Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Stereoselective annulation between an allene, an alkene, and two nitrosoarenes to access bis(isoxazoliodine) derivatives

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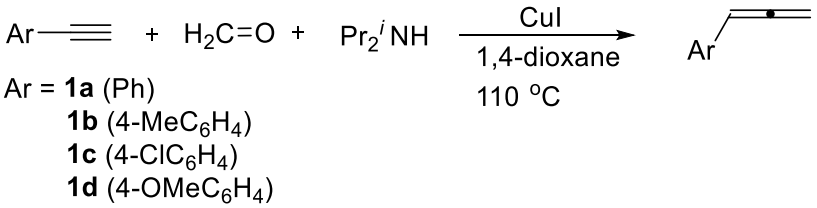
TABLE OF CONTENTS

[1] General Synthetic procedures

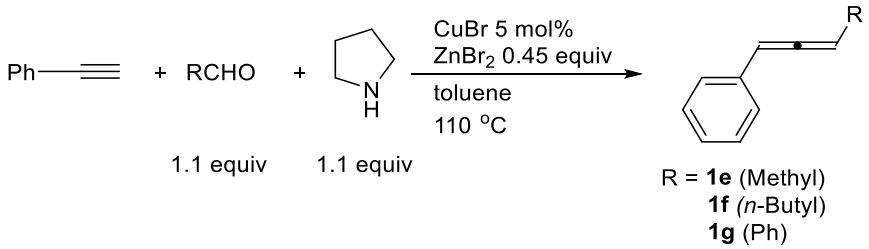
The nitrosobenzene was purchased from Sigma-Aldrich and other nitrosoarene were prepared according to literature procedure.[1]

1.1 General procedures for the synthesis of mono-substituted allenes:



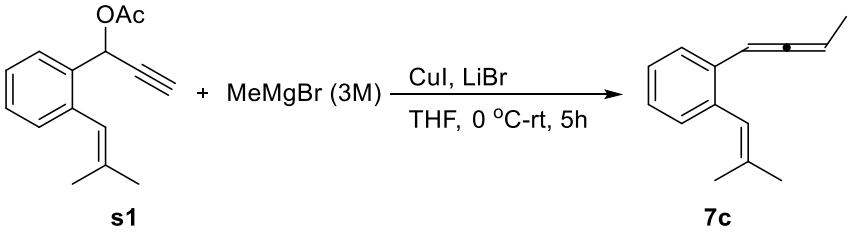
All mono-substituted allenes **1a-1d** were prepared according to above literature reported procedure.[2]

1.2 General procedure for the synthesis of 1,3-disubstituted allenes:



All 1,3-disubstituted allenes **1e-1g** were prepared according to above literature reported procedure.[2]

1.3 General procedure for the synthesis of 1-(buta-1,2-dien-1-yl)-2-(2-methylprop-1-en-1-yl)benzene (7c):

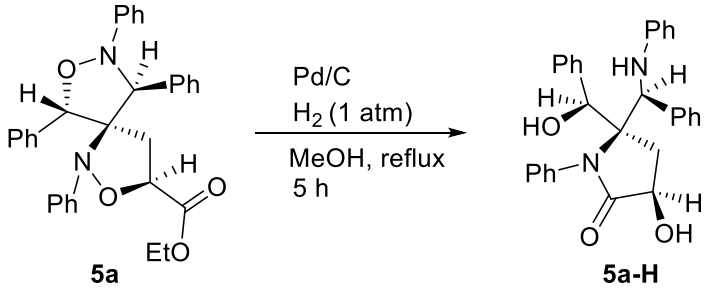


Compound **s1** was prepared according to literature procedure [3]

To a dry THF (30 mL) solution of CuI (1.16 g, 6.09 mmol) and LiBr (0.532 g, 6.13 mmol) was added MeMgCl 3M sol (2.0 mL, 6.09 mmol) at 0 ^{o}C and stirred for 1 h. Then added dry THF solution (5 mL) of compound 1-(2-(2-methylprop-1-en-1-yl)phenyl)prop-2-yn-1-yl acetate (**s1**) **(**1.0 g, 4.38 mmol) to the above reaction mixture at 0 ^{o}C and stirred for 4 h at room temperature. The reaction mixture was quenched with sat. Na_2SO_3 sol (20 mL) and extracted with ethylacetate (2 x 30 mL). The combined organic layer was dried over anhy. $MgSO_4$ and concentrated under reduced pressure. The crude reaction mixture was purified on a silica gel column using 1% ethyl acetate/hexane to yield 1-(buta-1,2-dien-1-yl)-2-(2-methylprop-1-en-1-yl)benzene **7c** (0.69 g, 3.71 mmol, 70 %) as colorless oil.

The substrates **7a, 7b, 7d,**[3] **7e, 7f, 7g** were prepared according to above procedure. The substrate **7a** was quickly pass through a silica gel column and used as such for next to avoid its further decomposition.

1.4 Synthesis of (*3R,5R*)-3-hydroxy-5-((*S*)-hydroxy(phenyl)methyl)-1-phenyl-5-((*S*)-phenyl(phenylamino)methyl)pyrrolidin-2-one (5a-H)

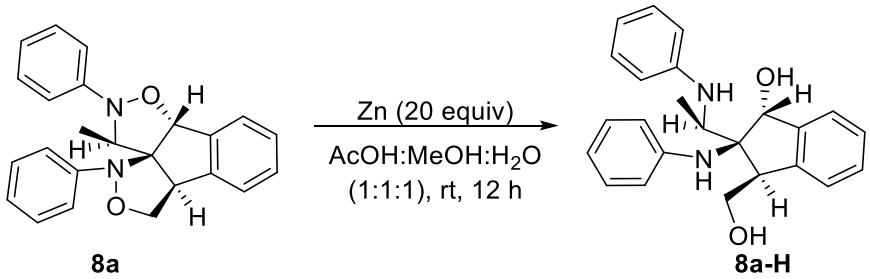


5a **5a-H**

To a methanol (15 mL) solution of 10% palladium on carbon (20.0 mg), was added ethyl (*3S,5R,6S,9S*)-1,6,8,9-tetraphenyl-2,7-dioxa-1,8-diazaspiro[4.4]nonane-3-carboxylate **5a** (100 mg, 0.259 mmol) and reaction mixture was refluxed under H_2 (1 atm) for 5 h. After complete consumption of starting material, the reaction mixture was filtered through celite, concentrated and residue was purified by flash silica gel column chromatography using 20% ethyl acetate/hexane as eluents to give (*3R,5R*)-3-hydroxy-5-((*S*)-hydroxy(phenyl)methyl)-1-phenyl-5-((*S*)-phenyl(phenylamino)methyl)pyrrolidin -2-one **5a-H** (91.9 mg, 0.235 mmol, 86%) as off white solid.

Synthesis of compound **5i-H** followed the same procedure as **5a-H**.

1.5 Typical procedure for (*1R,2S,3R*)-3-(hydroxymethyl)-2-(phenylamino)-2-((*R*)-1-(phenylamino)ethyl)-2,3-dihydro-*1H*-inden-1-ol (8a-H)



To a MeOH/H_2O (3 mL, 1:1) solution of (*3R,3aS,6aR,10bR*)-3-methyl-2,4-diphenyl-2,3,6a,10b-tetrahydro-*4H,6H*-indeno[2,1-*c*:2,3-*d'*]diisoxazole **8a** (0.1 g, 0.27 mmol) was added acetic acid (2 mL). To this reaction mixture was added Zn dust (0.352g, 5.38 mmol) portion wise and allowed to stir for 12 h at room temperature. After completion of reaction, saturated aqueous solution of $NaHCO_3$ was added carefully, filtered through celite, extracted with ethyl acetate, dried over $MgSO_4$, concentrated, eluted through silica gel column using ethyl acetate/hexane as eluents to afford **8a-H** (37.8 mg, 0.084 mmol, 83.0%) as white solid.

[2] References

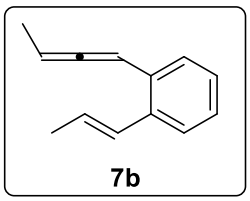
(1) D. Zhao, M. Johansson, J. -E. Bäckvall, *Eur. J. Org. Chem.* 2007, 4431–4436.

(2) J. Liu, M. Skaria, P. Sharma, Y. –W. Chiang, R. -S. Liu, *Chem. Sci.* 2017, **8**, 5482-5487.

(3) R. Chaudhuri, H. –Y. Liao, R. -S Liu, *Chem. Eur. J.* 2009, **15**, 8895 – 8901.

[3] Spectral Data of key Compounds

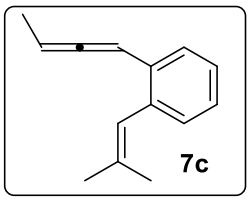
Spectral Data of (*E*)-1-(buta-1,2-dien-1-yl)-2-(prop-1-en-1-yl)benzene (7b)



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41-7.38 (m, 2H), 7.23-7.15 (m, 2H), 6.75 (d, *J* =16 Hz, 1H), 6.42-6.40 (m, 1H), 6.15-6.06 (m, 1H), 5.56-5.49 (m, 1H), 1.93 (dd, *J* =6.6, 1.7 Hz, 3H), 1.82 (dd,

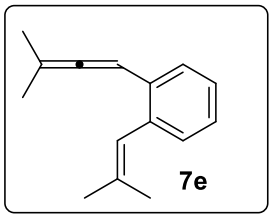
J =7.1, 3.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 206.9, 135.9, 131.7, 128.7, 128.0, 127.6, 126.8, 126.7, 126.6, 91.2, 88.5, 18.8, 14.1.

Spectral Data of 1-(buta-1,2-dien-1-yl)-2-(2-methylprop-1-en-1-yl)benzene (7c)



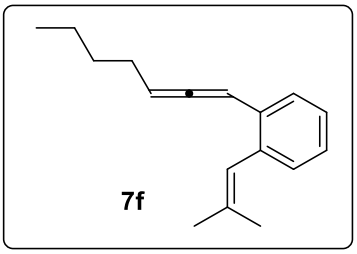
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.42 (d, *J* =1.2 Hz, 1H), 7.24-7.09 (m, 3H), 6.30 (s, 1H), 6.27-6.25 (m, 1H), 5.48 (q, *J* =7.0 Hz, 1H), 1.91 (d, *J* =1.8 Hz, 3H), 1.78 (dd, *J* =7.2, 3.6 Hz, 3H), 1.60 (d, *J* =1.2 Hz, 3H), ^{13}C NMR (150 MHz, $CDCl_3$): 206.5, 136.5, 136.1, 133.0, 130.0, 126.8, 126.4, 126.1, 12.5, 91.8, 88.7, 25.9, 19.3, 14.2.

Spectral Data of 1-(3-methylbuta-1,2-dien-1-yl)-2-(2-methylprop-1-en-1-yl)benzene (7e)



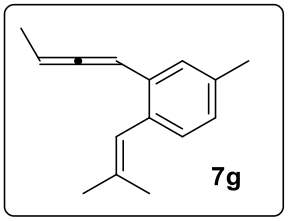
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.38 (dd, *J* =7.8, 1.4 Hz, 1H), 7.24-7.10 (m, 3H), 6.32 (s, 1H), 6.17 (t, *J* =2.9 Hz, 1H), 1.93 (d, *J* =1.5 Hz, 3H), 1.83-1.82 (m, 6H), 1.70 (d, *J* =1.3 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$); δ 203.7, 136.4, 135.7, 133.8, 130.0, 127.0, 126.4, 125.8, 123.7, 98.0, 90.5, 26.0, 20.4, 19.3 one carbon merged; EI^+-MS calcd for $C_{15}H_{18}$[M+]: 198.1409 found: 198.1408.

Spectral Data of 1-(hepta-1,2-dien-1-yl)-2-(2-methylprop-1-en-1-yl)benzene (7f)



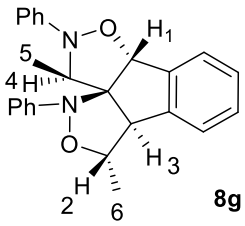
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.42 (dd, *J* =7.7, 1.1 Hz, 1H), 7.16 (d, *J* =1.6 Hz, 1H), 7.12-7.09 (m, 2H), 6.28 (m, 2H), 5.50-5.46 (m, 1H), 2.13-2.11 (m, 2H), 1.90 (d, *J* =1.3 Hz, 3H), 1.66 (d, *J* =1.1 Hz, 3H), 1.45 (t, *J* =6.2 Hz, 2H), 1.40-1.37 (m, 2H), 0.91 (t, *J* =7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$); 205.6, 136.4, 136.2, 133.1, 130.0, 126.7, 126.4, 126.0, 123.6, 94.2, 92.3, 31.4, 28.5, 25.9, 22.3, 19.3, 13.9; EI^{+}-MS calcd for $C_{17}H_{22}$[M+]: 226.1722 found: 226.1720

Spectral Data of 2-(buta-1,2-dien-1-yl)-4-methyl-1-(2-methylprop-1-en-1-yl)benzene (7g)



^{1}H NMR (600 MHz, $CDCl_3$): 7.22 (s, 1H), 6.99 (d, *J* = 2.6 Hz, 1H), 6.95 (d, J = 6.0 Hz, 1H), 6.26 (s, 1H), 6.25 ~ 6.22 (m, 1H), 5.51-5.46 (m, 1H), 2.32 (s, 3H), 1.90 (d, *J* = 1.4 Hz, 3H), 1.78 (dd, *J* = 7.1, 3.3 Hz, 3H), 1.66 (d, J = 1.2 Hz, 3H), ^{13}C NMR (150 MHz, $CDCl_3$): 206.3, 135.9, 135.8, 133.7, 132.7, 129.9, 127.3, 127.1, 123.4, 91.8, 88.6, 25.9, 21.1, 19.3, 14.2; EI^{+}-MS calcd for $C_{15}H_{18}$[M+]: 198.1409 found: 198.1406.

NOE Data of Compound 8g

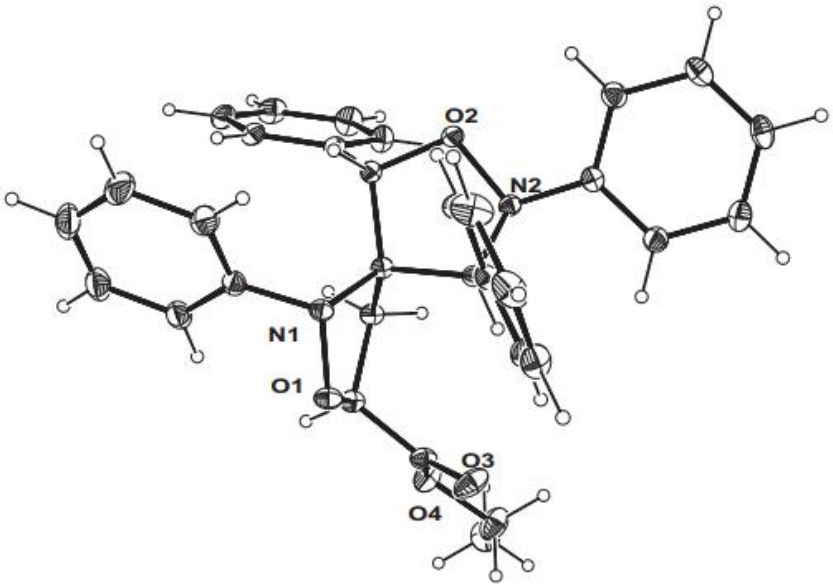


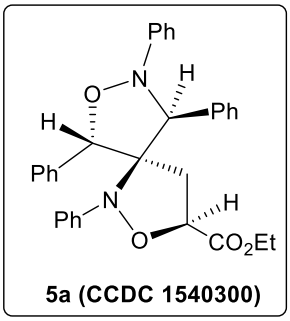
8g

Irradiation	Enhancement(%)
H^2 (δ 3.93-3.91)	H^1(δ 5.81, 1.27%), H^5 (δ 1.59, 4.83%)
H^3 (δ 3.81)	H^1(δ 5.81, 0.58%), H^4 (δ 3.32, 8.81%), H^5 (δ 1.59, 4.04%), H^6 (δ 1.40, 1.12%)
H^4 (δ 3.32)	H^3 (δ 3.81, 10.70%), H^6 (δ 1.40,4.78%)
H^5 (δ 1.59)	H^2 (δ 3.93-3.91, 3.35%, H^3 (δ 3.81, 2.55%)
H^6 (δ 1.40)	H^3 (δ 3.81, 0.91%), H^4 (δ 3.32, 3.32%)

[4] Crystallographic data

4.1 Crystallographic data for compound 5a:





5a (CCDC 1540300)

Table 1. Crystal data and structure refinement for d18485b.

Identification code	d18485b
Empirical formula	C32 H30 N2 O4
Formula weight	506.58
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 9.2140(3) Å □= 100.1170(10)°.
	b = 10.2240(3) Å □= 95.0210(10)°.

c = 14.5971(5) Å □ = 94.0310(10)°.

Volume 1343.37(7) Å3

Z 2

Density (calculated) 1.252 Mg/m3

Absorption coefficient 0.083 mm-1

F(000) 536

Crystal size 0.58 x 0.53 x 0.24 mm3

Theta range for data collection 2.23 to 25.04°.

Index ranges -10<=h<=10, -12<=k<=12, -17<=l<=17

Reflections collected 34042

Independent reflections 4699 [R(int) = 0.0362]

Completeness to theta = 25.04° 99.2 %

Absorption correction multi-scan

Max. and min. transmission 0.9804 and 0.9536

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 4699 / 0 / 344

Goodness-of-fit on F2 1.001

Final R indices [I>2sigma(I)] R1 = 0.0385, wR2 = 0.0898

R indices (all data) R1 = 0.0487, wR2 = 0.0980

Largest diff. peak and hole 0.221 and -0.183 e.Å-3

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103)

for d18485b. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	10205(2)	2569(2)	2587(1)	37(1)
C(2)	9946(2)	1240(2)	2664(1)	48(1)
C(3)	10966(3)	646(2)	3171(1)	66(1)
C(4)	12233(3)	1351(3)	3600(2)	74(1)
C(5)	12522(2)	2655(3)	3501(1)	69(1)
C(6)	11520(2)	3270(2)	2984(1)	50(1)
C(7)	8049(1)	3907(1)	2614(1)	28(1)
C(8)	8574(2)	4626(1)	3637(1)	29(1)
C(9)	8088(2)	3911(1)	4397(1)	30(1)
C(10)	8991(2)	3064(2)	4764(1)	37(1)
C(11)	8517(2)	2349(2)	5422(1)	46(1)
C(12)	7155(2)	2488(2)	5725(1)	51(1)
C(13)	6264(2)	3342(2)	5374(1)	52(1)
C(14)	6722(2)	4053(2)	4710(1)	42(1)
C(15)	6440(2)	7107(1)	2909(1)	30(1)

C(16)	6835(2)	8194(2)	3621(1)	41(1)
C(17)	6275(2)	9408(2)	3561(1)	49(1)
C(18)	5339(2)	9549(2)	2804(1)	45(1)
C(19)	4962(2)	8471(2)	2093(1)	43(1)
C(20)	5502(2)	7256(2)	2140(1)	39(1)
C(21)	7484(2)	5060(1)	2155(1)	28(1)
C(22)	8596(2)	5816(1)	1700(1)	31(1)
C(23)	9859(2)	6504(2)	2187(1)	49(1)
C(24)	10875(2)	7138(2)	1728(1)	59(1)
C(25)	10639(2)	7092(2)	779(1)	53(1)
C(26)	9394(2)	6423(2)	291(1)	50(1)
C(27)	8369(2)	5786(2)	747(1)	40(1)
C(28)	6853(2)	2764(1)	2533(1)	31(1)
C(29)	6995(2)	1941(1)	1570(1)	34(1)
C(30)	5806(2)	2130(1)	833(1)	37(1)
C(31)	3308(2)	1549(2)	317(2)	62(1)
C(32)	2095(2)	641(2)	510(2)	62(1)
N(1)	9208(1)	3287(1)	2091(1)	31(1)
N(2)	6868(1)	5817(1)	2967(1)	29(1)
O(1)	8390(1)	2380(1)	1311(1)	37(1)
O(2)	8038(1)	5924(1)	3727(1)	32(1)

O(3)	5905(1)	2840(1)	268(1)	57(1)
O(4)	4601(1)	1387(1)	916(1)	48(1)

Table 3. Bond lengths [Å] and angles [°] for d18485b.

C(1)-C(6)	1.388(2)
C(1)-C(2)	1.389(2)
C(1)-N(1)	1.4391(19)
C(2)-C(3)	1.384(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.367(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.376(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.394(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-N(1)	1.4814(17)
C(7)-C(28)	1.5305(18)
C(7)-C(21)	1.5531(19)
C(7)-C(8)	1.5622(18)

C(8)-O(2)	1.4369(16)
C(8)-C(9)	1.5133(19)
C(8)-H(8)	1.0000
C(9)-C(10)	1.384(2)
C(9)-C(14)	1.385(2)
C(10)-C(11)	1.386(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.375(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.374(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.386(2)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-C(16)	1.385(2)
C(15)-C(20)	1.392(2)
C(15)-N(2)	1.4170(18)
C(16)-C(17)	1.391(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.376(2)
C(17)-H(17)	0.9500

C(18)-C(19) 1.376(2)

C(18)-H(18) 0.9500

C(19)-C(20) 1.381(2)

C(19)-H(19) 0.9500

C(20)-H(20) 0.9500

C(21)-N(2) 1.4779(17)

C(21)-C(22) 1.5093(19)

C(21)-H(21) 1.0000

C(22)-C(27) 1.383(2)

C(22)-C(23) 1.385(2)

C(23)-C(24) 1.387(2)

C(23)-H(23) 0.9500

C(24)-C(25) 1.375(3)

C(24)-H(24) 0.9500

C(25)-C(26) 1.366(3)

C(25)-H(25) 0.9500

C(26)-C(27) 1.390(2)

C(26)-H(26) 0.9500

C(27)-H(27) 0.9500

C(28)-C(29) 1.5278(19)

C(28)-H(28A) 0.9900

C(28)-H(28B) 0.9900

C(29)-O(1) 1.4360(17)

C(29)-C(30) 1.514(2)

C(29)-H(29) 1.0000

C(30)-O(3) 1.1950(18)

C(30)-O(4) 1.3271(18)

C(31)-O(4) 1.452(2)

C(31)-C(32) 1.480(3)

C(31)-H(31A) 0.9900

C(31)-H(31B) 0.9900

C(32)-H(32A) 0.9800

C(32)-H(32B) 0.9800

C(32)-H(32C) 0.9800

N(1)-O(1) 1.4502(15)

N(2)-O(2) 1.4613(14)

C(6)-C(1)-C(2) 119.31(15)

C(6)-C(1)-N(1) 116.25(14)

C(2)-C(1)-N(1) 124.42(15)

C(3)-C(2)-C(1) 119.95(19)

C(3)-C(2)-H(2) 120.0

C(1)-C(2)-H(2) 120.0

C(4)-C(3)-C(2)	120.9(2)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
C(3)-C(4)-C(5)	119.62(19)
C(3)-C(4)-H(4)	120.2
C(5)-C(4)-H(4)	120.2
C(4)-C(5)-C(6)	120.5(2)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(5)-C(6)-C(1)	119.62(19)
C(5)-C(6)-H(6)	120.2
C(1)-C(6)-H(6)	120.2
N(1)-C(7)-C(28)	103.77(11)
N(1)-C(7)-C(21)	110.14(10)
C(28)-C(7)-C(21)	111.18(11)
N(1)-C(7)-C(8)	114.68(11)
C(28)-C(7)-C(8)	114.71(11)
C(21)-C(7)-C(8)	102.53(10)
O(2)-C(8)-C(9)	110.90(11)
O(2)-C(8)-C(7)	105.68(10)
C(9)-C(8)-C(7)	115.31(11)

O(2)-C(8)-H(8)	108.2
C(9)-C(8)-H(8)	108.2
C(7)-C(8)-H(8)	108.2
C(10)-C(9)-C(14)	119.03(13)
C(10)-C(9)-C(8)	120.07(13)
C(14)-C(9)-C(8)	120.85(13)
C(9)-C(10)-C(11)	120.27(15)
C(9)-C(10)-H(10)	119.9
C(11)-C(10)-H(10)	119.9
C(12)-C(11)-C(10)	120.40(15)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	119.59(15)
C(11)-C(12)-H(12)	120.2
C(13)-C(12)-H(12)	120.2
C(12)-C(13)-C(14)	120.45(16)
C(12)-C(13)-H(13)	119.8
C(14)-C(13)-H(13)	119.8
C(13)-C(14)-C(9)	120.24(15)
C(13)-C(14)-H(14)	119.9
C(9)-C(14)-H(14)	119.9

C(16)-C(15)-C(20)	119.24(14)
C(16)-C(15)-N(2)	122.18(13)
C(20)-C(15)-N(2)	118.40(13)
C(15)-C(16)-C(17)	119.54(15)
C(15)-C(16)-H(16)	120.2
C(17)-C(16)-H(16)	120.2
C(18)-C(17)-C(16)	121.03(16)
C(18)-C(17)-H(17)	119.5
C(16)-C(17)-H(17)	119.5
C(17)-C(18)-C(19)	119.27(15)
C(17)-C(18)-H(18)	120.4
C(19)-C(18)-H(18)	120.4
C(18)-C(19)-C(20)	120.58(15)
C(18)-C(19)-H(19)	119.7
C(20)-C(19)-H(19)	119.7
C(19)-C(20)-C(15)	120.32(15)
C(19)-C(20)-H(20)	119.8
C(15)-C(20)-H(20)	119.8
N(2)-C(21)-C(22)	116.80(11)
N(2)-C(21)-C(7)	98.90(10)
C(22)-C(21)-C(7)	115.89(11)

N(2)-C(21)-H(21)	108.2
C(22)-C(21)-H(21)	108.2
C(7)-C(21)-H(21)	108.2
C(27)-C(22)-C(23)	118.42(14)
C(27)-C(22)-C(21)	118.55(13)
C(23)-C(22)-C(21)	123.00(13)
C(24)-C(23)-C(22)	120.65(16)
C(24)-C(23)-H(23)	119.7
C(22)-C(23)-H(23)	119.7
C(25)-C(24)-C(23)	120.25(17)
C(25)-C(24)-H(24)	119.9
C(23)-C(24)-H(24)	119.9
C(26)-C(25)-C(24)	119.67(15)
C(26)-C(25)-H(25)	120.2
C(24)-C(25)-H(25)	120.2
C(25)-C(26)-C(27)	120.44(16)
C(25)-C(26)-H(26)	119.8
C(27)-C(26)-H(26)	119.8
C(22)-C(27)-C(26)	120.57(16)
C(22)-C(27)-H(27)	119.7
C(26)-C(27)-H(27)	119.7

C(29)-C(28)-C(7) 102.63(11)

C(29)-C(28)-H(28A) 111.2

C(7)-C(28)-H(28A) 111.2

C(29)-C(28)-H(28B) 111.2

C(7)-C(28)-H(28B) 111.2

H(28A)-C(28)-H(28B) 109.2

O(1)-C(29)-C(30) 109.19(11)

O(1)-C(29)-C(28) 106.15(11)

C(30)-C(29)-C(28) 113.07(12)

O(1)-C(29)-H(29) 109.4

C(30)-C(29)-H(29) 109.4

C(28)-C(29)-H(29) 109.4

O(3)-C(30)-O(4) 124.43(14)

O(3)-C(30)-C(29) 126.56(14)

O(4)-C(30)-C(29) 109.00(12)

O(4)-C(31)-C(32) 107.95(15)

O(4)-C(31)-H(31A) 110.1

C(32)-C(31)-H(31A) 110.1

O(4)-C(31)-H(31B) 110.1

C(32)-C(31)-H(31B) 110.1

H(31A)-C(31)-H(31B) 108.4

C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(1)-N(1)-O(1)	109.70(11)
C(1)-N(1)-C(7)	116.91(11)
O(1)-N(1)-C(7)	103.27(10)
C(15)-N(2)-O(2)	109.20(10)
C(15)-N(2)-C(21)	118.27(11)
O(2)-N(2)-C(21)	103.48(9)
C(29)-O(1)-N(1)	110.14(9)
C(8)-O(2)-N(2)	105.58(9)
C(30)-O(4)-C(31)	116.14(13)

Symmetry transformations used to generate equivalent atoms: Table 4. Anisotropic displacement parameters (Å2x 103)for d18485b. The anisotropic

displacement factor exponent takes the form: -2□2[h2a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12

C(1)	38(1)	44(1)	30(1)	6(1)	10(1)	14(1)
C(2)	62(1)	45(1)	42(1)	11(1)	10(1)	17(1)
C(3)	90(2)	63(1)	53(1)	19(1)	12(1)	40(1)
C(4)	79(2)	99(2)	53(1)	17(1)	11(1)	58(1)
C(5)	41(1)	105(2)	59(1)	1(1)	0(1)	27(1)
C(6)	36(1)	63(1)	50(1)	4(1)	8(1)	11(1)
C(7)	28(1)	29(1)	26(1)	7(1)	5(1)	0(1)
C(8)	29(1)	28(1)	28(1)	7(1)	4(1)	2(1)
C(9)	36(1)	31(1)	23(1)	5(1)	1(1)	0(1)
C(10)	41(1)	41(1)	29(1)	8(1)	-1(1)	5(1)
C(11)	64(1)	44(1)	33(1)	15(1)	-4(1)	6(1)
C(12)	70(1)	52(1)	33(1)	19(1)	8(1)	-6(1)
C(13)	53(1)	65(1)	44(1)	21(1)	20(1)	5(1)
C(14)	42(1)	49(1)	39(1)	18(1)	11(1)	9(1)
C(15)	31(1)	30(1)	33(1)	11(1)	12(1)	2(1)
C(16)	46(1)	35(1)	41(1)	8(1)	5(1)	2(1)
C(17)	58(1)	31(1)	58(1)	5(1)	11(1)	3(1)
C(18)	45(1)	36(1)	63(1)	22(1)	21(1)	10(1)
C(19)	40(1)	49(1)	48(1)	21(1)	11(1)	11(1)
C(20)	41(1)	40(1)	38(1)	8(1)	5(1)	6(1)

C(21)	31(1)	29(1)	25(1)	5(1)	4(1)	0(1)
C(22)	37(1)	28(1)	31(1)	9(1)	10(1)	4(1)
C(23)	54(1)	54(1)	37(1)	7(1)	11(1)	-18(1)
C(24)	61(1)	54(1)	59(1)	5(1)	22(1)	-22(1)
C(25)	67(1)	39(1)	60(1)	18(1)	35(1)	0(1)
C(26)	67(1)	53(1)	42(1)	25(1)	23(1)	14(1)
C(27)	45(1)	43(1)	35(1)	16(1)	9(1)	9(1)
C(28)	35(1)	31(1)	28(1)	7(1)	5(1)	-3(1)
C(29)	40(1)	30(1)	30(1)	6(1)	5(1)	-4(1)
C(30)	45(1)	32(1)	31(1)	5(1)	3(1)	-7(1)
C(31)	48(1)	65(1)	72(1)	29(1)	-16(1)	-11(1)
C(32)	46(1)	60(1)	79(1)	14(1)	4(1)	-6(1)
N(1)	33(1)	32(1)	27(1)	4(1)	6(1)	1(1)
N(2)	31(1)	31(1)	26(1)	6(1)	3(1)	2(1)
O(1)	41(1)	40(1)	27(1)	2(1)	7(1)	-2(1)
O(2)	40(1)	30(1)	26(1)	5(1)	-1(1)	3(1)
O(3)	61(1)	66(1)	44(1)	28(1)	-11(1)	-21(1)
O(4)	42(1)	50(1)	53(1)	23(1)	-3(1)	-9(1)

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 103) for d18485b.

	x	y	z	U(eq)
H(2)	9070	740	2370	58
H(3)	10784	-264	3220	79
H(4)	12911	942	3963	89
H(5)	13411	3141	3788	83
H(6)	11735	4163	2904	60
H(8)	9667	4742	3706	34
H(10)	9939	2973	4565	44
H(11)	9137	1759	5664	55
H(12)	6834	1995	6176	61
H(13)	5326	3447	5587	62
H(14)	6096	4639	4468	50
H(16)	7483	8111	4146	49
H(17)	6542	10152	4051	59
H(18)	4958	10381	2772	54
H(19)	4325	8564	1565	52
H(20)	5231	6518	1646	47
H(21)	6657	4679	1670	34

H(23)	10031	6541	2843	59
H(24)	11737	7607	2070	71
H(25)	11338	7522	465	63
H(26)	9228	6392	-364	60
H(27)	7506	5327	401	48
H(28A)		7029	2235	3033	38
H(28B)		5874	3102	2564	38
H(29)	6977	975	1615	40
H(31A)		3491	1327	-348	74
H(31B)		3055	2484	449	74
H(32A)		1206	734	114	93
H(32B)		1922	870	1170	93
H(32C)		2353	-282	373	93

4.2 Crystallographic data for compound 5c':

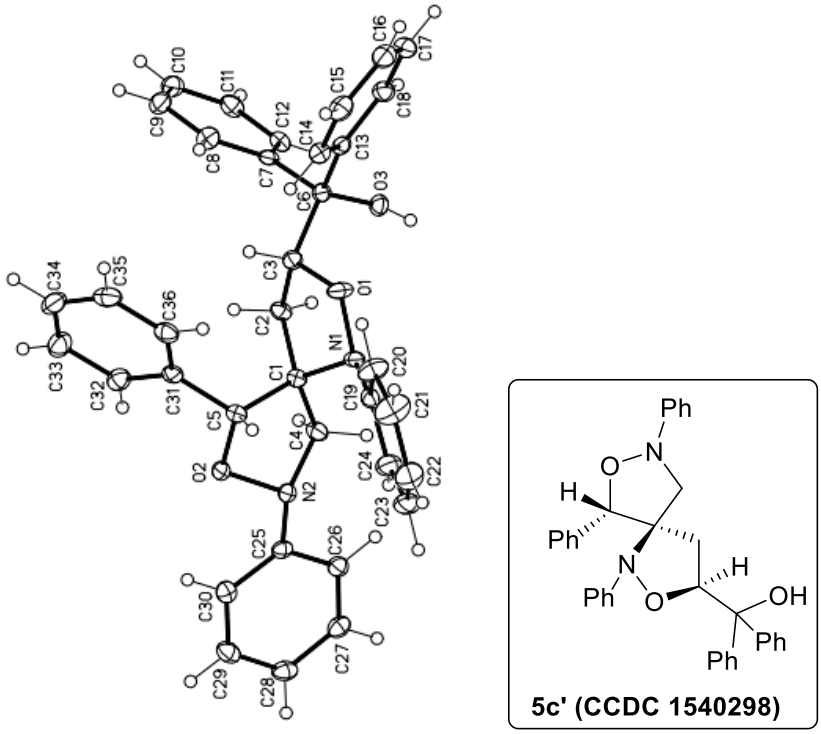


Table 1. Crystal data and structure refinement for mo_170254lt_0m_a.

Identification code mo_170254LT_0m_a

Empirical formula C36 H32 N2 O3

Formula weight 540.63

Temperature 99(2) K

Wavelength 0.71073 Å

Crystal system Triclinic

Space group P -1

Unit cell dimensions a = 9.6369(10) Å a= 86.914(3)°.

b = 12.1697(13) Å b= 73.831(3)°.

c = 12.3161(12) Å g = 85.494(3)°.

Volume 1382.2(2) Å3

Z 2

Density (calculated) 1.299 Mg/m3

Absorption coefficient 0.083 mm-1

F(000) 572

Crystal size 0.30 x 0.25 x 0.22 mm3

Theta range for data collection 1.679 to 26.478°.

