Supporting Information

N-Heterocyclic Pyridylmethylamines: Synthesis, Complexation, Molecular Structure and Application to Asymmetric Suzuki and Oxidative Coupling Reactions

Guillaume Grach,[a] Grégory Pieters,[a] Aurélia Dinut,[a,b] Vincent Terrasson,[a] Raouf Medimagh,[a] Alexandre Bridoux,[a] Vanessa Razafimahaleo,[a] Anne Gaucher,[a] Sylvain Marque,[a] Jérôme Marrot,[a] Damien Prim,*[a] Richard Gil,[b] José Giner Planas,[c] Clara Viñas,[c] Francesc Teixidor,[c] Isabelle Thomas,[d] Jean-Philippe Roblin[d] and Yves Troin[d]

[a] *Institut Lavoisier de Versailles – UMR CNRS 8180, Université de Versailles – Saint-Quentin-en-Yvelines, 45 avenue des Etats-Unis, 78035 Versailles, France Fax: +33 1 3925 4452. E-mail: prim@chimie.uvsq.fr*
[b] *Equipe de Catalyse Moléculaire, Institut de Chimie Moléculaire et des Matériaux d'Orsay (ICMMO), UMR 8182, bât. 420, Université Paris-Sud 11, 91405 Orsay Cedex, France.*
[c] *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus U.A.B. 08193 Bellaterra, Spain.*
[d] *Clermont Université, ENSCCF, EA 987, LCHG, BP 10448, F-63000 Clermont-Ferrand, Ensemble scientifique des Cézeaux, 24, Avenue des Landais, BP10187, 63174 Aubière Cedex, France.*

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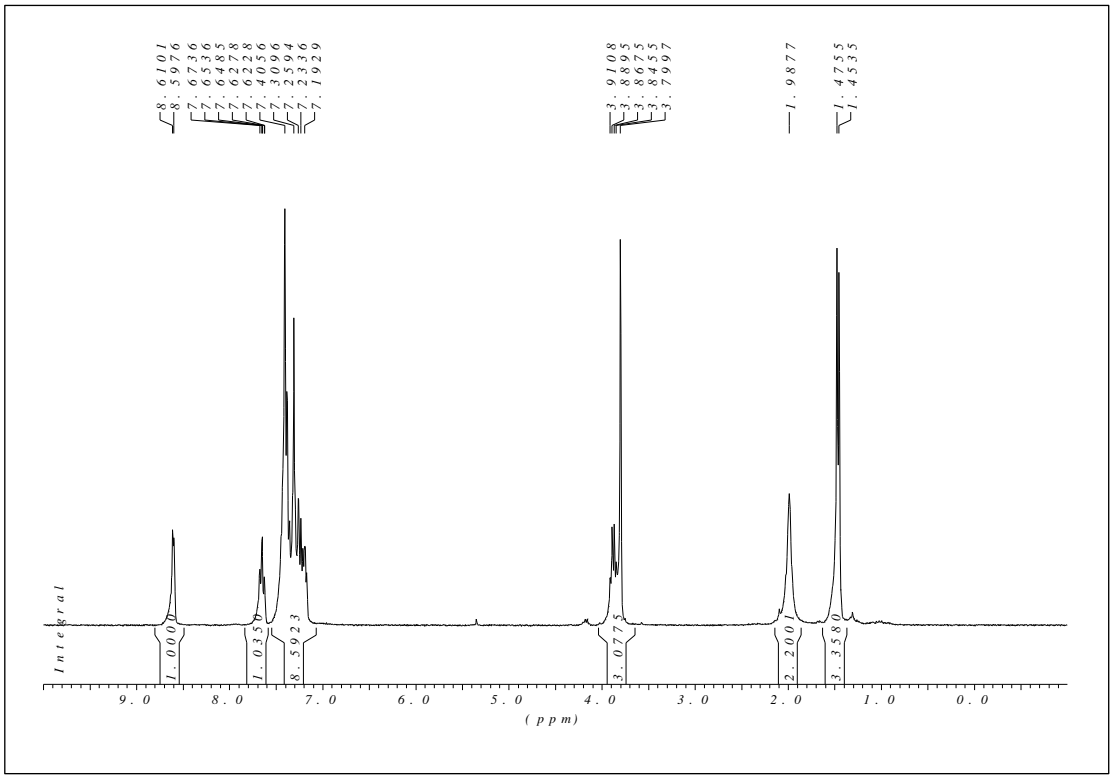
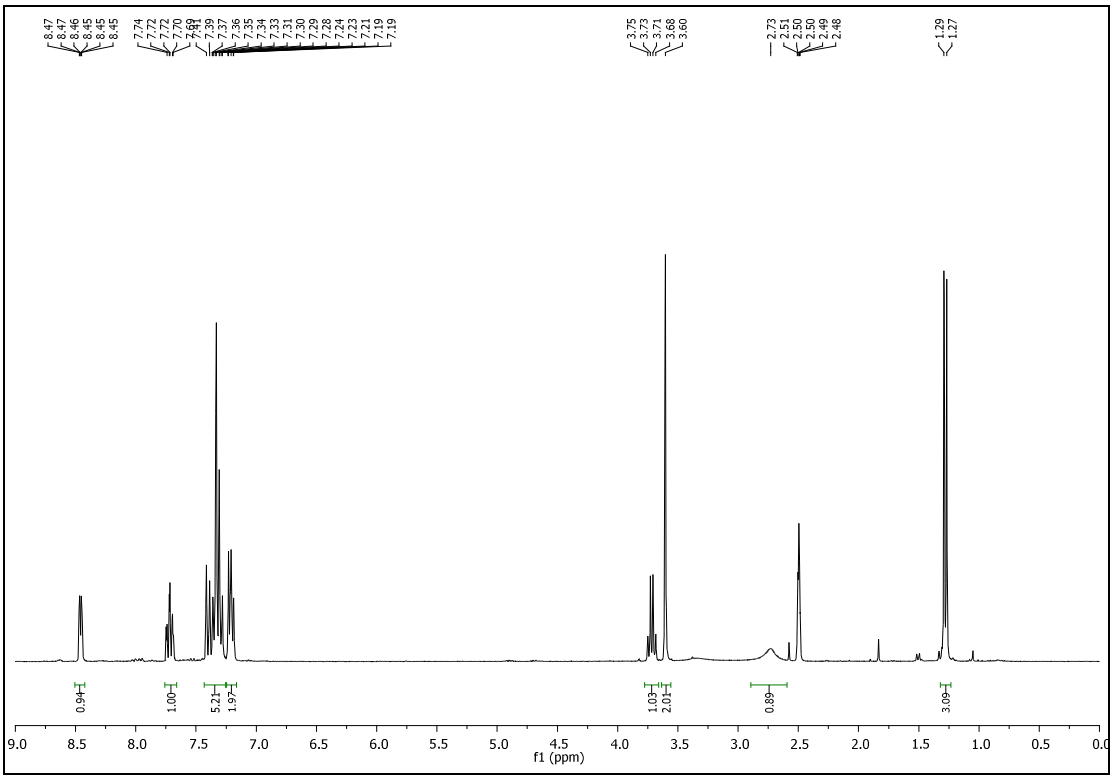
^{1}H NMR ($CDCl_3$, 300 MHz) of L7



^{1}H NMR ([D_6]dmso, 300 MHz) of L7



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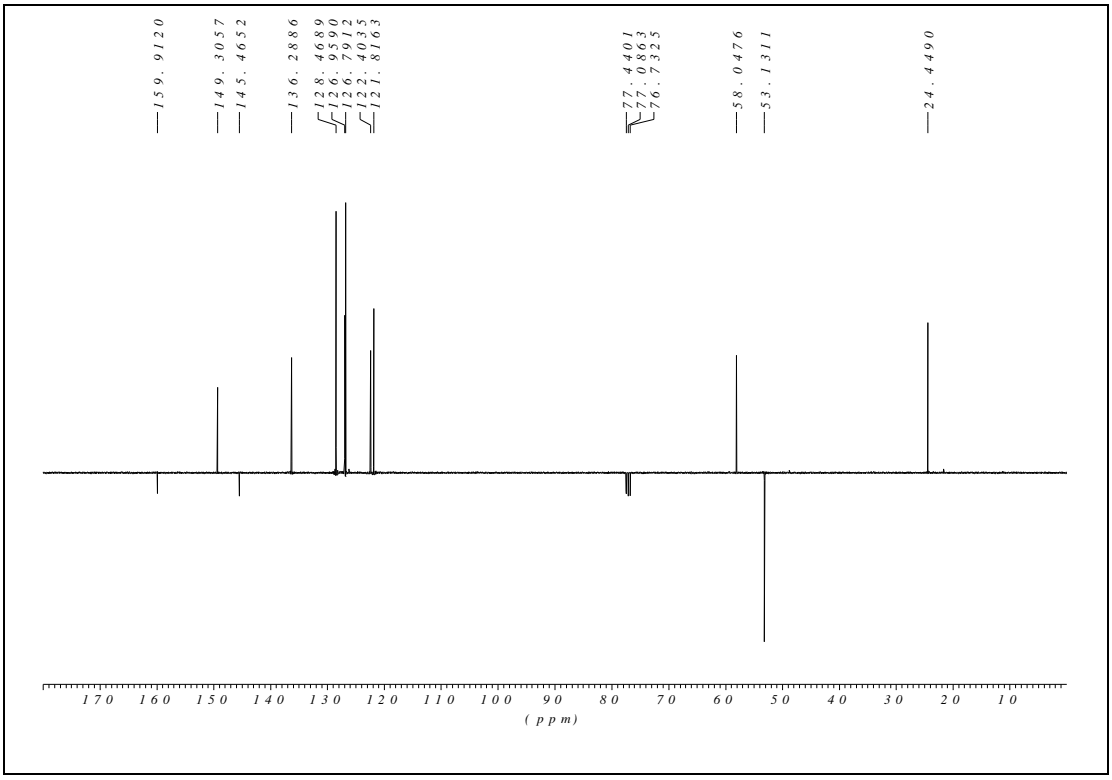

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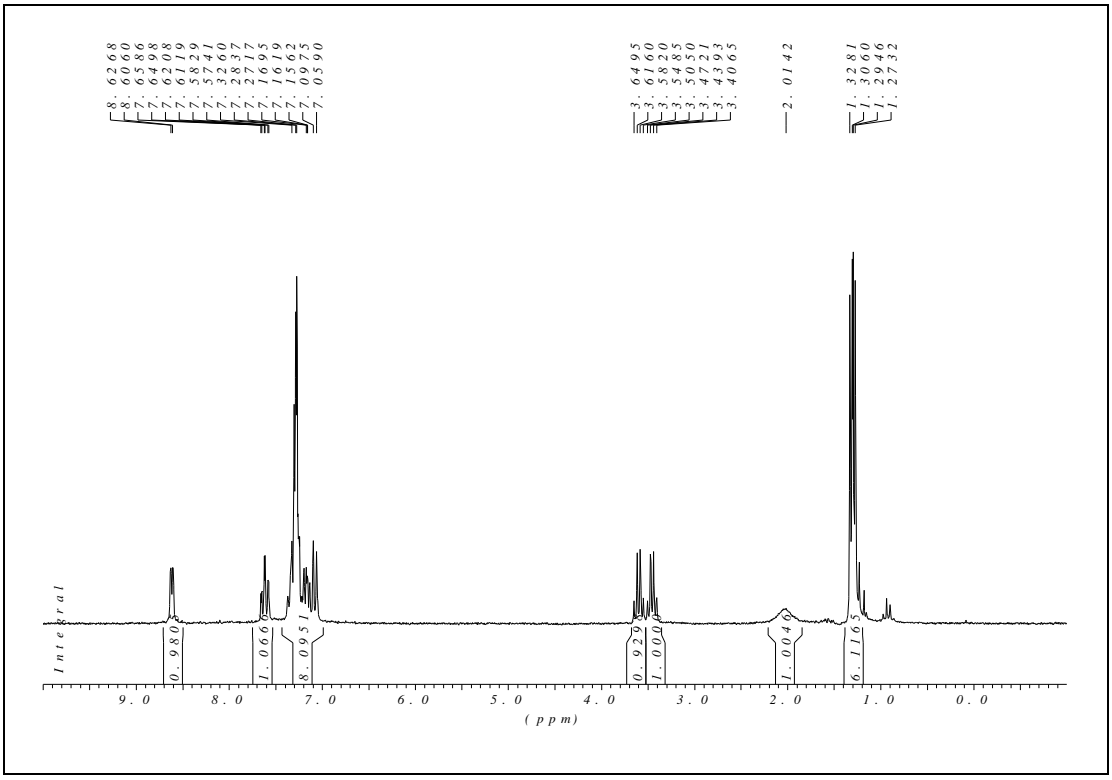

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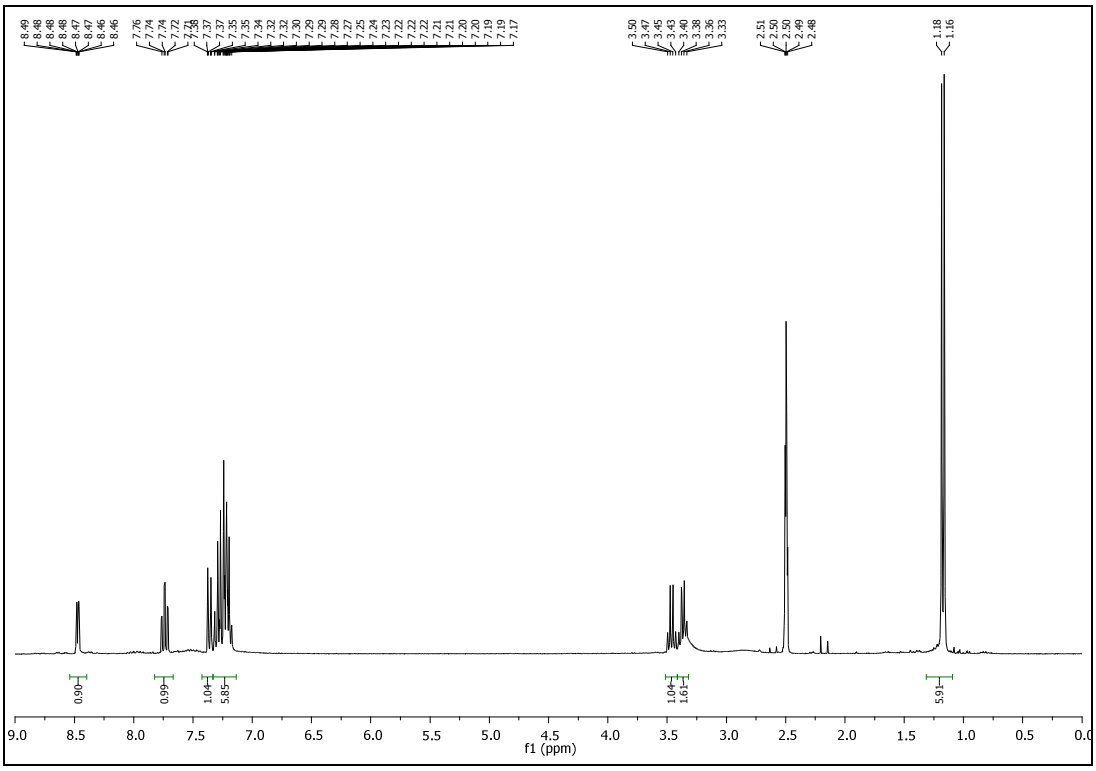

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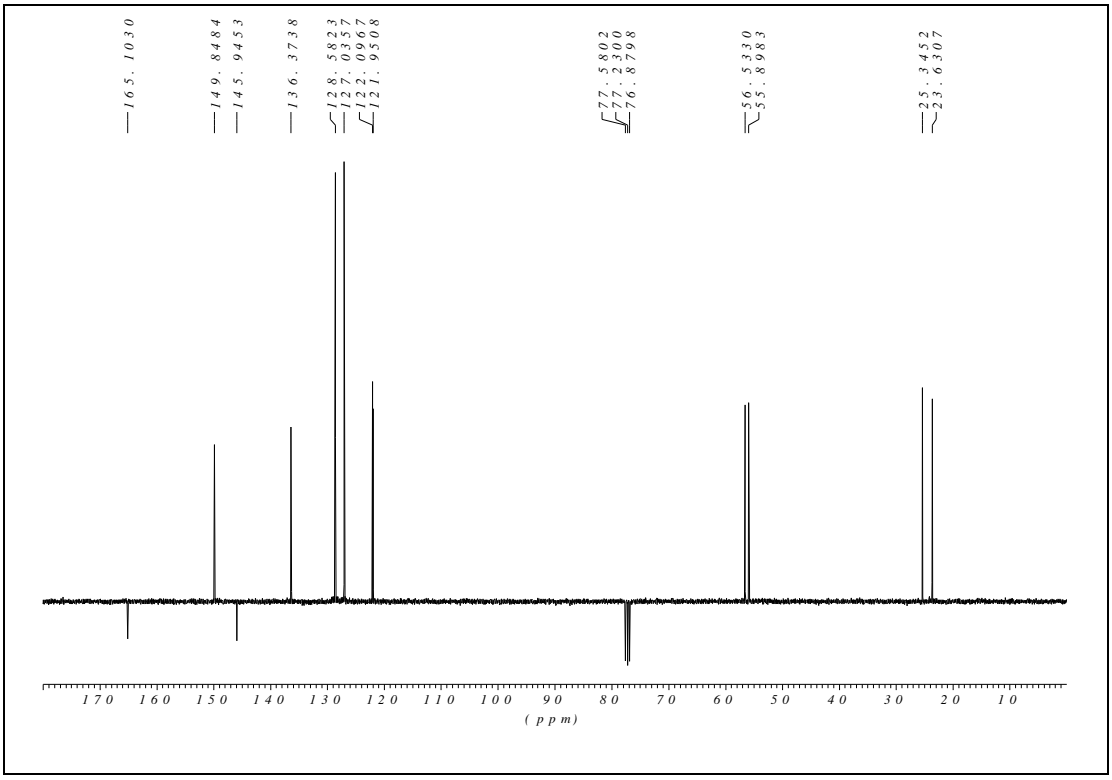

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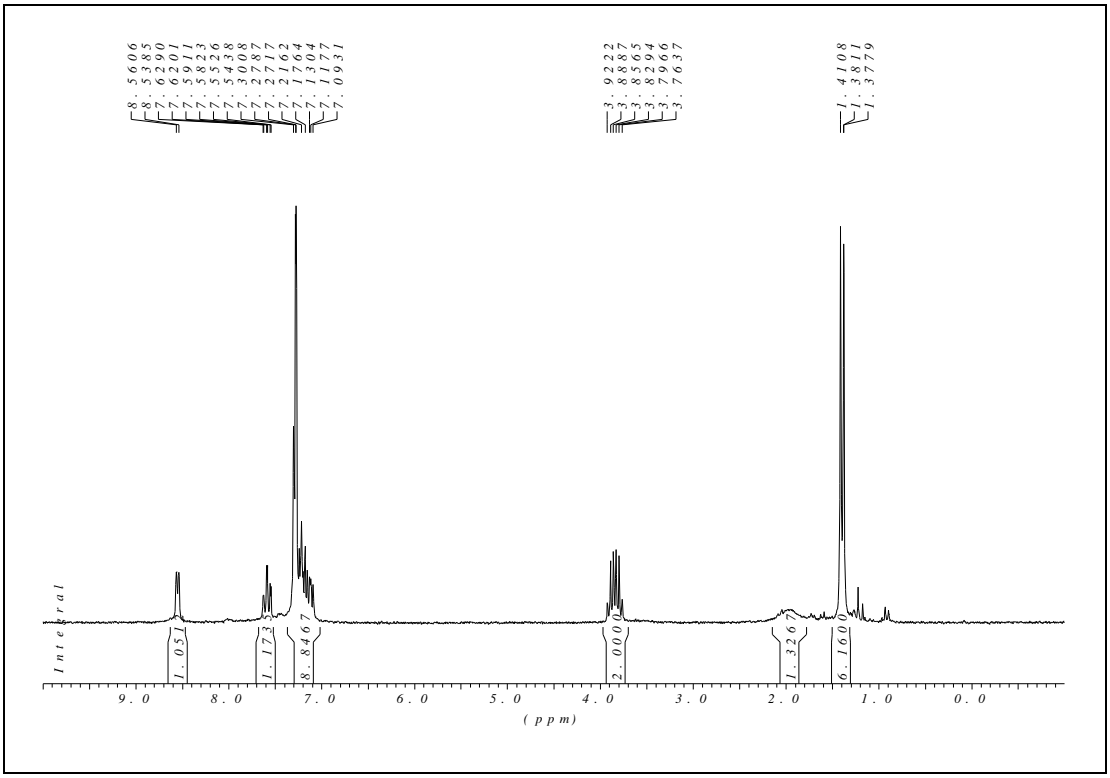

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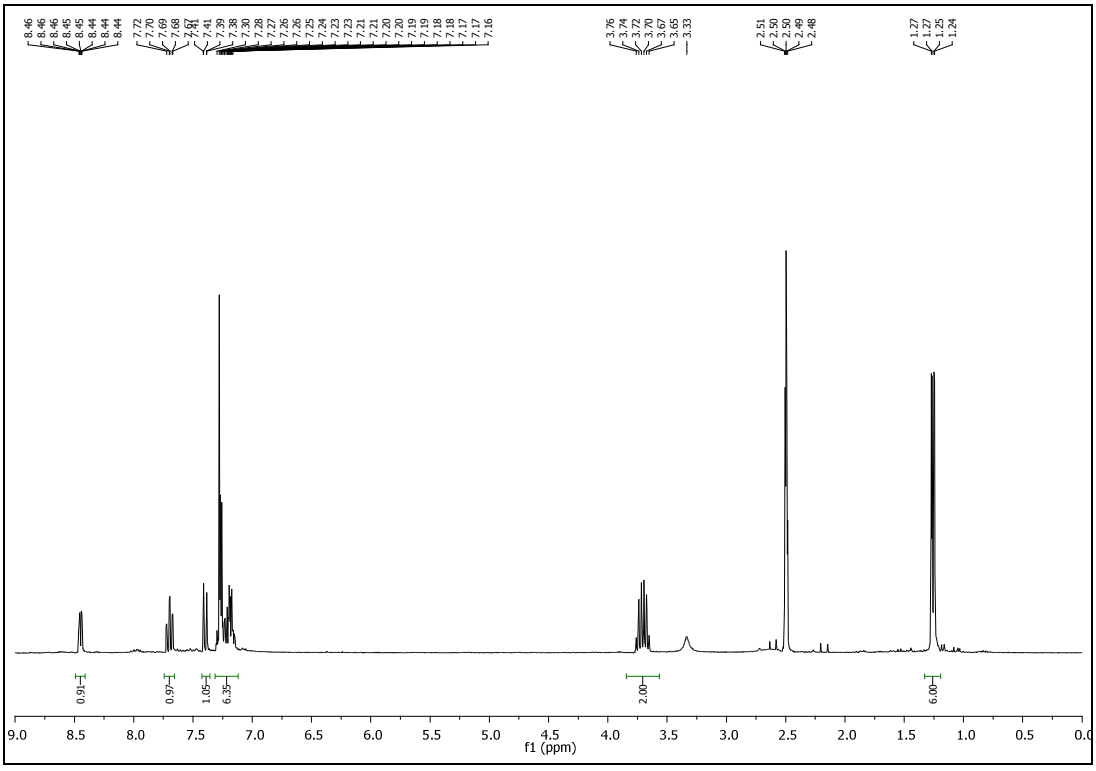

