-Ru(1)-N(1)-C(5)	-151.1(2)	C(14)-Ru(1)-C(17)-C(18)	-108.9(2)
C(21)-Ru(1)-N(1)-C(5)	-121.5(2)	O(2)-Ru(1)-C(17)-C(18)	-0.9(2)
C(5)-N(1)-C(1)-C(2)	1.8(4)	C(21)-Ru(1)-C(17)-C(18)	-4.5(4)
Ru(1)-N(1)-C(1)-C(2)	-177.6(2)	N(1)-Ru(1)-C(17)-C(16)	-155.6(3)
N(1)-C(1)-C(2)-C(3)	0.8(4)	C(7)-Ru(1)-C(17)-C(16)	-78.2(3)
C(1)-C(2)-C(3)-C(4)	-2.2(5)	C(18)-Ru(1)-C(17)-C(16)	119.1(4)
C(2)-C(3)-C(4)-C(5)	1.1(5)	O(1)-Ru(1)-C(17)-C(16)	-50.5(7)
C(1)-N(1)-C(5)-C(4)	-2.9(4)	C(13)-Ru(1)-C(17)-C(16)	44.9(3)
Ru(1)-N(1)-C(5)-C(4)	176.6(2)	C(14)-Ru(1)-C(17)-C(16)	10.2(3)
C(1)-N(1)-C(5)-C(6)	179.7(2)	O(2)-Ru(1)-C(17)-C(16)	118.1(3)
Ru(1)-N(1)-C(5)-C(6)	-0.9(3)	C(21)-Ru(1)-C(17)-C(16)	114.6(4)
C(3)-C(4)-C(5)-N(1)	1.4(4)	C(16)-C(17)-C(18)-C(19)	-2.1(5)
C(3)-C(4)-C(5)-C(6)	178.5(3)	Ru(1)-C(17)-C(18)-C(19)	103.4(3)
N(1)-C(5)-C(6)-C(11)	179.3(2)	C(16)-C(17)-C(18)-Ru(1)	-105.5(3)
C(4)-C(5)-C(6)-C(11)	2.1(4)	N(1)-Ru(1)-C(18)-C(17)	-95.01(19)
N(1)-C(5)-C(6)-C(7)	1.1(3)	C(7)-Ru(1)-C(18)-C(17)	-18.7(2)
C(4)-C(5)-C(6)-C(7)	-176.0(3)	O(1)-Ru(1)-C(18)-C(17)	175.85(18)
C(11)-C(6)-C(7)-C(8)	-4.4(4)	C(13)-Ru(1)-C(18)-C(17)	103.59(19)
C(5)-C(6)-C(7)-C(8)	173.8(2)	C(14)-Ru(1)-C(18)-C(17)	68.67(19)

C(11)-C(6)-C(7)-Ru(1)	-179.1(2)	O(2)-Ru(1)-C(18)-C(17)	179.28(18)
C(5)-C(6)-C(7)-Ru(1)	-0.9(3)	C(21)-Ru(1)-C(18)-C(17)	178.21(16)
N(1)-Ru(1)-C(7)-C(8)	-173.8(3)	N(1)-Ru(1)-C(18)-C(19)	143.1(4)
C(18)-Ru(1)-C(7)-C(8)	103.1(3)	C(7)-Ru(1)-C(18)-C(19)	-140.6(4)
C(17)-Ru(1)-C(7)-C(8)	91.5(3)	C(17)-Ru(1)-C(18)-C(19)	-121.9(4)
O(1)-Ru(1)-C(7)-C(8)	-83.5(2)	O(1)-Ru(1)-C(18)-C(19)	53.9(5)
C(13)-Ru(1)-C(7)-C(8)	7.2(3)	C(13)-Ru(1)-C(18)-C(19)	-18.3(4)
C(14)-Ru(1)-C(7)-C(8)	11.5(3)	C(14)-Ru(1)-C(18)-C(19)	-53.2(4)
O(2)-Ru(1)-C(7)-C(8)	-111.6(3)	O(2)-Ru(1)-C(18)-C(19)	57.4(4)
C(21)-Ru(1)-C(7)-C(8)	-93.4(3)	C(21)-Ru(1)-C(18)-C(19)	56.3(4)
N(1)-Ru(1)-C(7)-C(6)	0.34(19)	C(17)-C(18)-C(19)-C(20)	-63.1(7)
C(18)-Ru(1)-C(7)-C(6)	-82.8(2)	Ru(1)-C(18)-C(19)-C(20)	19.7(7)
C(17)-Ru(1)-C(7)-C(6)	-94.4(2)	C(18)-C(19)-C(20)-C(13)	-7.2(8)
O(1)-Ru(1)-C(7)-C(6)	90.57(19)	C(14)-C(13)-C(20)-C(19)	74.4(5)
C(13)-Ru(1)-C(7)-C(6)	-178.74(18)	Ru(1)-C(13)-C(20)-C(19)	-8.4(5)
C(14)-Ru(1)-C(7)-C(6)	-174.4(2)	N(1)-Ru(1)-O(1)-C(21)	-84.67(17)
O(2)-Ru(1)-C(7)-C(6)	62.5(3)	C(7)-Ru(1)-O(1)-C(21)	-162.82(17)
C(21)-Ru(1)-C(7)-C(6)	80.7(2)	C(18)-Ru(1)-O(1)-C(21)	4.0(3)
C(6)-C(7)-C(8)-C(9)	3.2(4)	C(17)-Ru(1)-O(1)-C(21)	170.0(5)
Ru(1)-C(7)-C(8)-C(9)	177.1(2)	C(13)-Ru(1)-O(1)-C(21)	74.45(17)
C(7)-C(8)-C(9)-C(10)	0.4(5)	C(14)-Ru(1)-O(1)-C(21)	110.66(17)
C(8)-C(9)-C(10)-C(11)	-2.8(5)	O(2)-Ru(1)-O(1)-C(21)	0.03(15)
C(9)-C(10)-C(11)-C(6)	1.5(4)	Ru(1)-O(1)-C(21)-O(2)	0.0(3)
C(9)-C(10)-C(11)-C(12)	-178.2(3)	Ru(1)-O(1)-C(21)-C(22)	-179.4(2)
C(7)-C(6)-C(11)-C(10)	2.2(4)	N(1)-Ru(1)-C(21)-O(2)	-85.09(16)
C(5)-C(6)-C(11)-C(10)	-175.9(3)	C(7)-Ru(1)-C(21)-O(2)	-160.00(16)
C(7)-C(6)-C(11)-C(12)	-178.1(3)	C(18)-Ru(1)-C(21)-O(2)	2.2(2)
C(5)-C(6)-C(11)-C(12)	3.8(4)	C(17)-Ru(1)-C(21)-O(2)	5.5(4)
N(1)-Ru(1)-C(13)-C(14)	-170.1(2)	O(1)-Ru(1)-C(21)-O(2)	180.0(3)
C(7)-Ru(1)-C(13)-C(14)	7.3(2)	C(13)-Ru(1)-C(21)-O(2)	76.67(17)
C(18)-Ru(1)-C(13)-C(14)	-106.61(18)	C(14)-Ru(1)-C(21)-O(2)	105.53(17)
C(17)-Ru(1)-C(13)-C(14)	-69.89(18)	N(1)-Ru(1)-C(21)-O(1)	94.96(16)
O(1)-Ru(1)-C(13)-C(14)	99.53(17)	C(7)-Ru(1)-C(21)-O(1)	20.0(2)
O(2)-Ru(1)-C(13)-C(14)	158.18(18)	C(18)-Ru(1)-C(21)-O(1)	-177.80(16)
C(21)-Ru(1)-C(13)-C(14)	128.50(17)	C(17)-Ru(1)-C(21)-O(1)	-174.5(3)

N(1)-Ru(1)-C(13)-C(20)	-48.8(4)	C(13)-Ru(1)-C(21)-O(1)	-103.28(17)
C(7)-Ru(1)-C(13)-C(20)	128.7(2)	C(14)-Ru(1)-C(21)-O(1)	-74.43(17)
C(18)-Ru(1)-C(13)-C(20)	14.7(2)	O(2)-Ru(1)-C(21)-O(1)	-180.0(3)
C(17)-Ru(1)-C(13)-C(20)	51.4(2)	N(1)-Ru(1)-C(21)-C(22)	109(6)
O(1)-Ru(1)-C(13)-C(20)	-139.2(2)	C(7)-Ru(1)-C(21)-C(22)	34(6)
C(14)-Ru(1)-C(13)-C(20)	121.3(3)	C(18)-Ru(1)-C(21)-C(22)	-163(6)
O(2)-Ru(1)-C(13)-C(20)	-80.5(2)	C(17)-Ru(1)-C(21)-C(22)	-160(5)
C(21)-Ru(1)-C(13)-C(20)	-110.2(2)	O(1)-Ru(1)-C(21)-C(22)	14(5)
C(20)-C(13)-C(14)-C(15)	2.3(4)	C(13)-Ru(1)-C(21)-C(22)	-89(6)
Ru(1)-C(13)-C(14)-C(15)	104.9(3)	C(14)-Ru(1)-C(21)-C(22)	-60(6)
C(20)-C(13)-C(14)-Ru(1)	-102.7(3)	O(2)-Ru(1)-C(21)-C(22)	-166(6)
N(1)-Ru(1)-C(14)-C(13)	167.5(3)	O(1)-C(21)-O(2)-Ru(1)	0.0(3)
C(7)-Ru(1)-C(14)-C(13)	-173.82(18)	C(22)-C(21)-O(2)-Ru(1)	179.4(2)
C(18)-Ru(1)-C(14)-C(13)	71.67(18)	N(1)-Ru(1)-O(2)-C(21)	93.25(17)
C(17)-Ru(1)-C(14)-C(13)	107.31(18)	C(7)-Ru(1)-O(2)-C(21)	33.1(3)
O(1)-Ru(1)-C(14)-C(13)	-81.98(17)	C(18)-Ru(1)-O(2)-C(21)	-178.18(17)
O(2)-Ru(1)-C(14)-C(13)	-22.66(18)	C(17)-Ru(1)-O(2)-C(21)	-177.60(17)
C(21)-Ru(1)-C(14)-C(13)	-53.21(18)	O(1)-Ru(1)-O(2)-C(21)	-0.03(15)
N(1)-Ru(1)-C(14)-C(15)	50.4(4)	C(13)-Ru(1)-O(2)-C(21)	-97.57(17)
C(7)-Ru(1)-C(14)-C(15)	69.1(2)	C(14)-Ru(1)-O(2)-C(21)	-83.89(17)
C(18)-Ru(1)-C(14)-C(15)	-45.4(2)		

Table S8. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2× 10^3) for **39a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	5478(1)	3942(1)	2453(1)	15(1)
N(1)	4047(4)	3409(3)	1938(2)	17(1)
C(1)	2660(5)	3266(5)	2394(3)	23(1)
C(2)	1719(5)	2827(5)	2084(3)	26(1)
C(3)	2245(5)	2494(5)	1280(3)	27(1)
C(4)	3645(5)	2641(4)	787(3)	22(1)
C(5)	4177(6)	2176(6)	-51(3)	39(1)
C(6)	4540(5)	3165(4)	1123(2)	16(1)
C(7)	6042(5)	3437(4)	726(2)	16(1)
C(8)	6726(5)	3467(4)	-148(3)	20(1)
C(9)	8179(5)	3663(4)	-461(3)	23(1)
C(10)	8978(5)	3835(4)	90(3)	24(1)
C(11)	8279(5)	3866(4)	938(3)	20(1)
C(12)	6812(5)	3709(4)	1277(3)	18(1)
N(2)	6935(4)	4558(3)	2959(2)	15(1)
C(13)	7591(5)	5516(4)	2438(3)	18(1)
C(14)	8715(5)	5905(5)	2634(3)	22(1)
C(15)	9237(5)	5232(4)	3384(3)	21(1)
C(16)	8569(5)	4258(4)	3950(3)	18(1)
C(17)	9249(5)	3522(5)	4745(3)	24(1)
C(18)	7306(5)	4011(4)	3754(2)	15(1)
C(19)	6269(5)	3265(4)	4413(2)	16(1)
C(20)	5947(5)	3477(4)	5257(3)	18(1)
C(21)	4896(5)	2929(4)	5902(3)	22(1)
C(22)	4094(5)	2198(5)	5718(3)	28(1)
C(23)	4349(5)	1997(4)	4901(3)	23(1)
C(24)	5433(5)	2496(4)	4230(3)	17(1)
C(25)	5610(5)	2168(4)	3391(3)	21(1)
C(26)	6990(5)	1934(4)	2775(3)	19(1)
C(27)	7374(5)	947(4)	2218(3)	20(1)
C(28)	6303(5)	341(4)	2122(3)	23(1)

C(29)	6728(6)	-559(5)	1576(3)	28(1)
C(30)	8235(6)	-885(5)	1111(3)	28(1)
C(31)	9290(6)	-319(5)	1217(3)	27(1)
C(32)	8871(5)	581(4)	1763(3)	23(1)
O(1)	4466(3)	6035(3)	1983(2)	21(1)
C(33)	3429(5)	6163(4)	2648(3)	19(1)
O(2)	3380(3)	5158(3)	3274(2)	21(1)
C(34)	2250(6)	7485(5)	2695(3)	31(1)
C(35)	-2390(14)	-180(13)	6166(8)	52(3)
C(36)	-992(6)	-63(8)	5480(4)	37(2)
C(37)	319(8)	-112(8)	5749(4)	36(3)
C(38)	1665(6)	-28(8)	5151(6)	50(3)
C(39)	1700(7)	104(9)	4284(5)	59(4)
C(40)	388(9)	152(8)	4014(3)	47(3)
C(41)	-958(7)	69(7)	4613(4)	20(2)

Table S9. Bond lengths [Å] and angles [°] for **39a**.

Ru(1)-N(1)	2.039(3)	C(13)-C(14)	1.379(6)
Ru(1)-C(12)	2.040(4)	C(14)-C(15)	1.380(6)
Ru(1)-C(25)	2.098(4)	C(15)-C(16)	1.389(6)
Ru(1)-N(2)	2.103(3)	C(16)-C(18)	1.416(6)
Ru(1)-O(1)	2.157(3)	C(16)-C(17)	1.521(6)
Ru(1)-C(26)	2.188(4)	C(18)-C(19)	1.491(6)
Ru(1)-O(2)	2.306(3)	C(19)-C(20)	1.406(6)
Ru(1)-C(33)	2.581(4)	C(19)-C(24)	1.425(6)
N(1)-C(1)	1.348(5)	C(20)-C(21)	1.384(6)
N(1)-C(6)	1.366(5)	C(21)-C(22)	1.370(6)
C(1)-C(2)	1.368(6)	C(22)-C(23)	1.366(6)
C(2)-C(3)	1.387(6)	C(23)-C(24)	1.403(6)
C(3)-C(4)	1.377(6)	C(24)-C(25)	1.470(6)
C(4)-C(6)	1.420(6)	C(25)-C(26)	1.415(6)
C(4)-C(5)	1.500(6)	C(26)-C(27)	1.481(6)
C(6)-C(7)	1.467(6)	C(27)-C(32)	1.390(6)
C(7)-C(8)	1.409(6)	C(27)-C(28)	1.409(6)
C(7)-C(12)	1.428(6)	C(28)-C(29)	1.388(6)
C(8)-C(9)	1.380(6)	C(29)-C(30)	1.400(7)
C(9)-C(10)	1.394(6)	C(30)-C(31)	1.374(7)
C(10)-C(11)	1.382(6)	C(31)-C(32)	1.389(6)
C(11)-C(12)	1.381(6)	O(1)-C(33)	1.264(5)
N(2)-C(13)	1.346(5)	C(33)-O(2)	1.280(5)
N(2)-C(18)	1.370(5)	C(33)-C(34)	1.505(6)
N(1)-Ru(1)-C(12)	79.58(15)	C(11)-C(12)-C(7)	117.4(4)
N(1)-Ru(1)-C(25)	89.97(15)	C(11)-C(12)-Ru(1)	129.1(3)
C(12)-Ru(1)-C(25)	114.78(16)	C(7)-C(12)-Ru(1)	113.4(3)
N(1)-Ru(1)-N(2)	178.06(14)	C(13)-N(2)-C(18)	118.9(3)
C(12)-Ru(1)-N(2)	100.01(15)	C(13)-N(2)-Ru(1)	116.4(3)
C(25)-Ru(1)-N(2)	91.92(15)	C(18)-N(2)-Ru(1)	124.7(3)
N(1)-Ru(1)-O(1)	90.33(12)	N(2)-C(13)-C(14)	123.2(4)
C(12)-Ru(1)-O(1)	92.16(13)	C(13)-C(14)-C(15)	118.0(4)

C(25)-Ru(1)-O(1)	152.63(14)	C(14)-C(15)-C(16)	120.7(4)
N(2)-Ru(1)-O(1)	87.80(12)	C(15)-C(16)-C(18)	118.3(4)
N(1)-Ru(1)-C(26)	97.27(15)	C(15)-C(16)-C(17)	117.5(4)
C(12)-Ru(1)-C(26)	79.01(15)	C(18)-C(16)-C(17)	124.2(4)
C(25)-Ru(1)-C(26)	38.47(16)	N(2)-C(18)-C(16)	119.8(3)
N(2)-Ru(1)-C(26)	84.49(15)	N(2)-C(18)-C(19)	118.1(3)
O(1)-Ru(1)-C(26)	167.06(13)	C(16)-C(18)-C(19)	121.8(3)
N(1)-Ru(1)-O(2)	89.97(12)	C(20)-C(19)-C(24)	117.7(4)
C(12)-Ru(1)-O(2)	149.36(13)	C(20)-C(19)-C(18)	117.2(4)
C(25)-Ru(1)-O(2)	93.74(14)	C(24)-C(19)-C(18)	124.6(4)
N(2)-Ru(1)-O(2)	89.47(12)	C(21)-C(20)-C(19)	122.0(4)
O(1)-Ru(1)-O(2)	58.90(10)	C(22)-C(21)-C(20)	119.8(4)
C(26)-Ru(1)-O(2)	131.21(13)	C(23)-C(22)-C(21)	119.9(4)
N(1)-Ru(1)-C(33)	89.86(13)	C(22)-C(23)-C(24)	122.5(4)
C(12)-Ru(1)-C(33)	120.75(15)	C(23)-C(24)-C(19)	118.1(4)
C(25)-Ru(1)-C(33)	123.42(15)	C(23)-C(24)-C(25)	116.3(4)
N(2)-Ru(1)-C(33)	88.74(13)	C(19)-C(24)-C(25)	125.6(4)
O(1)-Ru(1)-C(33)	29.22(12)	C(26)-C(25)-C(24)	126.0(4)
C(26)-Ru(1)-C(33)	160.03(14)	C(26)-C(25)-Ru(1)	74.2(2)
O(2)-Ru(1)-C(33)	29.69(11)	C(24)-C(25)-Ru(1)	108.6(3)
C(1)-N(1)-C(6)	120.4(4)	C(25)-C(26)-C(27)	123.1(4)
C(1)-N(1)-Ru(1)	121.1(3)	C(25)-C(26)-Ru(1)	67.3(2)
C(6)-N(1)-Ru(1)	118.4(3)	C(27)-C(26)-Ru(1)	121.0(3)
N(1)-C(1)-C(2)	122.3(4)	C(32)-C(27)-C(28)	117.4(4)
C(1)-C(2)-C(3)	117.9(4)	C(32)-C(27)-C(26)	118.9(4)
C(4)-C(3)-C(2)	121.7(4)	C(28)-C(27)-C(26)	123.6(4)
C(3)-C(4)-C(6)	117.9(4)	C(29)-C(28)-C(27)	120.8(4)
C(3)-C(4)-C(5)	118.4(4)	C(28)-C(29)-C(30)	120.5(4)
C(6)-C(4)-C(5)	123.6(4)	C(31)-C(30)-C(29)	118.8(4)
N(1)-C(6)-C(4)	119.5(4)	C(30)-C(31)-C(32)	120.9(5)
N(1)-C(6)-C(7)	111.8(3)	C(31)-C(32)-C(27)	121.5(4)
C(4)-C(6)-C(7)	128.6(4)	C(33)-O(1)-Ru(1)	94.4(2)
C(8)-C(7)-C(12)	119.7(4)	O(1)-C(33)-O(2)	119.6(4)
C(8)-C(7)-C(6)	124.2(4)	O(1)-C(33)-C(34)	120.0(4)
C(12)-C(7)-C(6)	116.1(3)	O(2)-C(33)-C(34)	120.4(4)

C(9)-C(8)-C(7)	120.5(4)	O(1)-C(33)-Ru(1)	56.4(2)
C(8)-C(9)-C(10)	119.9(4)	O(2)-C(33)-Ru(1)	63.2(2)
C(11)-C(10)-C(9)	119.5(4)	C(34)-C(33)-Ru(1)	176.1(3)
C(12)-C(11)-C(10)	122.8(4)	C(33)-O(2)-Ru(1)	87.1(2)

Table S10. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **39a**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	13(1)	21(1)	13(1)	-7(1)	-2(1)	-4(1)
N(1)	16(2)	20(2)	15(2)	-4(2)	-3(1)	-4(2)
C(1)	12(2)	39(3)	18(2)	-11(2)	4(2)	-8(2)
C(2)	17(3)	37(3)	29(3)	-9(2)	-4(2)	-10(2)
C(3)	21(3)	37(3)	29(3)	-6(2)	-11(2)	-12(2)
C(4)	22(3)	29(2)	18(2)	-4(2)	-9(2)	-7(2)
C(5)	49(4)	63(4)	27(3)	-17(3)	-4(2)	-39(3)
C(6)	19(2)	17(2)	13(2)	-2(2)	-4(2)	-4(2)
C(7)	16(2)	18(2)	12(2)	-4(2)	-3(2)	-3(2)
C(8)	20(2)	26(2)	17(2)	-6(2)	-5(2)	-6(2)
C(9)	24(3)	30(3)	17(2)	-9(2)	-1(2)	-8(2)
C(10)	24(3)	27(3)	22(2)	-9(2)	1(2)	-7(2)
C(11)	12(2)	27(2)	23(2)	-12(2)	-4(2)	-4(2)
C(12)	21(2)	15(2)	16(2)	-1(2)	-7(2)	-3(2)
N(2)	17(2)	18(2)	10(2)	-2(1)	0(1)	-6(2)
C(13)	20(2)	20(2)	14(2)	-5(2)	-2(2)	-3(2)
C(14)	15(2)	28(2)	26(2)	-11(2)	0(2)	-7(2)
C(15)	13(2)	27(2)	27(2)	-13(2)	-7(2)	-4(2)
C(16)	23(3)	16(2)	14(2)	-3(2)	-5(2)	-2(2)
C(17)	21(3)	27(2)	28(2)	-7(2)	-10(2)	-6(2)
C(18)	15(2)	16(2)	14(2)	-6(2)	-2(2)	-2(2)
C(19)	16(2)	15(2)	14(2)	-3(2)	-5(2)	1(2)
C(20)	18(2)	16(2)	19(2)	-5(2)	-9(2)	2(2)
C(21)	28(3)	25(2)	11(2)	-5(2)	-3(2)	-1(2)
C(22)	25(3)	35(3)	19(2)	-1(2)	2(2)	-12(2)
C(23)	24(3)	27(2)	21(2)	-3(2)	-4(2)	-12(2)
C(24)	21(2)	14(2)	16(2)	-2(2)	-7(2)	-2(2)
C(25)	21(3)	23(2)	24(2)	-8(2)	-6(2)	-8(2)
C(26)	20(2)	23(2)	14(2)	-2(2)	-6(2)	-8(2)
C(27)	24(3)	20(2)	13(2)	1(2)	-6(2)	-5(2)
C(28)	26(3)	22(2)	19(2)	-5(2)	-4(2)	-3(2)

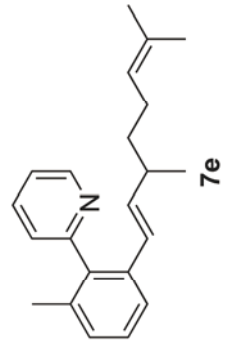
C(29)	33(3)	28(3)	29(3)	-11(2)	-12(2)	-7(2)
C(30)	40(3)	23(2)	21(2)	-10(2)	-10(2)	0(2)
C(31)	27(3)	27(3)	22(2)	-9(2)	-4(2)	2(2)
C(32)	23(3)	21(2)	23(2)	-3(2)	-5(2)	-4(2)
O(1)	22(2)	27(2)	14(2)	-5(1)	-4(1)	-6(1)
C(33)	19(2)	24(2)	18(2)	-7(2)	-9(2)	-5(2)
O(2)	23(2)	24(2)	18(2)	-7(1)	-5(1)	-5(1)
C(34)	28(3)	32(3)	30(3)	-10(2)	-9(2)	3(2)

Table S11. Torsion angles [°] for **39a**.