Index ranges -12<=h<=12, -15<=k<=15, -15<=l<=15

Reflections collected 21891

Independent reflections 5689 [R(int) = 0.0312]

Completeness to theta = 25.242° 99.8 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.9485 and 0.9031

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 5689 / 0 / 371

Goodness-of-fit on F2 1.038

Final R indices [I>2sigma(I)] R1 = 0.0371, wR2 = 0.0856

R indices (all data) R1 = 0.0479, wR2 = 0.0916

Extinction coefficient n/a

Largest diff. peak and hole 0.300 and -0.233 e.Å-3

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103)

for mo_170254lt_0m_a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	7191(1)	5646(1)	3322(1)	15(1)
C(2)	7311(1)	6880(1)	3376(1)	16(1)
C(3)	6458(1)	7392(1)	2593(1)	15(1)
C(4)	7406(1)	5024(1)	4386(1)	17(1)
C(5)	8375(1)	5037(1)	2354(1)	15(1)
C(6)	5640(1)	8500(1)	2978(1)	14(1)
C(7)	6744(1)	9355(1)	2903(1)	14(1)
C(8)	7661(1)	9633(1)	1851(1)	19(1)
C(9)	8621(1)	10446(1)	1736(1)	21(1)
C(10)	8678(1)	10997(1)	2678(1)	21(1)
C(11)	7790(1)	10714(1)	3730(1)	20(1)
C(12)	6824(1)	9895(1)	3845(1)	17(1)
C(13)	4625(1)	8924(1)	2262(1)	15(1)
C(14)	4705(1)	8539(1)	1202(1)	18(1)
C(15)	3732(1)	8959(1)	613(1)	23(1)

C(16)	2665(1)	9763(1)	1079(1)	24(1)
C(17)	2592(1)	10166(1)	2124(1)	23(1)
C(18)	3568(1)	9758(1)	2704(1)	19(1)
C(19)	5233(1)	4711(1)	2764(1)	17(1)
C(20)	4634(2)	4839(1)	1860(1)	27(1)
C(21)	4152(2)	3932(1)	1468(1)	37(1)
C(22)	4251(2)	2899(1)	1962(1)	33(1)
C(23)	4835(2)	2772(1)	2868(1)	32(1)
C(24)	5306(2)	3665(1)	3282(1)	26(1)
C(25)	8874(1)	3322(1)	4636(1)	15(1)
C(26)	8101(1)	3133(1)	5766(1)	17(1)
C(27)	8639(1)	2355(1)	6430(1)	19(1)
C(28)	9949(1)	1759(1)	5990(1)	21(1)
C(29)	10740(1)	1984(1)	4886(1)	21(1)
C(30)	10222(1)	2762(1)	4204(1)	18(1)
C(31)	9356(1)	5732(1)	1464(1)	17(1)
C(32)	10722(1)	5960(1)	1531(1)	21(1)
C(33)	11619(2)	6566(1)	666(1)	27(1)
C(34)	11165(2)	6959(1)	-258(1)	28(1)
C(35)	9800(2)	6745(1)	-324(1)	26(1)
C(36)	8905(1)	6126(1)	526(1)	20(1)

N(1)	5673(1)	5622(1)	3240(1)	16(1)
N(2)	8198(1)	3996(1)	3944(1)	16(1)
O(1)	5421(1)	6610(1)	2567(1)	20(1)
O(2)	9256(1)	4371(1)	2934(1)	18(1)
O(3)	4815(1)	8386(1)	4132(1)	17(1)

Table 3. Bond lengths [Å] and angles [°] for mo_170254lt_0m_a.

C(1)-N(1)	1.4963(15)
C(1)-C(2)	1.5216(17)
C(1)-C(4)	1.5339(17)
C(1)-C(5)	1.5737(16)
C(2)-C(3)	1.5140(17)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-O(1)	1.4408(14)
C(3)-C(6)	1.5362(17)
C(3)-H(3)	1.0000
C(4)-N(2)	1.4620(16)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900

C(5)-O(2)	1.4345(14)
C(5)-C(31)	1.5030(17)
C(5)-H(5)	1.0000
C(6)-O(3)	1.4268(13)
C(6)-C(7)	1.5264(16)
C(6)-C(13)	1.5333(17)
C(7)-C(12)	1.3872(17)
C(7)-C(8)	1.3927(17)
C(8)-C(9)	1.3823(18)
C(8)-H(8)	0.9500
C(9)-C(10)	1.3868(19)
C(9)-H(9)	0.9500
C(10)-C(11)	1.3825(18)
C(10)-H(10)	0.9500
C(11)-C(12)	1.3913(18)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(14)	1.3903(17)
C(13)-C(18)	1.3972(17)
C(14)-C(15)	1.3902(18)
C(14)-H(14)	0.9500

C(15)-C(16) 1.384(2)

C(15)-H(15) 0.9500

C(16)-C(17) 1.383(2)

C(16)-H(16) 0.9500

C(17)-C(18) 1.3814(18)

C(17)-H(17) 0.9500

C(18)-H(18) 0.9500

C(19)-C(20) 1.3865(18)

C(19)-C(24) 1.3982(18)

C(19)-N(1) 1.4272(16)

C(20)-C(21) 1.390(2)

C(20)-H(20) 0.9500

C(21)-C(22) 1.376(2)

C(21)-H(21) 0.9500

C(22)-C(23) 1.380(2)

C(22)-H(22) 0.9500

C(23)-C(24) 1.383(2)

C(23)-H(23) 0.9500

C(24)-H(24) 0.9500

C(25)-C(30) 1.3962(17)

C(25)-C(26) 1.3992(17)

C(25)-N(2) 1.4048(15)

C(26)-C(27) 1.3829(17)

C(26)-H(26) 0.9500

C(27)-C(28) 1.3891(18)

C(27)-H(27) 0.9500

C(28)-C(29) 1.3863(18)

C(28)-H(28) 0.9500

C(29)-C(30) 1.3875(18)

C(29)-H(29) 0.9500

C(30)-H(30) 0.9500

C(31)-C(32) 1.3922(18)

C(31)-C(36) 1.3926(18)

C(32)-C(33) 1.3883(19)

C(32)-H(32) 0.9500

C(33)-C(34) 1.379(2)

C(33)-H(33) 0.9500

C(34)-C(35) 1.385(2)

C(34)-H(34) 0.9500

C(35)-C(36) 1.3869(19)

C(35)-H(35) 0.9500

C(36)-H(36) 0.9500

N(1)-O(1)	1.4655(13)
N(2)-O(2)	1.4488(12)
O(3)-H(3A)	0.8400
N(1)-C(1)-C(2)	100.93(9)
N(1)-C(1)-C(4)	112.13(10)
C(2)-C(1)-C(4)	111.51(10)
N(1)-C(1)-C(5)	114.74(9)
C(2)-C(1)-C(5)	115.98(10)
C(4)-C(1)-C(5)	101.98(9)
C(3)-C(2)-C(1)	104.10(10)
C(3)-C(2)-H(2A)	110.9
C(1)-C(2)-H(2A)	110.9
C(3)-C(2)-H(2B)	110.9
C(1)-C(2)-H(2B)	110.9
H(2A)-C(2)-H(2B)	109.0
O(1)-C(3)-C(2)	105.85(9)
O(1)-C(3)-C(6)	108.72(9)
C(2)-C(3)-C(6)	114.27(10)
O(1)-C(3)-H(3)	109.3
C(2)-C(3)-H(3)	109.3
C(6)-C(3)-H(3)	109.3

N(2)-C(4)-C(1)	103.08(9)
N(2)-C(4)-H(4A)	111.1
C(1)-C(4)-H(4A)	111.1
N(2)-C(4)-H(4B)	111.1
C(1)-C(4)-H(4B)	111.1
H(4A)-C(4)-H(4B)	109.1
O(2)-C(5)-C(31)	107.85(9)
O(2)-C(5)-C(1)	104.46(9)
C(31)-C(5)-C(1)	117.89(10)
O(2)-C(5)-H(5)	108.8
C(31)-C(5)-H(5)	108.8
C(1)-C(5)-H(5)	108.8
O(3)-C(6)-C(7)	108.08(9)
O(3)-C(6)-C(13)	109.10(9)
C(7)-C(6)-C(13)	108.65(10)
O(3)-C(6)-C(3)	109.13(9)
C(7)-C(6)-C(3)	108.62(9)
C(13)-C(6)-C(3)	113.15(10)
C(12)-C(7)-C(8)	118.83(11)
C(12)-C(7)-C(6)	122.07(11)
C(8)-C(7)-C(6)	119.04(11)

C(9)-C(8)-C(7)	120.93(12)
C(9)-C(8)-H(8)	119.5
C(7)-C(8)-H(8)	119.5
C(8)-C(9)-C(10)	119.92(12)
C(8)-C(9)-H(9)	120.0
C(10)-C(9)-H(9)	120.0
C(11)-C(10)-C(9)	119.63(12)
C(11)-C(10)-H(10)	120.2
C(9)-C(10)-H(10)	120.2
C(10)-C(11)-C(12)	120.41(12)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(7)-C(12)-C(11)	120.25(12)
C(7)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(14)-C(13)-C(18)	118.42(11)
C(14)-C(13)-C(6)	124.13(11)
C(18)-C(13)-C(6)	117.44(11)
C(15)-C(14)-C(13)	120.50(12)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8

C(16)-C(15)-C(14)	120.27(12)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(17)-C(16)-C(15)	119.74(12)
C(17)-C(16)-H(16)	120.1
C(15)-C(16)-H(16)	120.1
C(18)-C(17)-C(16)	120.03(12)
C(18)-C(17)-H(17)	120.0
C(16)-C(17)-H(17)	120.0
C(17)-C(18)-C(13)	121.00(12)
C(17)-C(18)-H(18)	119.5
C(13)-C(18)-H(18)	119.5
C(20)-C(19)-C(24)	118.79(12)
C(20)-C(19)-N(1)	122.29(11)
C(24)-C(19)-N(1)	118.73(11)
C(19)-C(20)-C(21)	119.95(14)
C(19)-C(20)-H(20)	120.0
C(21)-C(20)-H(20)	120.0
C(22)-C(21)-C(20)	121.26(15)
C(22)-C(21)-H(21)	119.4
C(20)-C(21)-H(21)	119.4

C(21)-C(22)-C(23)	118.86(13)
C(21)-C(22)-H(22)	120.6
C(23)-C(22)-H(22)	120.6
C(22)-C(23)-C(24)	120.87(14)
C(22)-C(23)-H(23)	119.6
C(24)-C(23)-H(23)	119.6
C(23)-C(24)-C(19)	120.23(14)
C(23)-C(24)-H(24)	119.9
C(19)-C(24)-H(24)	119.9
C(30)-C(25)-C(26)	119.63(11)
C(30)-C(25)-N(2)	121.88(11)
C(26)-C(25)-N(2)	118.20(10)
C(27)-C(26)-C(25)	119.97(11)
C(27)-C(26)-H(26)	120.0
C(25)-C(26)-H(26)	120.0
C(26)-C(27)-C(28)	120.65(12)
C(26)-C(27)-H(27)	119.7
C(28)-C(27)-H(27)	119.7
C(29)-C(28)-C(27)	119.09(12)
C(29)-C(28)-H(28)	120.5
C(27)-C(28)-H(28)	120.5

C(28)-C(29)-C(30)	121.21(12)
C(28)-C(29)-H(29)	119.4
C(30)-C(29)-H(29)	119.4
C(29)-C(30)-C(25)	119.33(11)
C(29)-C(30)-H(30)	120.3
C(25)-C(30)-H(30)	120.3
C(32)-C(31)-C(36)	119.11(12)
C(32)-C(31)-C(5)	121.88(11)
C(36)-C(31)-C(5)	118.97(11)
C(33)-C(32)-C(31)	120.01(13)
C(33)-C(32)-H(32)	120.0
C(31)-C(32)-H(32)	120.0
C(34)-C(33)-C(32)	120.66(13)
C(34)-C(33)-H(33)	119.7
C(32)-C(33)-H(33)	119.7
C(33)-C(34)-C(35)	119.63(13)
C(33)-C(34)-H(34)	120.2
C(35)-C(34)-H(34)	120.2
C(34)-C(35)-C(36)	120.18(13)
C(34)-C(35)-H(35)	119.9
C(36)-C(35)-H(35)	119.9

C(35)-C(36)-C(31)	120.41(13)
C(35)-C(36)-H(36)	119.8
C(31)-C(36)-H(36)	119.8
C(19)-N(1)-O(1)	107.06(9)
C(19)-N(1)-C(1)	120.90(10)
O(1)-N(1)-C(1)	106.03(8)
C(25)-N(2)-O(2)	110.73(9)
C(25)-N(2)-C(4)	118.97(10)
O(2)-N(2)-C(4)	102.59(9)
C(3)-O(1)-N(1)	108.73(8)
C(5)-O(2)-N(2)	102.44(8)
C(6)-O(3)-H(3A)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103) for mo_170254lt_0m_a. The anisotropic

displacement factor exponent takes the form: -2p2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	15(1)	14(1)	15(1)	-1(1)	-4(1)	0(1)

C(2)	17(1)	14(1)	18(1)	-3(1)	-5(1)	1(1)
C(3)	15(1)	13(1)	17(1)	-2(1)	-5(1)	-2(1)
C(4)	18(1)	17(1)	16(1)	-2(1)	-4(1)	4(1)
C(5)	16(1)	13(1)	16(1)	-1(1)	-5(1)	2(1)
C(6)	16(1)	14(1)	12(1)	-1(1)	-2(1)	0(1)
C(7)	15(1)	10(1)	19(1)	0(1)	-6(1)	2(1)
C(8)	22(1)	19(1)	17(1)	-1(1)	-6(1)	-3(1)
C(9)	21(1)	21(1)	21(1)	4(1)	-4(1)	-4(1)
C(10)	17(1)	17(1)	31(1)	1(1)	-10(1)	-3(1)
C(11)	18(1)	19(1)	24(1)	-7(1)	-9(1)	2(1)
C(12)	14(1)	17(1)	18(1)	-2(1)	-4(1)	3(1)
C(13)	15(1)	12(1)	19(1)	2(1)	-5(1)	-4(1)
C(14)	19(1)	17(1)	19(1)	1(1)	-5(1)	-2(1)
C(15)	26(1)	26(1)	19(1)	4(1)	-9(1)	-7(1)
C(16)	20(1)	26(1)	28(1)	8(1)	-12(1)	-4(1)
C(17)	19(1)	18(1)	31(1)	3(1)	-7(1)	1(1)
C(18)	20(1)	16(1)	22(1)	-1(1)	-6(1)	-1(1)
C(19)	14(1)	15(1)	20(1)	-3(1)	-1(1)	-1(1)
C(20)	40(1)	20(1)	26(1)	2(1)	-15(1)	-8(1)
C(21)	54(1)	31(1)	34(1)	-4(1)	-22(1)	-14(1)
C(22)	33(1)	22(1)	44(1)	-11(1)	-8(1)	-10(1)

C(23)	25(1)	15(1)	55(1)	2(1)	-12(1)	-4(1)
C(24)	24(1)	18(1)	38(1)	6(1)	-13(1)	-4(1)
C(25)	17(1)	12(1)	18(1)	-1(1)	-7(1)	-3(1)
C(26)	17(1)	16(1)	20(1)	-1(1)	-6(1)	-2(1)
C(27)	22(1)	18(1)	19(1)	2(1)	-8(1)	-6(1)
C(28)	23(1)	17(1)	26(1)	3(1)	-14(1)	-2(1)
C(29)	17(1)	20(1)	28(1)	-4(1)	-10(1)	2(1)
C(30)	17(1)	19(1)	18(1)	-2(1)	-5(1)	-2(1)
C(31)	20(1)	12(1)	15(1)	-4(1)	-1(1)	2(1)
C(32)	24(1)	18(1)	20(1)	-1(1)	-6(1)	-3(1)
C(33)	27(1)	22(1)	30(1)	-2(1)	-2(1)	-7(1)
C(34)	37(1)	16(1)	23(1)	1(1)	5(1)	-3(1)
C(35)	40(1)	18(1)	16(1)	0(1)	-3(1)	7(1)
C(36)	24(1)	18(1)	17(1)	-4(1)	-4(1)	4(1)
N(1)	17(1)	11(1)	19(1)	2(1)	-6(1)	1(1)
N(2)	15(1)	16(1)	14(1)	2(1)	-1(1)	1(1)
O(1)	23(1)	11(1)	31(1)	4(1)	-16(1)	-2(1)
O(2)	15(1)	18(1)	16(1)	4(1)	-1(1)	2(1)
O(3)	17(1)	18(1)	15(1)	-1(1)	-1(1)	-2(1)

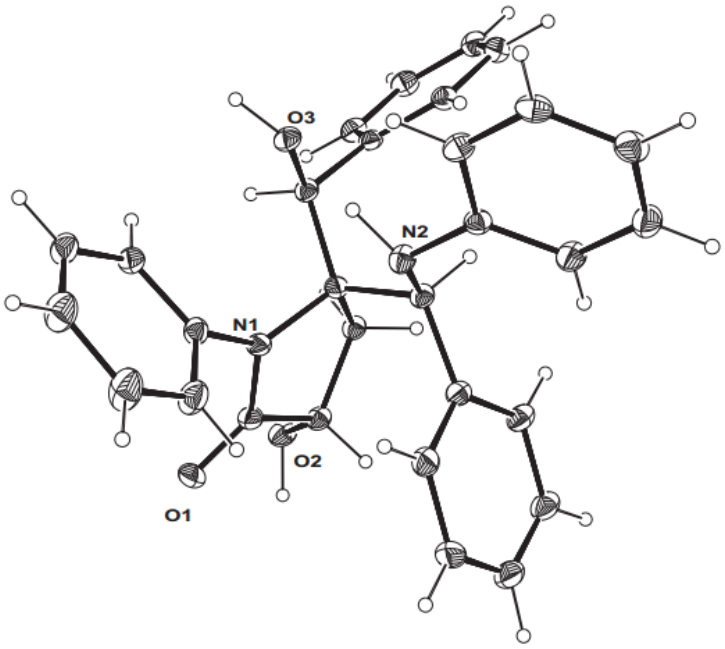
Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3)

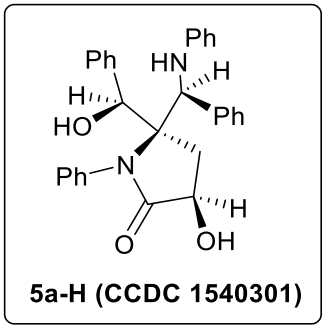
for mo_170254lt_0m_a.

	x	y	z	U(eq)
H(2A)	6890	7133	4157	19
H(2B)	8335	7068	3113	19
H(3)	7125	7492	1817	18
H(4A)	7977	5443	4757	21
H(4B)	6465	4881	4934	21
H(5)	7887	4542	1974	18
H(8)	7627	9259	1202	23
H(9)	9241	10628	1013	25
H(10)	9323	11566	2601	25
H(11)	7839	11081	4379	24
H(12)	6218	9706	4571	20
H(14)	5429	7984	879	22
H(15)	3799	8694	-113	27
H(16)	1987	10036	683	29
H(17)	1869	10724	2442	28
H(18)	3521	10048	3415	23
H(20)	4552	5547	1510	33

H(21)	3747	4027	846	45
H(22)	3922	2284	1685	39
H(23)	4915	2061	3213	38
H(24)	5680	3568	3920	31
H(26)	7207	3540	6075	21
H(27)	8108	2226	7195	23
H(28)	10298	1206	6441	25
H(29)	11652	1597	4590	25
H(30)	10779	2913	3450	21
H(32)	11041	5701	2168	25
H(33)	12555	6711	712	33
H(34)	11784	7373	-846	33
H(35)	9477	7024	-953	31
H(36)	7978	5970	469	24
H(3A)	4136	7977	4178	26

4.3 Crystallographic data for compound 5a-H:





5a-H (CCDC 1540301)

Table 1. Crystal data and structure refinement for d18714.

Identification code d18714

Empirical formula C31 H32 N2 O4

Formula weight 496.59

Temperature 200(2) K

Wavelength 0.71073 Å

Crystal system Monoclinic

Space group C 2/c

Unit cell dimensions a = 24.087(3) Å □= 90°.

b = 9.7374(11) Å □= 107.805(4)°.

c = 23.807(3) Å □ = 90°.

Volume 5316.5(11) Å3

Z 8

Density (calculated) 1.241 Mg/m3

Absorption coefficient 0.082 mm-1

F(000) 2112

Crystal size 0.10 x 0.07 x 0.03 mm3

Theta range for data collection 2.27 to 25.05°.

Index ranges -20<=h<=28, -11<=k<=11, -28<=l<=28

Reflections collected 19936

Independent reflections 4704 [R(int) = 0.0752]

Completeness to theta = 25.05° 99.6 %

Absorption correction multi-scan

Max. and min. transmission 0.9975 and 0.9918

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 4704 / 0 / 335

Goodness-of-fit on F2 1.078

Final R indices [I>2sigma(I)] R1 = 0.0567, wR2 = 0.1343

R indices (all data) R1 = 0.1157, wR2 = 0.1691

Largest diff. peak and hole 0.246 and -0.333 e.Å-3

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103)

for d18714. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	5361(1)	2001(3)	5532(1)	35(1)
C(2)	5834(1)	1043(3)	5482(1)	34(1)
C(3)	6375(1)	1919(3)	5691(1)	32(1)
C(4)	6247(1)	3076(3)	6079(1)	30(1)
C(5)	6482(1)	2685(3)	6749(1)	31(1)
C(6)	6282(1)	1258(3)	6865(1)	33(1)
C(7)	5747(1)	1053(3)	6957(1)	45(1)
C(8)	5539(2)	-279(4)	6972(2)	60(1)
C(9)	5867(2)	-1395(4)	6920(2)	61(1)
C(10)	6416(2)	-1203(3)	6874(1)	49(1)
C(11)	6622(2)	114(3)	6847(1)	40(1)
C(12)	6661(1)	3963(3)	7690(1)	33(1)
C(13)	6963(2)	2910(3)	8043(1)	43(1)
C(14)	7258(2)	3142(3)	8630(1)	50(1)
C(15)	7265(2)	4428(3)	8876(1)	47(1)
C(16)	6976(1)	5494(3)	8524(1)	42(1)

C(17)	6678(1)	5266(3)	7940(1)	39(1)
C(18)	6517(1)	4409(3)	5917(1)	31(1)
C(19)	7160(1)	4281(3)	5970(1)	31(1)
C(20)	7591(1)	4434(3)	6509(1)	36(1)
C(21)	8175(1)	4405(3)	6548(1)	43(1)
C(22)	8339(2)	4230(3)	6041(2)	43(1)
C(23)	7917(2)	4081(3)	5507(1)	43(1)
C(24)	7333(2)	4113(3)	5469(1)	39(1)
C(25)	5204(1)	4141(3)	5971(1)	35(1)
C(26)	5168(1)	5440(3)	5734(1)	38(1)
C(27)	4777(2)	6379(3)	5837(1)	46(1)
C(28)	4420(2)	6015(4)	6160(2)	59(1)
C(29)	4435(2)	4695(4)	6367(2)	66(1)
C(30)	4825(2)	3762(4)	6275(2)	53(1)
C(31)	3421(2)	2606(5)	5088(2)	90(1)
N(1)	5591(1)	3116(2)	5855(1)	32(1)
N(2)	6321(1)	3758(2)	7101(1)	36(1)
O(1)	4833(1)	1801(2)	5301(1)	46(1)
O(2)	5745(1)	627(2)	4891(1)	43(1)
O(3)	6436(1)	5561(2)	6257(1)	36(1)
O(4)	3722(1)	2666(3)	4673(1)	69(1)

Table 3. Bond lengths [Å] and angles [°] for d18714.

C(1)-O(1)	1.236(3)
C(1)-N(1)	1.349(4)
C(1)-C(2)	1.505(4)
C(2)-O(2)	1.417(3)
C(2)-C(3)	1.509(4)
C(2)-H(2)	1.0000
C(3)-C(4)	1.547(4)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-N(1)	1.504(4)
C(4)-C(18)	1.553(4)
C(4)-C(5)	1.567(4)
C(5)-N(2)	1.464(3)
C(5)-C(6)	1.524(4)
C(5)-H(5)	1.0000
C(6)-C(7)	1.386(4)
C(6)-C(11)	1.392(4)
C(7)-C(8)	1.395(5)

C(7)-H(7)	0.9500
C(8)-C(9)	1.371(5)
C(8)-H(8)	0.9500
C(9)-C(10)	1.371(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.384(4)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(13)	1.382(4)
C(12)-C(17)	1.396(4)
C(12)-N(2)	1.406(4)
C(13)-C(14)	1.380(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.380(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.380(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.374(4)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-O(3)	1.432(3)

C(18)-C(19) 1.519(4)

C(18)-H(18) 1.0000

C(19)-C(24) 1.387(4)

C(19)-C(20) 1.391(4)

C(20)-C(21) 1.382(4)

C(20)-H(20) 0.9500

C(21)-C(22) 1.391(4)

C(21)-H(21) 0.9500

C(22)-C(23) 1.370(4)

C(22)-H(22) 0.9500

C(23)-C(24) 1.384(4)

C(23)-H(23) 0.9500

C(24)-H(24) 0.9500

C(25)-C(26) 1.377(4)

C(25)-C(30) 1.378(4)

C(25)-N(1) 1.450(4)

C(26)-C(27) 1.387(4)

C(26)-H(26) 0.9500

C(27)-C(28) 1.364(5)

C(27)-H(27) 0.9500

C(28)-C(29) 1.372(5)

C(28)-H(28) 0.9500

C(29)-C(30) 1.371(5)

C(29)-H(29) 0.9500

C(30)-H(30) 0.9500

C(31)-O(4) 1.394(5)

C(31)-H(31A) 0.9800

C(31)-H(31B) 0.9800

C(31)-H(31C) 0.9800

N(2)-H(2') 0.9945

O(2)-H(2A) 0.9747

O(3)-H(3') 0.9833

O(4)-H(4') 0.8805

O(1)-C(1)-N(1) 124.7(3)

O(1)-C(1)-C(2) 124.5(3)

N(1)-C(1)-C(2) 110.8(3)

O(2)-C(2)-C(1) 111.6(2)

O(2)-C(2)-C(3) 110.0(2)

C(1)-C(2)-C(3) 102.8(2)

O(2)-C(2)-H(2) 110.7

C(1)-C(2)-H(2) 110.7

C(3)-C(2)-H(2) 110.7

C(2)-C(3)-C(4)	107.4(2)
C(2)-C(3)-H(3A)	110.2
C(4)-C(3)-H(3A)	110.2
C(2)-C(3)-H(3B)	110.2
C(4)-C(3)-H(3B)	110.2
H(3A)-C(3)-H(3B)	108.5
N(1)-C(4)-C(3)	100.8(2)
N(1)-C(4)-C(18)	111.4(2)
C(3)-C(4)-C(18)	106.5(2)
N(1)-C(4)-C(5)	112.4(2)
C(3)-C(4)-C(5)	110.8(2)
C(18)-C(4)-C(5)	114.0(2)
N(2)-C(5)-C(6)	113.1(2)
N(2)-C(5)-C(4)	109.5(2)
C(6)-C(5)-C(4)	111.7(2)
N(2)-C(5)-H(5)	107.4
C(6)-C(5)-H(5)	107.4
C(4)-C(5)-H(5)	107.4
C(7)-C(6)-C(11)	118.3(3)
C(7)-C(6)-C(5)	121.4(3)
C(11)-C(6)-C(5)	120.2(3)

C(6)-C(7)-C(8)	119.7(3)
C(6)-C(7)-H(7)	120.1
C(8)-C(7)-H(7)	120.1
C(9)-C(8)-C(7)	120.9(4)
C(9)-C(8)-H(8)	119.6
C(7)-C(8)-H(8)	119.6
C(10)-C(9)-C(8)	119.7(3)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(9)-C(10)-C(11)	119.9(3)
C(9)-C(10)-H(10)	120.0
C(11)-C(10)-H(10)	120.0
C(10)-C(11)-C(6)	121.1(3)
C(10)-C(11)-H(11)	119.5
C(6)-C(11)-H(11)	119.5
C(13)-C(12)-C(17)	118.3(3)
C(13)-C(12)-N(2)	122.6(2)
C(17)-C(12)-N(2)	119.1(3)
C(14)-C(13)-C(12)	120.4(3)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8

C(15)-C(14)-C(13)	120.9(3)
C(15)-C(14)-H(14)	119.6
C(13)-C(14)-H(14)	119.6
C(14)-C(15)-C(16)	119.1(3)
C(14)-C(15)-H(15)	120.4
C(16)-C(15)-H(15)	120.4
C(17)-C(16)-C(15)	120.2(3)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(16)-C(17)-C(12)	121.1(3)
C(16)-C(17)-H(17)	119.5
C(12)-C(17)-H(17)	119.5
O(3)-C(18)-C(19)	109.3(2)
O(3)-C(18)-C(4)	112.0(2)
C(19)-C(18)-C(4)	113.9(2)
O(3)-C(18)-H(18)	107.1
C(19)-C(18)-H(18)	107.1
C(4)-C(18)-H(18)	107.1
C(24)-C(19)-C(20)	118.0(3)
C(24)-C(19)-C(18)	120.4(3)
C(20)-C(19)-C(18)	121.5(3)

C(21)-C(20)-C(19)	121.3(3)
C(21)-C(20)-H(20)	119.4
C(19)-C(20)-H(20)	119.4
C(20)-C(21)-C(22)	119.8(3)
C(20)-C(21)-H(21)	120.1
C(22)-C(21)-H(21)	120.1
C(23)-C(22)-C(21)	119.5(3)
C(23)-C(22)-H(22)	120.3
C(21)-C(22)-H(22)	120.3
C(22)-C(23)-C(24)	120.6(3)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
C(23)-C(24)-C(19)	121.0(3)
C(23)-C(24)-H(24)	119.5
C(19)-C(24)-H(24)	119.5
C(26)-C(25)-C(30)	119.5(3)
C(26)-C(25)-N(1)	121.2(3)
C(30)-C(25)-N(1)	119.0(3)
C(25)-C(26)-C(27)	119.7(3)
C(25)-C(26)-H(26)	120.2
C(27)-C(26)-H(26)	120.2

C(28)-C(27)-C(26) 120.4(3)

C(28)-C(27)-H(27) 119.8

C(26)-C(27)-H(27) 119.8

C(27)-C(28)-C(29) 119.6(3)

C(27)-C(28)-H(28) 120.2

C(29)-C(28)-H(28) 120.2

C(30)-C(29)-C(28) 120.6(4)

C(30)-C(29)-H(29) 119.7

C(28)-C(29)-H(29) 119.7

C(29)-C(30)-C(25) 120.1(3)

C(29)-C(30)-H(30) 120.0

C(25)-C(30)-H(30) 120.0

O(4)-C(31)-H(31A) 109.5

O(4)-C(31)-H(31B) 109.5

H(31A)-C(31)-H(31B) 109.5

O(4)-C(31)-H(31C) 109.5

H(31A)-C(31)-H(31C) 109.5

H(31B)-C(31)-H(31C) 109.5

C(1)-N(1)-C(25) 119.1(3)

C(1)-N(1)-C(4) 112.7(2)

C(25)-N(1)-C(4) 128.1(2)

C(12)-N(2)-C(5)	119.8(2)
C(12)-N(2)-H(2')	108.2
C(5)-N(2)-H(2')	109.2
C(2)-O(2)-H(2A)	98.2
C(18)-O(3)-H(3')	107.1
C(31)-O(4)-H(4')	103.4

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103)for d18714. The anisotropic displacement factor exponent takes the form: -2□2[h2a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	39(2)	29(2)	35(2)	-1(1)	6(1)	-5(1)
C(2)	43(2)	26(2)	31(2)	-3(1)	10(1)	-1(1)
C(3)	37(2)	26(2)	32(2)	-3(1)	10(1)	3(1)
C(4)	30(2)	26(2)	32(2)	-2(1)	8(1)	-1(1)
C(5)	35(2)	26(2)	33(2)	-2(1)	10(1)	2(1)
C(6)	41(2)	30(2)	28(2)	-1(1)	9(1)	-2(1)
C(7)	41(2)	51(2)	41(2)	10(2)	11(2)	-1(2)
C(8)	45(2)	70(3)	60(2)	23(2)	8(2)	-18(2)

C(9)	76(3)	41(2)	50(2)	9(2)	-4(2)	-18(2)
C(10)	70(3)	31(2)	41(2)	-1(2)	8(2)	-4(2)
C(11)	57(2)	29(2)	36(2)	0(1)	14(2)	0(2)
C(12)	37(2)	30(2)	33(2)	-3(1)	11(1)	-3(1)
C(13)	58(2)	32(2)	35(2)	-6(1)	8(2)	-1(2)
C(14)	62(2)	41(2)	39(2)	2(2)	5(2)	0(2)
C(15)	57(2)	49(2)	33(2)	-9(2)	11(2)	-11(2)
C(16)	47(2)	38(2)	46(2)	-16(2)	21(2)	-9(2)
C(17)	47(2)	31(2)	42(2)	-2(1)	20(2)	1(1)
C(18)	35(2)	26(2)	31(2)	-2(1)	9(1)	2(1)
C(19)	37(2)	22(1)	34(2)	-1(1)	10(1)	-4(1)
C(20)	40(2)	31(2)	36(2)	-3(1)	12(2)	-3(1)
C(21)	38(2)	37(2)	48(2)	-1(2)	6(2)	-1(2)
C(22)	38(2)	36(2)	59(2)	4(2)	20(2)	3(2)
C(23)	49(2)	40(2)	47(2)	2(2)	25(2)	-1(2)
C(24)	50(2)	31(2)	35(2)	1(1)	14(2)	-2(2)
C(25)	33(2)	33(2)	37(2)	-1(1)	9(1)	5(1)
C(26)	39(2)	32(2)	39(2)	-1(1)	7(1)	0(1)
C(27)	49(2)	33(2)	53(2)	-1(2)	9(2)	9(2)
C(28)	59(3)	52(2)	73(3)	3(2)	29(2)	22(2)
C(29)	60(3)	69(3)	81(3)	18(2)	39(2)	26(2)

C(30)	49(2)	47(2)	68(2)	16(2)	28(2)	14(2)
C(31)	72(3)	101(4)	93(3)	11(3)	17(3)	3(3)
N(1)	31(2)	25(1)	40(1)	-2(1)	11(1)	0(1)
N(2)	44(2)	31(1)	34(1)	-4(1)	11(1)	5(1)
O(1)	34(1)	37(1)	58(1)	-5(1)	2(1)	-7(1)
O(2)	58(2)	32(1)	35(1)	-7(1)	12(1)	-6(1)
O(3)	43(1)	24(1)	42(1)	-4(1)	12(1)	1(1)
O(4)	58(2)	74(2)	77(2)	37(2)	21(2)	18(1)

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 103) for d18714.

	x	y	z	U(eq)
H(2)	5863	227	5744	40
H(3A)	6471	2317	5349	38
H(3B)	6710	1359	5922	38
H(5)	6917	2667	6861	37
H(7)	5522	1818	7009	54
H(8)	5165	-416	7019	72
H(9)	5715	-2296	6916	73
H(10)	6653	-1973	6861	59

H(11)	7002	239	6815	49
H(13)	6966	2021	7880	52
H(14)	7460	2407	8869	60
H(15)	7466	4579	9281	56
H(16)	6982	6387	8687	51
H(17)	6480	6006	7703	46
H(18)	6305	4616	5495	37
H(20)	7482	4560	6857	43
H(21)	8464	4504	6921	51
H(22)	8740	4213	6064	52
H(23)	8027	3956	5160	51
H(24)	7046	4018	5095	47
H(26)	5409	5691	5501	45
H(27)	4757	7282	5680	56
H(28)	4164	6671	6243	71
H(29)	4173	4426	6575	79
H(30)	4833	2852	6422	63
H(31A)		3427	1662	5233 136
H(31B)		3016	2897	4905 136
H(31C)		3608	3217	5419 136
H(2')	6288	4650	6890	83

H(2A)	5485	-145	4881	83
H(3')	6367	6368	5996	83
H(4')	4076	2396	4873	83

4.4 Crystallographic data for compound 8a:

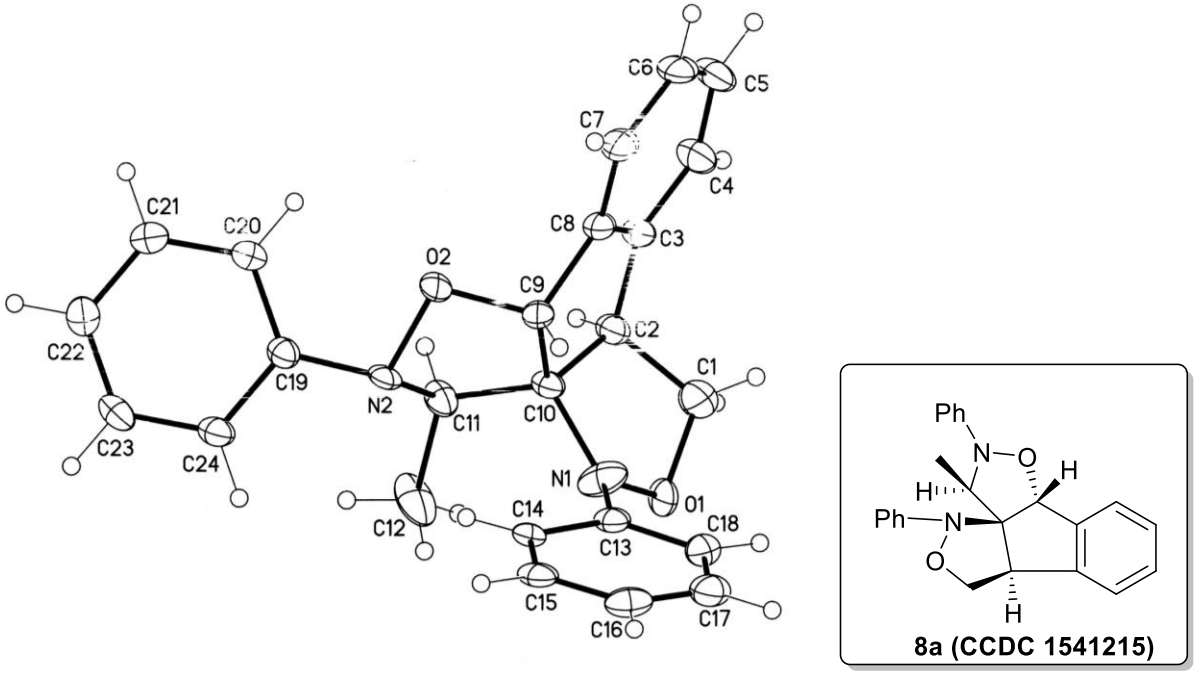


Table 1. Crystal data and structure refinement for 160816LT_0M_A.