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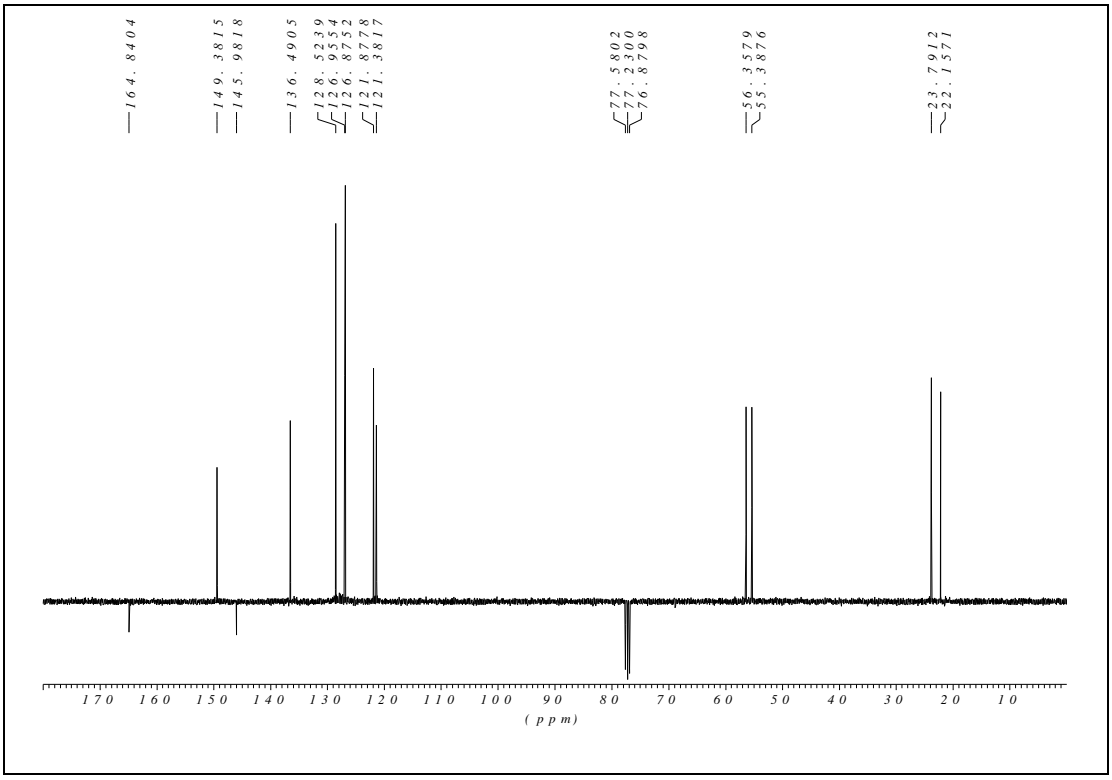

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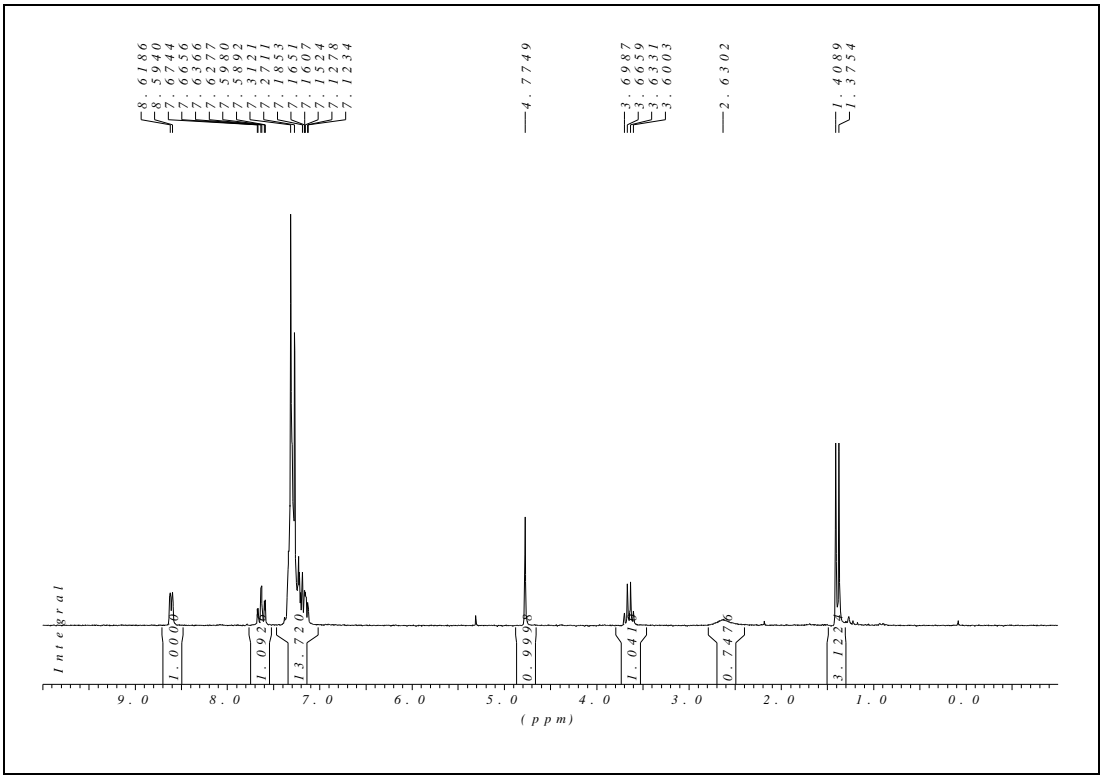

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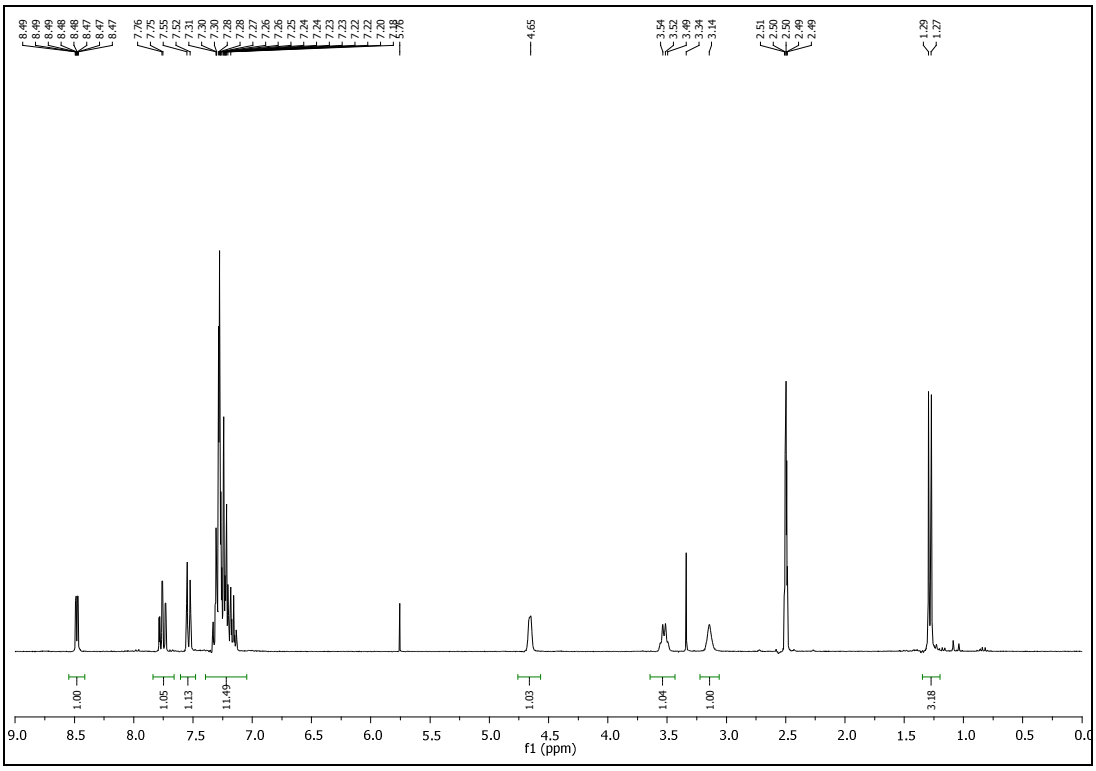

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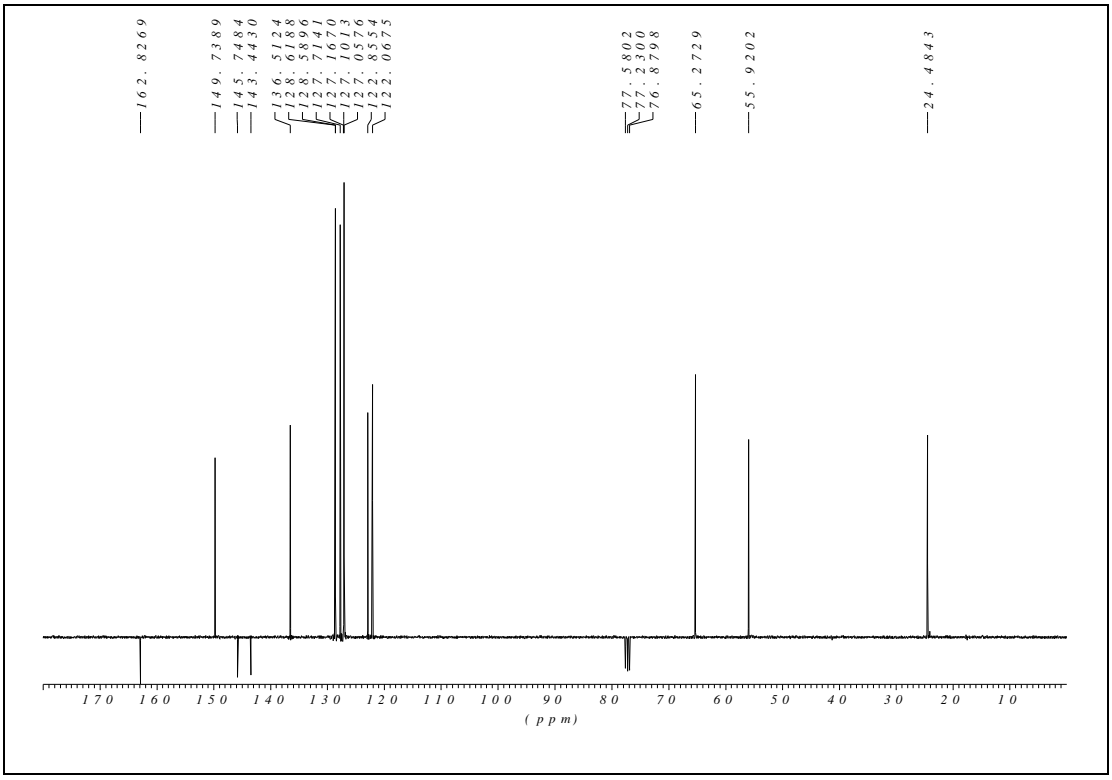

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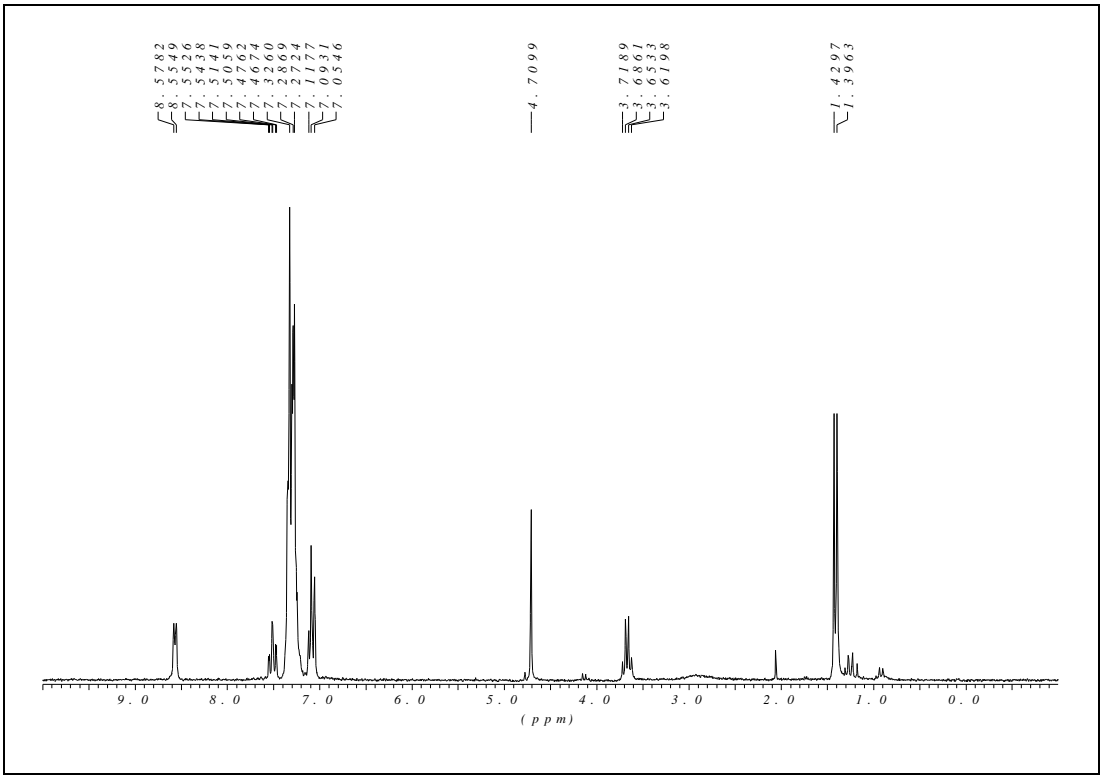

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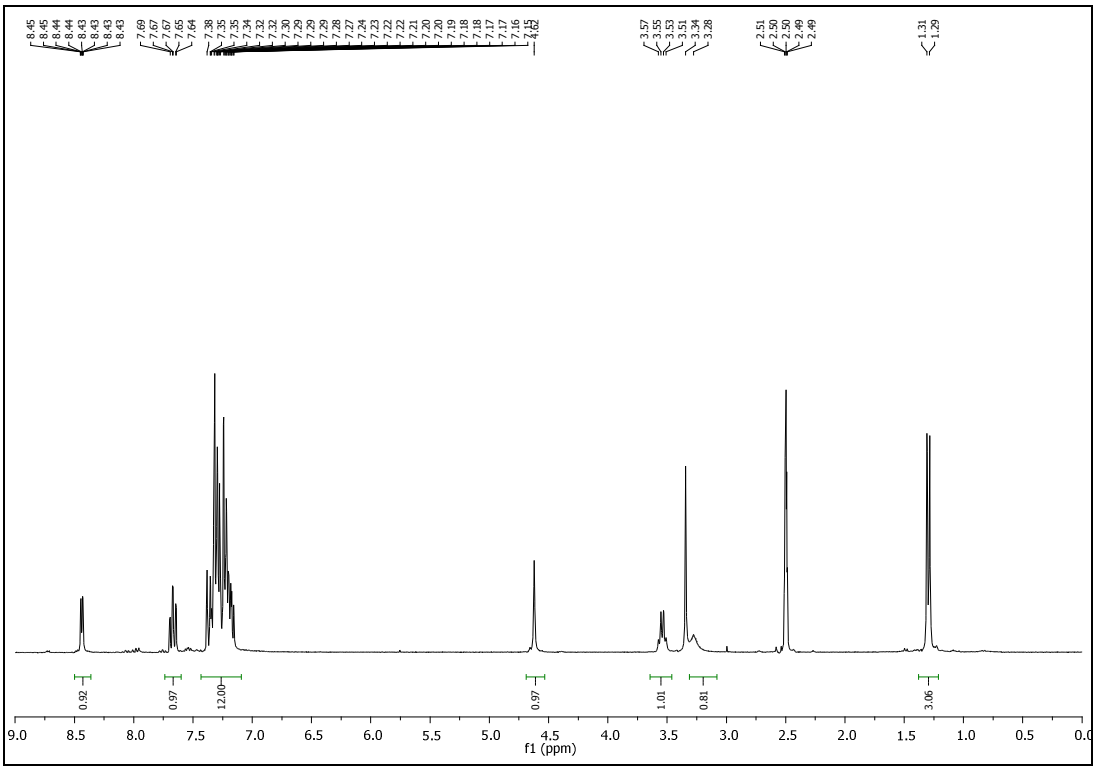

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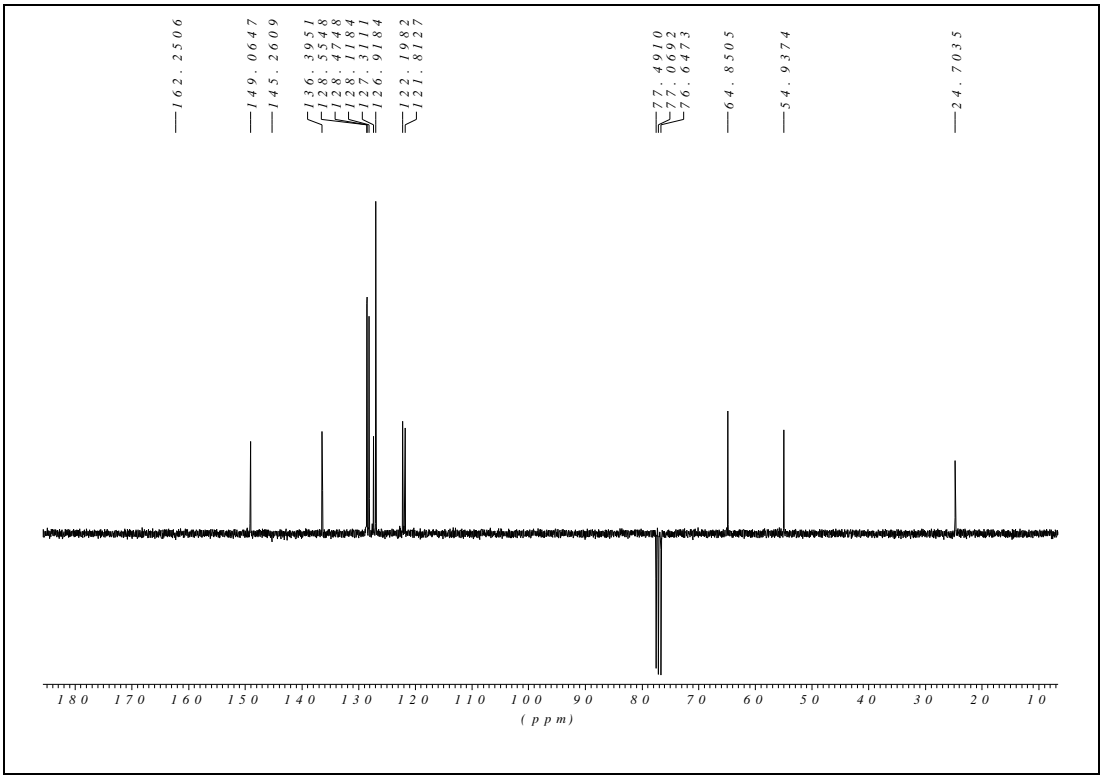

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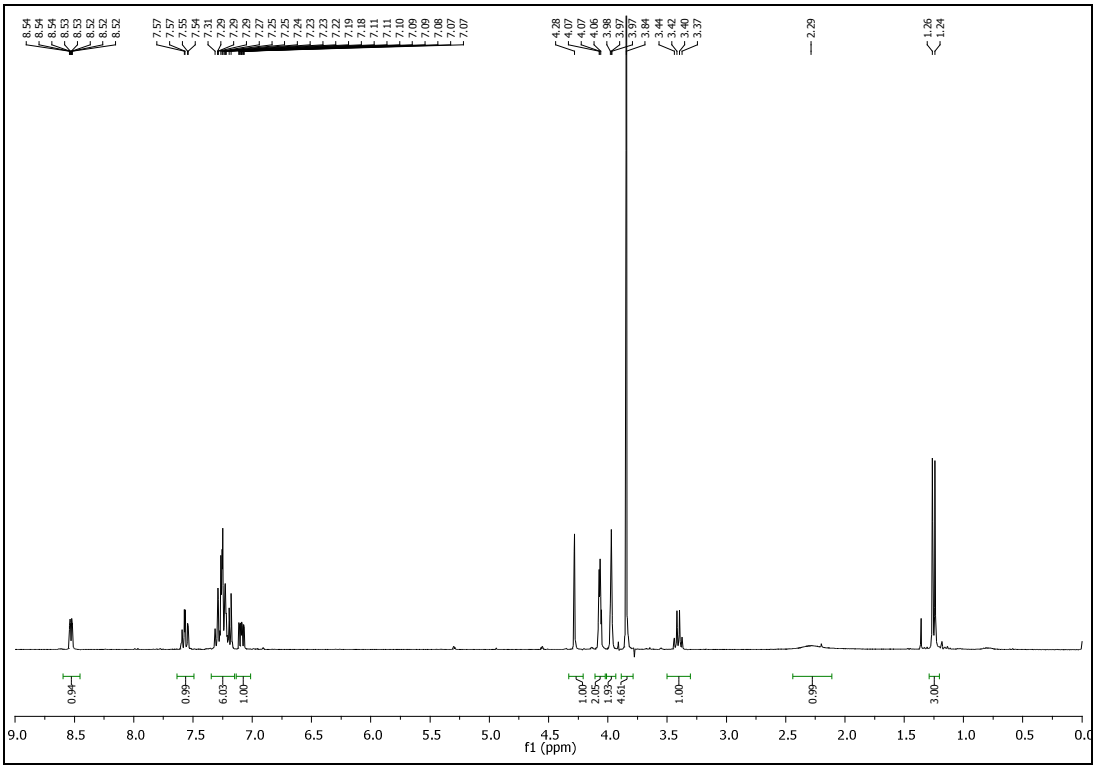

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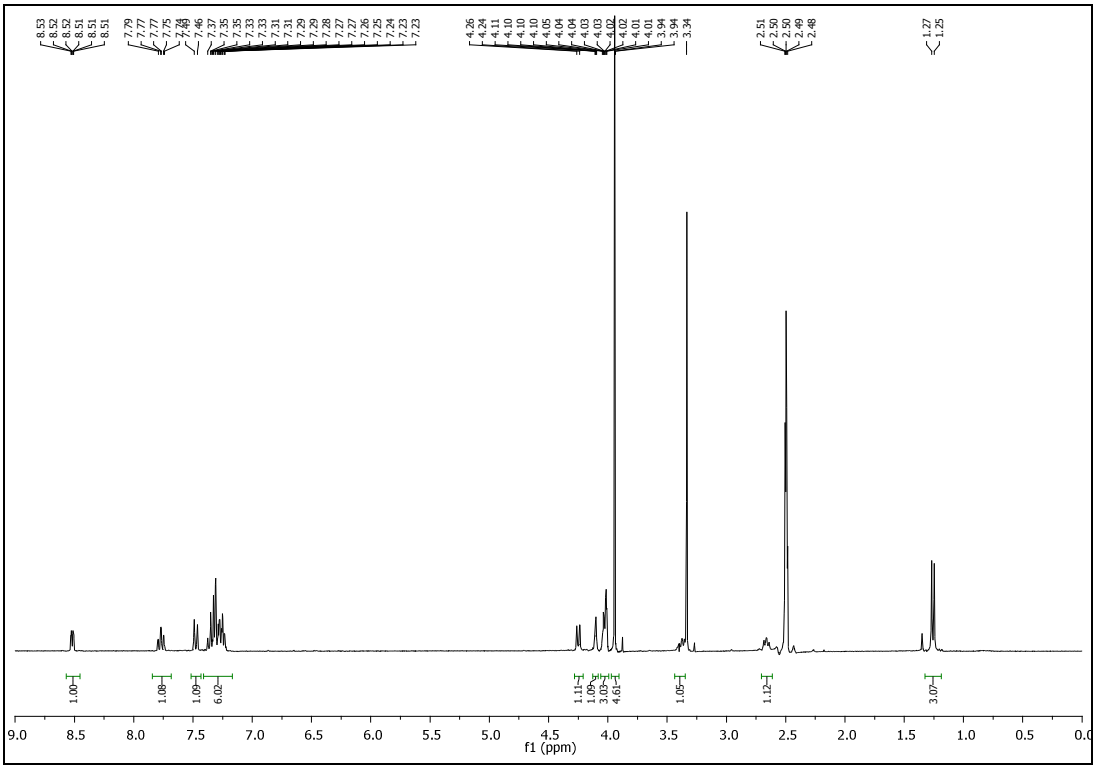