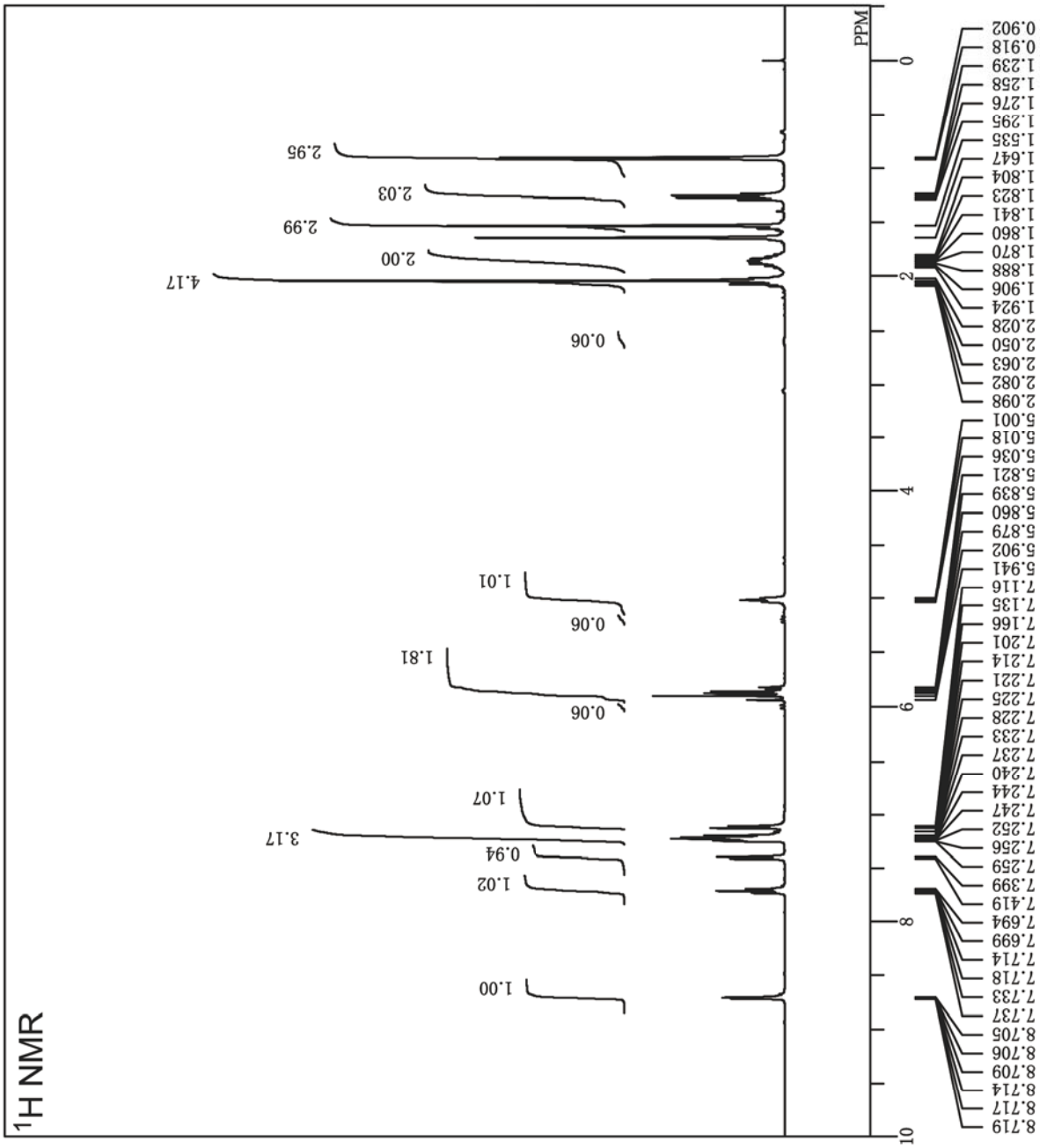
C(12)-Ru(1)-N(1)-C(1)	178.0(4)	C(18)-C(19)-C(20)-C(21)	174.3(4)
C(25)-Ru(1)-N(1)-C(1)	62.7(3)	C(19)-C(20)-C(21)-C(22)	-2.5(6)
N(2)-Ru(1)-N(1)-C(1)	-104(4)	C(20)-C(21)-C(22)-C(23)	0.9(7)
O(1)-Ru(1)-N(1)-C(1)	-89.9(3)	C(21)-C(22)-C(23)-C(24)	1.1(7)
C(26)-Ru(1)-N(1)-C(1)	100.6(3)	C(22)-C(23)-C(24)-C(19)	-1.4(7)
O(2)-Ru(1)-N(1)-C(1)	-31.0(3)	C(22)-C(23)-C(24)-C(25)	178.4(4)
C(33)-Ru(1)-N(1)-C(1)	-60.7(3)	C(20)-C(19)-C(24)-C(23)	-0.2(6)
C(12)-Ru(1)-N(1)-C(6)	-0.4(3)	C(18)-C(19)-C(24)-C(23)	-171.7(4)
C(25)-Ru(1)-N(1)-C(6)	-115.6(3)	C(20)-C(19)-C(24)-C(25)	-179.9(4)
N(2)-Ru(1)-N(1)-C(6)	77(4)	C(18)-C(19)-C(24)-C(25)	8.6(7)
O(1)-Ru(1)-N(1)-C(6)	91.8(3)	C(23)-C(24)-C(25)-C(26)	-146.3(4)
C(26)-Ru(1)-N(1)-C(6)	-77.7(3)	C(19)-C(24)-C(25)-C(26)	33.4(7)
O(2)-Ru(1)-N(1)-C(6)	150.7(3)	C(23)-C(24)-C(25)-Ru(1)	130.0(3)
C(33)-Ru(1)-N(1)-C(6)	121.0(3)	C(19)-C(24)-C(25)-Ru(1)	-50.3(5)
C(6)-N(1)-C(1)-C(2)	2.6(7)	N(1)-Ru(1)-C(25)-C(26)	101.8(3)
Ru(1)-N(1)-C(1)-C(2)	-175.7(3)	C(12)-Ru(1)-C(25)-C(26)	23.3(3)
N(1)-C(1)-C(2)-C(3)	1.5(7)	N(2)-Ru(1)-C(25)-C(26)	-78.7(3)
C(1)-C(2)-C(3)-C(4)	-2.3(7)	O(1)-Ru(1)-C(25)-C(26)	-167.6(3)
C(2)-C(3)-C(4)-C(6)	-0.8(7)	O(2)-Ru(1)-C(25)-C(26)	-168.3(2)
C(2)-C(3)-C(4)-C(5)	176.2(5)	C(33)-Ru(1)-C(25)-C(26)	-168.4(2)
C(1)-N(1)-C(6)-C(4)	-5.7(6)	N(1)-Ru(1)-C(25)-C(24)	-134.9(3)
Ru(1)-N(1)-C(6)-C(4)	172.6(3)	C(12)-Ru(1)-C(25)-C(24)	146.7(3)
C(1)-N(1)-C(6)-C(7)	177.4(4)	N(2)-Ru(1)-C(25)-C(24)	44.7(3)
Ru(1)-N(1)-C(6)-C(7)	-4.2(4)	O(1)-Ru(1)-C(25)-C(24)	-44.2(5)
C(3)-C(4)-C(6)-N(1)	4.8(6)	C(26)-Ru(1)-C(25)-C(24)	123.4(4)
C(5)-C(4)-C(6)-N(1)	-172.0(4)	O(2)-Ru(1)-C(25)-C(24)	-44.9(3)
C(3)-C(4)-C(6)-C(7)	-178.9(4)	C(33)-Ru(1)-C(25)-C(24)	-45.0(4)
C(5)-C(4)-C(6)-C(7)	4.3(7)	C(24)-C(25)-C(26)-C(27)	145.0(4)
N(1)-C(6)-C(7)-C(8)	-170.2(4)	Ru(1)-C(25)-C(26)-C(27)	-113.2(4)
C(4)-C(6)-C(7)-C(8)	13.4(7)	C(24)-C(25)-C(26)-Ru(1)	-101.8(4)
N(1)-C(6)-C(7)-C(12)	8.6(5)	N(1)-Ru(1)-C(26)-C(25)	-80.7(3)
C(4)-C(6)-C(7)-C(12)	-167.9(4)	C(12)-Ru(1)-C(26)-C(25)	-158.6(3)
C(12)-C(7)-C(8)-C(9)	4.6(6)	N(2)-Ru(1)-C(26)-C(25)	100.1(3)

C(6)-C(7)-C(8)-C(9)	-176.7(4)	O(1)-Ru(1)-C(26)-C(25)	153.8(5)
C(7)-C(8)-C(9)-C(10)	-0.1(7)	O(2)-Ru(1)-C(26)-C(25)	15.7(3)
C(8)-C(9)-C(10)-C(11)	-2.8(7)	C(33)-Ru(1)-C(26)-C(25)	29.4(6)
C(9)-C(10)-C(11)-C(12)	1.1(7)	N(1)-Ru(1)-C(26)-C(27)	35.3(3)
C(10)-C(11)-C(12)-C(7)	3.3(6)	C(12)-Ru(1)-C(26)-C(27)	-42.5(3)
C(10)-C(11)-C(12)-Ru(1)	-171.8(3)	C(25)-Ru(1)-C(26)-C(27)	116.1(4)
C(8)-C(7)-C(12)-C(11)	-6.1(6)	N(2)-Ru(1)-C(26)-C(27)	-143.8(3)
C(6)-C(7)-C(12)-C(11)	175.1(4)	O(1)-Ru(1)-C(26)-C(27)	-90.1(7)
C(8)-C(7)-C(12)-Ru(1)	169.8(3)	O(2)-Ru(1)-C(26)-C(27)	131.7(3)
C(6)-C(7)-C(12)-Ru(1)	-9.0(5)	C(33)-Ru(1)-C(26)-C(27)	145.4(4)
N(1)-Ru(1)-C(12)-C(11)	-179.7(4)	C(25)-C(26)-C(27)-C(32)	-166.7(4)
C(25)-Ru(1)-C(12)-C(11)	-94.6(4)	Ru(1)-C(26)-C(27)-C(32)	111.6(4)
N(2)-Ru(1)-C(12)-C(11)	2.3(4)	C(25)-C(26)-C(27)-C(28)	12.9(6)
O(1)-Ru(1)-C(12)-C(11)	90.4(4)	Ru(1)-C(26)-C(27)-C(28)	-68.8(5)
C(26)-Ru(1)-C(12)-C(11)	-80.1(4)	C(32)-C(27)-C(28)-C(29)	-1.7(6)
O(2)-Ru(1)-C(12)-C(11)	108.5(4)	C(26)-C(27)-C(28)-C(29)	178.7(4)
C(33)-Ru(1)-C(12)-C(11)	96.8(4)	C(27)-C(28)-C(29)-C(30)	0.3(7)
N(1)-Ru(1)-C(12)-C(7)	5.1(3)	C(28)-C(29)-C(30)-C(31)	1.2(7)
C(25)-Ru(1)-C(12)-C(7)	90.2(3)	C(29)-C(30)-C(31)-C(32)	-1.2(7)
N(2)-Ru(1)-C(12)-C(7)	-173.0(3)	C(30)-C(31)-C(32)-C(27)	-0.3(7)
O(1)-Ru(1)-C(12)-C(7)	-84.9(3)	C(28)-C(27)-C(32)-C(31)	1.7(6)
C(26)-Ru(1)-C(12)-C(7)	104.7(3)	C(26)-C(27)-C(32)-C(31)	-178.7(4)
O(2)-Ru(1)-C(12)-C(7)	-66.8(4)	N(1)-Ru(1)-O(1)-C(33)	89.1(3)
C(33)-Ru(1)-C(12)-C(7)	-78.5(3)	C(12)-Ru(1)-O(1)-C(33)	168.7(3)
N(1)-Ru(1)-N(2)-C(13)	-31(4)	C(25)-Ru(1)-O(1)-C(33)	-1.4(4)
C(12)-Ru(1)-N(2)-C(13)	46.4(3)	N(2)-Ru(1)-O(1)-C(33)	-91.4(3)
C(25)-Ru(1)-N(2)-C(13)	162.0(3)	C(26)-Ru(1)-O(1)-C(33)	-144.7(6)
O(1)-Ru(1)-N(2)-C(13)	-45.4(3)	O(2)-Ru(1)-O(1)-C(33)	-0.6(2)
C(26)-Ru(1)-N(2)-C(13)	124.2(3)	Ru(1)-O(1)-C(33)-O(2)	1.1(4)
O(2)-Ru(1)-N(2)-C(13)	-104.3(3)	Ru(1)-O(1)-C(33)-C(34)	-178.1(4)
C(33)-Ru(1)-N(2)-C(13)	-74.6(3)	N(1)-Ru(1)-C(33)-O(1)	-90.9(2)
N(1)-Ru(1)-N(2)-C(18)	152(4)	C(12)-Ru(1)-C(33)-O(1)	-13.2(3)
C(12)-Ru(1)-N(2)-C(18)	-130.4(3)	C(25)-Ru(1)-C(33)-O(1)	179.2(2)
C(25)-Ru(1)-N(2)-C(18)	-14.8(3)	N(2)-Ru(1)-C(33)-O(1)	87.7(2)
O(1)-Ru(1)-N(2)-C(18)	137.8(3)	C(26)-Ru(1)-C(33)-O(1)	157.8(4)

C(26)-Ru(1)-N(2)-C(18)	-52.6(3)	O(2)-Ru(1)-C(33)-O(1)	178.9(4)
O(2)-Ru(1)-N(2)-C(18)	78.9(3)	N(1)-Ru(1)-C(33)-O(2)	90.2(2)
C(33)-Ru(1)-N(2)-C(18)	108.6(3)	C(12)-Ru(1)-C(33)-O(2)	167.9(2)
C(18)-N(2)-C(13)-C(14)	5.4(6)	C(25)-Ru(1)-C(33)-O(2)	0.3(3)
Ru(1)-N(2)-C(13)-C(14)	-171.7(3)	N(2)-Ru(1)-C(33)-O(2)	-91.2(2)
N(2)-C(13)-C(14)-C(15)	3.1(7)	O(1)-Ru(1)-C(33)-O(2)	-178.9(4)
C(13)-C(14)-C(15)-C(16)	-4.4(6)	C(26)-Ru(1)-C(33)-O(2)	-21.1(5)
C(14)-C(15)-C(16)-C(18)	-2.3(6)	N(1)-Ru(1)-C(33)-C(34)	-66(5)
C(14)-C(15)-C(16)-C(17)	177.6(4)	C(12)-Ru(1)-C(33)-C(34)	12(5)
C(13)-N(2)-C(18)-C(16)	-12.3(6)	C(25)-Ru(1)-C(33)-C(34)	-156(5)
Ru(1)-N(2)-C(18)-C(16)	164.5(3)	N(2)-Ru(1)-C(33)-C(34)	113(5)
C(13)-N(2)-C(18)-C(19)	162.5(4)	O(1)-Ru(1)-C(33)-C(34)	25(5)
Ru(1)-N(2)-C(18)-C(19)	-20.7(5)	C(26)-Ru(1)-C(33)-C(34)	-177(5)
C(15)-C(16)-C(18)-N(2)	10.8(6)	O(2)-Ru(1)-C(33)-C(34)	-156(5)
C(17)-C(16)-C(18)-N(2)	-169.1(4)	O(1)-C(33)-O(2)-Ru(1)	-1.1(4)
C(15)-C(16)-C(18)-C(19)	-163.8(4)	C(34)-C(33)-O(2)-Ru(1)	178.2(4)
C(17)-C(16)-C(18)-C(19)	16.3(6)	N(1)-Ru(1)-O(2)-C(33)	-89.8(2)
N(2)-C(18)-C(19)-C(20)	-138.4(4)	C(12)-Ru(1)-O(2)-C(33)	-20.6(4)
C(16)-C(18)-C(19)-C(20)	36.3(6)	C(25)-Ru(1)-O(2)-C(33)	-179.7(3)
N(2)-C(18)-C(19)-C(24)	33.1(6)	N(2)-Ru(1)-O(2)-C(33)	88.4(2)
C(16)-C(18)-C(19)-C(24)	-152.2(4)	O(1)-Ru(1)-O(2)-C(33)	0.6(2)
C(24)-C(19)-C(20)-C(21)	2.1(6)	C(26)-Ru(1)-O(2)-C(33)	170.6(2)



7e


1H NMR
PPM
10
8
6
4
2
0
1.00
1.02
0.94
3.17
1.07
0.06
1.81
0.06
1.01
0.06
4.17
2.00
2.99
2.03
2.95
8.719
8.717
8.714
8.709
8.706
8.705
7.737
7.733
7.718
7.714
7.699
7.694
7.419
7.399
7.259
7.256
7.252
7.247
7.244
7.240
7.237
7.233
7.228
7.225
7.221
7.214
7.201
7.166
7.135
7.116
5.941
5.902
5.879
5.860
5.839
5.821
5.036
5.018
5.001
2.098
2.082
2.063
2.050
2.028
1.924
1.906
1.888
1.870
1.860
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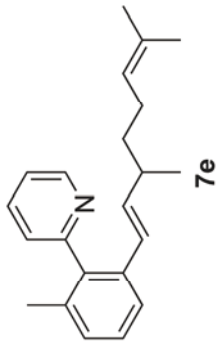
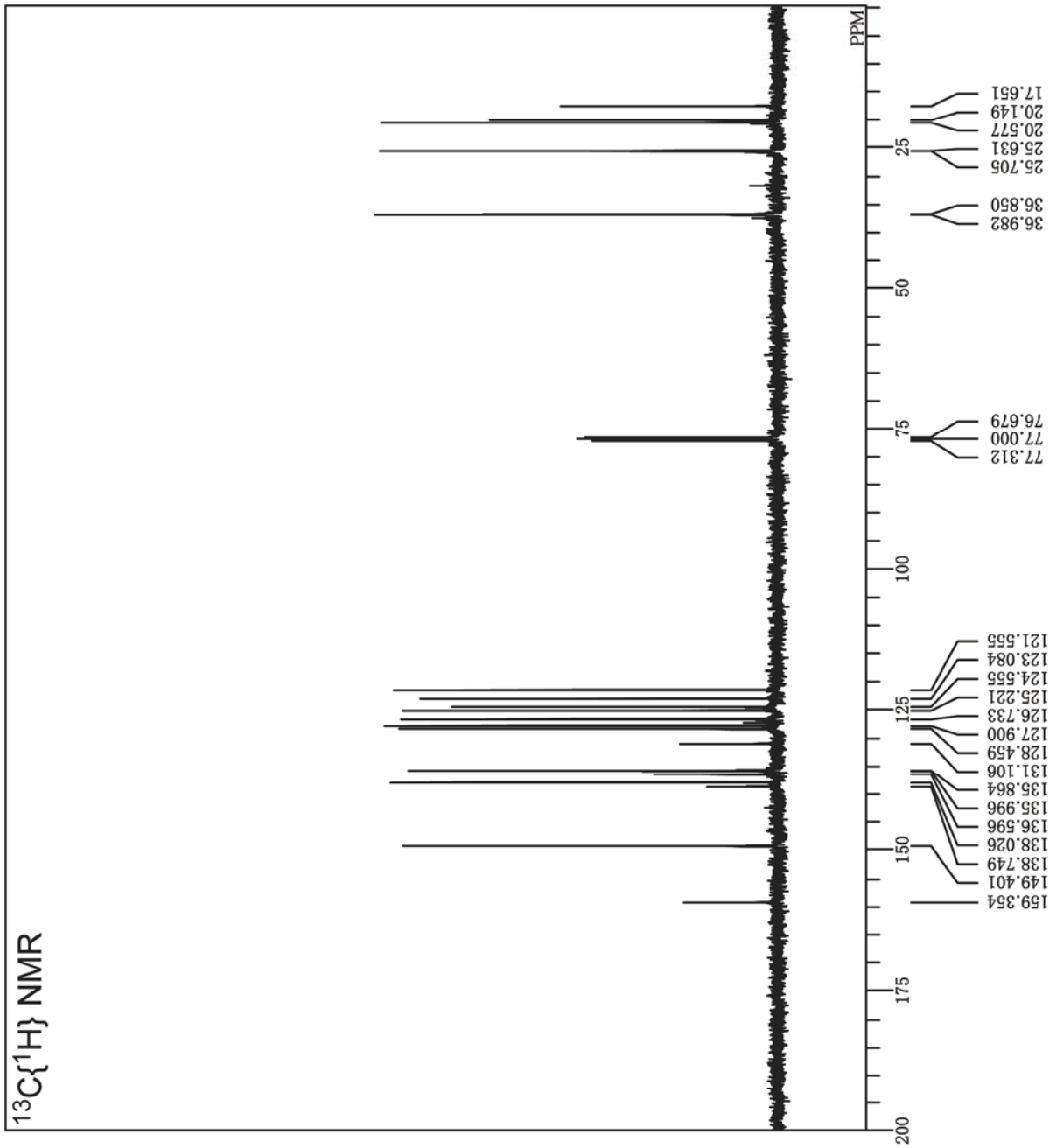
1.804
1.647
1.535
1.295
1.276
1.258
1.239
0.918
0.902


N
7e


$^{13}C\{^{1}H\}$ NMR
PPM
200
175
150
125
100
75
50
25
17.651
20.149
20.577
25.631
25.705
36.850
36.982
76.679
77.000
77.312
121.555
123.084
124.555
125.221
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128.459
131.106
135.864
135.996
136.596
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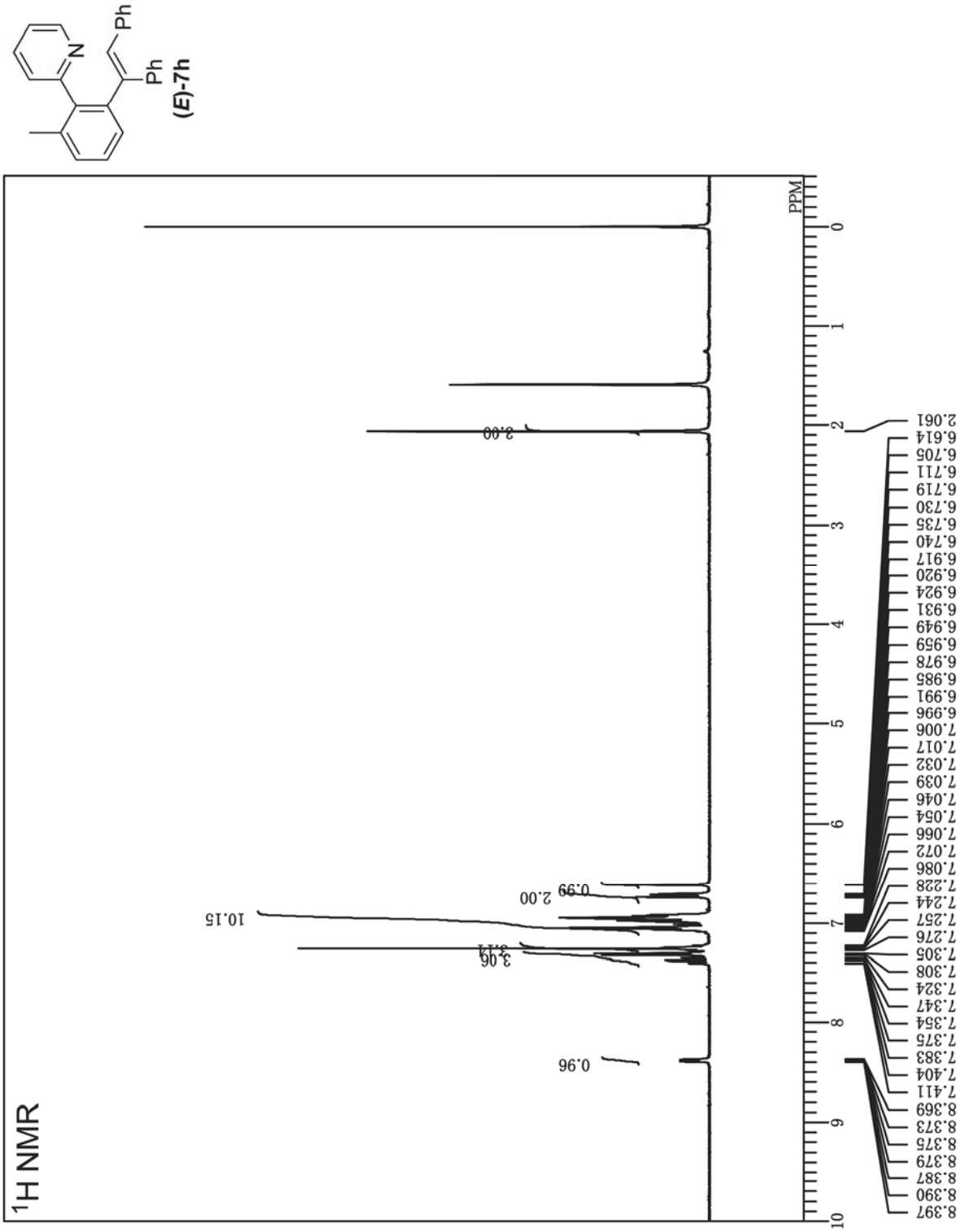
138.749
149.401
159.354