Identification code	160816LT_0m_a
Empirical formula	C24 H22 N2 O2
Formula weight	370.43
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic

Space group P 21/n

Unit cell dimensions a = 13.7372(10) Å a= 90°.

b = 7.3706(5) Å b= 106.653(4)°.

c = 19.7024(14) Å g = 90°.

Volume 1911.2(2) Å3

Z 4

Density (calculated) 1.287 Mg/m3

Absorption coefficient 0.082 mm-1

F(000) 784

Crystal size 0.15 x 0.04 x 0.01 mm3

Theta range for data collection 1.613 to 26.397°.

Index ranges -17<=h<=17, -8<=k<=8, -24<=l<=24

Reflections collected 11858

Independent reflections 3834 [R(int) = 0.0475]

Completeness to theta = 25.242° 98.4 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.9485 and 0.8028

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 3834 / 0 / 258

Goodness-of-fit on F2 1.086

Final R indices [I>2sigma(I)] R1 = 0.0607, wR2 = 0.1533

R indices (all data) R1 = 0.1143, wR2 = 0.1968

Extinction coefficient n/a

Largest diff. peak and hole 0.714 and -0.774 e.Å-3

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103)

for 160816LT_0M_A. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	4388(2)	5212(4)	7771(1)	33(1)
N(2)	3994(2)	8542(3)	6593(1)	20(1)
O(1)	4180(5)	3497(8)	7816(3)	24(1)
O(1')	5023(2)	3422(4)	7974(2)	24(1)
O(2)	5030(1)	8259(3)	6538(1)	25(1)
C(1)	4731(3)	2493(5)	7380(2)	41(1)
C(2)	4746(2)	3769(4)	6783(2)	23(1)
C(3)	5773(2)	4002(4)	6657(2)	25(1)
C(4)	6320(2)	2694(5)	6405(2)	35(1)
C(5)	7275(3)	3155(6)	6353(2)	44(1)
C(6)	7679(2)	4866(6)	6549(2)	40(1)
C(7)	7135(2)	6170(5)	6797(2)	32(1)

C(8)	6167(2)	5718(4)	6834(1)	23(1)
C(9)	5440(2)	6899(4)	7070(2)	21(1)
C(10)	4525(2)	5648(4)	7063(1)	19(1)
C(11)	3619(2)	6643(4)	6554(2)	24(1)
C(12)	2612(2)	6495(5)	6727(2)	48(1)
C(13)	4796(2)	6346(4)	8369(1)	21(1)
C(14)	4591(2)	8198(4)	8322(2)	20(1)
C(15)	4985(2)	9309(4)	8902(2)	24(1)
C(16)	5566(2)	8594(5)	9538(2)	29(1)
C(17)	5743(2)	6758(5)	9591(2)	33(1)
C(18)	5360(2)	5624(4)	9015(2)	29(1)
C(19)	3480(2)	9721(4)	6022(1)	20(1)
C(20)	3820(2)	10035(4)	5431(2)	25(1)
C(21)	3335(2)	11307(4)	4934(2)	30(1)
C(22)	2505(2)	12264(4)	5016(2)	28(1)
C(23)	2151(2)	11923(4)	5592(2)	26(1)
C(24)	2640(2)	10677(4)	6101(2)	23(1)

Table 3. Bond lengths [Å] and angles [°] for 160816LT_0M_A.

N(1)-O(1)	1.305(7)

N(1)-C(13)	1.421(4)
N(1)-C(10)	1.496(4)
N(1)-O(1')	1.569(4)
N(2)-C(19)	1.436(4)
N(2)-O(2)	1.472(3)
N(2)-C(11)	1.486(4)
O(1)-C(1)	1.493(7)
O(2)-C(9)	1.442(3)
C(1)-C(2)	1.511(4)
C(1)-H(1A)	0.9789
C(1)-H(1B)	0.9686
C(2)-C(3)	1.512(4)
C(2)-C(10)	1.552(4)
C(2)-H(2)	1.0000
C(3)-C(8)	1.381(4)
C(3)-C(4)	1.398(4)
C(4)-C(5)	1.387(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.387(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.389(5)

C(6)-H(6)	0.9500
C(7)-C(8)	1.394(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.496(4)
C(9)-C(10)	1.556(4)
C(9)-H(9)	1.0000
C(10)-C(11)	1.543(4)
C(11)-C(12)	1.521(4)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.392(4)
C(13)-C(18)	1.393(4)
C(14)-C(15)	1.385(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.382(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.373(5)
C(16)-H(16)	0.9500
C(17)-C(18)	1.386(4)

C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(20)	1.393(4)
C(19)-C(24)	1.398(4)
C(20)-C(21)	1.382(4)
C(20)-H(20)	0.9500
C(21)-C(22)	1.390(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.379(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.383(4)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500

O(1)-N(1)-C(13)	123.8(4)
O(1)-N(1)-C(10)	111.1(3)
C(13)-N(1)-C(10)	121.4(2)
C(13)-N(1)-O(1')	103.0(2)
C(10)-N(1)-O(1')	102.0(2)
C(19)-N(2)-O(2)	107.30(18)
C(19)-N(2)-C(11)	116.4(2)

O(2)-N(2)-C(11)	100.99(19)
N(1)-O(1)-C(1)	106.5(5)
C(9)-O(2)-N(2)	103.27(17)
O(1)-C(1)-C(2)	105.2(3)
O(1)-C(1)-H(1A)	111.1
C(2)-C(1)-H(1A)	110.8
O(1)-C(1)-H(1B)	111.6
C(2)-C(1)-H(1B)	111.6
H(1A)-C(1)-H(1B)	106.7
C(1)-C(2)-C(3)	114.9(2)
C(1)-C(2)-C(10)	103.4(2)
C(3)-C(2)-C(10)	104.1(2)
C(1)-C(2)-H(2)	111.3
C(3)-C(2)-H(2)	111.3
C(10)-C(2)-H(2)	111.3
C(8)-C(3)-C(4)	120.7(3)
C(8)-C(3)-C(2)	112.3(2)
C(4)-C(3)-C(2)	127.1(3)
C(5)-C(4)-C(3)	118.2(3)
C(5)-C(4)-H(4)	120.9
C(3)-C(4)-H(4)	120.9

C(4)-C(5)-C(6)	120.9(3)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(5)-C(6)-C(7)	121.0(3)
C(5)-C(6)-H(6)	119.5
C(7)-C(6)-H(6)	119.5
C(6)-C(7)-C(8)	118.0(3)
C(6)-C(7)-H(7)	121.0
C(8)-C(7)-H(7)	121.0
C(3)-C(8)-C(7)	121.1(3)
C(3)-C(8)-C(9)	111.3(2)
C(7)-C(8)-C(9)	127.5(3)
O(2)-C(9)-C(8)	109.6(2)
O(2)-C(9)-C(10)	105.1(2)
C(8)-C(9)-C(10)	105.2(2)
O(2)-C(9)-H(9)	112.2
C(8)-C(9)-H(9)	112.2
C(10)-C(9)-H(9)	112.2
N(1)-C(10)-C(11)	114.5(2)
N(1)-C(10)-C(2)	103.3(2)
C(11)-C(10)-C(2)	113.3(2)

N(1)-C(10)-C(9)	115.9(2)
C(11)-C(10)-C(9)	102.9(2)
C(2)-C(10)-C(9)	107.0(2)
N(2)-C(11)-C(12)	112.3(2)
N(2)-C(11)-C(10)	102.2(2)
C(12)-C(11)-C(10)	115.8(2)
N(2)-C(11)-H(11)	108.7
C(12)-C(11)-H(11)	108.7
C(10)-C(11)-H(11)	108.7
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	119.0(3)
C(14)-C(13)-N(1)	119.8(3)
C(18)-C(13)-N(1)	121.1(3)
C(15)-C(14)-C(13)	120.1(3)
C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9

C(16)-C(15)-C(14)	120.7(3)
C(16)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7
C(17)-C(16)-C(15)	119.2(3)
C(17)-C(16)-H(16)	120.4
C(15)-C(16)-H(16)	120.4
C(16)-C(17)-C(18)	121.0(3)
C(16)-C(17)-H(17)	119.5
C(18)-C(17)-H(17)	119.5
C(17)-C(18)-C(13)	119.9(3)
C(17)-C(18)-H(18)	120.0
C(13)-C(18)-H(18)	120.0
C(20)-C(19)-C(24)	119.6(3)
C(20)-C(19)-N(2)	123.2(2)
C(24)-C(19)-N(2)	117.1(2)
C(21)-C(20)-C(19)	119.8(3)
C(21)-C(20)-H(20)	120.1
C(19)-C(20)-H(20)	120.1
C(20)-C(21)-C(22)	120.4(3)
C(20)-C(21)-H(21)	119.8
C(22)-C(21)-H(21)	119.8

C(23)-C(22)-C(21)	119.9(3)
C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1
C(22)-C(23)-C(24)	120.4(3)
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-H(23)	119.8
C(23)-C(24)-C(19)	119.9(3)
C(23)-C(24)-H(24)	120.0
C(19)-C(24)-H(24)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103) for 160816LT_0M_A. The anisotropic

displacement factor exponent takes the form: -2p2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	47(2)	25(2)	33(2)	-5(1)	23(1)	-15(1)
N(2)	14(1)	22(1)	30(1)	3(1)	14(1)	2(1)
O(1)	29(1)	13(2)	32(2)	6(1)	11(1)	3(1)
O(1')	29(1)	13(2)	32(2)	6(1)	11(1)	3(1)

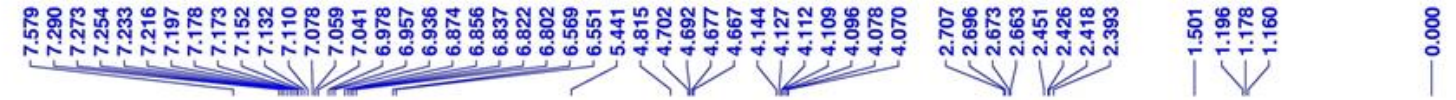
O(2)	12(1)	32(1)	36(1)	13(1)	13(1)	4(1)
C(1)	52(2)	33(2)	48(2)	10(2)	30(2)	16(2)
C(2)	22(1)	20(2)	31(2)	2(1)	14(1)	2(1)
C(3)	21(1)	35(2)	22(2)	4(1)	11(1)	7(1)
C(4)	33(2)	43(2)	32(2)	0(2)	16(1)	14(2)
C(5)	32(2)	68(3)	36(2)	7(2)	18(2)	25(2)
C(6)	20(2)	73(3)	32(2)	17(2)	16(1)	14(2)
C(7)	18(1)	50(2)	31(2)	13(2)	10(1)	4(1)
C(8)	17(1)	34(2)	20(2)	7(1)	9(1)	4(1)
C(9)	16(1)	25(2)	25(2)	7(1)	10(1)	0(1)
C(10)	17(1)	20(2)	24(2)	-1(1)	10(1)	0(1)
C(11)	18(1)	18(2)	35(2)	2(1)	9(1)	0(1)
C(12)	17(2)	33(2)	95(3)	20(2)	21(2)	1(1)
C(13)	20(1)	22(2)	24(2)	0(1)	14(1)	-2(1)
C(14)	17(1)	25(2)	24(2)	2(1)	13(1)	3(1)
C(15)	25(2)	22(2)	33(2)	-1(1)	21(1)	-3(1)
C(16)	25(2)	38(2)	29(2)	-6(1)	15(1)	-10(1)
C(17)	21(2)	55(2)	22(2)	4(2)	8(1)	5(1)
C(18)	33(2)	26(2)	33(2)	7(1)	19(1)	6(1)
C(19)	18(1)	18(2)	25(2)	0(1)	9(1)	0(1)
C(20)	24(2)	28(2)	28(2)	3(1)	15(1)	6(1)

C(21)	29(2)	38(2)	26(2)	6(1)	15(1)	5(1)
C(22)	27(2)	28(2)	30(2)	5(1)	8(1)	5(1)
C(23)	18(1)	25(2)	36(2)	-2(1)	10(1)	4(1)
C(24)	21(1)	24(2)	28(2)	-1(1)	13(1)	0(1)

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3) for 160816LT_0M_A.

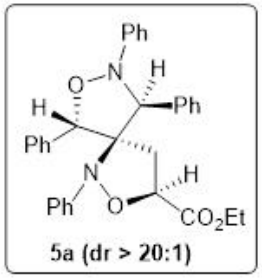
	x	y	z	U(eq)
H(1A)	4381	1362	7196	49
H(1B)	5412	2164	7657	49
H(2)	4214	3437	6337	28
H(4)	6045	1520	6274	42
H(5)	7657	2288	6181	52
H(6)	8337	5149	6514	48
H(7)	7416	7337	6937	38
H(9)	5756	7444	7547	25
H(11)	3527	6175	6063	28
H(12A)		2676	7056	7189	71
H(12B)		2429	5214	6742	71

H(12C)	2082	7121	6362	71
H(14)	4181	8701	7890	24
H(15)	4854	10576	8863	29
H(16)	5841	9363	9934	35
H(17)	6132	6258	10029	39
H(18)	5483	4355	9061	35
H(20)	4384	9377	5370	30
H(21)	3570	11528	4532	36
H(22)	2181	13151	4677	34
H(23)	1570	12547	5640	31
H(24)	2404	10471	6503	28

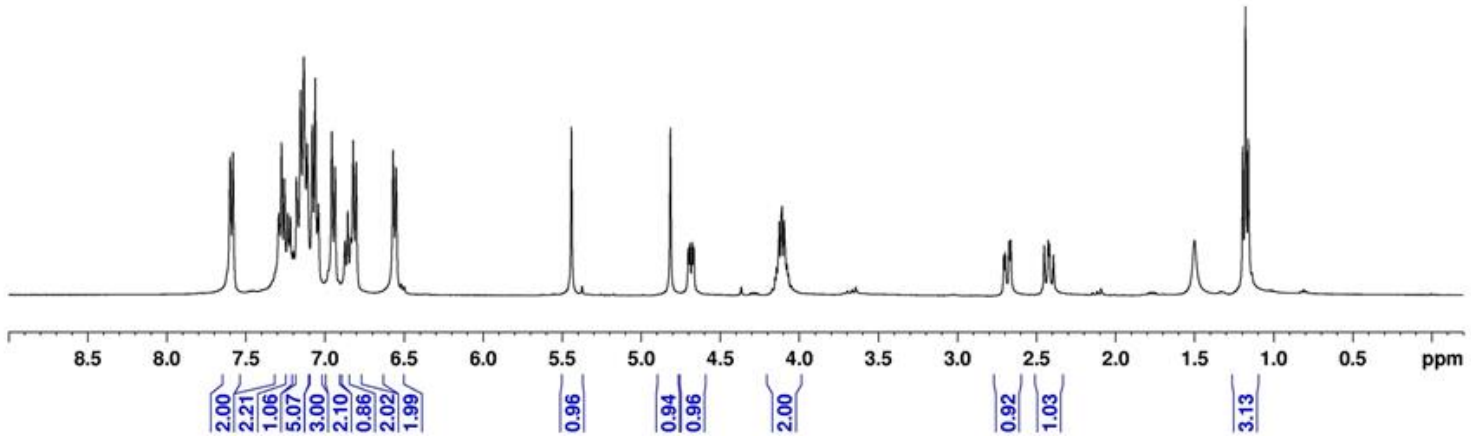


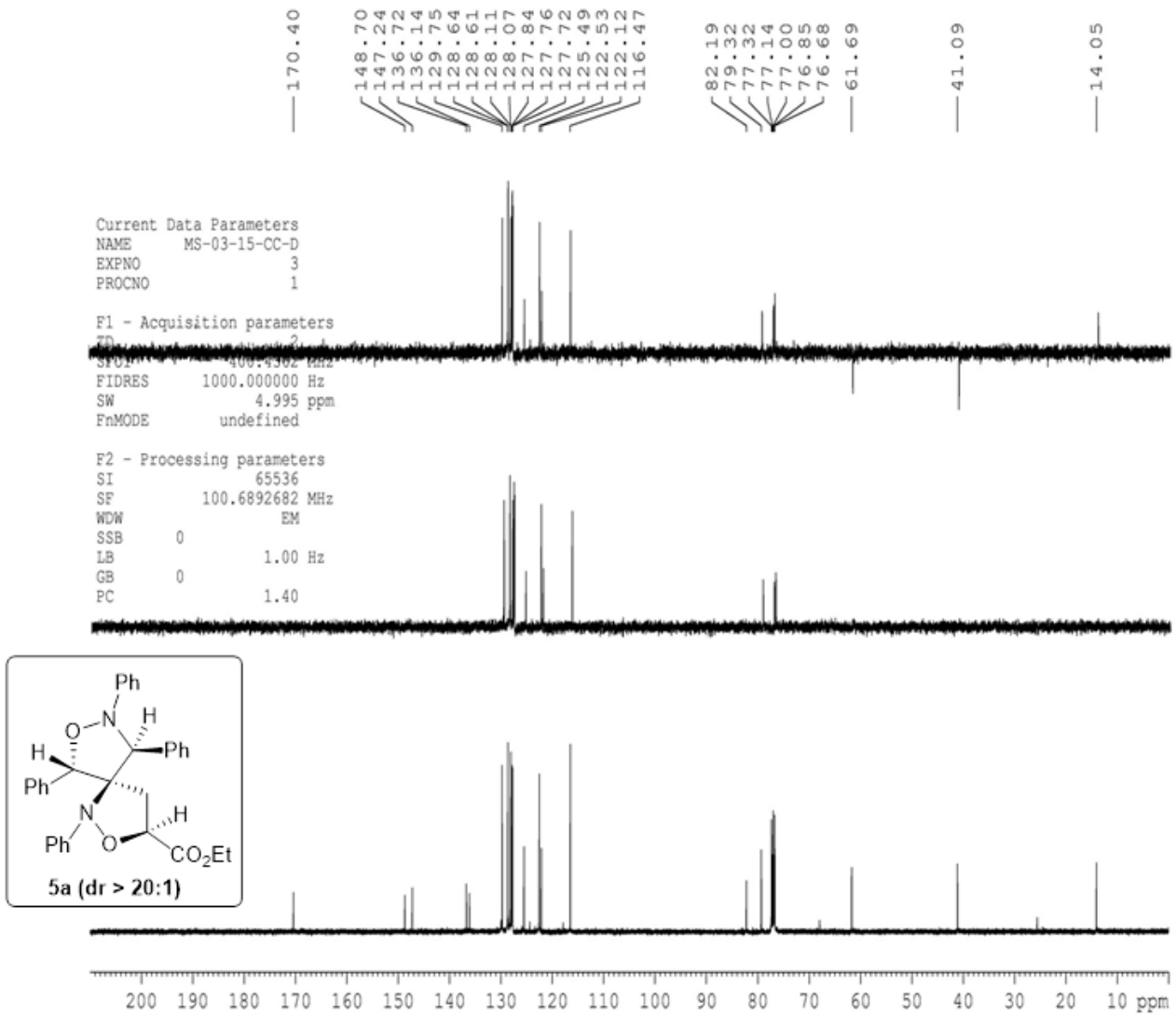

```
Current Data Parameters
NAME          MS-03-15-PP
EXPNO                   1
PROCNO                  1

F2 - Processing parameters
SI                  32768
SF          400.4342541 MHz
WDW                    EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



5a (dr > 20:1)




170.40
148.70
147.24
136.72
136.14
129.75
128.64
128.61
128.11
128.07
127.84
127.76
127.72
125.49
122.53
122.12
116.47
82.19
79.32
77.32
77.14
77.00
76.85
76.68
61.69
41.09
14.05
Current Data Parameters
NAME MS-03-15-CC-D
EXPNO 3
PROCNO 1
F1 - Acquisition parameters
FIDRES 1000.000000 Hz
SW 4.995 ppm
FnMODE undefined
F2 - Processing parameters
SI 65536
SF 100.6892682 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph
N
O
H
Ph
H
Ph
N
H
Ph
O
CO2Et
5a (dr > 20:1)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

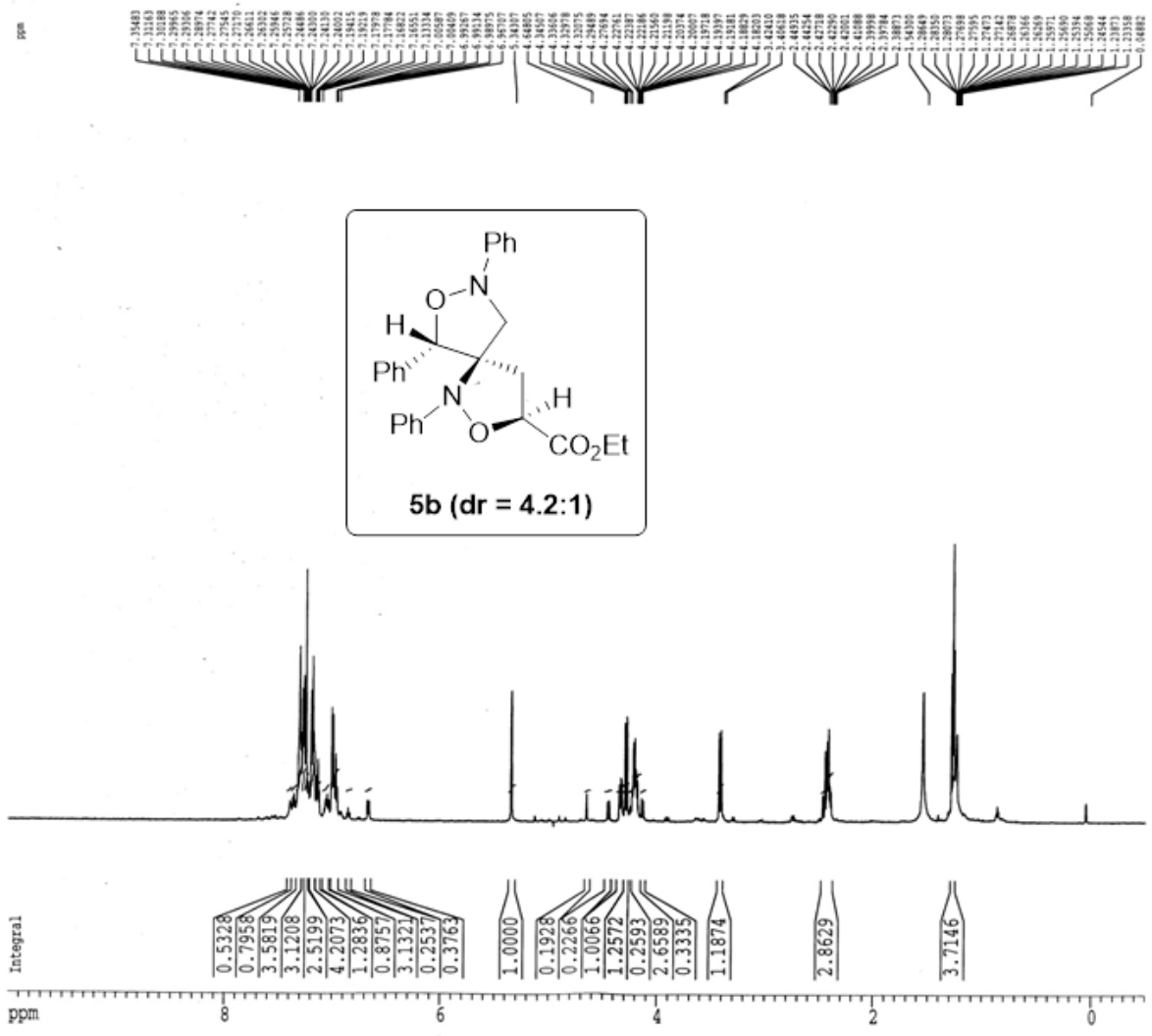
```
Current Data Parameters
NAME       PDJ-B-166-2nd
EXPNO                 1
PROCNO                1

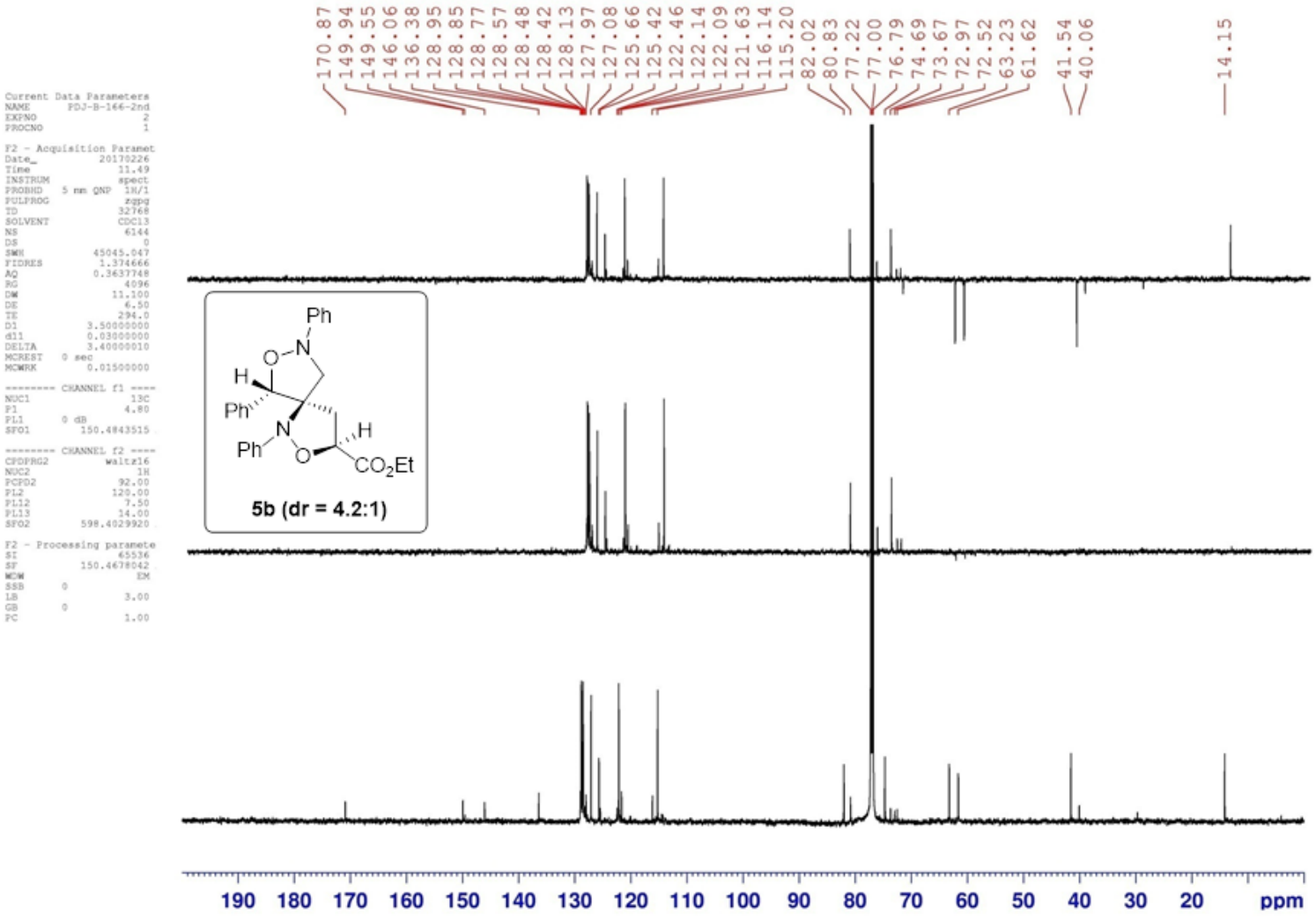
F2 - Acquisition Parameters
Date_          20170224
Time               9.48
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG             zg
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    0
SWH            9541.984 Hz
FIDRES         0.291198 Hz
AQ             1.7170932 sec
RG                  512
DW               52.400 usec
DE                6.50 usec
TE                295.2 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

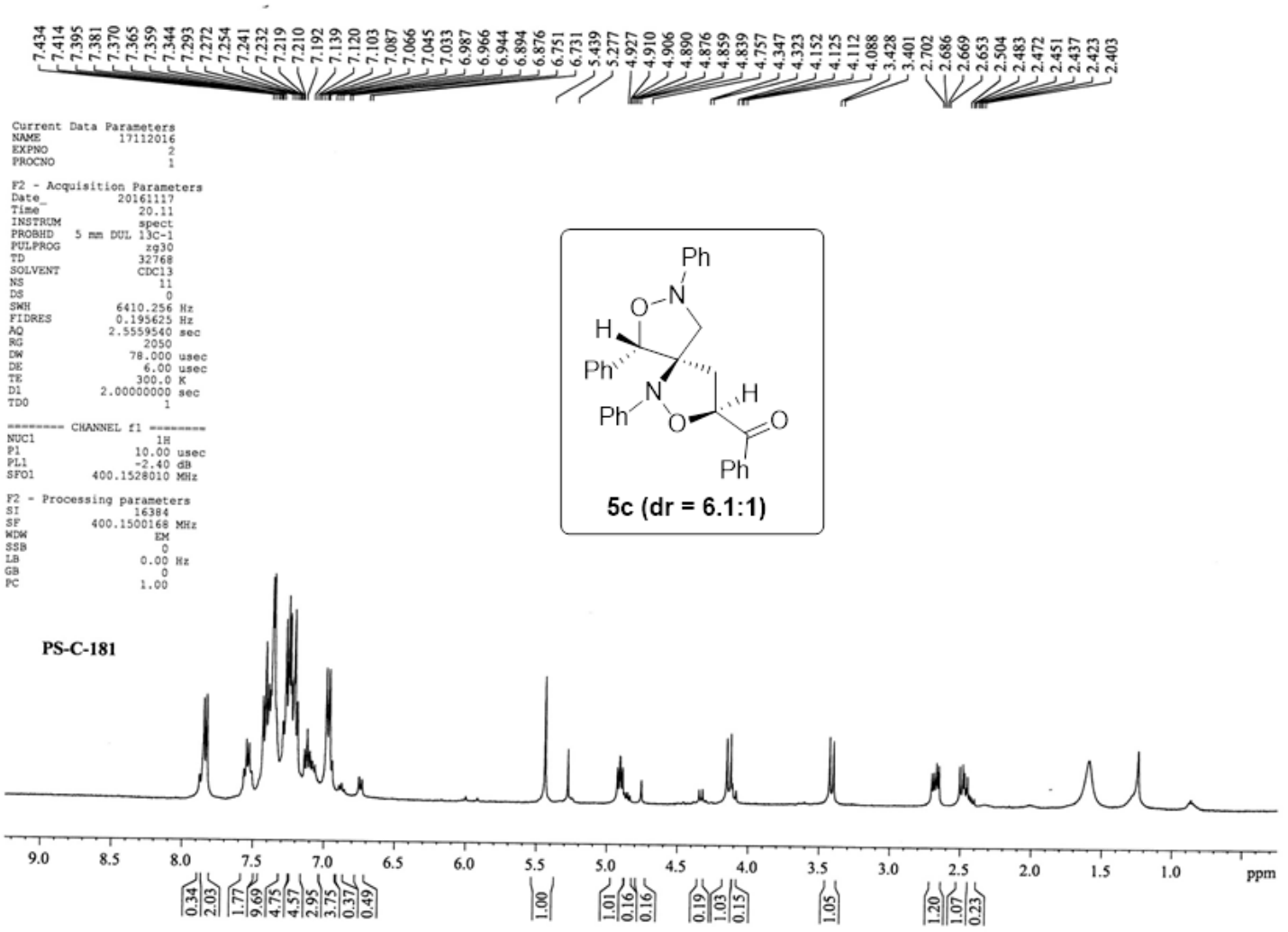
======== CHANNEL f1 ========
NUC1                 1H
P1                10.00 usec
PL1                0.00 dB
SFO1        598.4029920 MHz

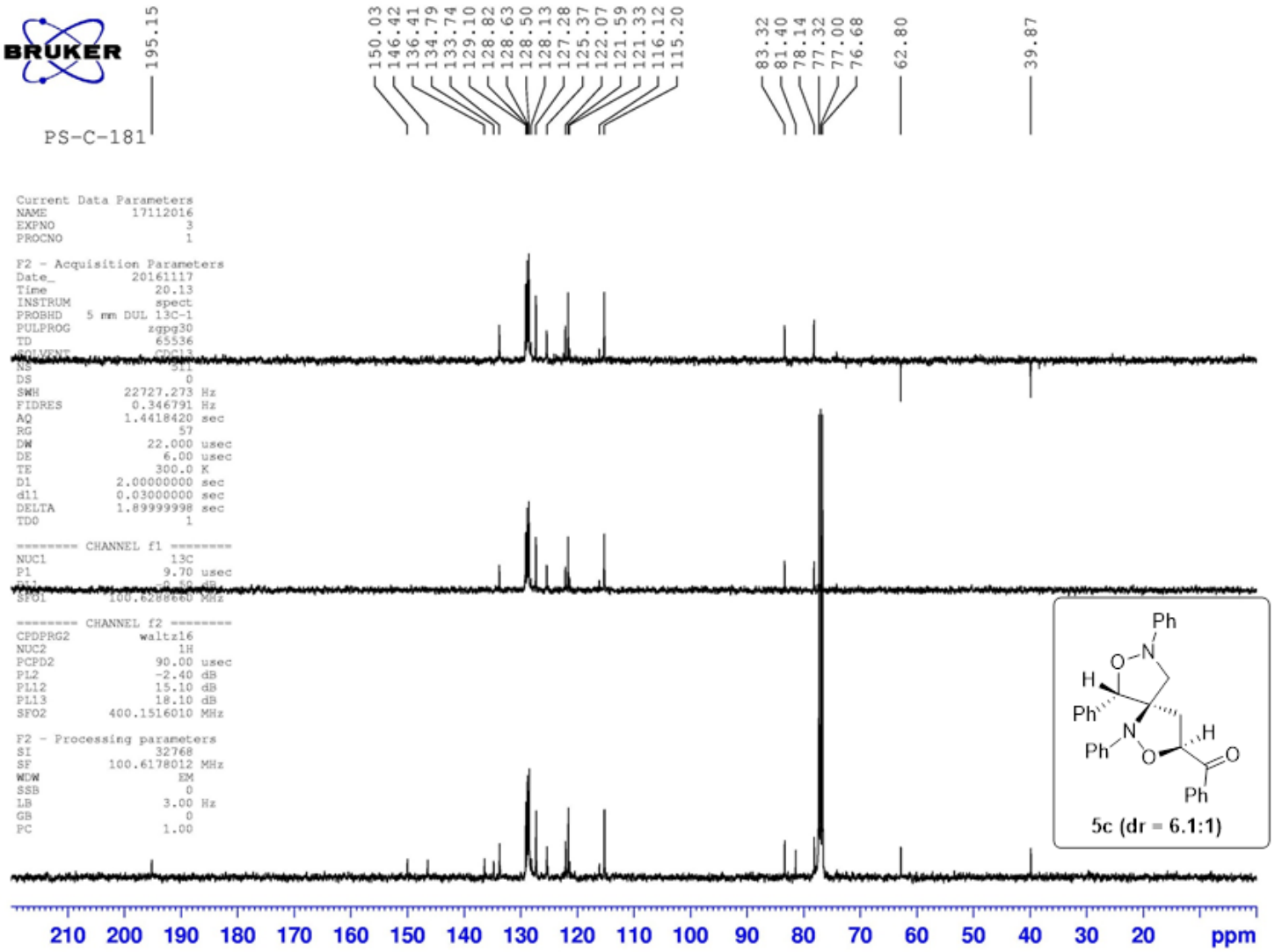
F2 - Processing parameters
SI                32768
SF          598.4000256 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00

