

Supporting Information

NH-Type of chiral Ni(II) complexes of glycine Schiff base: design, structural evaluation, reactivity and synthetic applications

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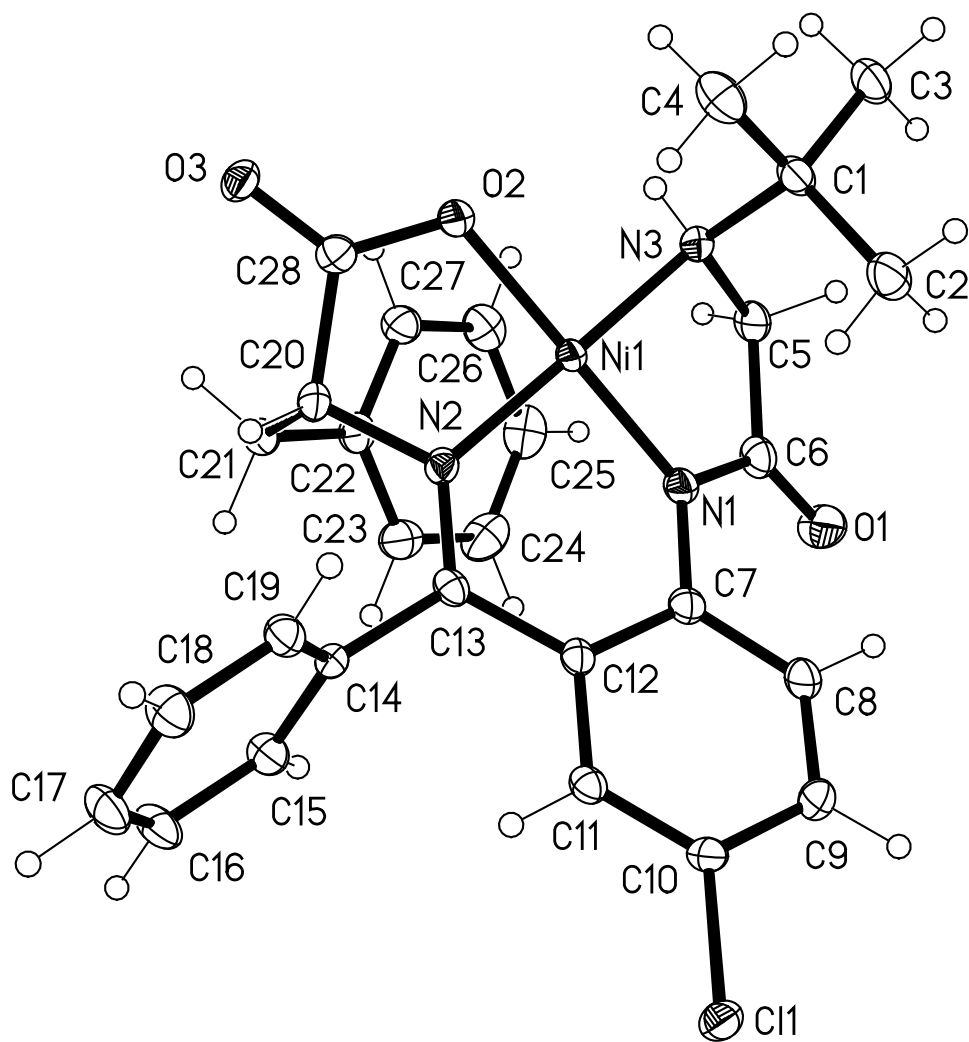
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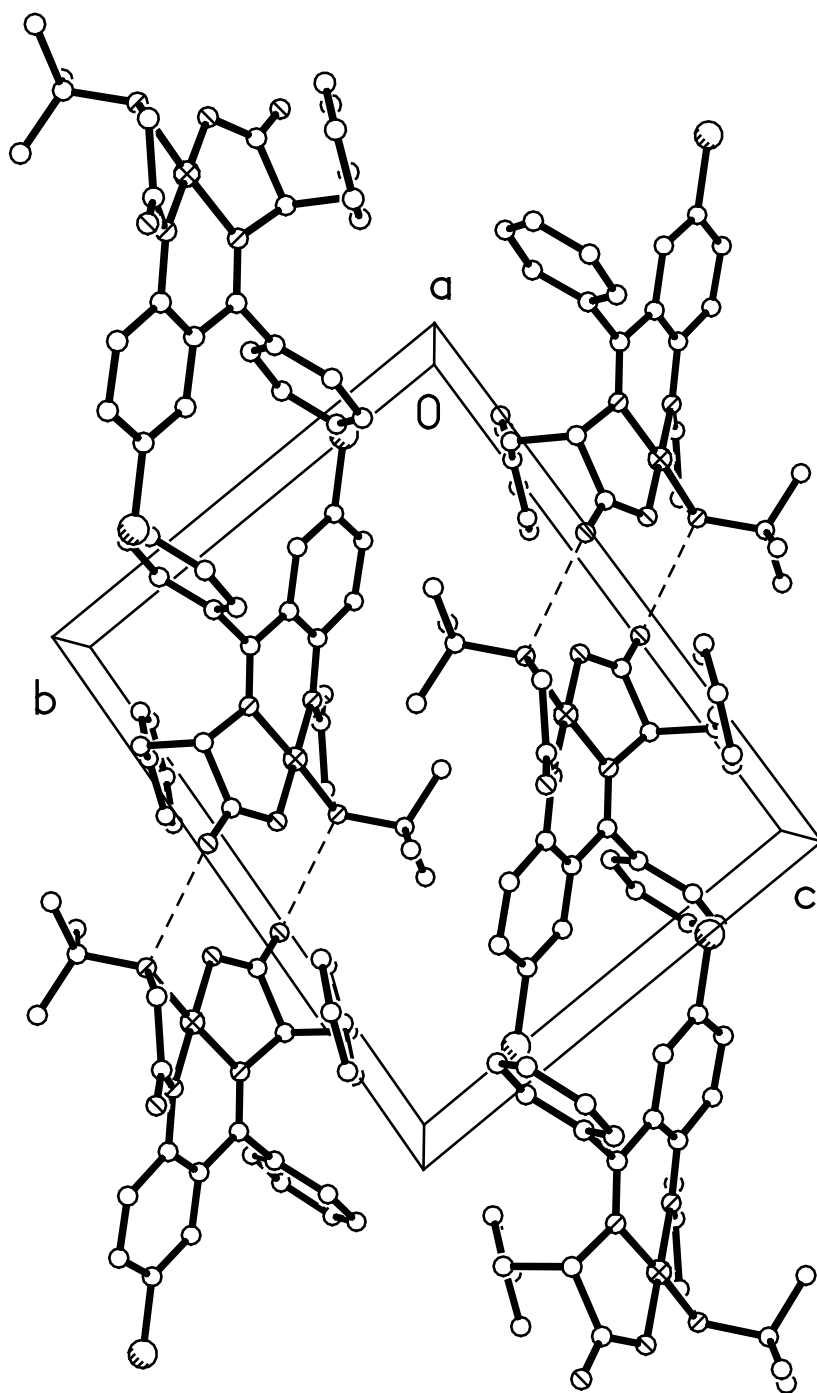
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Comment

The displacement ellipsoids were drawn at the 50% probability level.

Experimental

A red prism-shaped crystal of dimensions 0.47 x 0.15 x 0.13 mm was selected for structural analysis. Intensity data for this compound were collected using an instrument with a Bruker APEX ccd area detector (1) with graphite-monochromated Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$). The sample was cooled to 100(2) K. Cell parameters were determined from a non-linear least squares fit of 7600 peaks in the range $2.27 < \theta < 28.27^\circ$. A total of 9916 data were measured in the range $1.98 < \theta < 26.00^\circ$ using ω oscillation frames. The data were corrected for absorption by the semi-empirical method (2) giving minimum and maximum transmission factors of 0.6730 and 0.8903. The data were merged to form a set of 4890 independent data with $R(\text{int}) = 0.0200$ and a coverage of 98.7 %.

The triclinic space group $P\bar{1}$ was determined by statistical tests and verified by subsequent refinement. The structure was solved by direct methods and refined by full-matrix least-squares methods on F^2 (3). Hydrogen atom positions were initially determined by geometry and refined by a riding model. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atom displacement parameters were set to 1.2 (1.5 for methyl) times the displacement parameters of the bonded atoms. A total of 331 parameters were refined against 4890 data to give $wR(F^2) = 0.0813$ and $S = 1.006$ for weights of $w = 1/[\sigma^2(F^2) + (0.0420 P)^2 + 0.9000 P]$, where $P = [F_o^2 + 2F_c^2] / 3$. The final $R(F)$ was 0.0321 for the 4458 observed, $[F > 4\sigma(F)]$, data. The largest shift/s.u. was 0.001 in the final refinement cycle. The final difference map had maxima and minima of 0.392 and -0.230 e/ \AA^3 , respectively.

Acknowledgment

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Table 1. Crystal data and structure refinement for 06087.

Empirical formula	C ₂₈ H ₂₈ Cl N ₃ Ni O ₃	
Formula weight	548.69	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	$a = 9.263(2) \text{ \AA}$	$\alpha = 86.448(7)^\circ$
	$b = 10.294(2) \text{ \AA}$	$\beta = 75.238(7)^\circ$
	$c = 13.643(3) \text{ \AA}$	$\gamma = 89.471(7)^\circ$
Volume	1255.5(5) Å ³	
Z, Z'	2, 1	
Density (calculated)	1.451 Mg/m ³	
Wavelength	0.71073 Å	
Temperature	100(2) K	
$F(000)$	572	
Absorption coefficient	0.915 mm ⁻¹	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8903 and 0.6730	
Theta range for data collection	1.98 to 26.00°	
Reflections collected	9916	
Independent reflections	4890 [R(int) = 0.0200]	
Data / restraints / parameters	4890 / 0 / 331	
$wR(F^2 \text{ all data})$	$wR2 = 0.0813$	
$R(F \text{ obsd data})$	$R1 = 0.0321$	
Goodness-of-fit on F^2	1.006	
Observed data [$I > 2\sigma(I)$]	4458	
Largest and mean shift / s.u.	0.001 and 0.000	
Largest diff. peak and hole	0.392 and -0.230 e/Å ³	

$$wR2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$$

$$R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$$

Table 2. Atomic coordinates and equivalent isotropic displacement parameters for 06087. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ni(1)	0.56214(3)	0.24272(2)	0.612657(17)	0.01300(8)
Cl(1)	0.42132(5)	0.72839(5)	0.97526(4)	0.01921(11)
O(1)	0.92509(16)	0.36666(16)	0.67183(12)	0.0278(4)
O(2)	0.44743(15)	0.13973(13)	0.55160(10)	0.0170(3)
O(3)	0.24907(15)	0.00521(13)	0.59338(11)	0.0196(3)
N(1)	0.67491(17)	0.34274(16)	0.67261(12)	0.0159(3)
N(2)	0.40168(17)	0.23225(15)	0.72605(12)	0.0140(3)
N(3)	0.73452(18)	0.24374(16)	0.49762(12)	0.0152(3)
C(1)	0.7411(2)	0.34434(19)	0.41029(15)	0.0190(4)
C(2)	0.7531(3)	0.4809(2)	0.44548(17)	0.0273(5)
C(3)	0.8747(2)	0.3160(2)	0.32155(16)	0.0246(5)
C(4)	0.5980(2)	0.3300(2)	0.37652(16)	0.0258(5)
C(5)	0.8639(2)	0.2487(2)	0.54287(15)	0.0185(4)
C(6)	0.8258(2)	0.3273(2)	0.63658(15)	0.0192(4)
C(7)	0.6158(2)	0.42995(19)	0.74632(14)	0.0161(4)
C(8)	0.6983(2)	0.5400(2)	0.75767(15)	0.0208(4)
C(9)	0.6390(2)	0.6323(2)	0.82523(15)	0.0203(4)
C(10)	0.4953(2)	0.61422(18)	0.88689(14)	0.0161(4)
C(11)	0.4103(2)	0.50874(18)	0.87892(14)	0.0150(4)
C(12)	0.4671(2)	0.41570(18)	0.80752(14)	0.0140(4)
C(13)	0.3684(2)	0.30825(18)	0.80047(14)	0.0140(4)
C(14)	0.2224(2)	0.29316(17)	0.87907(14)	0.0144(4)
C(15)	0.2139(2)	0.24061(19)	0.97688(15)	0.0184(4)
C(16)	0.0767(2)	0.2343(2)	1.04830(15)	0.0227(4)
C(17)	-0.0504(2)	0.2801(2)	1.02286(16)	0.0234(4)
C(18)	-0.0424(2)	0.3306(2)	0.92512(16)	0.0224(4)
C(19)	0.0934(2)	0.33698(19)	0.85305(15)	0.0182(4)
C(20)	0.3130(2)	0.11428(18)	0.72536(14)	0.0167(4)
C(21)	0.3656(2)	0.00019(19)	0.78750(15)	0.0196(4)
C(22)	0.5339(2)	-0.01037(18)	0.76791(15)	0.0193(4)
C(23)	0.6037(3)	0.02920(19)	0.84022(16)	0.0231(4)
C(24)	0.7580(3)	0.0259(2)	0.82321(18)	0.0289(5)
C(25)	0.8449(3)	-0.0195(2)	0.73360(18)	0.0276(5)
C(26)	0.7768(2)	-0.0608(2)	0.66181(17)	0.0253(5)
C(27)	0.6225(2)	-0.05533(19)	0.67795(15)	0.0211(4)
C(28)	0.3352(2)	0.08263(18)	0.61454(15)	0.0165(4)

Table 3. Bond lengths [Å] and angles [°] for 06087.

Ni(1)-N(1)	1.8384(16)	C(9)-H(9)	0.9500
Ni(1)-N(2)	1.8506(16)	C(10)-C(11)	1.373(3)
Ni(1)-O(2)	1.8784(13)	C(11)-C(12)	1.410(3)
Ni(1)-N(3)	1.9324(17)	C(11)-H(11)	0.9500
Cl(1)-C(10)	1.745(2)	C(12)-C(13)	1.465(3)
O(1)-C(6)	1.224(2)	C(13)-C(14)	1.498(2)
O(2)-C(28)	1.287(2)	C(14)-C(15)	1.392(3)
O(3)-C(28)	1.230(2)	C(14)-C(19)	1.394(3)
N(1)-C(6)	1.370(2)	C(15)-C(16)	1.390(3)
N(1)-C(7)	1.393(3)	C(15)-H(15)	0.9500
N(2)-C(13)	1.293(3)	C(16)-C(17)	1.381(3)
N(2)-C(20)	1.474(2)	C(16)-H(16)	0.9500
N(3)-C(5)	1.484(2)	C(17)-C(18)	1.385(3)
N(3)-C(1)	1.519(2)	C(17)-H(17)	0.9500
N(3)-H(3N)	0.80(2)	C(18)-C(19)	1.385(3)
C(1)-C(4)	1.521(3)	C(18)-H(18)	0.9500
C(1)-C(2)	1.527(3)	C(19)-H(19)	0.9500
C(1)-C(3)	1.535(3)	C(20)-C(28)	1.528(3)
C(2)-H(2A)	0.9800	C(20)-C(21)	1.553(3)
C(2)-H(2B)	0.9800	C(20)-H(20)	1.0000
C(2)-H(2C)	0.9800	C(21)-C(22)	1.517(3)
C(3)-H(3A)	0.9800	C(21)-H(21A)	0.9900
C(3)-H(3B)	0.9800	C(21)-H(21B)	0.9900
C(3)-H(3C)	0.9800	C(22)-C(23)	1.392(3)
C(4)-H(4A)	0.9800	C(22)-C(27)	1.394(3)
C(4)-H(4B)	0.9800	C(23)-C(24)	1.389(3)
C(4)-H(4C)	0.9800	C(23)-H(23)	0.9500
C(5)-C(6)	1.519(3)	C(24)-C(25)	1.387(3)
C(5)-H(5A)	0.9900	C(24)-H(24)	0.9500
C(5)-H(5B)	0.9900	C(25)-C(26)	1.381(3)
C(7)-C(8)	1.410(3)	C(25)-H(25)	0.9500
C(7)-C(12)	1.421(3)	C(26)-C(27)	1.392(3)
C(8)-C(9)	1.377(3)	C(26)-H(26)	0.9500
C(8)-H(8)	0.9500	C(27)-H(27)	0.9500
C(9)-C(10)	1.388(3)		
N(1)-Ni(1)-N(2)	93.68(7)	C(7)-N(1)-Ni(1)	124.27(13)
N(1)-Ni(1)-O(2)	179.70(7)	C(13)-N(2)-C(20)	121.53(16)
N(2)-Ni(1)-O(2)	86.35(6)	C(13)-N(2)-Ni(1)	128.71(13)
N(1)-Ni(1)-N(3)	86.36(7)	C(20)-N(2)-Ni(1)	109.68(12)
N(2)-Ni(1)-N(3)	176.38(7)	C(5)-N(3)-C(1)	114.02(15)
O(2)-Ni(1)-N(3)	93.59(7)	C(5)-N(3)-Ni(1)	104.40(12)
C(28)-O(2)-Ni(1)	114.18(12)	C(1)-N(3)-Ni(1)	118.10(12)
C(6)-N(1)-C(7)	121.64(16)	C(5)-N(3)-H(3N)	110.4(17)
C(6)-N(1)-Ni(1)	114.08(13)	C(1)-N(3)-H(3N)	105.6(17)

Ni(1)-N(3)-H(3N)	103.9(17)	C(12)-C(11)-H(11)	119.7
N(3)-C(1)-C(4)	107.10(16)	C(11)-C(12)-C(7)	119.04(17)
N(3)-C(1)-C(2)	109.98(16)	C(11)-C(12)-C(13)	117.76(17)
C(4)-C(1)-C(2)	110.51(18)	C(7)-C(12)-C(13)	123.20(17)
N(3)-C(1)-C(3)	109.46(16)	N(2)-C(13)-C(12)	121.42(17)
C(4)-C(1)-C(3)	108.85(17)	N(2)-C(13)-C(14)	120.49(16)
C(2)-C(1)-C(3)	110.86(17)	C(12)-C(13)-C(14)	117.99(16)
C(1)-C(2)-H(2A)	109.5	C(15)-C(14)-C(19)	119.90(18)
C(1)-C(2)-H(2B)	109.5	C(15)-C(14)-C(13)	121.79(17)
H(2A)-C(2)-H(2B)	109.5	C(19)-C(14)-C(13)	118.28(17)
C(1)-C(2)-H(2C)	109.5	C(16)-C(15)-C(14)	119.51(18)
H(2A)-C(2)-H(2C)	109.5	C(16)-C(15)-H(15)	120.2
H(2B)-C(2)-H(2C)	109.5	C(14)-C(15)-H(15)	120.2
C(1)-C(3)-H(3A)	109.5	C(17)-C(16)-C(15)	120.45(18)
C(1)-C(3)-H(3B)	109.5	C(17)-C(16)-H(16)	119.8
H(3A)-C(3)-H(3B)	109.5	C(15)-C(16)-H(16)	119.8
C(1)-C(3)-H(3C)	109.5	C(16)-C(17)-C(18)	120.07(19)
H(3A)-C(3)-H(3C)	109.5	C(16)-C(17)-H(17)	120.0
H(3B)-C(3)-H(3C)	109.5	C(18)-C(17)-H(17)	120.0
C(1)-C(4)-H(4A)	109.5	C(19)-C(18)-C(17)	120.11(19)
C(1)-C(4)-H(4B)	109.5	C(19)-C(18)-H(18)	119.9
H(4A)-C(4)-H(4B)	109.5	C(17)-C(18)-H(18)	119.9
C(1)-C(4)-H(4C)	109.5	C(18)-C(19)-C(14)	119.94(18)
H(4A)-C(4)-H(4C)	109.5	C(18)-C(19)-H(19)	120.0
H(4B)-C(4)-H(4C)	109.5	C(14)-C(19)-H(19)	120.0
N(3)-C(5)-C(6)	110.42(16)	N(2)-C(20)-C(28)	107.32(15)
N(3)-C(5)-H(5A)	109.6	N(2)-C(20)-C(21)	109.91(15)
C(6)-C(5)-H(5A)	109.6	C(28)-C(20)-C(21)	111.06(16)
N(3)-C(5)-H(5B)	109.6	N(2)-C(20)-H(20)	109.5
C(6)-C(5)-H(5B)	109.6	C(28)-C(20)-H(20)	109.5
H(5A)-C(5)-H(5B)	108.1	C(21)-C(20)-H(20)	109.5
O(1)-C(6)-N(1)	127.81(19)	C(22)-C(21)-C(20)	114.06(16)
O(1)-C(6)-C(5)	120.26(18)	C(22)-C(21)-H(21A)	108.7
N(1)-C(6)-C(5)	111.92(16)	C(20)-C(21)-H(21A)	108.7
N(1)-C(7)-C(8)	120.89(17)	C(22)-C(21)-H(21B)	108.7
N(1)-C(7)-C(12)	121.01(17)	C(20)-C(21)-H(21B)	108.7
C(8)-C(7)-C(12)	117.96(18)	H(21A)-C(21)-H(21B)	107.6
C(9)-C(8)-C(7)	122.11(19)	C(23)-C(22)-C(27)	118.4(2)
C(9)-C(8)-H(8)	118.9	C(23)-C(22)-C(21)	119.50(19)
C(7)-C(8)-H(8)	118.9	C(27)-C(22)-C(21)	122.05(18)
C(8)-C(9)-C(10)	119.02(18)	C(24)-C(23)-C(22)	121.2(2)
C(8)-C(9)-H(9)	120.5	C(24)-C(23)-H(23)	119.4
C(10)-C(9)-H(9)	120.5	C(22)-C(23)-H(23)	119.4
C(11)-C(10)-C(9)	121.15(18)	C(25)-C(24)-C(23)	119.9(2)
C(11)-C(10)-Cl(1)	119.55(15)	C(25)-C(24)-H(24)	120.1
C(9)-C(10)-Cl(1)	119.30(15)	C(23)-C(24)-H(24)	120.1
C(10)-C(11)-C(12)	120.64(18)	C(26)-C(25)-C(24)	119.5(2)
C(10)-C(11)-H(11)	119.7	C(26)-C(25)-H(25)	120.2