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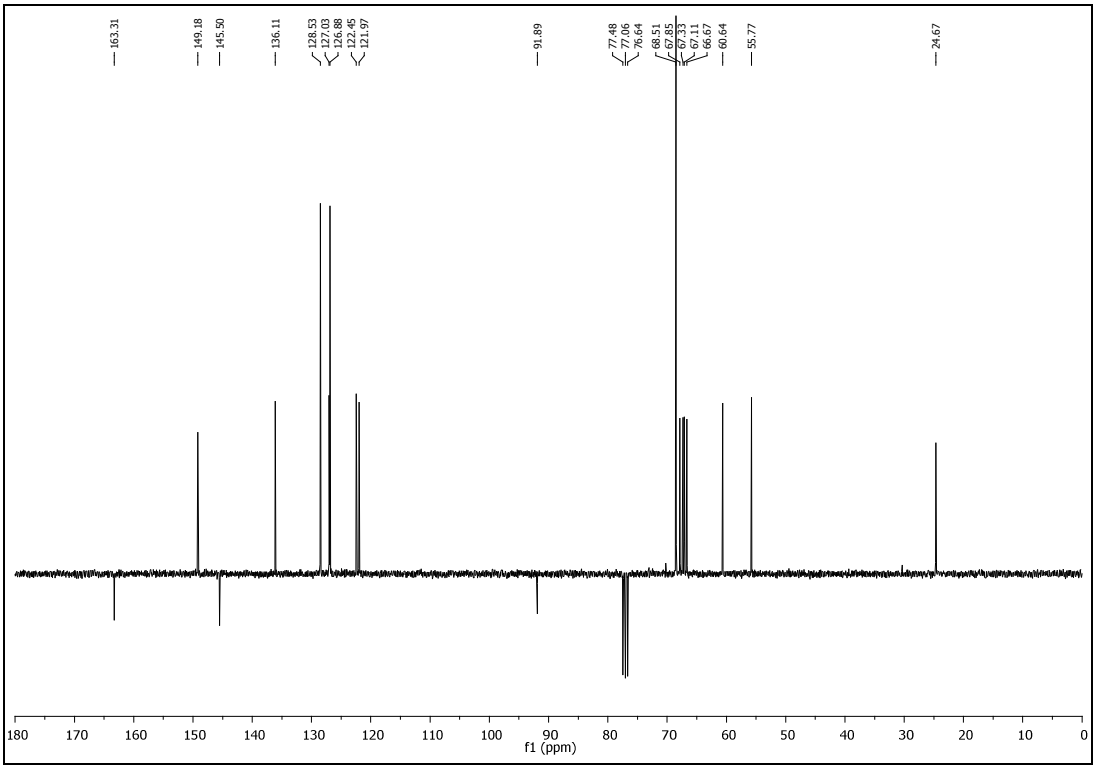

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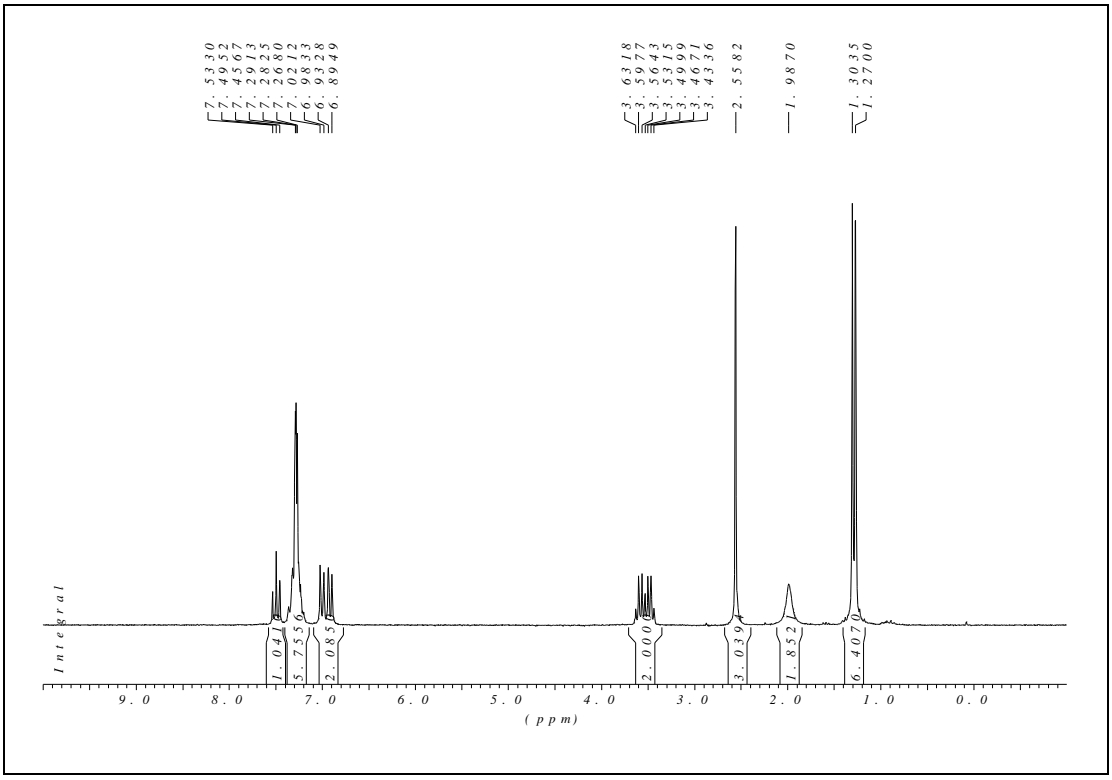

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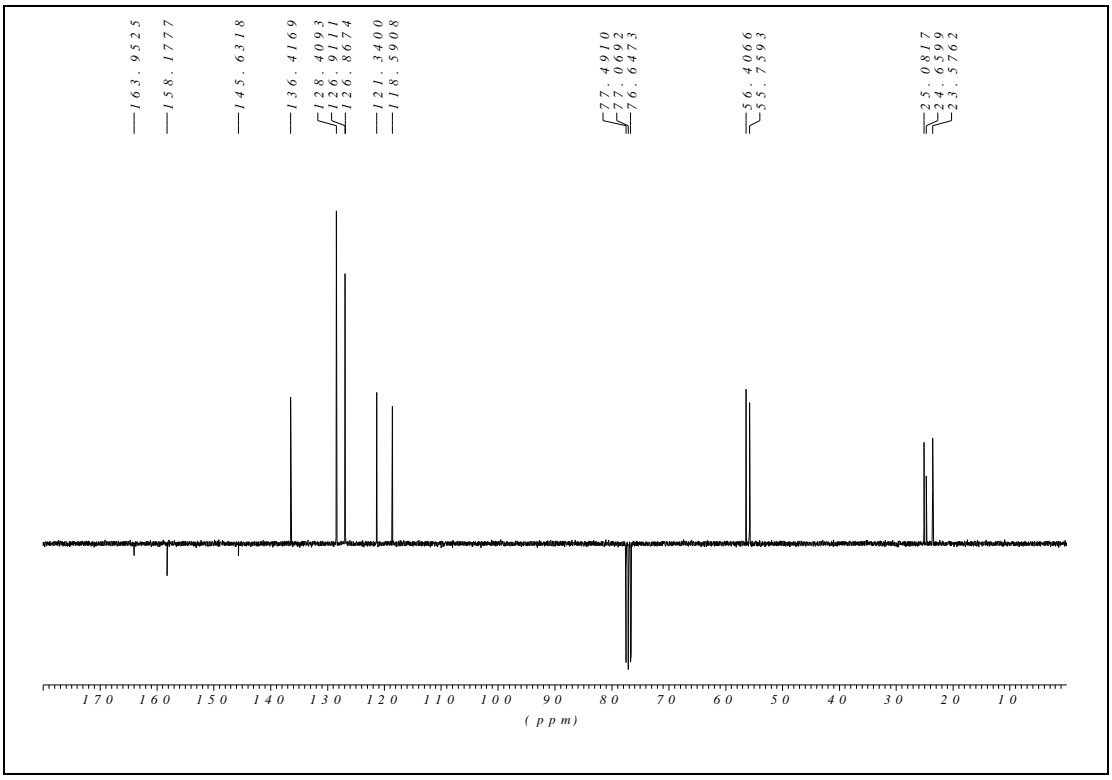

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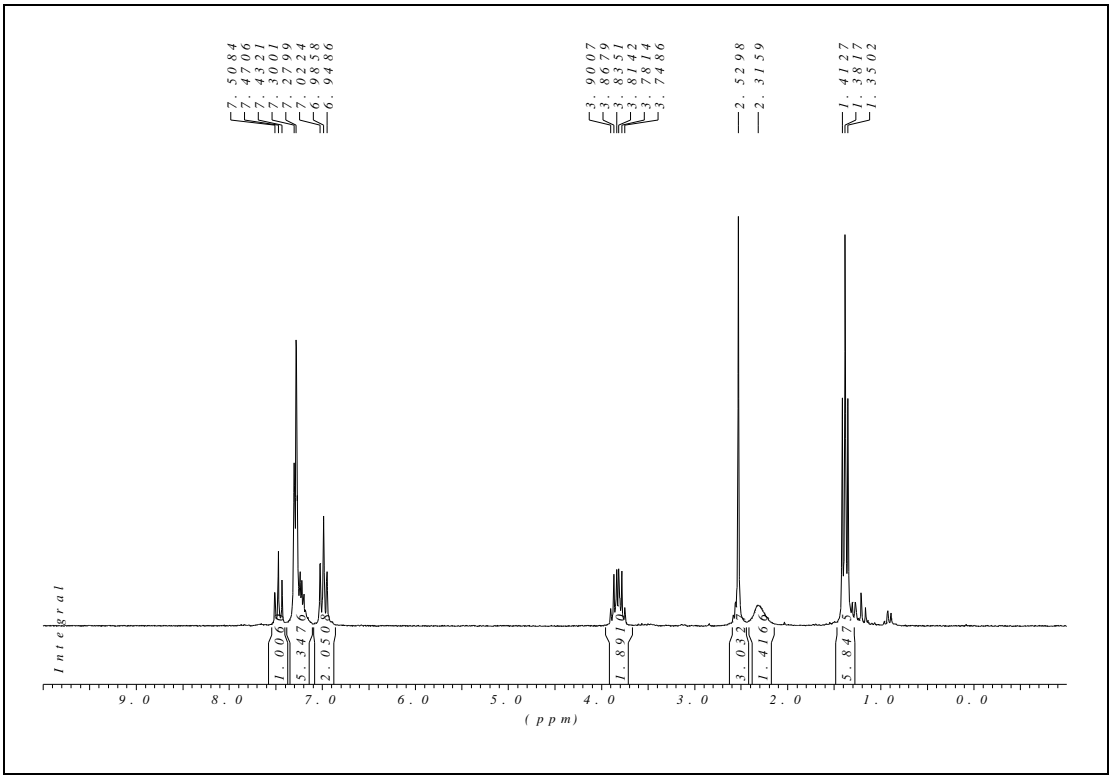

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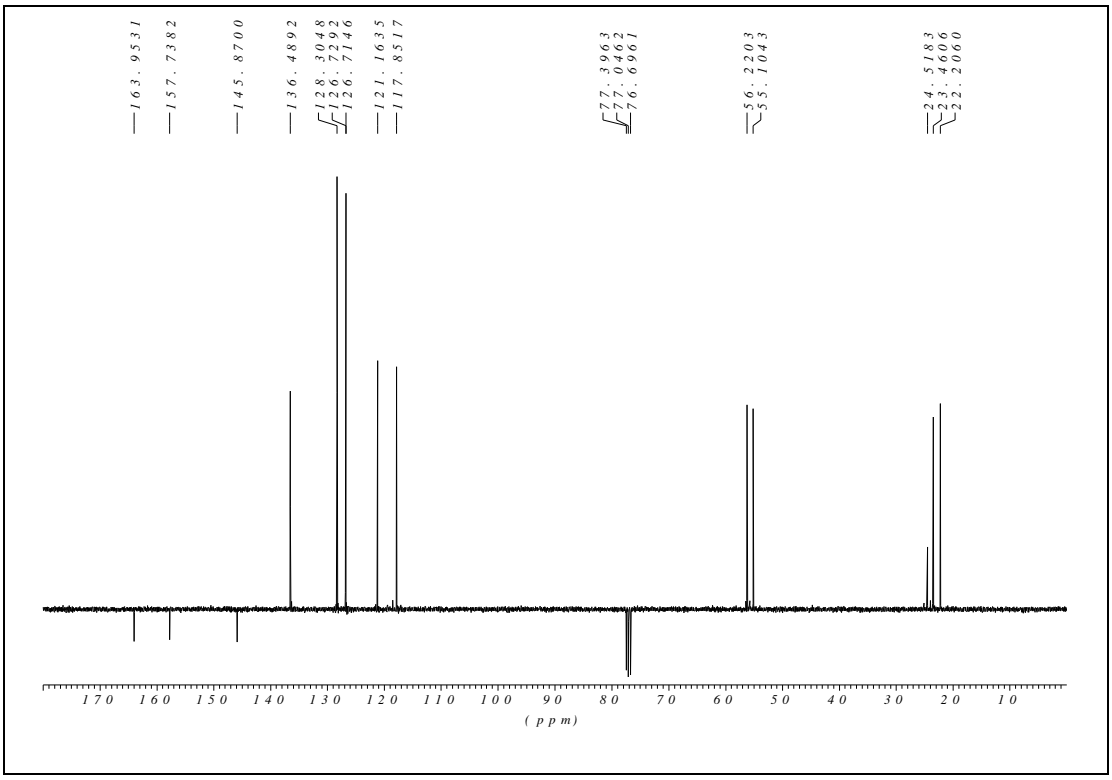

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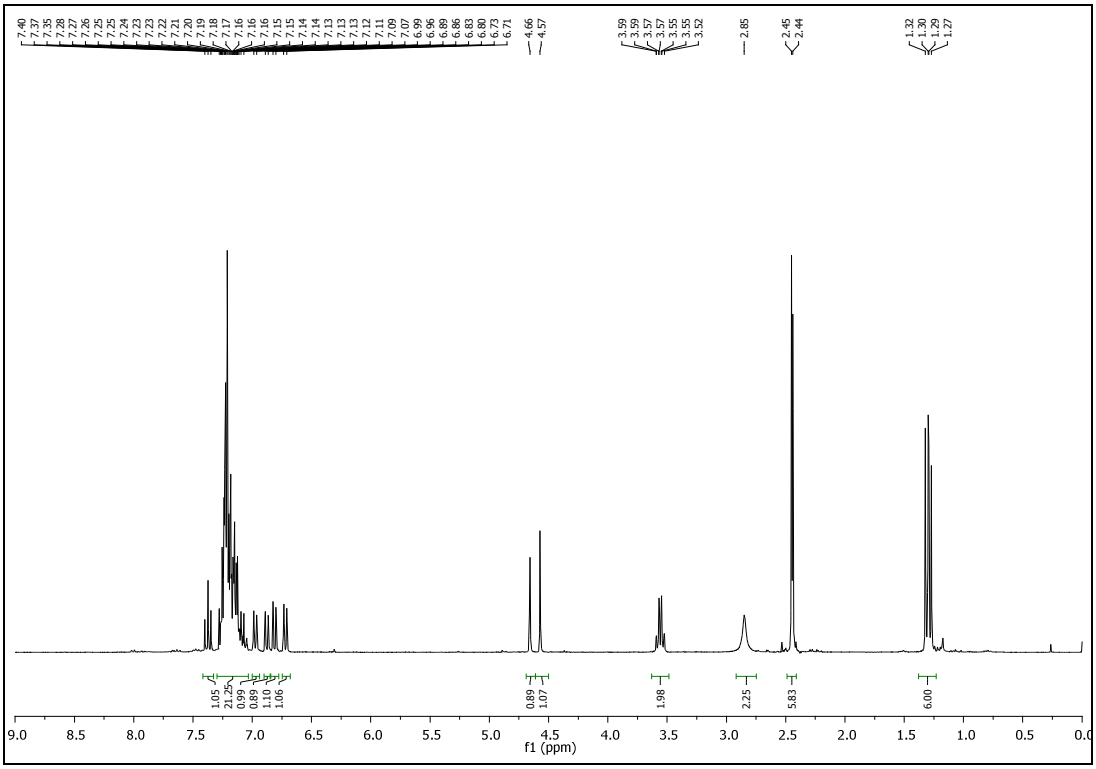

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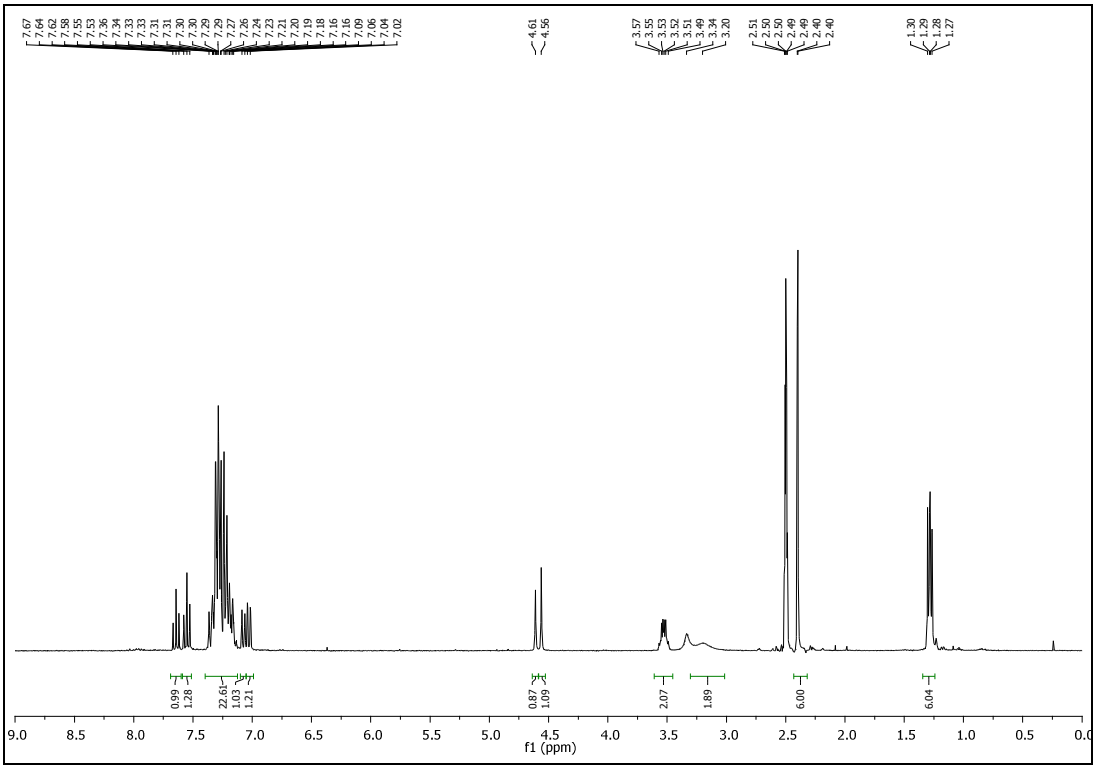

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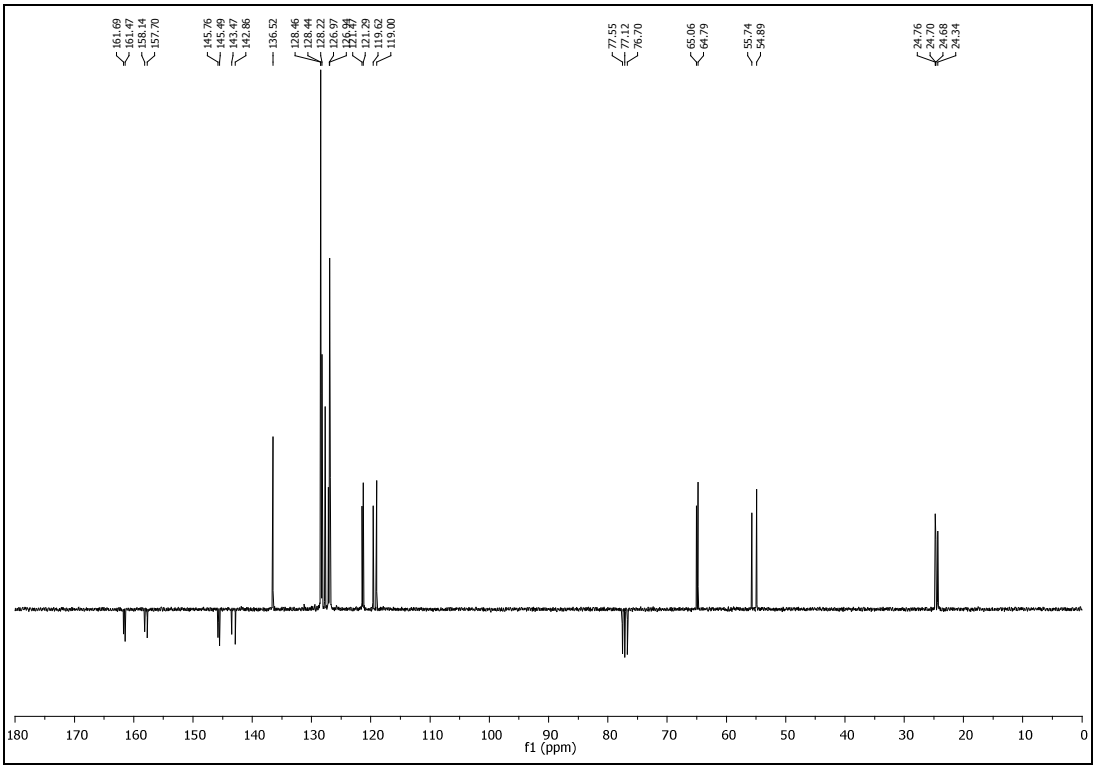

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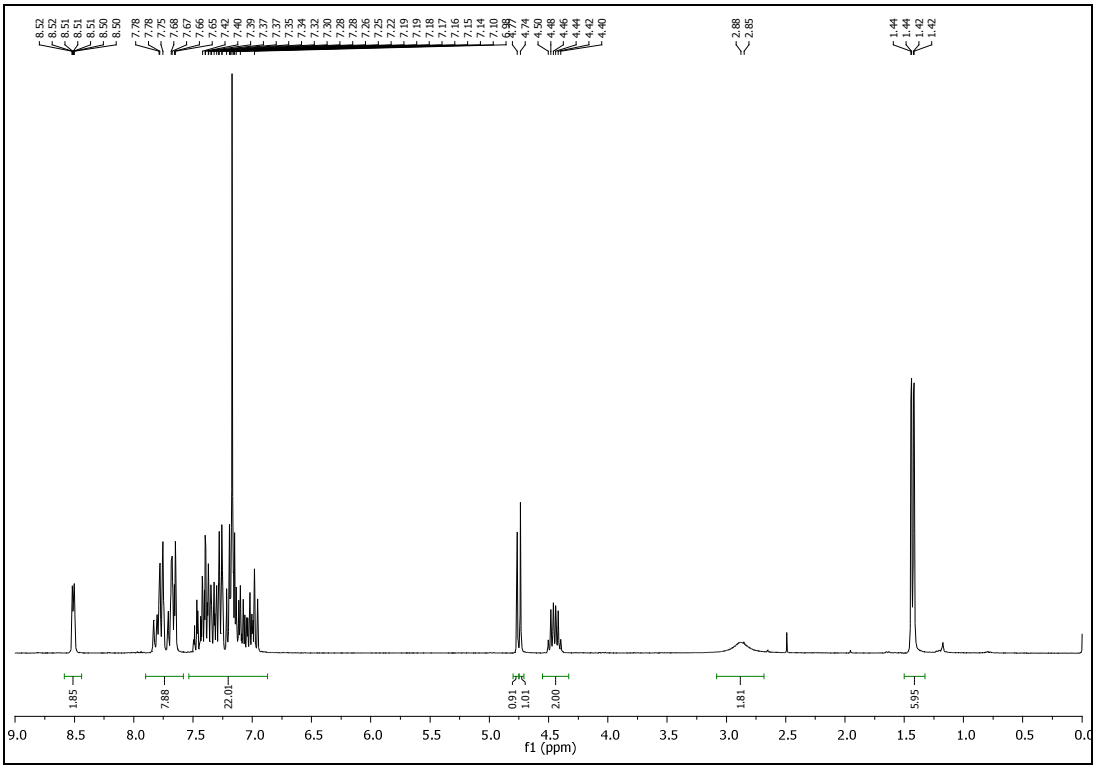