Ph
Ph
N
(E)-7h
1H NMR
PPM
0.96
3.06
3.14
10.15
0.99
2.00
3.00
2.061
6.614
6.705
6.711
6.719
6.730
6.735
6.740
6.917
6.920
6.924
6.931
6.949
6.959
6.978
6.985
6.991
6.996
7.006
7.017
7.032
7.039
7.046
7.054
7.066
7.072
7.086
7.228
7.244
7.257
7.276
7.305
7.308
7.324
7.347
7.354
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7.404
7.411
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8.373
8.375
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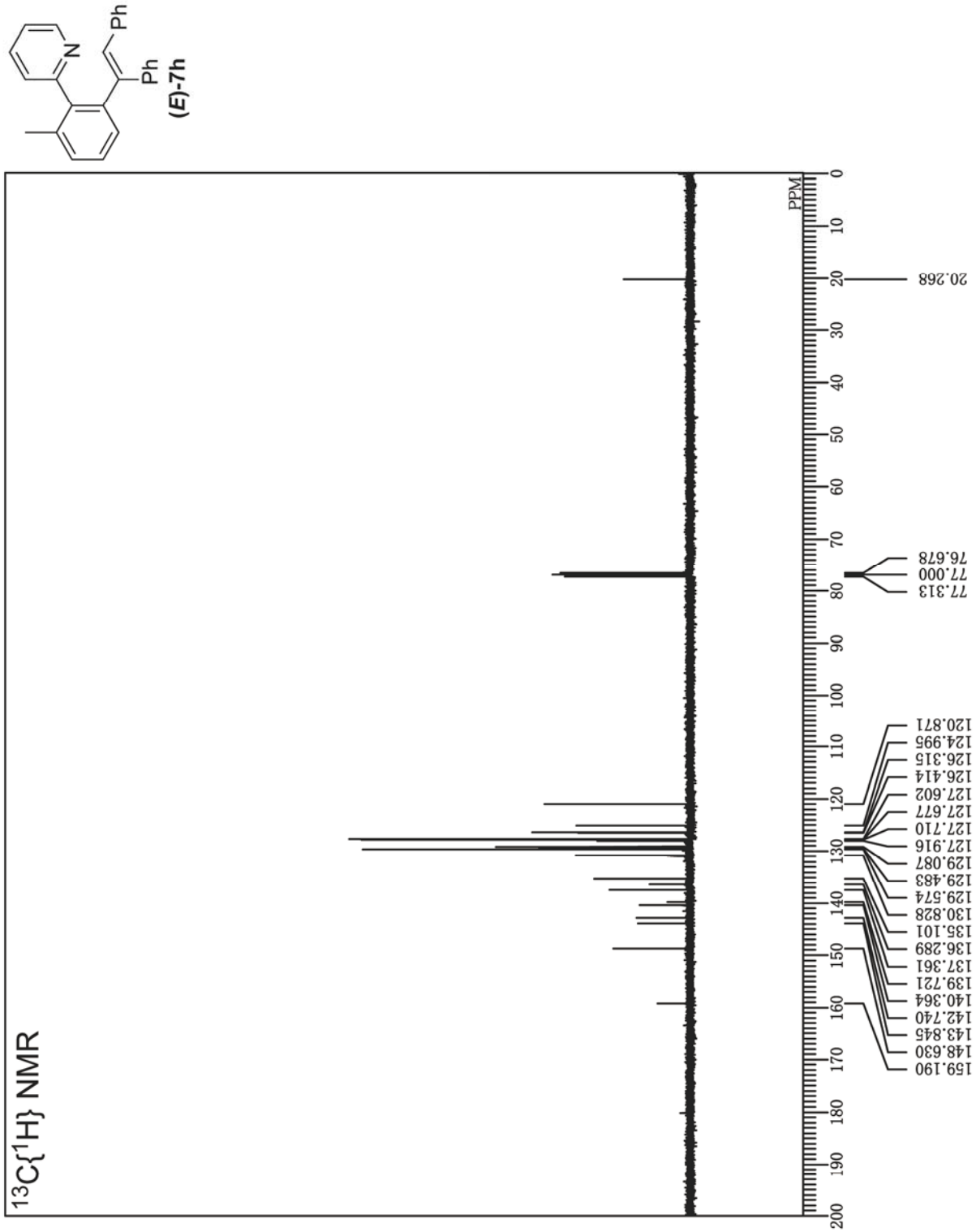
8.387
8.390
8.397


(E)-7h
13C{1H} NMR
PPM
20.268
76.678
77.000
77.313
120.871
124.995
126.315
126.414
127.602
127.677
127.710
127.916
129.087
129.483
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136.289
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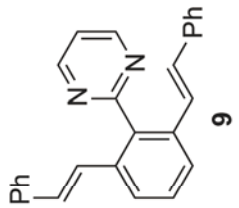
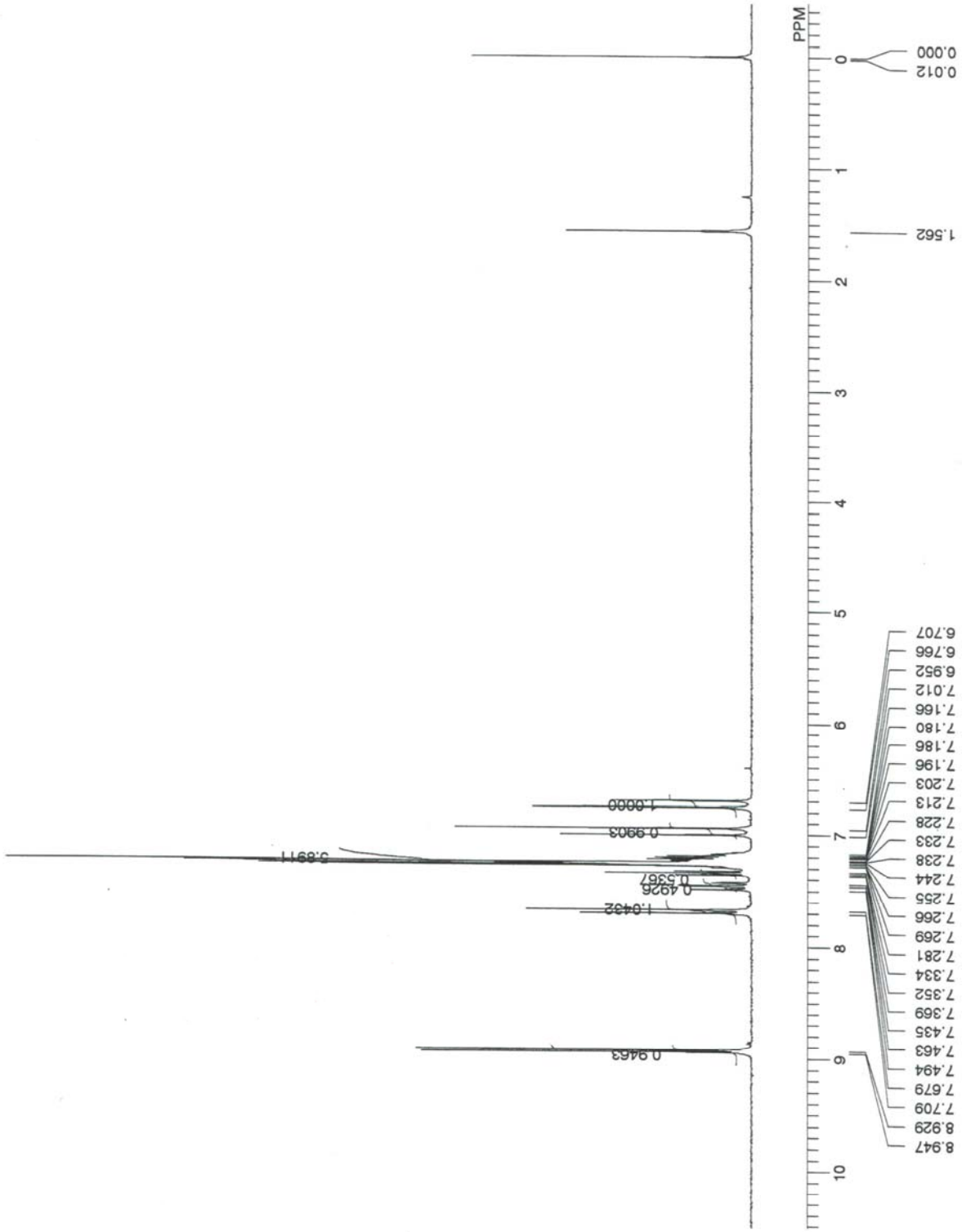
159.190


Ph
N
N
Ph

9

^{1}H NMR


PPM
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8.929
7.709
7.679
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7.463
7.435
7.369
7.352
7.334
7.281
7.269
7.266
7.255
7.244
7.238
7.233
7.228
7.213
7.203
7.196
7.186
7.180
7.166
7.012
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6.707
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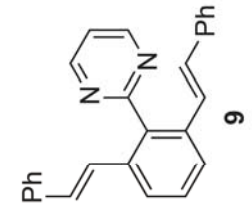
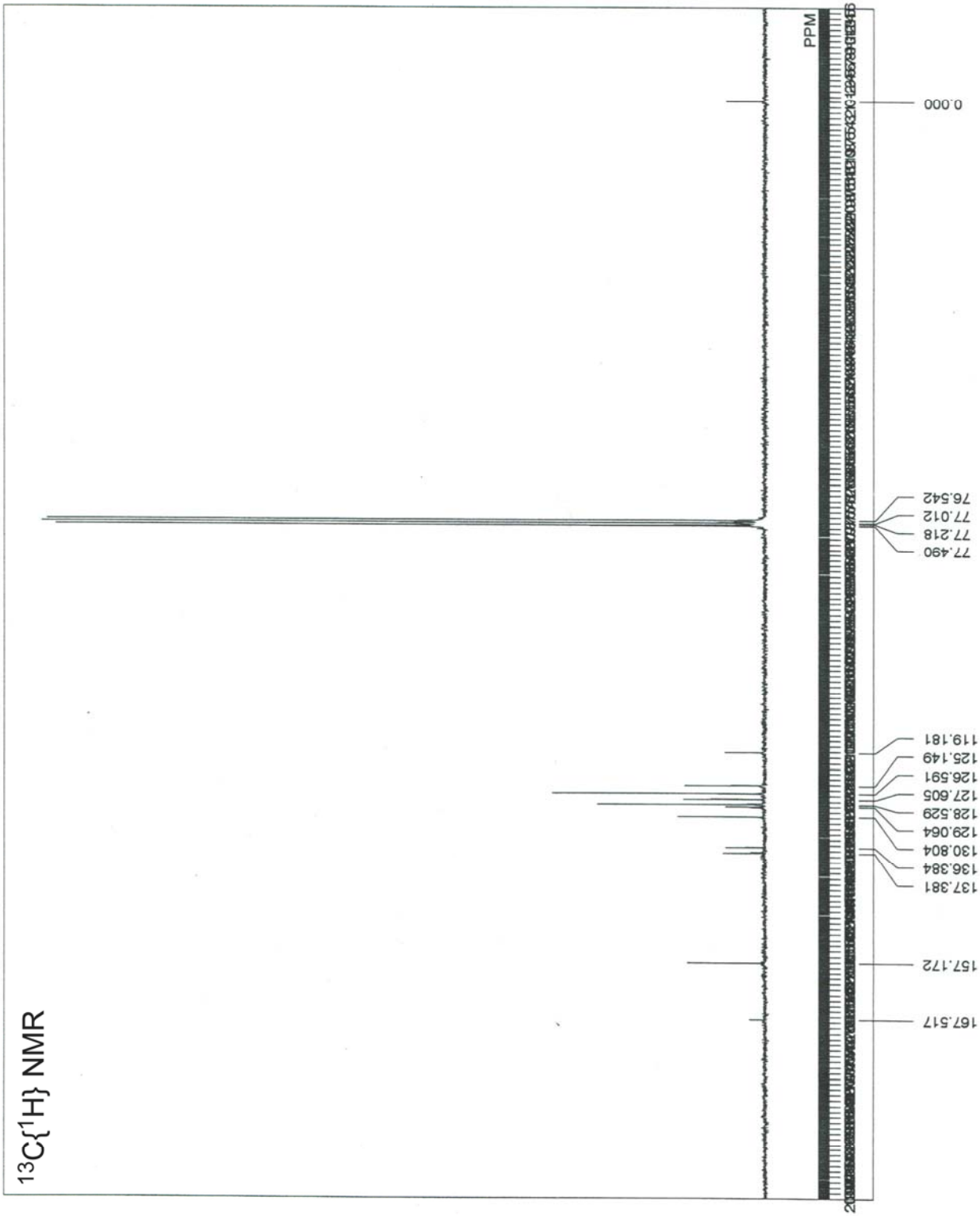
0.5567
0.4926
1.0432
0.9463


Ph
N
N
Ph
6


$^{13}C\{^{1}H\}$ NMR
PPM
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77.012
77.218
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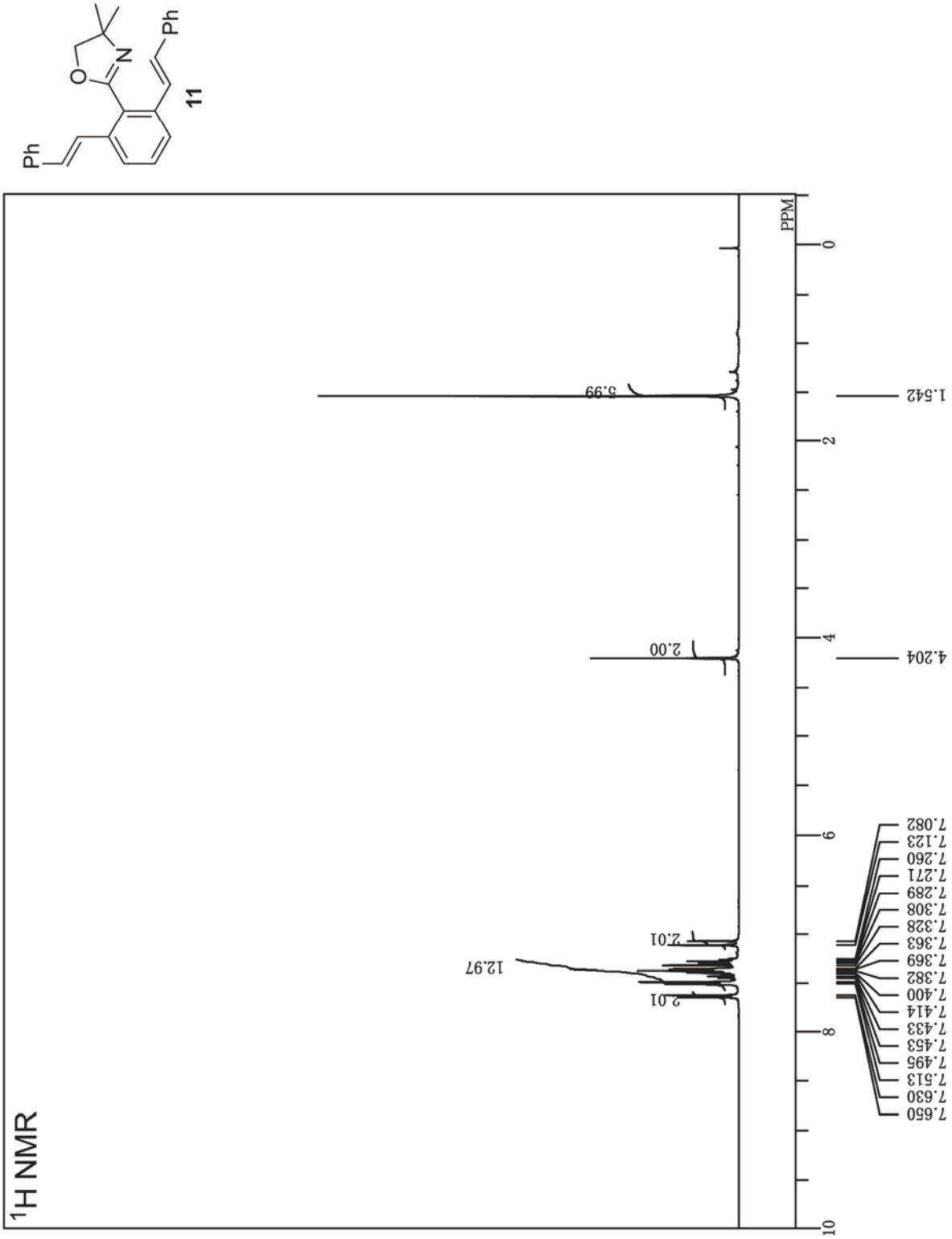
125.149
126.591
127.605
128.529
129.064
130.804
136.384
137.381
157.172
167.517


Ph
Ph
O
N
11
1H NMR
PPM
10
8
6
4
2
0
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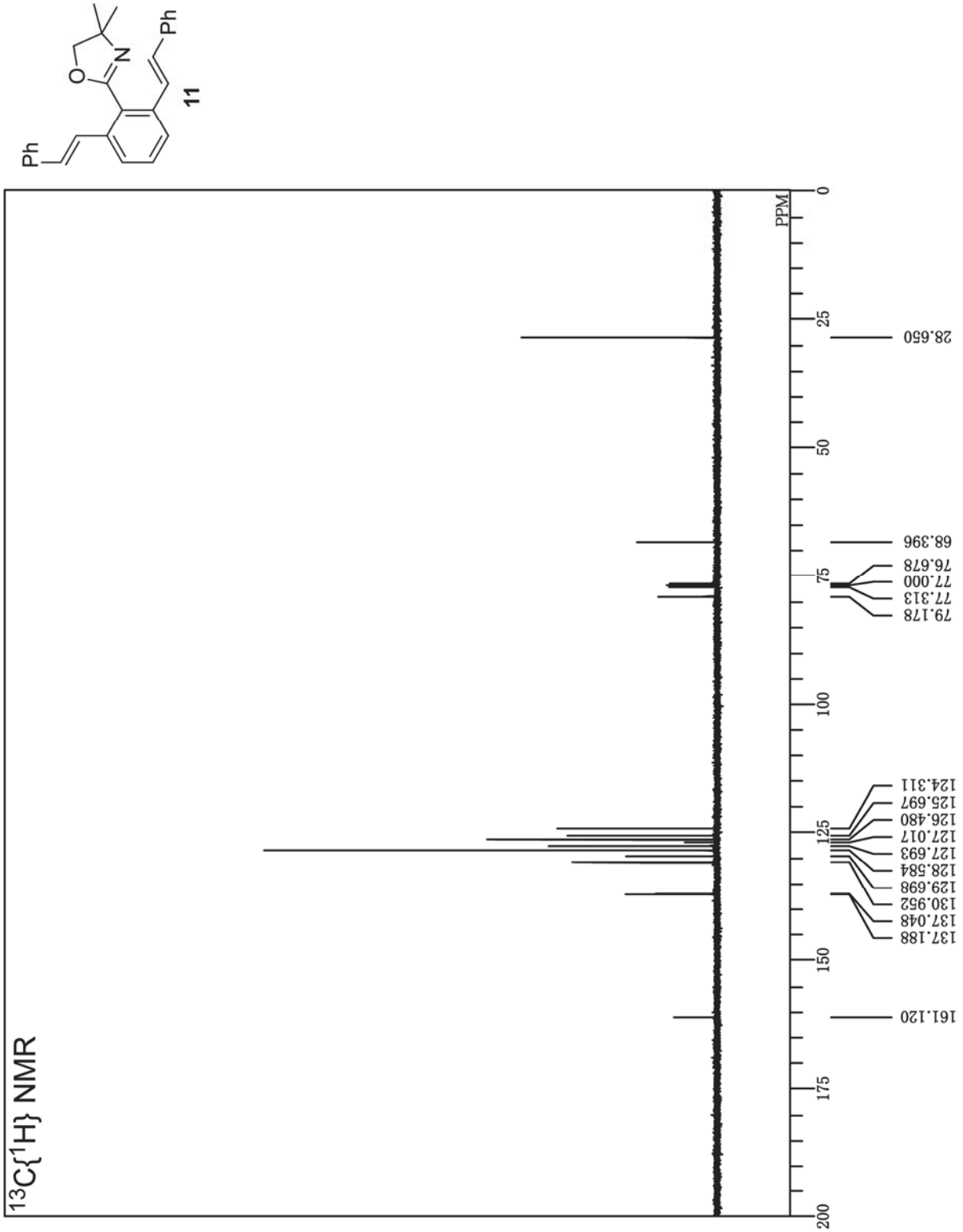
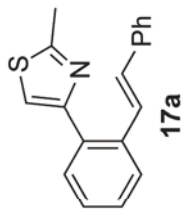
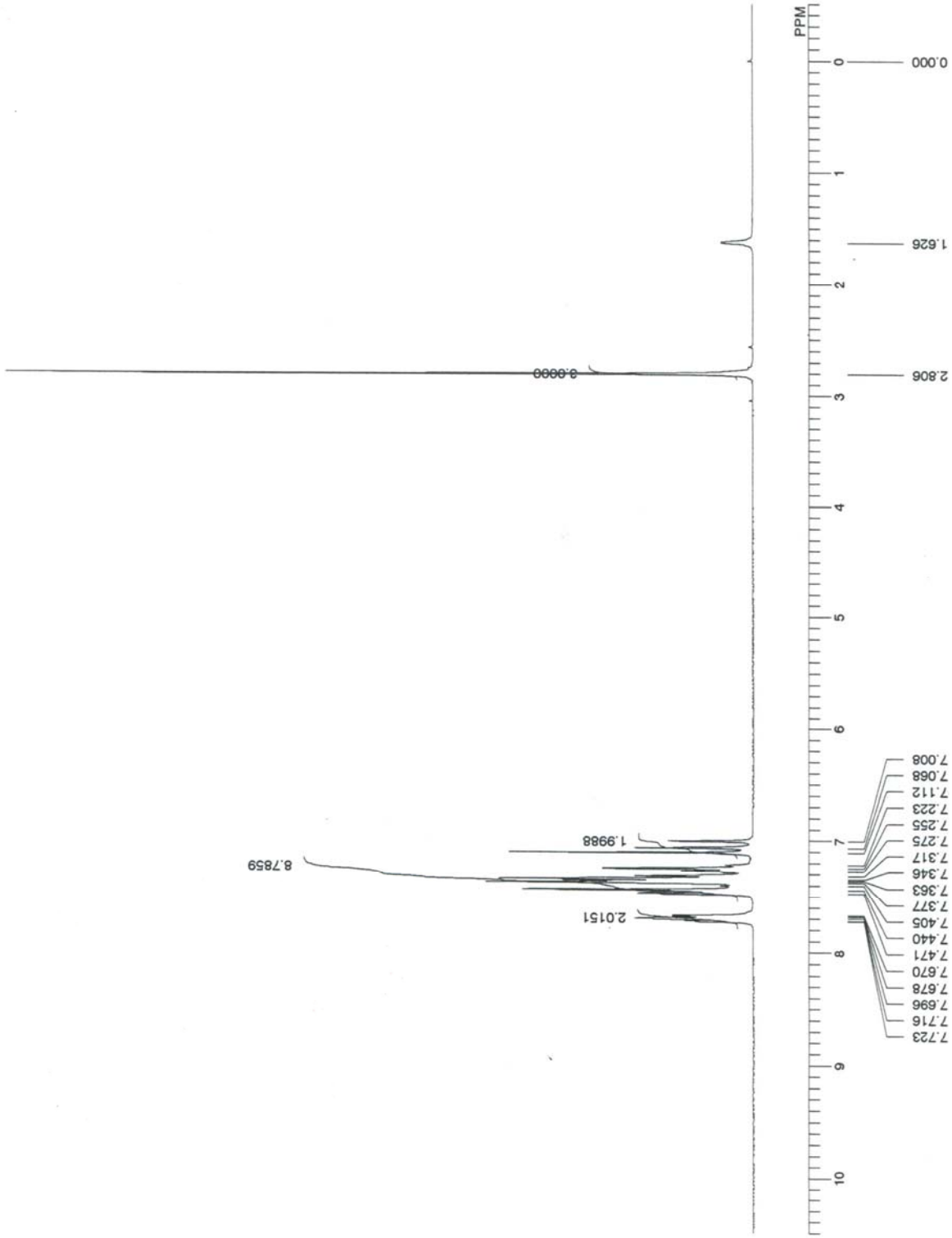
7.630
7.513
7.495
7.453
7.433
7.414
7.400
7.382
7.369
7.363
7.328
7.308
7.289
7.271
7.260
7.123
7.082
4.204
1.542
2.01
12.97
2.01
2.00
5.99


Ph
Ph
N
O
11
13C{1H} NMR
PPM
0
25
50
75
100
125
150
175
200
28.650
68.396
76.678
77.000
77.313
79.178
124.311
125.697
126.480
127.017
127.693
128.584
129.698
130.952
137.048
137.188
161.120