C(24)-C(25)-H(25)	120.2	C(26)-C(27)-H(27)	119.8
C(25)-C(26)-C(27)	120.6(2)	C(22)-C(27)-H(27)	119.8
C(25)-C(26)-H(26)	119.7	O(3)-C(28)-O(2)	126.06(18)
C(27)-C(26)-H(26)	119.7	O(3)-C(28)-C(20)	118.79(17)
C(26)-C(27)-C(22)	120.3(2)	O(2)-C(28)-C(20)	115.13(16)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 06087. The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni(1)	11(1)	16(1)	11(1)	-1(1)	-1(1)	-3(1)
Cl(1)	18(1)	19(1)	21(1)	-6(1)	-4(1)	-1(1)
O(1)	15(1)	43(1)	27(1)	-9(1)	-6(1)	-4(1)
O(2)	15(1)	21(1)	15(1)	-2(1)	-2(1)	-3(1)
O(3)	15(1)	21(1)	23(1)	-7(1)	-4(1)	-4(1)
N(1)	13(1)	20(1)	14(1)	-1(1)	-2(1)	-3(1)
N(2)	13(1)	16(1)	14(1)	0(1)	-5(1)	-2(1)
N(3)	15(1)	15(1)	15(1)	-2(1)	-2(1)	-2(1)
C(1)	23(1)	18(1)	14(1)	0(1)	1(1)	-1(1)
C(2)	39(1)	16(1)	21(1)	-1(1)	2(1)	-1(1)
C(3)	25(1)	25(1)	18(1)	-1(1)	4(1)	-4(1)
C(4)	25(1)	30(1)	21(1)	5(1)	-4(1)	3(1)
C(5)	11(1)	24(1)	20(1)	-2(1)	-2(1)	-2(1)
C(6)	14(1)	23(1)	20(1)	1(1)	-3(1)	-3(1)
C(7)	17(1)	19(1)	13(1)	1(1)	-5(1)	-3(1)
C(8)	15(1)	28(1)	18(1)	-2(1)	-1(1)	-7(1)
C(9)	21(1)	22(1)	18(1)	-1(1)	-6(1)	-8(1)
C(10)	18(1)	17(1)	13(1)	-3(1)	-4(1)	0(1)
C(11)	14(1)	19(1)	12(1)	1(1)	-4(1)	-1(1)
C(12)	14(1)	17(1)	12(1)	3(1)	-5(1)	-3(1)
C(13)	13(1)	17(1)	12(1)	2(1)	-3(1)	1(1)
C(14)	15(1)	13(1)	14(1)	-3(1)	-2(1)	-3(1)
C(15)	14(1)	25(1)	17(1)	-1(1)	-5(1)	1(1)
C(16)	20(1)	34(1)	13(1)	2(1)	-2(1)	0(1)
C(17)	14(1)	34(1)	19(1)	-1(1)	2(1)	1(1)
C(18)	15(1)	29(1)	22(1)	0(1)	-5(1)	2(1)
C(19)	18(1)	22(1)	15(1)	1(1)	-4(1)	-2(1)
C(20)	14(1)	17(1)	18(1)	-2(1)	-2(1)	-4(1)
C(21)	25(1)	18(1)	15(1)	0(1)	-2(1)	-5(1)
C(22)	26(1)	13(1)	19(1)	3(1)	-6(1)	-2(1)
C(23)	32(1)	18(1)	20(1)	-1(1)	-9(1)	1(1)
C(24)	35(1)	24(1)	34(1)	1(1)	-21(1)	-1(1)
C(25)	22(1)	24(1)	38(1)	5(1)	-12(1)	2(1)
C(26)	27(1)	21(1)	26(1)	2(1)	-4(1)	4(1)
C(27)	25(1)	20(1)	18(1)	0(1)	-6(1)	-1(1)
C(28)	15(1)	17(1)	18(1)	-4(1)	-3(1)	2(1)

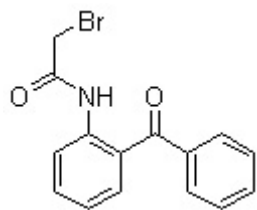
Table 5. Hydrogen coordinates and isotropic displacement parameters for 06087.

	x	y	z	U(eq)
H(3N)	0.730(3)	0.175(2)	0.4746(18)	0.018
H(2A)	0.6691	0.4955	0.5039	0.041
H(2B)	0.7508	0.5454	0.3900	0.041
H(2C)	0.8471	0.4893	0.4651	0.041
H(3A)	0.9676	0.3272	0.3420	0.037
H(3B)	0.8741	0.3764	0.2632	0.037
H(3C)	0.8676	0.2264	0.3027	0.037
H(4A)	0.5899	0.2409	0.3569	0.039
H(4B)	0.5998	0.3914	0.3184	0.039
H(4C)	0.5120	0.3484	0.4326	0.039
H(5A)	0.9506	0.2888	0.4923	0.022
H(5B)	0.8915	0.1591	0.5616	0.022
H(8)	0.7980	0.5508	0.7174	0.025
H(9)	0.6955	0.7073	0.8296	0.024
H(11)	0.3123	0.4983	0.9219	0.018
H(15)	0.3012	0.2093	0.9947	0.022
H(16)	0.0703	0.1982	1.1151	0.027
H(17)	-0.1435	0.2770	1.0725	0.028
H(18)	-0.1302	0.3608	0.9075	0.027
H(19)	0.0987	0.3712	0.7859	0.022
H(20)	0.2050	0.1318	0.7559	0.020
H(21A)	0.3226	0.0114	0.8607	0.024
H(21B)	0.3258	-0.0824	0.7711	0.024
H(23)	0.5448	0.0590	0.9023	0.028
H(24)	0.8040	0.0547	0.8729	0.035
H(25)	0.9505	-0.0222	0.7217	0.033
H(26)	0.8360	-0.0932	0.6008	0.030
H(27)	0.5772	-0.0824	0.6274	0.025

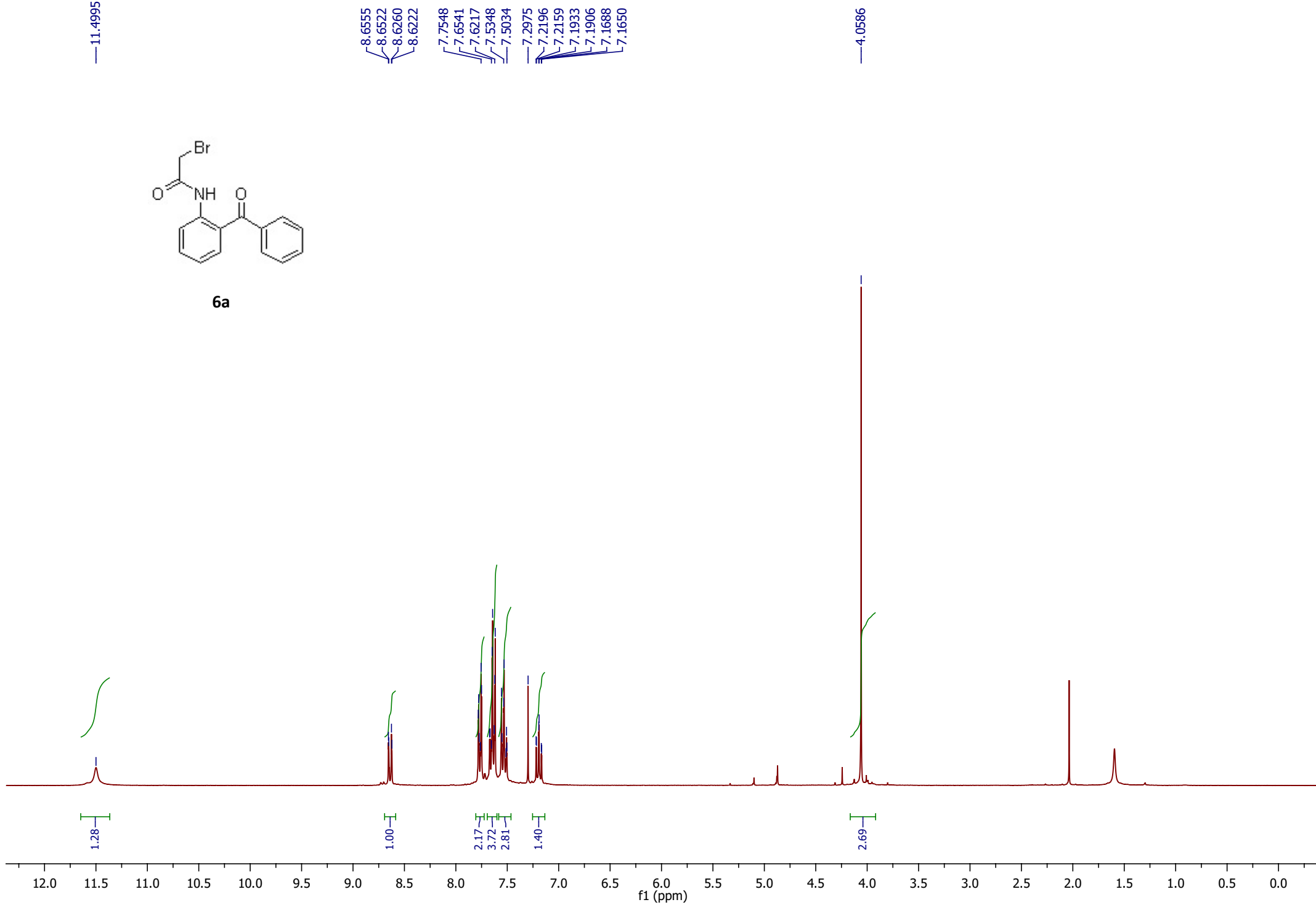
Table 6. Torsion angles [°] for 06087.

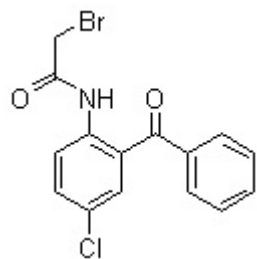
N(1)-Ni(1)-O(2)-C(28)	80(13)	Cl(1)-C(10)-C(11)-C(12)	179.46(14)
N(2)-Ni(1)-O(2)-C(28)	-15.81(13)	C(10)-C(11)-C(12)-C(7)	2.3(3)
N(3)-Ni(1)-O(2)-C(28)	160.56(13)	C(10)-C(11)-C(12)-C(13)	-177.75(17)
N(2)-Ni(1)-N(1)-C(6)	151.45(14)	N(1)-C(7)-C(12)-C(11)	-177.95(16)
O(2)-Ni(1)-N(1)-C(6)	56(13)	C(8)-C(7)-C(12)-C(11)	-2.2(3)
N(3)-Ni(1)-N(1)-C(6)	-24.92(14)	N(1)-C(7)-C(12)-C(13)	2.1(3)
N(2)-Ni(1)-N(1)-C(7)	-30.21(15)	C(8)-C(7)-C(12)-C(13)	177.88(17)
O(2)-Ni(1)-N(1)-C(7)	-126(13)	C(20)-N(2)-C(13)-C(12)	172.01(16)
N(3)-Ni(1)-N(1)-C(7)	153.42(15)	Ni(1)-N(2)-C(13)-C(12)	-4.3(3)
N(1)-Ni(1)-N(2)-C(13)	21.38(17)	C(20)-N(2)-C(13)-C(14)	-11.6(3)
O(2)-Ni(1)-N(2)-C(13)	-158.92(17)	Ni(1)-N(2)-C(13)-C(14)	172.16(13)
N(3)-Ni(1)-N(2)-C(13)	111.9(11)	C(11)-C(12)-C(13)-N(2)	167.87(17)
N(1)-Ni(1)-N(2)-C(20)	-155.26(12)	C(7)-C(12)-C(13)-N(2)	-12.2(3)
O(2)-Ni(1)-N(2)-C(20)	24.44(12)	C(11)-C(12)-C(13)-C(14)	-8.6(2)
N(3)-Ni(1)-N(2)-C(20)	-64.8(11)	C(7)-C(12)-C(13)-C(14)	171.28(16)
N(1)-Ni(1)-N(3)-C(5)	32.10(12)	N(2)-C(13)-C(14)-C(15)	106.8(2)
N(2)-Ni(1)-N(3)-C(5)	-58.6(11)	C(12)-C(13)-C(14)-C(15)	-76.6(2)
O(2)-Ni(1)-N(3)-C(5)	-147.60(12)	N(2)-C(13)-C(14)-C(19)	-75.1(2)
N(1)-Ni(1)-N(3)-C(1)	-95.74(14)	C(12)-C(13)-C(14)-C(19)	101.5(2)
N(2)-Ni(1)-N(3)-C(1)	173.5(10)	C(19)-C(14)-C(15)-C(16)	-1.0(3)
O(2)-Ni(1)-N(3)-C(1)	84.56(14)	C(13)-C(14)-C(15)-C(16)	177.04(18)
C(5)-N(3)-C(1)-C(4)	-177.40(16)	C(14)-C(15)-C(16)-C(17)	-0.2(3)
Ni(1)-N(3)-C(1)-C(4)	-54.27(19)	C(15)-C(16)-C(17)-C(18)	1.2(3)
C(5)-N(3)-C(1)-C(2)	-57.3(2)	C(16)-C(17)-C(18)-C(19)	-0.9(3)
Ni(1)-N(3)-C(1)-C(2)	65.85(19)	C(17)-C(18)-C(19)-C(14)	-0.3(3)
C(5)-N(3)-C(1)-C(3)	64.7(2)	C(15)-C(14)-C(19)-C(18)	1.3(3)
Ni(1)-N(3)-C(1)-C(3)	-172.12(13)	C(13)-C(14)-C(19)-C(18)	-176.83(18)
C(1)-N(3)-C(5)-C(6)	96.75(19)	C(13)-N(2)-C(20)-C(28)	155.64(17)
Ni(1)-N(3)-C(5)-C(6)	-33.55(17)	Ni(1)-N(2)-C(20)-C(28)	-27.44(17)
C(7)-N(1)-C(6)-O(1)	12.8(3)	C(13)-N(2)-C(20)-C(21)	-83.5(2)
Ni(1)-N(1)-C(6)-O(1)	-168.81(18)	Ni(1)-N(2)-C(20)-C(21)	93.44(15)
C(7)-N(1)-C(6)-C(5)	-168.48(16)	N(2)-C(20)-C(21)-C(22)	-43.1(2)
Ni(1)-N(1)-C(6)-C(5)	9.9(2)	C(28)-C(20)-C(21)-C(22)	75.5(2)
N(3)-C(5)-C(6)-O(1)	-164.11(18)	C(20)-C(21)-C(22)-C(23)	105.0(2)
N(3)-C(5)-C(6)-N(1)	17.1(2)	C(20)-C(21)-C(22)-C(27)	-73.1(2)
C(6)-N(1)-C(7)-C(8)	26.0(3)	C(27)-C(22)-C(23)-C(24)	0.8(3)
Ni(1)-N(1)-C(7)-C(8)	-152.26(15)	C(21)-C(22)-C(23)-C(24)	-177.38(18)
C(6)-N(1)-C(7)-C(12)	-158.41(18)	C(22)-C(23)-C(24)-C(25)	-1.1(3)
Ni(1)-N(1)-C(7)-C(12)	23.4(2)	C(23)-C(24)-C(25)-C(26)	0.2(3)
N(1)-C(7)-C(8)-C(9)	175.61(18)	C(24)-C(25)-C(26)-C(27)	1.0(3)
C(12)-C(7)-C(8)-C(9)	-0.2(3)	C(25)-C(26)-C(27)-C(22)	-1.3(3)
C(7)-C(8)-C(9)-C(10)	2.4(3)	C(23)-C(22)-C(27)-C(26)	0.3(3)
C(8)-C(9)-C(10)-C(11)	-2.3(3)	C(21)-C(22)-C(27)-C(26)	178.51(18)
C(8)-C(9)-C(10)-Cl(1)	178.17(15)	Ni(1)-O(2)-C(28)-O(3)	-175.89(16)
C(9)-C(10)-C(11)-C(12)	0.0(3)	Ni(1)-O(2)-C(28)-C(20)	2.6(2)

N(2)-C(20)-C(28)-O(3)	-165.04(17)
C(21)-C(20)-C(28)-O(3)	74.8(2)
N(2)-C(20)-C(28)-O(2)	16.3(2)
C(21)-C(20)-C(28)-O(2)	-103.83(19)