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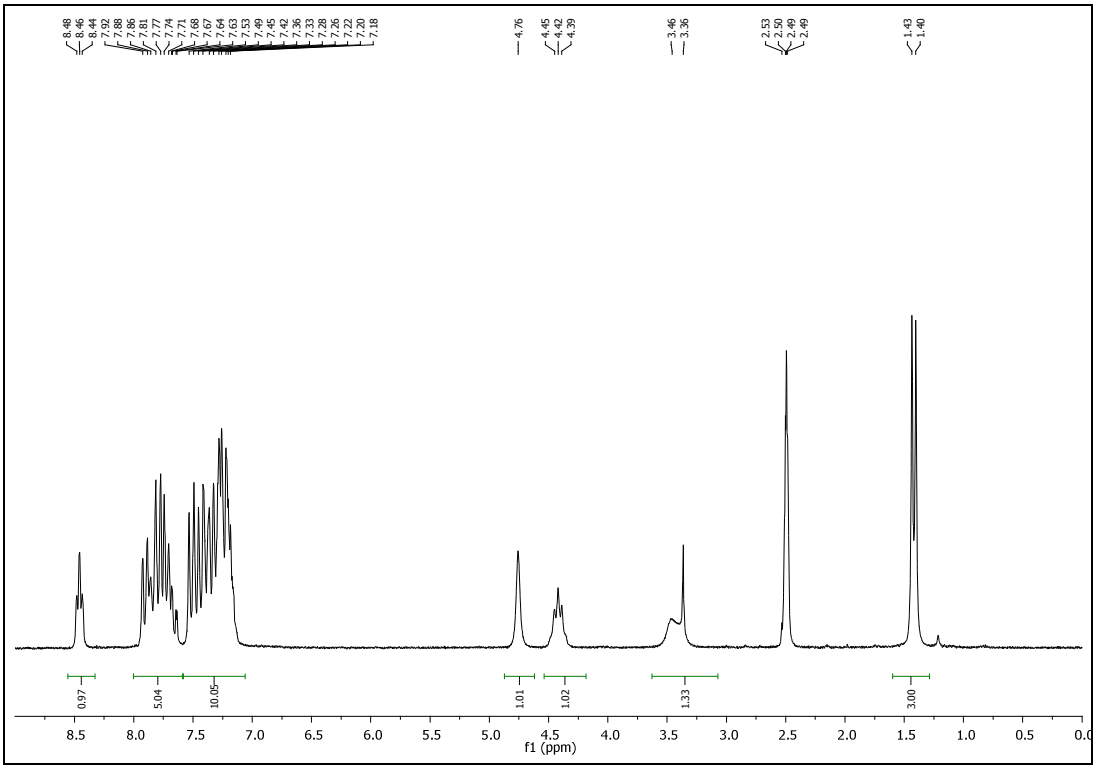
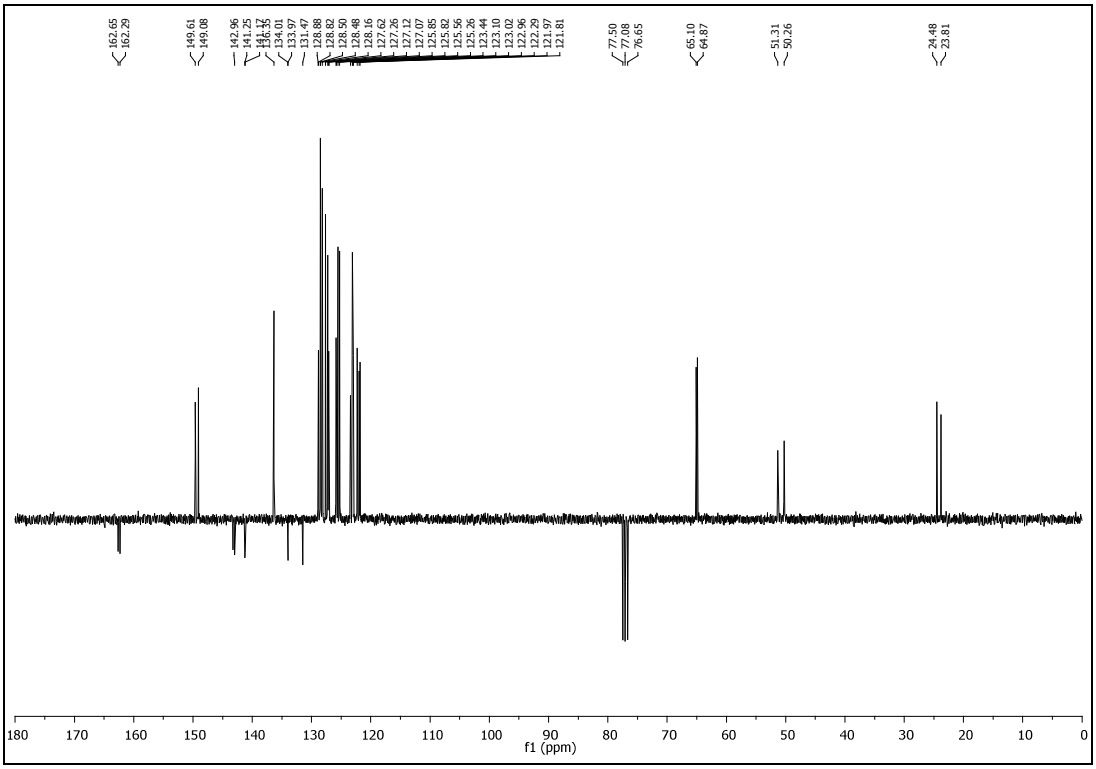


^{13}C NMR ($CDCl_3$, 75 MHz) of L13



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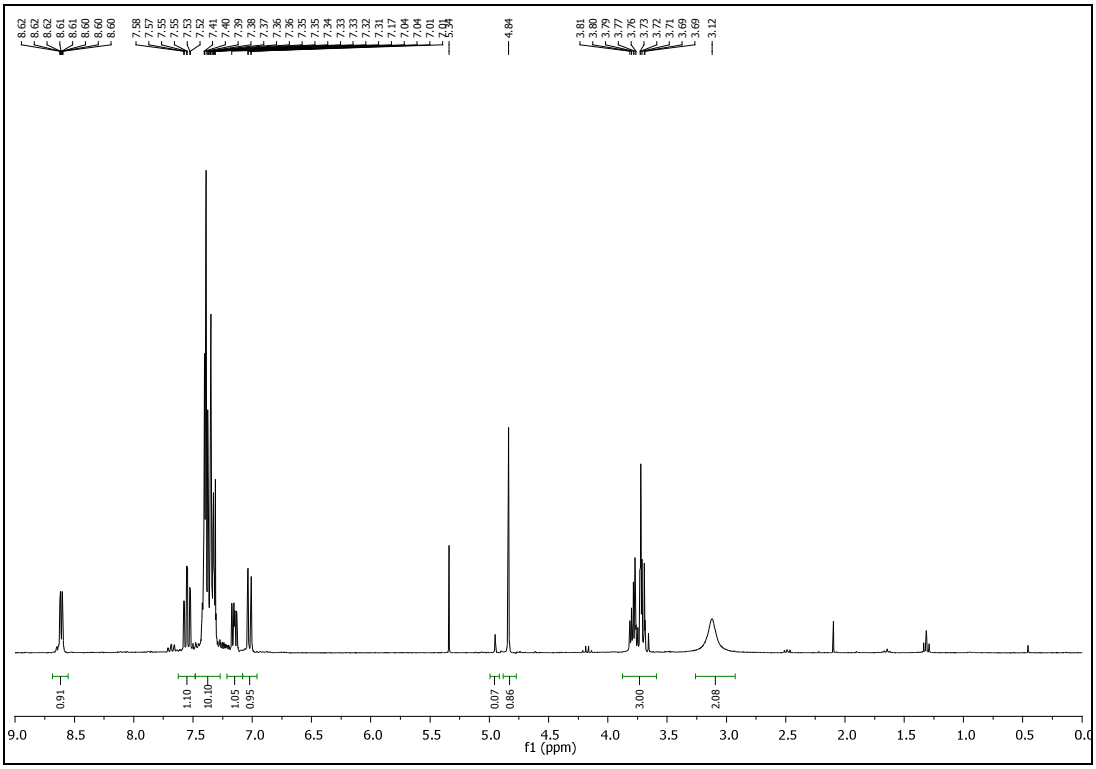

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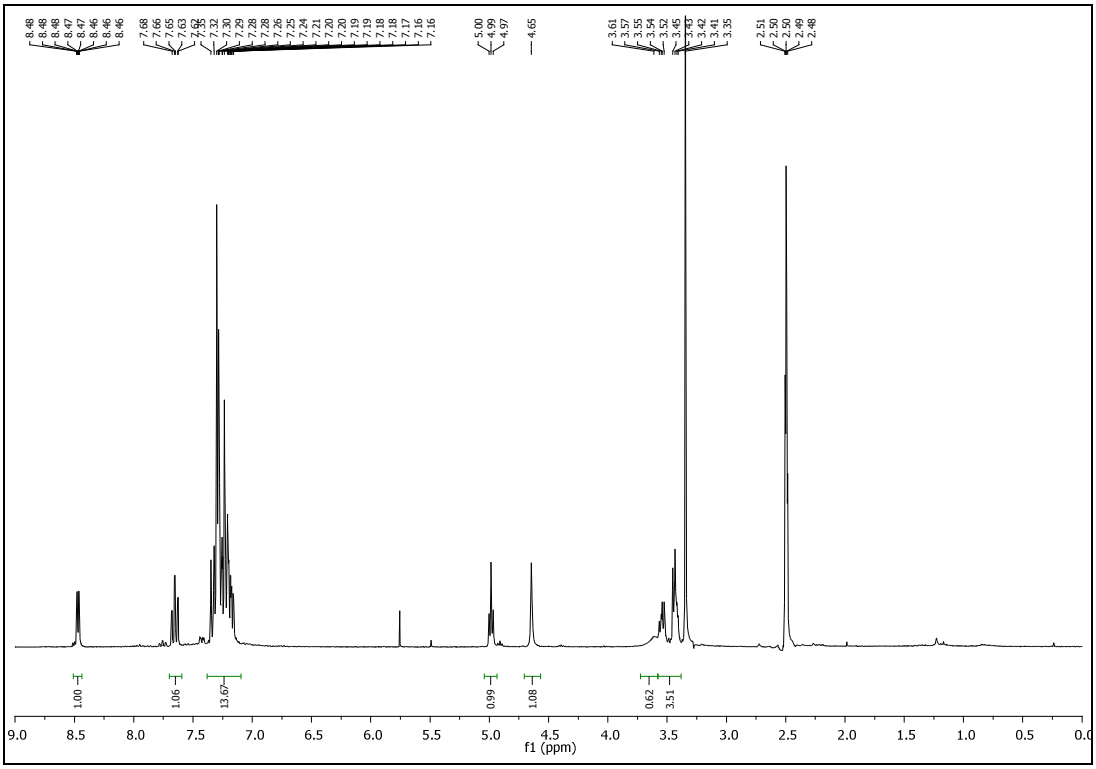

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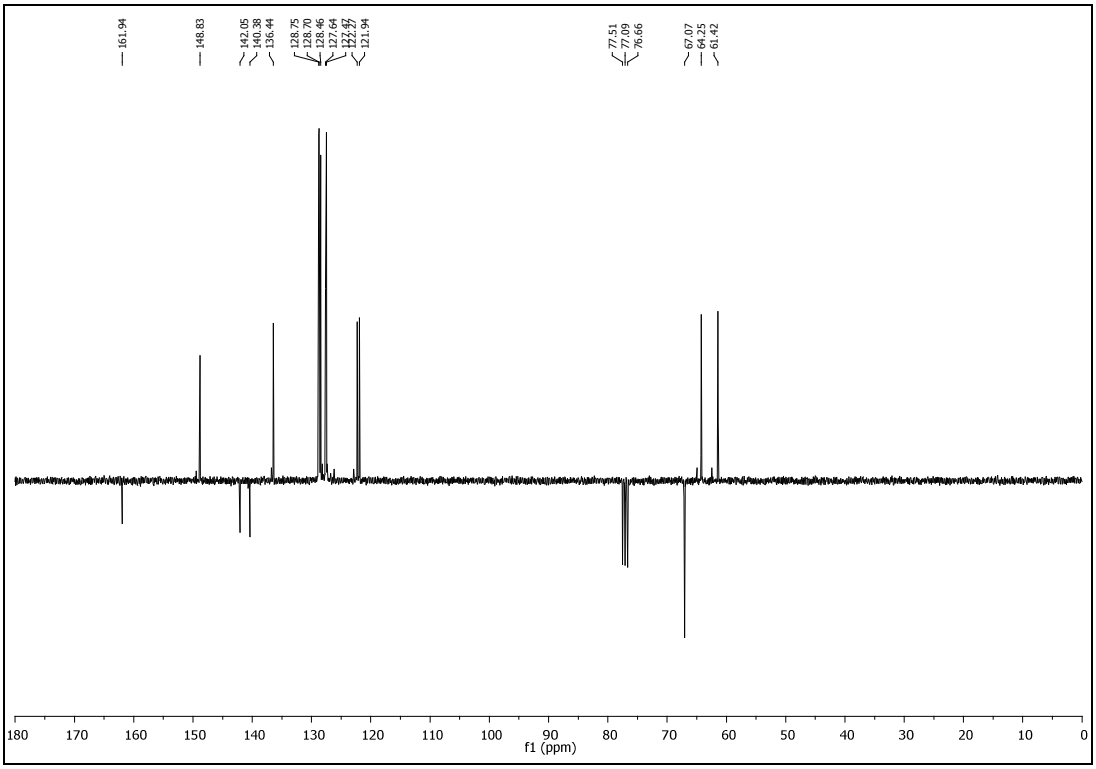

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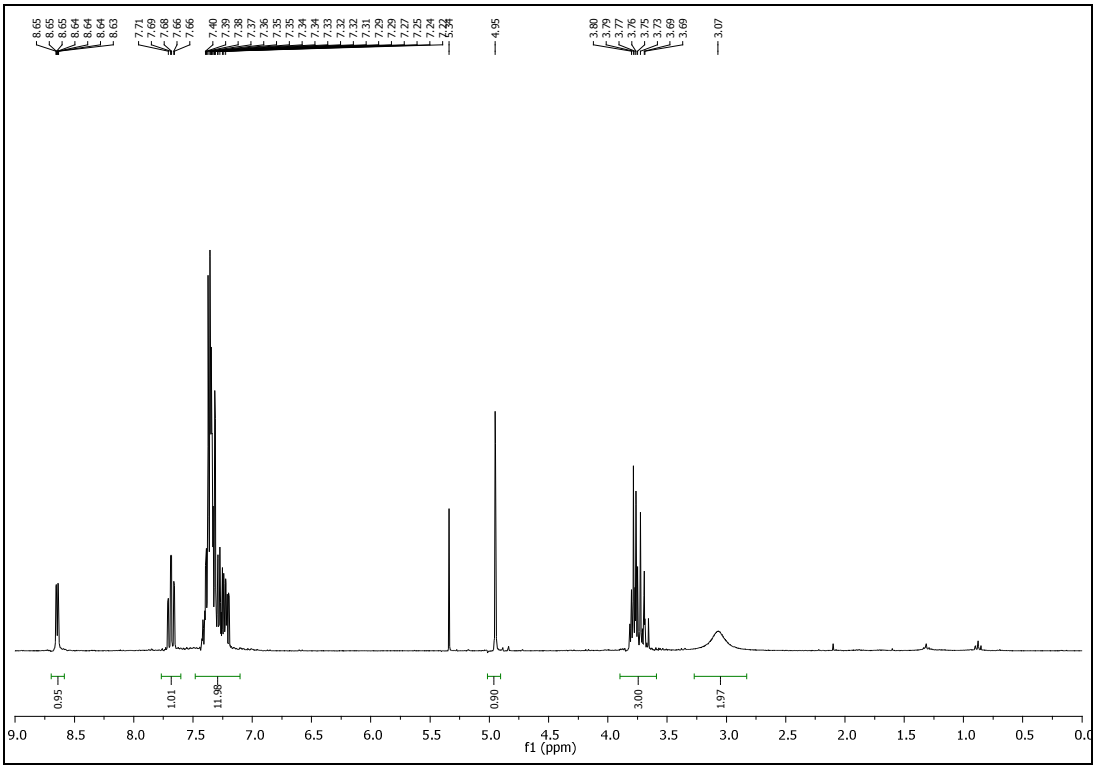

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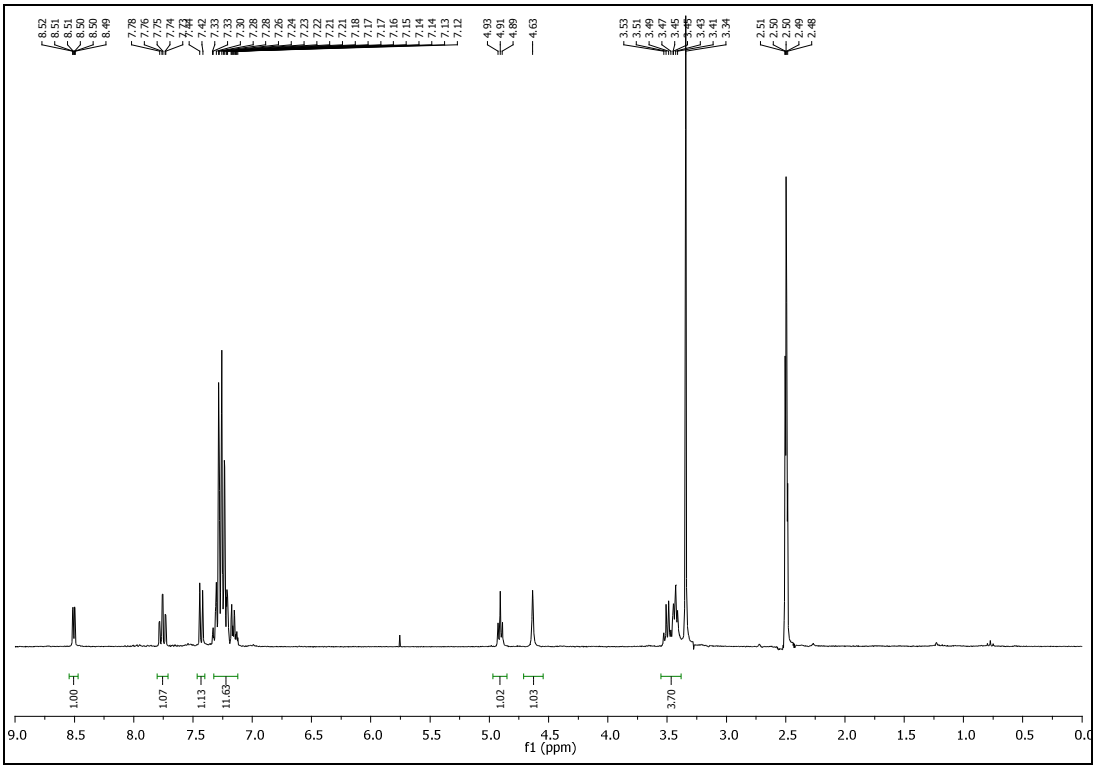

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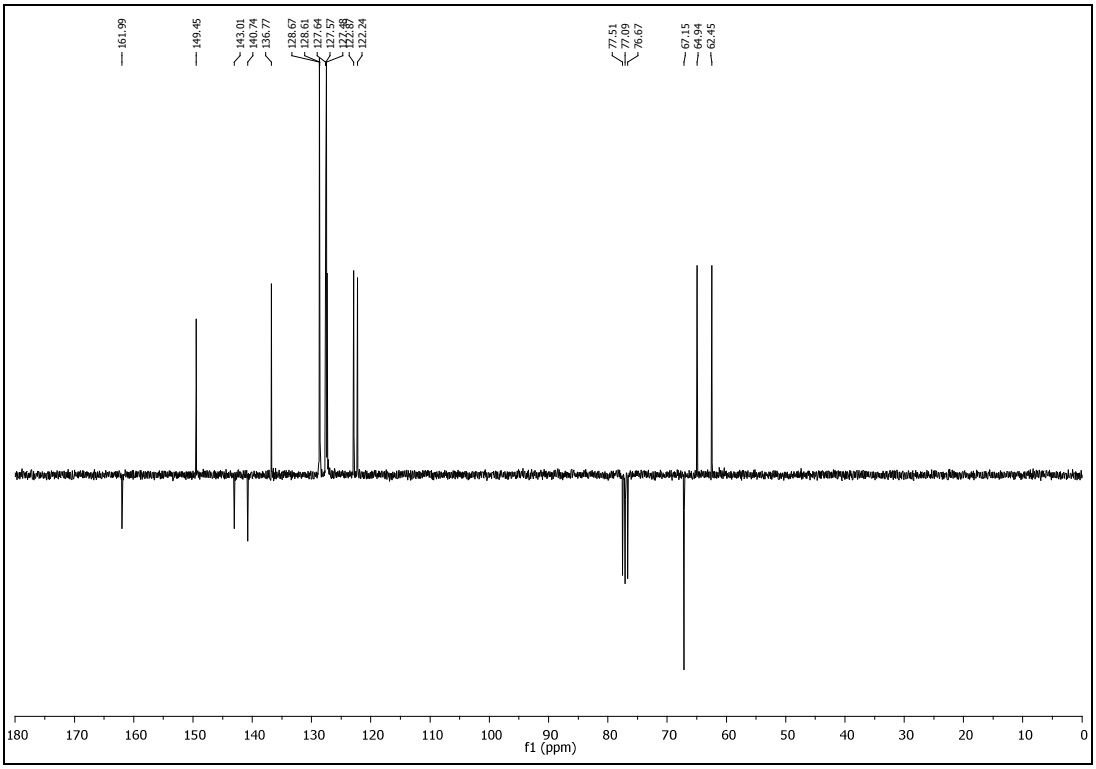

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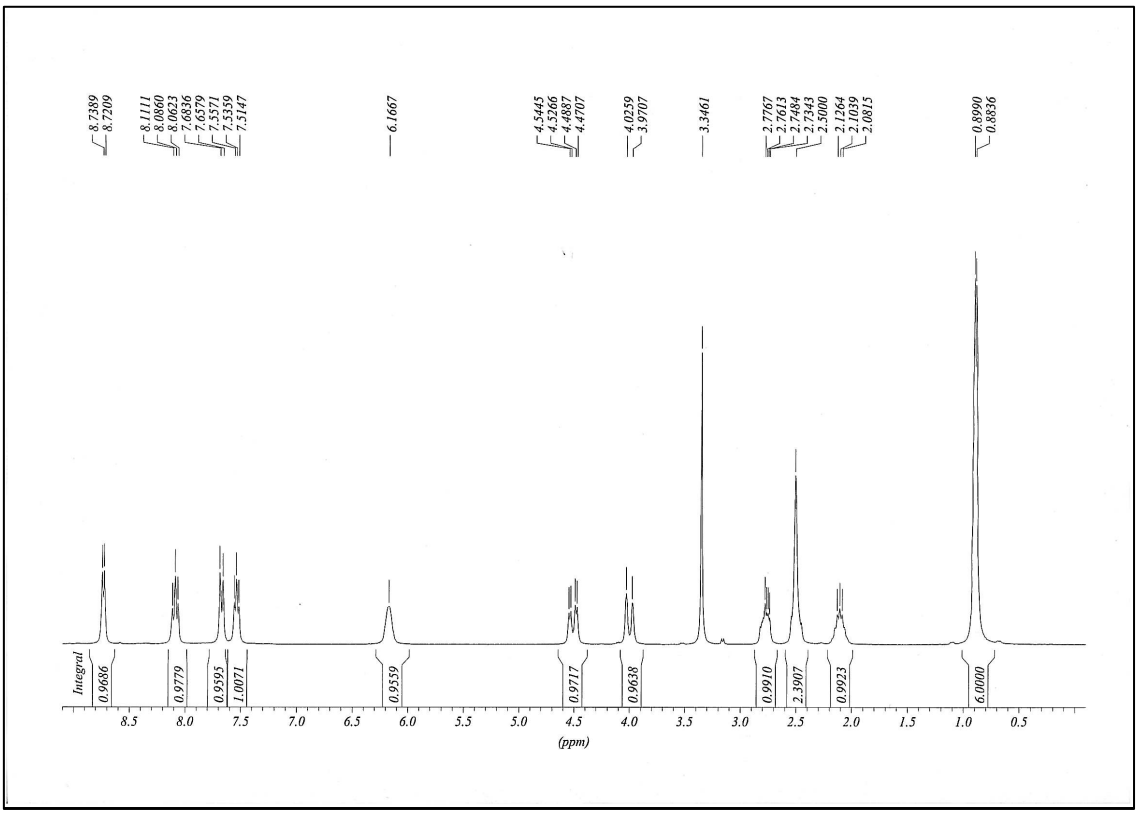