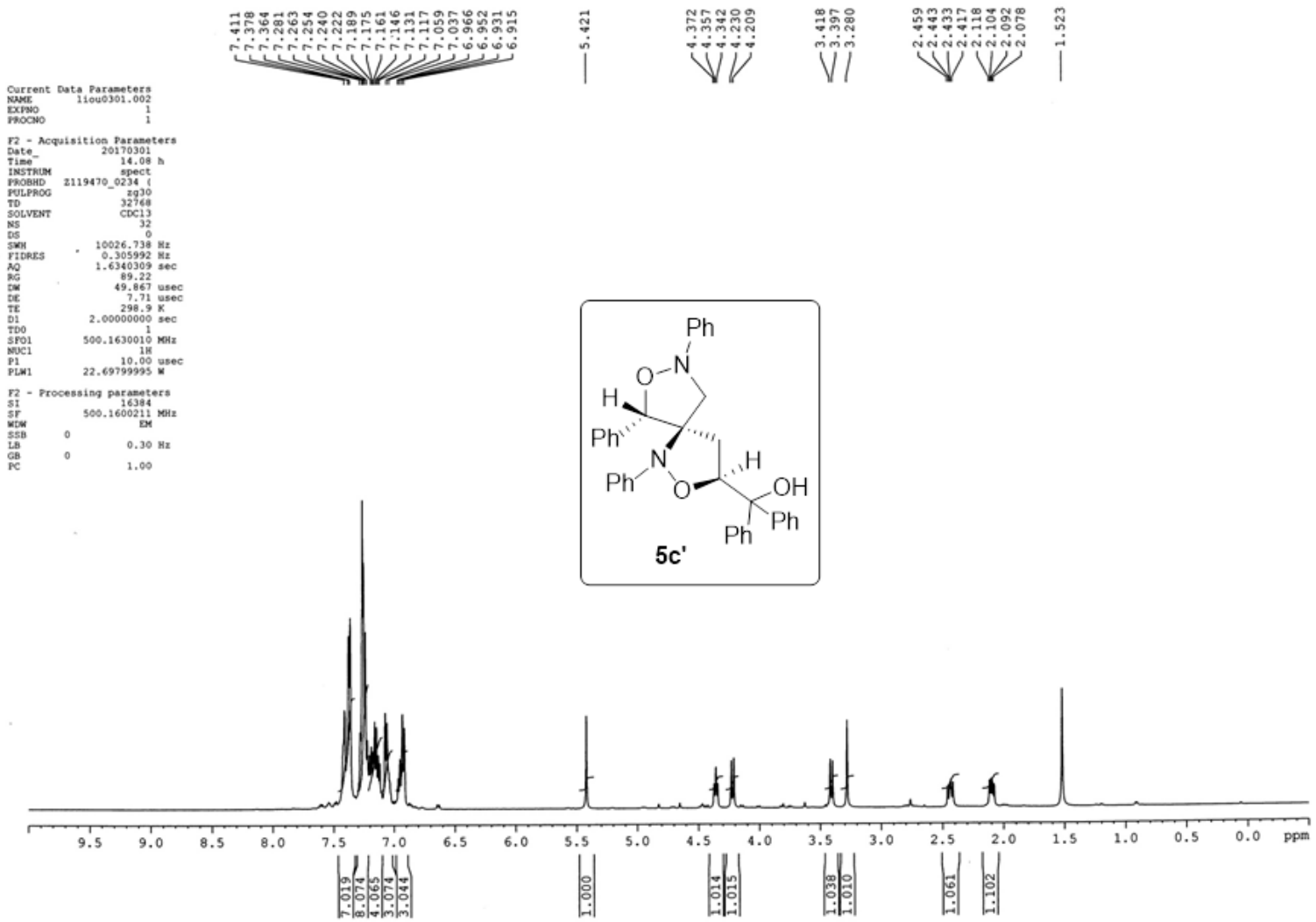
1D NMR plot parameters
CX                20.00 cm
CY                 5.00 cm
F1P               10.000 ppm
F1              5984.00 Hz
F2P               -0.500 ppm
F2              -299.20 Hz
PPMCM          0.52500 ppm/cm
HZCM         314.16000 Hz/cm
```

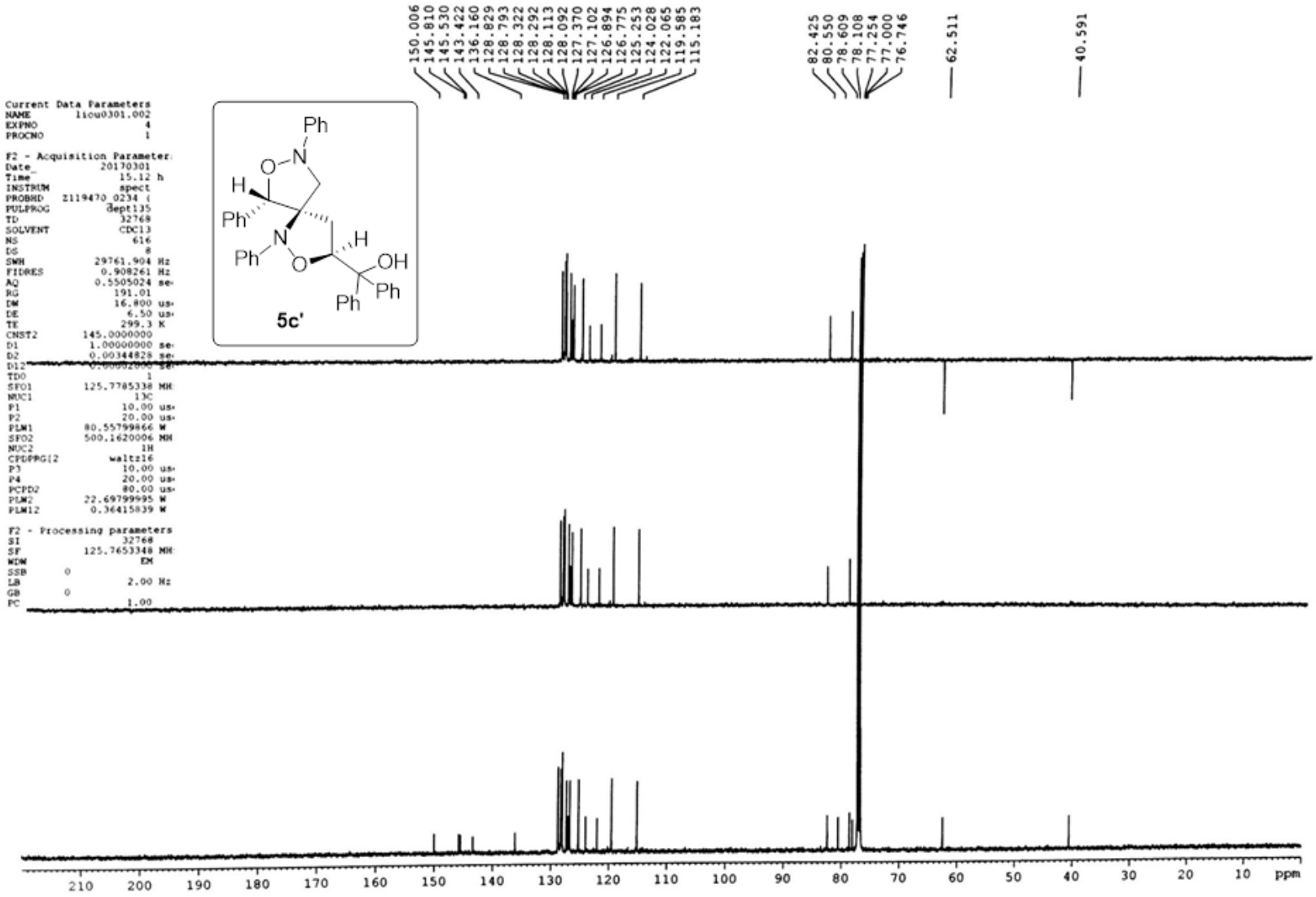


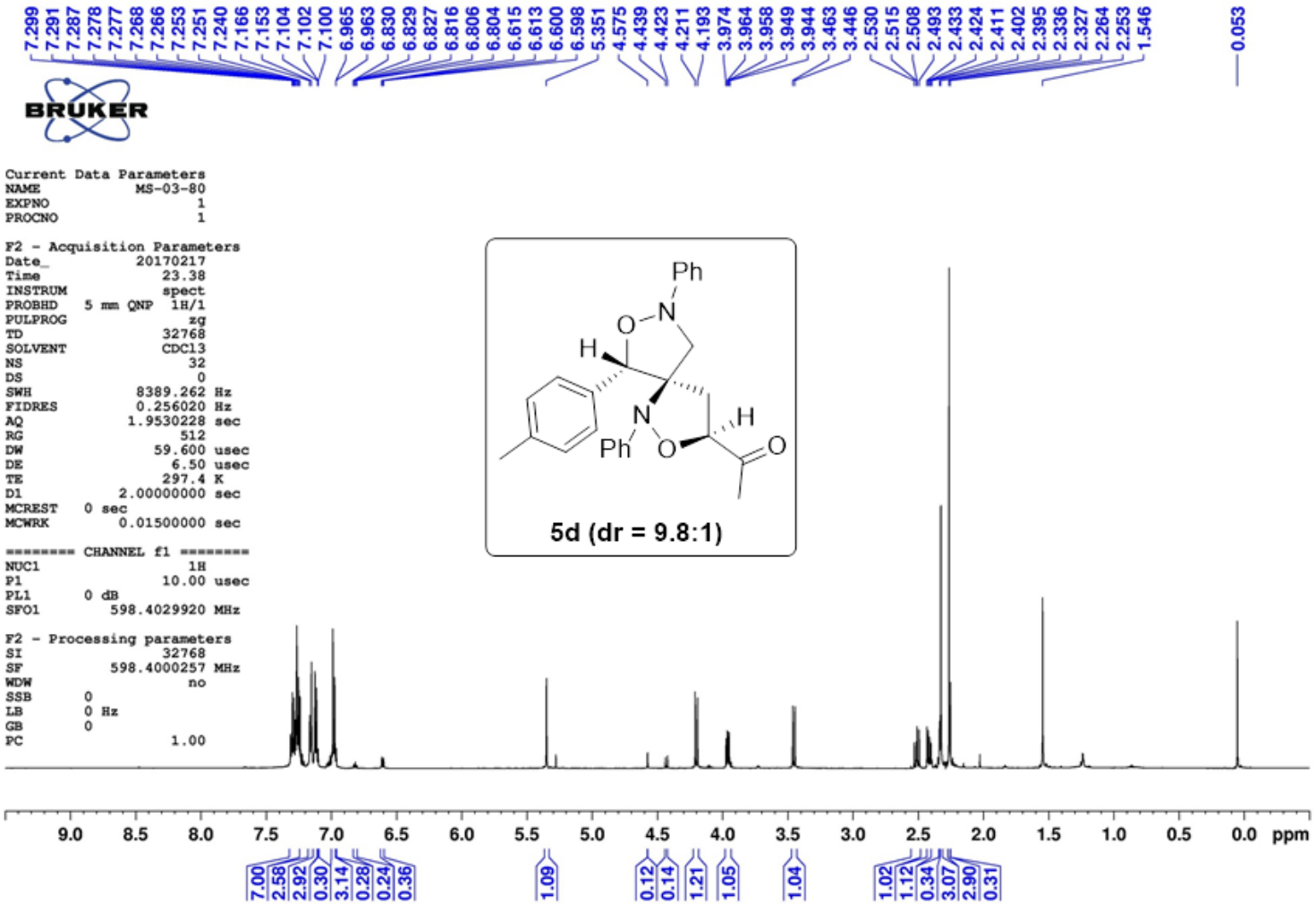

Current Data Parameters
NAME PDJ-B-166-2nd
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20170226
Time 11.49
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 294.0
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
-------- CHANNEL f1 ----
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.4843515
-------- CHANNEL f2 ----
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 7.50
PL13 14.00
SFO2 598.4029920
F2 - Processing paramete
SI 65536
SF 150.4678042
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
170.87
149.94
149.55
146.06
136.38
128.95
128.85
128.77
128.57
128.48
128.42
128.13
127.97
127.08
125.66
125.42
122.46
122.14
122.09
121.63
116.14
115.20
82.02
80.83
77.22
77.00
76.79
74.69
73.67
72.97
72.52
63.23
61.62
41.54
40.06
14.15
Ph
O
N
H
Ph
N
Ph
O
H
CO2Et
5b (dr = 4.2:1)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

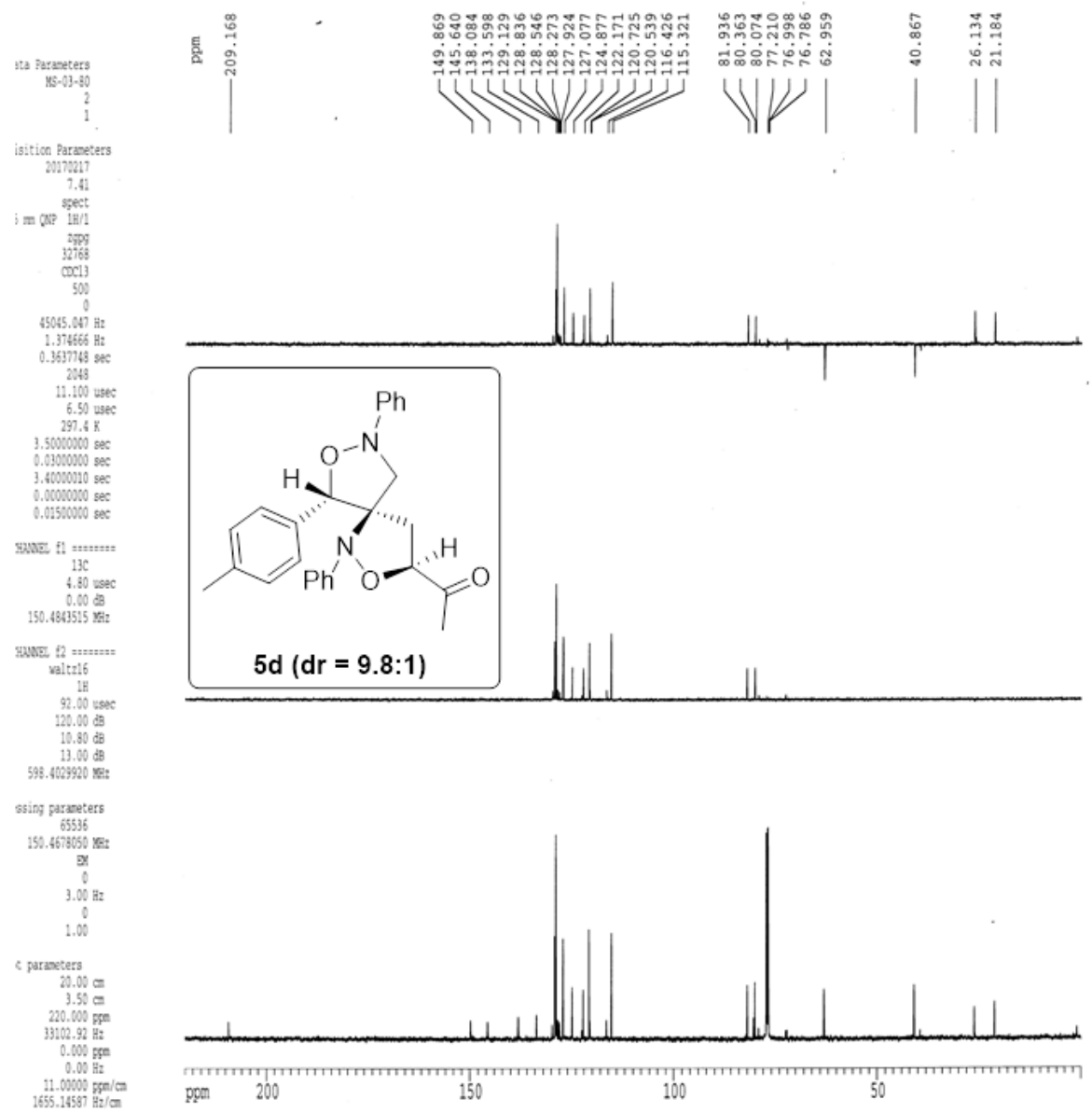

7.434
7.414
7.395
7.381
7.370
7.365
7.359
7.344
7.293
7.272
7.254
7.241
7.232
7.219
7.210
7.192
7.139
7.120
7.103
7.087
7.066
7.045
7.033
6.987
6.966
6.944
6.894
6.876
6.751
6.731
5.439
5.277
4.927
4.910
4.906
4.890
4.876
4.859
4.839
4.757
4.347
4.323
4.152
4.125
4.112
4.088
3.428
3.401
2.702
2.686
2.669
2.653
2.504
2.483
2.472
2.451
2.437
2.423
2.403
Current Data Parameters
NAME 17112016
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161117
Time 20.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 2050
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ph
O
N
H
Ph
N
H
Ph
O
O
Ph
5c (dr = 6.1:1)
PS-C-181
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
ppm
0.34
2.03
1.77
9.69
4.75
4.57
2.95
3.75
0.37
0.49
1.00
1.01
0.16
0.16
0.19
1.03
0.15
1.05
1.20
1.07
0.23

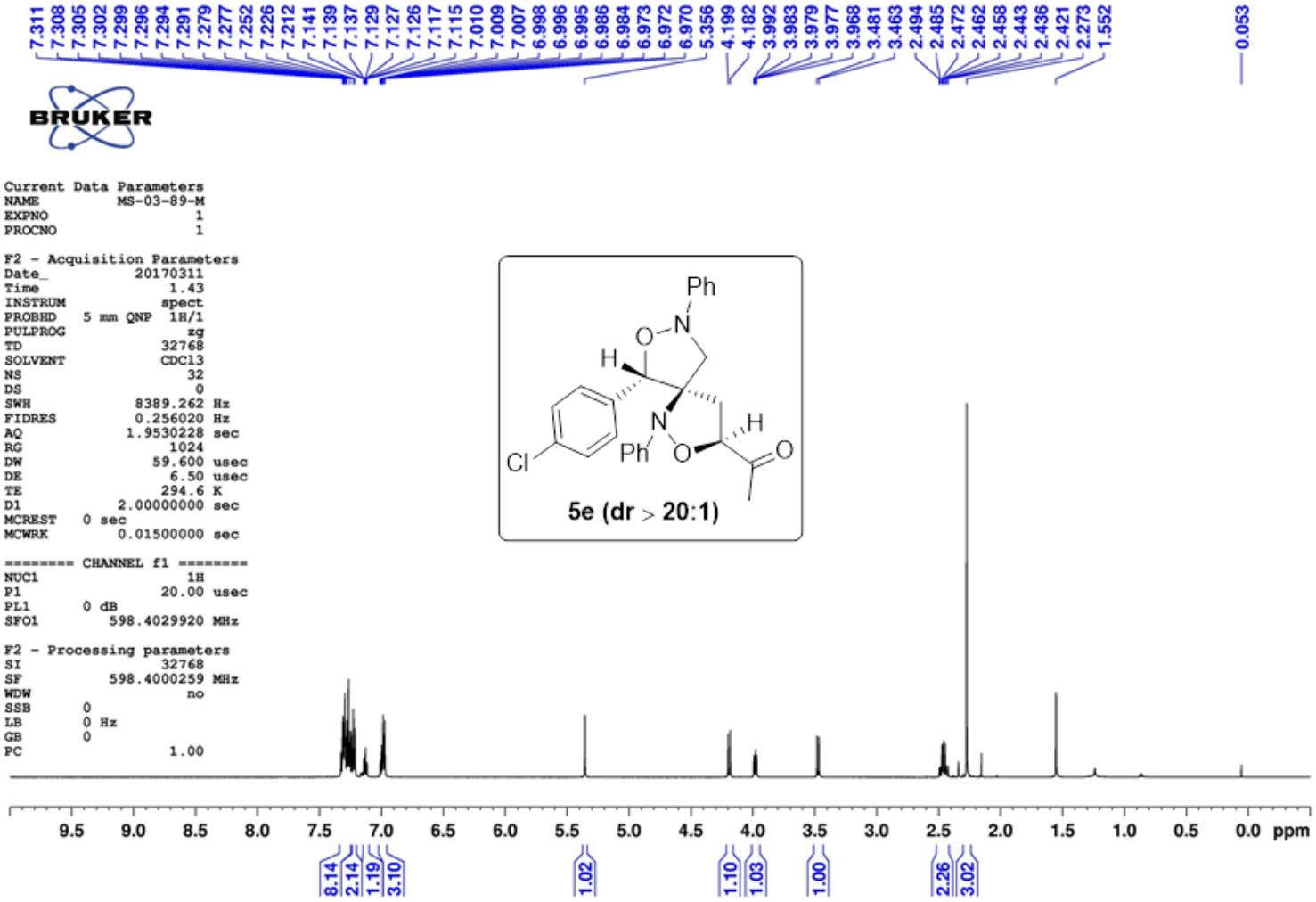

BRUKER
PS-C-181
195.15
150.03
146.42
136.41
134.79
133.74
129.10
128.82
128.63
128.50
128.13
127.28
125.37
122.07
121.59
121.33
116.12
115.20
83.32
81.40
78.14
77.32
77.00
76.68
62.80
39.87
Current Data Parameters
NAME 17112016
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161117
Time 20.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -2.58 dB
SFO1 100.6280660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178012 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
N
H
Ph
N
Ph
O
H
O
Ph
5c (dr = 6.1:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

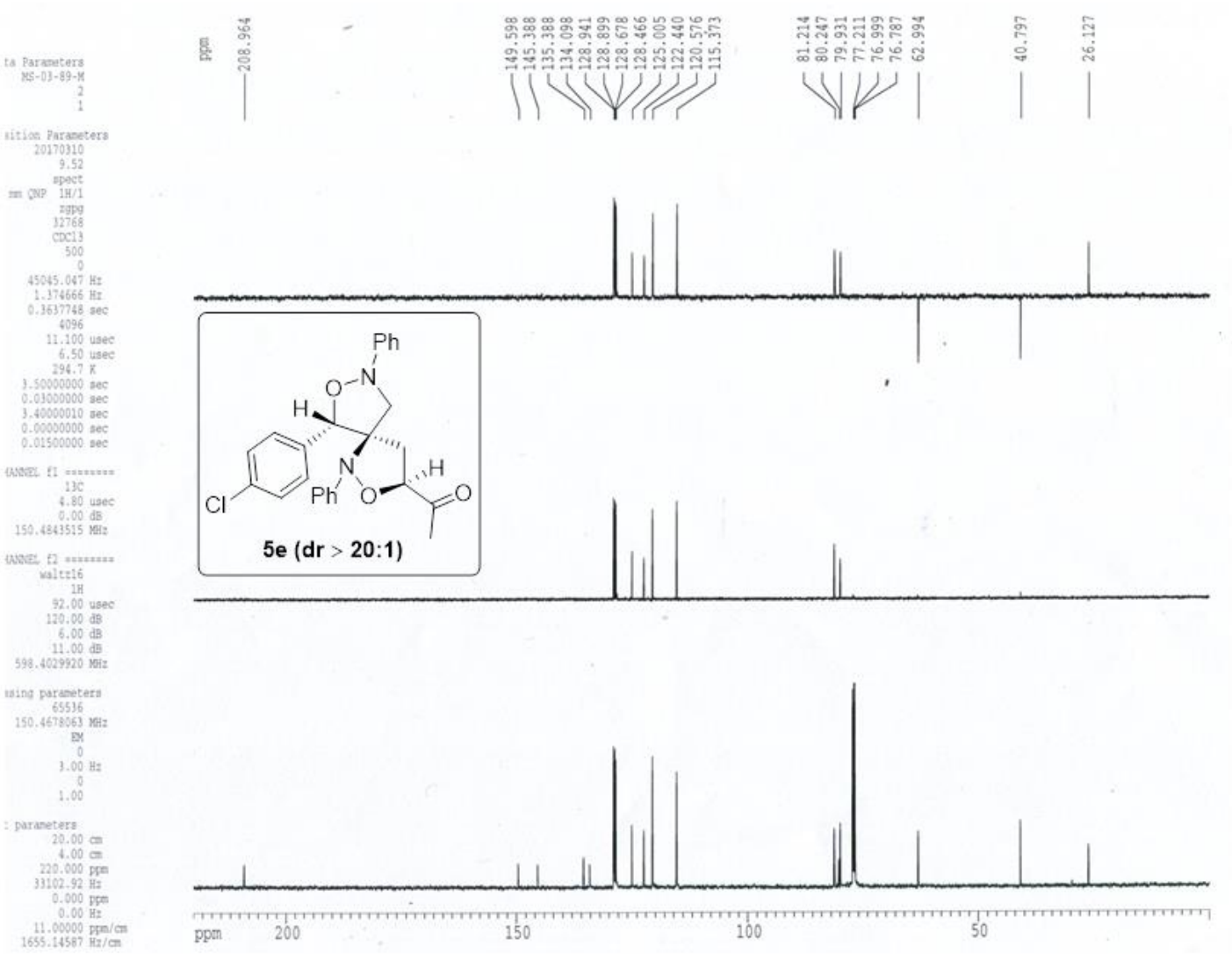

7.411
7.378
7.364
7.281
7.263
7.254
7.240
7.222
7.189
7.175
7.161
7.146
7.131
7.117
7.059
7.037
6.966
6.952
6.931
6.915
5.421
4.372
4.357
4.342
4.230
4.209
3.418
3.397
3.280
2.459
2.443
2.433
2.417
2.118
2.104
2.092
2.078
1.523
Current Data Parameters
NAME liou0301.002
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20170301
Time 14.08 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 10026.738 Hz
FIDRES 0.305992 Hz
AQ 1.6340309 sec
RG 89.22
DW 49.867 usec
DE 7.71 usec
TE 298.9 K
D1 2.00000000 sec
TD0 1
SFO1 500.1630010 MHz
NUC1 1H
P1 10.00 usec
PLW1 22.69799995 W
F2 - Processing parameters
SI 16384
SF 500.1600211 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
O
N
H
Ph
N
H
Ph
O
OH
Ph
Ph
5c'
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
ppm
7.019
8.074
4.065
3.074
3.044
1.000
1.014
1.015
1.038
1.010
1.061
1.102

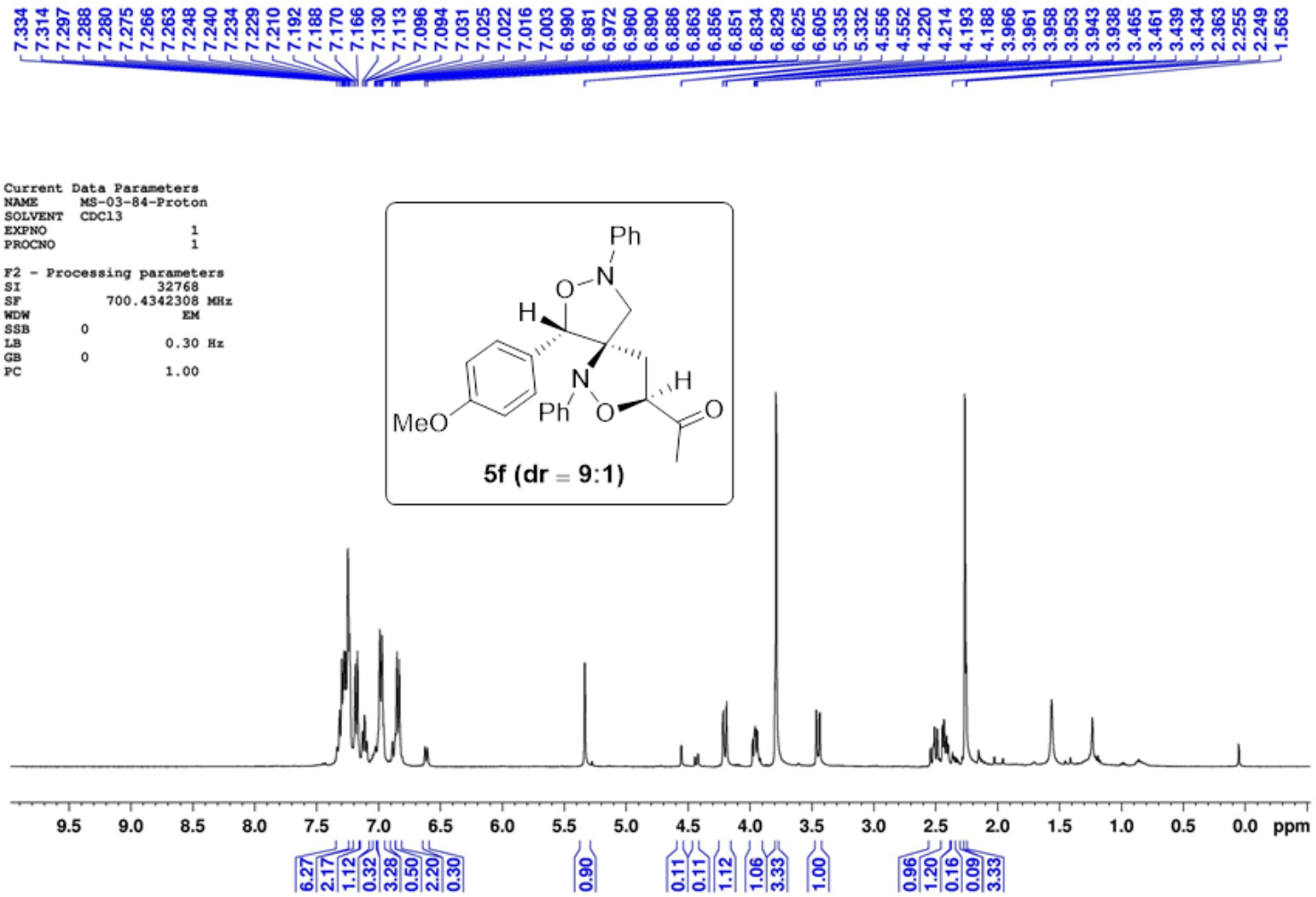

150.006
145.810
145.530
143.422
136.160
128.829
128.793
128.322
128.292
128.113
128.092
127.370
127.102
126.894
126.775
125.253
124.028
122.065
119.585
115.183
82.425
80.550
78.609
78.108
77.254
77.000
76.746
62.511
40.591
Current Data Parameters
NAME 1icou0301.002
EXPNO 4
PROCNO 1
F2 - Acquisition Parameter
Date 20170301
Time 15.12 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG dept135
TD 32768
SOLVENT CDCl3
NS 616
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505024 se
RG 191.01
DW 16.800 us
DE 6.50 us
TE 299.3 K
CNST2 145.0000000
D1 1.00000000 se
D2 0.00344828 se
D12 0.00002000 se
TD0 1
SFO1 125.7785338 MH
NUC1 13C
P1 10.00 us
P2 20.00 us
PLW1 80.55799866 W
SFO2 500.1620006 MH
NUC2 1H
CPDPRG[2 waltz16
P3 10.00 us
P4 20.00 us
PCPD2 80.00 us
PLW2 22.69799995 W
PLW12 0.36415839 W
F2 - Processing parameters
SI 32768
SF 125.7653348 MH
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
Ph
O
N
H
Ph
N
Ph
O
H
OH
Ph
Ph
5c'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

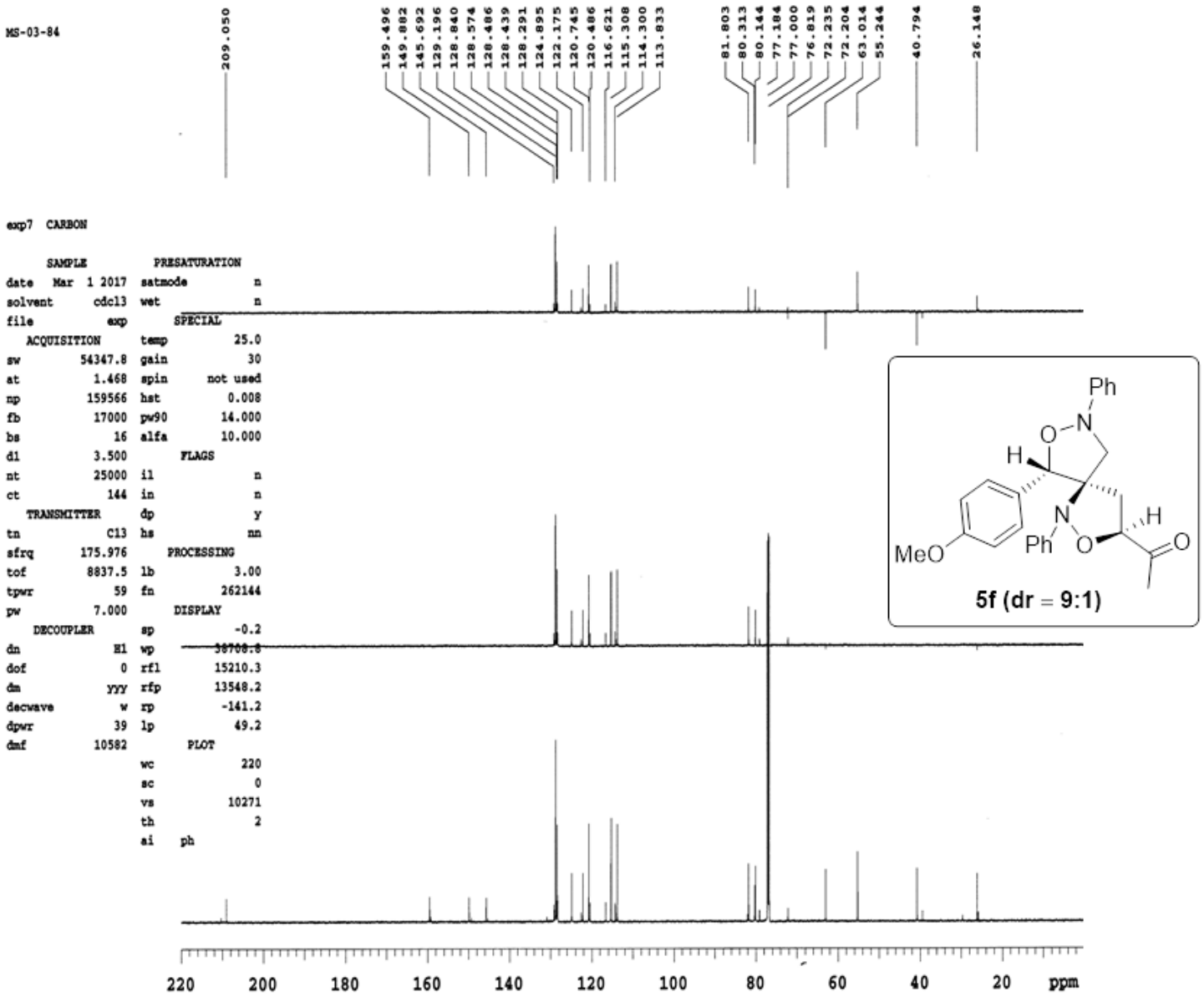

7.299
7.291
7.287
7.278
7.277
7.268
7.266
7.253
7.251
7.240
7.166
7.153
7.104
7.102
7.100
6.965
6.963
6.830
6.829
6.827
6.816
6.806
6.804
6.615
6.613
6.600
6.598
5.351
4.575
4.439
4.423
4.211
4.193
3.974
3.964
3.958
3.949
3.944
3.463
3.446
2.530
2.515
2.508
2.493
2.433
2.424
2.411
2.402
2.395
2.336
2.327
2.264
2.253
1.546
0.053
BRUKER
Current Data Parameters
NAME MS-03-80
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170217
Time 23.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000257 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
N
H
N
H
Ph
O
O
5d (dr = 9.8:1)
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
ppm
7.00
2.58
2.92
0.30
3.14
0.28
0.24
0.36
1.09
0.12
0.14
1.21
1.05
1.04
1.02
1.12
0.34
3.07
2.90
0.31

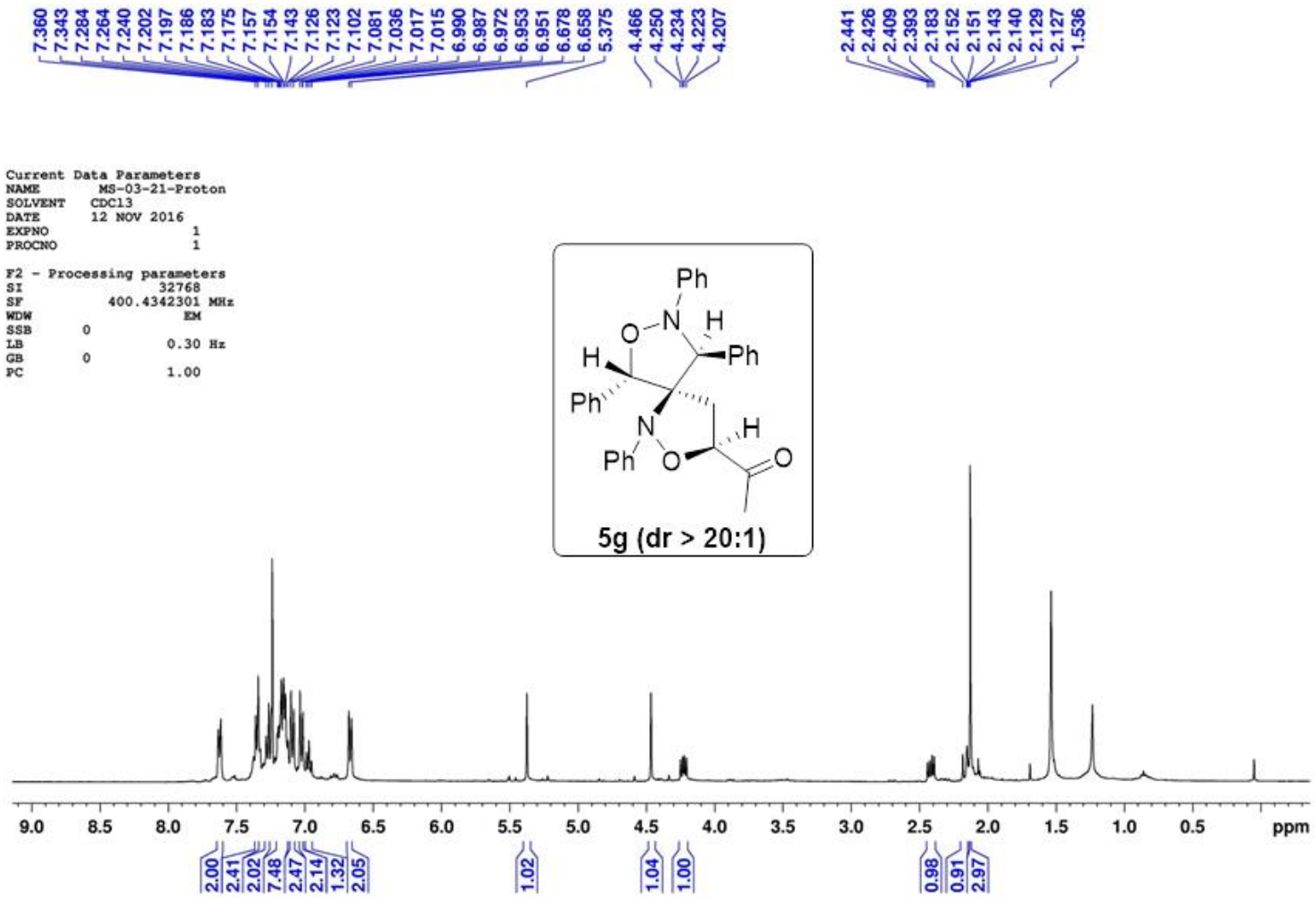

ppm
209.168
149.869
145.640
138.084
133.598
129.129
128.836
128.546
128.273
127.924
127.077
124.877
122.171
120.725
120.539
116.426
115.321
81.936
80.363
80.074
77.210
76.998
76.786
62.959
40.867
26.134
21.184
Ph
N
O
H
N
Ph
O
H
O
5d (dr = 9.8:1)
ppm
200
150
100
50

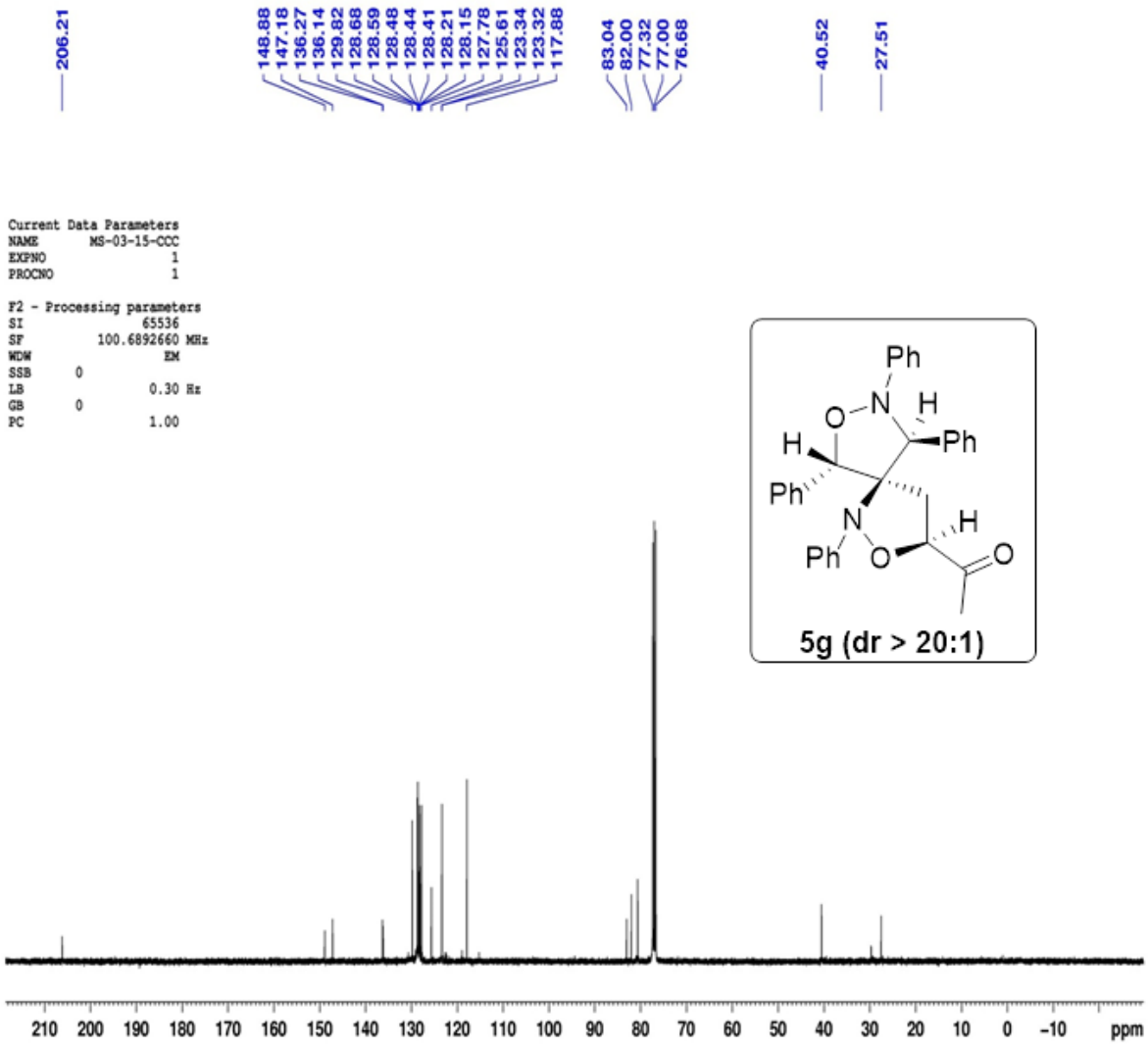

7.311
7.308
7.305
7.302
7.299
7.296
7.294
7.291
7.279
7.277
7.252
7.226
7.212
7.141
7.139
7.137
7.129
7.127
7.126
7.117
7.115
7.010
7.009
7.007
6.998
6.996
6.995
6.986
6.984
6.973
6.972
6.970
5.356
4.199
4.182
3.992
3.983
3.979
3.977
3.968
3.481
3.463
2.494
2.485
2.472
2.462
2.458
2.443
2.436
2.421
2.273
1.552
0.053
BRUKER
Current Data Parameters
NAME MS-03-89-M
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170311
Time 1.43
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 1024
DW 59.600 usec
DE 6.50 usec
TE 294.6 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 20.00 usec
PL1 0 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000259 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
N
H
N
H
Ph
O
O
Cl
5e (dr > 20:1)
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 ppm
8.14
2.14
1.19
3.10
1.02
1.10
1.03
1.00
2.26
3.02

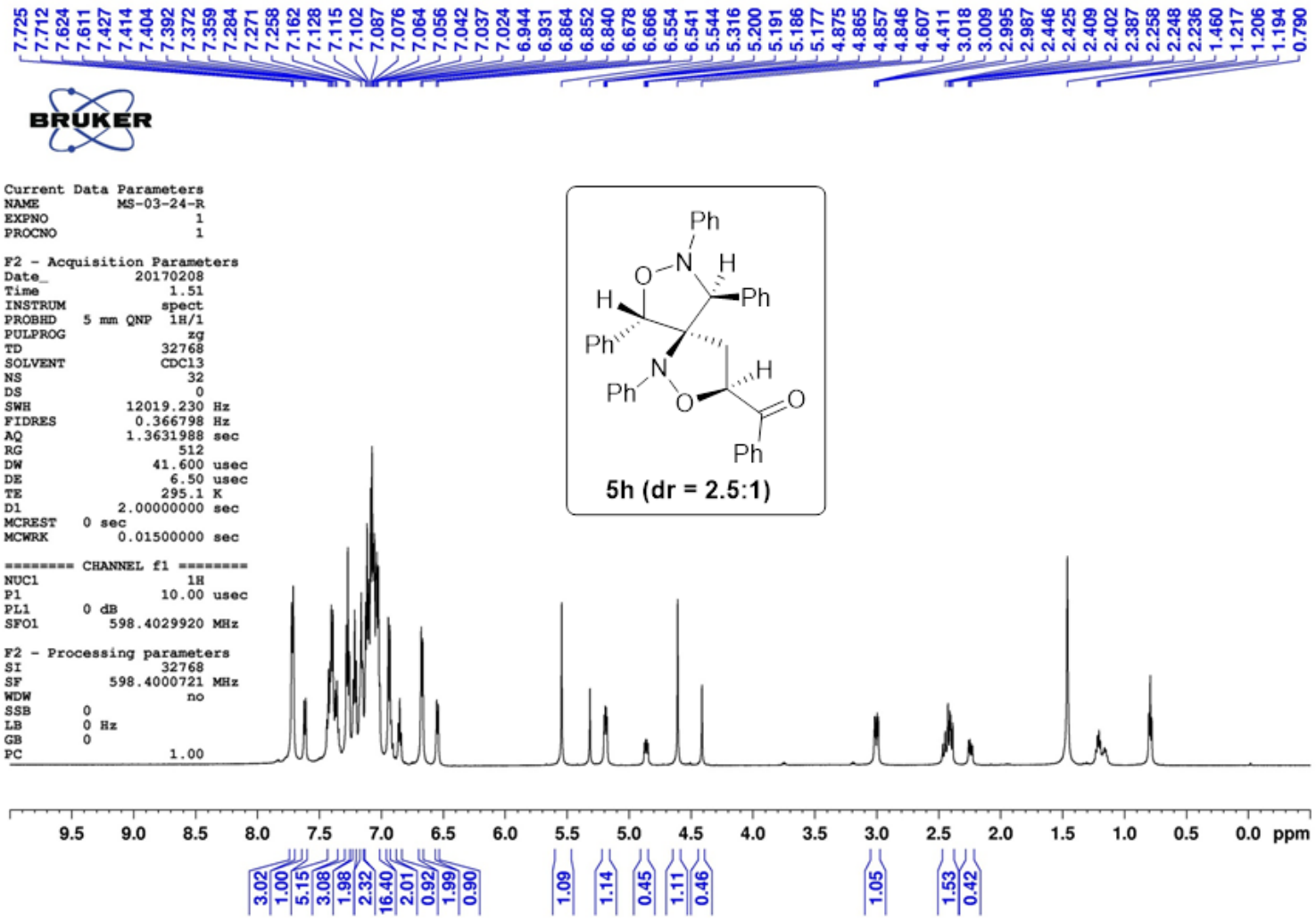

ppm
208.964
149.598
145.388
135.388
134.098
128.941
128.899
128.678
128.466
125.005
122.440
120.576
115.373
81.214
80.247
79.931
77.211
76.999
76.787
62.994
40.797
26.127
Ph
N
O
H
N
H
Ph
O
O
Cl
5e (dr > 20:1)
ppm
200
150
100
50

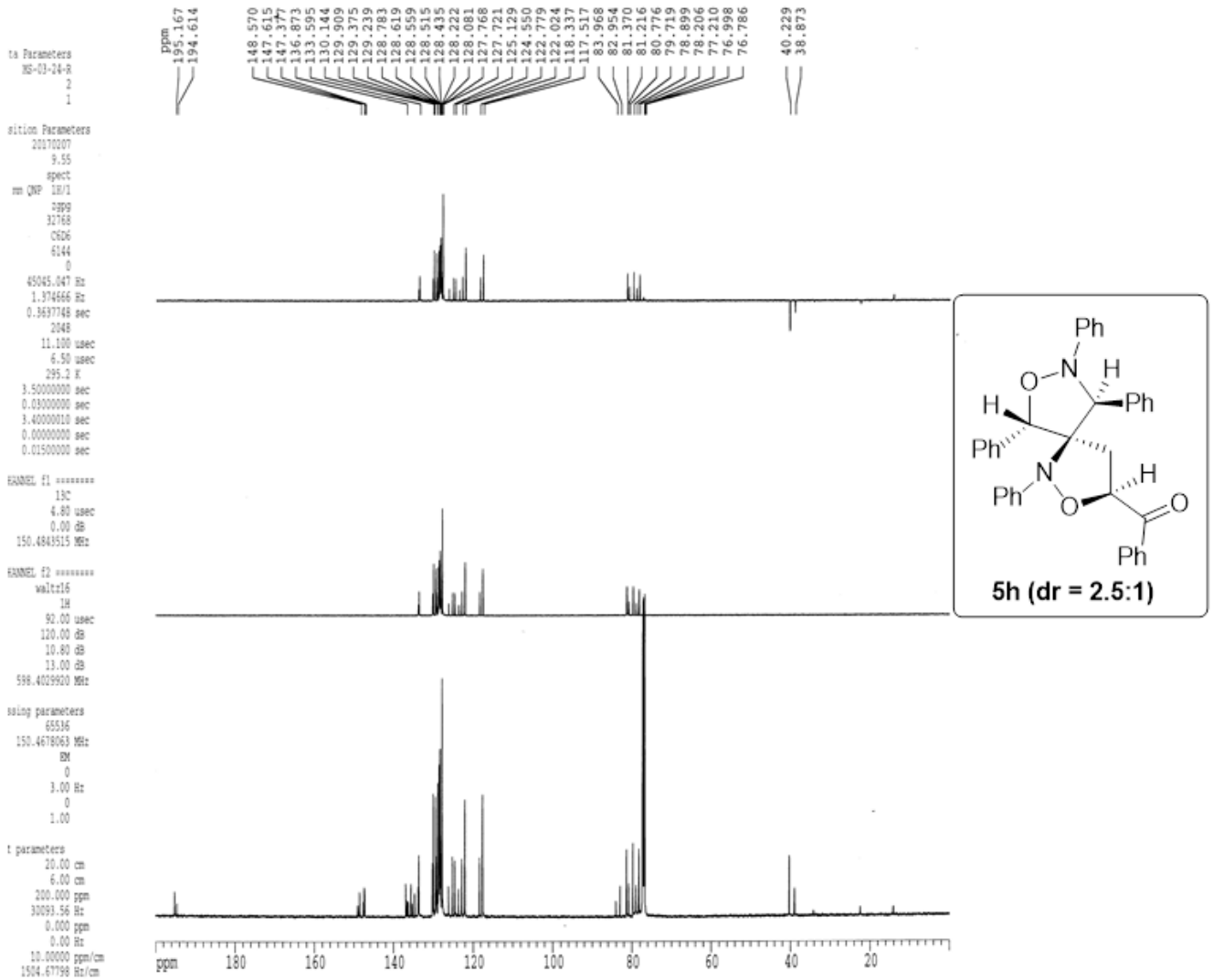

7.334 7.314 7.297 7.288 7.280 7.275 7.266 7.263 7.248 7.240 7.234 7.229 7.210 7.192 7.188 7.170 7.166 7.130 7.113 7.096 7.094 7.031 7.025 7.022 7.016 7.003 6.990 6.981 6.972 6.960 6.890 6.886 6.863 6.856 6.851 6.834 6.829 6.625 6.605 5.335 5.332 4.556 4.552 4.220 4.214 4.193 4.188 3.966 3.961 3.958 3.953 3.943 3.938 3.465 3.461 3.439 3.434 2.363 2.255 2.249 1.563
Current Data Parameters
NAME MS-03-84-Proton
SOLVENT CDCl3
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 700.4342308 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
O
N
H
N
H
Ph
O
O
MeO
5f (dr = 9:1)
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 ppm
6.27 2.17 1.12 0.32 3.28 0.50 2.20 0.30 0.90 0.11 0.11 1.12 1.06 3.33 1.00 0.96 1.20 0.16 0.09 3.33

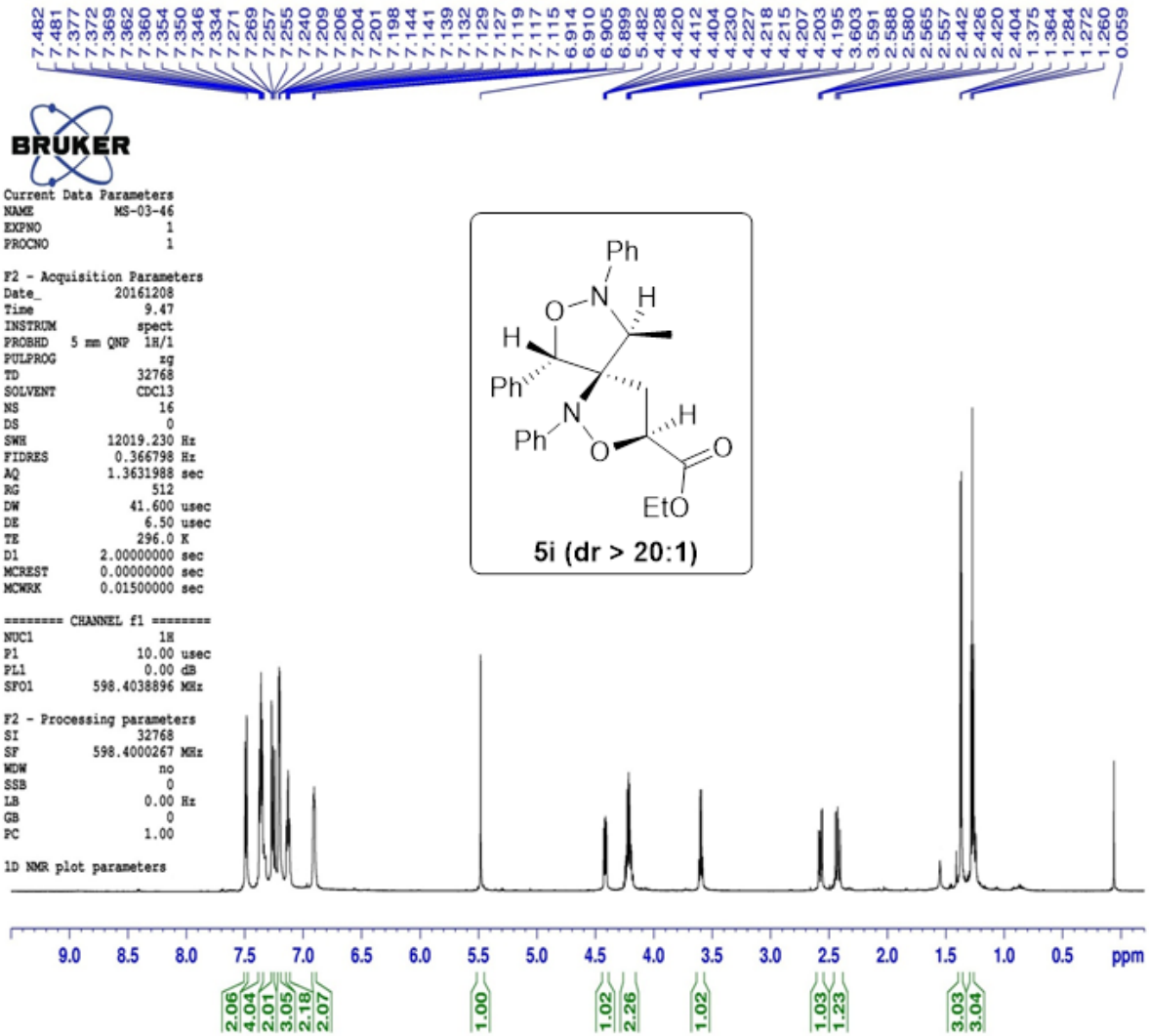

MS-03-84
209.050
159.496
149.882
145.692
129.196
128.840
128.574
128.486
128.439
128.291
124.895
122.175
120.745
120.486
116.621
115.308
114.300
113.833
81.803
80.313
80.144
77.184
77.000
76.819
72.235
72.204
63.014
55.244
40.794
26.148
exp7 CARBON
SAMPLE
date Mar 1 2017
solvent cdcl3
file exp
ACQUISITION
sw 54347.8
at 1.468
np 159566
fb 17000
bs 16
d1 3.500
nt 25000
ct 144
TRANSMITTER
tn C13
sfrq 175.976
tof 8837.5
tpwr 59
pw 7.000
DECOUPLER
dn H1
dof 0
dm yyy
decwave w
dpwr 39
dmf 10582
PRESATURATION
satmode n
wet n
SPECIAL
temp 25.0
gain 30
spin not used
hst 0.008
pw90 14.000
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 3.00
fn 262144
DISPLAY
sp -0.2
wp 38708.8
rfl 15210.3
rfp 13548.2
rp -141.2
lp 49.2
PLOT
wc 220
sc 0
vs 10271
th 2
ai ph
Ph
O
N
H
N
H
Ph
O
O
MeO
5f (dr = 9:1)
220
200
180
160
140
120
100
80
60
40
20
ppm

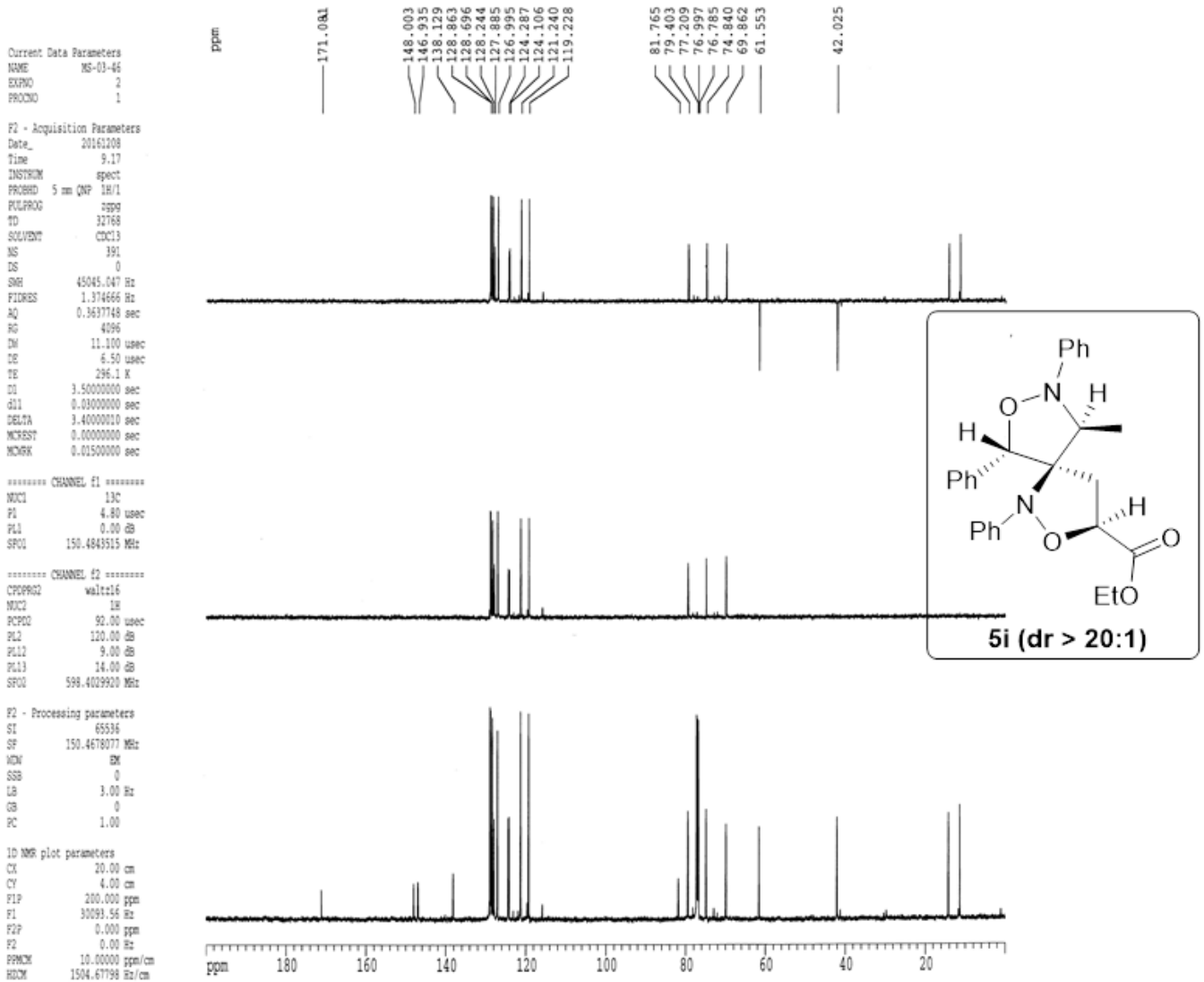

7.360
7.343
7.284
7.264
7.240
7.202
7.197
7.186
7.183
7.175
7.157
7.154
7.143
7.126
7.123
7.102
7.081
7.036
7.017
7.015
6.990
6.987
6.972
6.953
6.951
6.678
6.658
5.375
4.466
4.250
4.234
4.223
4.207
2.441
2.426
2.409
2.393
2.183
2.152
2.151
2.143
2.140
2.129
2.127
1.536
Current Data Parameters
NAME MS-03-21-Proton
SOLVENT CDCl3
DATE 12 NOV 2016
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 400.4342301 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
N
H
O
H
Ph
Ph
N
H
Ph
O
O
5g (dr > 20:1)
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
ppm
2.00
2.41
2.02
7.48
2.47
2.14
1.32
2.05
1.02
1.04
1.00
0.98
0.91
2.97


206.21
148.88
147.18
136.27
136.14
129.82
128.68
128.59
128.48
128.44
128.41
128.21
128.15
127.78
125.61
123.34
123.32
117.88
83.04
82.00
77.32
77.00
76.68
40.52
27.51
Current Data Parameters
NAME MS-03-15-CCC
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.6892660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
O
N
H
H
Ph
Ph
N
H
Ph
O
O
5g (dr > 20:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


7.725 7.712 7.624 7.611 7.427 7.414 7.404 7.392 7.372 7.359 7.284 7.271 7.258 7.162 7.128 7.115 7.102 7.087 7.076 7.064 7.056 7.042 7.037 7.024 6.944 6.931 6.864 6.852 6.840 6.678 6.666 6.554 6.541 5.544 5.316 5.200 5.191 5.186 5.177 4.875 4.865 4.857 4.846 4.607 4.411 3.018 3.009 2.995 2.987 2.446 2.425 2.409 2.402 2.387 2.258 2.248 2.236 1.460 1.217 1.206 1.194 0.790
BRUKER
Current Data Parameters
NAME MS-03-24-R
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170208
Time 1.51
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000721 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
N
H
O
Ph
H
Ph
N
H
Ph
O
O
Ph
5h (dr = 2.5:1)
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 ppm
3.02 1.00 5.15 3.08 1.98 2.32 16.40 2.01 0.92 1.99 0.90 1.09 1.14 0.45 1.11 0.46 1.05 1.53 0.42


ppm
195.167
194.614
148.570
147.615
147.377
136.873
133.595
130.144
129.909
129.375
129.239
128.783
128.619
128.559
128.515
128.435
128.222
128.081
127.768
127.721
125.129
124.550
122.779
122.024
118.337
117.517
83.968
82.954
81.370
81.216
80.776
79.719
78.899
78.206
77.210
76.998
76.786
40.229
38.873
ppm
180
160
140
120
100
80
60
40
20
Ph
N
H
O
Ph
H
Ph
Ph
N
H
Ph
O
O
Ph
5h (dr = 2.5:1)


7.482
7.481
7.377
7.372
7.369
7.362
7.360
7.354
7.350
7.346
7.334
7.271
7.269
7.257
7.255
7.240
7.209
7.206
7.204
7.201
7.198
7.144
7.141
7.139
7.132
7.129
7.127
7.119
7.117
7.115
6.914
6.910
6.905
6.899
5.482
4.428
4.420
4.412
4.404
4.230
4.227
4.218
4.215
4.207
4.203
4.195
3.603
3.591
2.588
2.580
2.565
2.557
2.442
2.426
2.420
2.404
1.375
1.364
1.284
1.272
1.260
0.059
BRUKER
Current Data Parameters
NAME MS-03-46
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161208
Time 9.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.4038896 MHz
F2 - Processing parameters
SI 32768
SF 598.4000267 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
Ph
N
H
O
H
Ph
Ph
N
H
O
O
EtO
5i (dr > 20:1)
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
ppm
2.06
4.04
2.01
3.05
2.18
2.07
1.00
1.02
2.26
1.02
1.03
1.23
3.03
3.04


Current Data Parameters
NAME MS-03-46
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161208
Time 9.17
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 391
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678077 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67798 Hz/cm
ppm
171.081
148.003
146.935
138.129
128.863
128.696
128.244
127.885
126.995
124.287
124.106
121.240
119.228
81.765
79.403
77.209
76.997
76.785
74.840
69.862
61.553
42.025
Ph
N
H
O
H
Ph
N
Ph
H
O
O
EtO
5i (dr > 20:1)
ppm
180
160
140
120
100
80
60
40
20

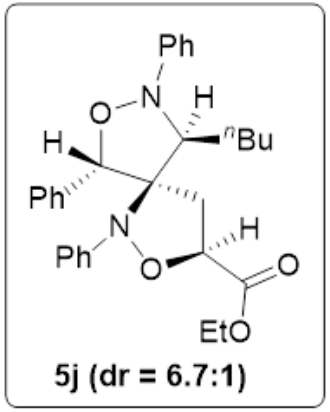
PS-C-199-A-