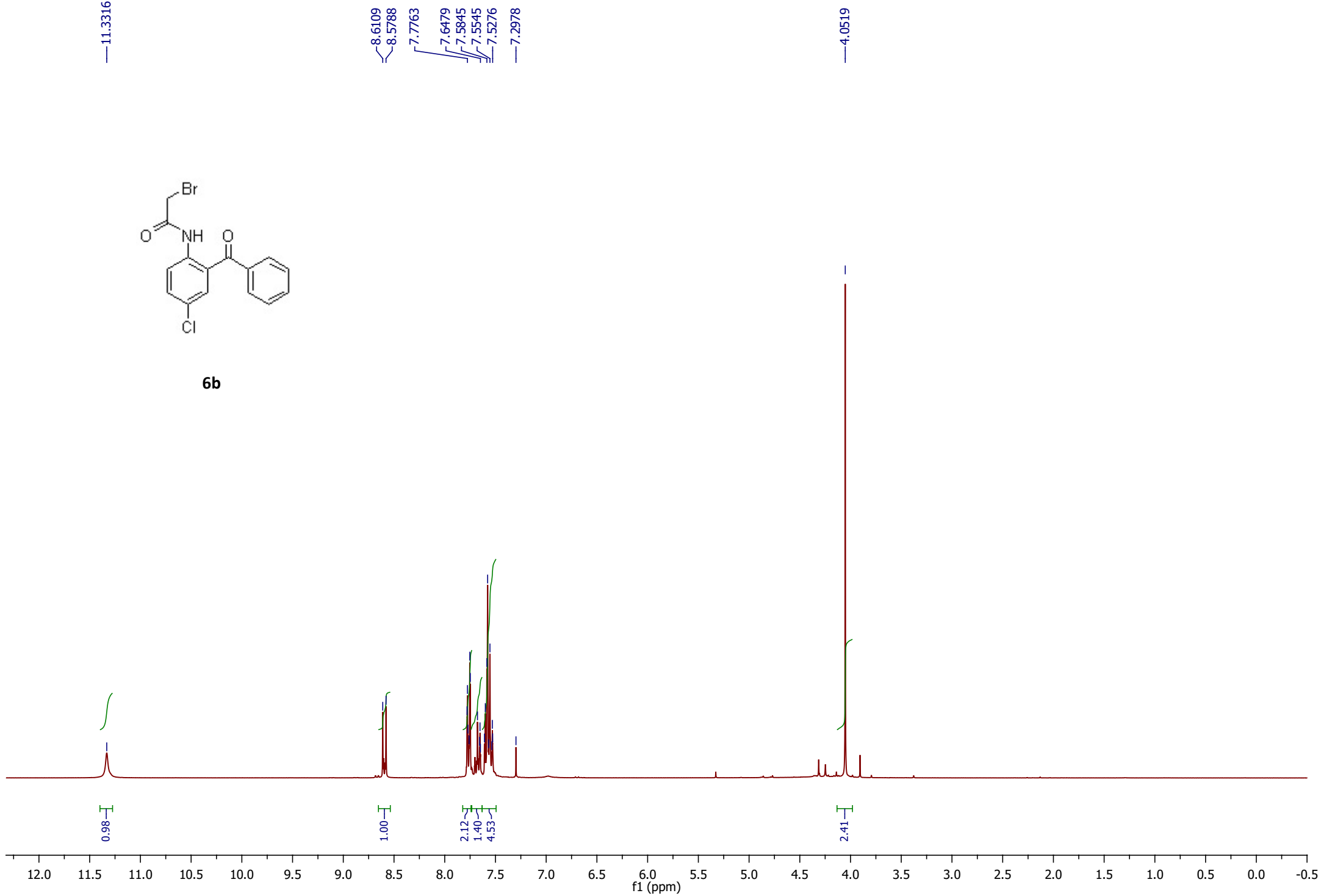


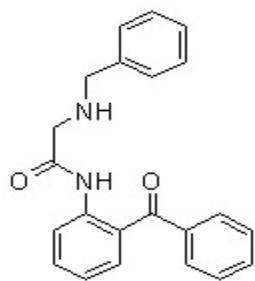
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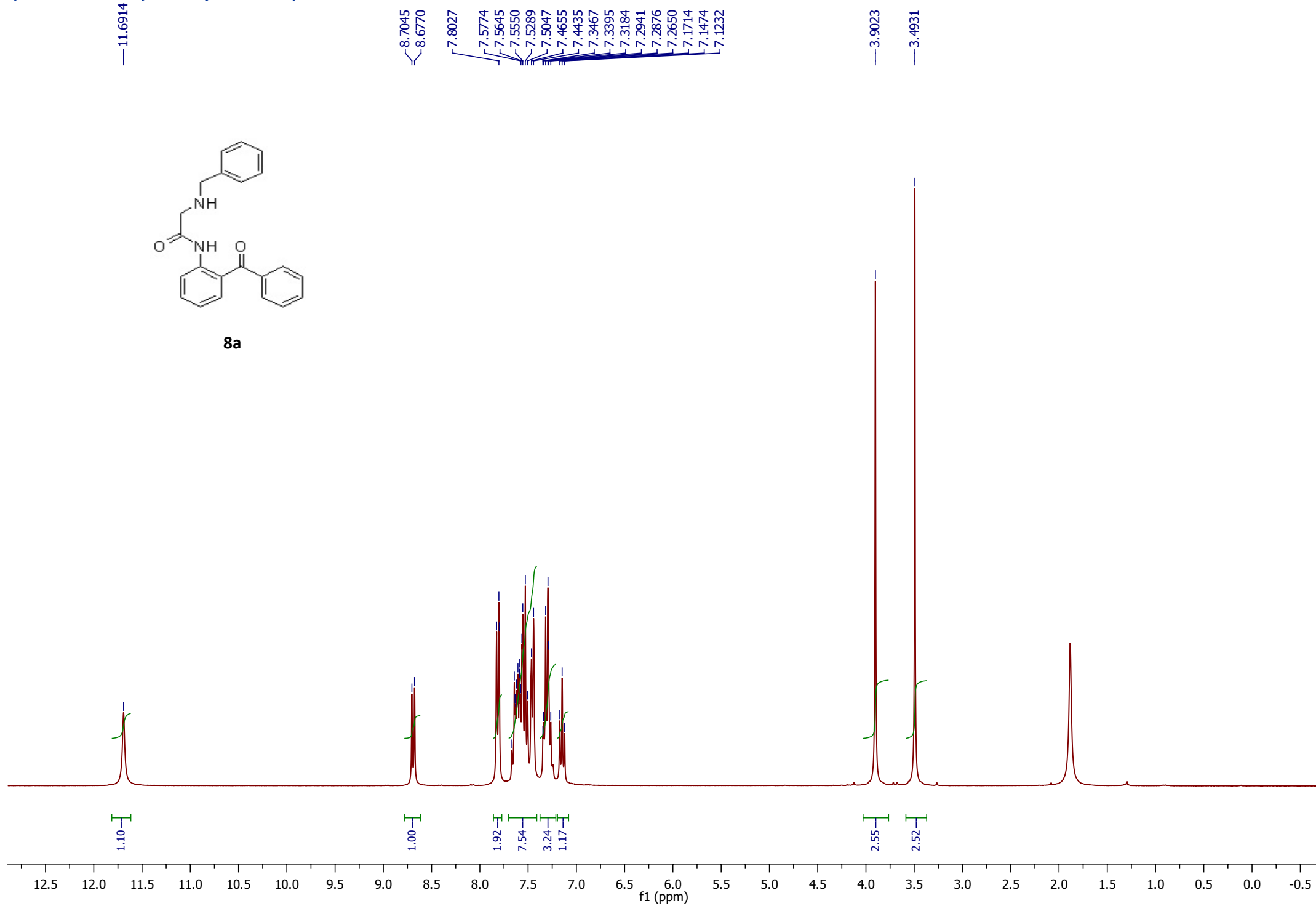


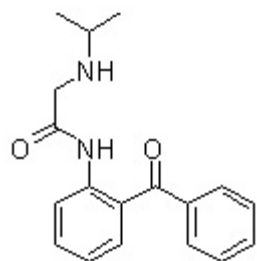
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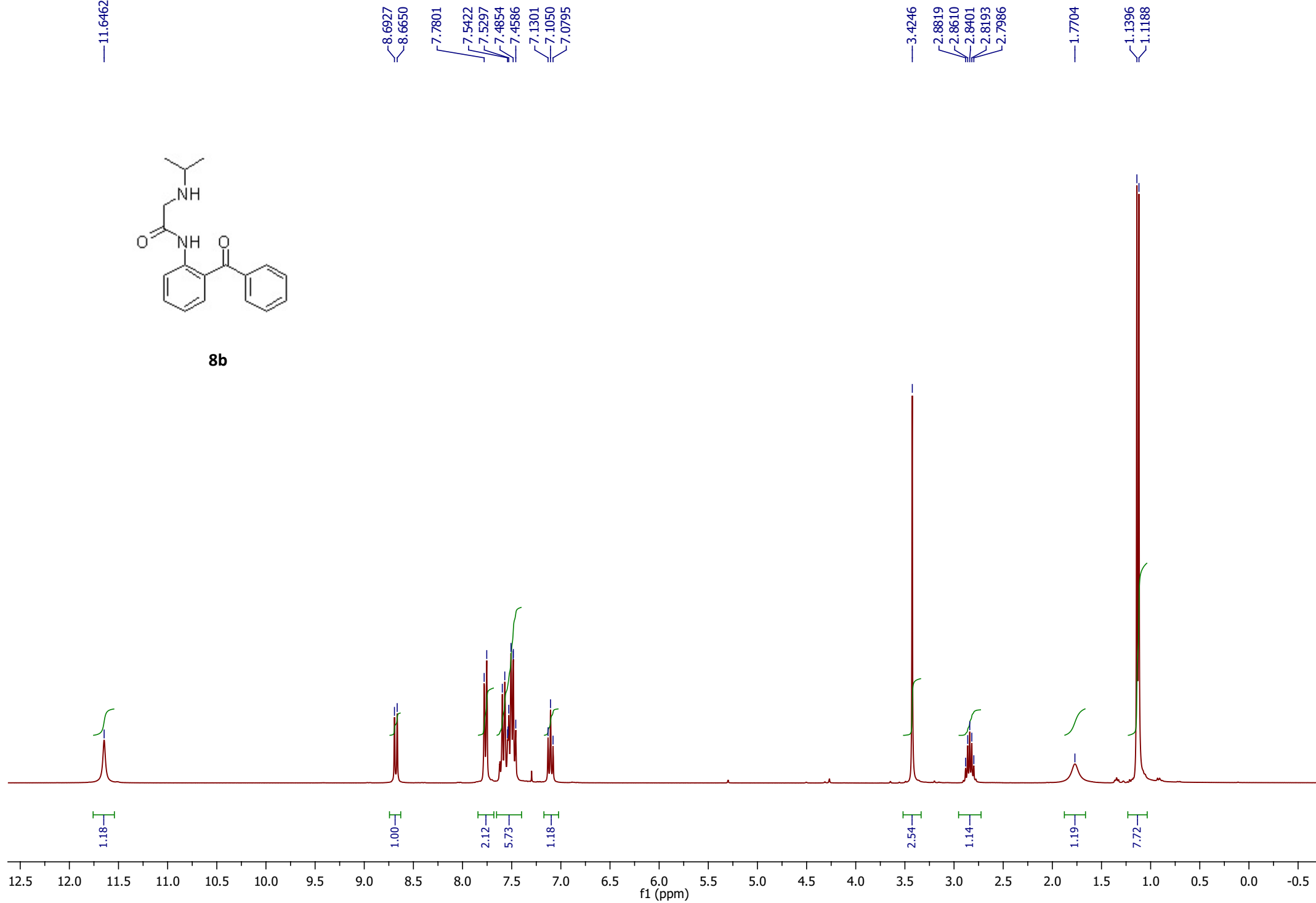


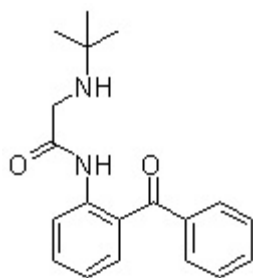
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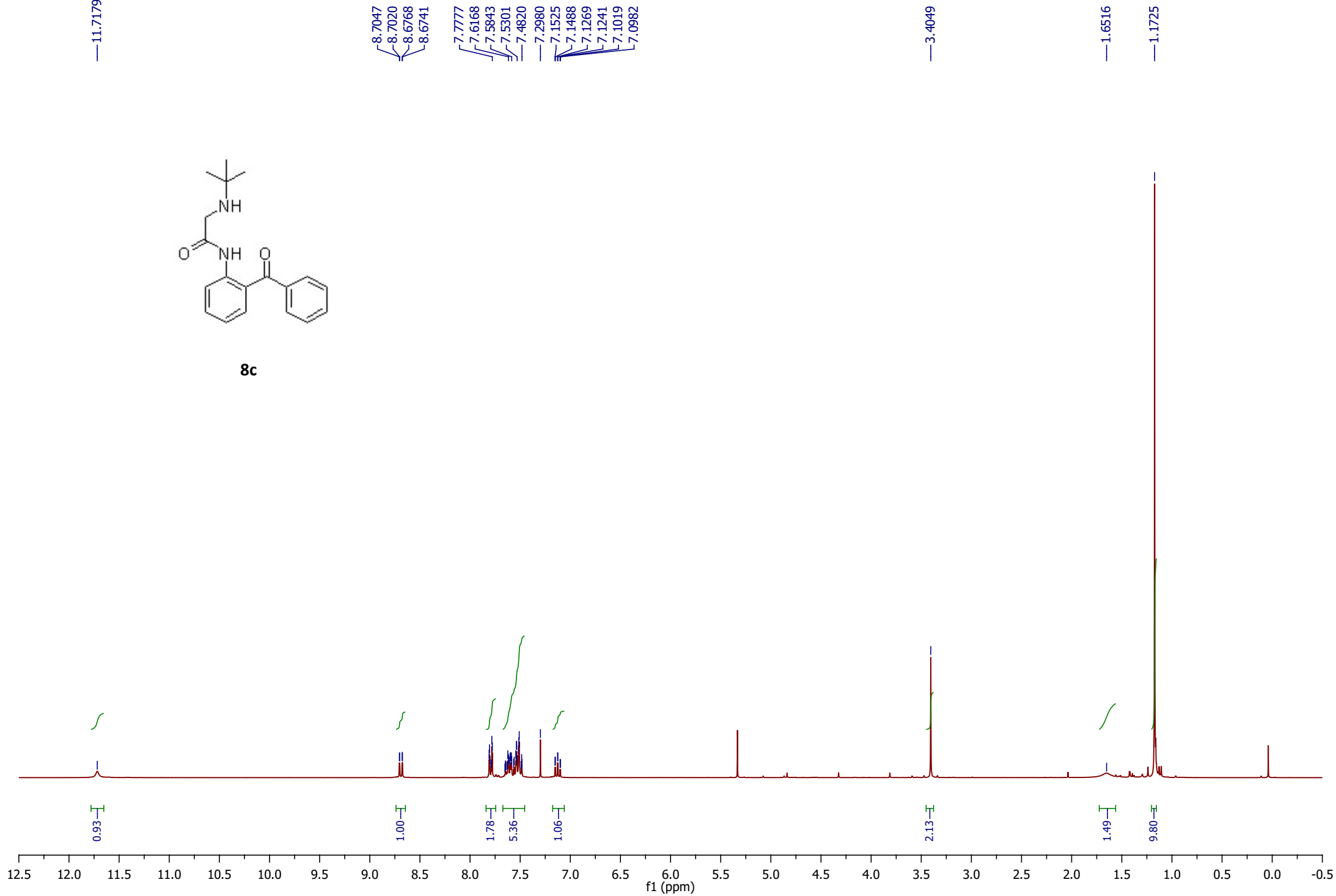


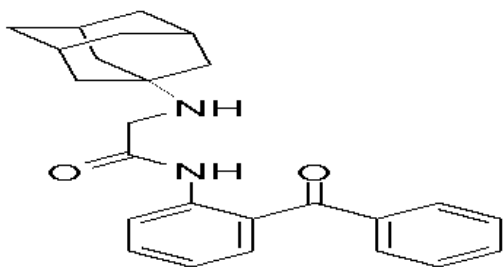
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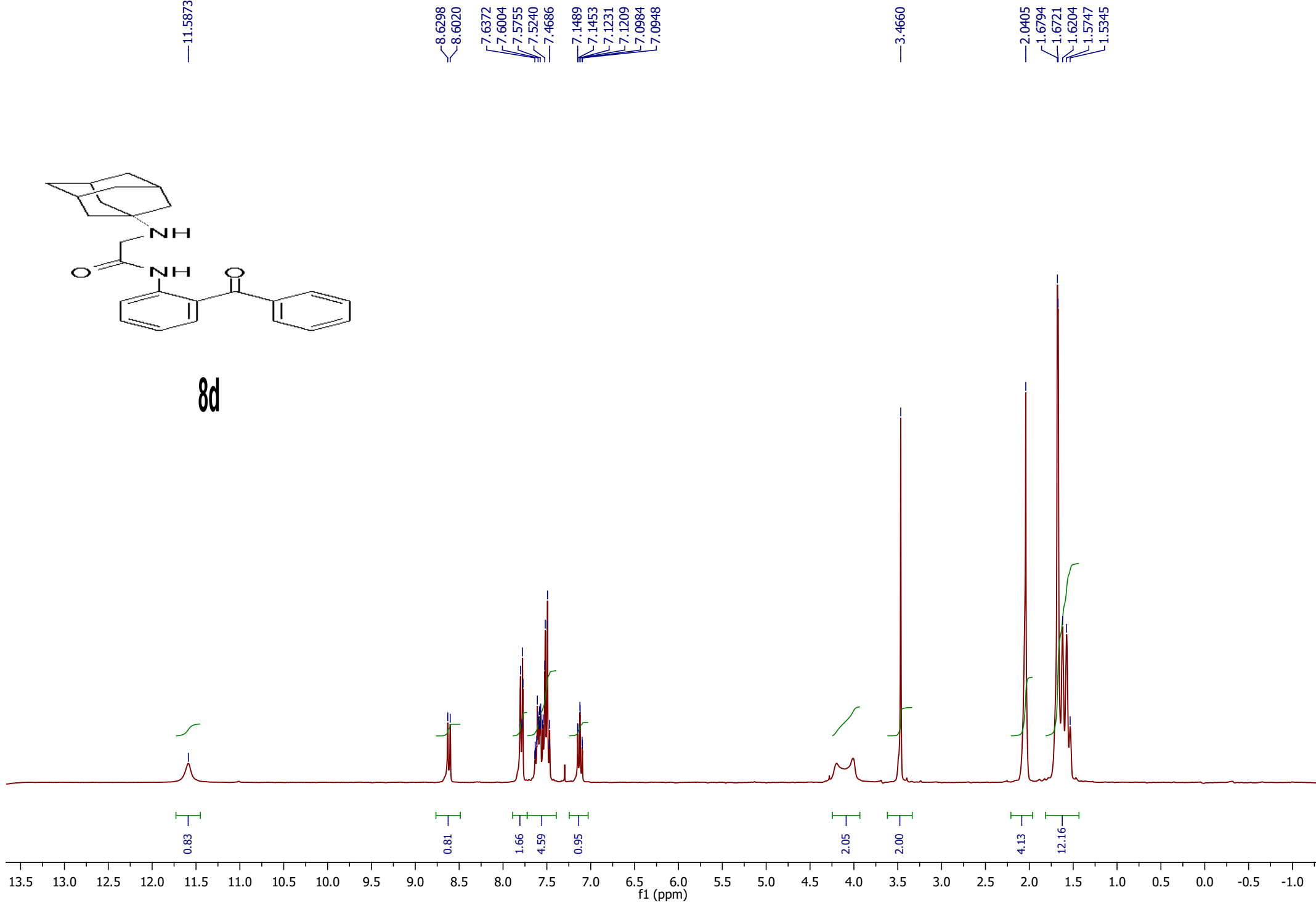


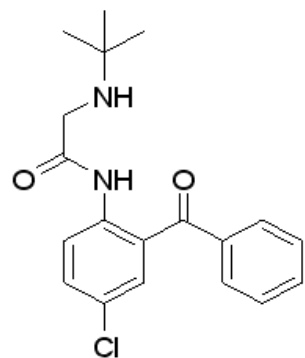
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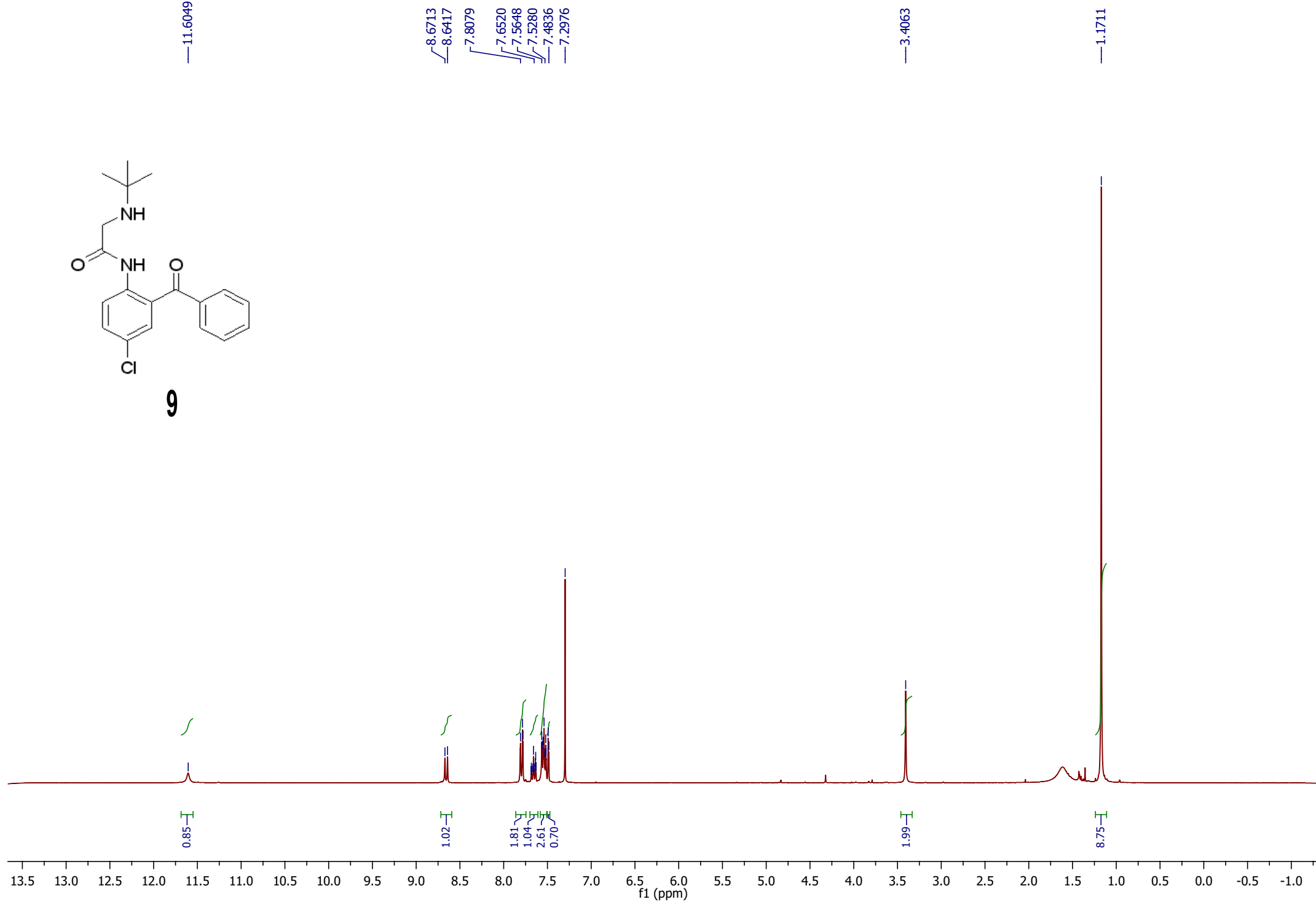


8d





9



8.6500
8.6218

7.4490
7.4281
7.4048
7.3828
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6.8352
6.8091