S
N
Ph

17a

^{1}H NMR


PPM
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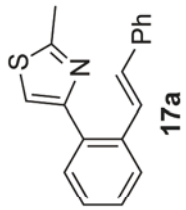
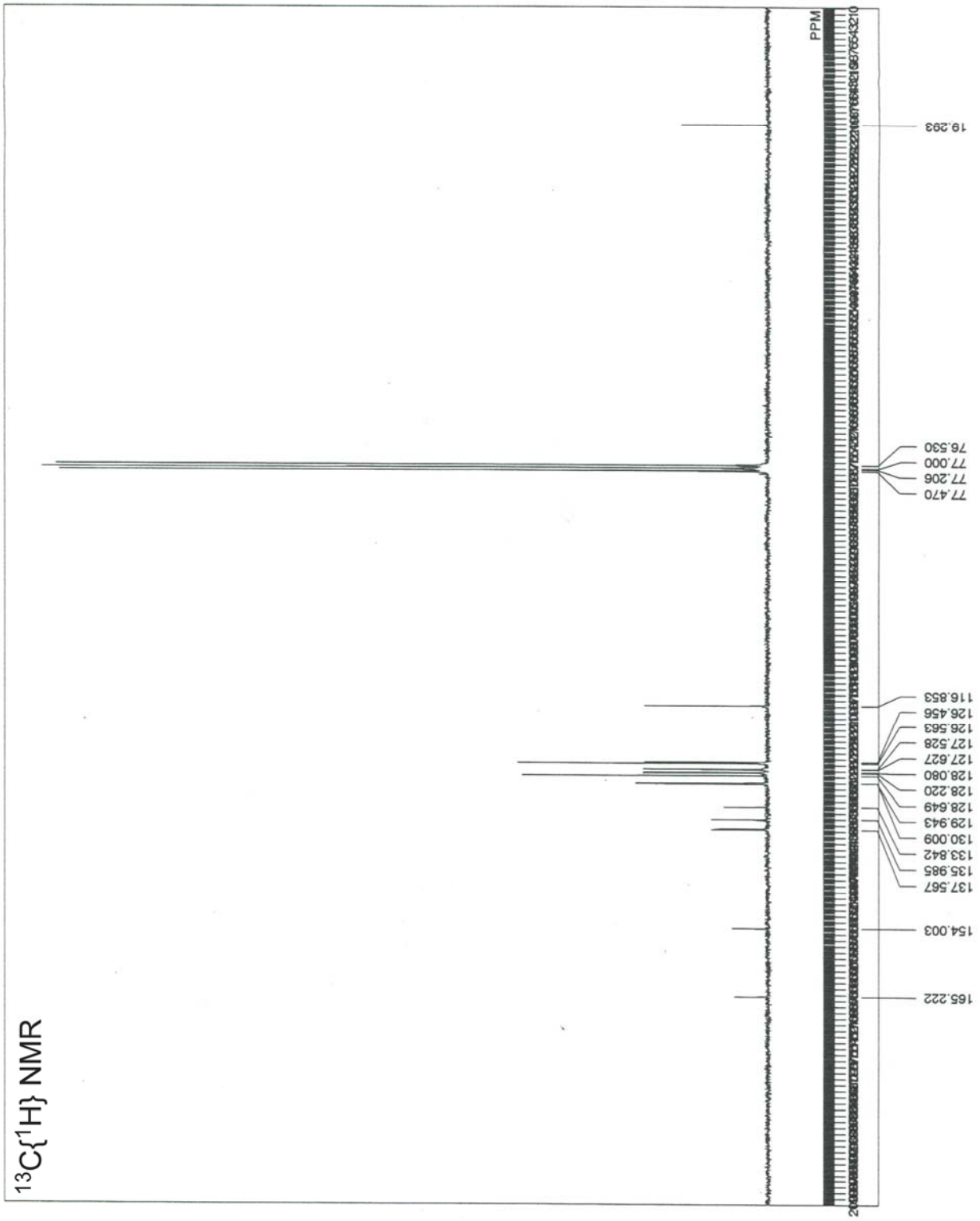
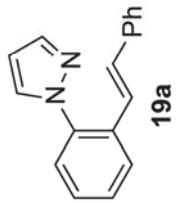
3.0000
1.9988
8.7859
2.0151
7.723
7.716
7.696
7.678
7.670
7.471
7.440
7.405
7.377
7.363
7.346
7.317
7.275
7.255
7.223
7.112
7.068
7.008

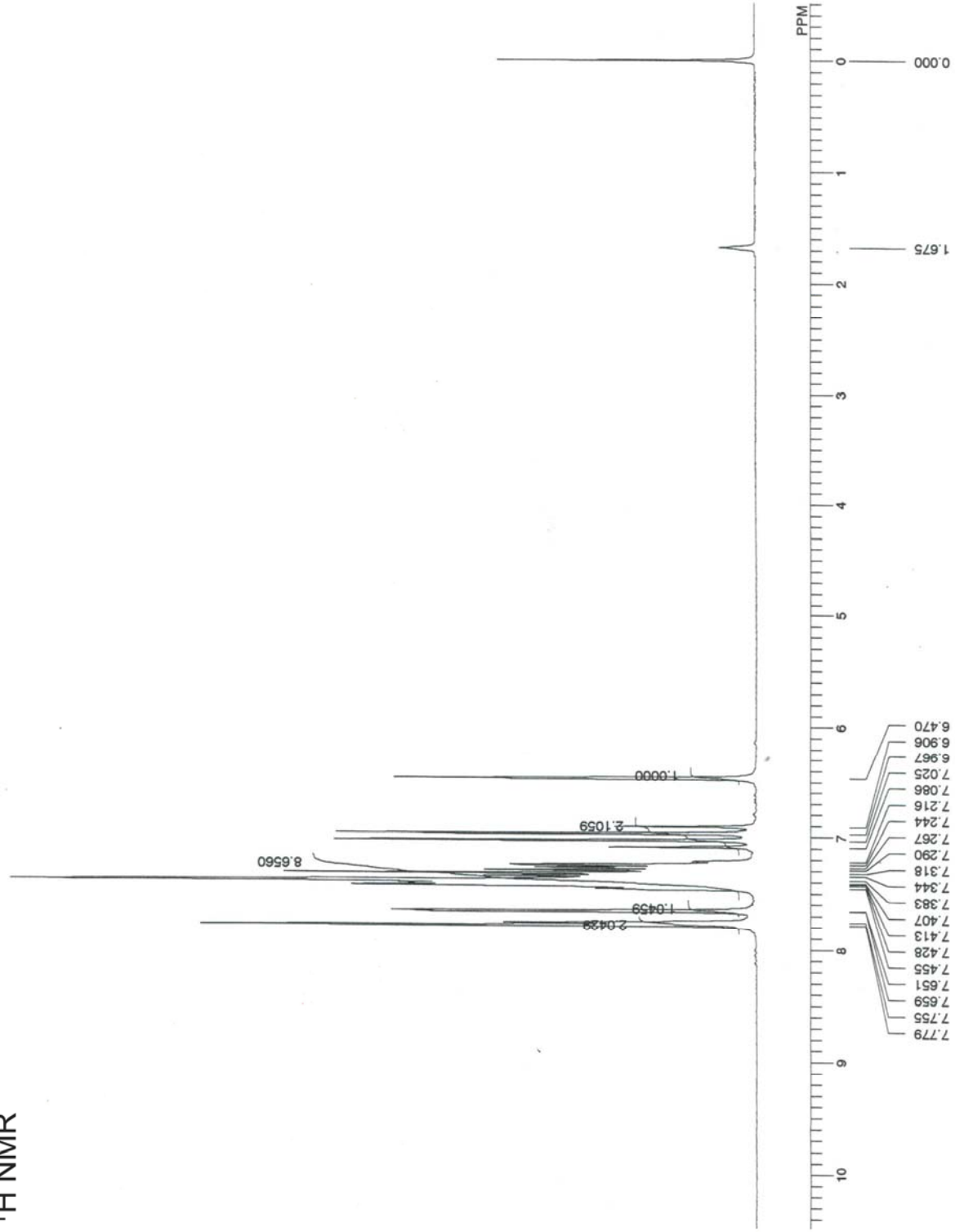

S
N
Ph

17a

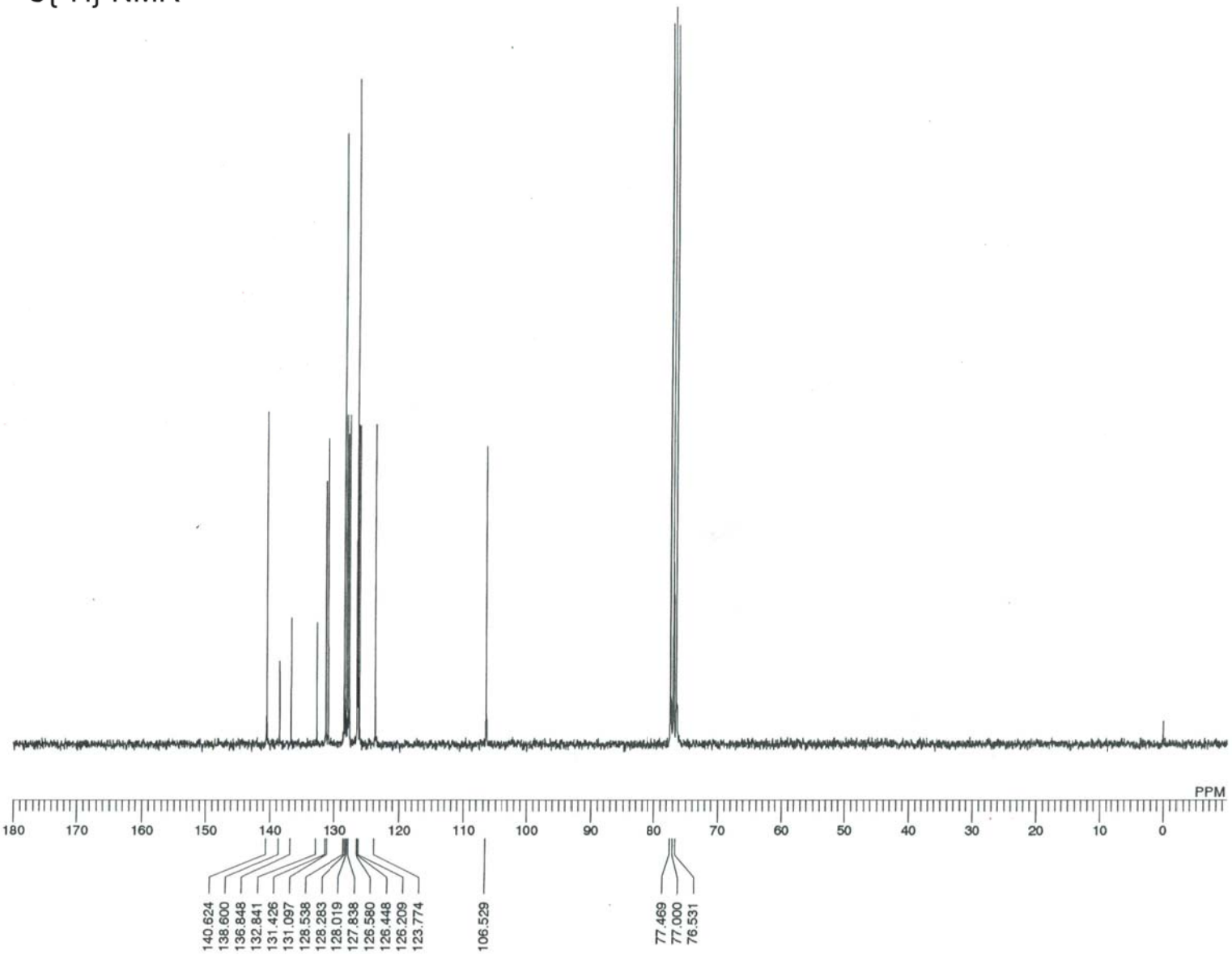

$^{13}C\{^{1}H\}$ NMR
PPM
19.293
76.530
77.000
77.206
77.470
116.853
126.456
126.563
127.528
127.627
128.080
128.220
128.649
129.943
130.009
133.842
135.985
137.567
154.003
165.222

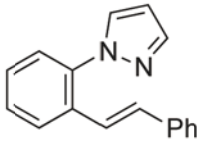

Ph
N
N
19a

^{1}H NMR

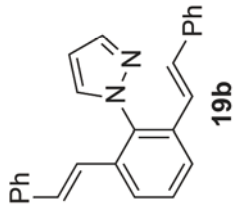

PPM
0.000
1.675
6.470
6.906
6.967
7.025
7.086
7.216
7.244
7.267
7.290
7.318
7.344
7.383
7.407
7.413
7.428
7.455
7.651
7.659
7.755
7.779
1.0000
2.1059
8.6560
1.0459
2.0429

$^{13}C\{^{1}H\}$ NMR

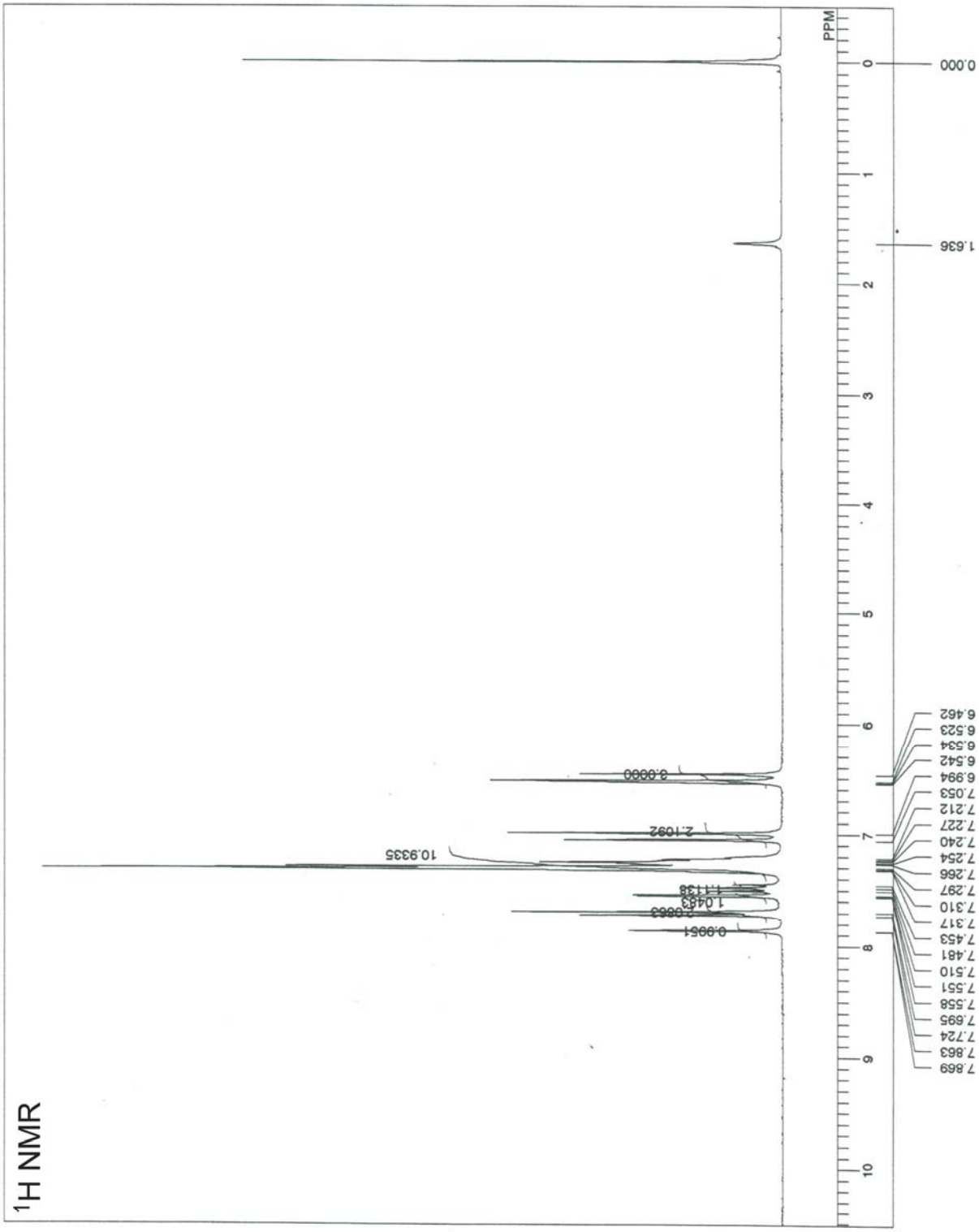


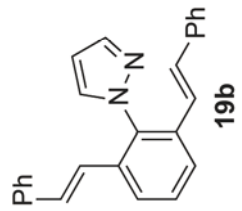


19a


Ph
N
N
Ph

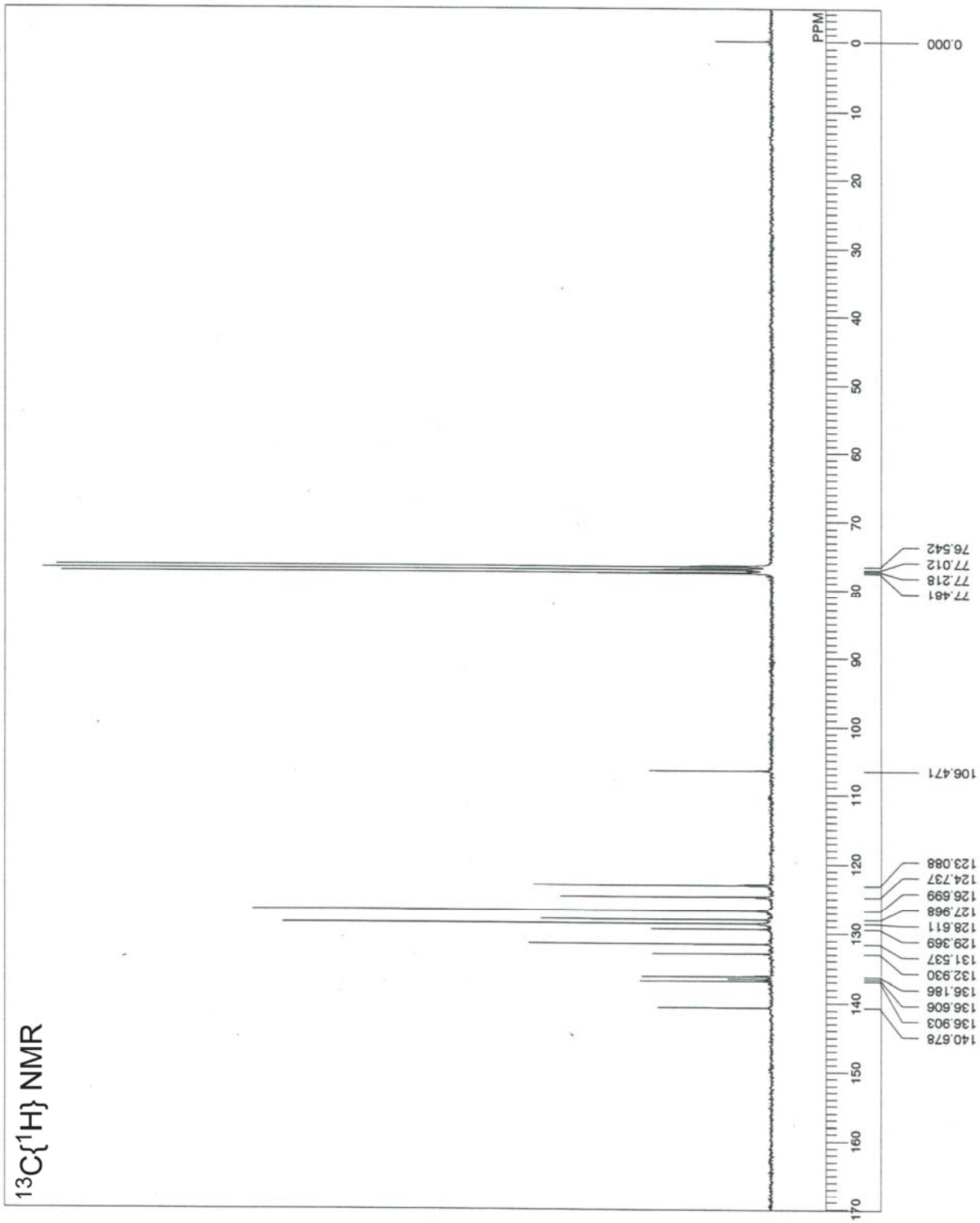
19b

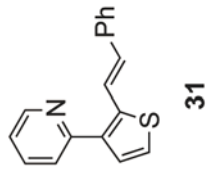

^{1}H NMR
PPM
0.000
1.636
6.462
6.523
6.534
6.542
6.994
7.053
7.212
7.227
7.240
7.254
7.266
7.297
7.310
7.317
7.453
7.481
7.510
7.551
7.558
7.695
7.724
7.863
7.869
0.0000
2.1092
10.9335
0.0061
2.0863
1.0483
1.1138



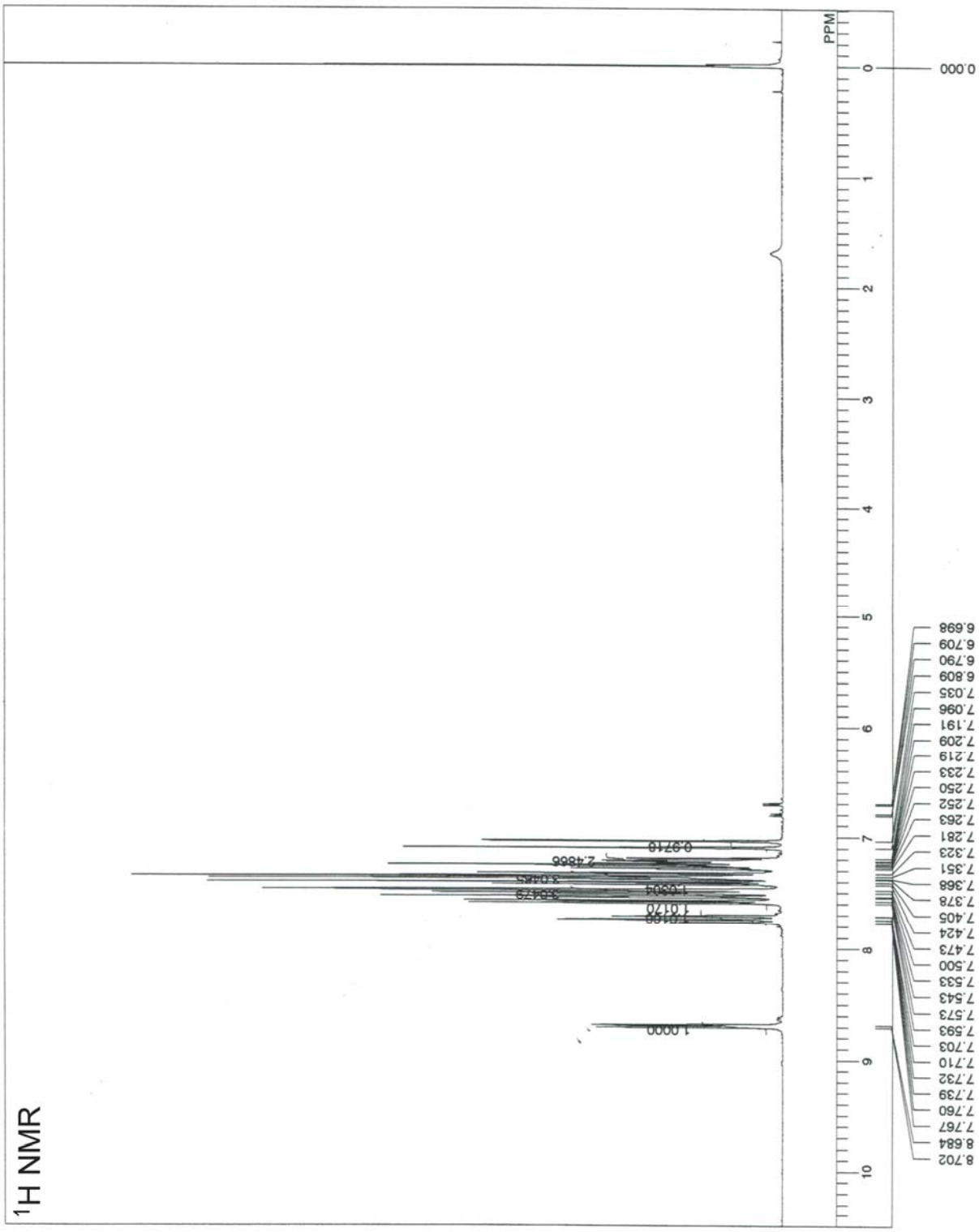
19b

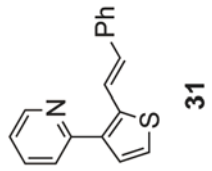
$^{13}C\{^{1}H\}$ NMR



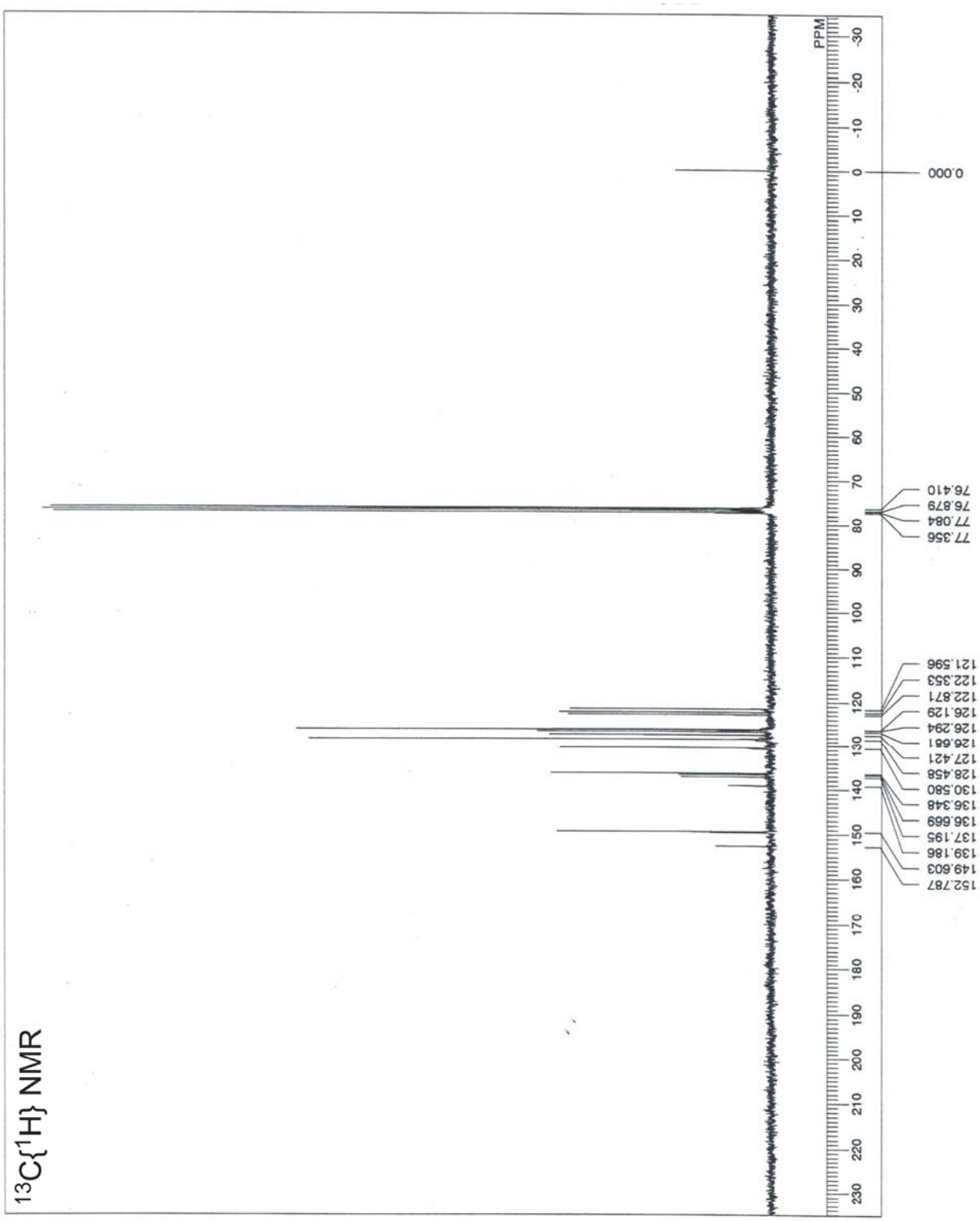

Ph
N
S

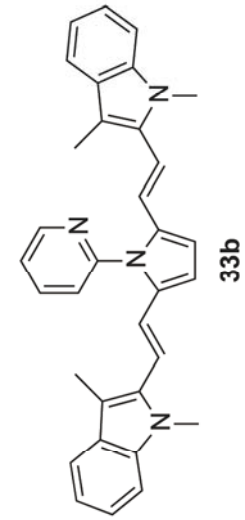
31


^{1}H NMR
PPM
0.000
6.698
6.709
6.790
6.809
7.035
7.096
7.191
7.209
7.219
7.233
7.250
7.252
7.263
7.281
7.323
7.351
7.368
7.378
7.405
7.424
7.473
7.500
7.533
7.543
7.573
7.593
7.703
7.710
7.732
7.739
7.760
7.767
8.684
8.702
1.0000
0.9710
2.1866
3.0465
3.0429
1.0804
1.0170
1.0159