```
Current Data Parameters
NAME                 09032017
EXPNO                       1
PROCNO                      1

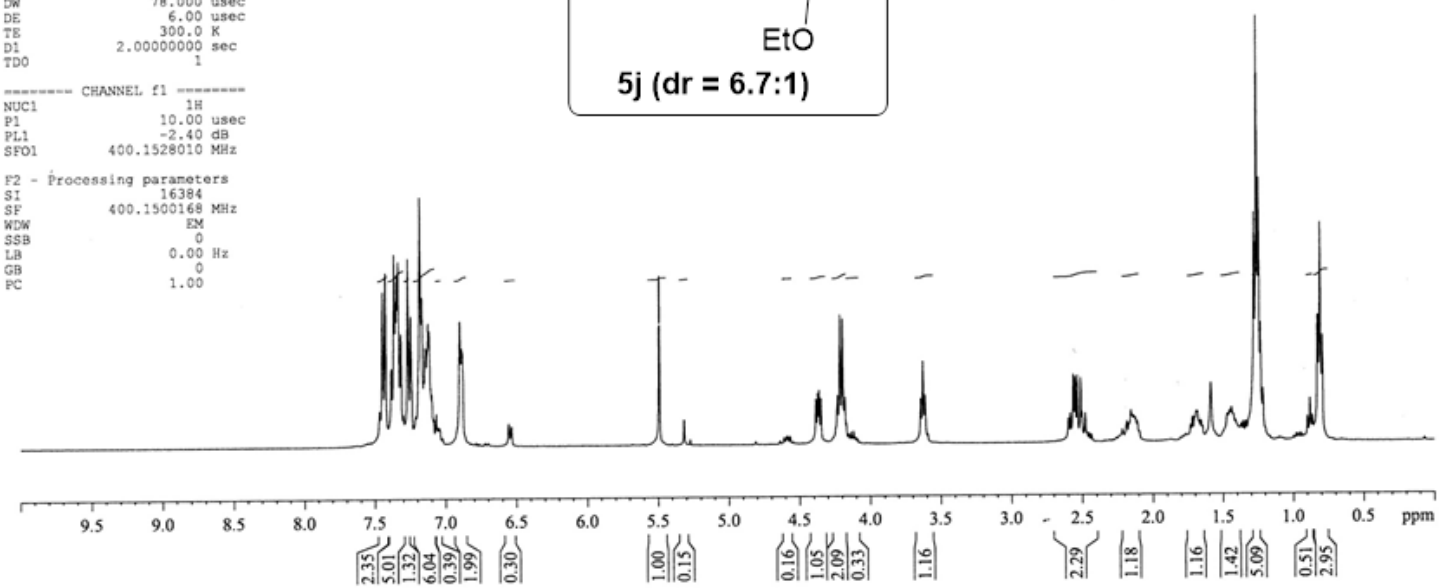
F2 - Acquisition Parameters
Date_               20170309
Time                   23.04
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                6410.256 Hz
FIDRES             0.195625 Hz
AQ                 2.5559540 sec
RG                      101
DW                   78.000 usec
DE                    6.00 usec
TE                   300.0 K
D1                2.00000000 sec
TD0                         1

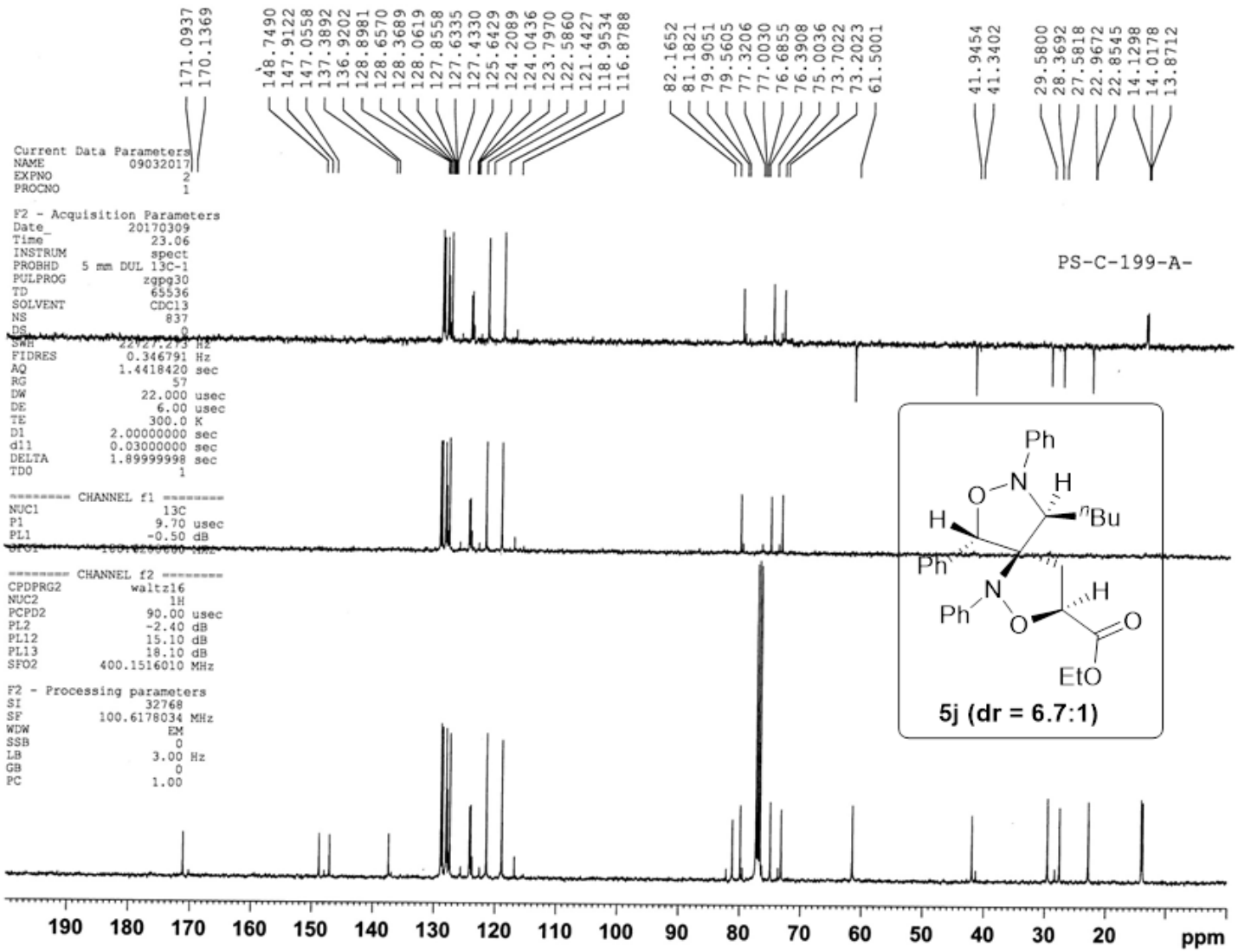
======== CHANNEL f1 ========
NUC1                       1H
P1                      10.00 usec
PL1                     -2.40 dB
SFO1              400.1528010 MHz