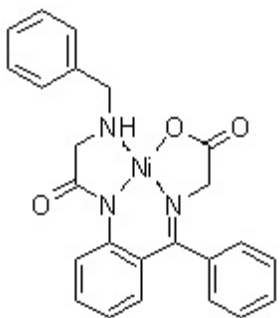
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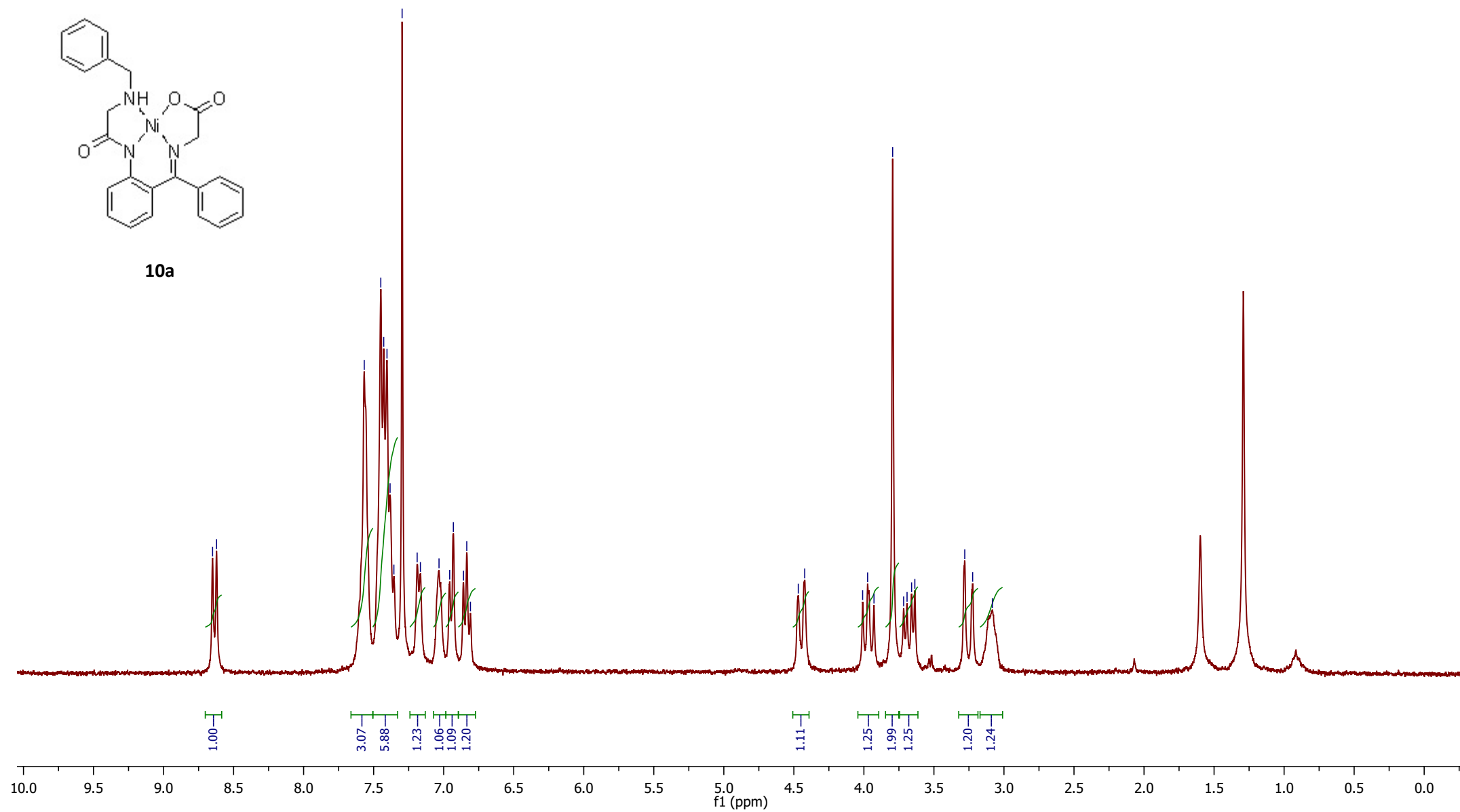
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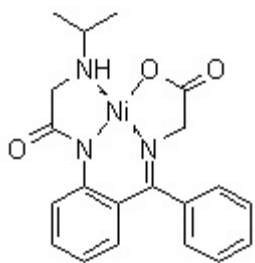
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3.2236

3.0827



10a



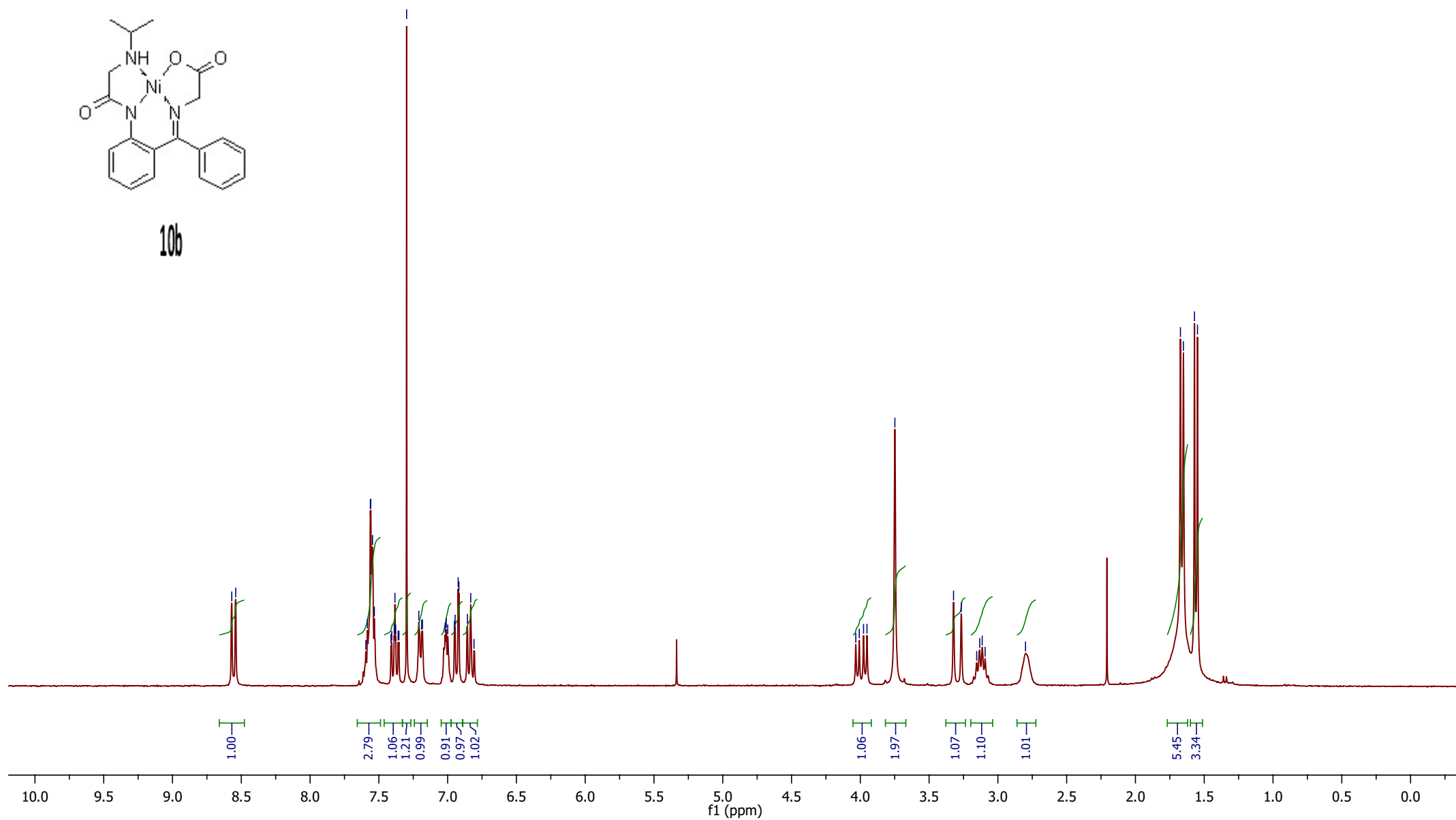


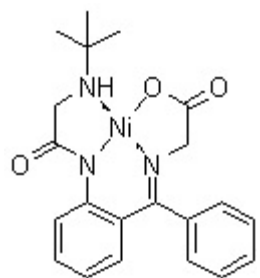
10b

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7.3776
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6.8321
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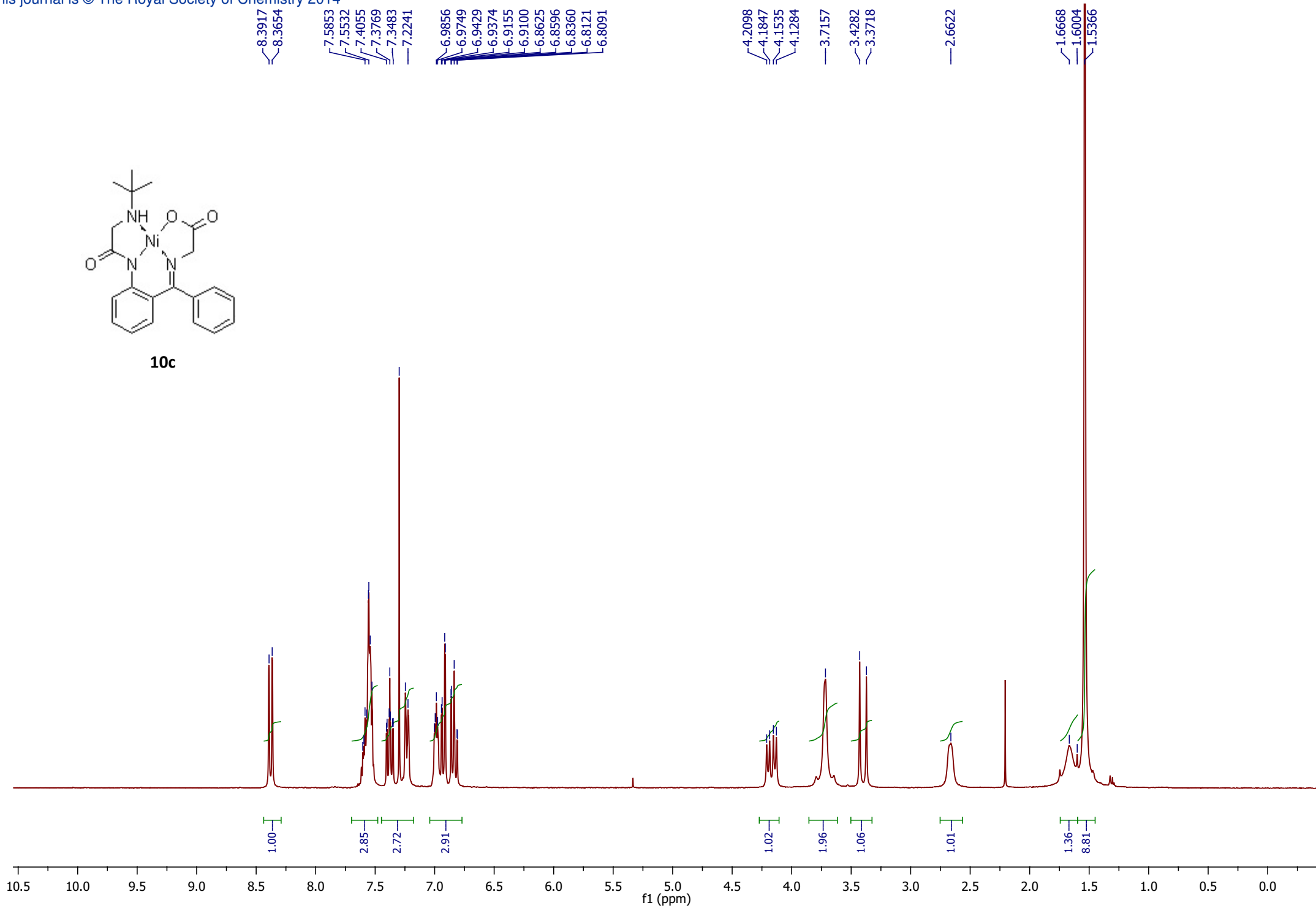
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2.7990

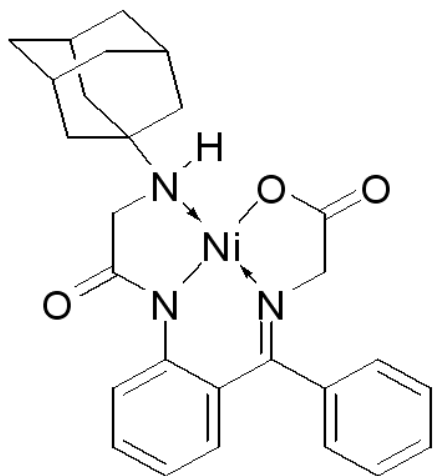
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1.6511
1.5707
1.5489



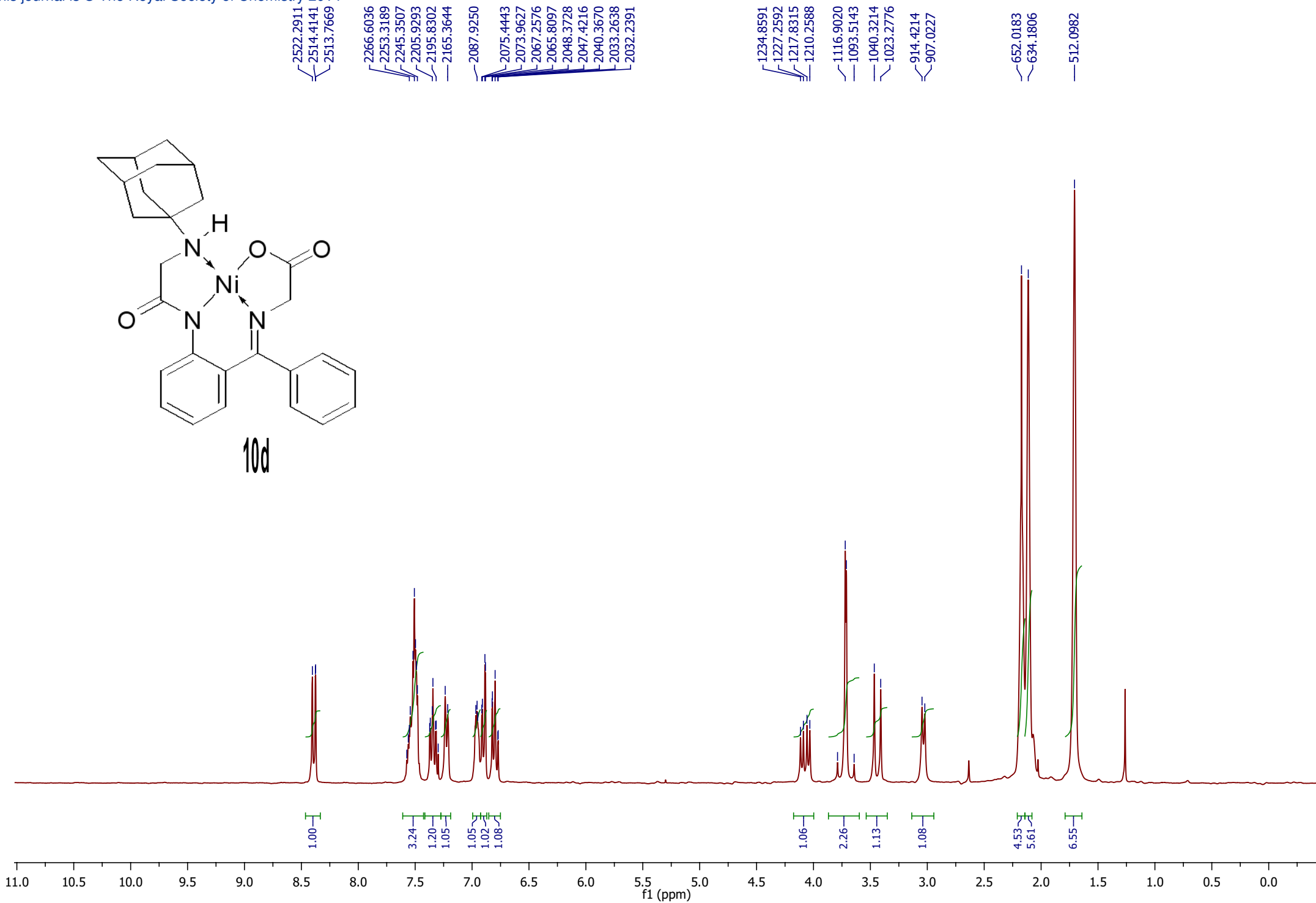


10c





10d



8.3953
8.3649

7.5724
7.5630
7.5536
7.5462

7.2107

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6.9718
6.9628
6.9497
6.8573
6.8489