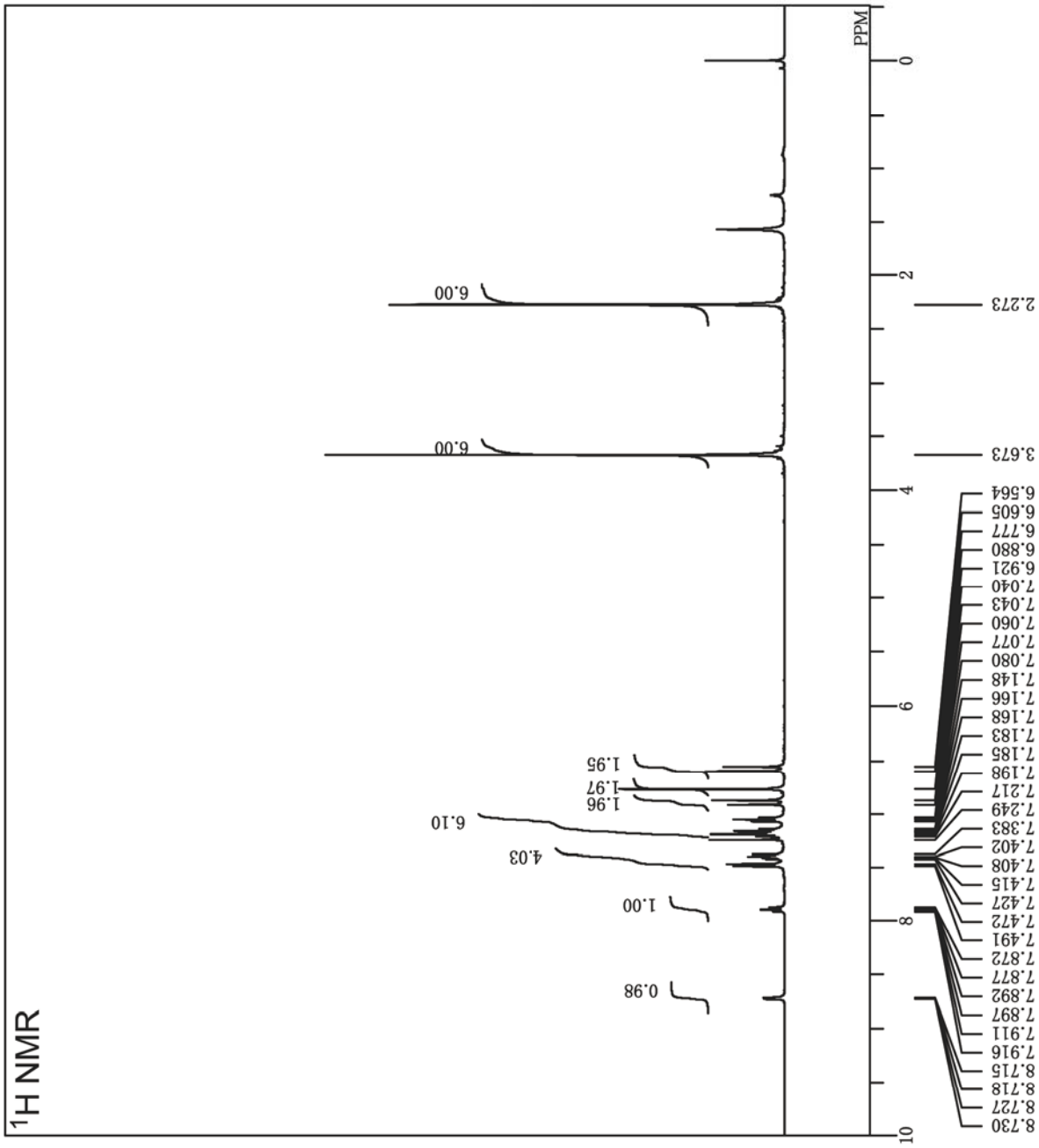

Ph
N
S

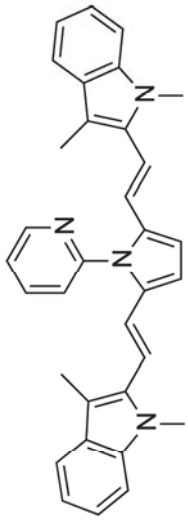
31


$^{13}C\{^{1}H\}$ NMR
PPM
0.000
76.410
76.879
77.084
77.356
121.596
122.353
122.871
126.129
126.294
126.661
127.421
128.458
130.580
136.348
136.669
137.195
139.186
149.603
152.787

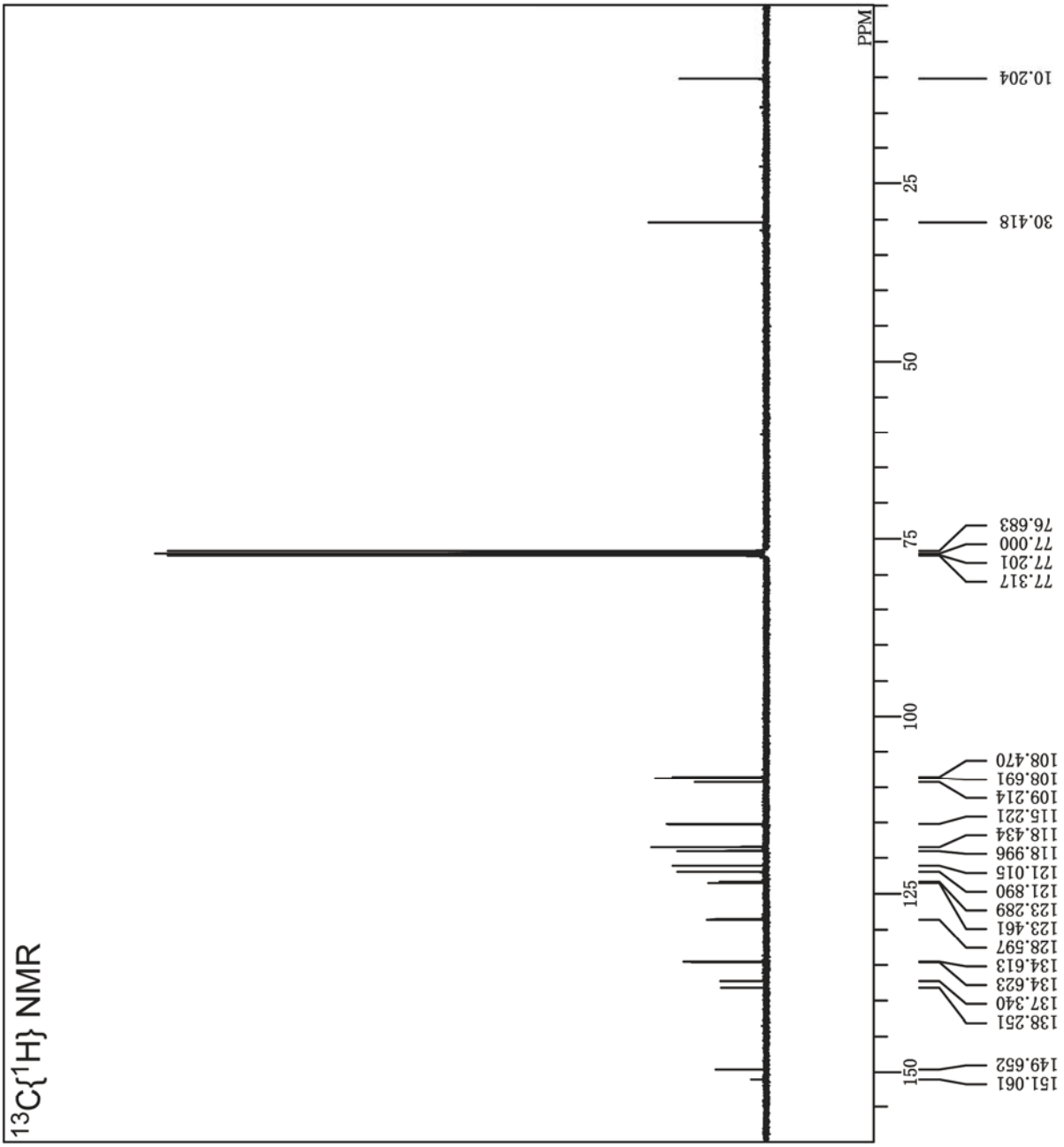


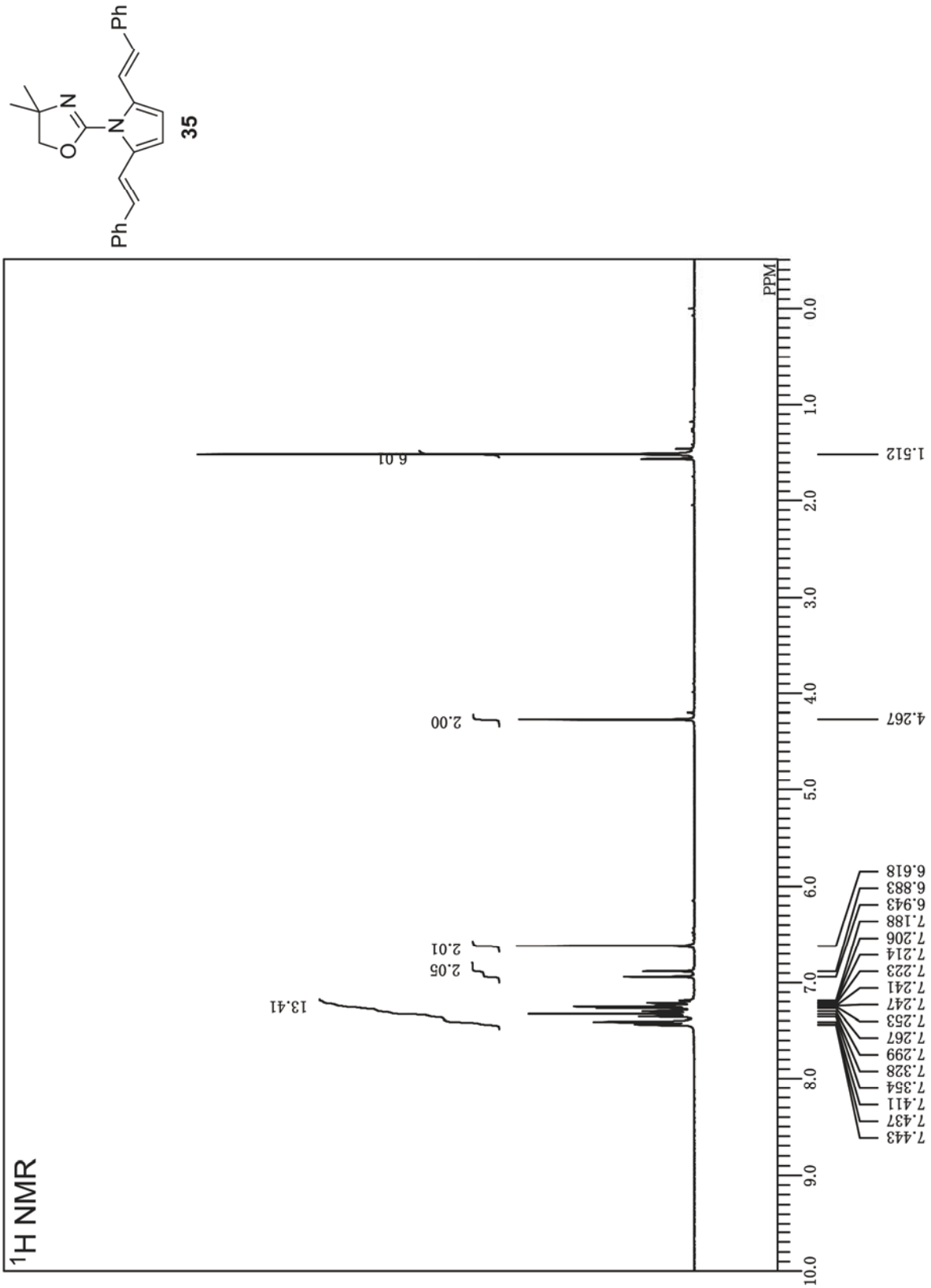
33b

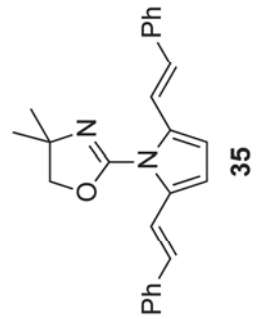

^{1}H NMR
PPM
0
2
4
6
8
10
0.98
1.00
4.03
6.10
1.96
1.97
1.95
6.00
6.00
2.273
3.673
6.564
6.605
6.777
6.880
6.921
7.040
7.043
7.060
7.077
7.080
7.148
7.166
7.168
7.183
7.185
7.198
7.217
7.249
7.383
7.402
7.408
7.415
7.427
7.472
7.491
7.872
7.877
7.892
7.897
7.911
7.916
8.715
8.718
8.727
8.730



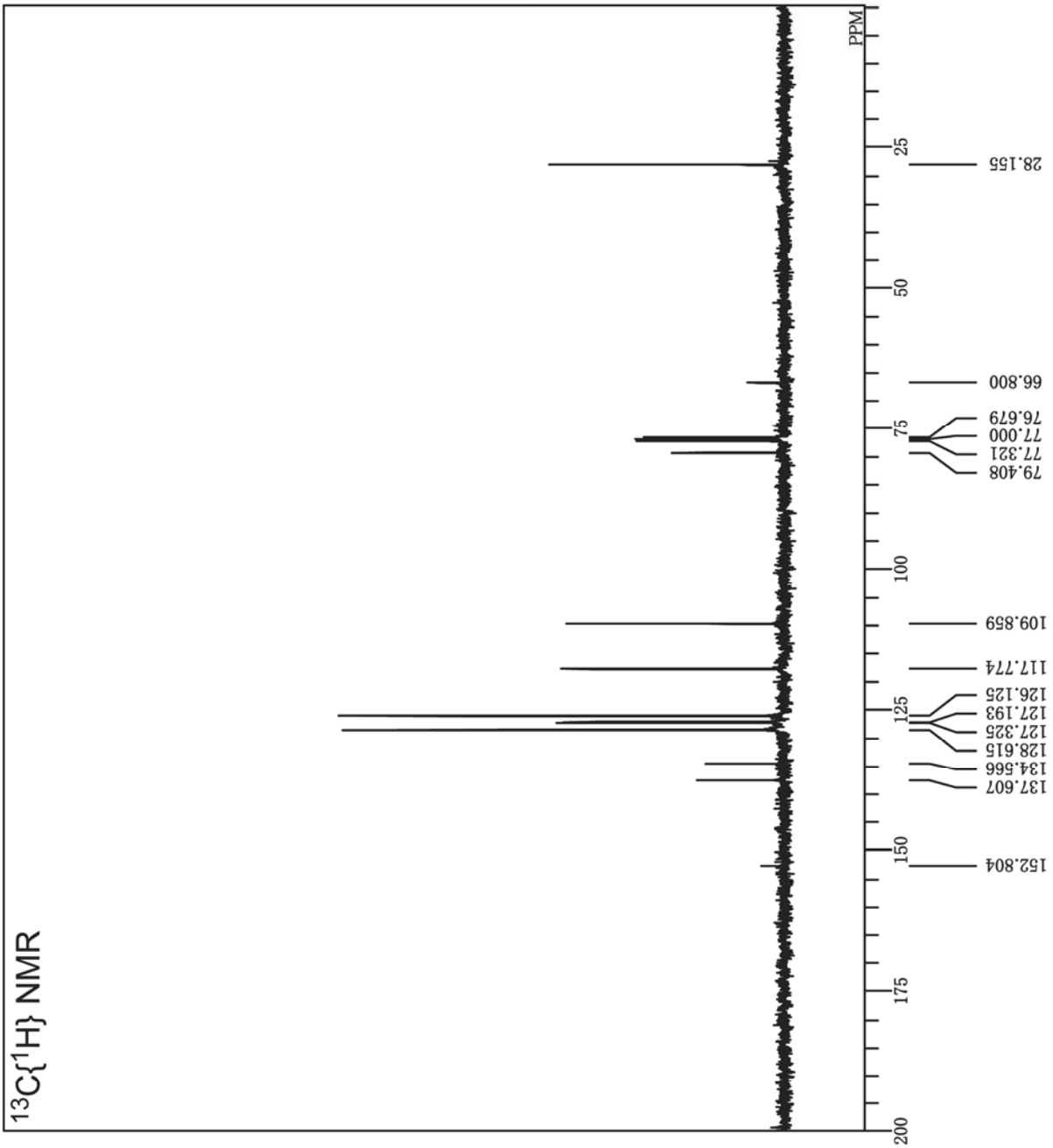
33b

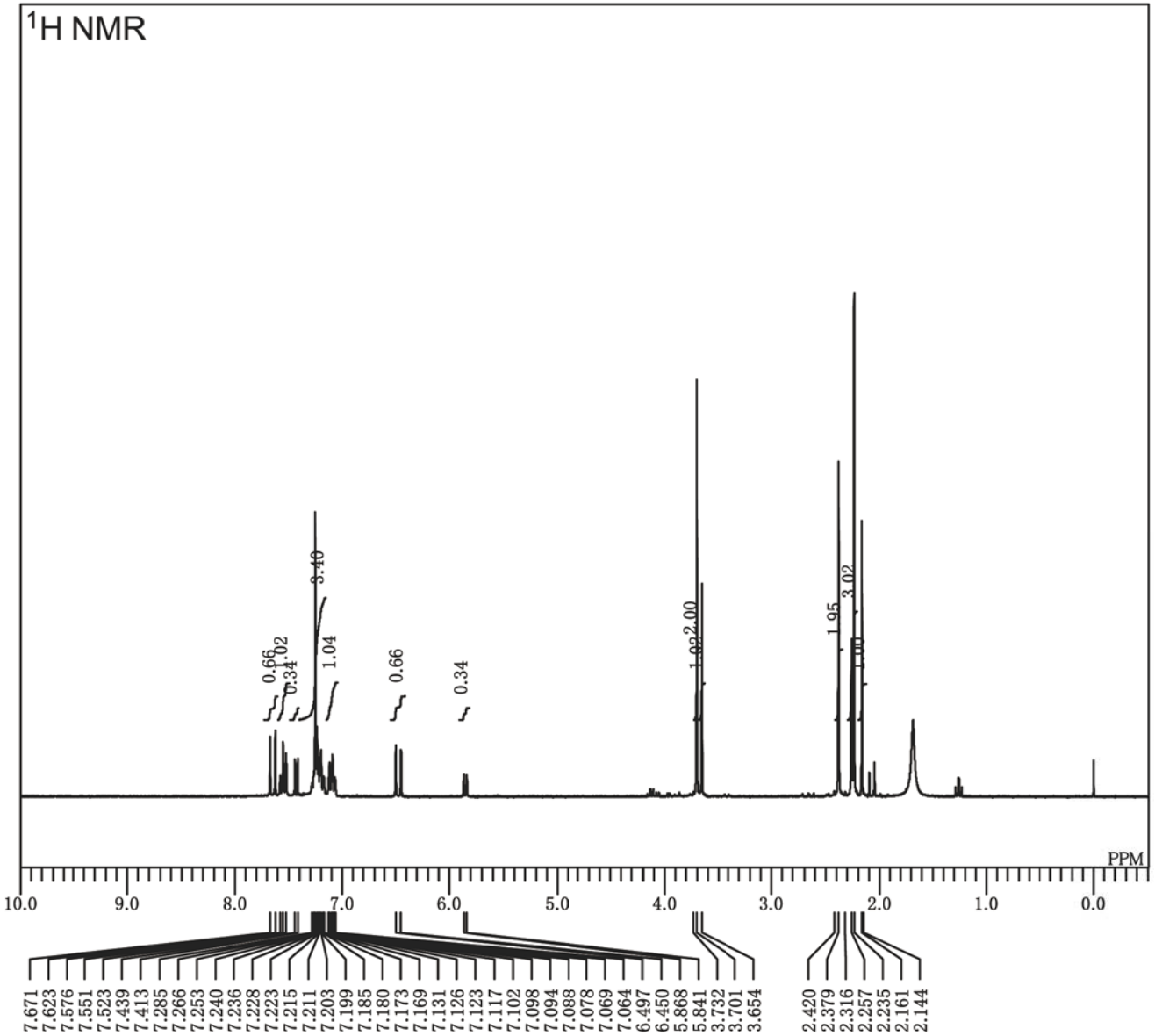

$^{13}C\{^{1}H\}$ NMR
PPM
10.204
30.418
76.683
77.000
77.201
77.317
108.470
108.691
109.214
115.221
118.434
118.996
121.015
121.890
123.289
123.461
128.597
134.613
134.623
137.340
138.251
149.652
151.061

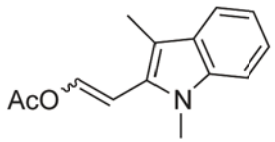

35
Ph
Ph
N
N
O
1H NMR
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
7.443
7.437
7.411
7.354
7.328
7.299
7.267
7.253
7.247
7.241
7.223
7.214
7.206
7.188
6.943
6.883
6.618
4.267
1.512
13.41
2.05
2.01
2.00
6.01