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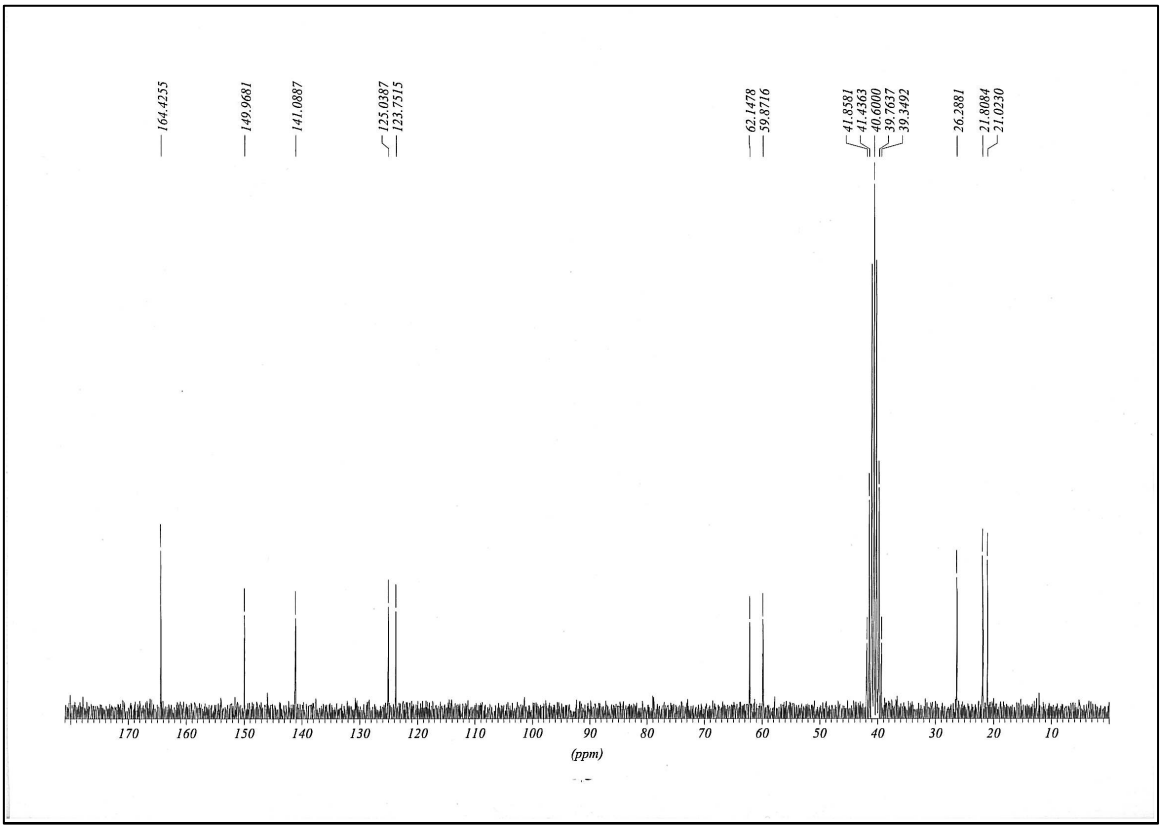

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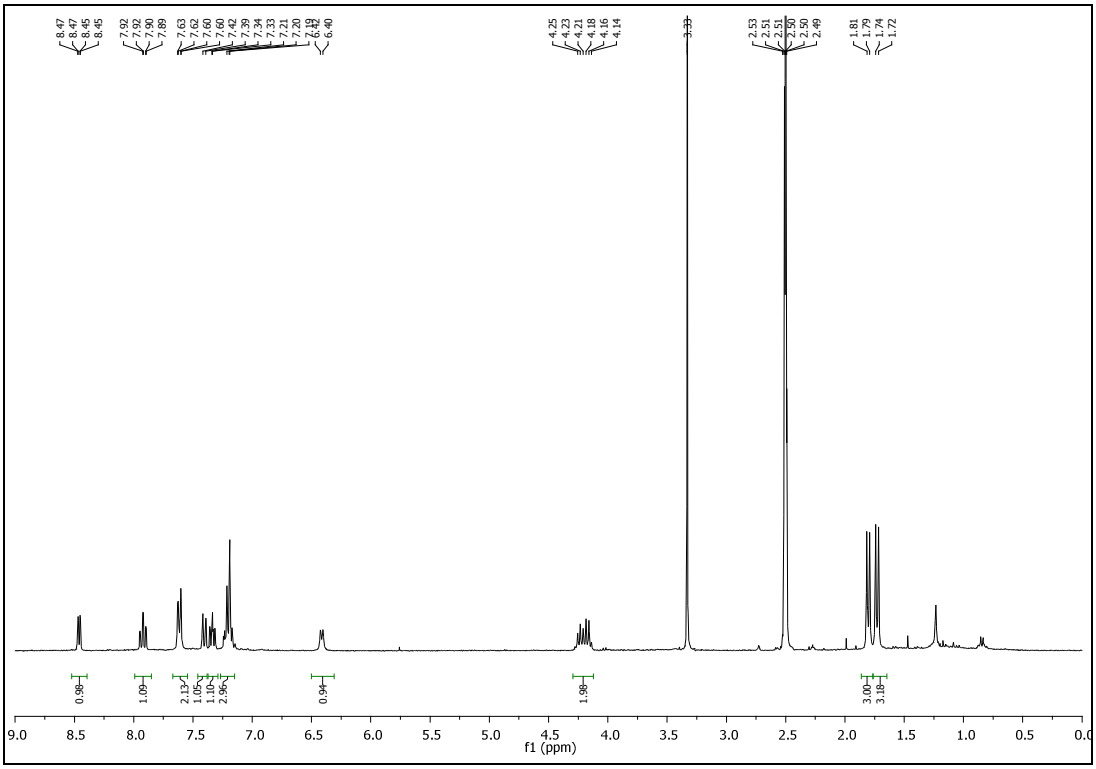

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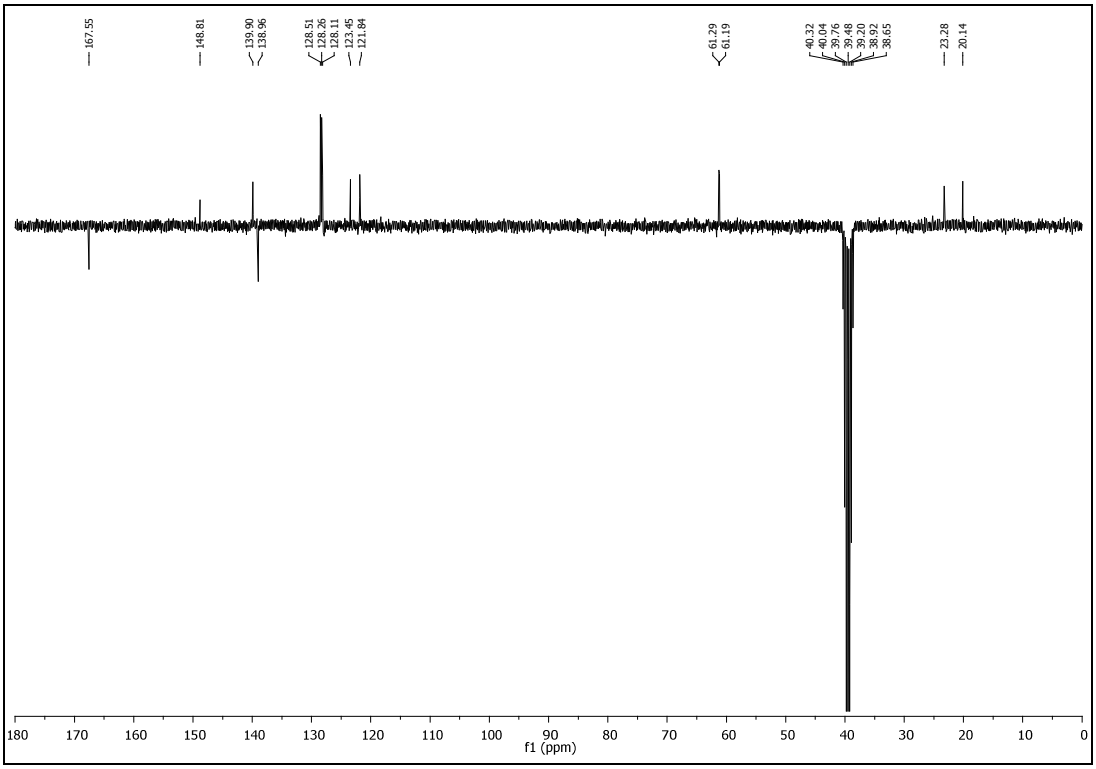

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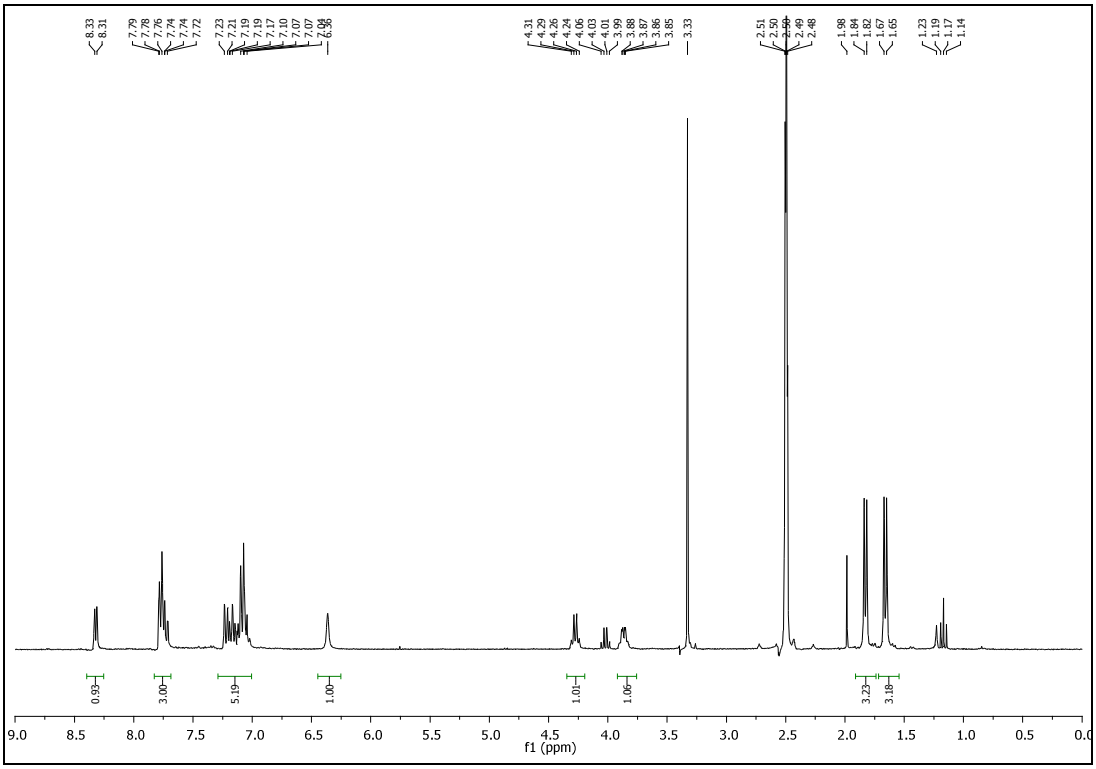

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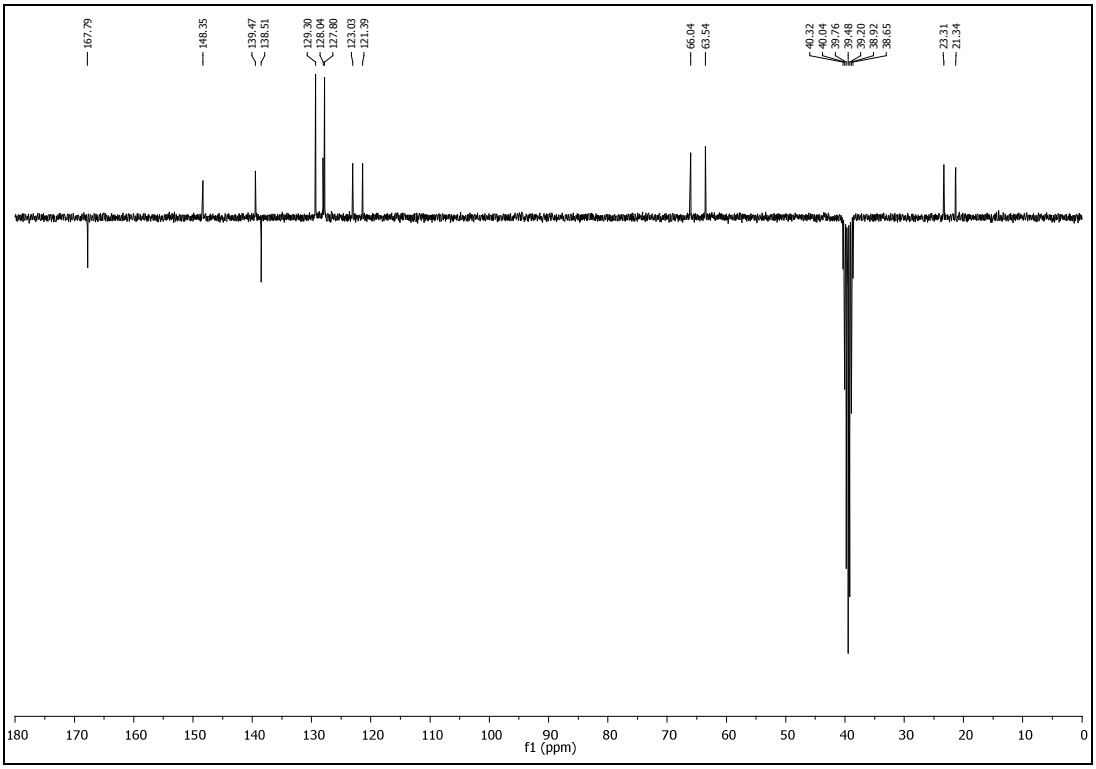

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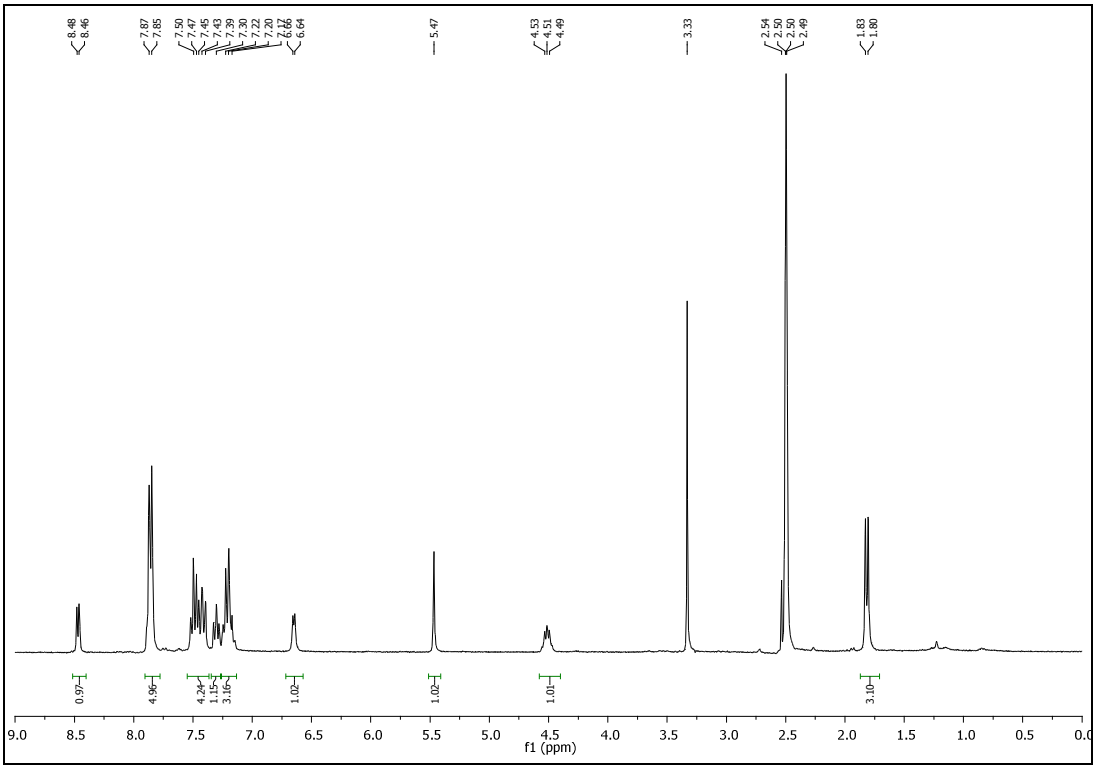

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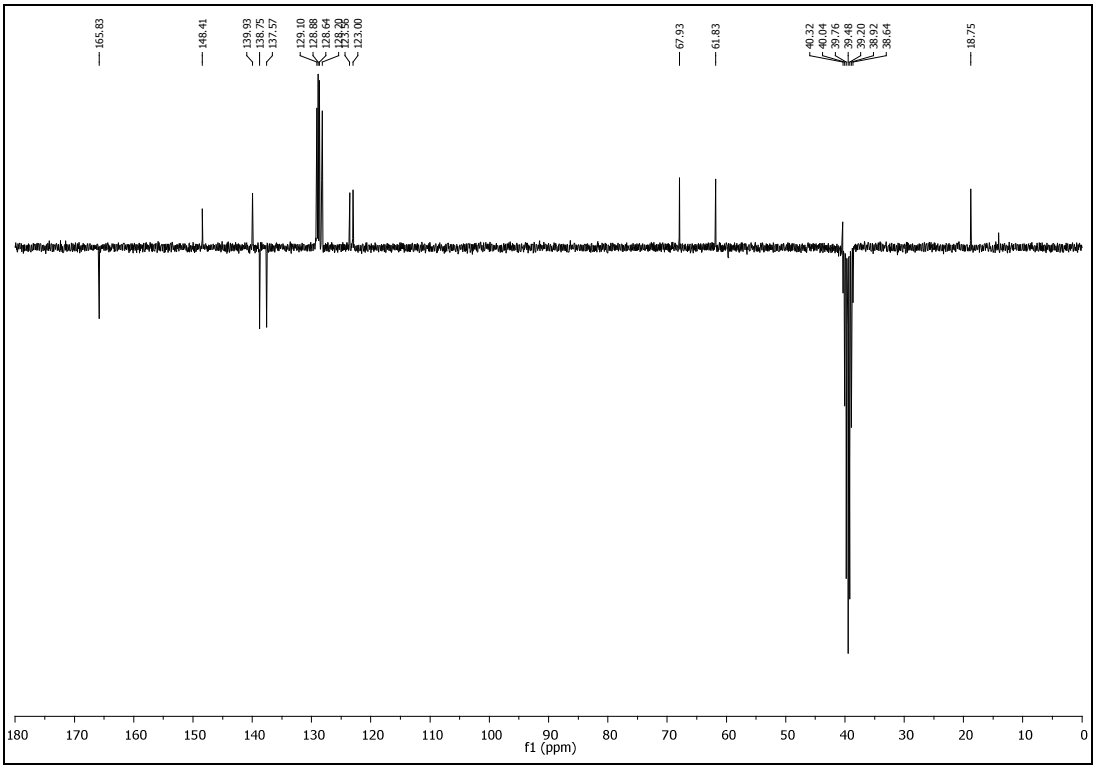

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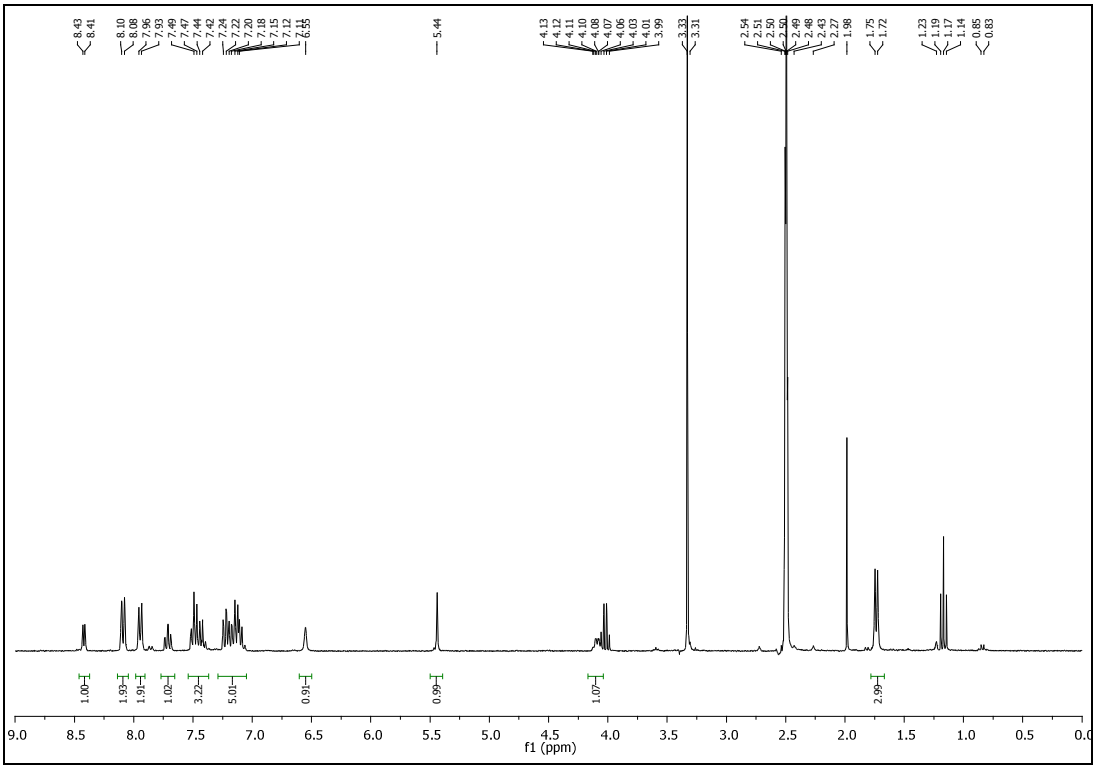

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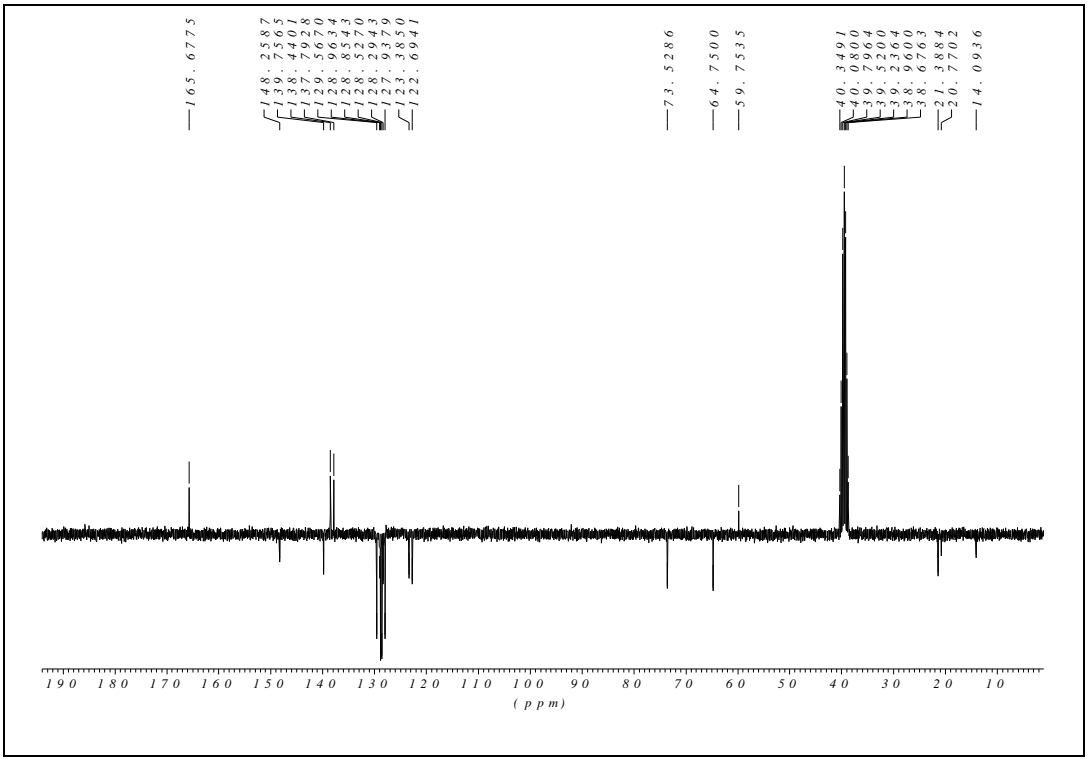