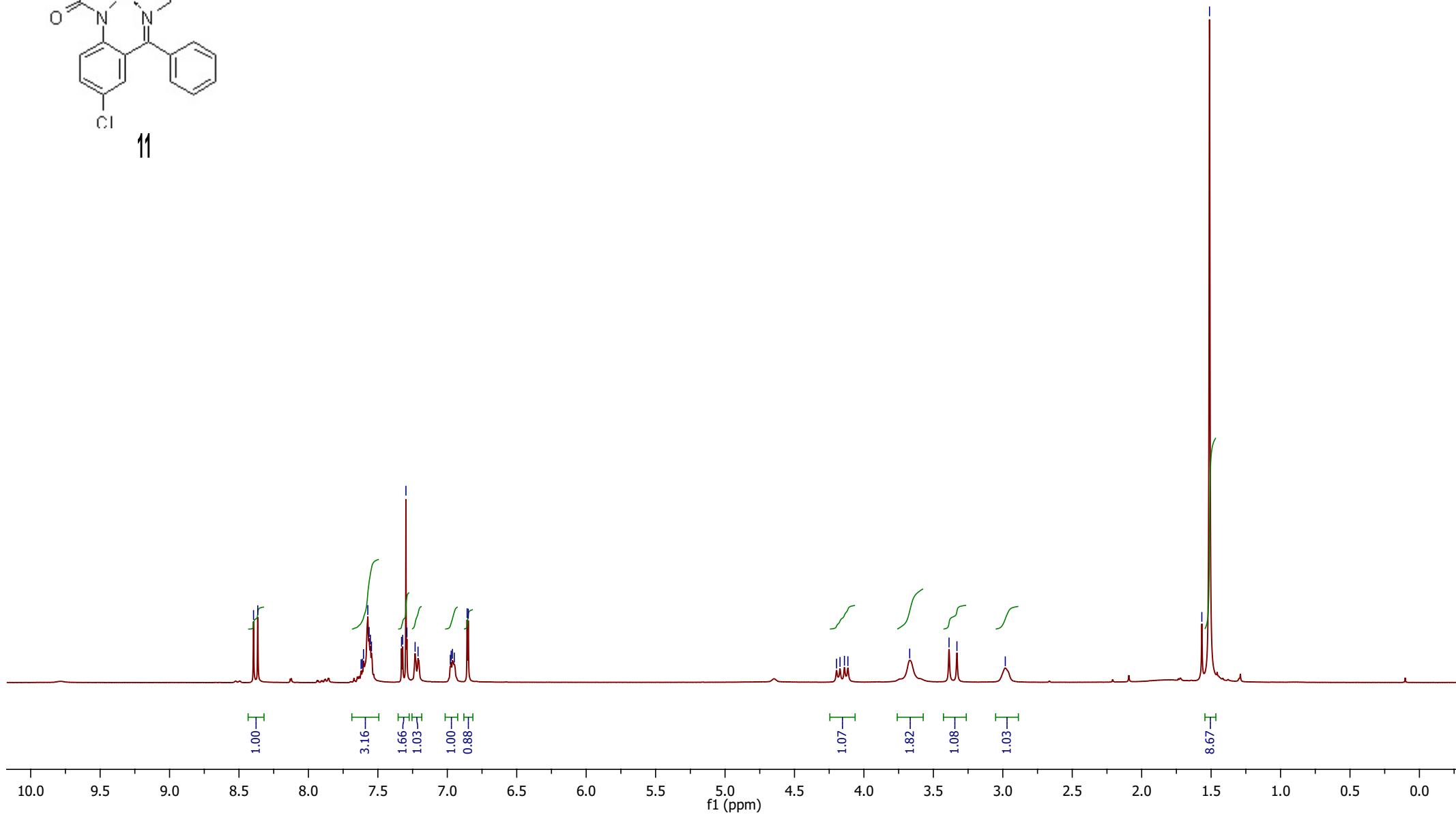
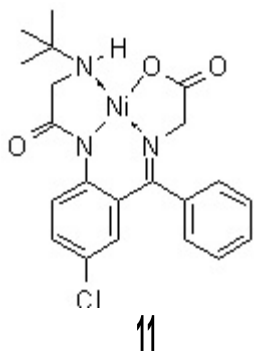
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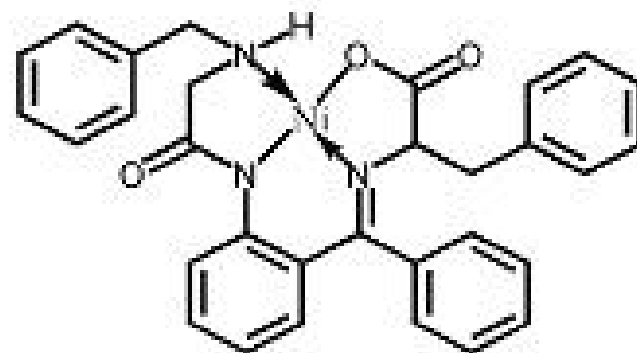
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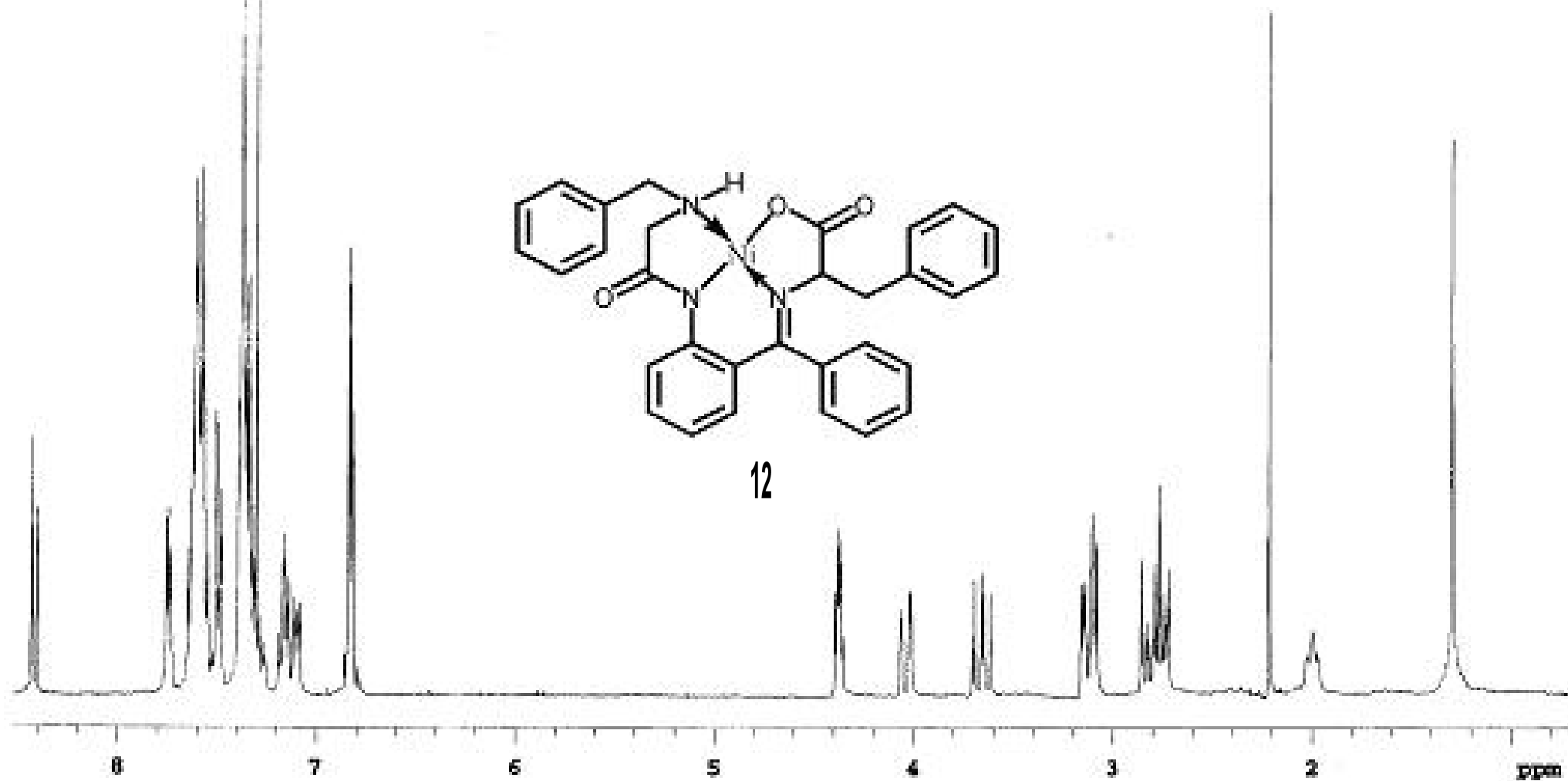
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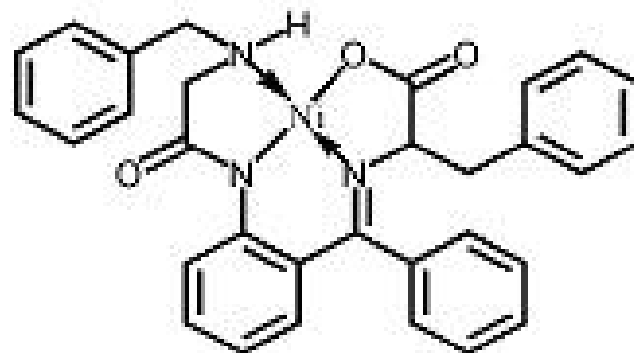
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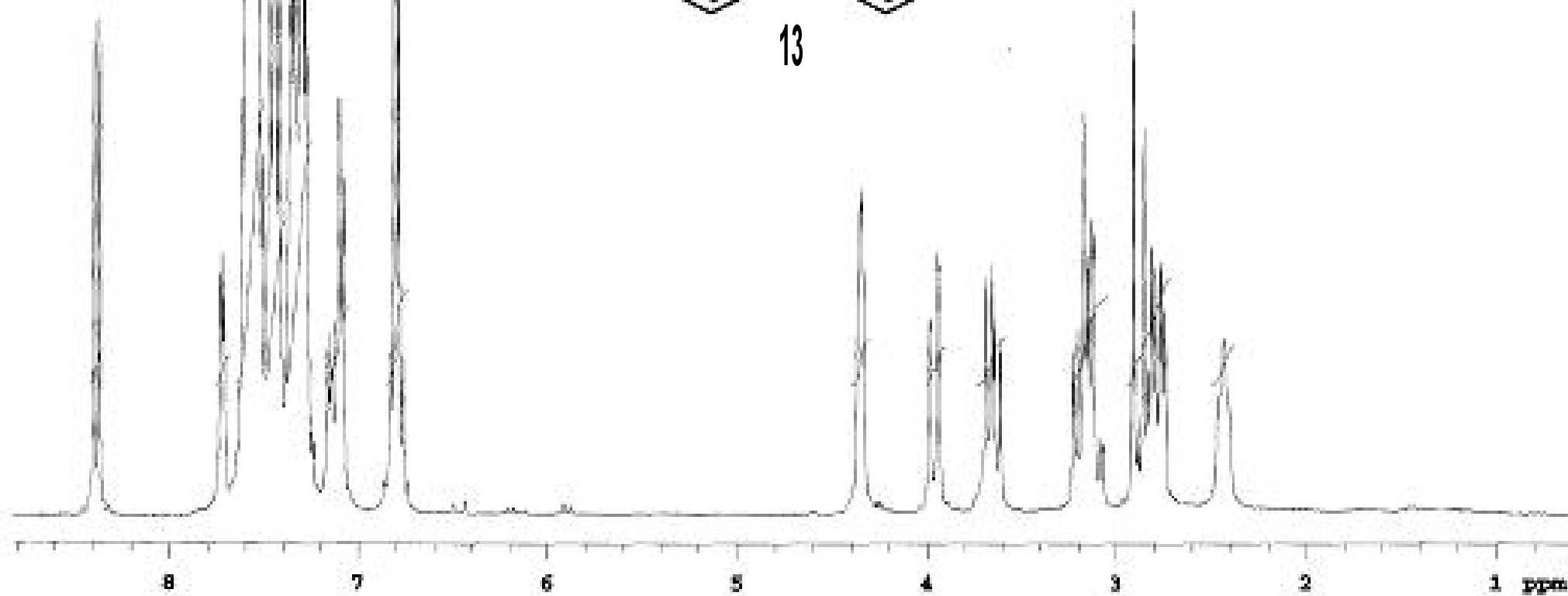


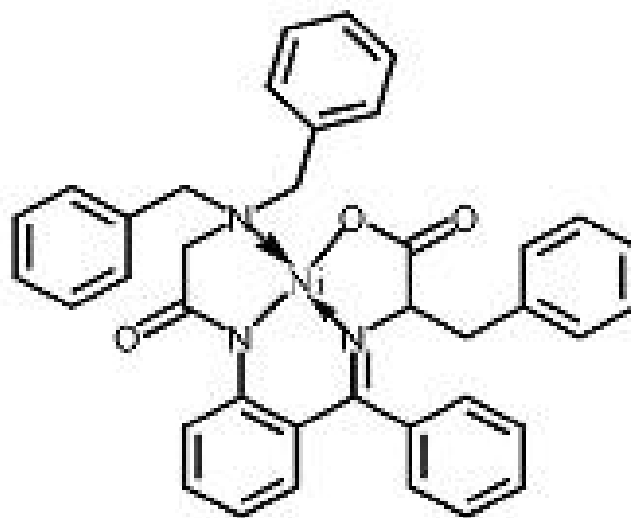
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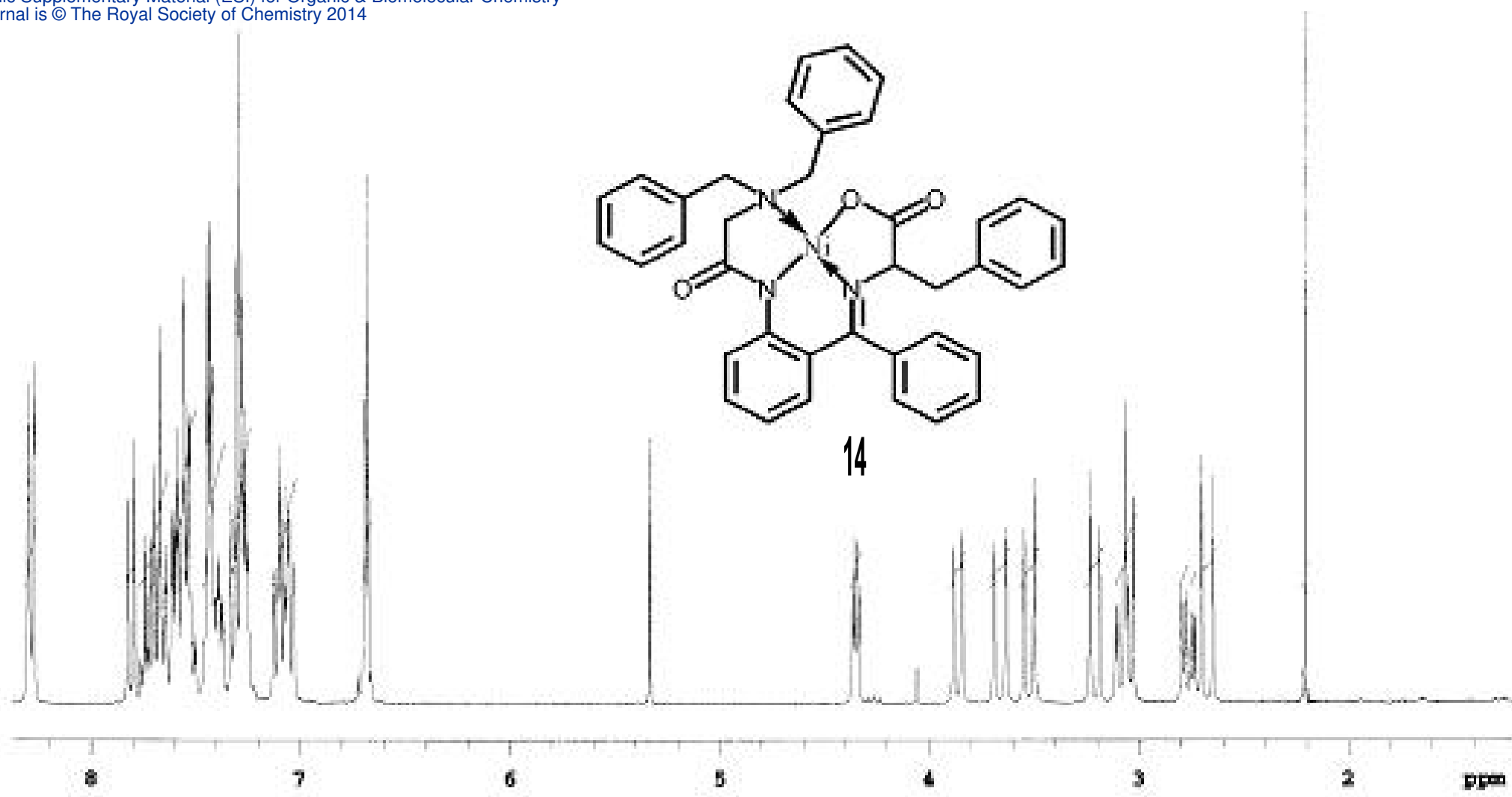


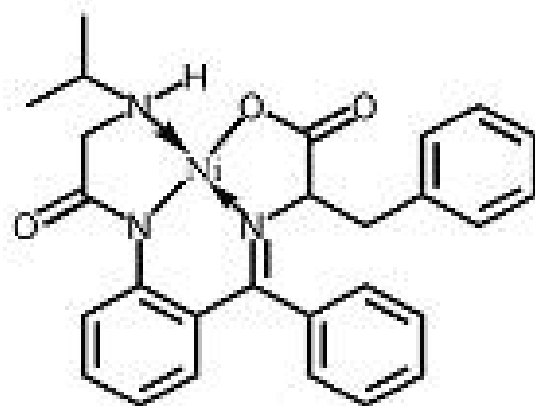
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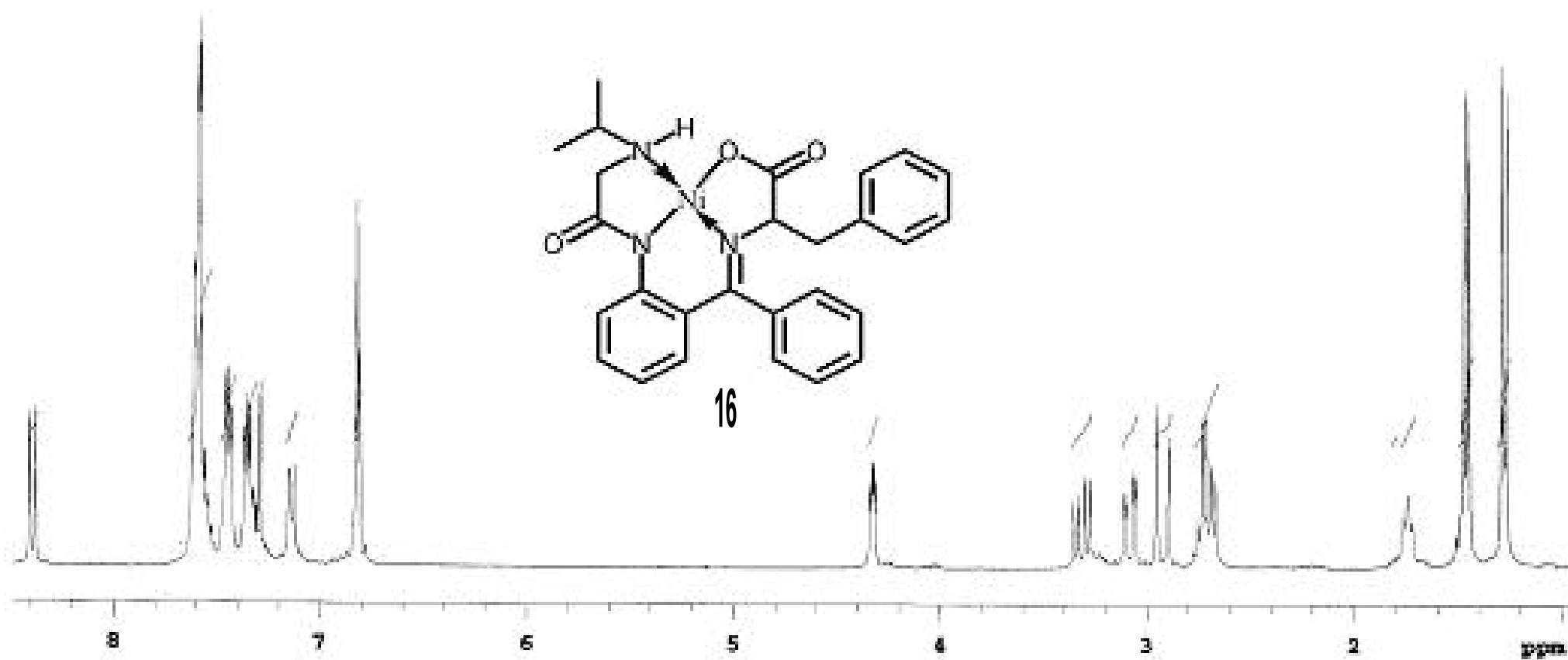


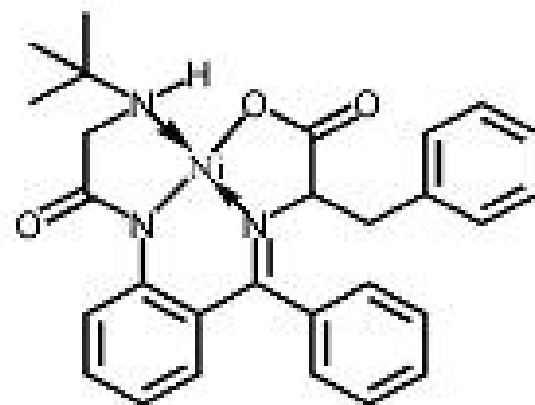
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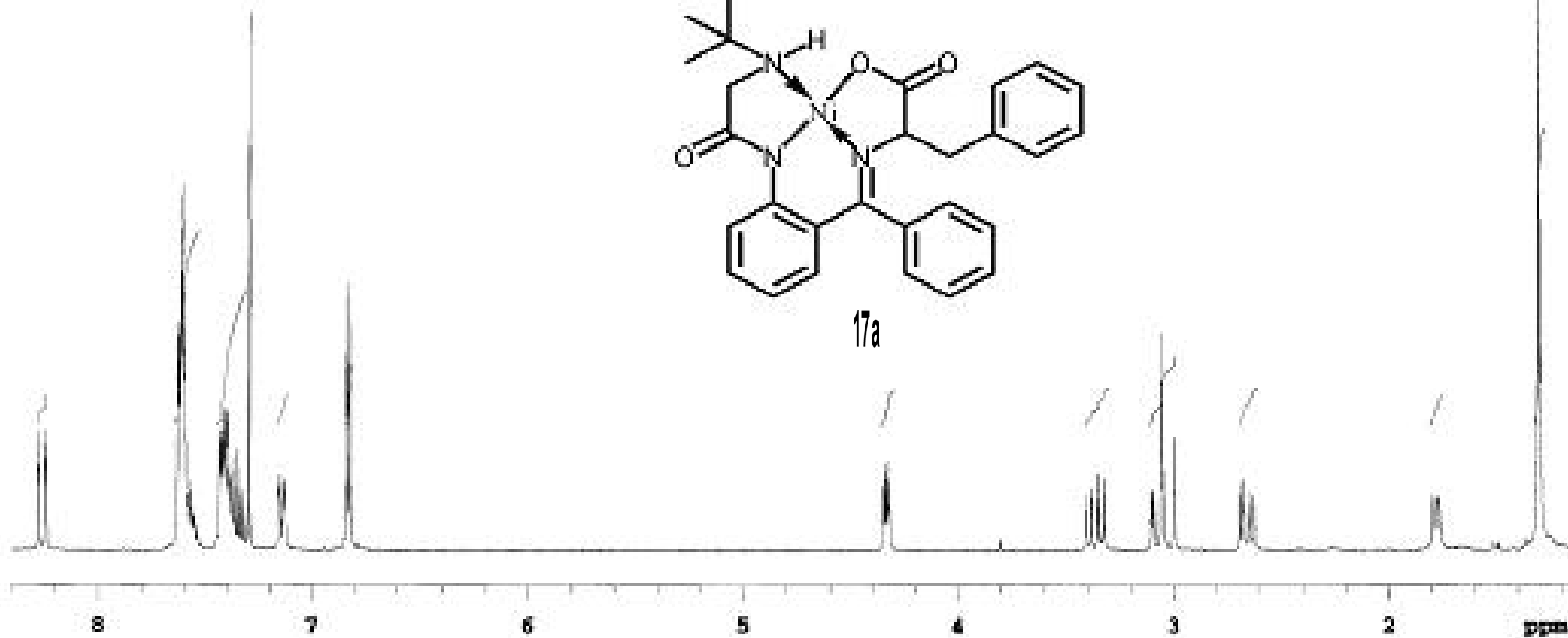