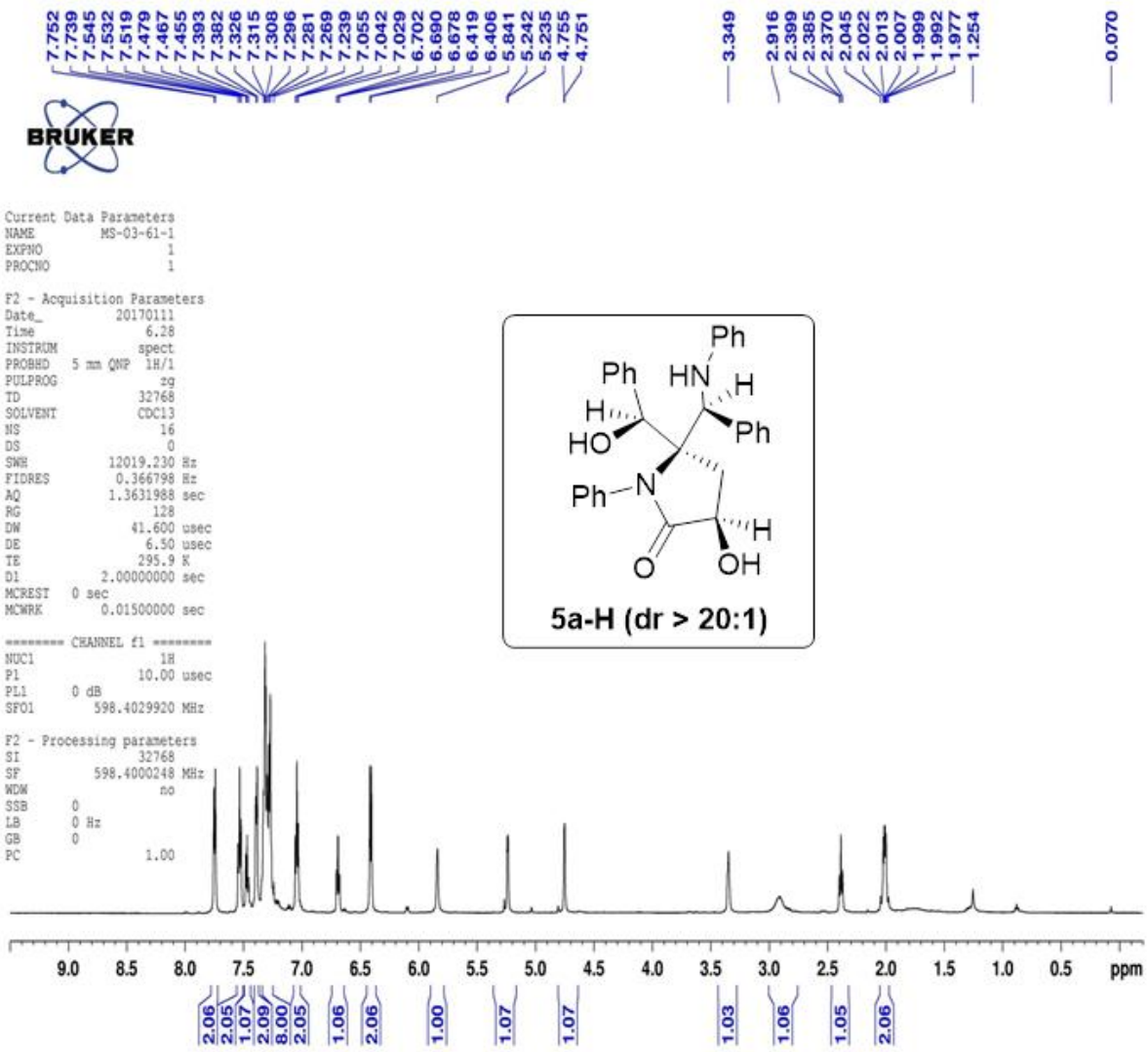
F2 - Processing parameters
SI                      16384
SF                400.1500168 MHz
WDW                        EM
SSB                         0
LB                       0.00 Hz
GB                          0
PC                       1.00
```

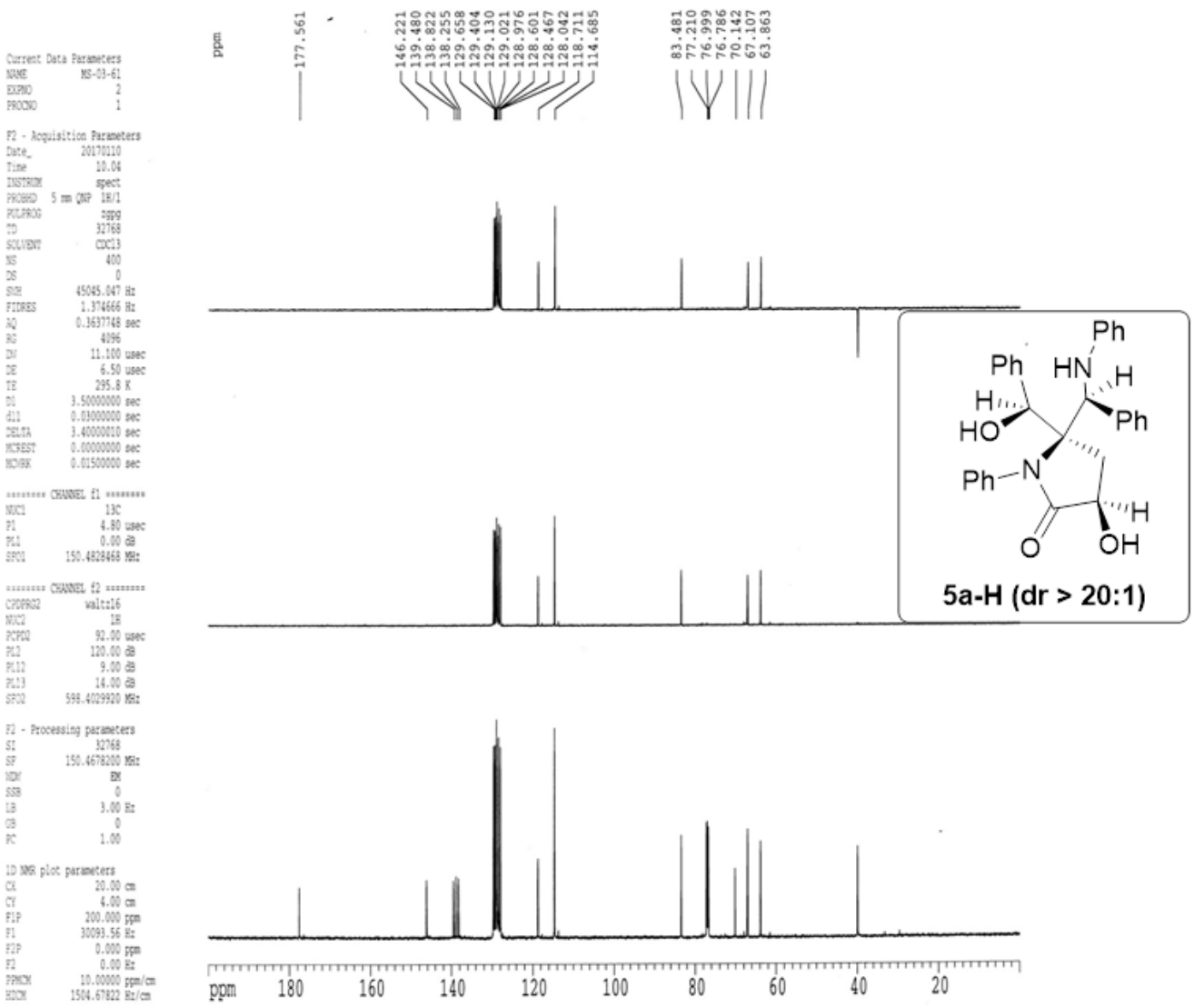


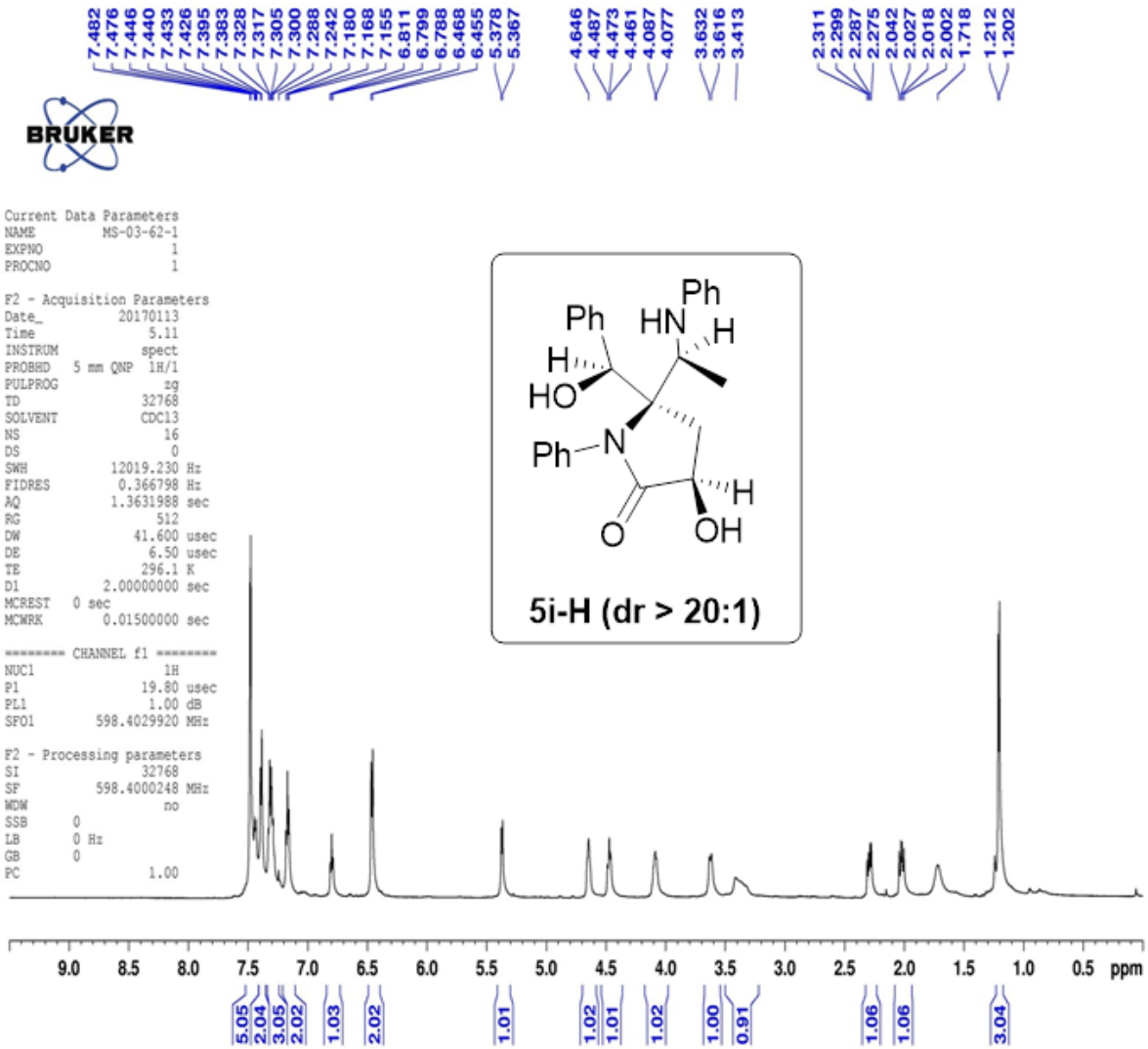
5j (dr = 6.7:1)

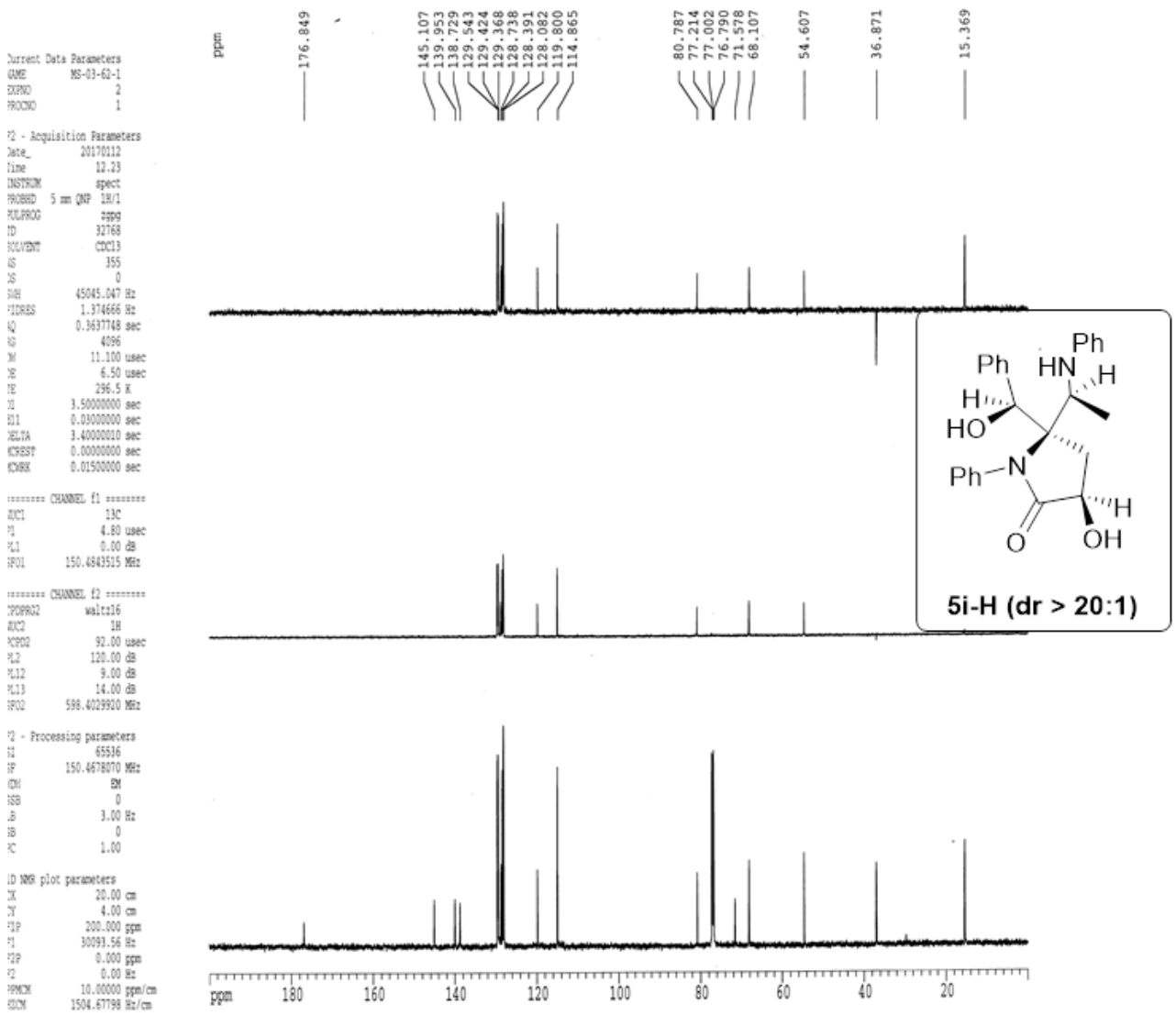



171.0937
170.1369
148.7490
147.9122
147.0558
137.3892
136.9202
128.8981
128.6570
128.3689
128.0619
127.8558
127.6335
127.4330
125.6429
124.2089
124.0436
123.7970
122.5860
121.4427
118.9534
116.8788
82.1652
81.1821
79.9051
79.5605
77.3206
77.0030
76.6855
76.3908
75.0036
73.7022
73.2023
61.5001
41.9454
41.3402
29.5800
28.3692
27.5818
22.9672
22.8545
14.1298
14.0178
13.8712
Current Data Parameters
NAME 09032017
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170309
Time 23.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 837
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6293600 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178034 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
PS-C-199-A-
Ph
N
H
O
H
nBu
Ph
Ph
N
H
O
O
EtO
5j (dr = 6.7:1)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.752
7.739
7.545
7.532
7.519
7.479
7.467
7.455
7.393
7.382
7.326
7.315
7.308
7.296
7.281
7.269
7.239
7.055
7.042
7.029
6.702
6.690
6.678
6.419
6.406
5.841
5.242
5.235
4.755
4.751
3.349
2.916
2.399
2.385
2.370
2.045
2.022
2.013
2.007
1.999
1.992
1.977
1.254
0.070
BRUKER
Current Data Parameters
NAME MS-03-61-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170111
Time 6.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 128
DW 41.600 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000248 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
Ph
HN
H
H
Ph
HO
Ph
N
H
O
OH
5a-H (dr > 20:1)
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
ppm
2.06
2.05
1.07
2.09
8.00
2.05
1.06
2.06
1.00
1.07
1.07
1.03
1.06
1.05
2.06


Current Data Parameters
NAME MS-03-61
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170110
Time 10.04
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 400
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.8 K
D1 3.50000000 sec
D11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.4828468 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 150.4678200 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67822 Hz/cm
ppm
177.561
146.221
139.480
138.822
138.255
129.658
129.404
129.130
129.021
128.976
128.601
128.467
128.042
118.711
114.685
83.481
77.210
76.999
76.786
70.142
67.107
63.863
ppm 180 160 140 120 100 80 60 40 20
Ph
HN
H
Ph
H
HO
Ph
Ph
N
H
O
OH
5a-H (dr > 20:1)


7.482
7.476
7.446
7.440
7.433
7.426
7.395
7.383
7.328
7.317
7.305
7.300
7.288
7.242
7.180
7.168
7.155
6.811
6.799
6.788
6.468
6.455
5.378
5.367
4.646
4.487
4.473
4.461
4.087
4.077
3.632
3.616
3.413
2.311
2.299
2.287
2.275
2.042
2.027
2.018
2.002
1.718
1.212
1.202
BRUKER
Current Data Parameters
NAME MS-03-62-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170113
Time 5.11
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 19.80 usec
PL1 1.00 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000248 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
HN
H
Ph
H
HO
Ph
N
H
O
OH
5i-H (dr > 20:1)
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
ppm
5.05
2.04
3.05
2.02
1.03
2.02
1.01
1.02
1.01
1.02
1.00
0.91
1.06
1.06
3.04




```
Current Data Parameters
NAME          MS-03-62-1
EXPNO                  2
PROCNO                 1

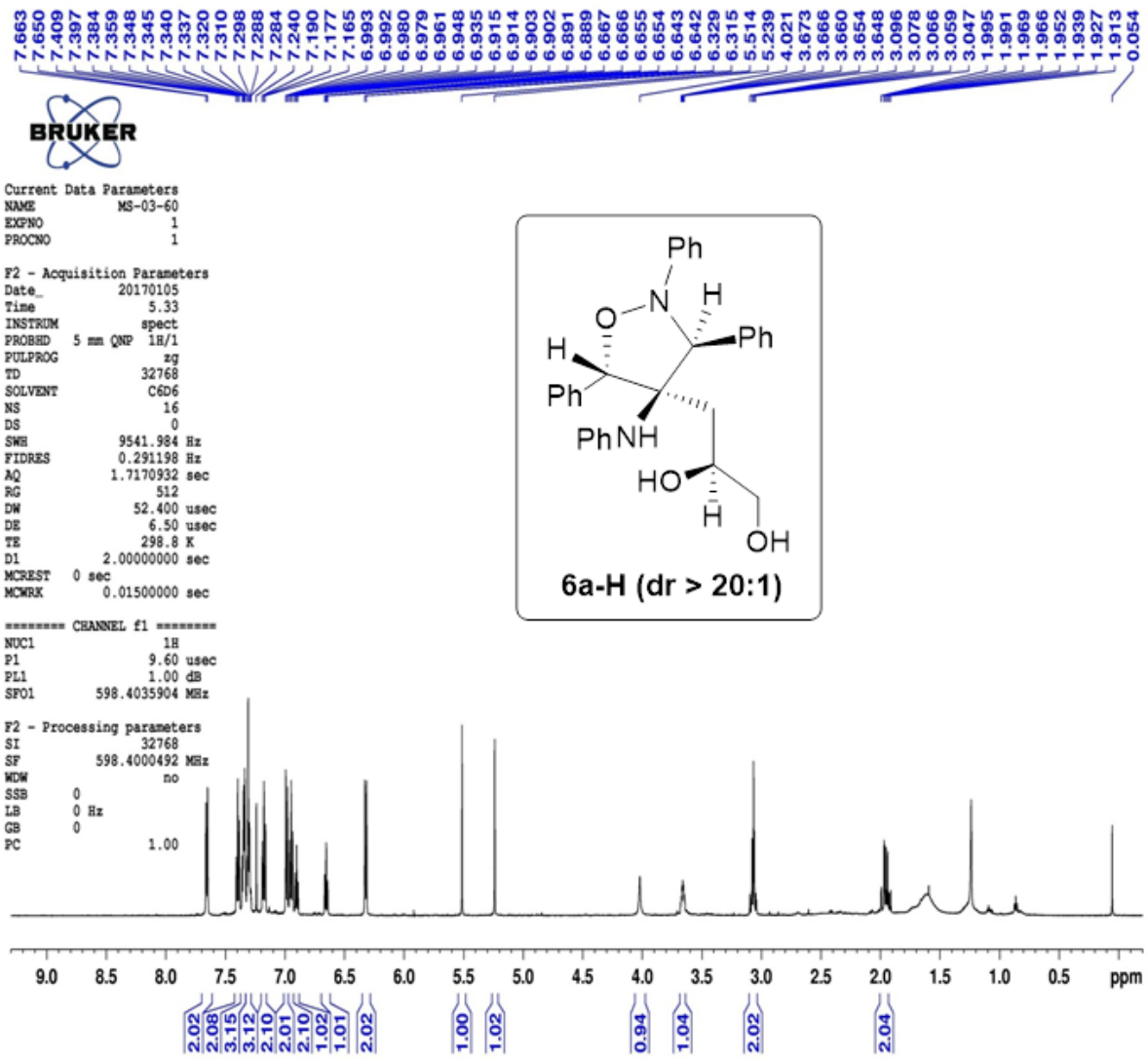
F2 - Acquisition Parameters
Date_          20170112
Time              12.23
INSTRUM           spect
PROBHD  5 mm CNP  1H/1
PULPROG           zgpg
TD                32768
SOLVENT           CDCl3
NS                  355
DS                    0
SWH           45045.047 Hz
FIDRES        1.374666 Hz
AQ            0.3637748 sec
RG                 4096
DW               11.100 usec
DE                6.50 usec
TE              296.5 K
D1            3.50000000 sec
D11           0.03000000 sec
DELTA         3.40000010 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

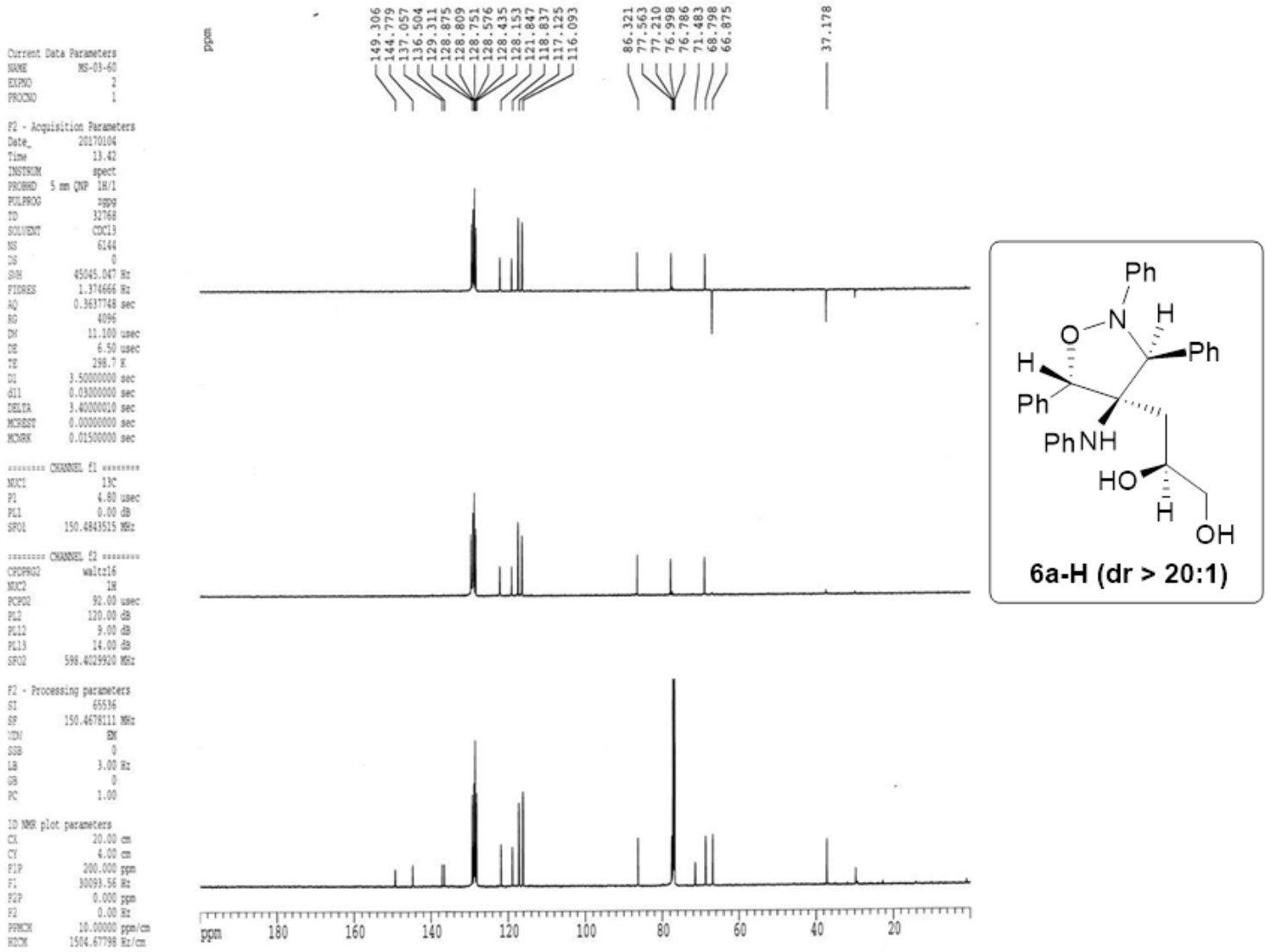
======== CHANNEL f1 ========
NUC1               13C
P1                4.80 usec
PL1               0.00 dB
SFO1        150.4843515 MHz

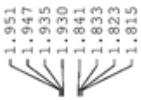
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             92.00 usec
PL2              120.00 dB
PL12               9.00 dB
PL13              14.00 dB
SFO2        598.4029920 MHz

F2 - Processing parameters
SI                 65536
SF          150.4678070 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                20.00 cm
CY                 4.00 cm
F1P             200.000 ppm
F1              30093.56 Hz
F2P               0.000 ppm
F2                0.00 Hz
PPMCM          10.00000 ppm/cm
HZCM         1504.67798 Hz/cm
```

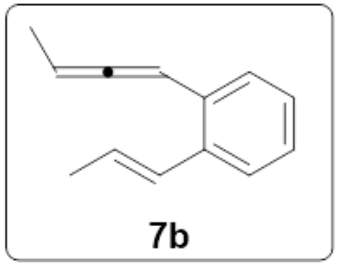

7.663 7.650 7.409 7.397 7.384 7.359 7.348 7.345 7.340 7.337 7.320 7.310 7.298 7.288 7.284 7.240 7.190 7.177 7.165 6.993 6.992 6.980 6.979 6.961 6.948 6.935 6.915 6.914 6.903 6.902 6.891 6.889 6.667 6.666 6.655 6.654 6.643 6.642 6.329 6.315 5.514 5.239 4.021 3.673 3.666 3.660 3.654 3.648 3.096 3.078 3.066 3.059 3.047 1.995 1.991 1.969 1.966 1.952 1.939 1.927 1.913 0.054
BRUKER
Current Data Parameters
NAME MS-03-60
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170105
Time 5.33
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT C6D6
NS 16
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 1.00 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000492 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
N
H
O
H
Ph
Ph
PhNH
HO
H
OH
6a-H (dr > 20:1)
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 ppm
2.02 2.08 3.15 3.12 2.10 2.01 2.10 1.02 1.01 2.02 1.00 1.02 0.94 1.04 2.02 2.04

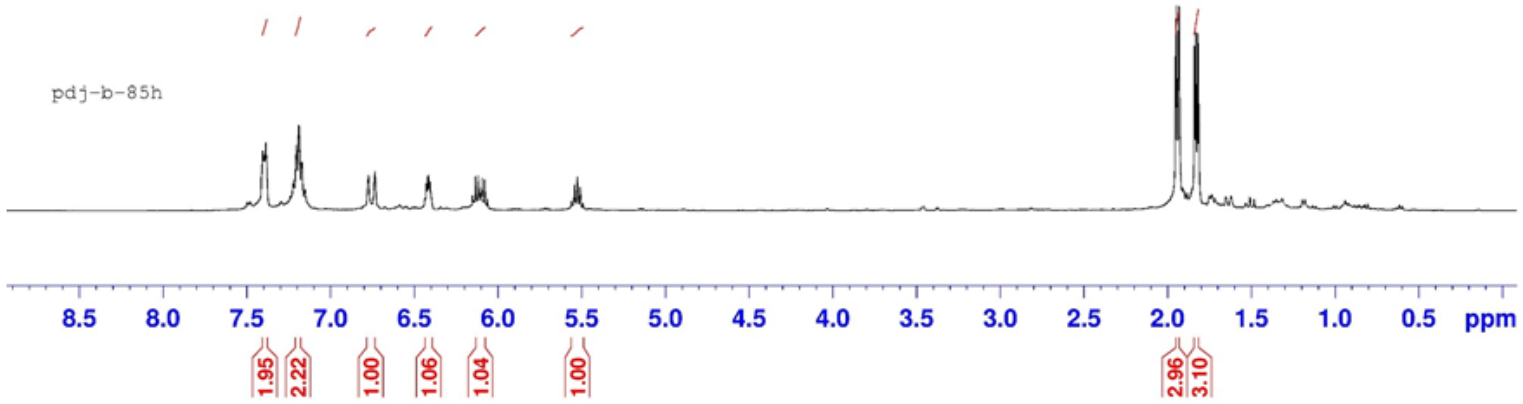

Current Data Parameters
NAME MS-03-60
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170104
Time 13.42
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG ppgp
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 298.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678111 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67798 Hz/cm
ppm
149.306
144.779
137.057
136.504
129.311
128.875
128.809
128.751
128.576
128.435
128.153
121.847
118.837
117.125
116.093
86.321
77.563
77.210
76.998
76.786
71.483
68.798
66.875
37.178
ppm
180
160
140
120
100
80
60
40
20
Ph
N
H
O
Ph
H
Ph
PhNH
HO
H
OH
6a-H (dr > 20:1)




```
Current Data Parameters
NAME       pdj_b_85h.fid
EXPNO                  1
PROCNO                 1

F2 - Processing parameters
SI                 32768
SF          399.7611794 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```