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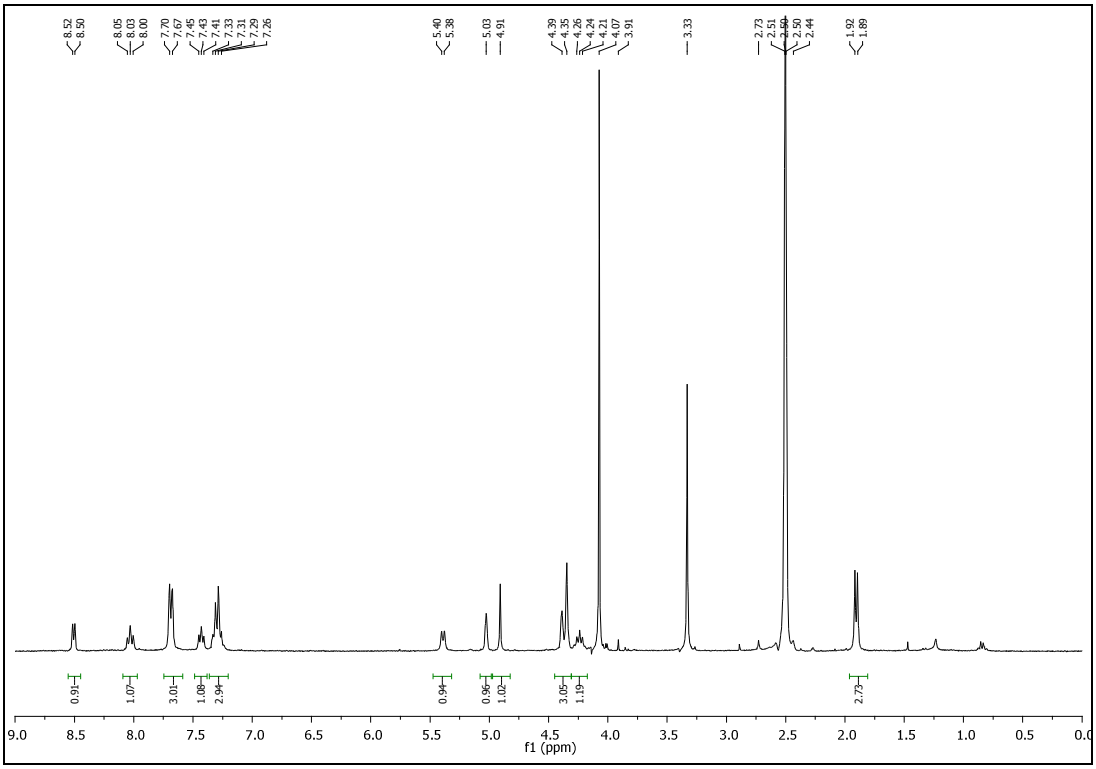

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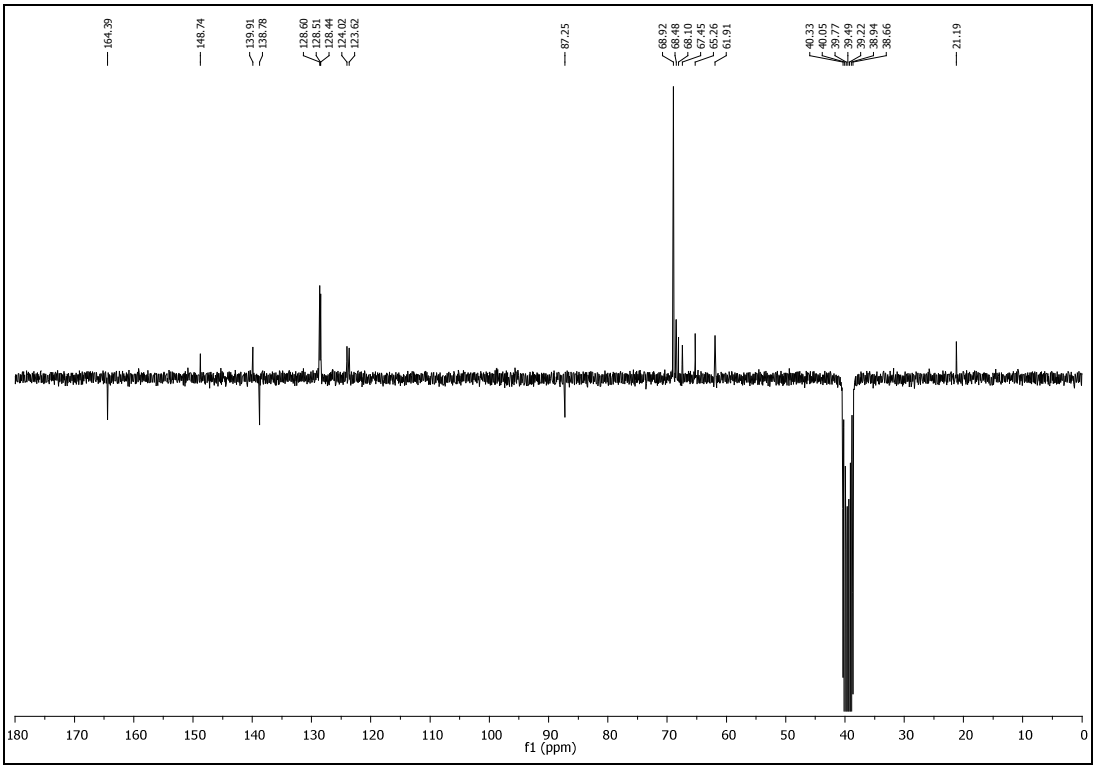

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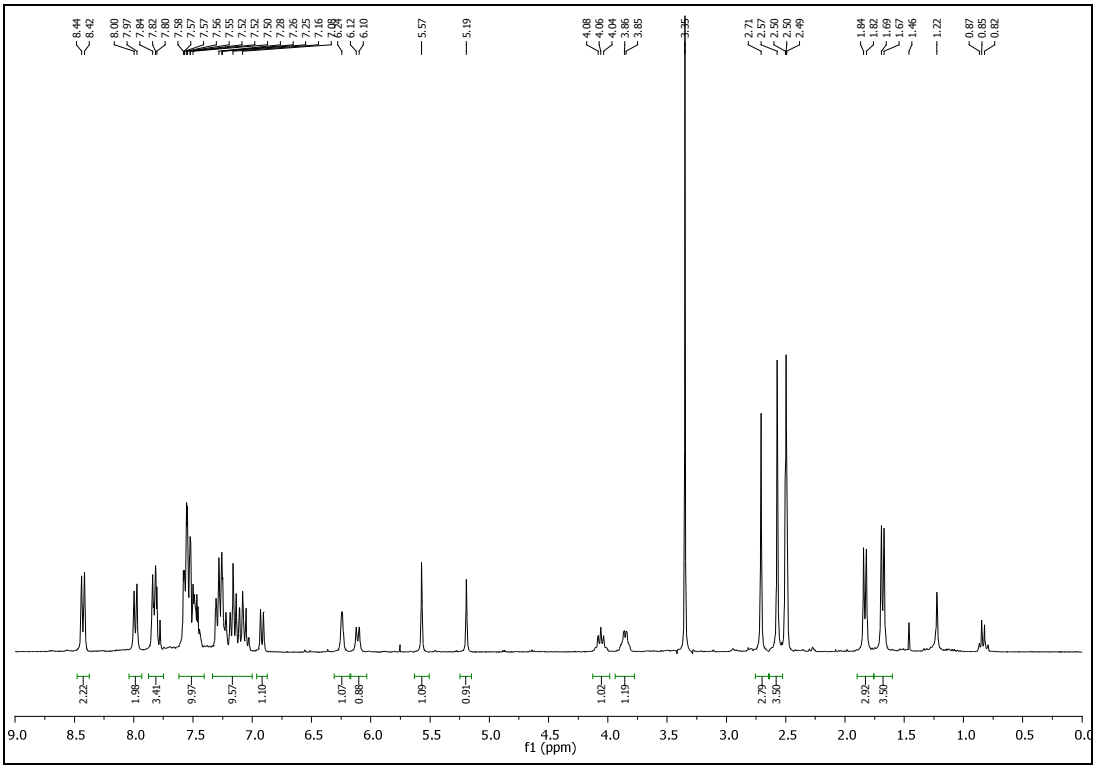
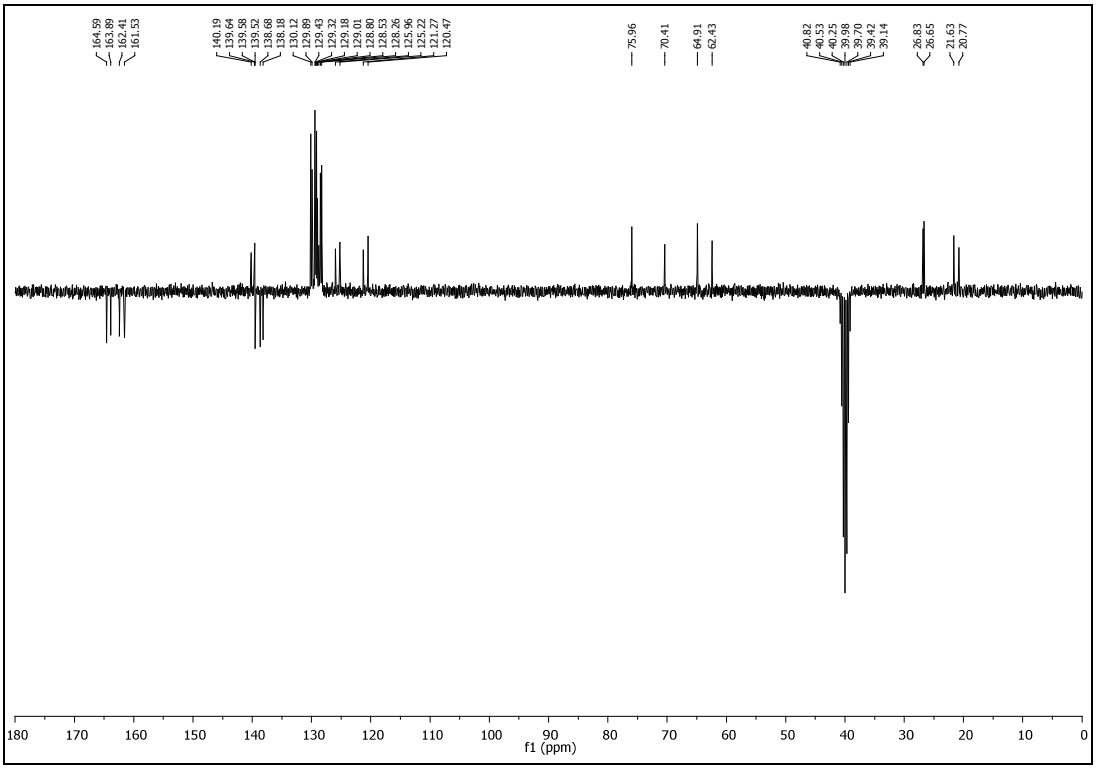
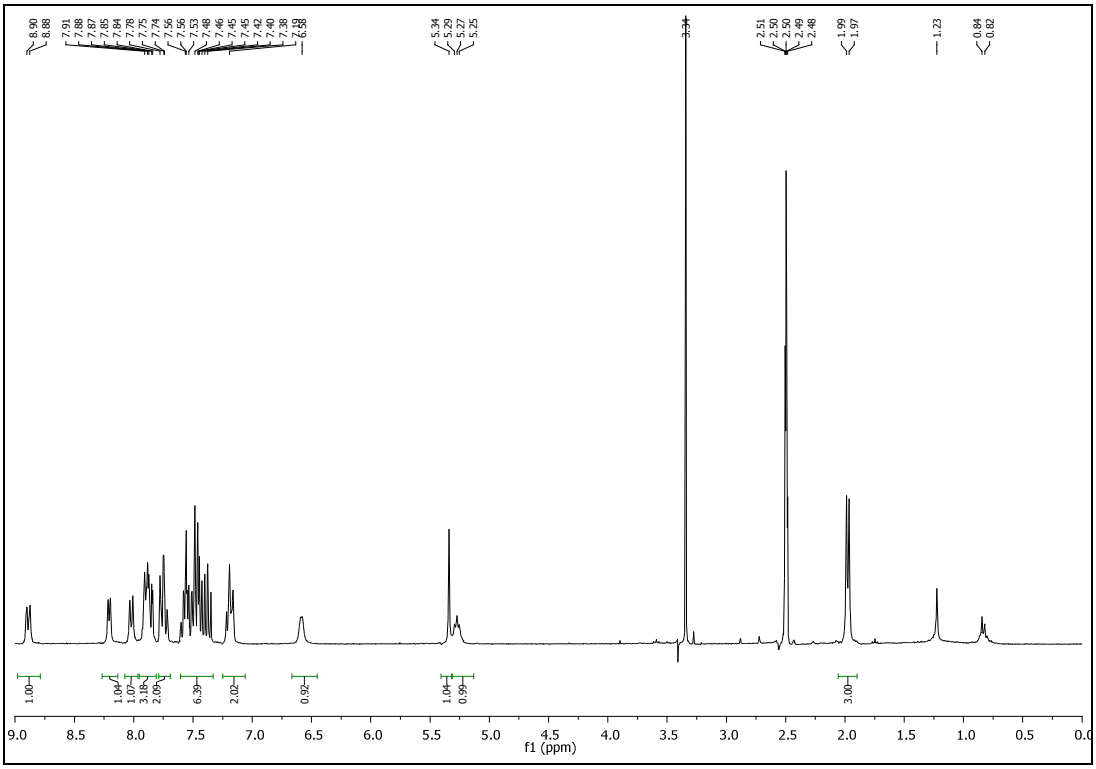


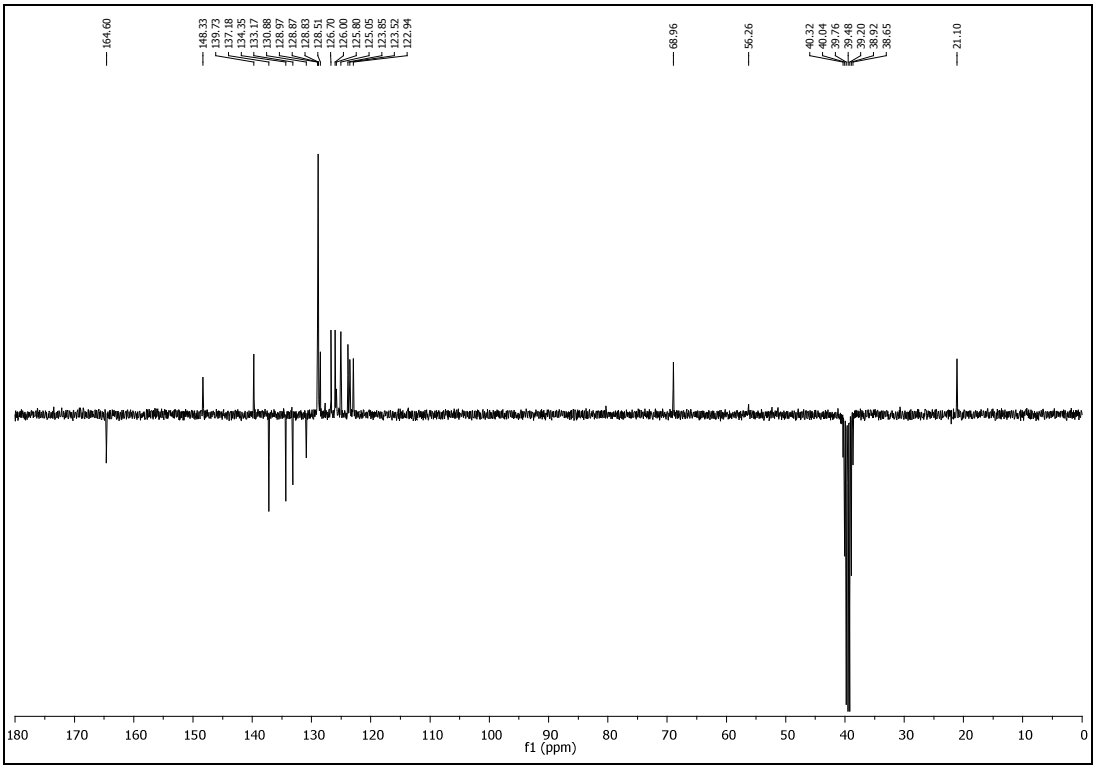
^{13}C NMR ([D$_6$]dmso, 75 MHz) of C12



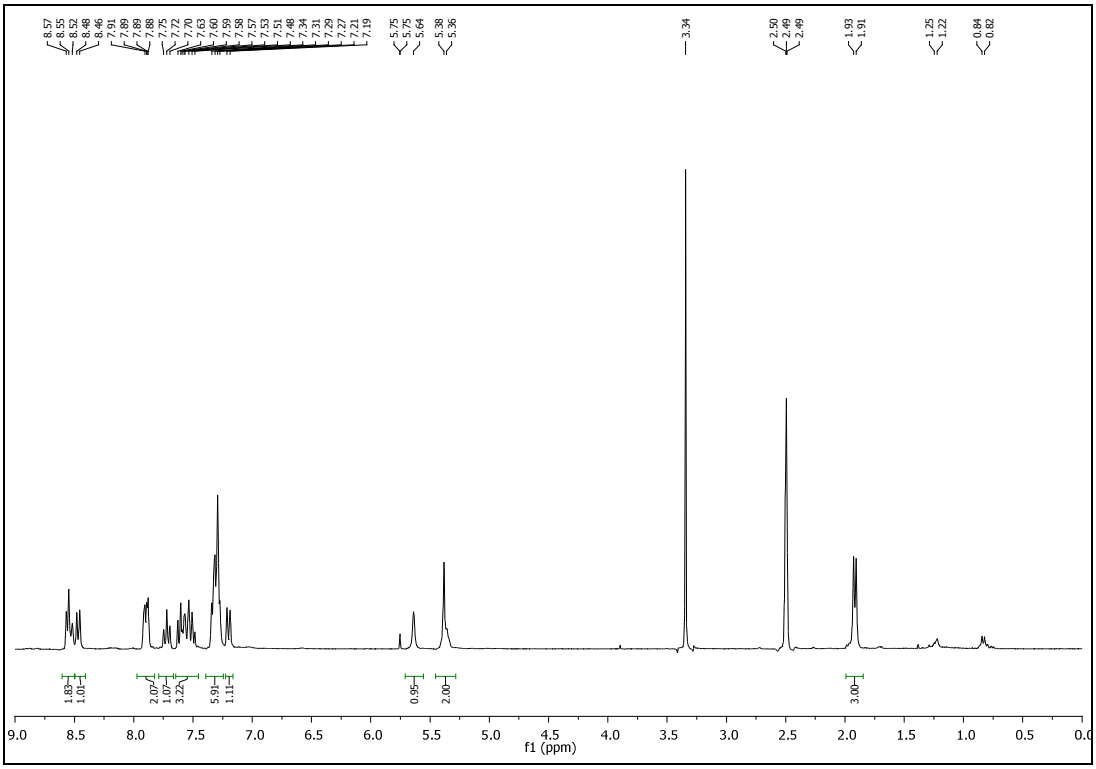
^{1}H NMR ([D$_6$]dmso, 200 MHz) of C13a



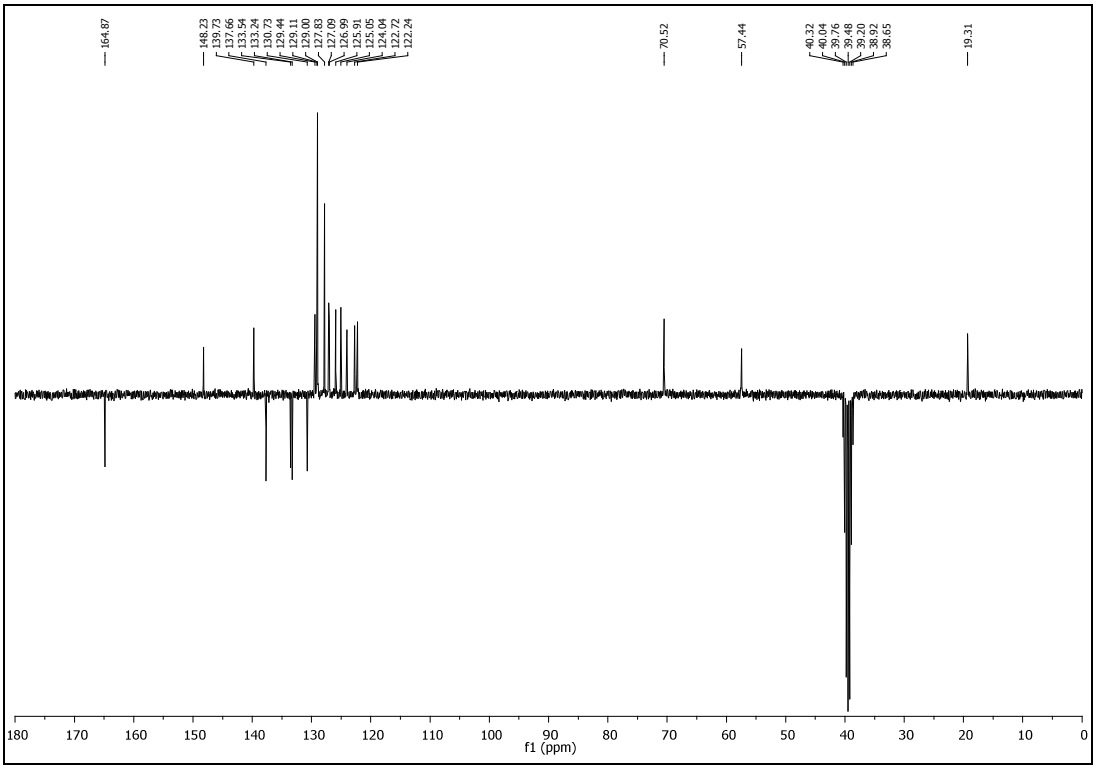
^{13}C NMR ([D$_6$]dmso, 75 MHz) of C13a



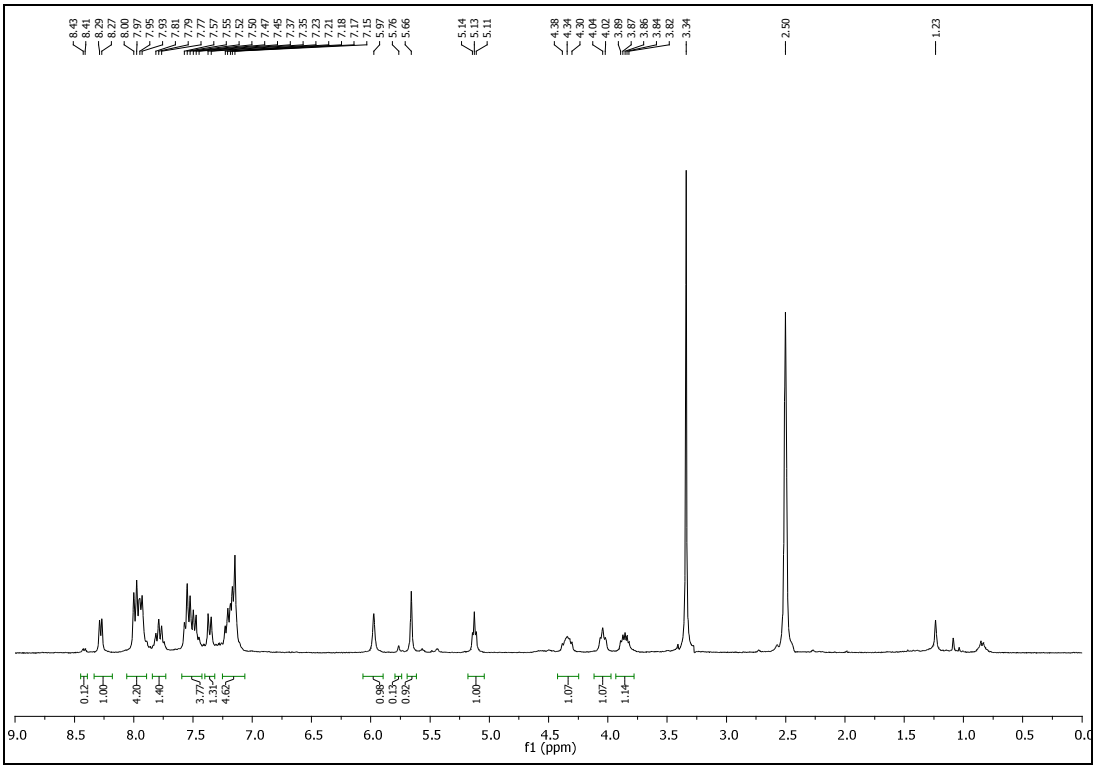
^{1}H NMR ([D$_6$]dmso, 200 MHz) of C13b