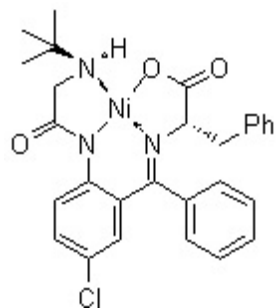
16





17a





18

8.2733
8.2430

7.6284
7.6051
7.5812
7.5610
7.4052

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7.1437
7.1157

6.7730
6.7646

4.3246
4.3148
4.3061
4.2962

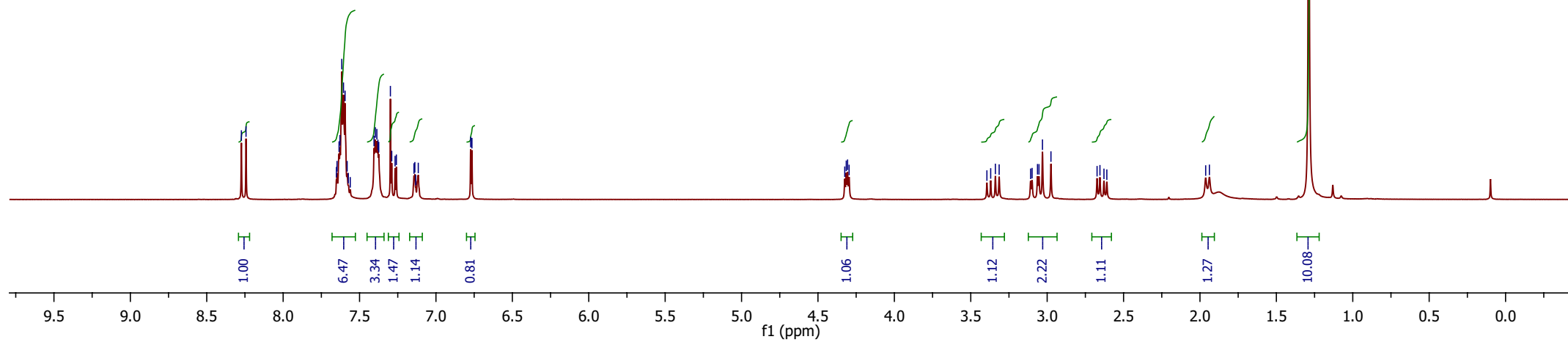
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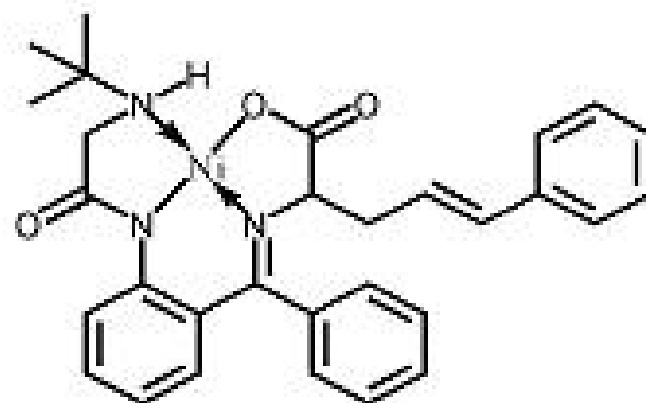
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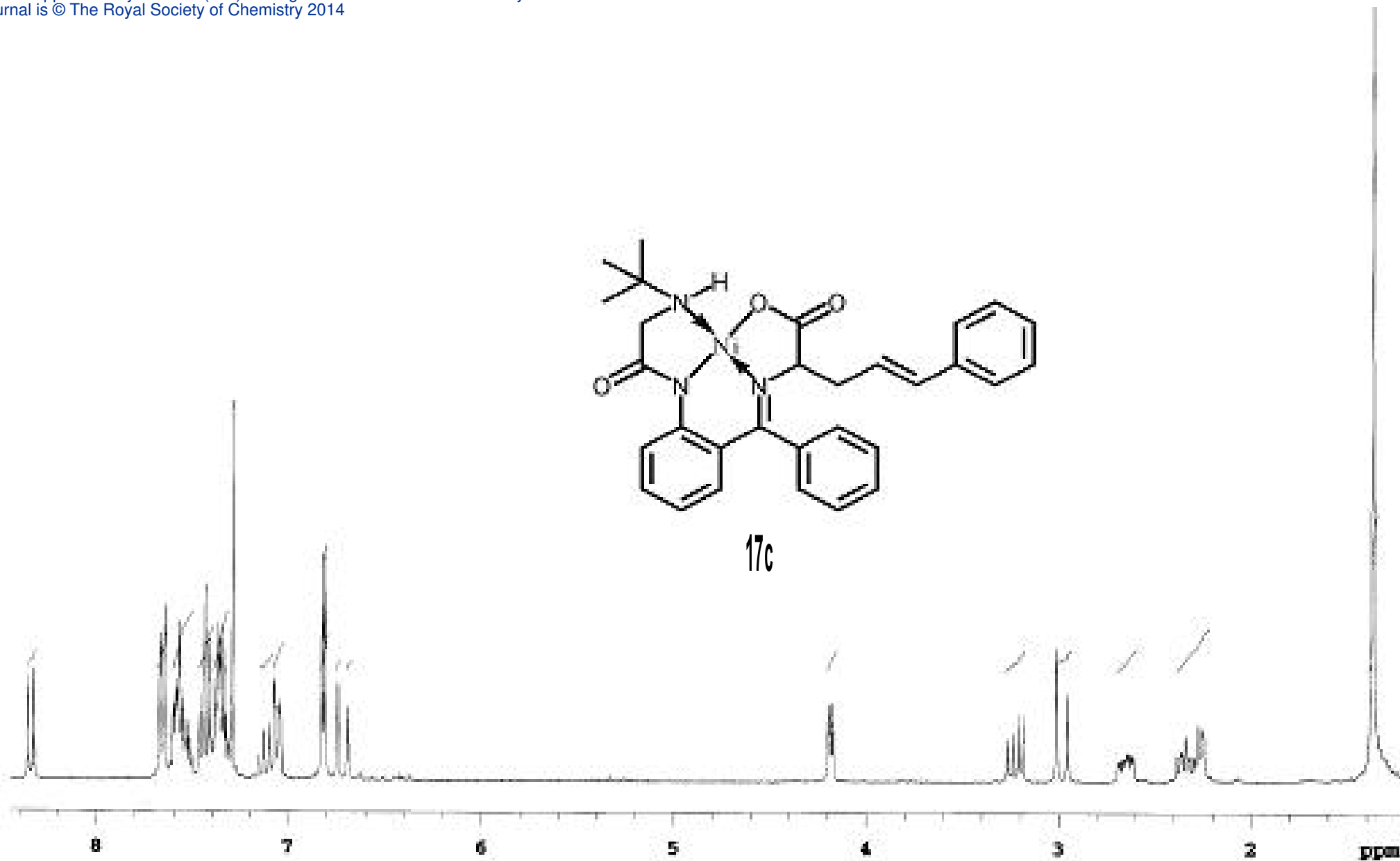
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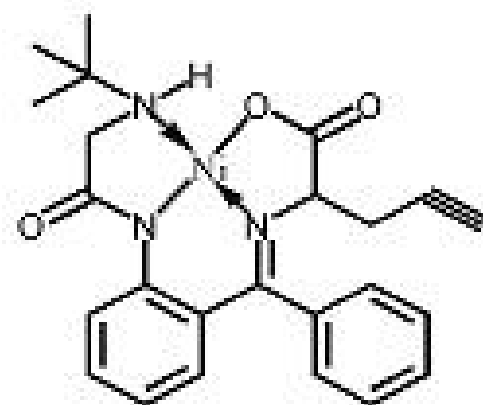
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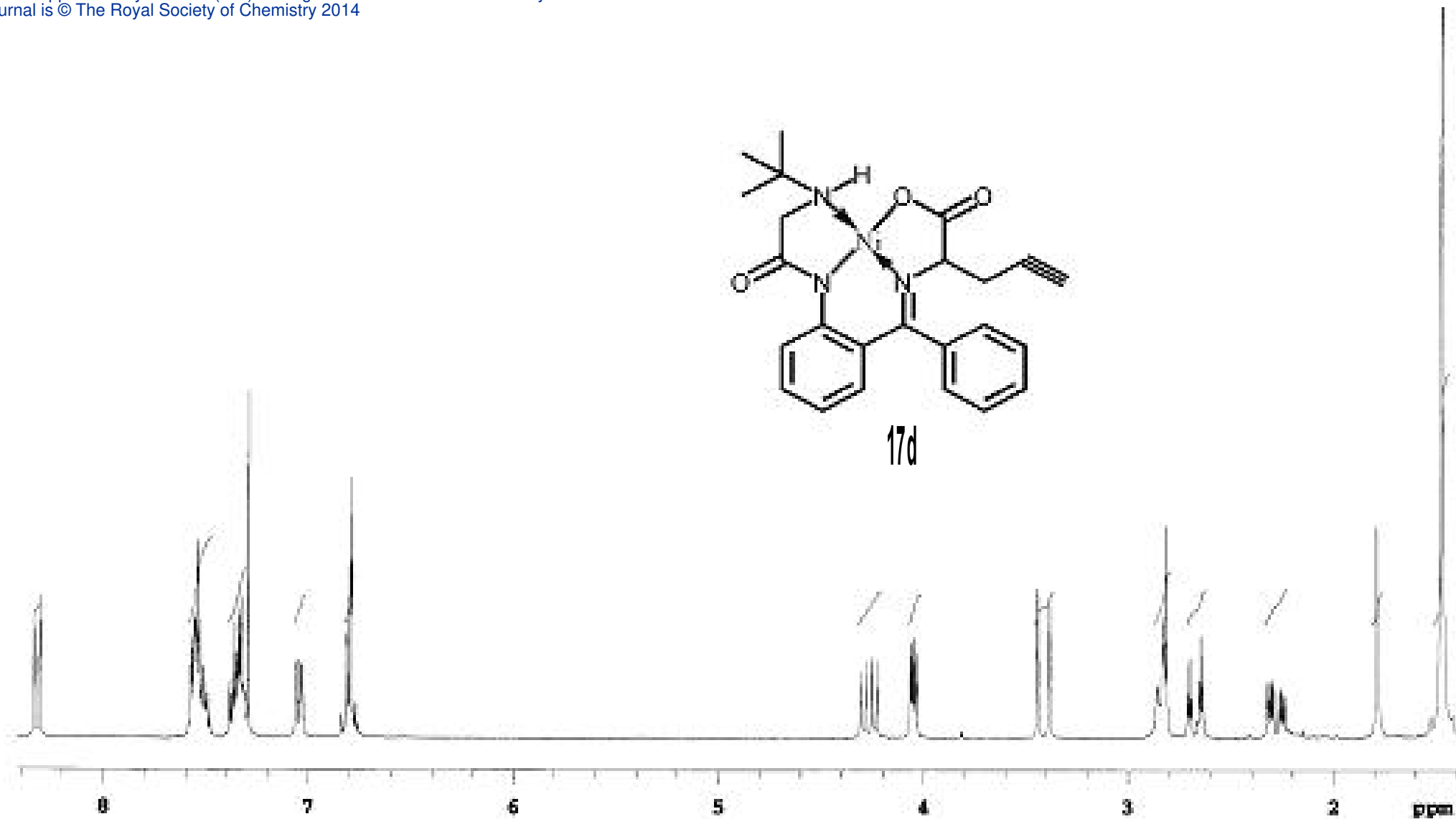


17c





17d



8.2959
8.2677

7.5929

7.3982

7.3471

7.3310

7.2980

7.1249

6.8385

6.8264

4.3203

4.3123

3.1594

3.1035

3.0938

3.0848

3.0481

3.0399

2.6973

2.6788

2.6526

2.6339

2.1095

1.9489

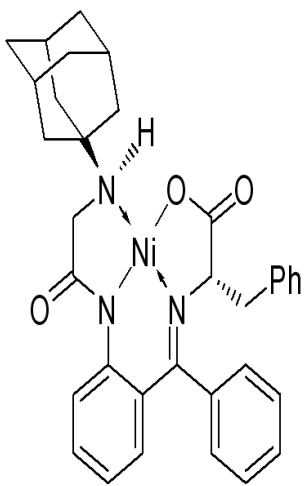
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1.7818

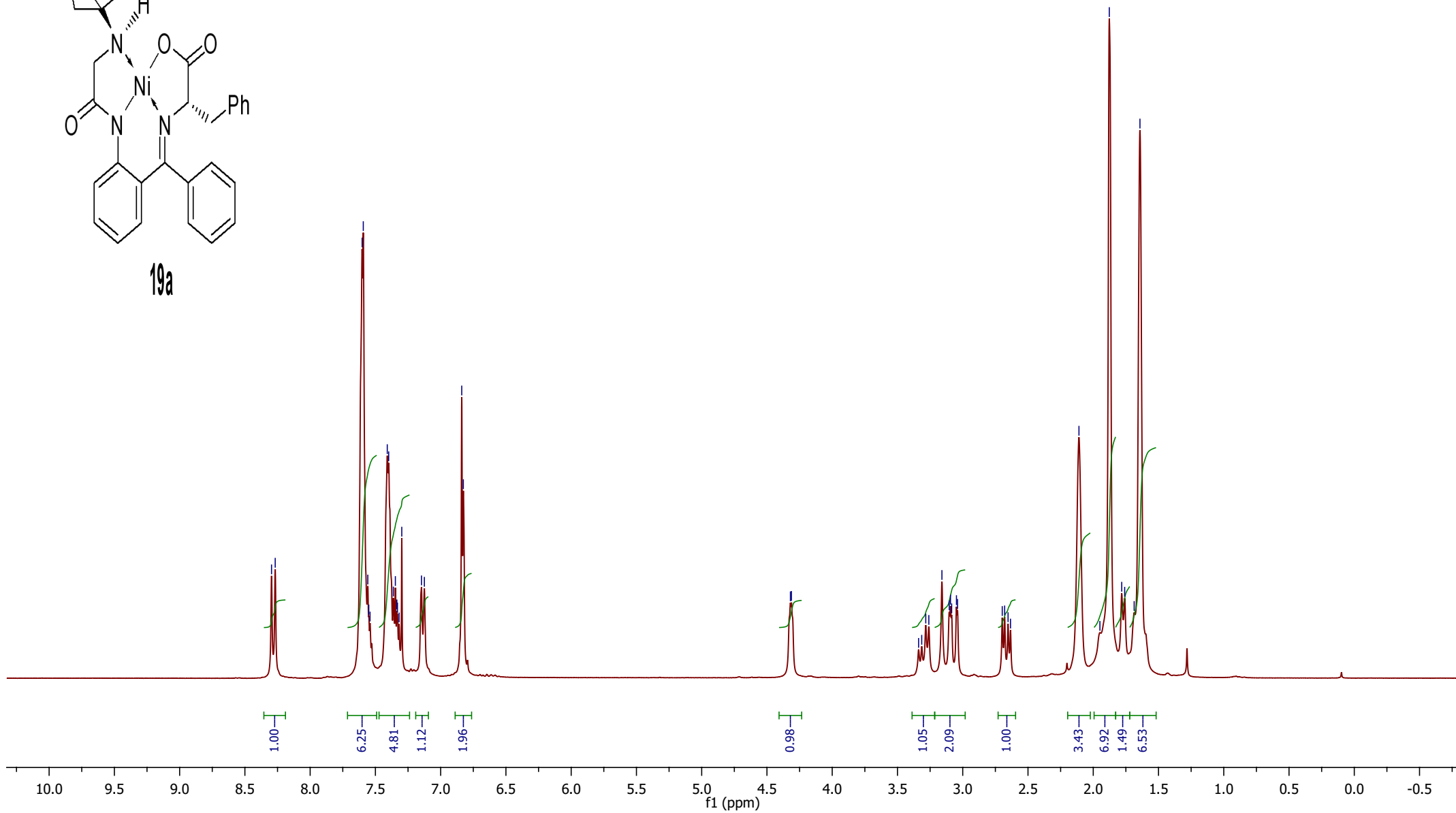
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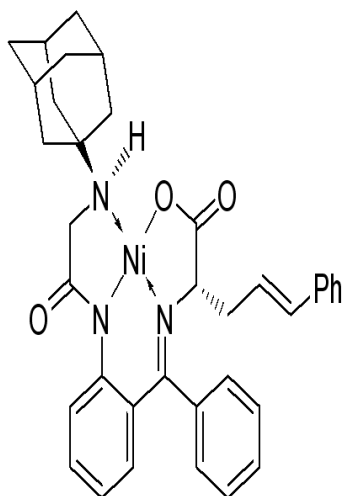
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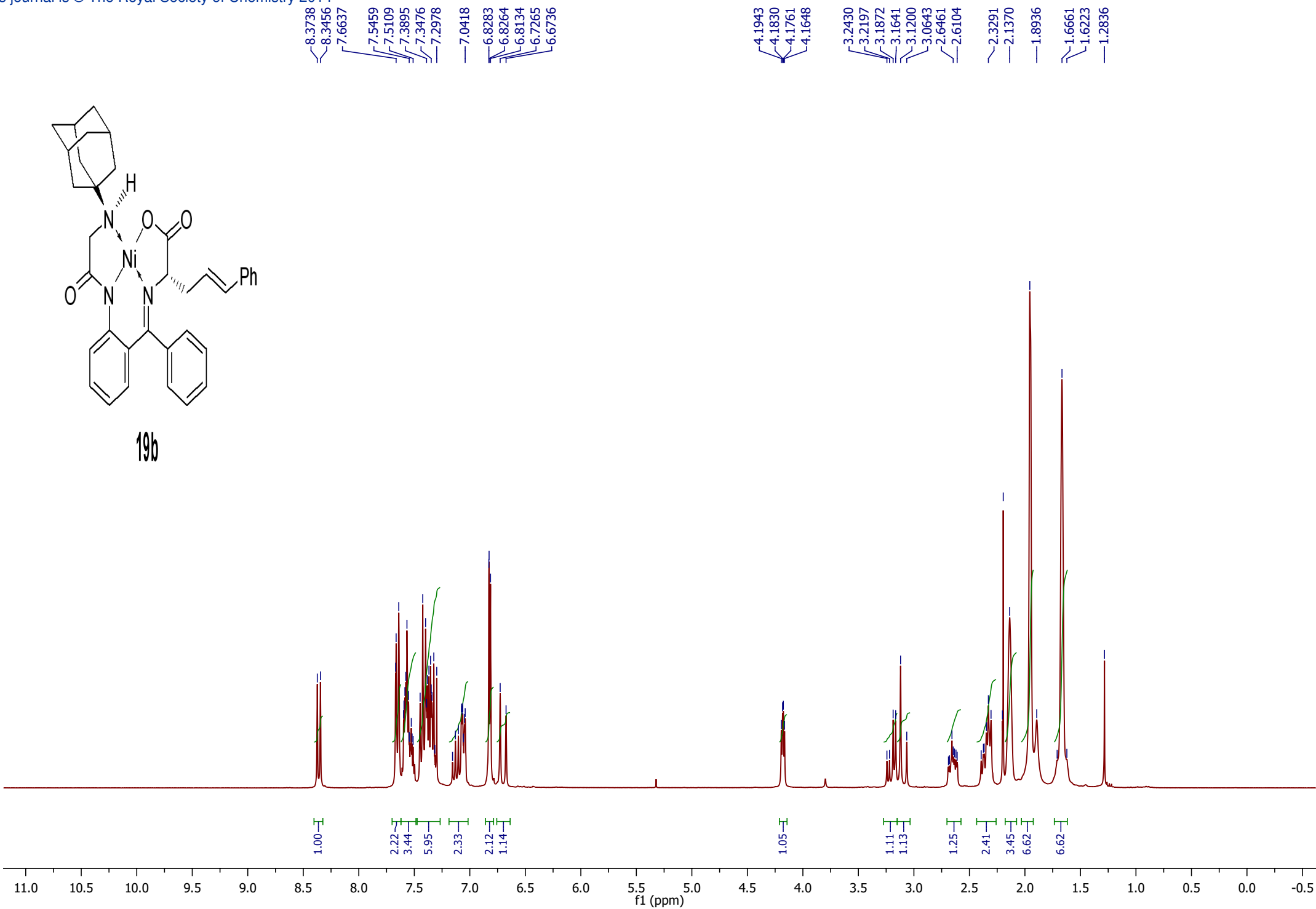