Ph
N
N
O
Ph

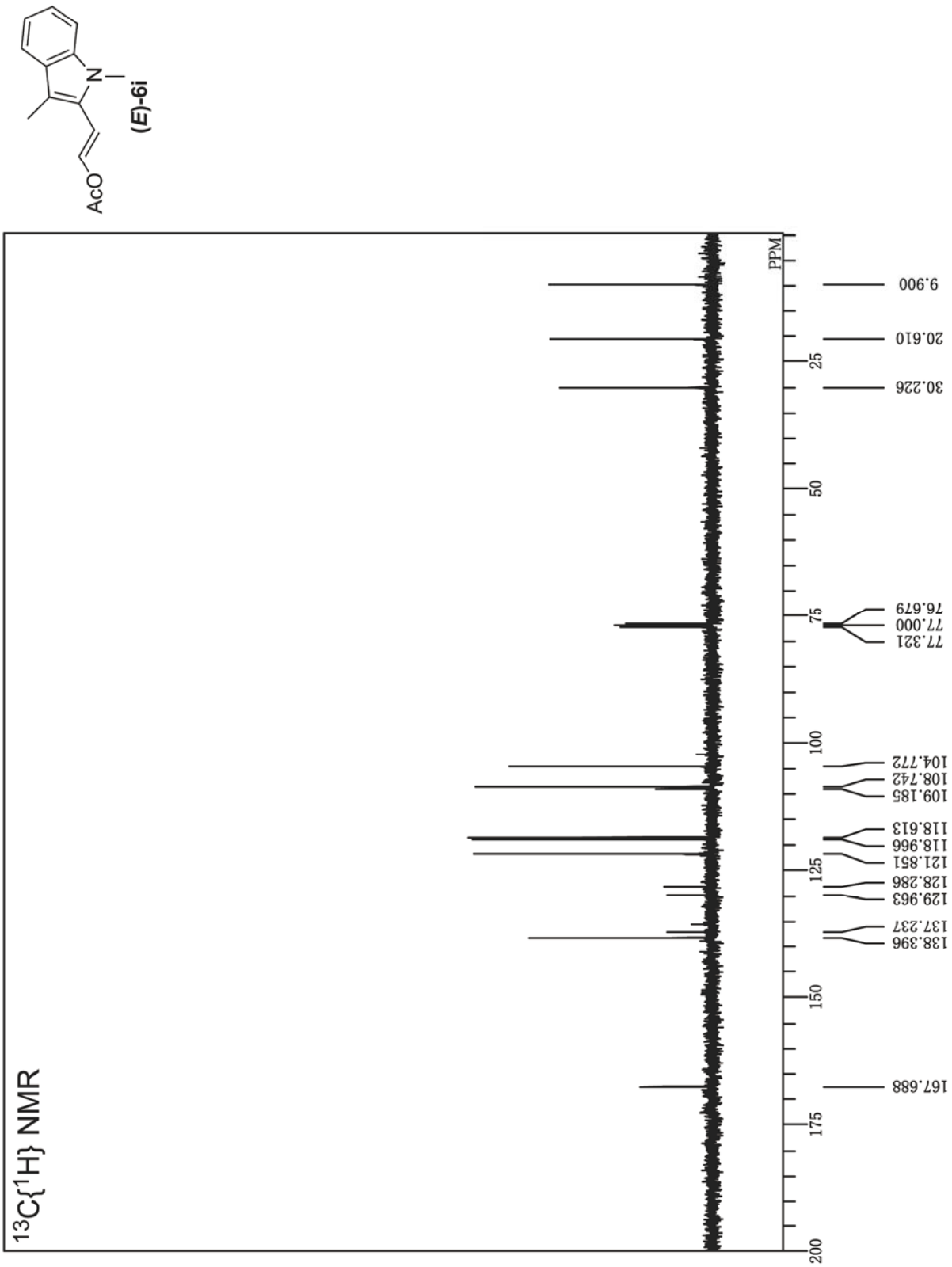
35

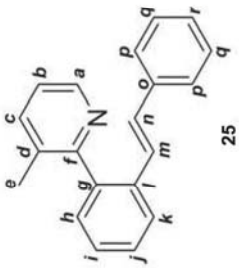

$^{13}C\{^{1}H\}$ NMR
PPM
200
175
150
125
100
75
50
25
152.804
137.607
134.566
128.615
127.325
127.193
126.125
117.774
109.859
79.408
77.321
77.000
76.679
66.800
28.155


1H NMR
0.66
1.02
0.34
3.40
1.04
0.66
0.34
1.02
2.00
1.95
3.02
1.00
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
7.671
7.623
7.576
7.551
7.523
7.439
7.413
7.285
7.266
7.253
7.240
7.236
7.228
7.223
7.215
7.211
7.203
7.199
7.185
7.180
7.173
7.169
7.131
7.126
7.123
7.117
7.102
7.098
7.094
7.088
7.078
7.069
7.064
6.497
6.450
5.868
5.841
3.732
3.701
3.654
2.420
2.379
2.316
2.257
2.235
2.161
2.144


AcO
N

6i


(E)-6i
AcO
N
13C{1H} NMR
PPM
200
175
150
125
100
75
50
25
9.900
20.610
30.226
76.679
77.000
77.321
104.772
108.742
109.185
118.613
118.966
121.851
128.286
129.963
137.237
138.396
167.688



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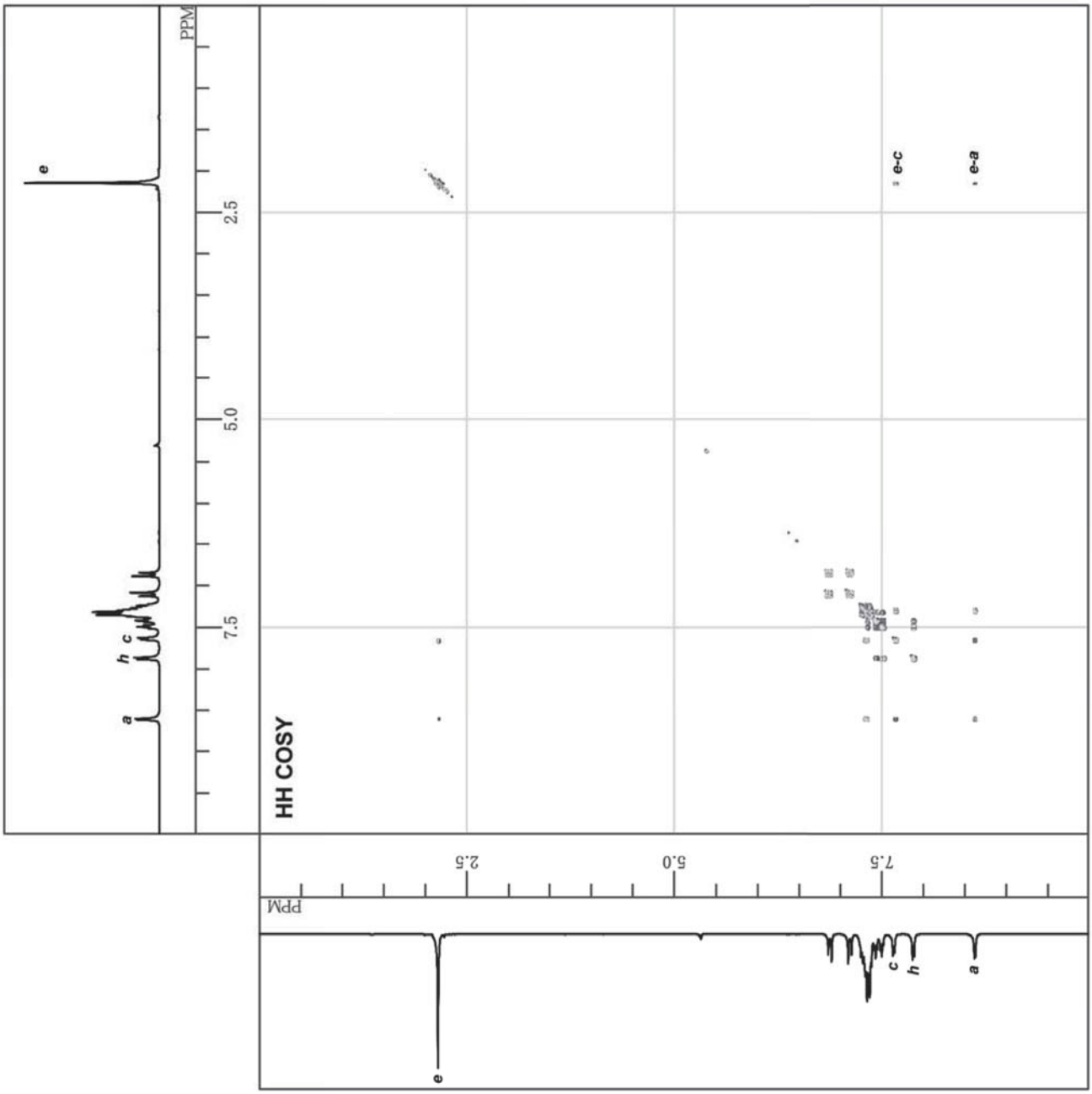

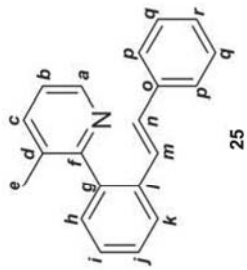

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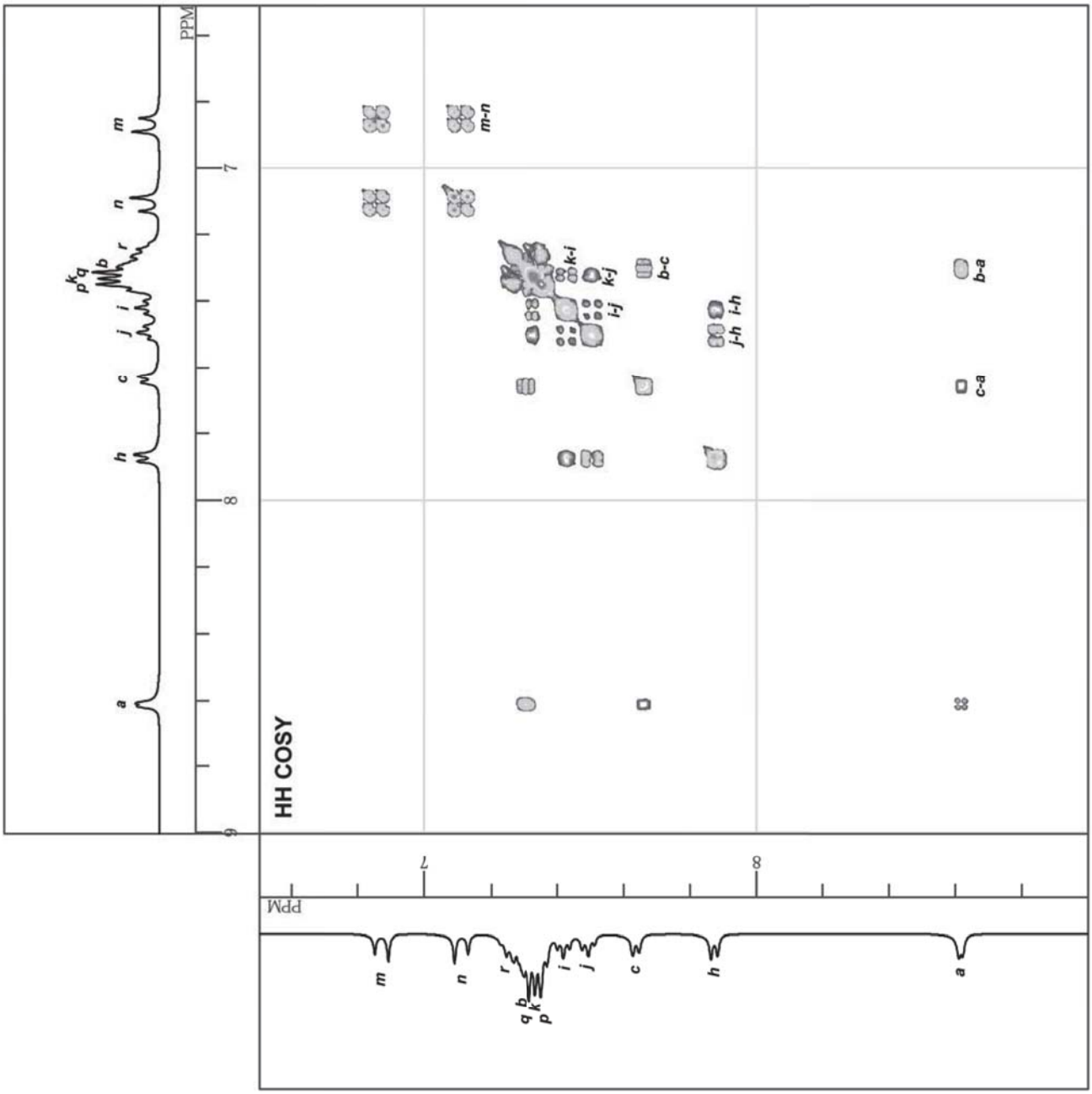

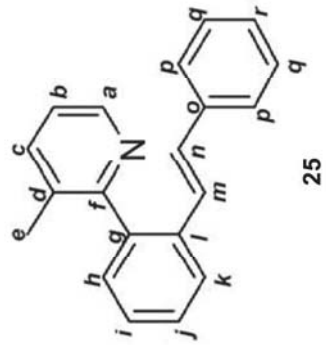

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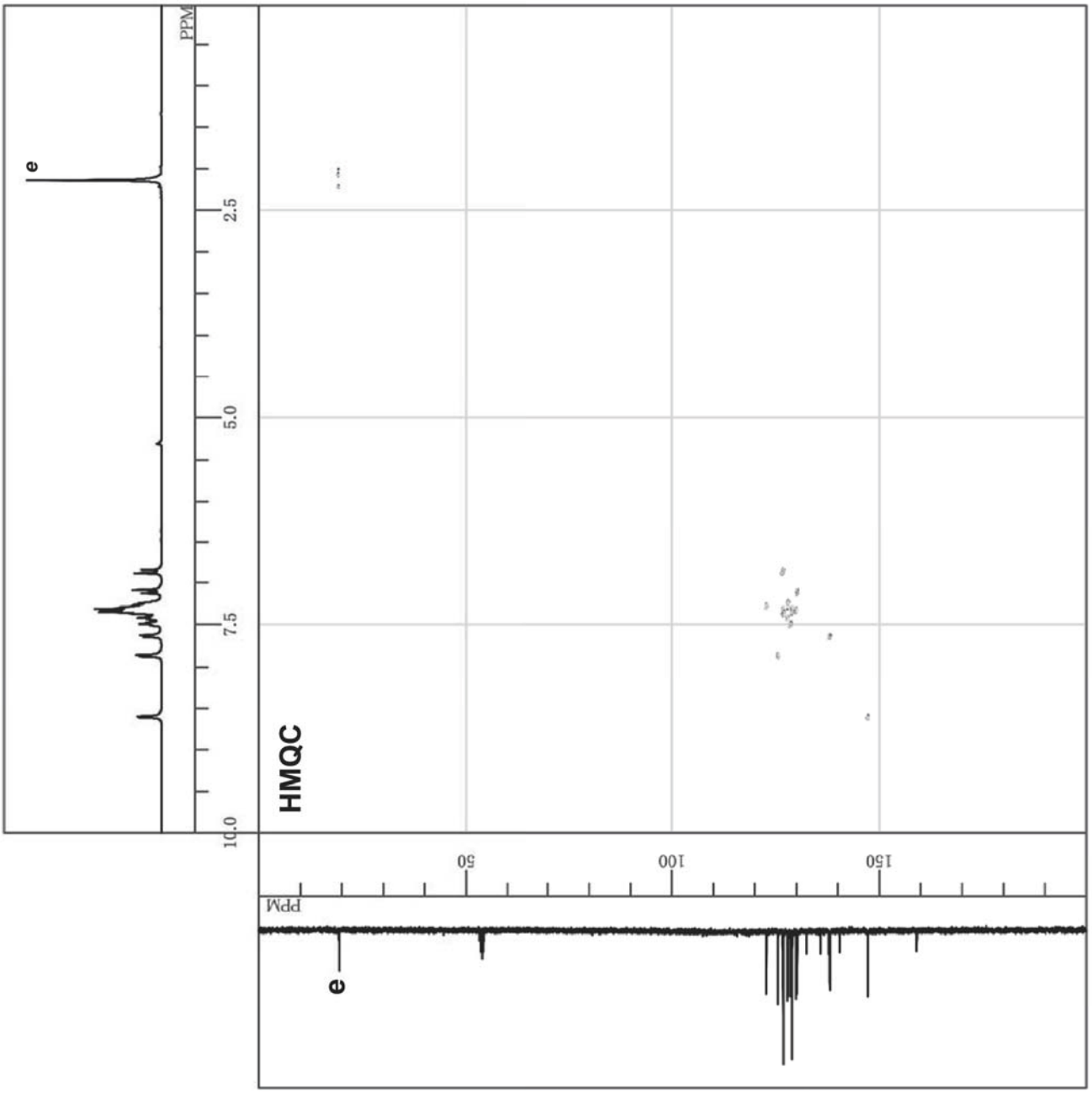

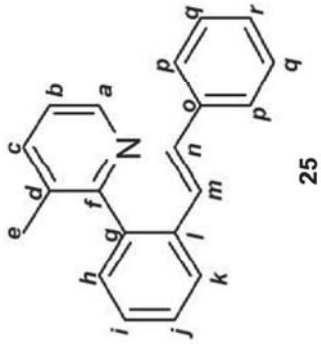

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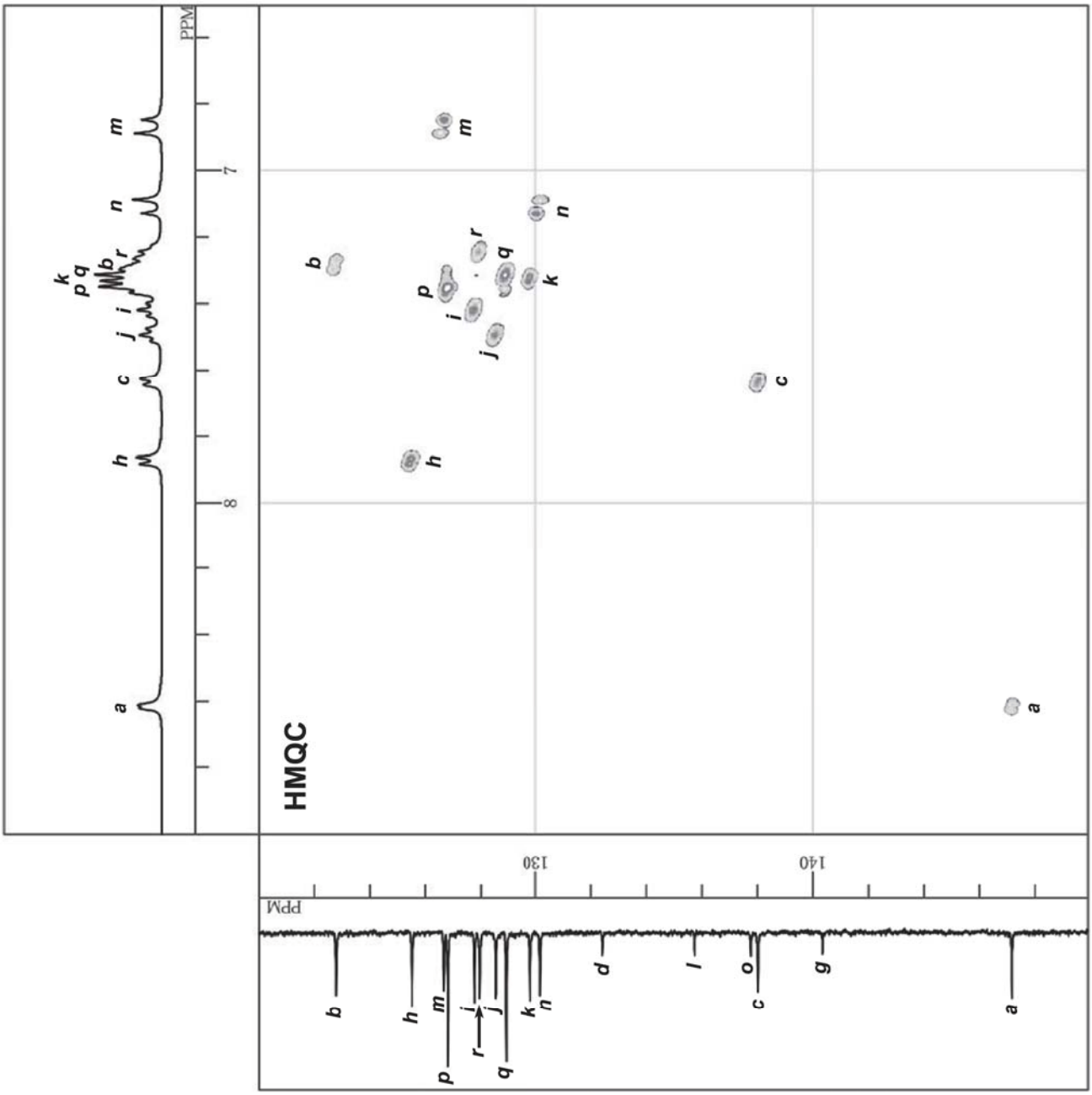
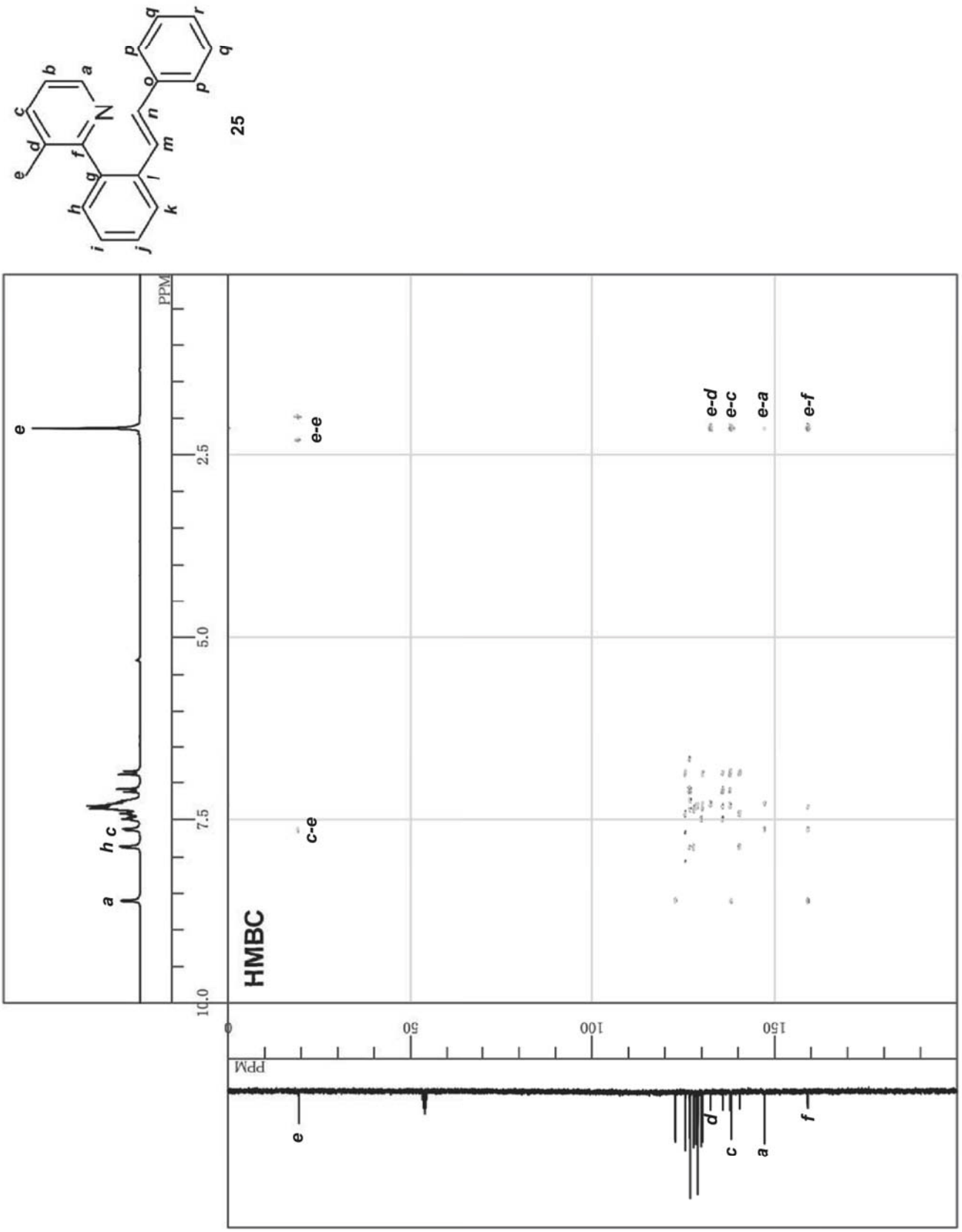
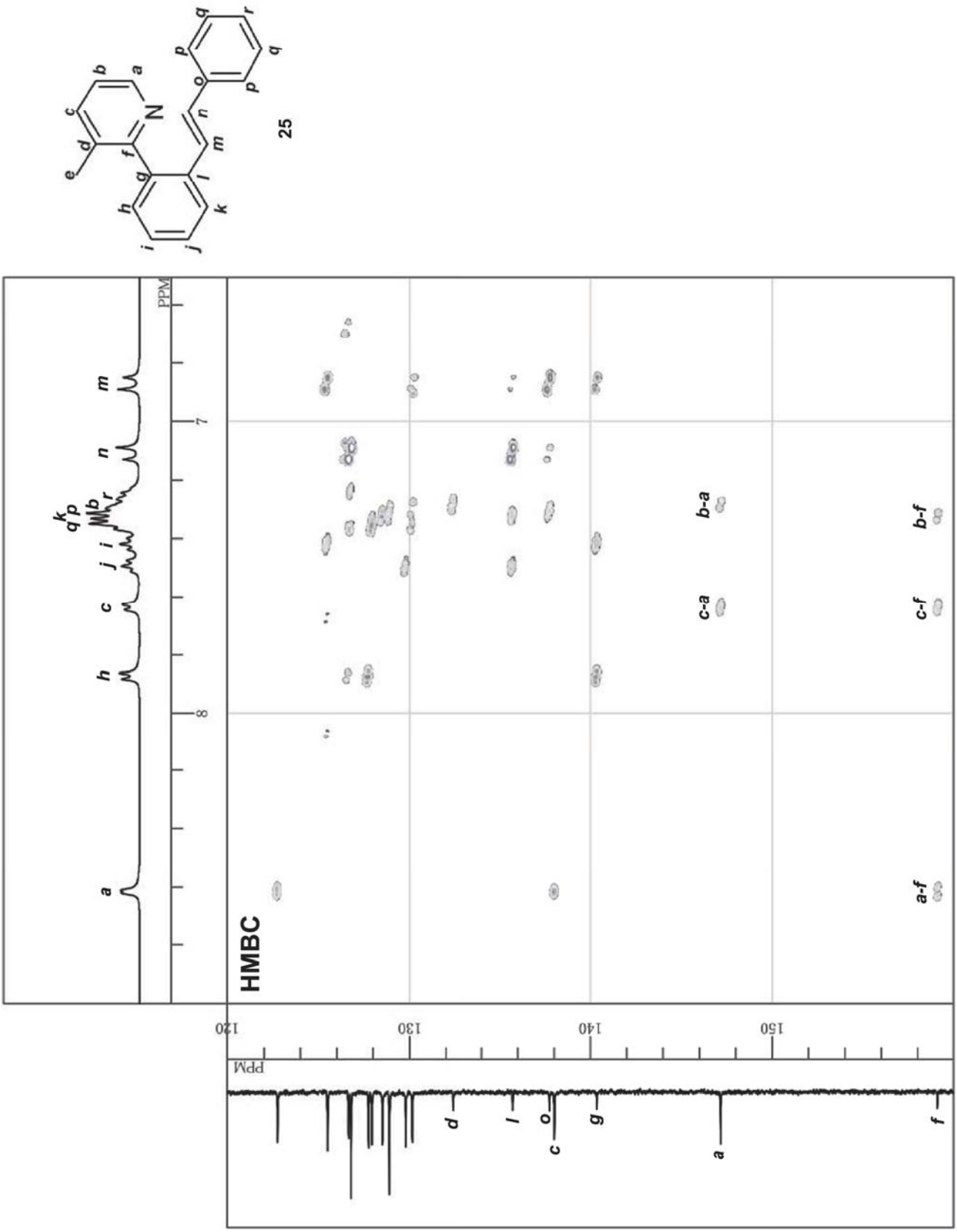
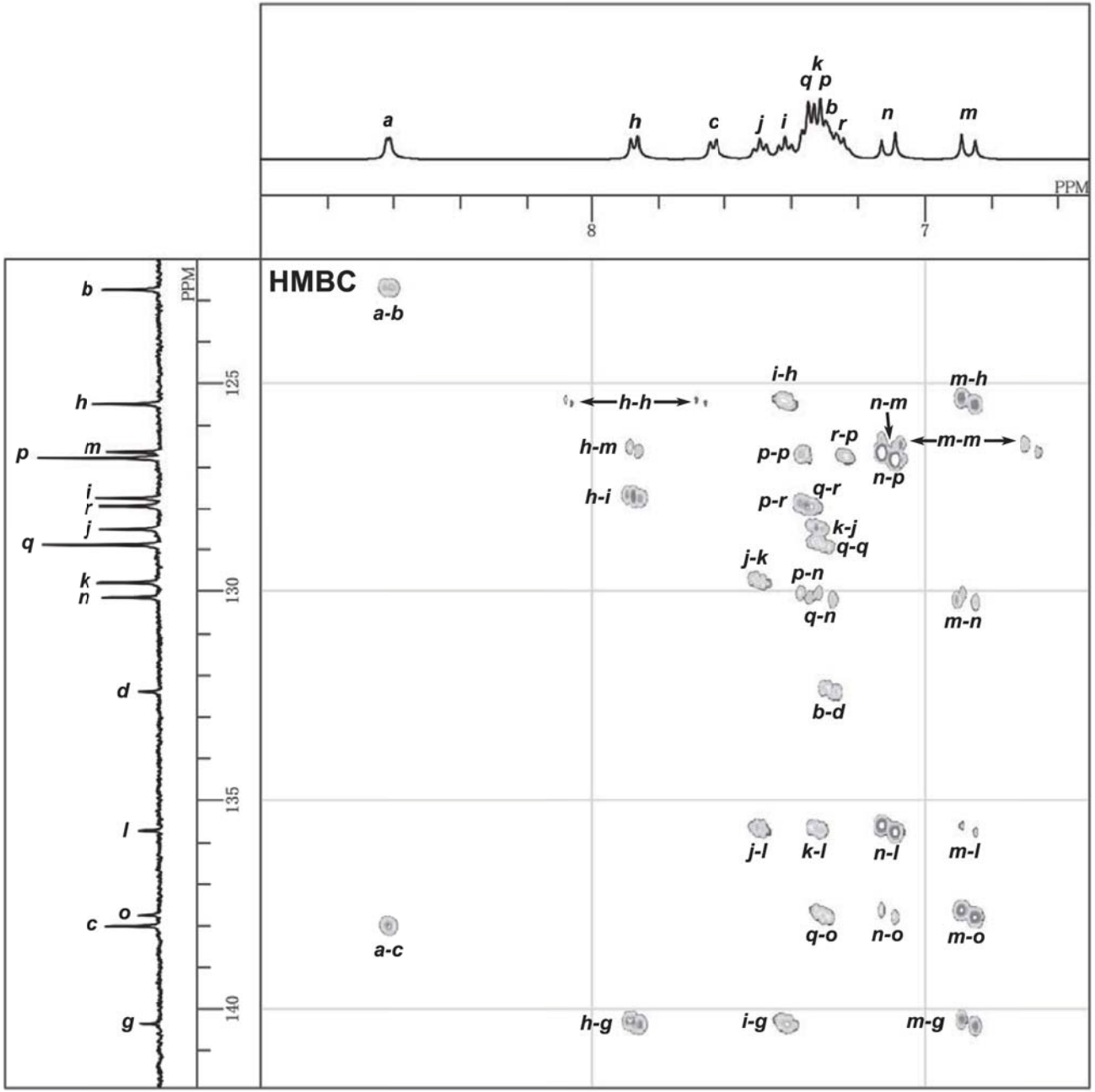
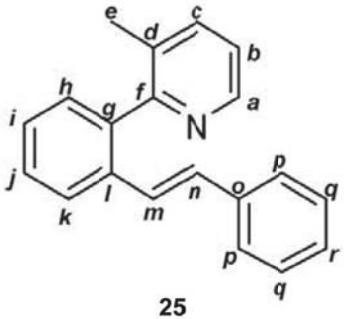