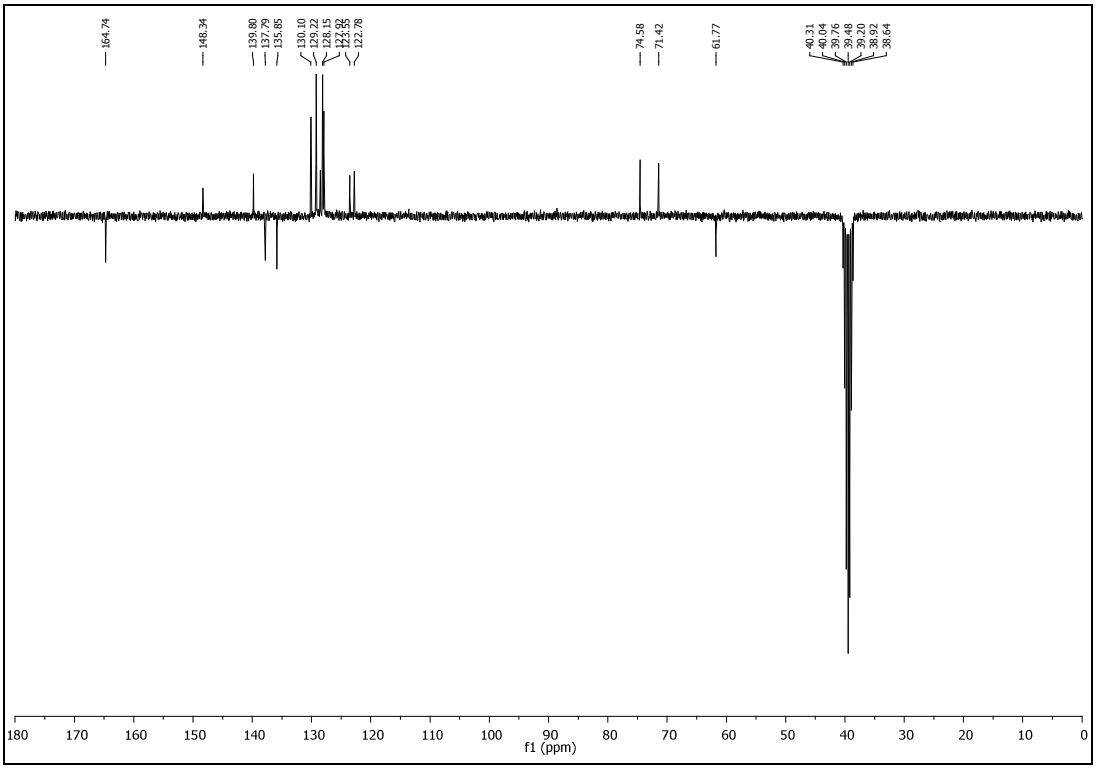
^{13}C NMR ([D$_6$]dmso, 75 MHz) of C13b



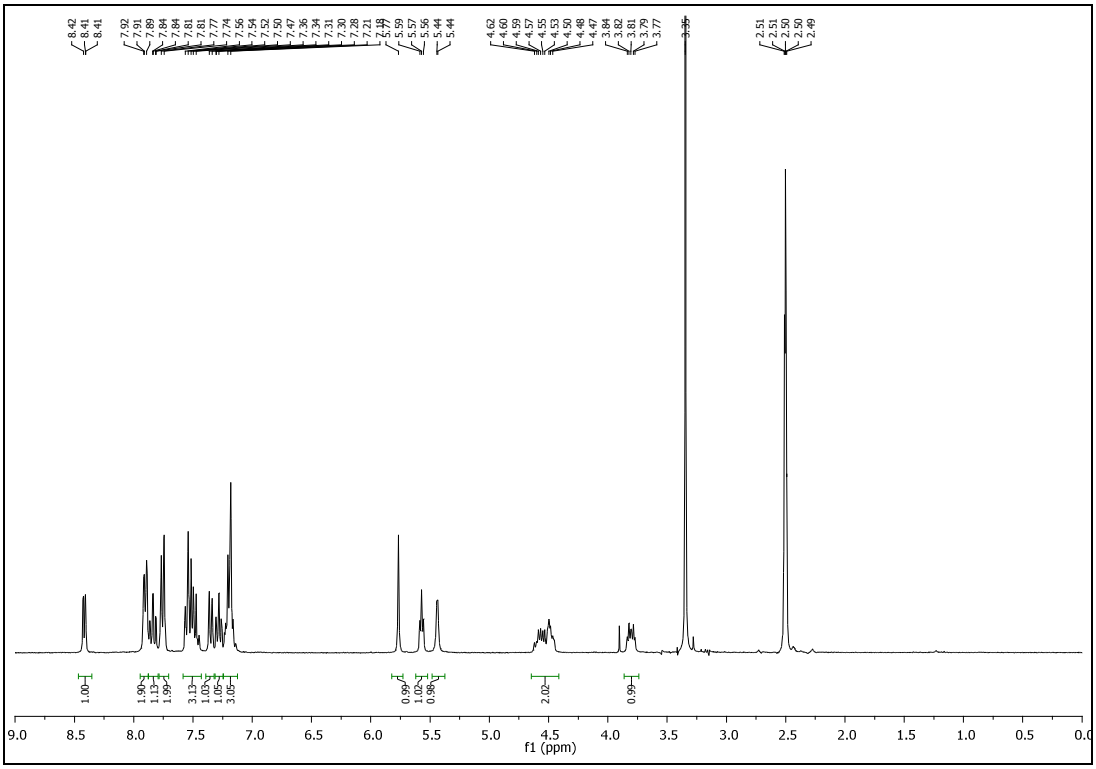
^{1}H NMR ([D$_6$]dmso, 300 MHz) of (1*S*,1'*S*)-C14



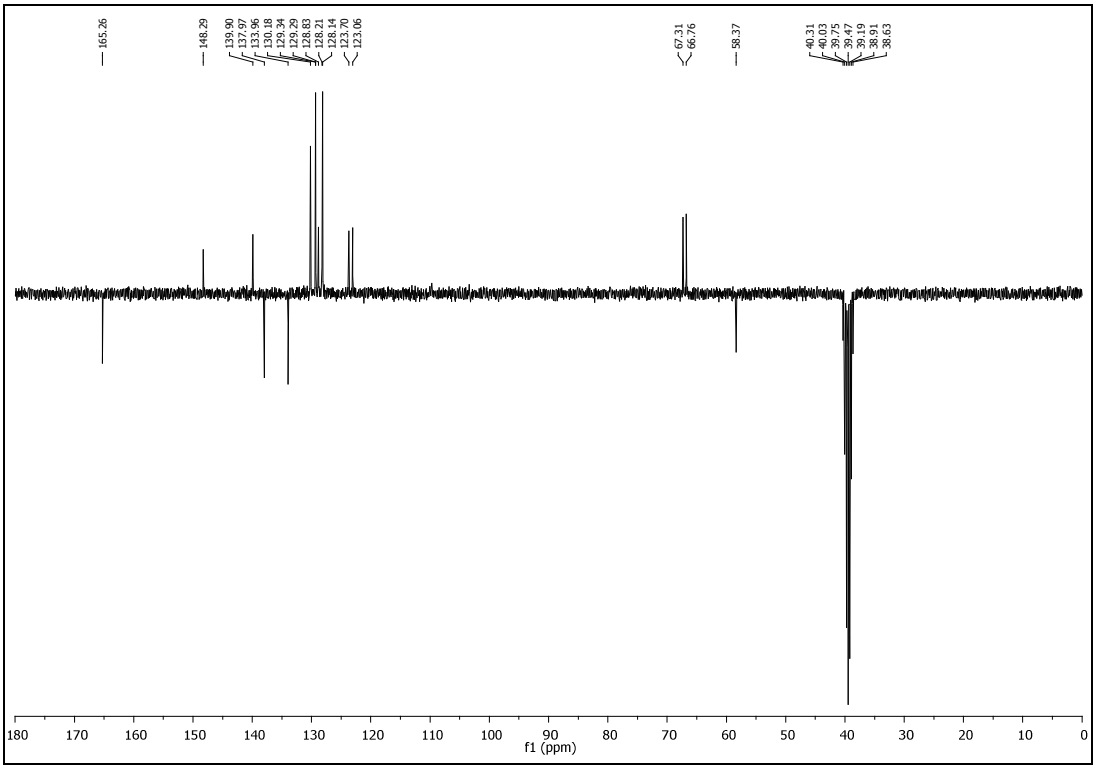
^{13}C NMR ([D$_6$]dmso, 75 MHz) of (1*S*,1'*S*)-C14



^{1}H NMR ([D$_6$]dmso, 300 MHz) of (1*R*,1'*S*)-C14



^{13}C NMR ([D$_6$]dmso, 75 MHz) of (1*R*,1'*S*)-C14



Xray data for C8

Table 1. Crystal data and structure refinement for C8.

Empirical formula	C15 H18 Cl2 N2 Pd
Formula weight	403.61
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 9.5902(5) A alpha = 90 deg. b = 11.5116(6) A beta = 90 deg. c = 14.6184(7) A gamma = 90 deg.
Volume	1613.85(14) A^3
Z, Calculated density	4, 1.661 Mg/m^3
Absorption coefficient	1.472 mm^-1
F(000)	808
Crystal size	0.24 x 0.14 x 0.12 mm
Theta range for data collection	2.25 to 29.98 deg.
Limiting indices	-13<=h<=13, -16<=k<=16, -20<=l<=20
Reflections collected / unique	113820 / 4698 [R(int) = 0.0316]
Completeness to theta = 29.98	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8431 and 0.7189
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4698 / 0 / 183
Goodness-of-fit on F^2	1.484
Final R indices [I>2sigma(I)]	R1 = 0.0166, wR2 = 0.0482
R indices (all data)	R1 = 0.0277, wR2 = 0.0732
Absolute structure parameter	0.07(2)
Largest diff. peak and hole	1.480 and -2.616 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for data3.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd(1)	9730(1)	415(1)	7875(1)	22(1)
Cl(1)	11861(1)	-386(1)	7582(1)	42(1)
Cl(2)	10660(1)	1710(1)	8917(1)	33(1)
N(1)	7721(2)	859(2)	8117(1)	24(1)
C(2)	7250(2)	1840(2)	8513(2)	30(1)
C(3)	5833(3)	2048(2)	8613(2)	38(1)
C(4)	4888(2)	1248(2)	8285(2)	38(1)
C(5)	5379(2)	244(2)	7867(2)	32(1)
C(6)	6800(2)	67(2)	7790(1)	24(1)
C(7)	7439(2)	-1021(2)	7394(1)	24(1)
N(8)	8810(2)	-699(1)	6970(1)	22(1)
C(9)	8678(2)	-352(2)	5975(1)	26(1)
C(10)	7542(2)	536(2)	5812(1)	25(1)
C(11)	7696(2)	1710(2)	6041(1)	29(1)
C(12)	6637(3)	2489(2)	5863(2)	35(1)
C(13)	5399(3)	2111(2)	5460(2)	38(1)
C(14)	5226(3)	959(2)	5232(2)	38(1)
C(15)	6301(2)	176(2)	5406(1)	30(1)
C(16)	7661(3)	-1937(2)	8130(2)	34(1)
C(17)	10088(3)	3(2)	5599(2)	37(1)

Table 3. Bond lengths [A] and angles [deg] for data3.

Pd(1)-N(1)	2.0250(17)
Pd(1)-N(8)	2.0431(17)
Pd(1)-Cl(1)	2.2822(6)
Pd(1)-Cl(2)	2.3103(5)
N(1)-C(2)	1.347(3)
N(1)-C(6)	1.356(3)
C(2)-C(3)	1.388(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.377(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.390(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.383(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.510(3)
C(7)-N(8)	1.501(3)
C(7)-C(16)	1.521(3)
C(7)-H(7)	1.0000
N(8)-C(9)	1.514(2)
N(8)-H(8)	0.9300
C(9)-C(10)	1.513(3)
C(9)-C(17)	1.515(3)
C(9)-H(9)	1.0000
C(10)-C(15)	1.392(3)
C(10)-C(11)	1.400(3)
C(11)-C(12)	1.380(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.394(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.377(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.393(3)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
N(1)-Pd(1)-N(8)	81.99(7)
N(1)-Pd(1)-Cl(1)	170.71(5)
N(8)-Pd(1)-Cl(1)	90.68(5)
N(1)-Pd(1)-Cl(2)	95.11(5)
N(8)-Pd(1)-Cl(2)	177.10(5)
Cl(1)-Pd(1)-Cl(2)	92.20(2)
C(2)-N(1)-C(6)	119.78(19)
C(2)-N(1)-Pd(1)	127.30(15)
C(6)-N(1)-Pd(1)	112.85(14)
N(1)-C(2)-C(3)	121.2(2)
N(1)-C(2)-H(2)	119.4
C(3)-C(2)-H(2)	119.4
C(4)-C(3)-C(2)	119.5(2)
C(4)-C(3)-H(3)	120.3
C(2)-C(3)-H(3)	120.3
C(3)-C(4)-C(5)	119.1(2)

C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
C(6)-C(5)-C(4)	119.5(2)
C(6)-C(5)-H(5)	120.3
C(4)-C(5)-H(5)	120.3
N(1)-C(6)-C(5)	120.9(2)
N(1)-C(6)-C(7)	115.40(17)
C(5)-C(6)-C(7)	123.58(19)
N(8)-C(7)-C(6)	107.99(15)
N(8)-C(7)-C(16)	109.91(17)
C(6)-C(7)-C(16)	111.14(17)
N(8)-C(7)-H(7)	109.3
C(6)-C(7)-H(7)	109.3
C(16)-C(7)-H(7)	109.3
C(7)-N(8)-C(9)	112.89(15)
C(7)-N(8)-Pd(1)	105.44(11)
C(9)-N(8)-Pd(1)	119.50(12)
C(7)-N(8)-H(8)	106.0
C(9)-N(8)-H(8)	106.0
Pd(1)-N(8)-H(8)	106.0
C(10)-C(9)-N(8)	112.94(15)
C(10)-C(9)-C(17)	113.76(18)
N(8)-C(9)-C(17)	110.16(17)
C(10)-C(9)-H(9)	106.5
N(8)-C(9)-H(9)	106.5
C(17)-C(9)-H(9)	106.5
C(15)-C(10)-C(11)	118.6(2)
C(15)-C(10)-C(9)	118.79(19)
C(11)-C(10)-C(9)	122.57(19)
C(12)-C(11)-C(10)	120.3(2)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(13)	120.2(2)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
C(14)-C(13)-C(12)	120.3(2)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(13)-C(14)-C(15)	119.3(2)
C(13)-C(14)-H(14)	120.3
C(15)-C(14)-H(14)	120.3
C(10)-C(15)-C(14)	121.2(2)
C(10)-C(15)-H(15)	119.4
C(14)-C(15)-H(15)	119.4
C(7)-C(16)-H(16A)	109.5
C(7)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(7)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(9)-C(17)-H(17A)	109.5
C(9)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(9)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for data3.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd(1)	20(1)	21(1)	26(1)	2(1)	-2(1)	-2(1)
Cl(1)	22(1)	45(1)	60(1)	-6(1)	-5(1)	5(1)
Cl(2)	37(1)	29(1)	33(1)	0(1)	-7(1)	-12(1)
N(1)	22(1)	26(1)	24(1)	-1(1)	0(1)	-1(1)
C(2)	34(1)	27(1)	30(1)	-4(1)	-1(1)	3(1)
C(3)	37(1)	38(1)	39(1)	-3(1)	4(1)	11(1)
C(4)	26(1)	48(1)	38(1)	2(1)	3(1)	10(1)
C(5)	24(1)	40(1)	33(1)	-1(1)	0(1)	-1(1)
C(6)	23(1)	26(1)	23(1)	1(1)	0(1)	0(1)
C(7)	22(1)	24(1)	26(1)	0(1)	0(1)	-4(1)
N(8)	22(1)	19(1)	25(1)	2(1)	0(1)	0(1)
C(9)	32(1)	24(1)	22(1)	0(1)	2(1)	3(1)
C(10)	29(1)	25(1)	22(1)	1(1)	1(1)	3(1)
C(11)	33(1)	26(1)	28(1)	1(1)	-1(1)	1(1)
C(12)	45(1)	30(1)	31(1)	3(1)	2(1)	10(1)
C(13)	38(1)	45(1)	30(1)	7(1)	3(1)	15(1)
C(14)	32(1)	52(1)	29(1)	4(1)	-5(1)	3(1)
C(15)	34(1)	32(1)	26(1)	2(1)	-3(1)	-3(1)
C(16)	43(1)	27(1)	31(1)	6(1)	3(1)	-4(1)
C(17)	33(1)	40(1)	37(1)	6(1)	12(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for data3.

	x	y	z	U(eq)
H(2)	7900	2399	8729	36
H(3)	5517	2736	8906	45
H(4)	3915	1382	8344	45
H(5)	4743	-317	7636	39
H(7)	6807	-1340	6911	29
H(8)	9348	-1372	6977	26
H(9)	8396	-1068	5634	31
H(11)	8533	1971	6321	35
H(12)	6752	3285	6015	42
H(13)	4672	2651	5343	45
H(14)	4382	702	4960	45
H(15)	6186	-617	5245	37
H(16A)	8167	-2598	7870	51
H(16B)	6755	-2200	8361	51
H(16C)	8203	-1603	8634	51
H(17A)	10445	666	5949	55
H(17B)	9991	223	4955	55
H(17C)	10740	-649	5652	55

Xray data for C9

Table 1. Crystal data and structure refinement for C9.

Empirical formula	C20 H20 Cl2 N2 Pd
Formula weight	465.68
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 10.1669(12) A alpha = 90 deg. b = 11.8011(13) A beta = 90 deg. c = 15.7914(18) A gamma = 90 deg.
Volume	1894.7(4) A^3
Z, Calculated density	4, 1.633 Mg/m^3
Absorption coefficient	1.266 mm^-1
F(000)	936
Crystal size	0.25 x 0.25 x 0.10 mm
Theta range for data collection	2.15 to 29.98 deg.
Limiting indices	-13<=h<=14, -16<=k<=14, -22<=l<=20
Reflections collected / unique	20922 / 5413 [R(int) = 0.0362]
Completeness to theta = 29.98	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8838 and 0.7425
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5413 / 0 / 227
Goodness-of-fit on F^2	1.114
Final R indices [I>2sigma(I)]	R1 = 0.0212, wR2 = 0.0497
R indices (all data)	R1 = 0.0217, wR2 = 0.0499
Absolute structure parameter	0.01(2)
Largest diff. peak and hole	0.335 and -0.450 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for data2.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd(1)	2393(1)	758(1)	9996(1)	11(1)
Cl(1)	426(1)	777(1)	10697(1)	17(1)
Cl(2)	3591(1)	1422(1)	11135(1)	17(1)
N(1)	3930(2)	715(1)	9186(1)	13(1)
C(2)	5038(2)	1341(2)	9246(1)	16(1)
C(3)	5901(2)	1445(2)	8572(1)	20(1)
C(4)	5616(2)	904(2)	7819(1)	19(1)
C(5)	4482(2)	240(2)	7758(1)	16(1)
C(6)	3660(2)	166(2)	8456(1)	12(1)
C(7)	2405(2)	-515(1)	8451(1)	12(1)
C(8)	2554(2)	-1702(2)	8821(1)	15(1)
C(9)	3687(2)	-2058(2)	9238(1)	17(1)
C(10)	3769(2)	-3152(2)	9561(1)	22(1)
C(11)	2711(2)	-3883(2)	9495(1)	21(1)
C(12)	1568(2)	-3532(2)	9095(1)	21(1)
C(13)	1498(2)	-2449(2)	8746(1)	19(1)
N(14)	1412(2)	123(1)	8977(1)	12(1)
C(15)	554(2)	951(2)	8490(1)	14(1)
C(16)	1394(2)	1699(2)	7929(1)	13(1)
C(17)	1616(2)	1455(2)	7075(1)	15(1)
C(18)	2444(2)	2132(2)	6591(1)	19(1)
C(19)	3050(2)	3070(2)	6950(1)	20(1)
C(20)	2826(2)	3322(2)	7800(1)	20(1)
C(21)	2003(2)	2646(2)	8285(1)	16(1)
C(22)	-530(2)	296(2)	8028(1)	20(1)

Table 3. Bond lengths [A] and angles [deg] for data2.

Pd(1)-N(1)	2.0201(15)
Pd(1)-N(14)	2.0377(15)
Pd(1)-Cl(1)	2.2850(5)
Pd(1)-Cl(2)	2.3090(5)
N(1)-C(2)	1.350(2)
N(1)-C(6)	1.352(2)
C(2)-C(3)	1.385(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.379(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.397(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.385(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.508(3)
C(7)-N(14)	1.508(2)
C(7)-C(8)	1.525(2)
C(7)-H(7)	1.0000
C(8)-C(9)	1.392(3)
C(8)-C(13)	1.394(3)
C(9)-C(10)	1.391(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.382(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.386(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.394(3)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
N(14)-C(15)	1.519(2)
N(14)-H(14)	0.9300
C(15)-C(16)	1.514(3)
C(15)-C(22)	1.531(3)
C(15)-H(15)	1.0000
C(16)-C(21)	1.395(3)
C(16)-C(17)	1.398(3)
C(17)-C(18)	1.389(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.388(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.393(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.387(3)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
N(1)-Pd(1)-N(14)	82.47(6)
N(1)-Pd(1)-Cl(1)	169.58(4)
N(14)-Pd(1)-Cl(1)	87.55(5)
N(1)-Pd(1)-Cl(2)	95.39(5)
N(14)-Pd(1)-Cl(2)	177.19(4)
Cl(1)-Pd(1)-Cl(2)	94.677(19)
C(2)-N(1)-C(6)	119.44(16)
C(2)-N(1)-Pd(1)	125.96(13)

C(6)-N(1)-Pd(1)	113.31(12)
N(1)-C(2)-C(3)	121.52(18)
N(1)-C(2)-H(2)	119.2
C(3)-C(2)-H(2)	119.2
C(4)-C(3)-C(2)	119.20(19)
C(4)-C(3)-H(3)	120.4
C(2)-C(3)-H(3)	120.4
C(3)-C(4)-C(5)	119.52(18)
C(3)-C(4)-H(4)	120.2
C(5)-C(4)-H(4)	120.2
C(6)-C(5)-C(4)	118.56(19)
C(6)-C(5)-H(5)	120.7
C(4)-C(5)-H(5)	120.7
N(1)-C(6)-C(5)	121.73(17)
N(1)-C(6)-C(7)	115.55(15)
C(5)-C(6)-C(7)	122.71(17)
C(6)-C(7)-N(14)	107.33(13)
C(6)-C(7)-C(8)	113.83(16)
N(14)-C(7)-C(8)	108.31(14)
C(6)-C(7)-H(7)	109.1
N(14)-C(7)-H(7)	109.1
C(8)-C(7)-H(7)	109.1
C(9)-C(8)-C(13)	119.13(17)
C(9)-C(8)-C(7)	122.74(17)
C(13)-C(8)-C(7)	118.12(17)
C(10)-C(9)-C(8)	120.23(19)
C(10)-C(9)-H(9)	119.9
C(8)-C(9)-H(9)	119.9
C(11)-C(10)-C(9)	120.30(19)
C(11)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	120.04(18)
C(10)-C(11)-H(11)	120.0
C(12)-C(11)-H(11)	120.0
C(11)-C(12)-C(13)	119.81(19)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(12)-C(13)-C(8)	120.44(19)
C(12)-C(13)-H(13)	119.8
C(8)-C(13)-H(13)	119.8
C(7)-N(14)-C(15)	115.28(14)
C(7)-N(14)-Pd(1)	106.88(11)
C(15)-N(14)-Pd(1)	116.39(11)
C(7)-N(14)-H(14)	105.8
C(15)-N(14)-H(14)	105.8
Pd(1)-N(14)-H(14)	105.8
C(16)-C(15)-N(14)	110.34(14)
C(16)-C(15)-C(22)	115.01(16)
N(14)-C(15)-C(22)	109.25(15)
C(16)-C(15)-H(15)	107.3
N(14)-C(15)-H(15)	107.3
C(22)-C(15)-H(15)	107.3
C(21)-C(16)-C(17)	118.80(18)
C(21)-C(16)-C(15)	118.85(16)
C(17)-C(16)-C(15)	122.31(17)
C(18)-C(17)-C(16)	120.67(18)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(19)-C(18)-C(17)	120.15(18)
C(19)-C(18)-H(18)	119.9
C(17)-C(18)-H(18)	119.9

C(18)-C(19)-C(20)	119.45(19)
C(18)-C(19)-H(19)	120.3
C(20)-C(19)-H(19)	120.3
C(21)-C(20)-C(19)	120.48(19)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(20)-C(21)-C(16)	120.44(18)
C(20)-C(21)-H(21)	119.8
C(16)-C(21)-H(21)	119.8
C(15)-C(22)-H(22A)	109.5
C(15)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(15)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for data2.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd(1)	12(1)	10(1)	10(1)	0(1)	0(1)	0(1)
Cl(1)	18(1)	18(1)	15(1)	0(1)	5(1)	-2(1)
Cl(2)	21(1)	17(1)	13(1)	-1(1)	-3(1)	-3(1)
N(1)	13(1)	13(1)	13(1)	0(1)	0(1)	1(1)
C(2)	16(1)	12(1)	20(1)	-2(1)	-1(1)	-1(1)
C(3)	14(1)	17(1)	29(1)	-1(1)	3(1)	-1(1)
C(4)	17(1)	18(1)	23(1)	3(1)	7(1)	4(1)
C(5)	17(1)	16(1)	16(1)	0(1)	2(1)	5(1)
C(6)	13(1)	12(1)	13(1)	0(1)	-1(1)	3(1)
C(7)	12(1)	11(1)	12(1)	-2(1)	1(1)	1(1)
C(8)	19(1)	12(1)	12(1)	-2(1)	1(1)	1(1)
C(9)	16(1)	15(1)	21(1)	1(1)	-2(1)	1(1)
C(10)	21(1)	20(1)	25(1)	3(1)	-5(1)	4(1)
C(11)	27(1)	14(1)	21(1)	1(1)	0(1)	2(1)
C(12)	22(1)	14(1)	28(1)	-1(1)	-3(1)	-4(1)
C(13)	18(1)	16(1)	23(1)	0(1)	-6(1)	-1(1)
N(14)	11(1)	10(1)	13(1)	-1(1)	0(1)	0(1)
C(15)	11(1)	15(1)	14(1)	0(1)	0(1)	2(1)
C(16)	11(1)	14(1)	16(1)	3(1)	-2(1)	3(1)
C(17)	14(1)	15(1)	16(1)	1(1)	-1(1)	1(1)
C(18)	20(1)	24(1)	14(1)	3(1)	2(1)	5(1)
C(19)	17(1)	20(1)	22(1)	8(1)	2(1)	-2(1)
C(20)	19(1)	15(1)	26(1)	2(1)	-3(1)	-3(1)
C(21)	18(1)	14(1)	15(1)	0(1)	-1(1)	3(1)
C(22)	14(1)	21(1)	25(1)	3(1)	-4(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for data2.

	x	y	z	U(eq)
H(2)	5231	1718	9763	19
H(3)	6680	1883	8626	24
H(4)	6186	982	7346	23
H(5)	4280	-153	7250	20
H(7)	2074	-576	7857	14
H(9)	4407	-1552	9302	21
H(10)	4556	-3399	9828	26
H(11)	2768	-4626	9723	25
H(12)	834	-4028	9059	25
H(13)	726	-2218	8454	23
H(14)	842	-423	9191	14
H(15)	116	1453	8914	16
H(17)	1197	819	6823	18
H(18)	2596	1952	6013	23
H(19)	3613	3536	6620	24
H(20)	3240	3962	8049	24
H(21)	1853	2828	8863	19
H(22A)	-1089	829	7716	31
H(22B)	-1064	-118	8442	31
H(22C)	-132	-241	7631	31

Xray data for C14

Table 1. Crystal data and structure refinement for C14.