206.93

135.87
131.73
128.75
128.00
127.56
126.84
126.72
126.64

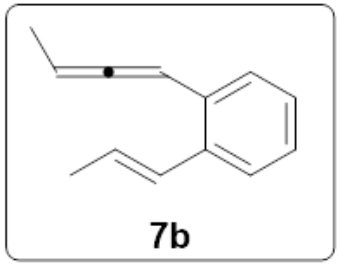
91.25
88.55

77.32
77.00
76.68

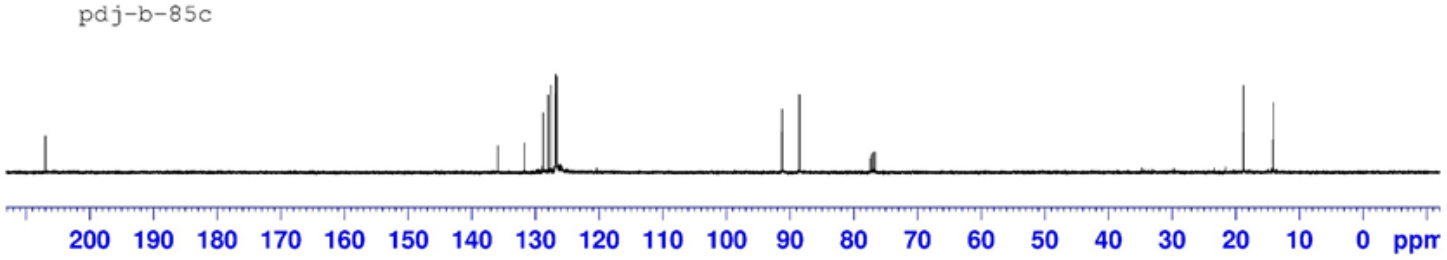
18.76
14.10

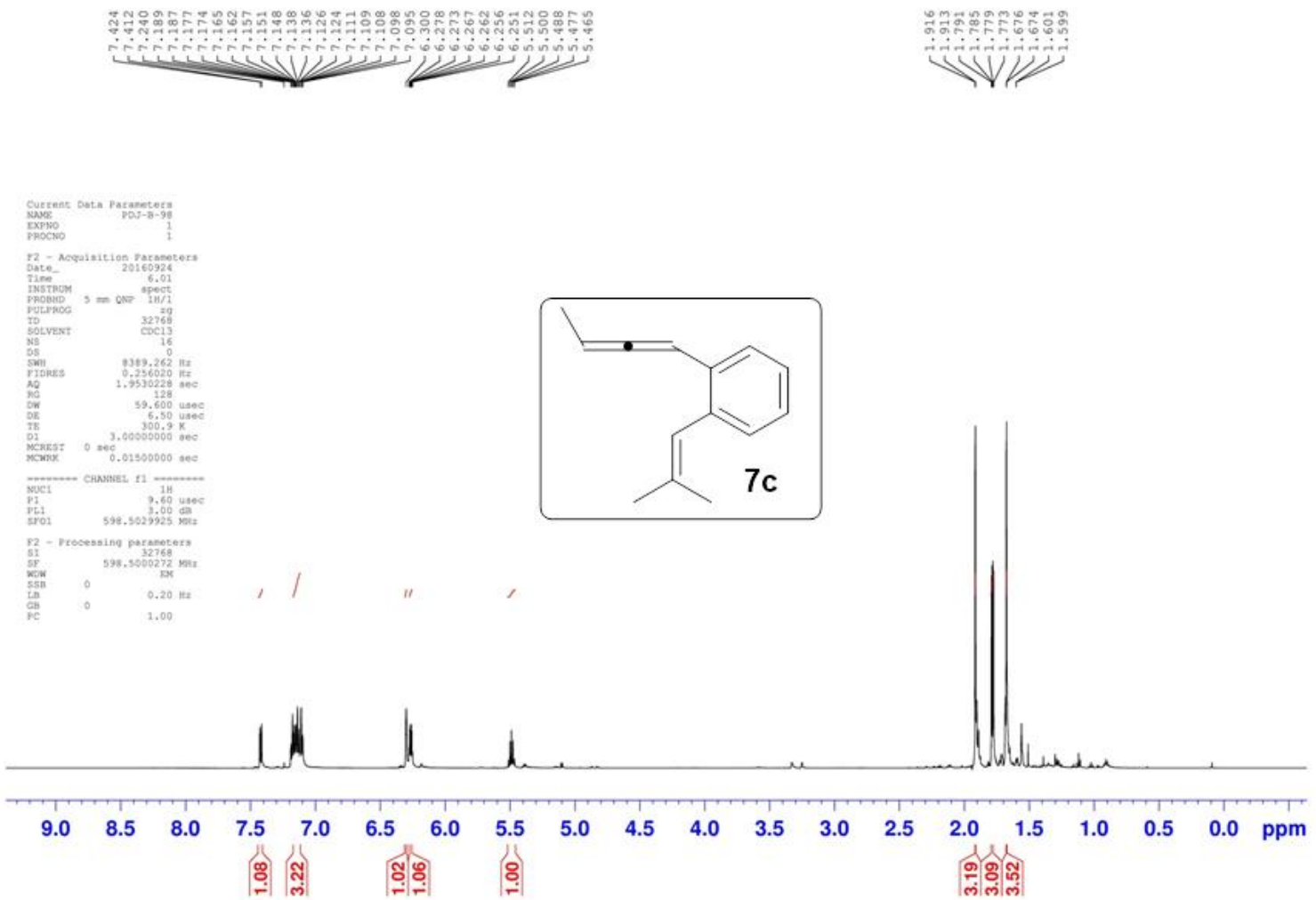
```
Current Data Parameters
NAME      pdj-b-85c.fid
EXPNO                1
PROCNO               1

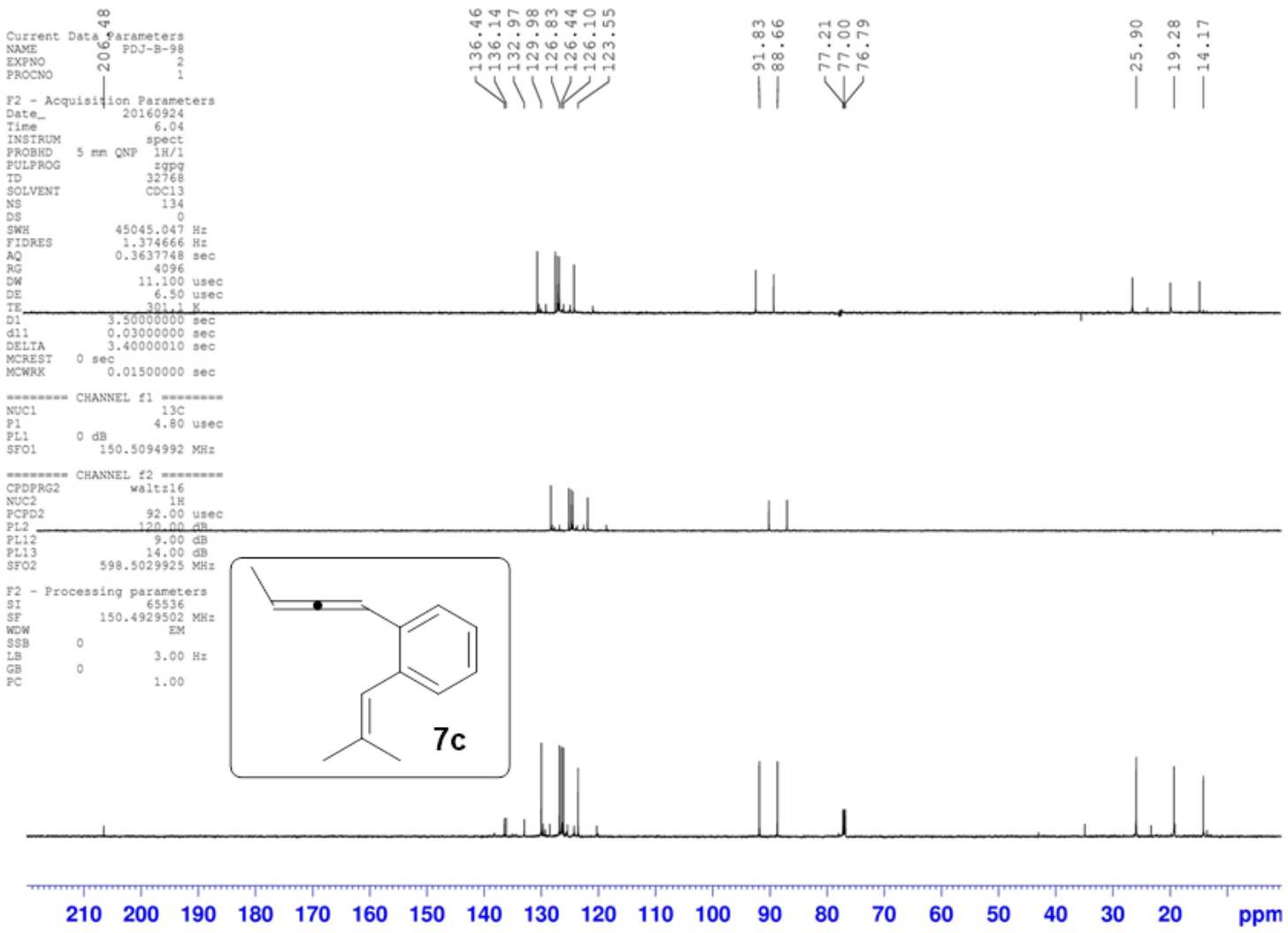
F2 - Processing parameters
SI                65536
SF          100.5214635 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

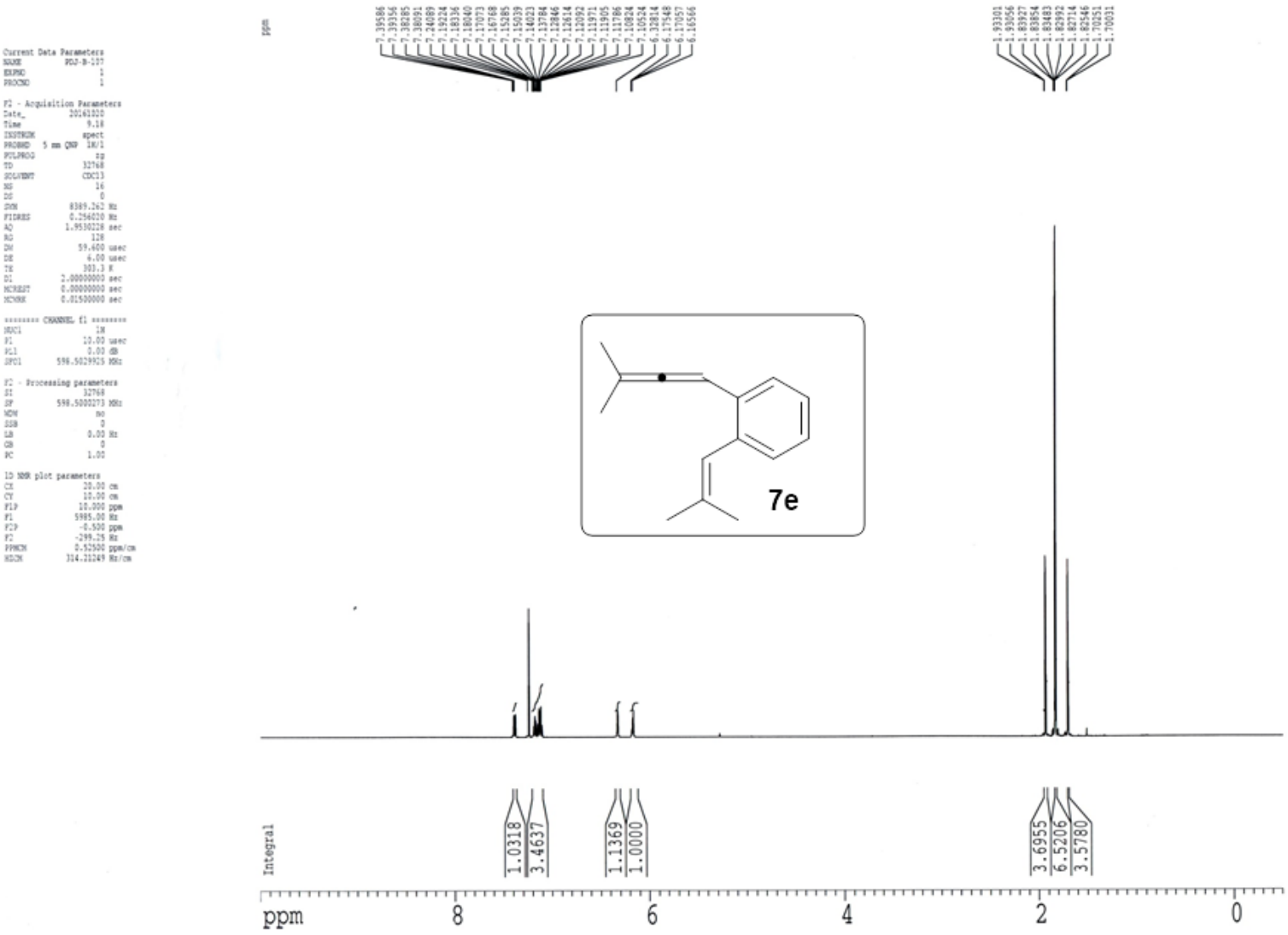


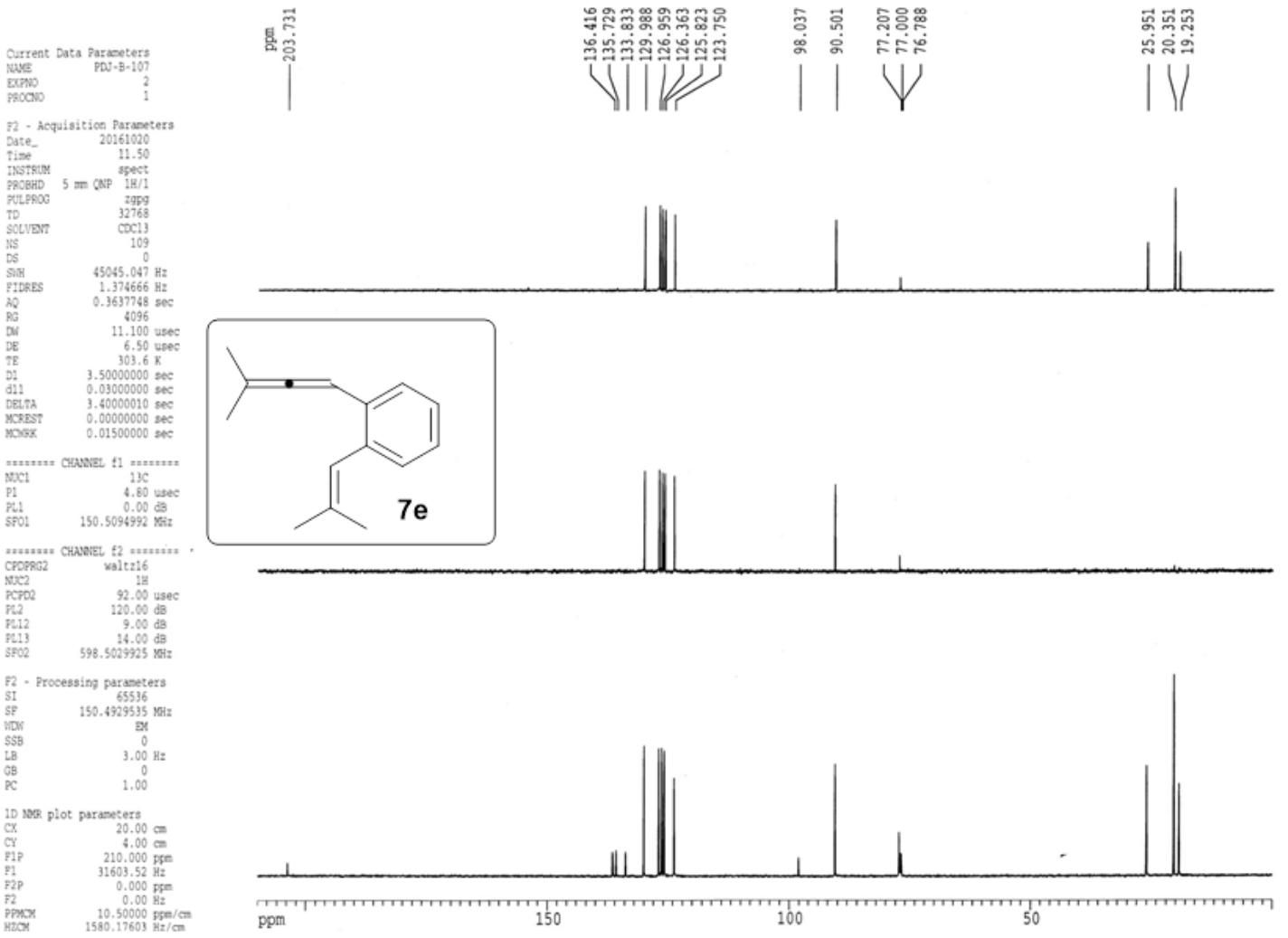
7b




7.424
7.412
7.240
7.189
7.187
7.177
7.174
7.165
7.162
7.157
7.151
7.148
7.138
7.136
7.126
7.124
7.111
7.109
7.108
7.098
7.095
6.300
6.278
6.273
6.267
6.262
6.256
6.251
5.512
5.500
5.488
5.477
5.465
1.916
1.913
1.791
1.785
1.779
1.773
1.676
1.674
1.601
1.599
Current Data Parameters
NAME PDJ-B-98
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160924
Time 6.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 300.9 K
D1 3.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 3.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000272 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
7c
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
ppm
1.08
3.22
1.02
1.06
1.00
3.19
3.09
3.52


206.48
136.46
136.14
132.97
129.98
126.83
126.44
126.10
123.55
91.83
88.66
77.21
77.00
76.79
25.90
19.28
14.17
Current Data Parameters
NAME PDJ-B-98
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160924
Time 6.04
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 134
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5094992 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.5029925 MHz
F2 - Processing parameters
SI 65536
SF 150.4929502 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
7c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


Current Data Parameters
NAME POZ-B-127
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161020
Time 9.18
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.00 usec
TE 303.3 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.5029915 MHz
F2 - Processing parameters
SI 32768
SF 598.5000273 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5985.00 Hz
F2P -0.500 ppm
F2 -299.25 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.21249 Hz/cm
ppm
7.39586
7.39356
7.38285
7.38091
7.24089
7.15224
7.14836
7.14040
7.11073
7.10768
7.10285
7.15039
7.14023
7.13784
7.12846
7.12614
7.12092
7.11971
7.11905
7.11786
7.10824
7.10524
6.32814
6.17548
6.17057
6.16566
1.93301
1.93056
1.83927
1.83854
1.83483
1.82992
1.82714
1.82546
1.70251
1.70031
7e
Integral
1.0318
3.4637
1.1369
1.0000
3.6955
6.5206
3.5780
ppm
8
6
4
2
0


Current Data Parameters
NAME PDJ-B-107
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161020
Time 11.50
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 109
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 303.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5094992 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.5029925 MHz
F2 - Processing parameters
SI 65536
SF 150.4929535 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 210.000 ppm
F1 31603.52 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.50000 ppm/cm
HZCM 1580.17603 Hz/cm
ppm
203.731
136.416
135.729
133.833
129.988
126.959
126.363
125.823
123.750
98.037
90.501
77.207
77.000
76.788
25.951
20.351
19.253
7e
ppm
150
100
50

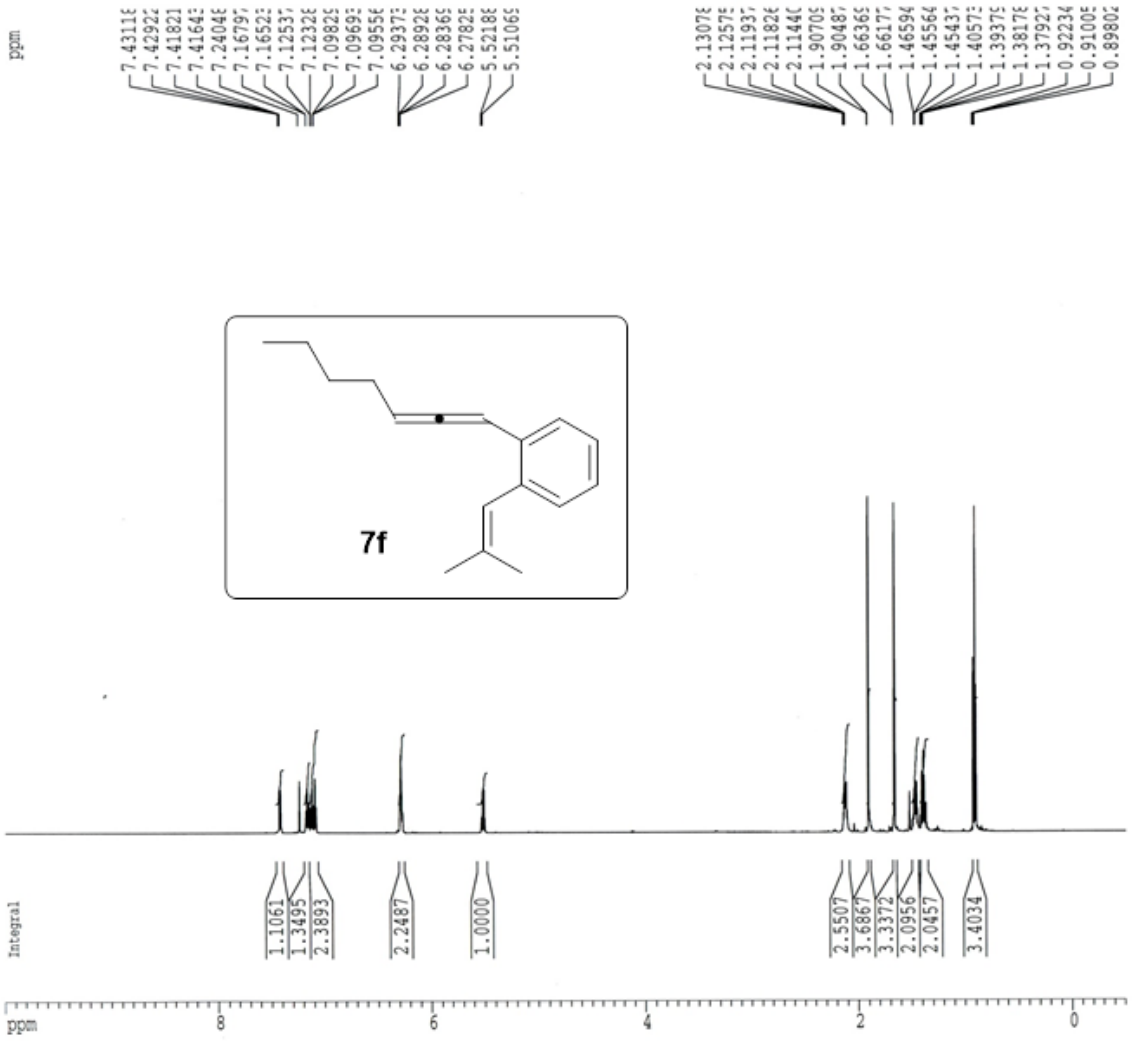
```
Current Data Parameters
NAME              PDJ-B-109
EXPNO                     1
PROCNO                    1

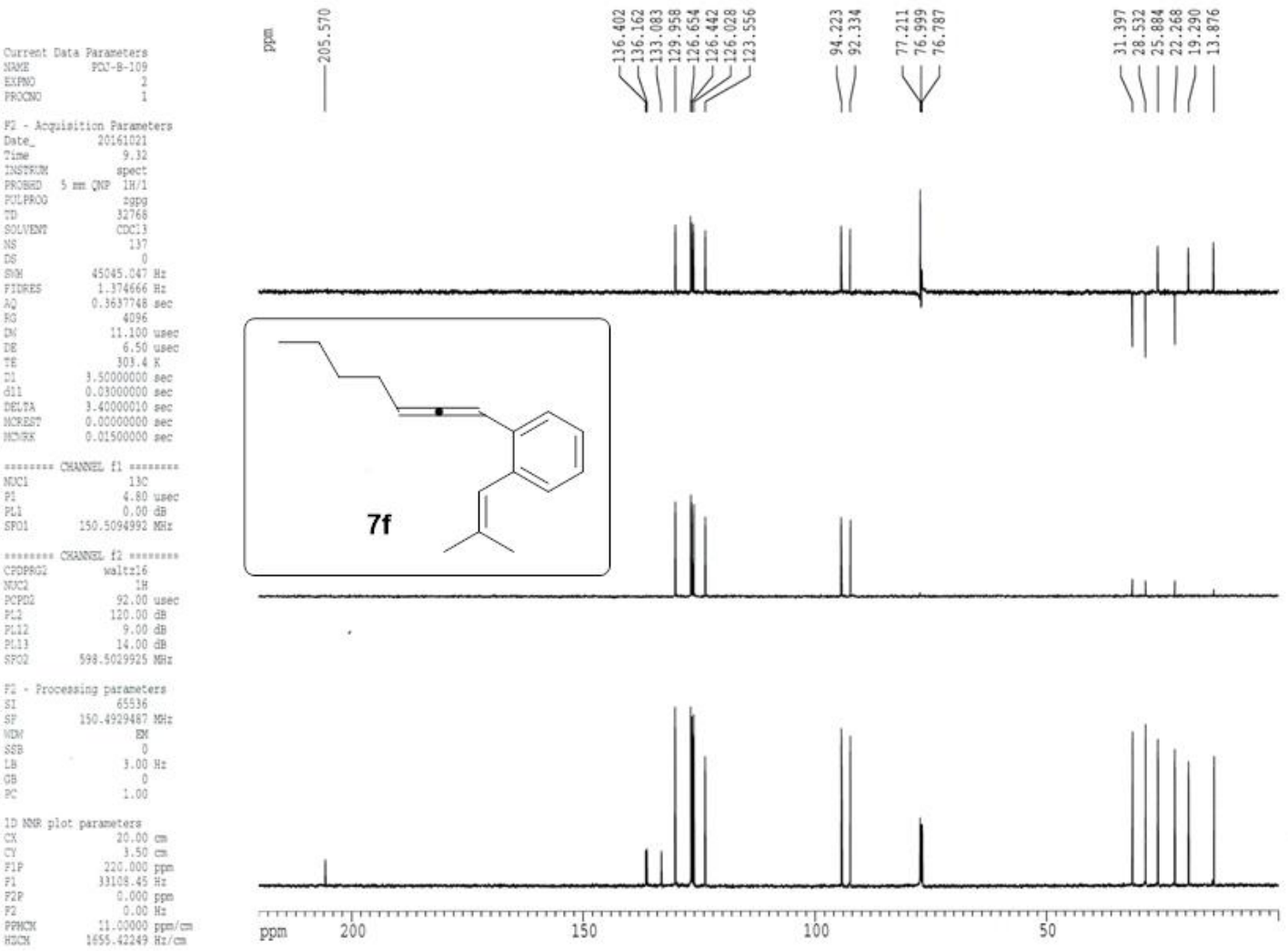
F2 - Acquisition Parameters
Date_              20161021
Time                   9.27
INSTRUM               spect
PROBHD   5 mm QNP  1H/1
PULPROG                  zg
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8389.262 Hz
FIDRES                0.256020 Hz
AQ                 1.9530228 sec
RG                      128
DW                   59.600 usec
DE                    6.50 usec
TE                   303.2 K
D1                 1.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

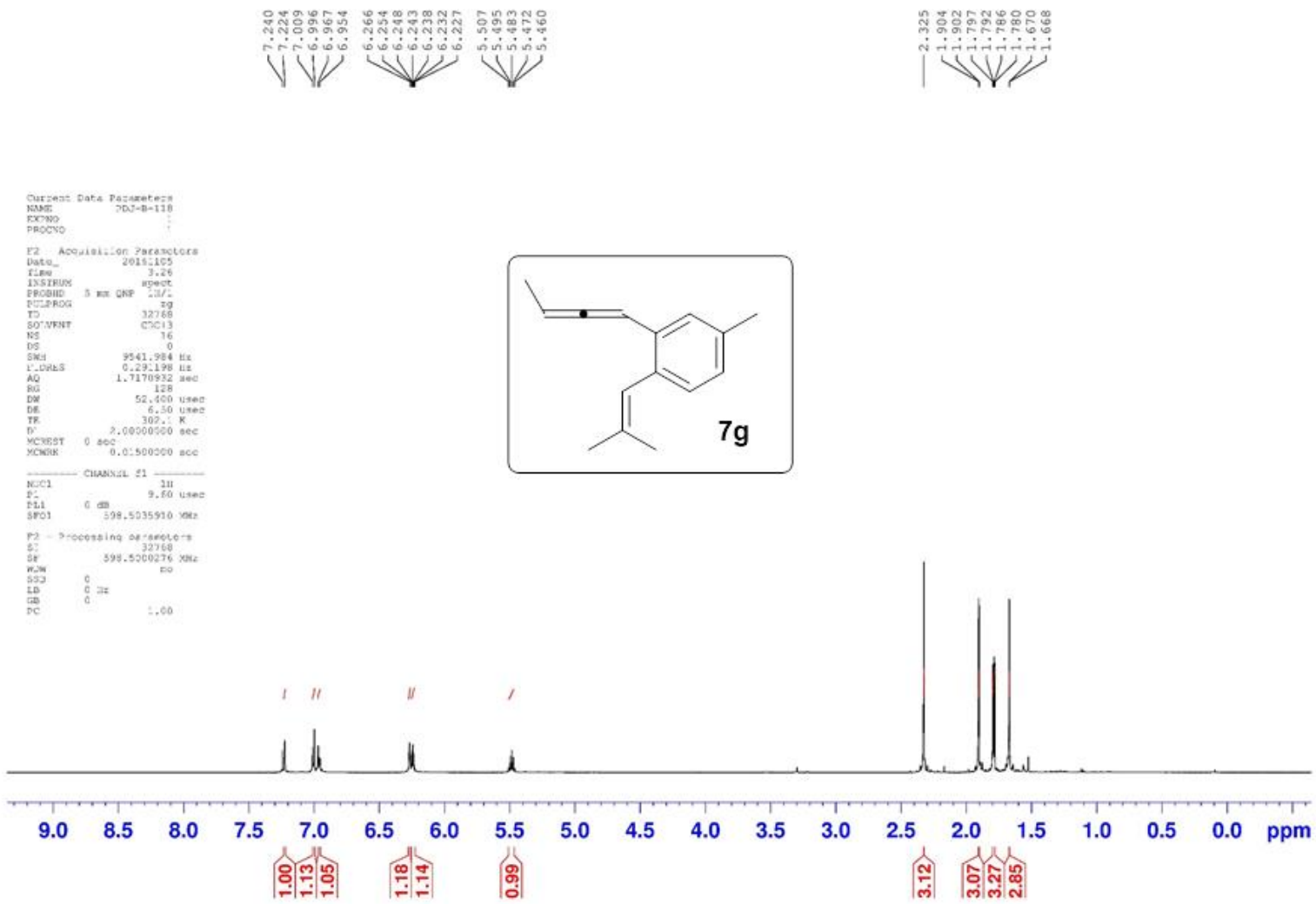
======== CHANNEL f1 ========
NUC1                      1H
P1                     12.30 usec
PL1                     3.00 dB
SFO1             598.5029925 MHz

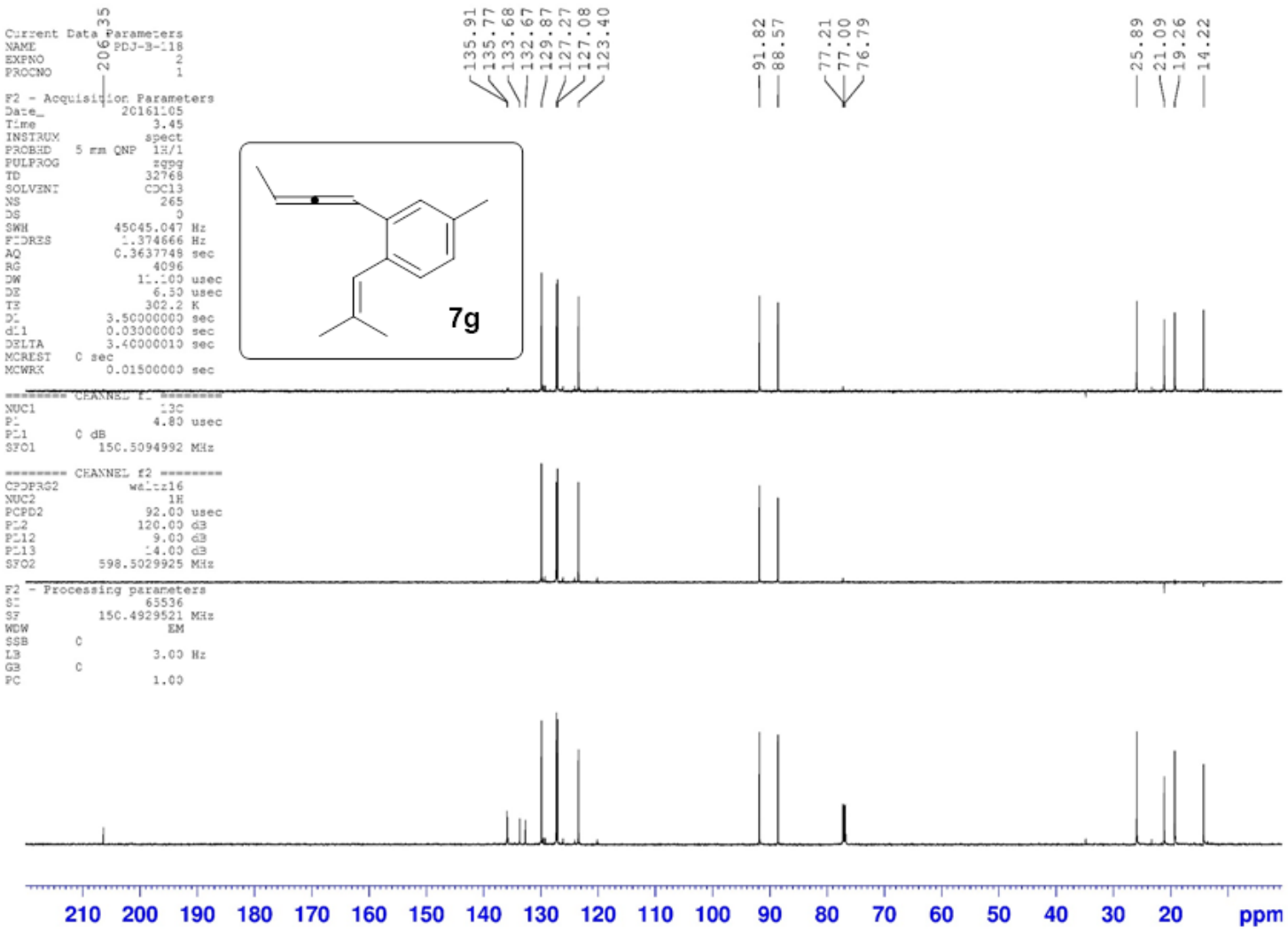
F2 - Processing parameters
SI                    32768
SF               598.5000273 MHz
WDW                      no
SSB                       0
LB                     0.00 Hz
GB                        0
PC                     1.00