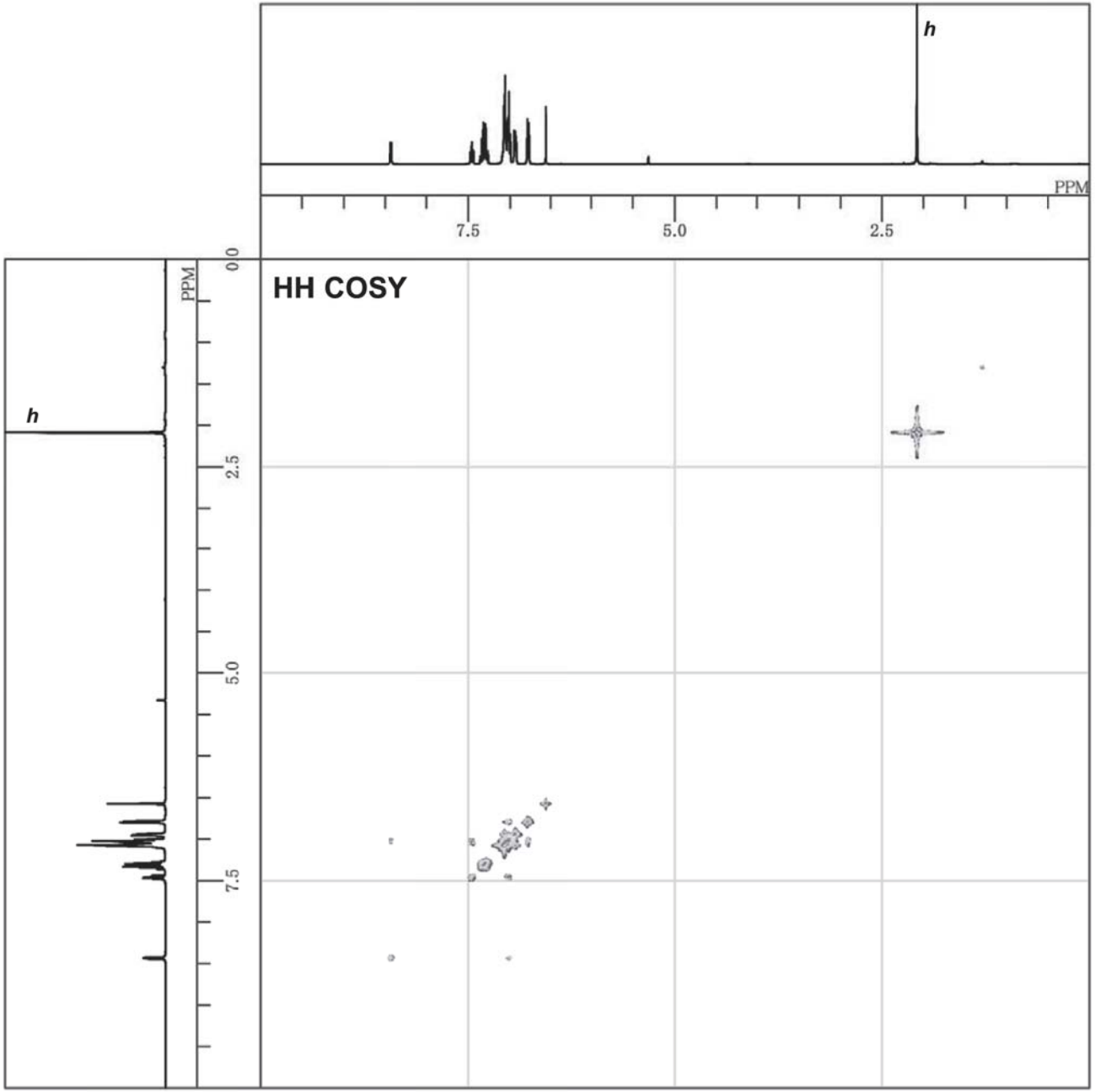

25
HMBC
PPM
e-e
c-e
e-d
e-c
e-a
e-f

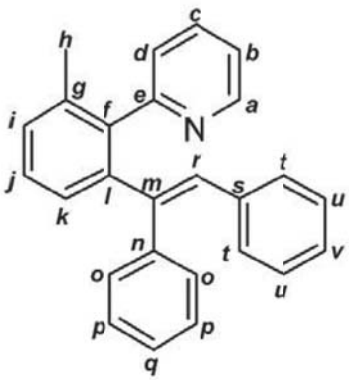

25
HMBC
PPM
a-f
b-f
c-f
b-a
c-a


HMBC
PPM
a-b
a-c
h-h
h-m
h-i
h-g
i-h
i-g
m-h
m-m
m-n
m-l
m-o
m-g
n-m
n-p
n-l
n-o
r-p
p-p
p-r
q-r
k-j
q-q
j-k
p-n
q-n
b-d
j-l
k-l
q-o
a
h
c
j
i
k
q
p
b
r
n
m
8
7
125
130
135
140