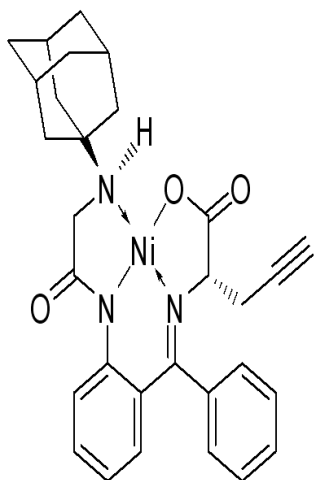
19a





19b





19c

8.3778
8.3497

7.5560
7.5211
7.4066
7.3778
7.3488
7.2981

7.0481

6.8264
6.8168
6.8078

4.2427
4.2180
4.1875
4.1628
4.0699
4.0612
4.0500
4.0412
3.7681
3.5697
3.5144

2.7867
2.7097
2.6619
2.6441
2.5554
2.3267
2.2613
2.2407
2.0875
1.7341
1.6363

1.00

3.09

2.11

1.05

1.98

1.17

1.03

1.17

0.87

1.22

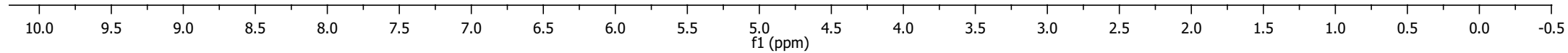
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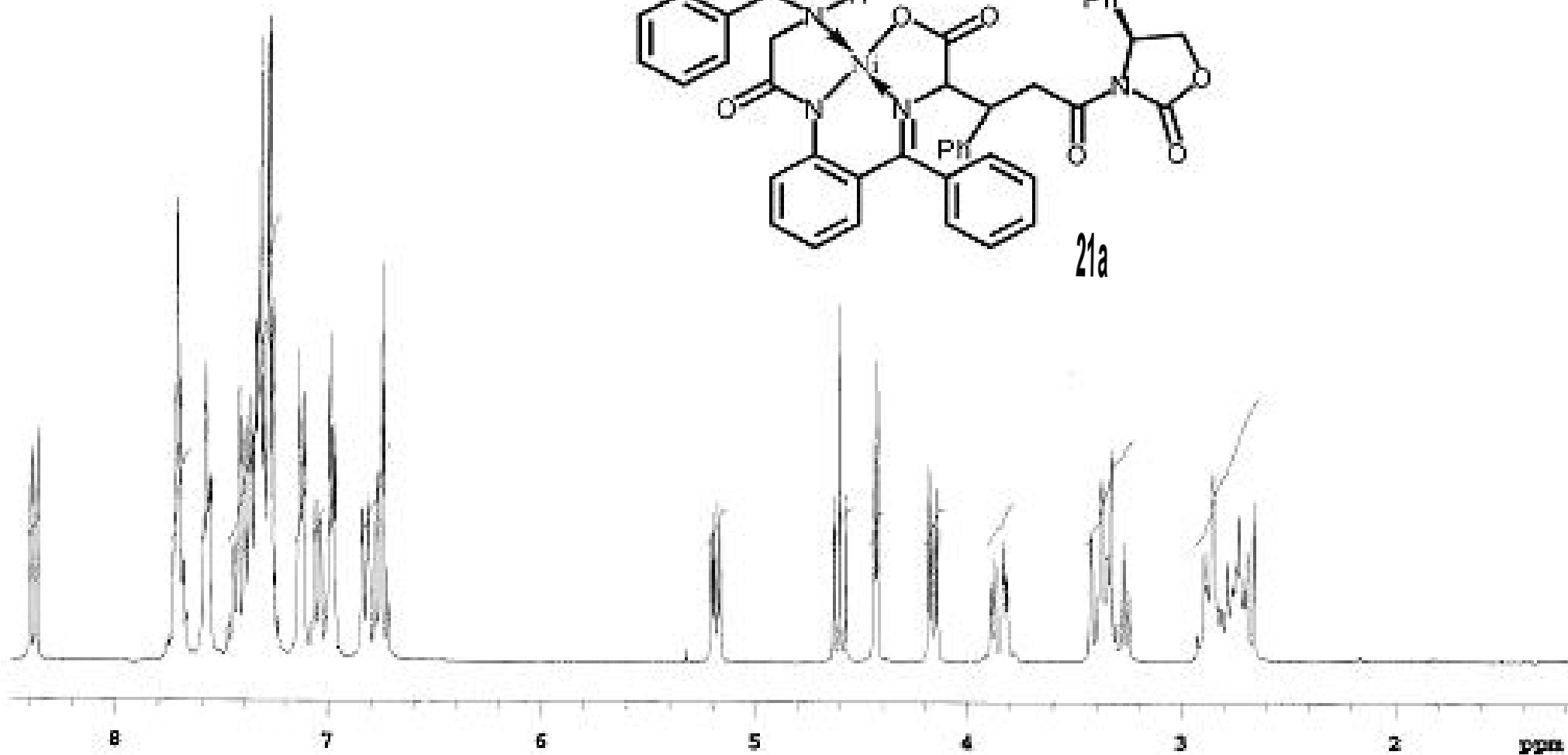
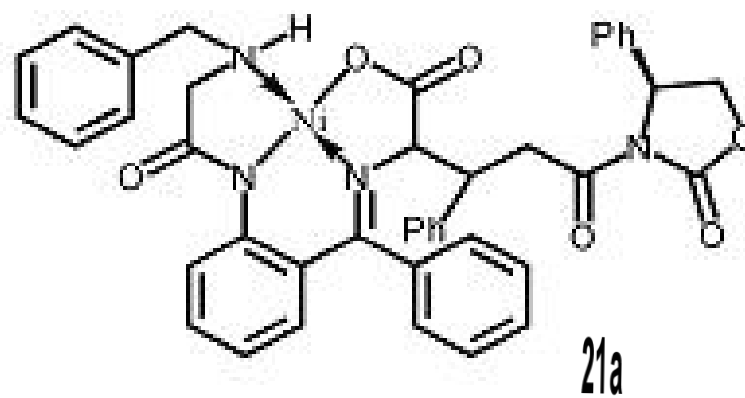
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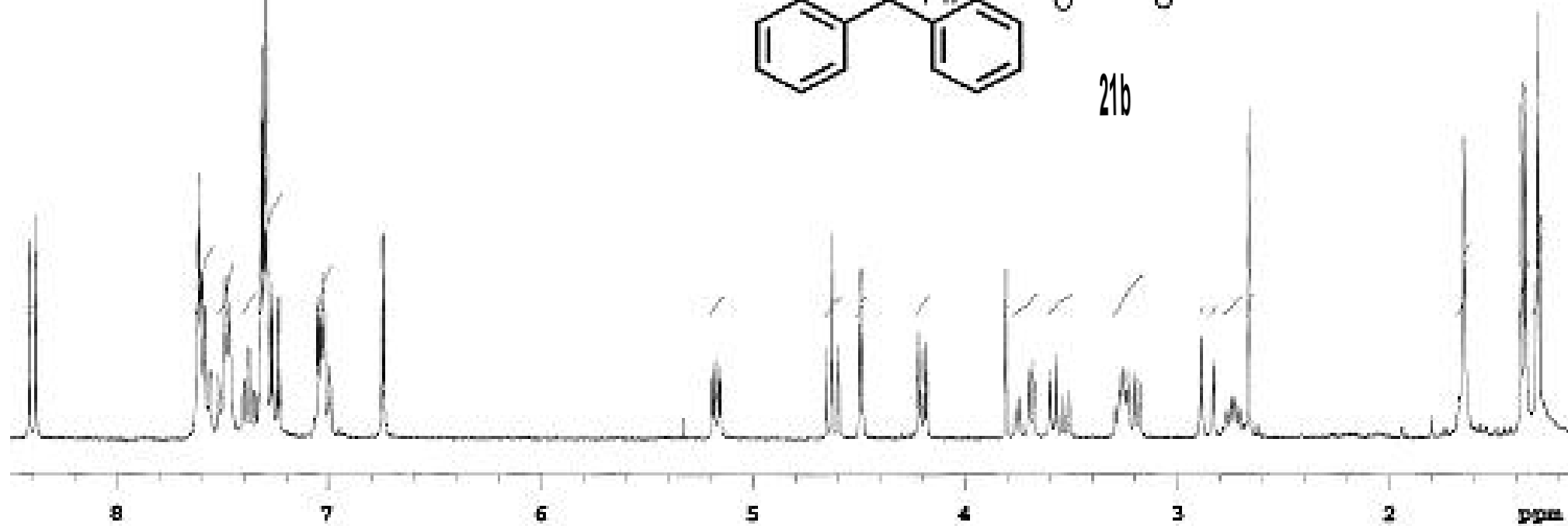
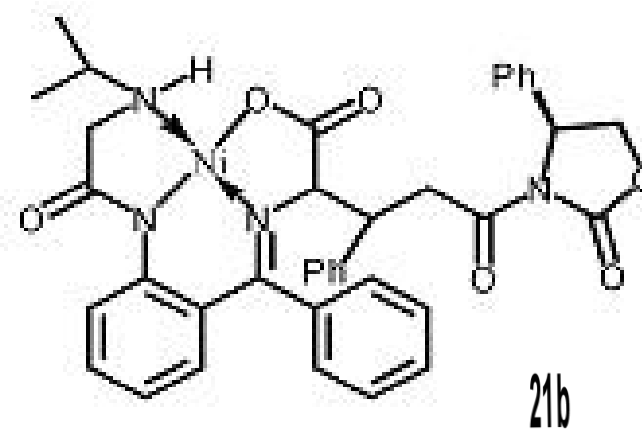
2.99

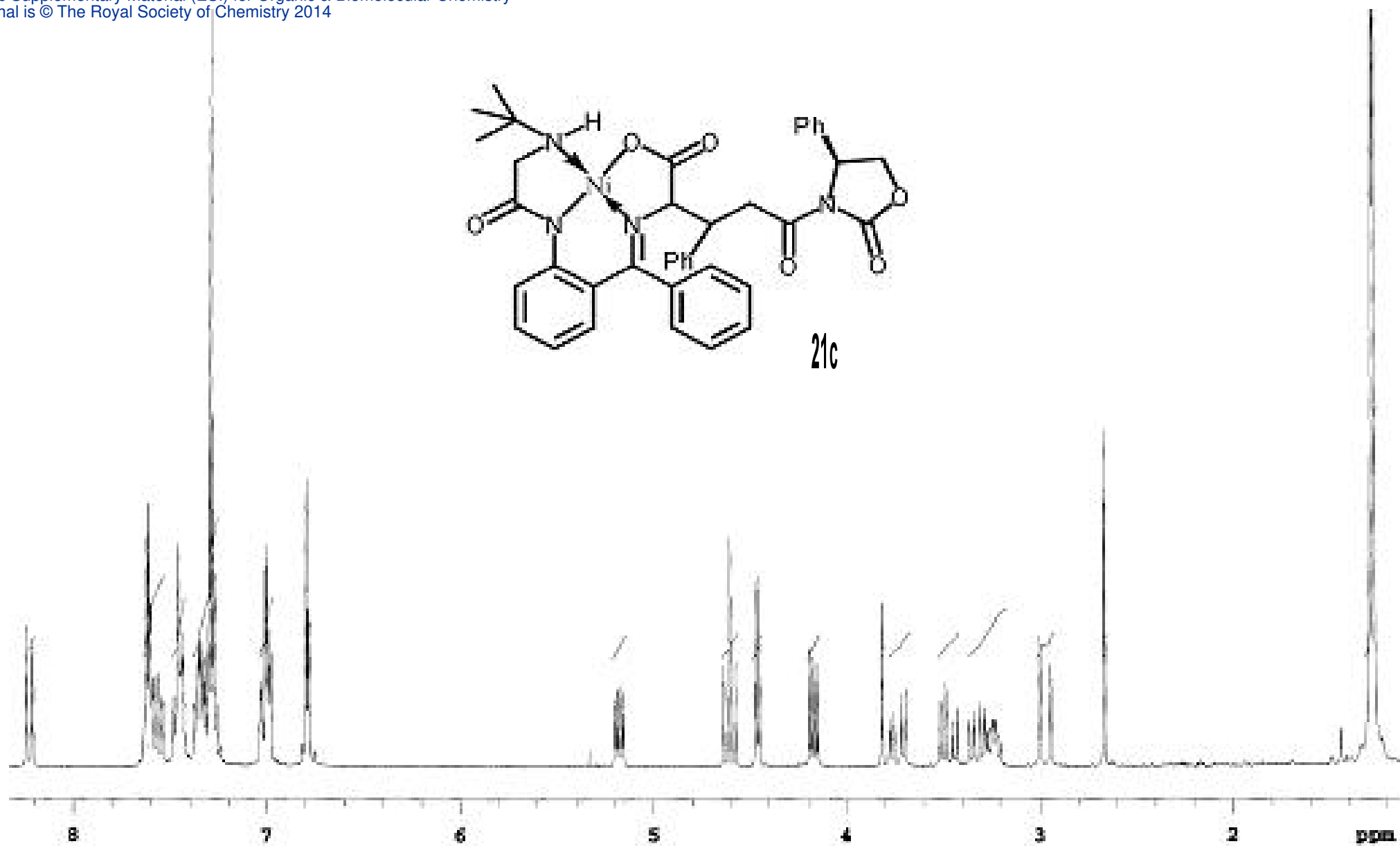
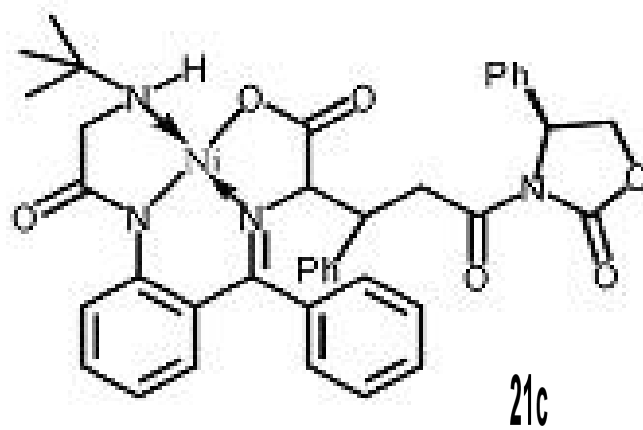
5.88

6.38







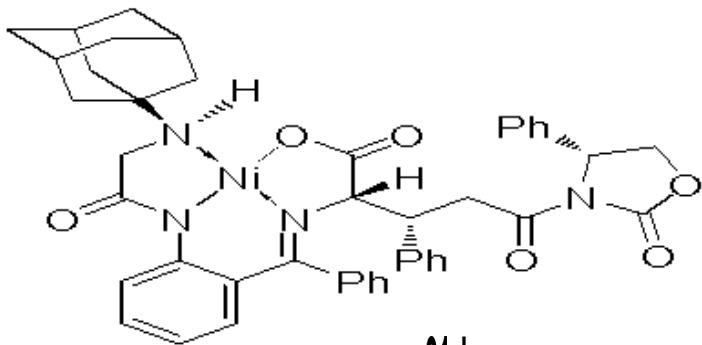


2483.5522
2475.1619
2287.6790
2214.8635
2200.1619
2189.0202
2178.4657
2094.1251
2048.2991
2043.0628
2040.4128
2037.6456

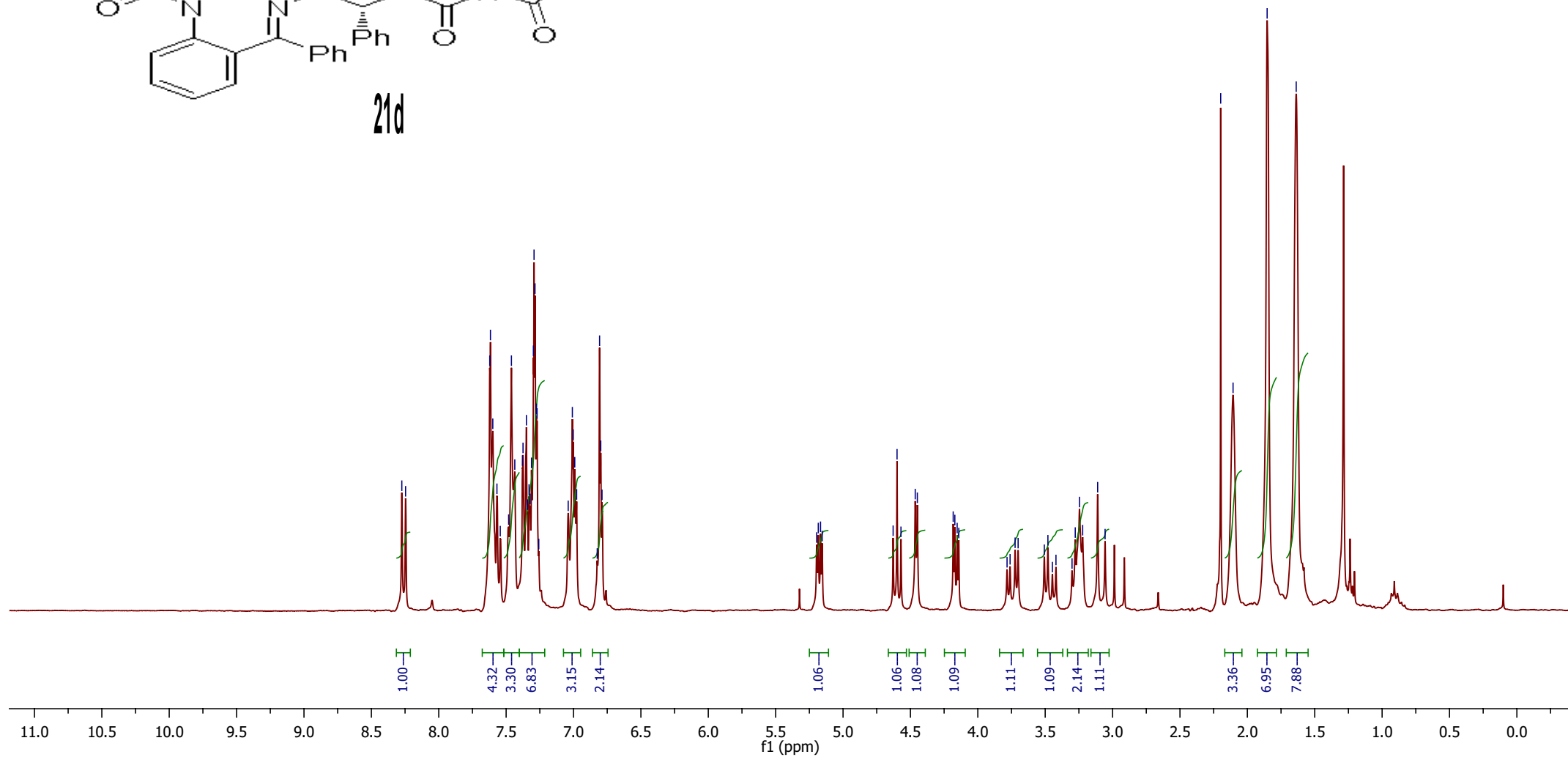
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1335.3444

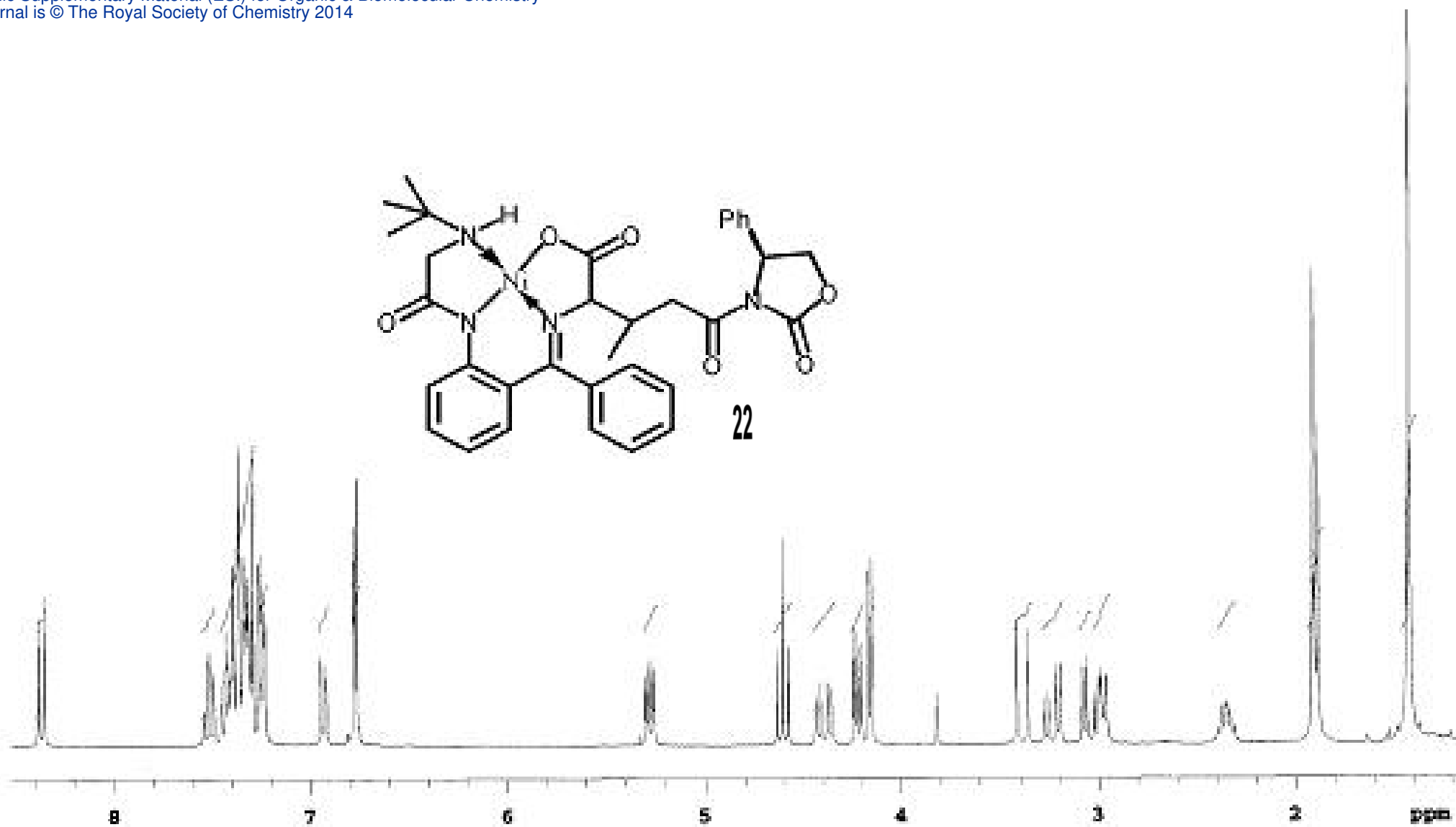
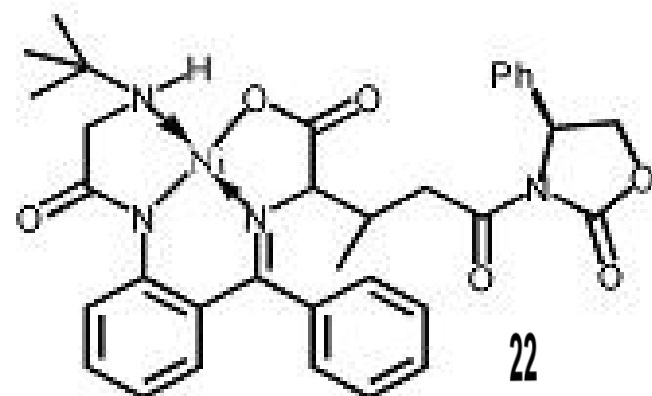
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1128.7672
1119.8593
1044.5302
990.7857
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974.2004
967.1139
933.7103
917.1798