Empirical formula	C20 H20 Cl2 N2 O Pd
Formula weight	481.68
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 10.286(2) A alpha = 90 deg. b = 12.912(3) A beta = 90 deg. c = 14.411(3) A gamma = 90 deg.
Volume	1914.0(7) A^3
Z, Calculated density	4, 1.672 Mg/m^3
Absorption coefficient	1.260 mm^-1
F(000)	968
Crystal size	0.30 x 0.25 x 0.06 mm
Theta range for data collection	2.12 to 30.08 deg.
Limiting indices	-14<=h<=14, -18<=k<=18, -20<=l<=20
Reflections collected / unique	81447 / 5584 [R(int) = 0.0305]
Completeness to theta = 30.08	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9282 and 0.7036
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5584 / 0 / 236
Goodness-of-fit on F^2	1.412
Final R indices [I>2sigma(I)]	R1 = 0.0157, wR2 = 0.0476
R indices (all data)	R1 = 0.0187, wR2 = 0.0627
Absolute structure parameter	0.036(16)
Largest diff. peak and hole	0.818 and -1.155 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for data1.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd(1)	6485(1)	4279(1)	6374(1)	13(1)
Cl(1)	5145(1)	4565(1)	7628(1)	21(1)
Cl(2)	6620(1)	2536(1)	6685(1)	22(1)
N(1)	6524(1)	5781(1)	5986(1)	14(1)
N(2)	7640(1)	4113(1)	5230(1)	14(1)
C(3)	5740(2)	6538(1)	6301(1)	19(1)
C(4)	5816(2)	7534(1)	5961(1)	22(1)
C(5)	6689(2)	7756(1)	5249(1)	21(1)
C(6)	7481(2)	6970(1)	4911(1)	18(1)
C(7)	7391(2)	5990(1)	5308(1)	14(1)
C(8)	8317(2)	5132(1)	5067(1)	14(1)
C(9)	9565(2)	5192(1)	5639(1)	15(1)
C(10)	9755(2)	5932(1)	6329(1)	17(1)
C(11)	10936(2)	5988(2)	6805(1)	21(1)
C(12)	11922(2)	5291(2)	6603(1)	24(1)
C(13)	11741(2)	4545(2)	5920(1)	23(1)
C(14)	10571(2)	4498(1)	5435(1)	20(1)
C(15)	6916(2)	3681(1)	4397(1)	16(1)
C(16)	5956(2)	4454(1)	4003(1)	16(1)
C(17)	4660(2)	4411(2)	4294(1)	20(1)
C(18)	3762(2)	5147(2)	3989(1)	25(1)
C(19)	4164(2)	5937(2)	3389(1)	23(1)
C(20)	5441(2)	5969(1)	3082(1)	21(1)
C(21)	6325(2)	5224(1)	3377(1)	18(1)
C(22)	7898(2)	3275(1)	3683(1)	20(1)
O(23)	8754(1)	2592(1)	4163(1)	22(1)

Table 3. Bond lengths [A] and angles [deg] for data1.

Pd(1)-N(1)	2.0197(14)
Pd(1)-N(2)	2.0429(14)
Pd(1)-Cl(2)	2.2986(7)
Pd(1)-Cl(1)	2.3031(6)
N(1)-C(3)	1.346(2)
N(1)-C(7)	1.350(2)
N(2)-C(8)	1.507(2)
N(2)-C(15)	1.519(2)
N(2)-H(2)	0.9300
C(3)-C(4)	1.377(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.393(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.390(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.392(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.502(2)
C(8)-C(9)	1.527(2)
C(8)-H(8)	1.0000
C(9)-C(10)	1.393(2)
C(9)-C(14)	1.400(2)
C(10)-C(11)	1.397(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.387(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.390(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.393(3)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-C(16)	1.515(2)
C(15)-C(22)	1.534(2)
C(15)-H(15)	1.0000
C(16)-C(21)	1.394(2)
C(16)-C(17)	1.399(2)
C(17)-C(18)	1.397(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.399(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.386(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.391(3)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-O(23)	1.426(2)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
O(23)-H(23)	0.8400
N(1)-Pd(1)-N(2)	82.30(5)
N(1)-Pd(1)-Cl(2)	173.37(4)
N(2)-Pd(1)-Cl(2)	91.14(4)
N(1)-Pd(1)-Cl(1)	94.28(4)
N(2)-Pd(1)-Cl(1)	176.44(4)
Cl(2)-Pd(1)-Cl(1)	92.296(18)
C(3)-N(1)-C(7)	119.69(14)

C(3)-N(1)-Pd(1)	126.34(12)
C(7)-N(1)-Pd(1)	113.87(11)
C(8)-N(2)-C(15)	115.09(12)
C(8)-N(2)-Pd(1)	107.65(10)
C(15)-N(2)-Pd(1)	112.97(10)
C(8)-N(2)-H(2)	106.9
C(15)-N(2)-H(2)	106.9
Pd(1)-N(2)-H(2)	106.9
N(1)-C(3)-C(4)	121.59(17)
N(1)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2
C(3)-C(4)-C(5)	119.37(17)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3
C(6)-C(5)-C(4)	119.07(16)
C(6)-C(5)-H(5)	120.5
C(4)-C(5)-H(5)	120.5
C(5)-C(6)-C(7)	118.73(16)
C(5)-C(6)-H(6)	120.6
C(7)-C(6)-H(6)	120.6
N(1)-C(7)-C(6)	121.49(15)
N(1)-C(7)-C(8)	116.07(14)
C(6)-C(7)-C(8)	122.26(15)
C(7)-C(8)-N(2)	108.36(13)
C(7)-C(8)-C(9)	111.78(13)
N(2)-C(8)-C(9)	110.41(13)
C(7)-C(8)-H(8)	108.7
N(2)-C(8)-H(8)	108.7
C(9)-C(8)-H(8)	108.7
C(10)-C(9)-C(14)	119.00(16)
C(10)-C(9)-C(8)	122.54(15)
C(14)-C(9)-C(8)	118.42(15)
C(9)-C(10)-C(11)	120.57(16)
C(9)-C(10)-H(10)	119.7
C(11)-C(10)-H(10)	119.7
C(12)-C(11)-C(10)	119.92(18)
C(12)-C(11)-H(11)	120.0
C(10)-C(11)-H(11)	120.0
C(11)-C(12)-C(13)	120.02(17)
C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0
C(12)-C(13)-C(14)	120.07(17)
C(12)-C(13)-H(13)	120.0
C(14)-C(13)-H(13)	120.0
C(13)-C(14)-C(9)	120.41(17)
C(13)-C(14)-H(14)	119.8
C(9)-C(14)-H(14)	119.8
C(16)-C(15)-N(2)	112.00(13)
C(16)-C(15)-C(22)	113.71(14)
N(2)-C(15)-C(22)	109.42(14)
C(16)-C(15)-H(15)	107.1
N(2)-C(15)-H(15)	107.1
C(22)-C(15)-H(15)	107.1
C(21)-C(16)-C(17)	118.82(16)
C(21)-C(16)-C(15)	122.33(16)
C(17)-C(16)-C(15)	118.82(16)
C(18)-C(17)-C(16)	120.60(18)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(17)-C(18)-C(19)	119.64(19)
C(17)-C(18)-H(18)	120.2

C(19)-C(18)-H(18)	120.2
C(20)-C(19)-C(18)	119.97(18)
C(20)-C(19)-H(19)	120.0
C(18)-C(19)-H(19)	120.0
C(19)-C(20)-C(21)	120.05(17)
C(19)-C(20)-H(20)	120.0
C(21)-C(20)-H(20)	120.0
C(20)-C(21)-C(16)	120.84(17)
C(20)-C(21)-H(21)	119.6
C(16)-C(21)-H(21)	119.6
O(23)-C(22)-C(15)	106.99(15)
O(23)-C(22)-H(22A)	110.3
C(15)-C(22)-H(22A)	110.3
O(23)-C(22)-H(22B)	110.3
C(15)-C(22)-H(22B)	110.3
H(22A)-C(22)-H(22B)	108.6
C(22)-O(23)-H(23)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for data1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd(1)	11(1)	14(1)	13(1)	2(1)	0(1)	-1(1)
Cl(1)	17(1)	29(1)	17(1)	3(1)	3(1)	-2(1)
Cl(2)	21(1)	16(1)	28(1)	8(1)	-3(1)	-3(1)
N(1)	14(1)	14(1)	14(1)	1(1)	-1(1)	1(1)
N(2)	13(1)	12(1)	15(1)	0(1)	0(1)	0(1)
C(3)	16(1)	21(1)	18(1)	-3(1)	-1(1)	4(1)
C(4)	21(1)	18(1)	27(1)	-5(1)	-8(1)	6(1)
C(5)	23(1)	13(1)	26(1)	2(1)	-10(1)	0(1)
C(6)	19(1)	16(1)	19(1)	4(1)	-5(1)	-2(1)
C(7)	12(1)	13(1)	18(1)	1(1)	-1(1)	0(1)
C(8)	13(1)	13(1)	15(1)	2(1)	1(1)	-1(1)
C(9)	12(1)	16(1)	17(1)	4(1)	0(1)	-1(1)
C(10)	16(1)	17(1)	18(1)	2(1)	0(1)	-1(1)
C(11)	20(1)	23(1)	21(1)	4(1)	-4(1)	-3(1)
C(12)	15(1)	29(1)	28(1)	10(1)	-4(1)	-3(1)
C(13)	16(1)	23(1)	30(1)	8(1)	3(1)	3(1)
C(14)	16(1)	17(1)	25(1)	2(1)	3(1)	0(1)
C(15)	17(1)	13(1)	18(1)	0(1)	1(1)	-1(1)
C(16)	16(1)	17(1)	15(1)	-2(1)	0(1)	0(1)
C(17)	18(1)	24(1)	19(1)	0(1)	1(1)	2(1)
C(18)	22(1)	31(1)	22(1)	0(1)	4(1)	8(1)
C(19)	26(1)	23(1)	21(1)	-1(1)	-2(1)	7(1)
C(20)	28(1)	18(1)	17(1)	0(1)	-4(1)	0(1)
C(21)	19(1)	19(1)	15(1)	0(1)	-1(1)	-2(1)
C(22)	22(1)	18(1)	20(1)	-2(1)	3(1)	2(1)
O(23)	21(1)	18(1)	28(1)	0(1)	6(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for data1.

	x	y	z	U(eq)
H(2)	8280	3634	5383	16
H(3)	5120	6383	6769	22
H(4)	5278	8063	6210	26
H(5)	6741	8435	4998	25
H(6)	8073	7100	4418	21
H(8)	8546	5186	4394	16
H(10)	9075	6402	6477	21
H(11)	11063	6503	7267	25
H(12)	12722	5324	6931	29
H(13)	12416	4066	5783	28
H(14)	10455	3993	4963	23
H(15)	6402	3072	4620	19
H(17)	4389	3877	4704	24
H(18)	2882	5111	4187	30
H(19)	3563	6451	3193	28
H(20)	5712	6501	2669	25
H(21)	7192	5239	3149	21
H(22A)	7442	2902	3179	24
H(22B)	8391	3857	3408	24
H(23)	9421	2488	3840	34

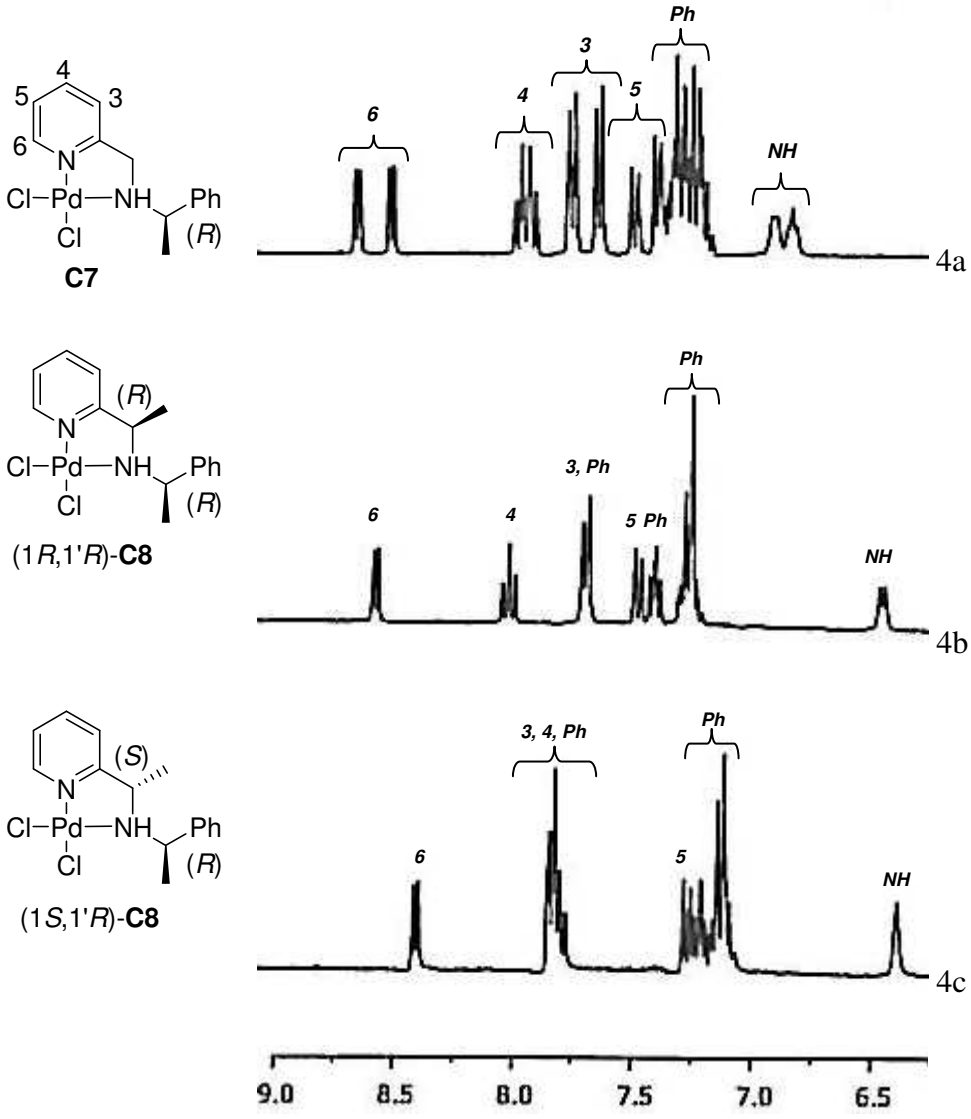
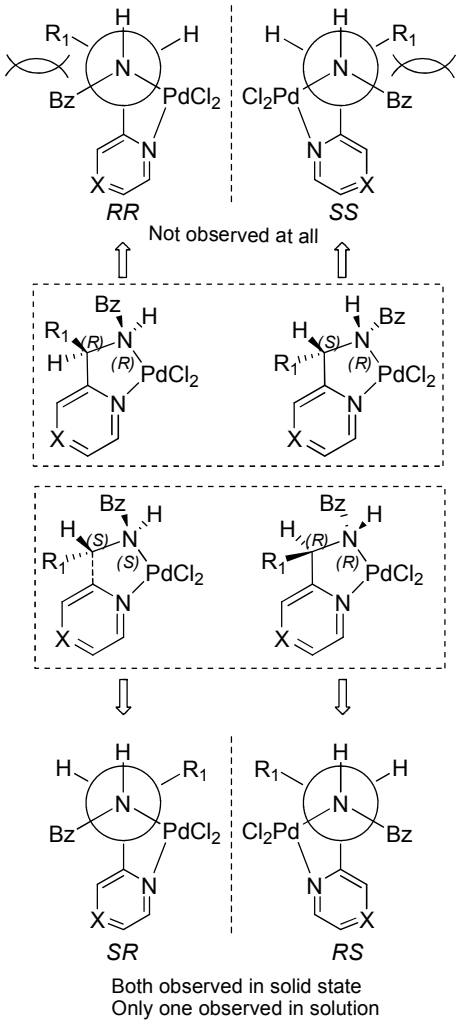
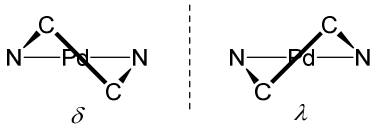


Figure 4. Set of characteristic ^{1}H NMR signals for **C7** (4a), (1*R*,1'*R*)-**C8** (4b) and (1*S*,1'*R*)-**C8** (4c).

Scheme 6. Possible configurations for the benzylic and nitrogen positions.
R_1 = Ph, Carboranyl; Bz = CH_2Ph



Scheme 7



δ λ

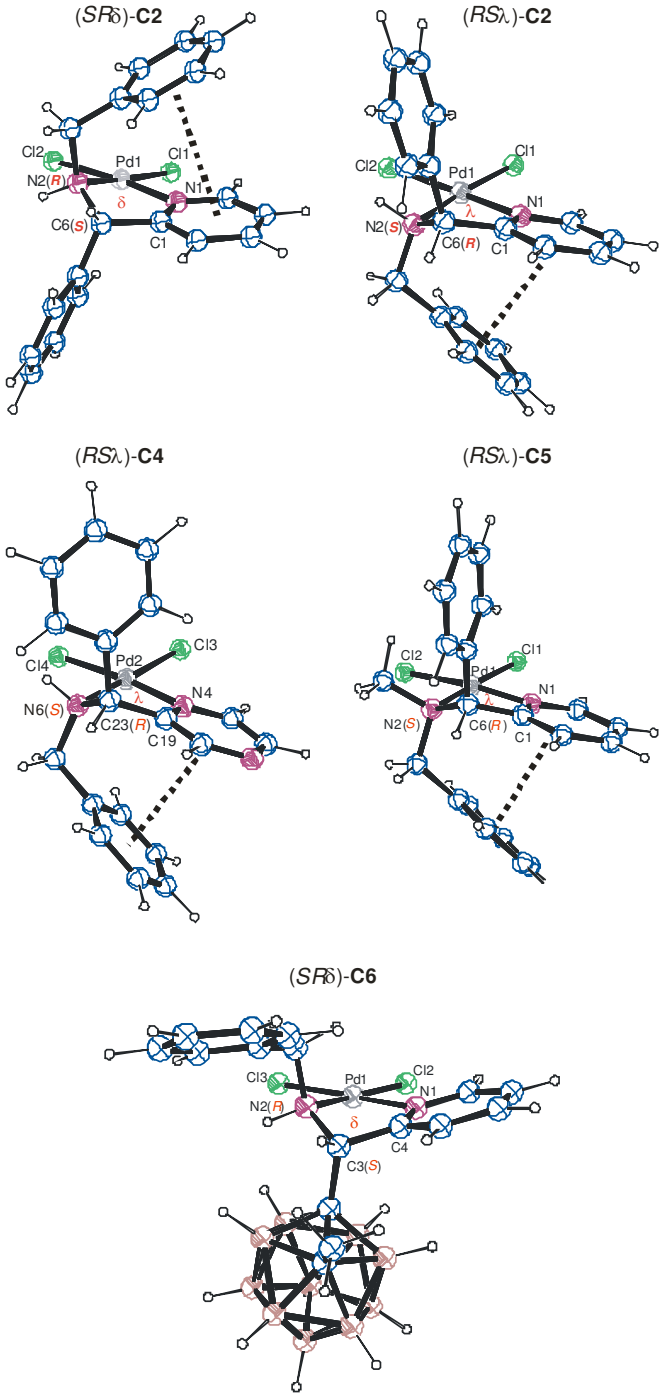


Figure S6. Molecular structures of **C2**, **C4**, **C5** and **C6** showing the intramolecular π–π interactions; thermal ellipsoids set at 50% probability. Both diasteromers are only shown for **C2** as example. Other isomers for **C4**-**C6** are also present in the crystal (see text).

Table 3. Crystallographic Parameters for compounds (1*S*, 1'*R*)-**C8**, (1*R*, 1'*R*)-**C9**, and (1*S*, 1'*R*)-**C14**

Compound	**C8**	**C9**	**C14**
Empirical formula	$C_{15}H_{18}Cl_2N_2Pd$	$C_{20}H_{20}Cl_2N_2Pd$	$C_{20}H_{20}Cl_2N_2OPd$
Formula weight	403.61	465.68	481.68
Temperature [K]	200	100	100
Wavelength [Å]	0.71073	0.71073	0.71073
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
a [Å]	9.5902(5)	10.1669(12)	10.286(2)
b [Å]	11.5116(6)	11.8011(13)	12.912 (3)
c [Å]	14.6184(7)	15.7914(18)	14.411(3)
Volume [Å^3]	1613.85(14)	1894.7(4)	1914.0(7)
Z	4	4	4
ρ_{calcd} [g cm^{-3}]	1.661	1.633	1.672
Absorption coefficient [mm^{-1}]	1.47	1.27	1.26
F(000)	808	936	968
Crystal	Block; orange	Block; Orange	Platelet; yellow
Crystal size [mm]	0.24 × 0.14 × 0.12	0.25 × 0.25 × 0.10	0.30 × 0.25 × 0.06
θ range for data collection [°]	2.5 – 29.9	2.9 – 29.9	2.4 – 30.1
Reflections collected	113820	20922	81447
Independent reflections	4698 [R_{int} = 0.032]	5413 [R_{int} = 0.036]	5584 [R_{int} = 0.031]
Max. and min. transmission	0.719 and 0.843	0.743 and 0.884	0.704 and 0.928
Data / restraints / parameters	4698 / 0 / 183	5413 / 0 / 227	5584 / 0 / 236
Goodness-of-fit on F^2	1.48	1.11	1.41
Final *R* indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.017, *wR2* = 0.073	*R1* = 0.021, *wR2* = 0.050	*R1* = 0.016, *wR2* = 0.063
Flack parameter	0.07(2)	0.01(2)	0.036(16)

CCDC 812300, 812301 and 812302 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.