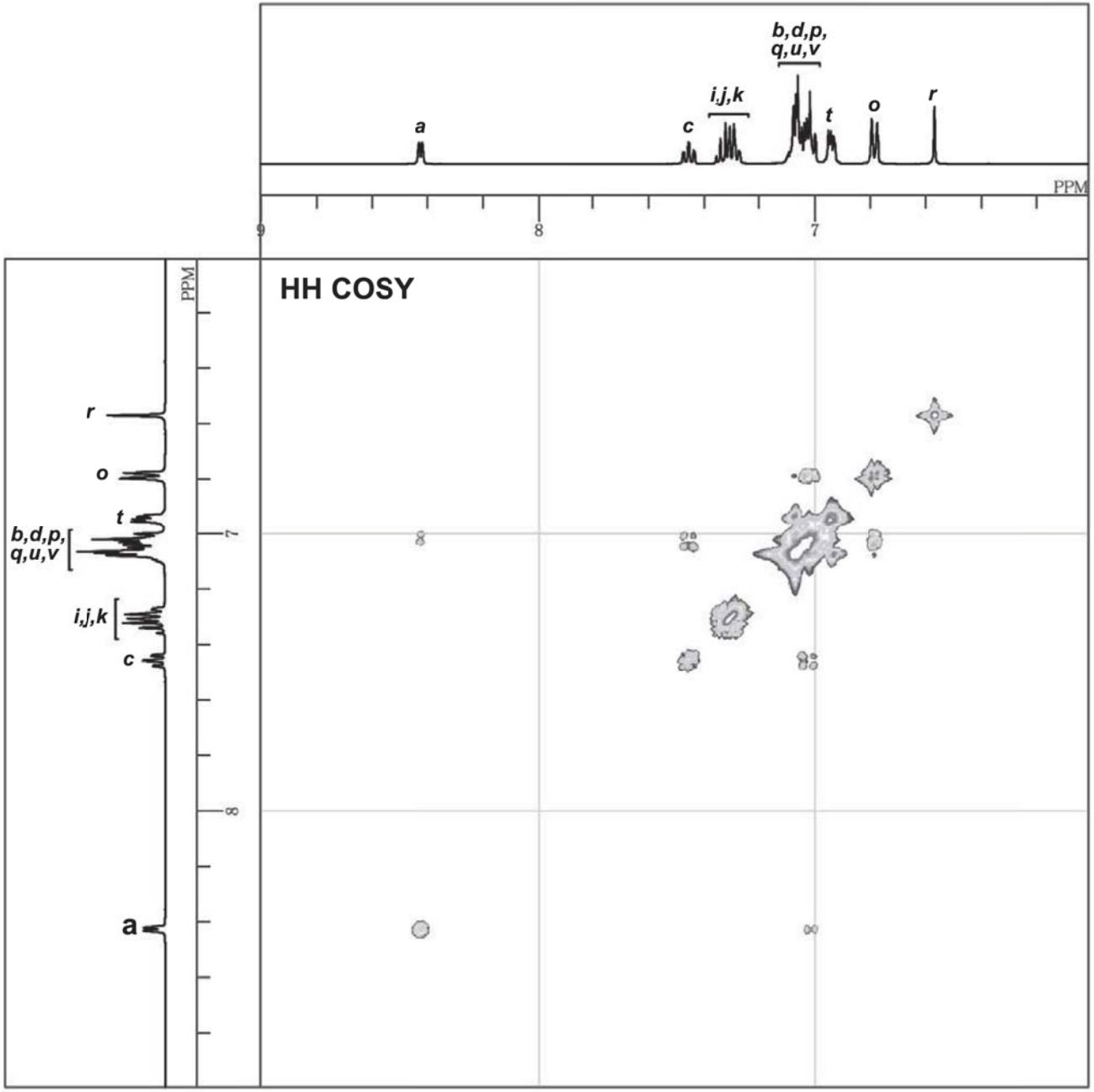

N

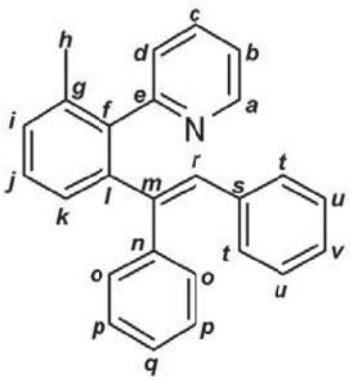
25



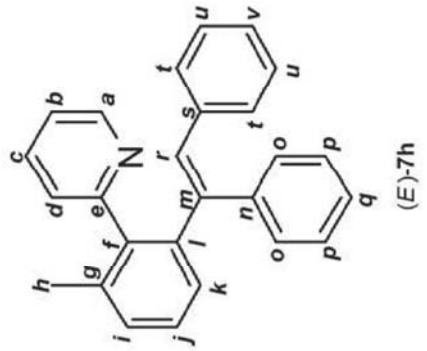


(*E*)-**7h**

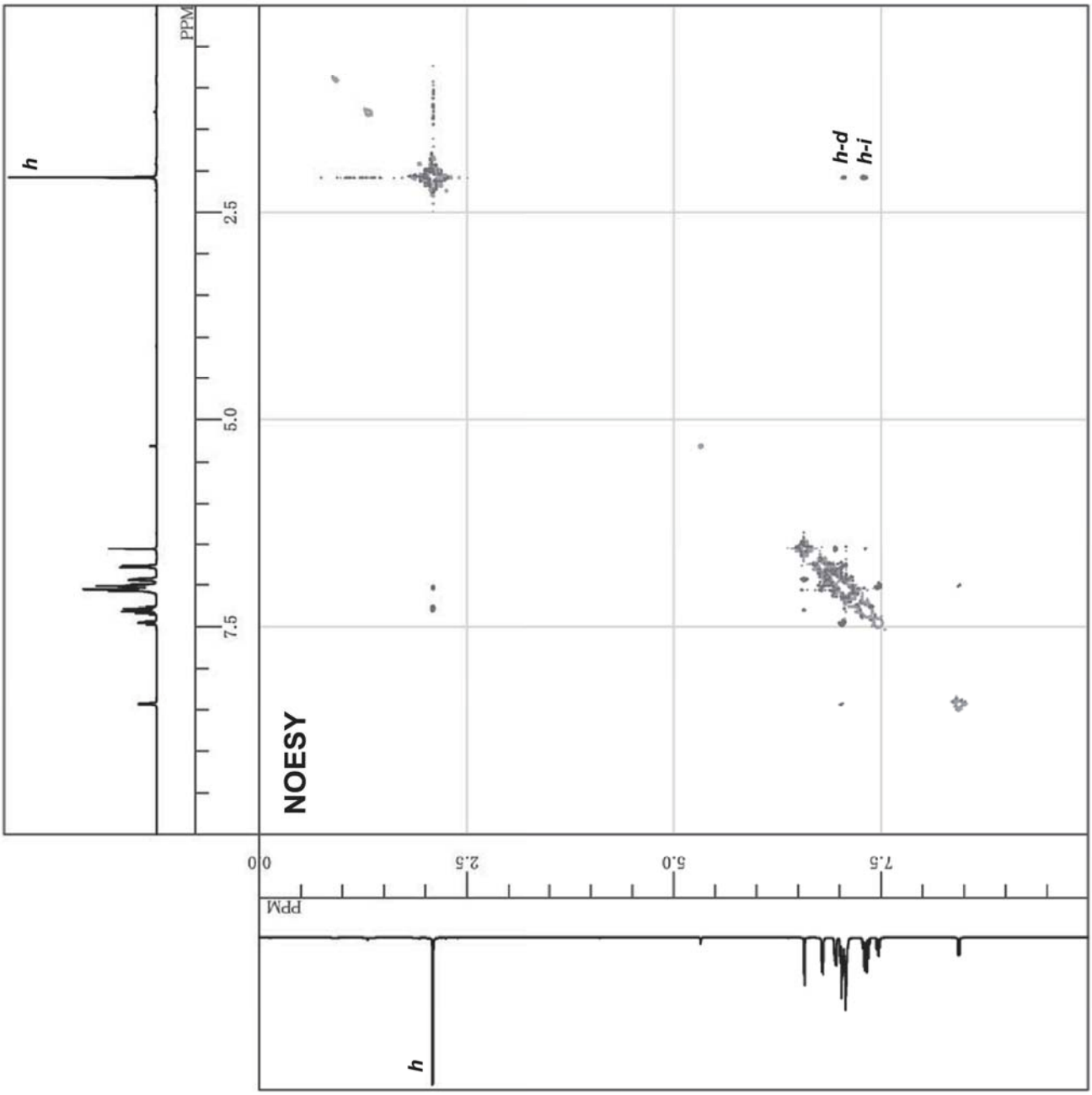


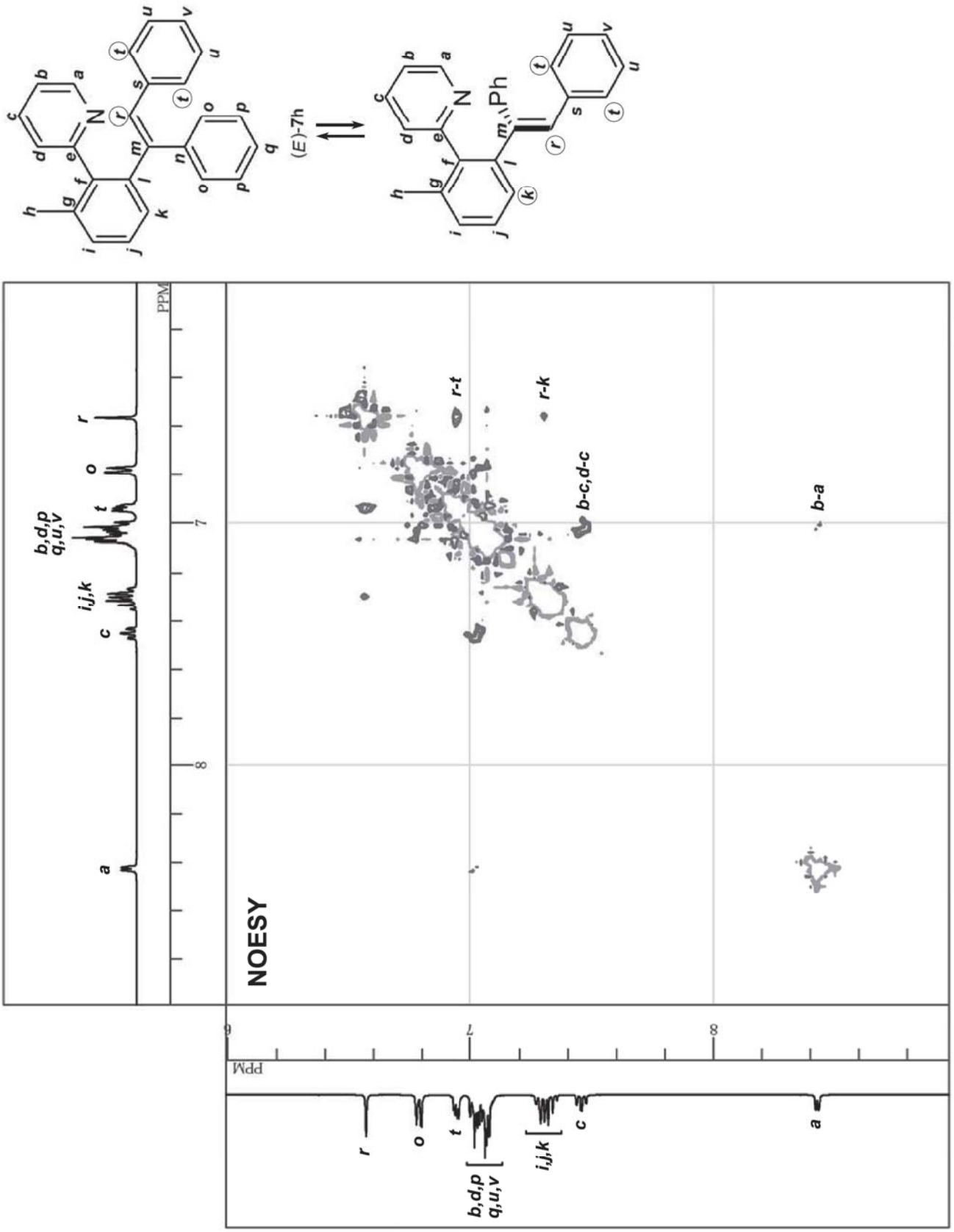


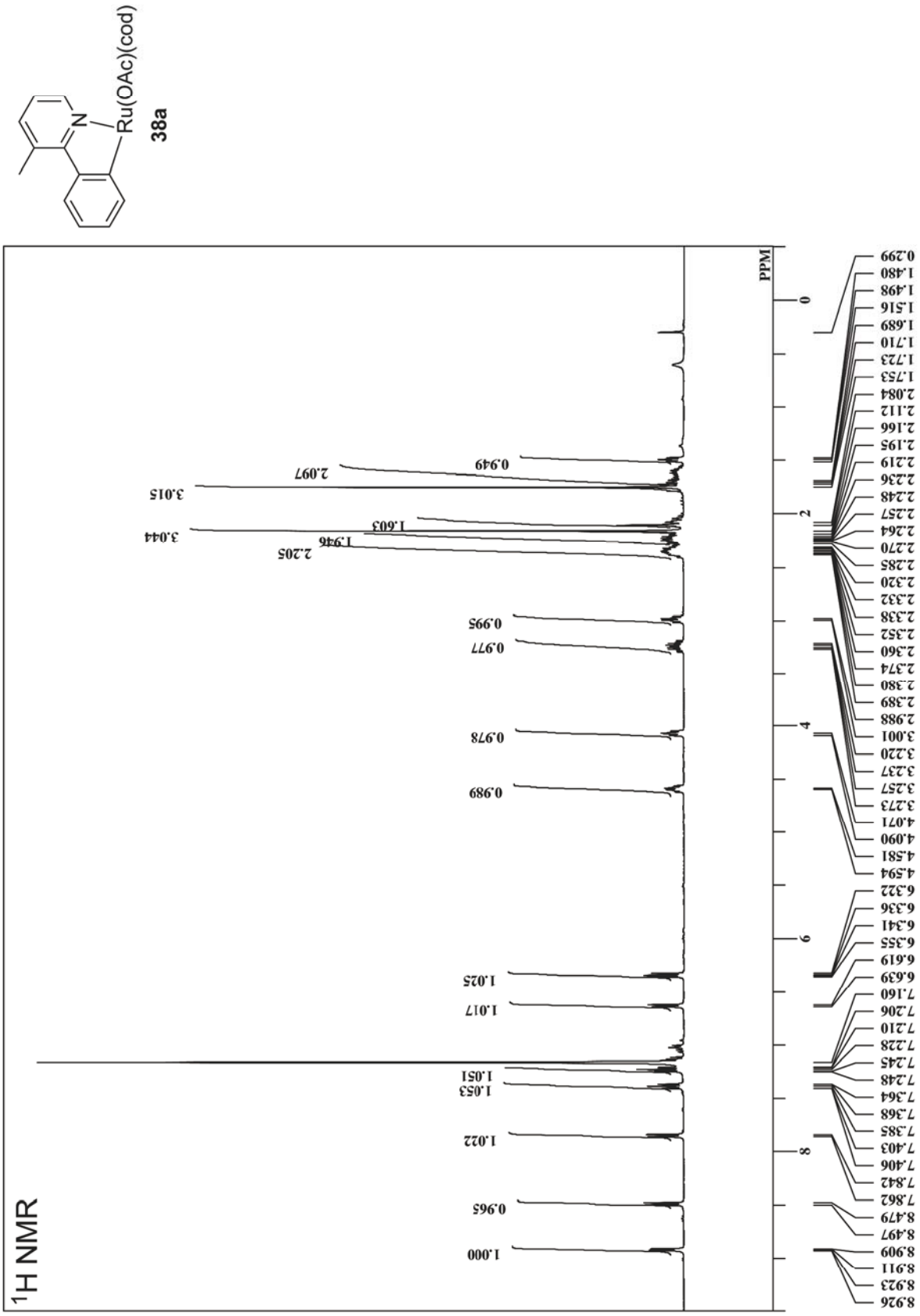
(*E*)-**7h**

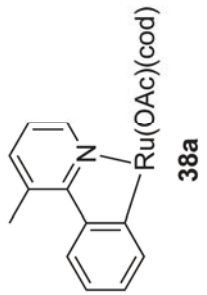


(*E*)-7h

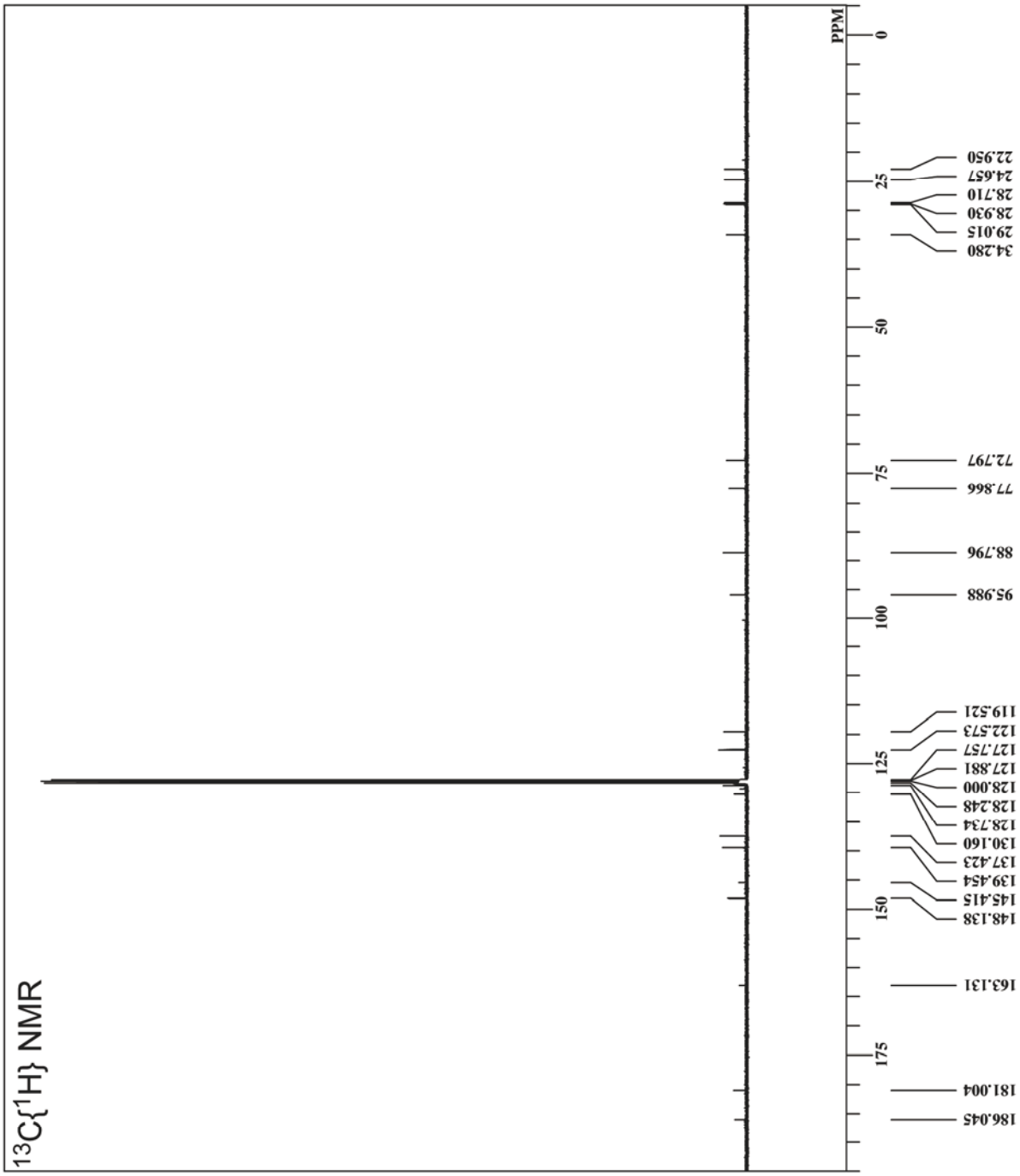


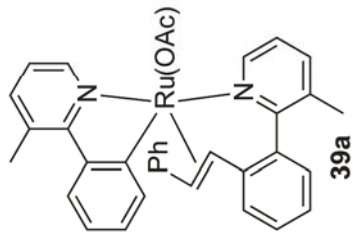

(E)-7h
Ph
NOESY
PPM
r-t
r-k
b-c,d-c
b-a
b,d,p
q,u,v
i,j,k

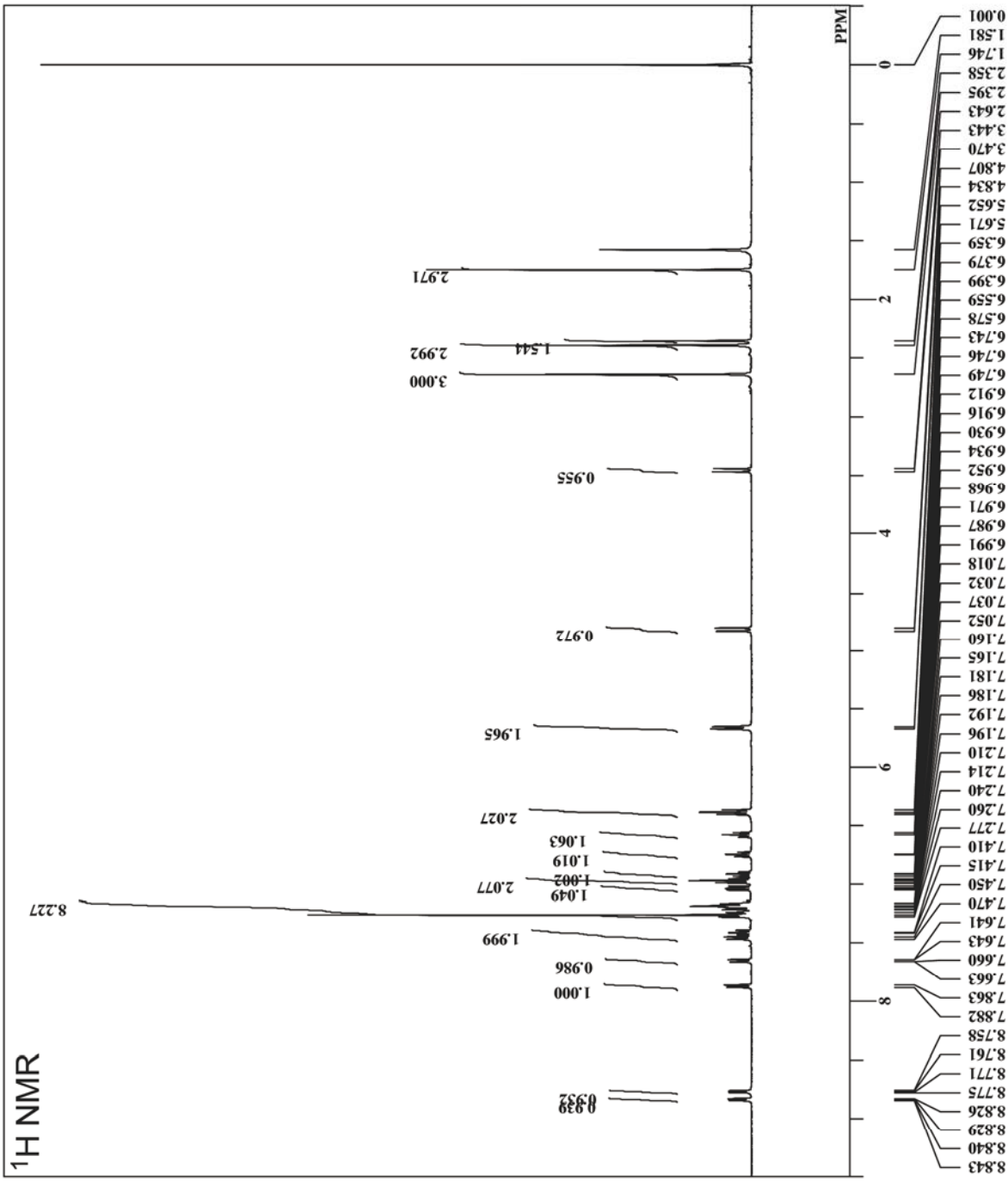

Ru(OAc)(cod)
N
38a
1H NMR
PPM
0
2
4
6
8
1.000
0.965
1.022
1.053
1.051
1.017
1.025
0.989
0.978
0.977
0.995
2.205
1.946
1.603
3.044
3.015
2.097
0.949
0.299
1.480
1.498
1.516
1.689
1.710
1.723
1.753
2.084
2.112
2.166
2.195
2.219
2.236
2.248
2.257
2.264
2.270
2.285
2.320
2.332
2.338
2.352
2.360
2.374
2.380
2.389
2.988
3.001
3.220
3.237
3.257
3.273
4.071
4.090
4.581
4.594
6.322
6.336
6.341
6.355
6.619
6.639
7.160
7.206
7.210
7.228
7.245
7.248
7.364
7.368
7.385
7.403
7.406
7.842
7.862
8.479
8.497
8.909
8.911
8.923
8.926

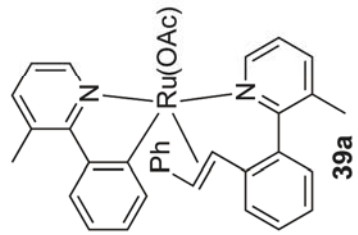

N
Ru(OAc)(cod)

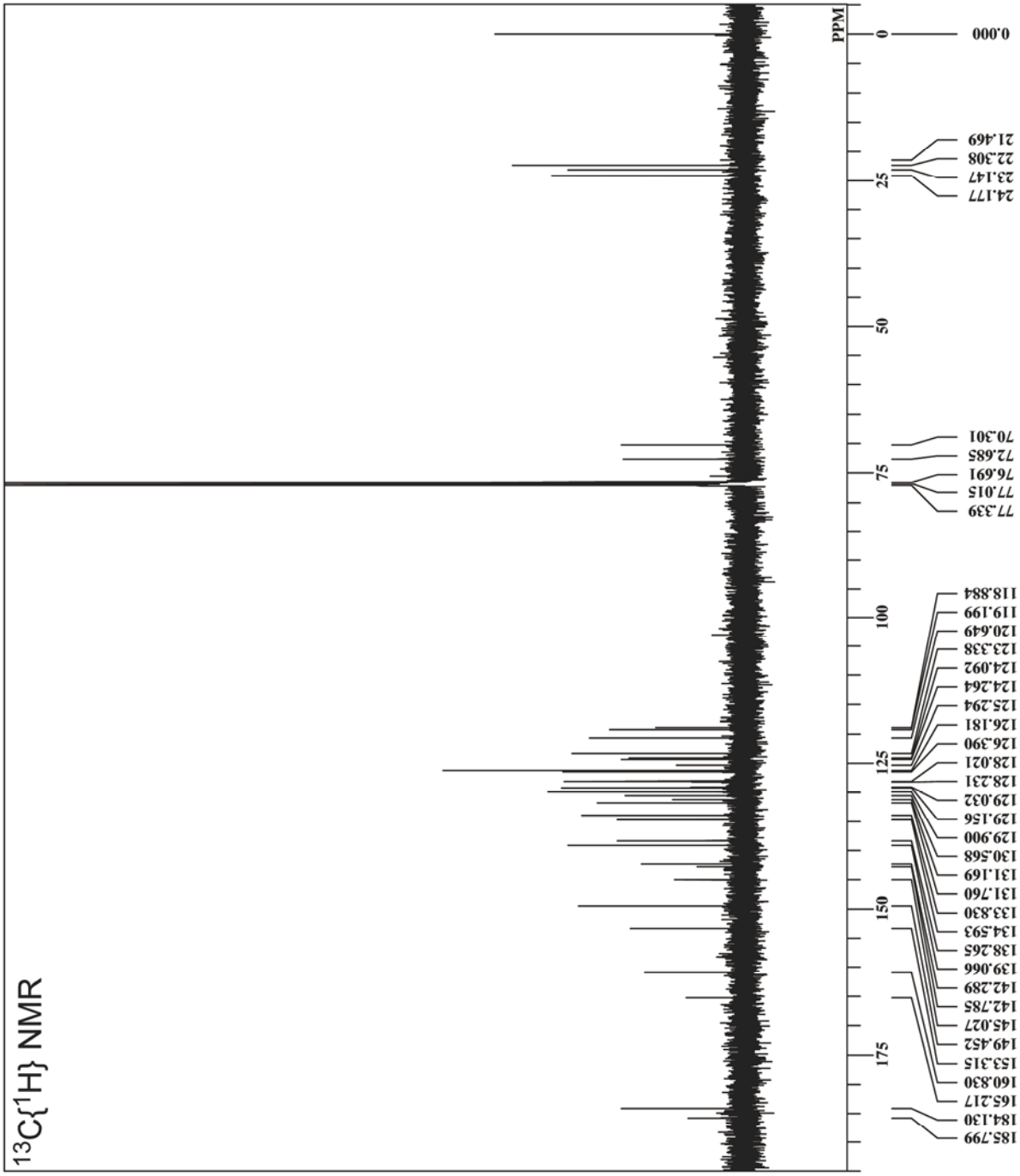
38a

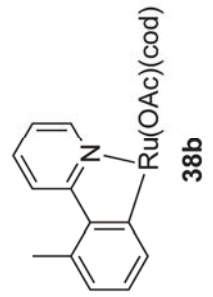

13C{1H} NMR
PPM
0
25
50
75
100
125
150
175
22.950
24.657
28.710
28.930
29.015
34.280
72.797
77.866
88.796
95.988
119.521
122.573
127.757
127.881
128.000
128.248
128.734
130.160
137.423
139.454
145.415
148.138
163.131
181.004
186.045


Ru(OAc)
N
N
Ph
39a

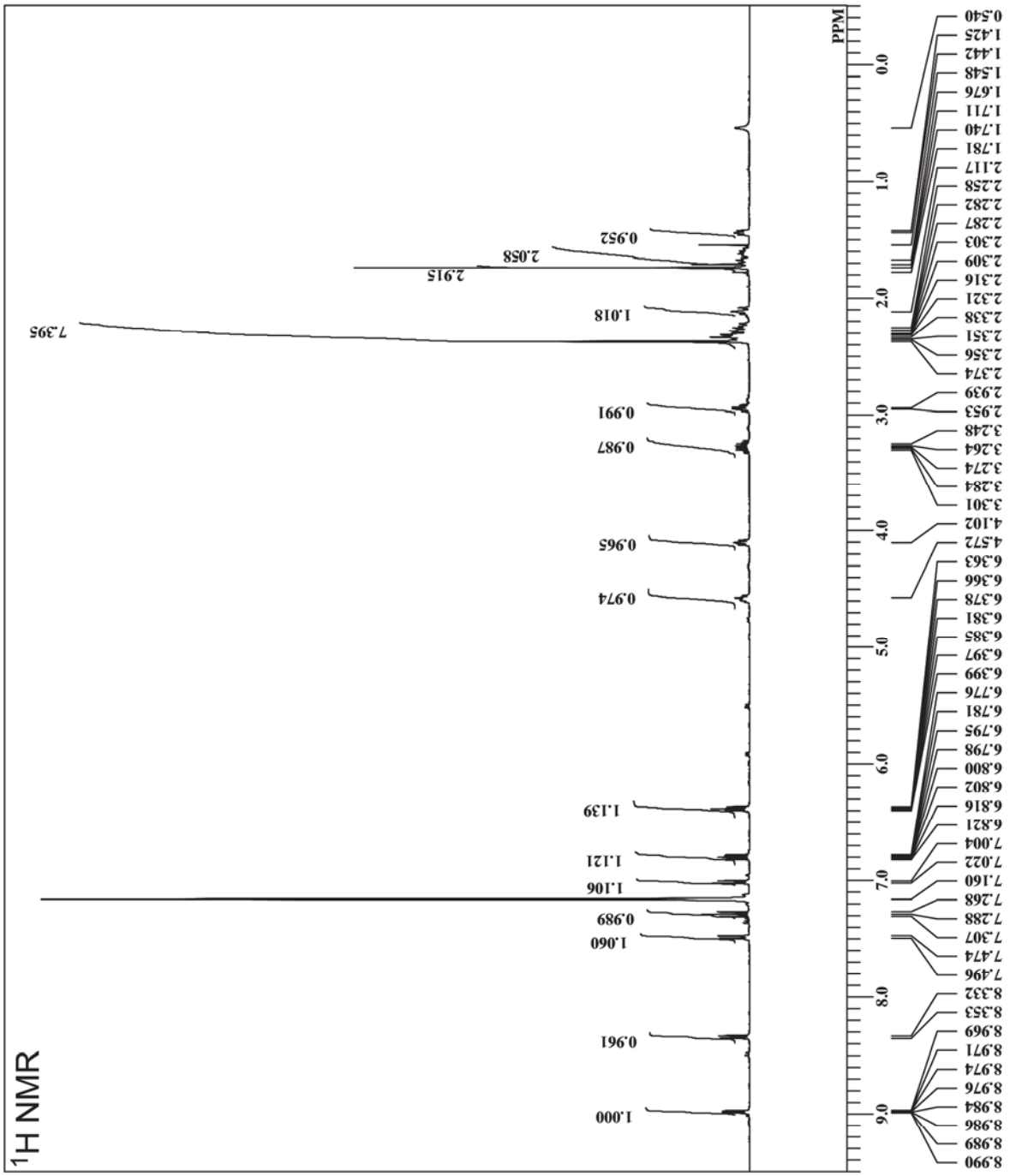

1H NMR
PPM
8.843
8.840
8.829
8.826
8.775
8.771
8.761
8.758
7.882
7.863
7.663
7.660
7.643
7.641
7.470
7.450
7.415
7.410
7.277
7.260
7.240
7.214
7.210
7.196
7.192
7.186
7.181
7.165
7.160
7.052
7.037
7.032
7.018
6.991
6.987
6.971
6.968
6.952
6.934
6.930
6.916
6.912
6.749
6.746
6.743
6.578
6.559
6.399
6.379
6.359
5.671
5.652
4.834
4.807
3.470
3.443
2.643
2.395
2.358
1.746
1.581
0.001
8.227
0.932
0.929
1.000
0.986
1.999
1.049
1.002
2.077
1.019
1.063
2.027
1.965
0.972
0.955
3.000
1.544
2.992
2.971

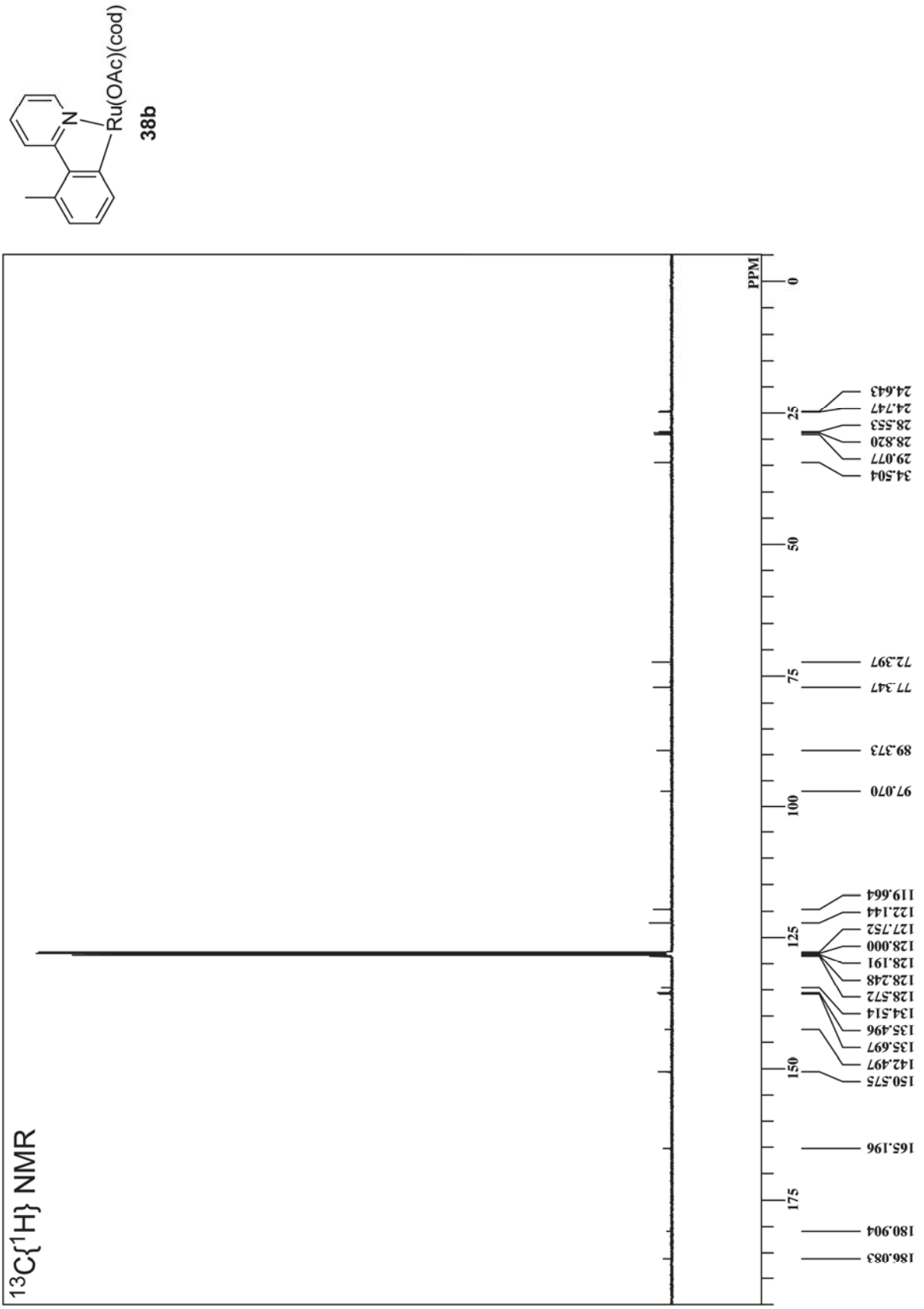

Ru(OAc)
N
N
Ph
39a


13C{1H} NMR
PPM
0.000
21.469
22.308
23.147
24.177
70.301
72.685
76.691
77.015
77.339
118.884
119.199
120.649
123.338
124.092
124.264
125.294
126.181
126.390
128.021
128.231
129.032
129.156
129.900
130.568
131.169
131.760
133.830
134.593
138.265
139.066
142.289
142.785
145.027
149.452
153.315
160.830
165.217
184.130
185.799


N
Ru(OAc)(cod)

38b


^{1}H NMR
PPM
0.540
1.425
1.442
1.548
1.676
1.711
1.740
1.781
2.117
2.258
2.282
2.287
2.303
2.309
2.316
2.321
2.338
2.351
2.356
2.374
2.939
2.953
3.248
3.264
3.274
3.284
3.301
4.102
4.572
6.363
6.366
6.378
6.381
6.385
6.397
6.399
6.776
6.781
6.795
6.798
6.800
6.802
6.816
6.821
7.004
7.022
7.160
7.268
7.288
7.307
7.474
7.496
8.332
8.353
8.969
8.971
8.974
8.976
8.984
8.986
8.989
8.990
1.000
0.961
1.060
0.989
1.106
1.121
1.139
0.974
0.965
0.987
0.991
7.395
1.018
2.915
2.058
0.952


Ru(OAc)(cod)
38b
13C{1H} NMR
PPM
0
25
50
75
100
125
150
175
186.083
180.904
165.196
150.575
142.497
135.697
135.496
134.514
128.572
128.248
128.191
128.000
127.752
122.144
119.664
97.070
89.373
77.347
72.397
34.504
29.077
28.820
28.553
24.747
24.643