659.6684
632.1476
556.2503
491.4952



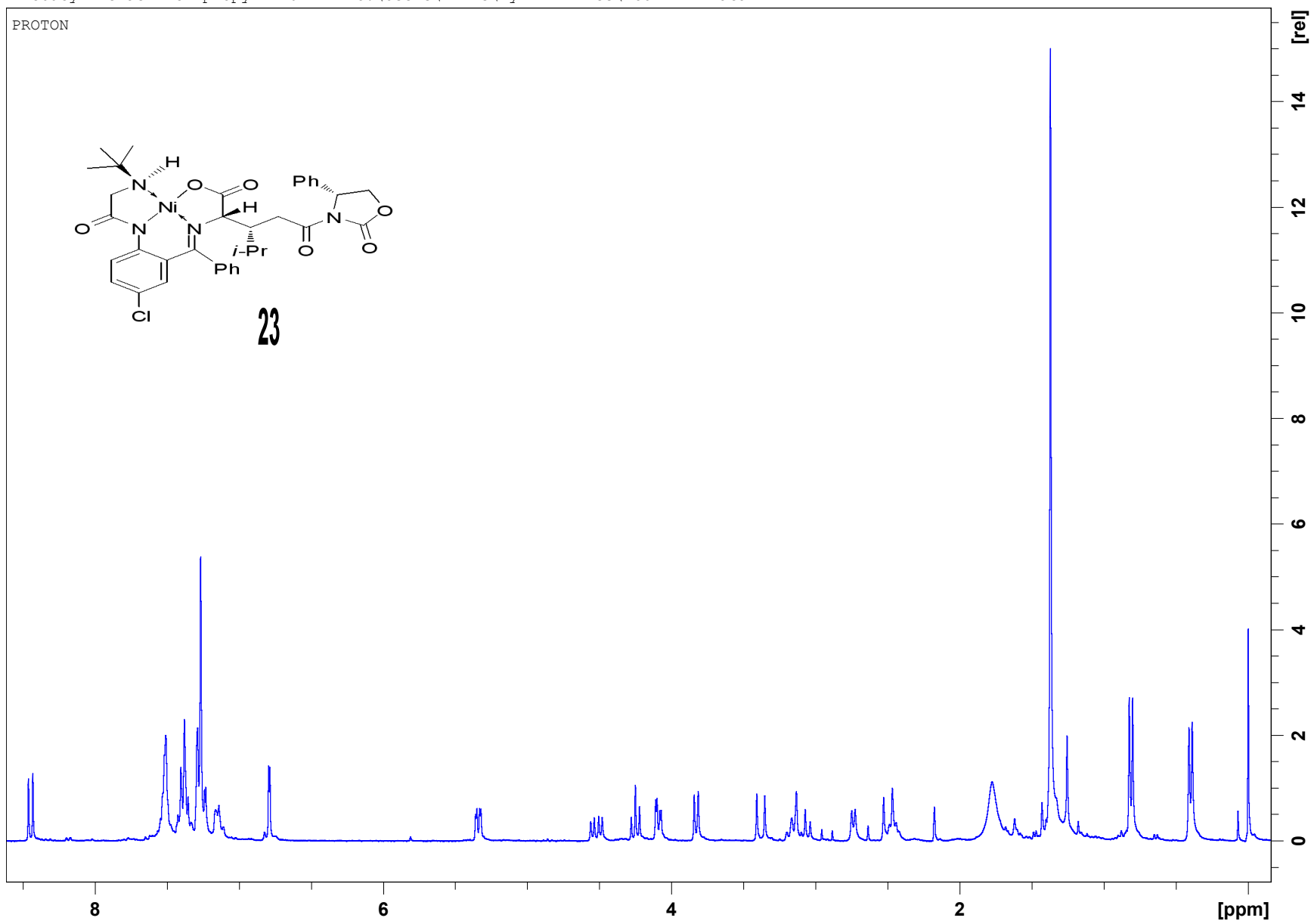
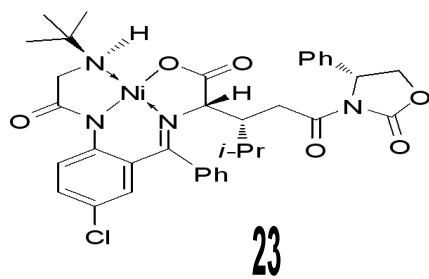
21d





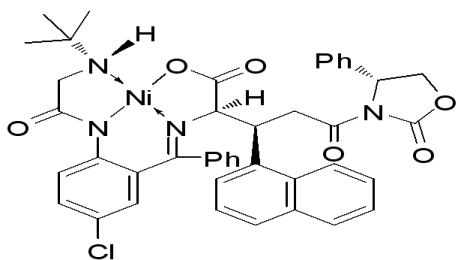
NHtbutylMichaelwithipropyl 10 1 "C:\Users\Ellis\My NMR Files\ICON-NMR Data"

PROTON

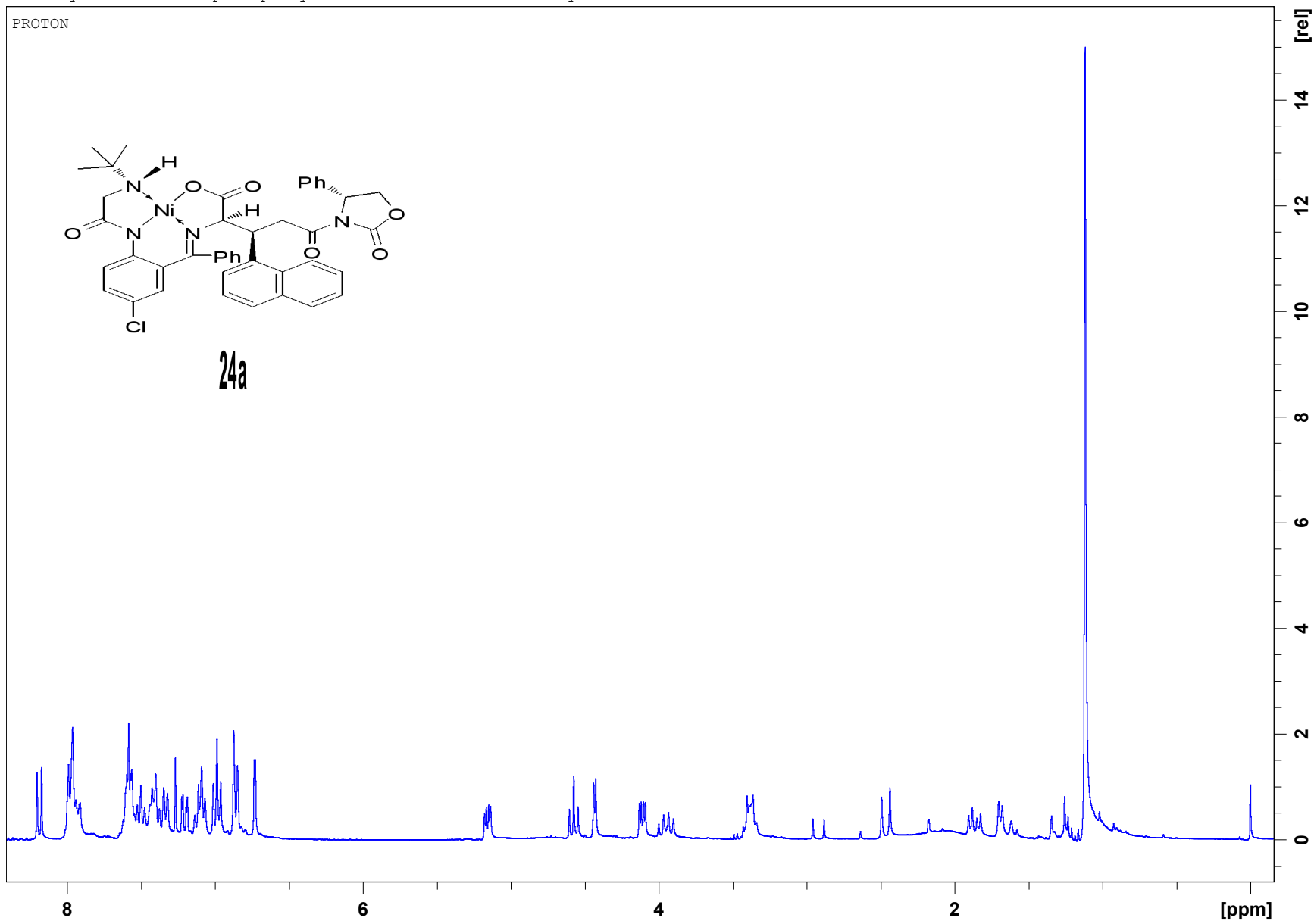


NHtbutylmichaelwithalphanaphthyl 10 1 "C:\Users\Ellis\My NMR Files\ICON-NMR Data"

PROTON

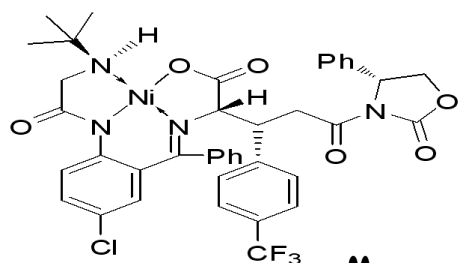


24a

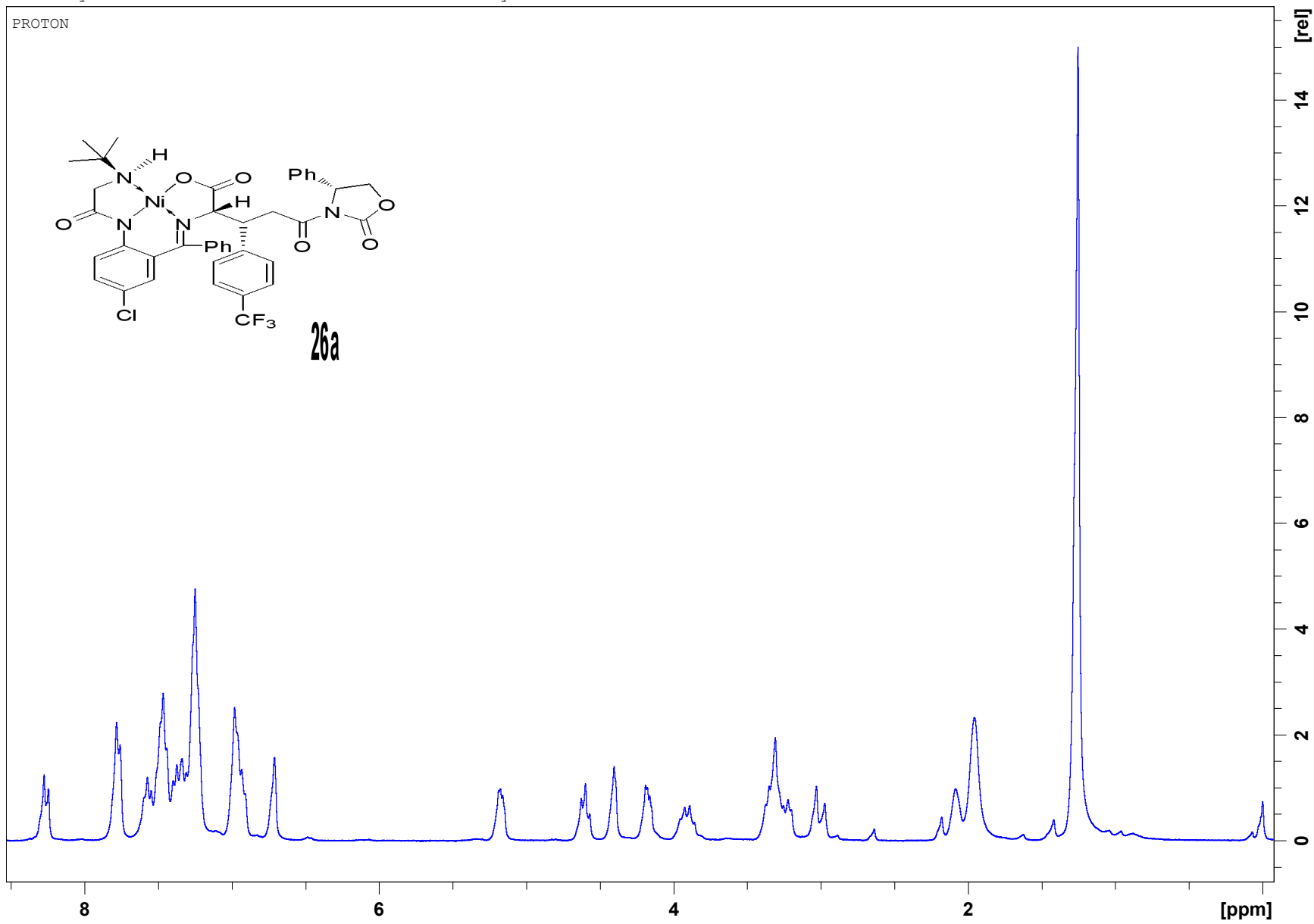


NHtButlymichaelwith4CF3Ph 10 1 "C:\Users\Hubin\My NMR Files\ICON-NMR Data"

PROTON

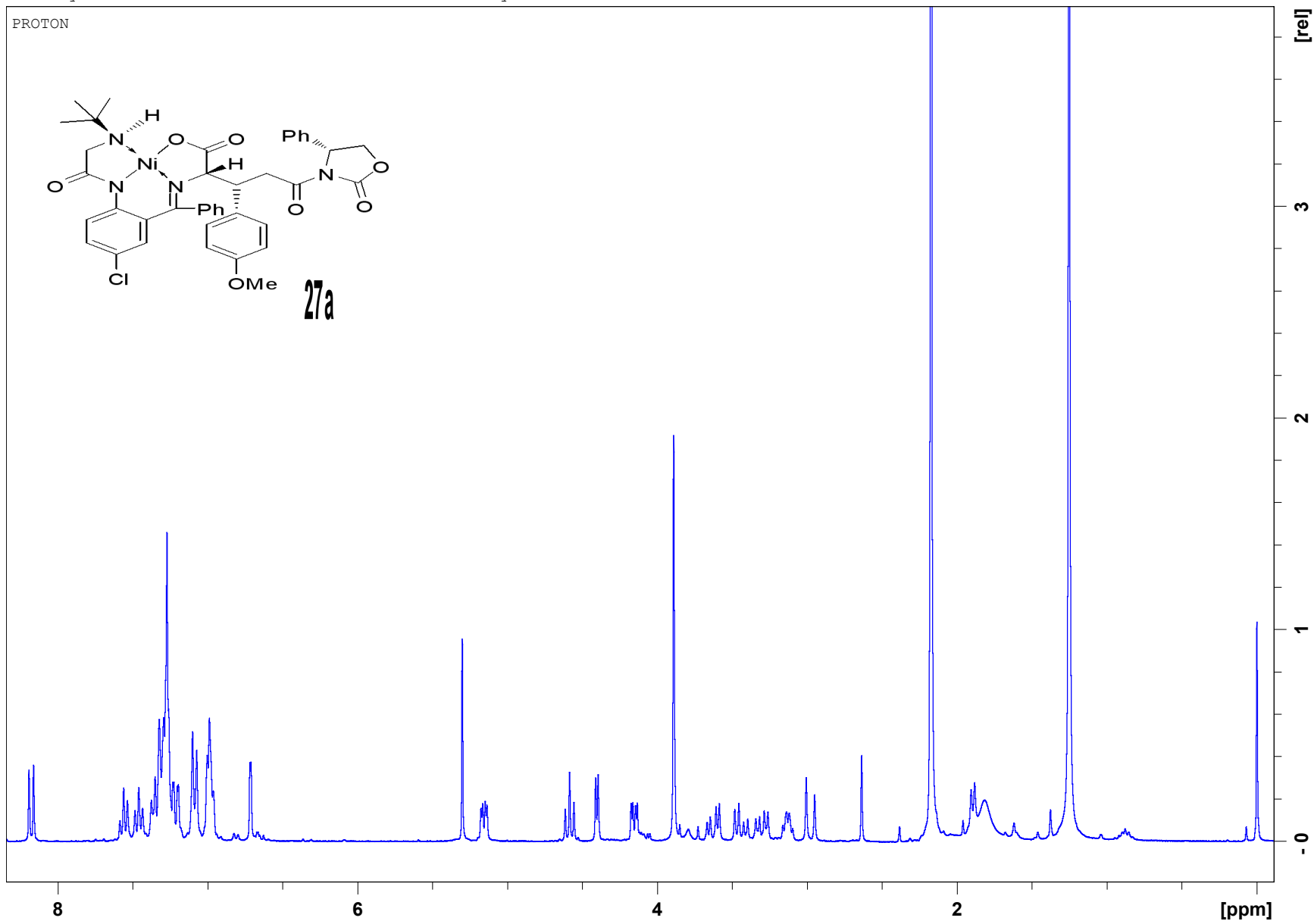
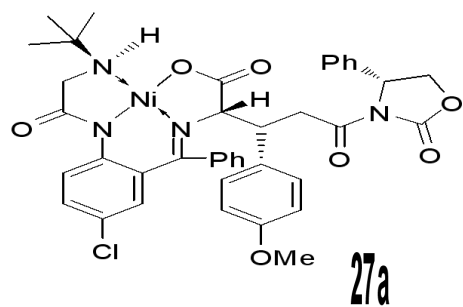


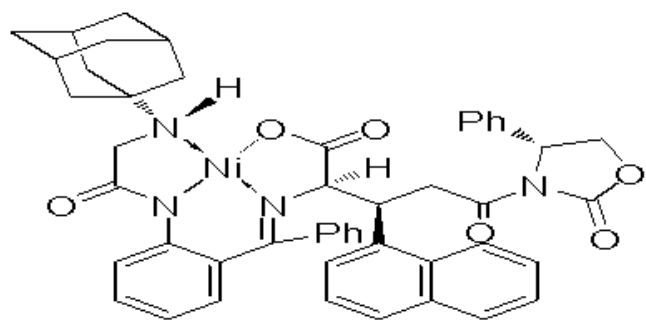
26a



NHtbutylMichaelwith4OMePH 10 1 "C:\Users\Ellis\My NMR Files\ICON-NMR Data"

PROTON





24b

8.3241
8.2961

7.8073
7.7804

7.4612
7.3071
7.2190

6.9527
6.8019
6.8005
6.7905
6.7849

5.2130
5.2001
5.1841
5.1713

4.6280
4.5986
4.5693

4.3976
4.1843

4.0223
3.9983
3.9664
3.9363

3.3131
3.2798
3.2575
3.2233

3.2018
3.1841
3.1285

2.1858
2.1001
2.0222
2.0022

1.8702

1.6324

0.95

2.04

4.98

7.39

3.01

2.06

1.00

1.12

1.04

1.08

1.11

4.42

3.37

1.16

6.69

6.46

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)

26b