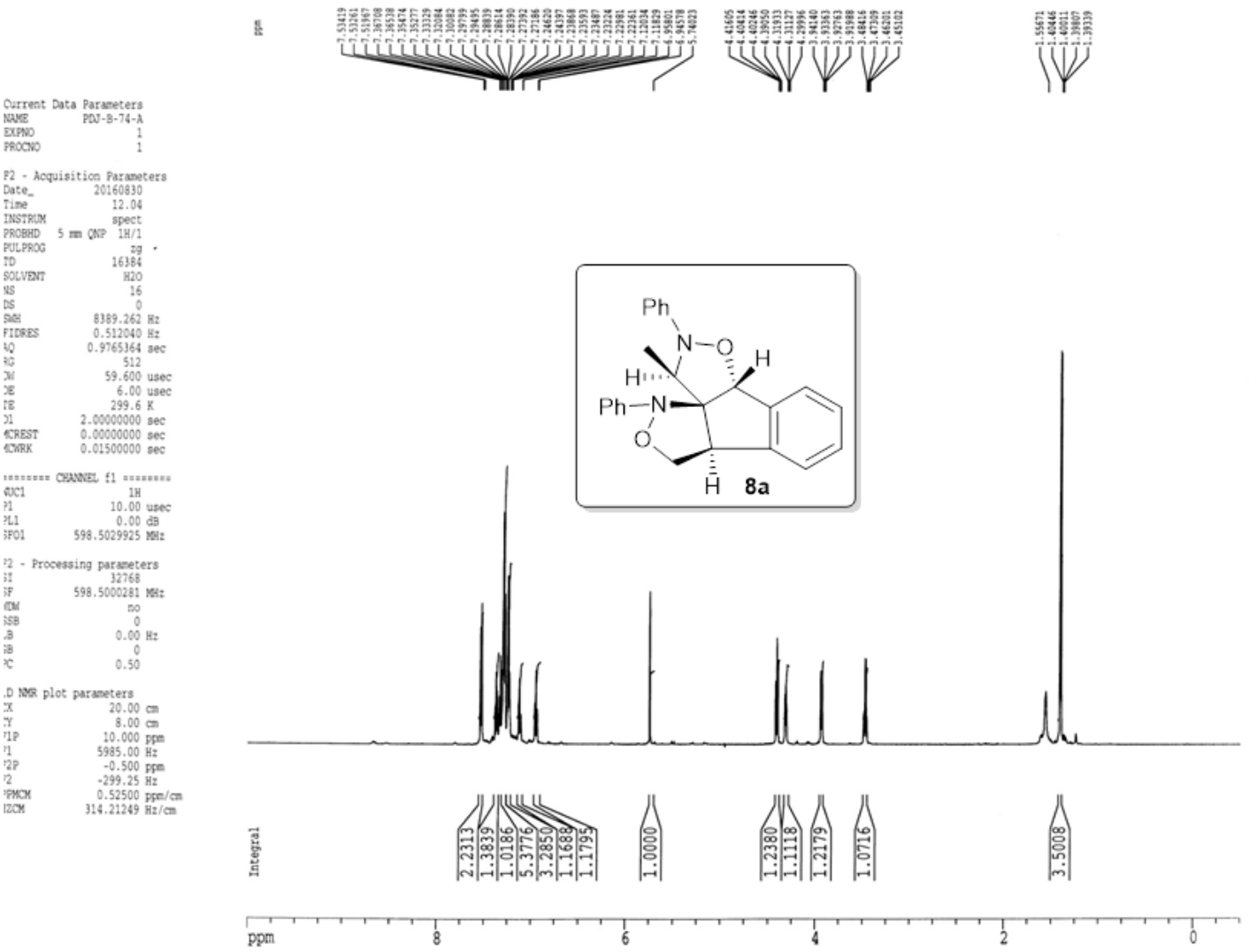
1D NMR plot parameters
CX                    20.00 cm
CY                     6.00 cm
F1P                  10.000 ppm
F1                 5985.00 Hz
F2P                  -0.500 ppm
F2                 -299.25 Hz
PPMCM                 0.52500 ppm/cm
HZCM               314.21249 Hz/cm
```

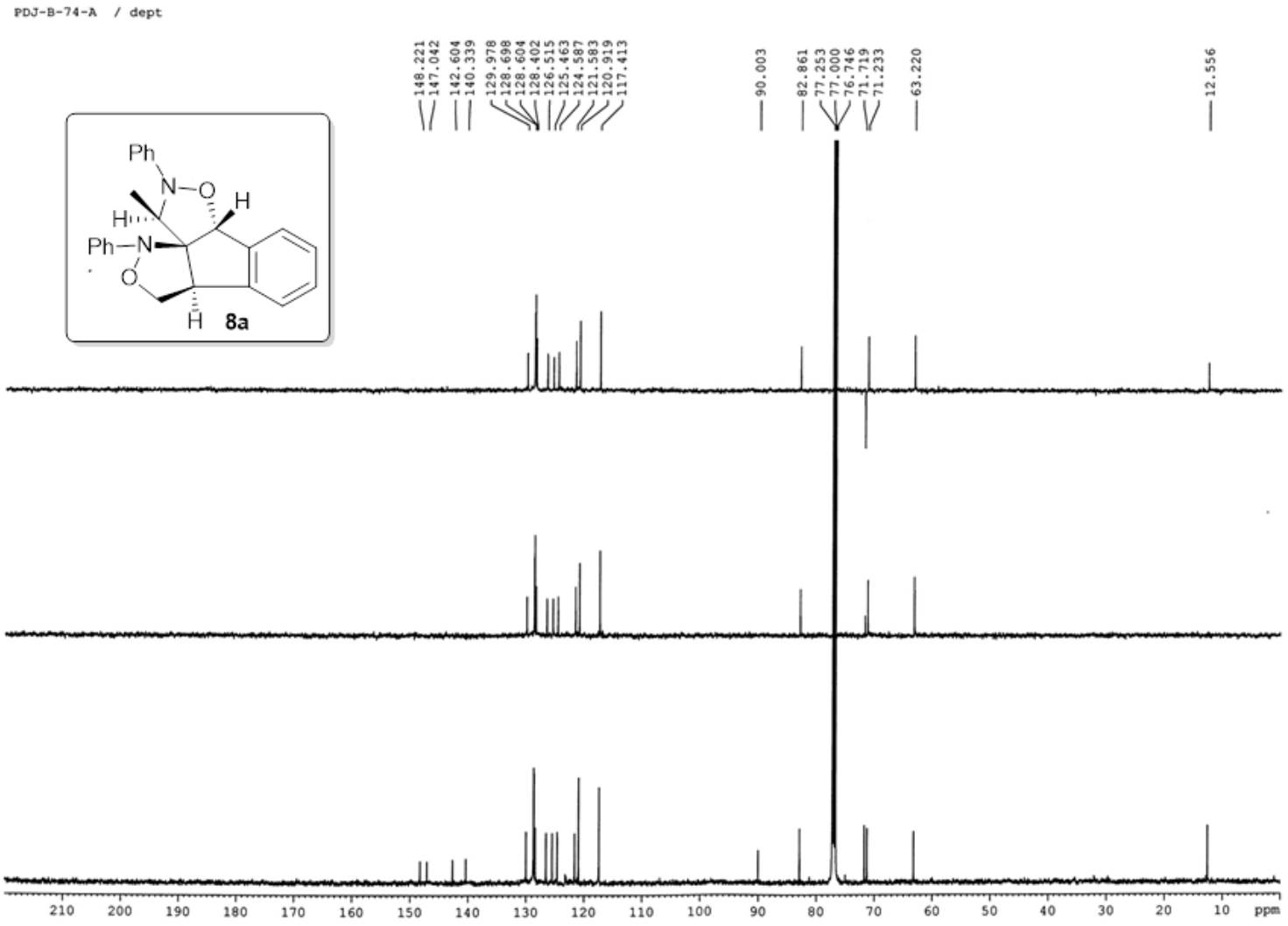


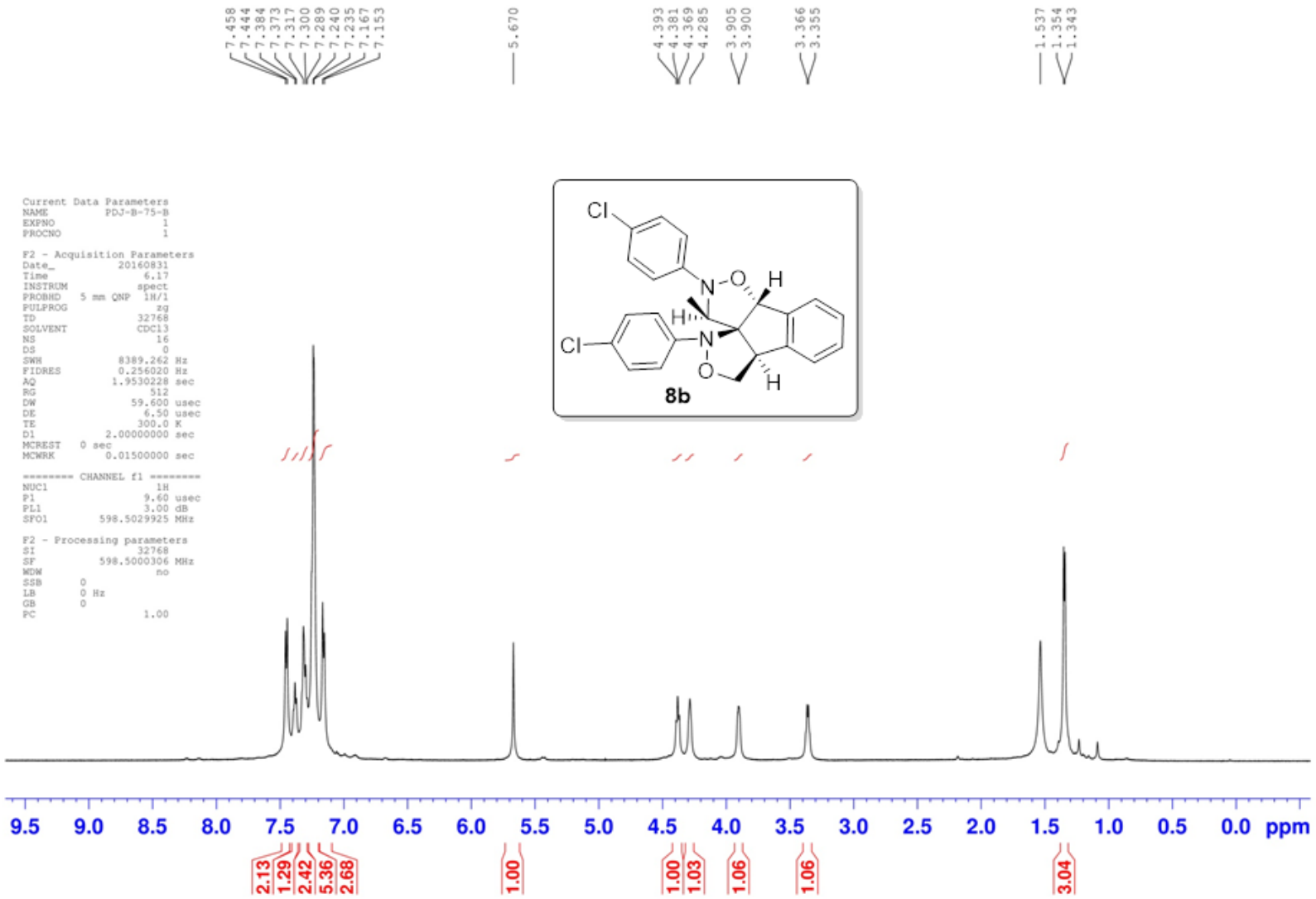

Current Data Parameters
NAME PDZ-B-109
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161021
Time 9.32
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 137
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 303.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5094992 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.5029925 MHz
F2 - Processing parameters
SI 65536
SF 150.4929487 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 3.50 cm
F1P 220.000 ppm
F1 33108.45 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 11.00000 ppm/cm
HZCM 1655.42249 Hz/cm
ppm
205.570
136.402
136.162
133.083
129.958
126.654
126.442
126.028
123.556
94.223
92.334
77.211
76.999
76.787
31.397
28.532
25.884
22.268
19.290
13.876
7f
ppm
200
150
100
50

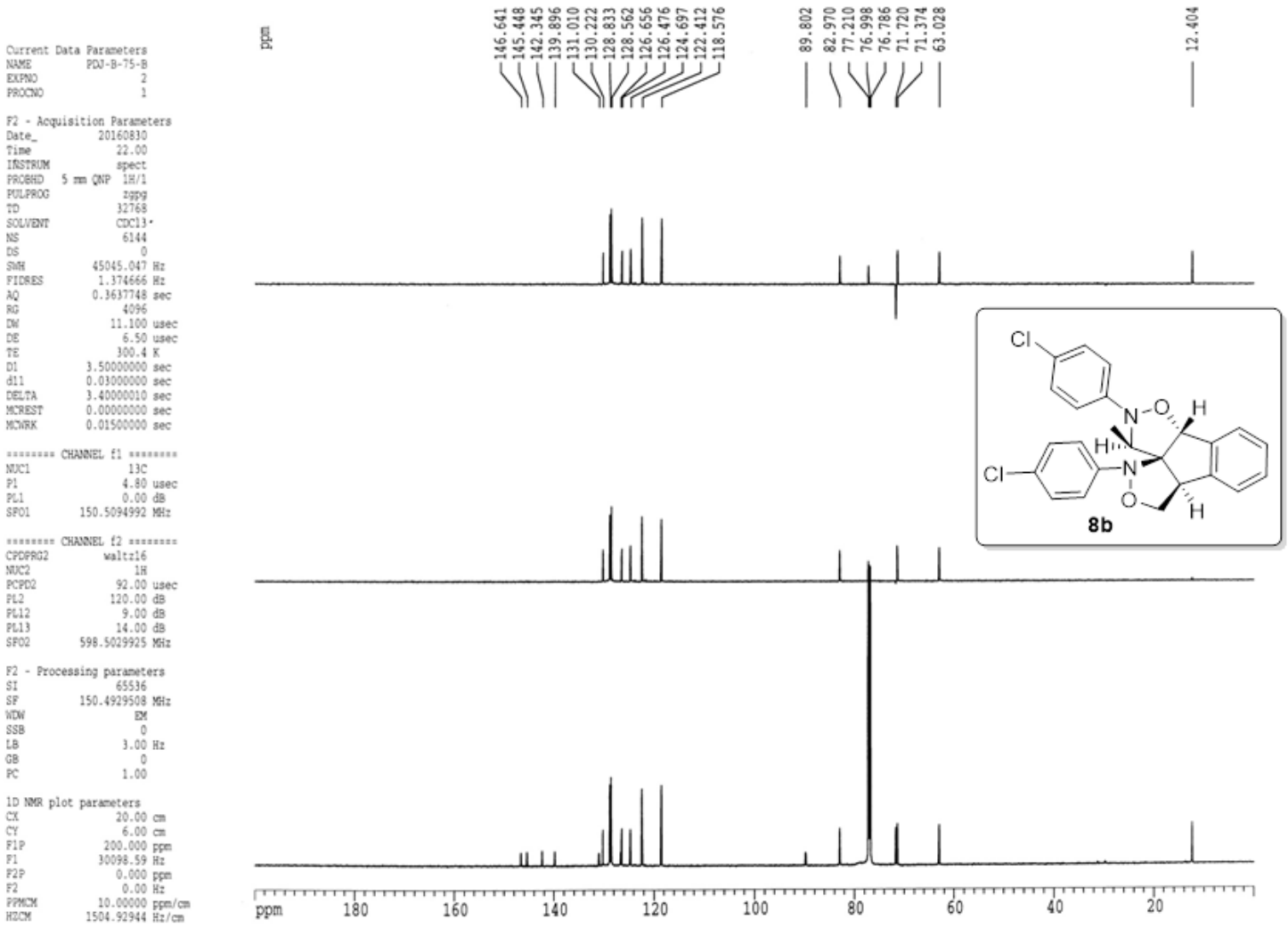

7.240
7.224
7.009
6.996
6.967
6.954
6.266
6.254
6.248
6.243
6.238
6.232
6.227
5.507
5.495
5.483
5.472
5.460
2.325
1.904
1.902
1.797
1.792
1.786
1.780
1.670
1.668
7g
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.13
1.05
1.18
1.14
0.99
3.12
3.07
3.27
2.85

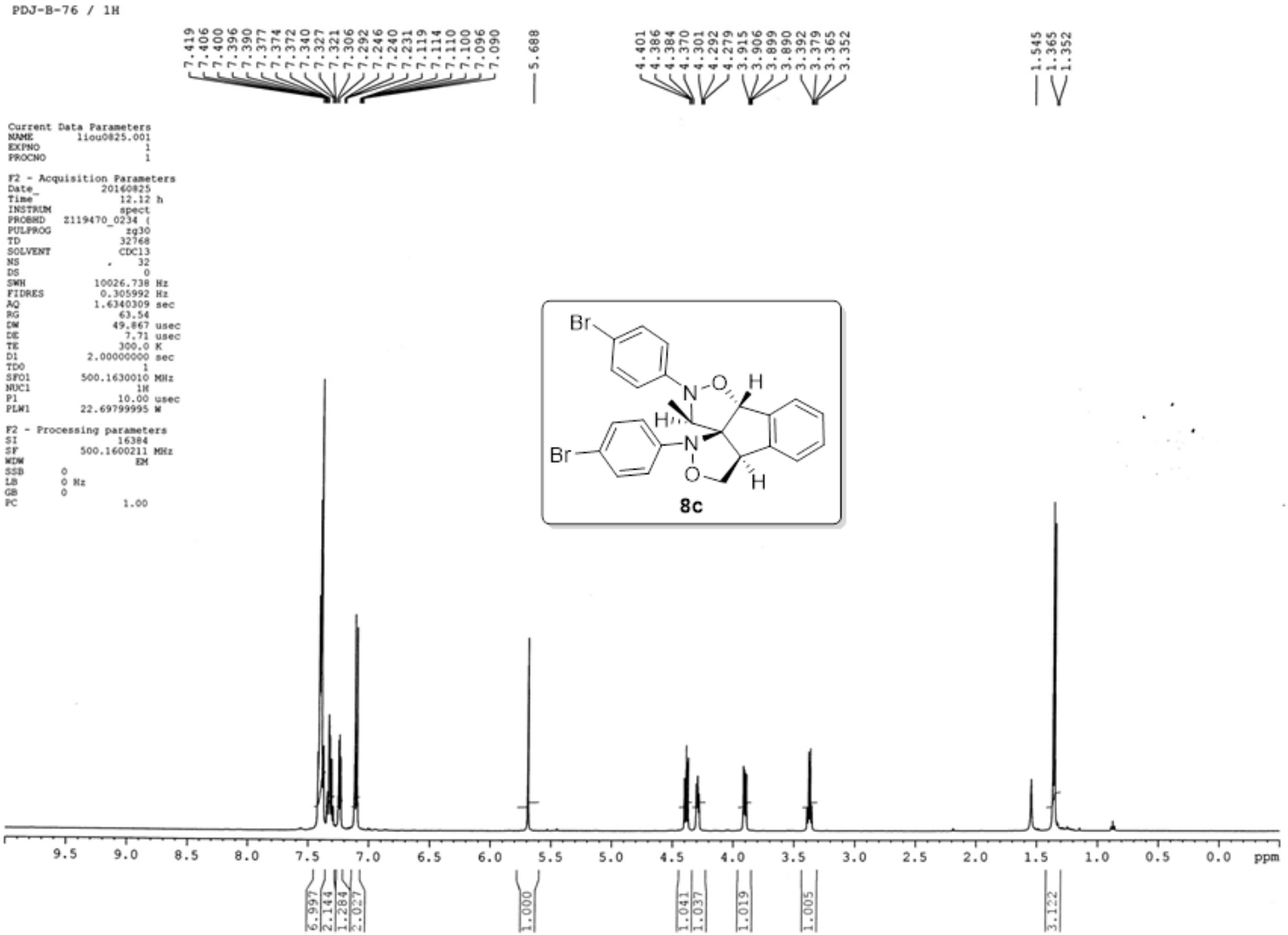

135.91
135.77
133.68
132.67
129.87
127.27
127.08
123.40
91.82
88.57
77.21
77.00
76.79
25.89
21.09
19.26
14.22
7g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

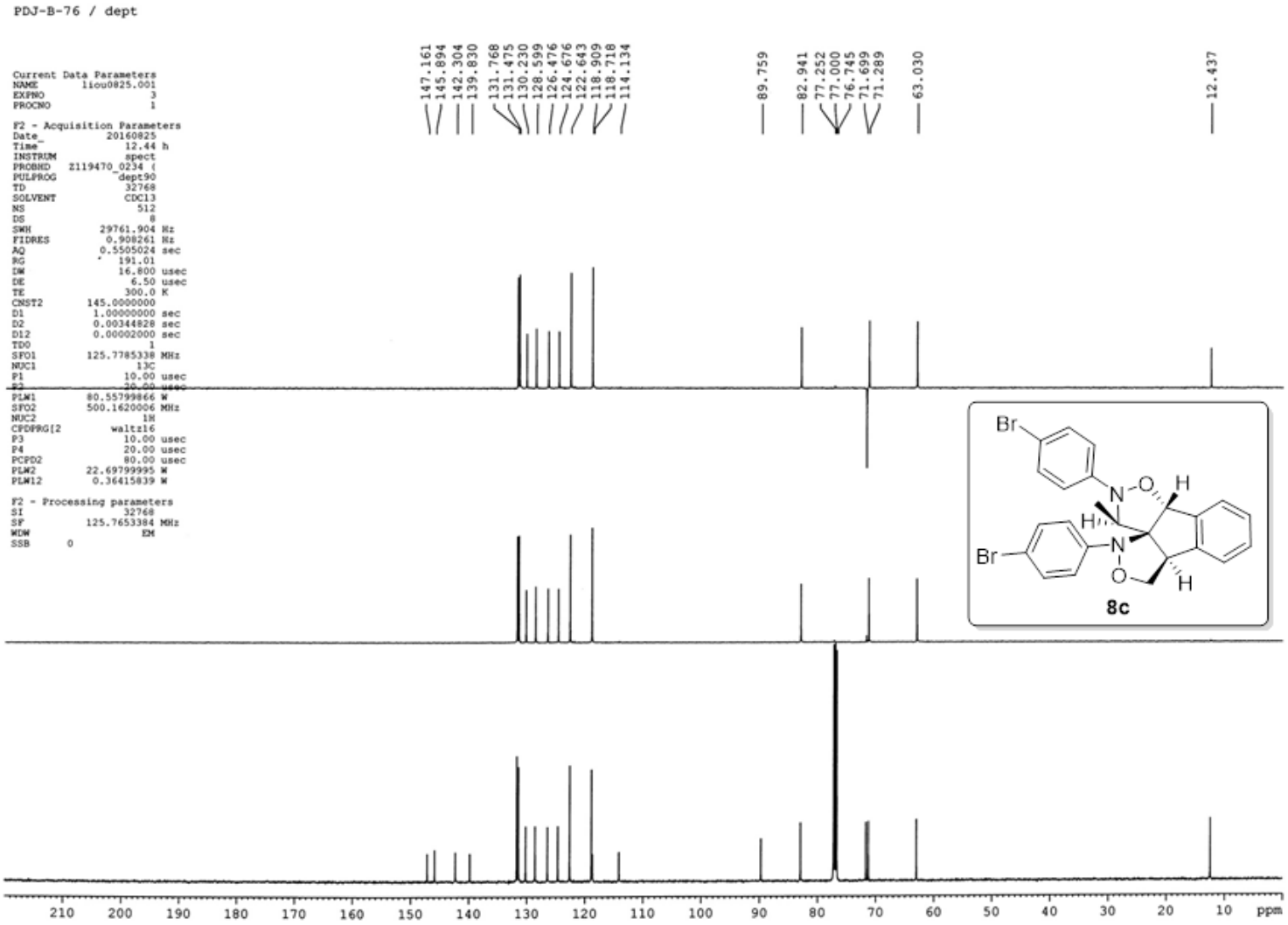

Current Data Parameters
NAME PDJ-B-74-A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160830
Time 12.04
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 16384
SOLVENT H2O
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.512040 Hz
AQ 0.9765364 sec
RG 512
DW 59.600 usec
DE 6.00 usec
TE 299.6 K
D1 2.00000000 sec
DCREST 0.00000000 sec
DCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000281 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.000 ppm
F1 5985.00 Hz
F2P -0.500 ppm
F2 -299.25 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.21249 Hz/cm
ppm
7.53419
7.53261
7.51967
7.36708
7.36538
7.35474
7.35277
7.33329
7.33084
7.33082
7.29799
7.29495
7.28839
7.28614
7.28390
7.27392
7.27186
7.24620
7.24397
7.23868
7.23593
7.23487
7.23224
7.22981
7.22361
7.22034
7.21829
6.95801
6.94578
6.94023
4.41605
4.40414
4.40244
4.39650
4.31933
4.31127
4.29996
3.94140
3.93363
3.92763
3.91988
3.48416
3.47309
3.46201
3.45102
1.56571
1.56446
1.40611
1.39803
1.39339
Ph
N
O
H
H
Ph
N
O
H
8a
Integral
2.2313
1.3839
1.0186
5.3776
3.2850
1.1688
1.1795
1.0000
1.2380
1.1118
1.2179
1.0716
3.5008
ppm
8
6
4
2
0

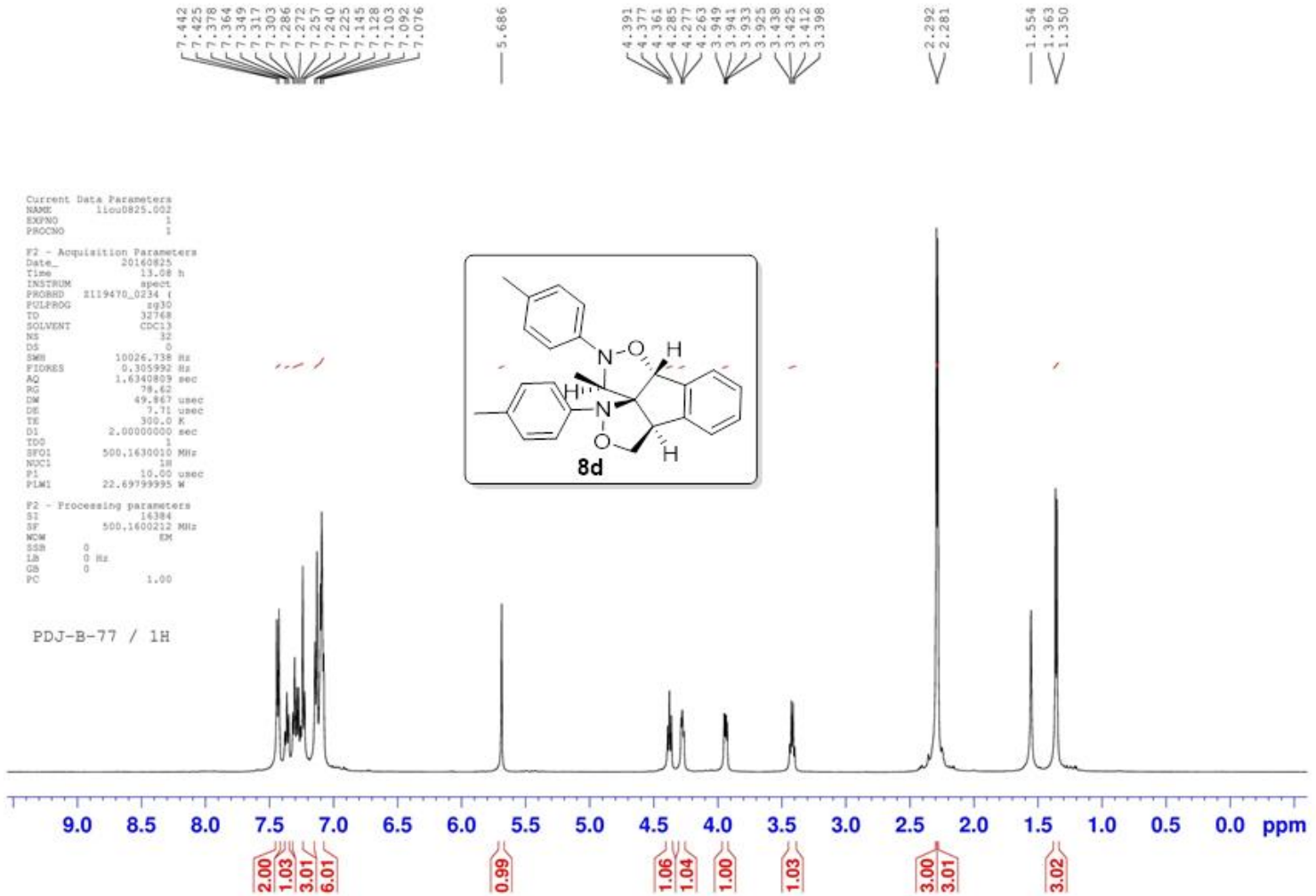

PDJ-B-74-A / dept
148.221
147.042
142.604
140.339
129.978
128.698
128.604
128.402
126.515
125.463
124.587
121.583
120.919
117.413
90.003
82.861
77.253
77.000
76.746
71.719
71.233
63.220
12.556
Ph
N
O
H
Ph
N
O
H
8a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

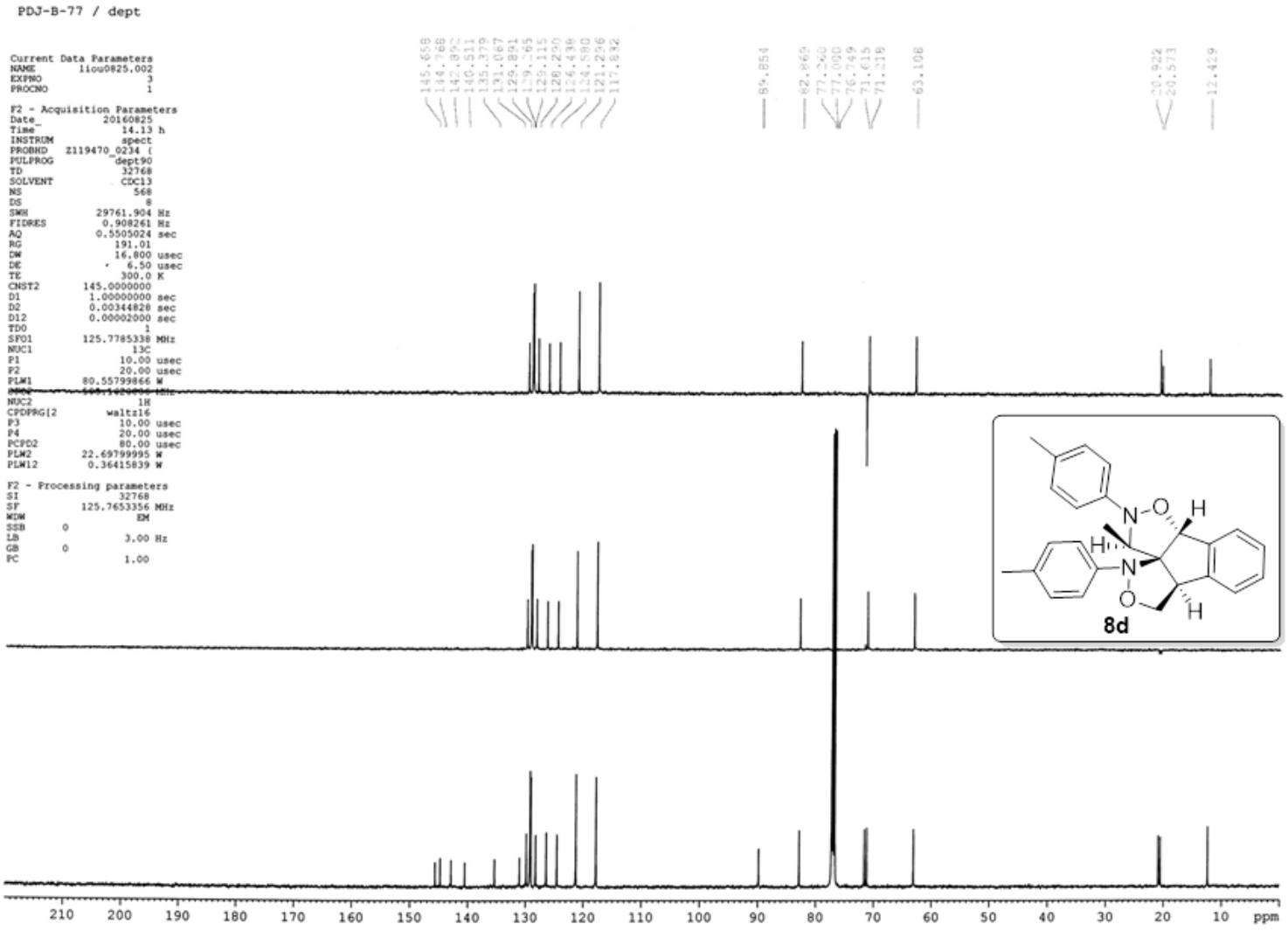

7.458
7.444
7.384
7.373
7.317
7.300
7.289
7.240
7.235
7.167
7.153
5.670
4.393
4.381
4.369
4.285
3.905
3.900
3.366
3.355
1.537
1.354
1.343
Current Data Parameters
NAME PDJ-B-75-B
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160831
Time 6.17
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 3.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000306 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Cl
N
O
H
Cl
N
O
H
8b
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 ppm
2.13
1.29
2.42
5.36
2.68
1.00
1.00
1.03
1.06
1.06
3.04

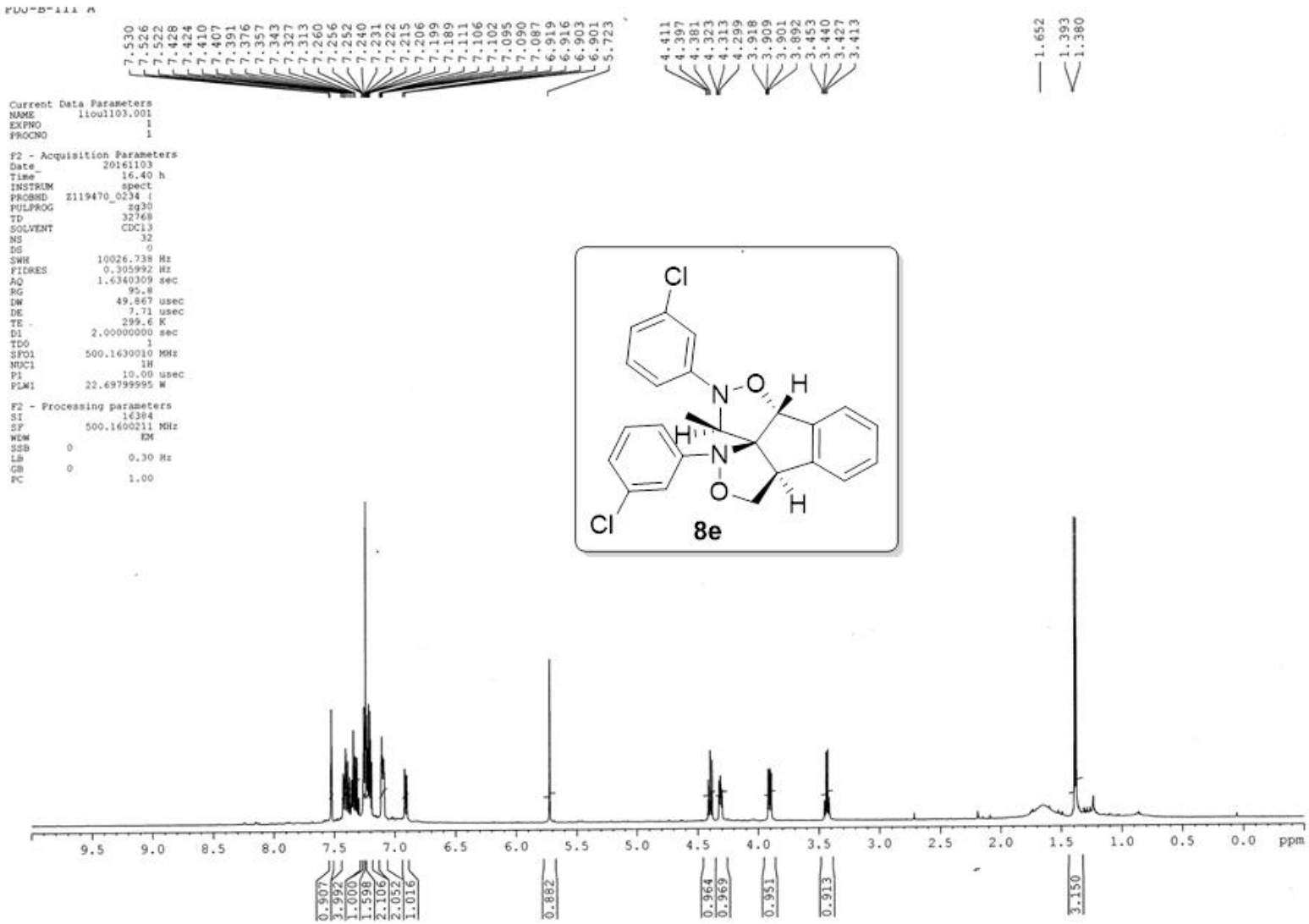

Current Data Parameters
NAME PDJ-B-75-B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160830
Time 22.00
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 300.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5094992 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.5029925 MHz
F2 - Processing parameters
SI 65536
SF 150.4929508 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 200.000 ppm
F1 30098.59 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.92944 Hz/cm
ppm
146.641
145.448
142.345
139.896
131.010
130.222
128.833
128.562
126.656
126.476
124.697
122.412
118.576
89.802
82.970
77.210
76.998
76.786
71.720
71.374
63.028
12.404
Cl
N
O
H
H
N
Cl
O
H
8b
ppm
180
160
140
120
100
80
60
40
20


PDJ-B-76 / 1H
7.419
7.406
7.400
7.396
7.390
7.377
7.374
7.372
7.340
7.327
7.321
7.306
7.292
7.246
7.240
7.231
7.119
7.114
7.110
7.100
7.096
7.090
5.688
4.401
4.386
4.384
4.370
4.301
4.292
4.279
3.915
3.906
3.899
3.890
3.392
3.379
3.365
3.352
1.545
1.365
1.352
Current Data Parameters
NAME liou0825.001
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160825
Time 12.12 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 10026.738 Hz
FIDRES 0.305992 Hz
AQ 1.6340309 sec
RG 63.54
DW 49.867 usec
DE 7.71 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
SFO1 500.1630010 MHz
NUC1 1H
P1 10.00 usec
PLW1 22.69799995 W
F2 - Processing parameters
SI 16384
SF 500.1600211 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Br
Br
N
O
H
8c
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
ppm
6.997
2.144
1.284
2.027
1.000
1.041
1.037
1.019
1.005
3.122


PDJ-B-76 / dept
Current Data Parameters
NAME liou0825.001
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160825
Time_ 12.44 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG dept90
TD 32768
SOLVENT CDCl3
NS 512
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505024 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7785338 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 80.55799866 W
SFO2 500.1620006 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 22.69799995 W
PLW12 0.36415839 W
F2 - Processing parameters
SI 32768
SF 125.7653384 MHz
WDW EM
SSB 0
147.161
145.894
142.304
139.830
131.768
131.475
130.230
128.599
126.476
124.676
122.643
118.909
118.718
114.134
89.759
82.941
77.252
77.000
76.745
71.699
71.289
63.030
12.437
Br
N
O
H
Br
8c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.442
7.425
7.378
7.364
7.349
7.317
7.303
7.286
7.272
7.257
7.240
7.225
7.145
7.128
7.103
7.092
7.076
5.686
4.391
4.377
4.361
4.285
4.277
4.263
3.949
3.941
3.933
3.925
3.438
3.425
3.412
3.398
2.292
2.281
1.554
1.363
1.350
Current Data Parameters
NAME 11ou0825.002
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160825
Time 13.08 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 10026.738 Hz
FIDRES 0.305992 Hz
AQ 1.6340809 sec
RG 78.62
DW 49.867 usec
DE 7.71 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
SFO1 500.1630010 MHz
NUC1 1H
P1 10.00 usec
PLW1 22.69799995 W
F2 - Processing parameters
SI 16384
SF 500.1600212 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
PDJ-B-77 / 1H
8d
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 ppm
2.00 1.03 3.01 6.01 0.99 1.06 1.04 1.00 1.03 3.00 3.01 3.02


PDJ-B-77 / dept
Current Data Parameters
NAME liou0825.002
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160825
Time 14.13 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG dept90
TD 32768
SOLVENT CDCl3
NS 568
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505024 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7785338 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 80.55799866 W
NUC2 1H
CPDPRG[2 waltz16
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 22.69799995 W
PLW12 0.36415839 W
F2 - Processing parameters
SI 32768
SF 125.7653356 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
145.658
144.768
142.852
140.511
135.379
134.067
129.891
129.765
129.115
126.200
124.498
124.580
121.256
117.692
89.854
82.865
77.360
77.000
76.749
71.615
71.318
63.108
20.922
20.573
12.429
8d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.530
7.526
7.522
7.428
7.424
7.410
7.407
7.391
7.376
7.357
7.343
7.327
7.313
7.260
7.256
7.252
7.240
7.231
7.222
7.215
7.206
7.199
7.189
7.111
7.106
7.102
7.095
7.090
7.087
6.919
6.916
6.903
6.901
5.723
4.411
4.397
4.381
4.323
4.313
4.299
3.918
3.909
3.901
3.892
3.453
3.440
3.427
3.413
1.652
1.393
1.380
Current Data Parameters
NAME liou1103.001
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161103
Time 16.40 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 10026.738 Hz
FIDRES 0.305992 Hz
AQ 1.6340309 sec
RG 95.8
DW 49.867 usec
DE 7.71 usec
TE 299.6 K
D1 2.00000000 sec
TD0 1
SFO1 500.1630010 MHz
NUC1 1H
P1 10.00 usec
PLW1 22.69799995 W
F2 - Processing parameters
SI 16384
SF 500.1600211 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
N
O
H
H
N
O
H
Cl
8e
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
ppm
0.907
3.992
1.000
1.598
2.106
2.052
1.016
0.882
0.964
0.969
0.951
0.913
3.150

```
Current Data Parameters
NAME          PDJ-B-111
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20161025
Time              13.14
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG           zgpg
TD                32768
SOLVENT           CDCl3
NS                 6144
DS                    0
SWH           45045.047 Hz
FIDRES        1.374666 Hz
AQ            0.3637748 sec
RG                 4096
DW               11.100 usec
DE                6.50 usec
TE               302.9 K
D1            3.50000000 sec
d11           0.03000000 sec
DELTA         3.40000010 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                  4.80 usec
PL1                 0.00 dB
SFO1         150.5094992 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              92.00 usec
PL2               120.00 dB
PL12               9.00 dB
PL13              14.00 dB
SFO2         598.5029925 MHz

F2 - Processing parameters
SI                  65536
SF          150.4929474 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                  10.00 cm
F1P                200.000 ppm
F1               30098.59 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM           10.00000 ppm/cm
HZCM          1504.92944 Hz/cm
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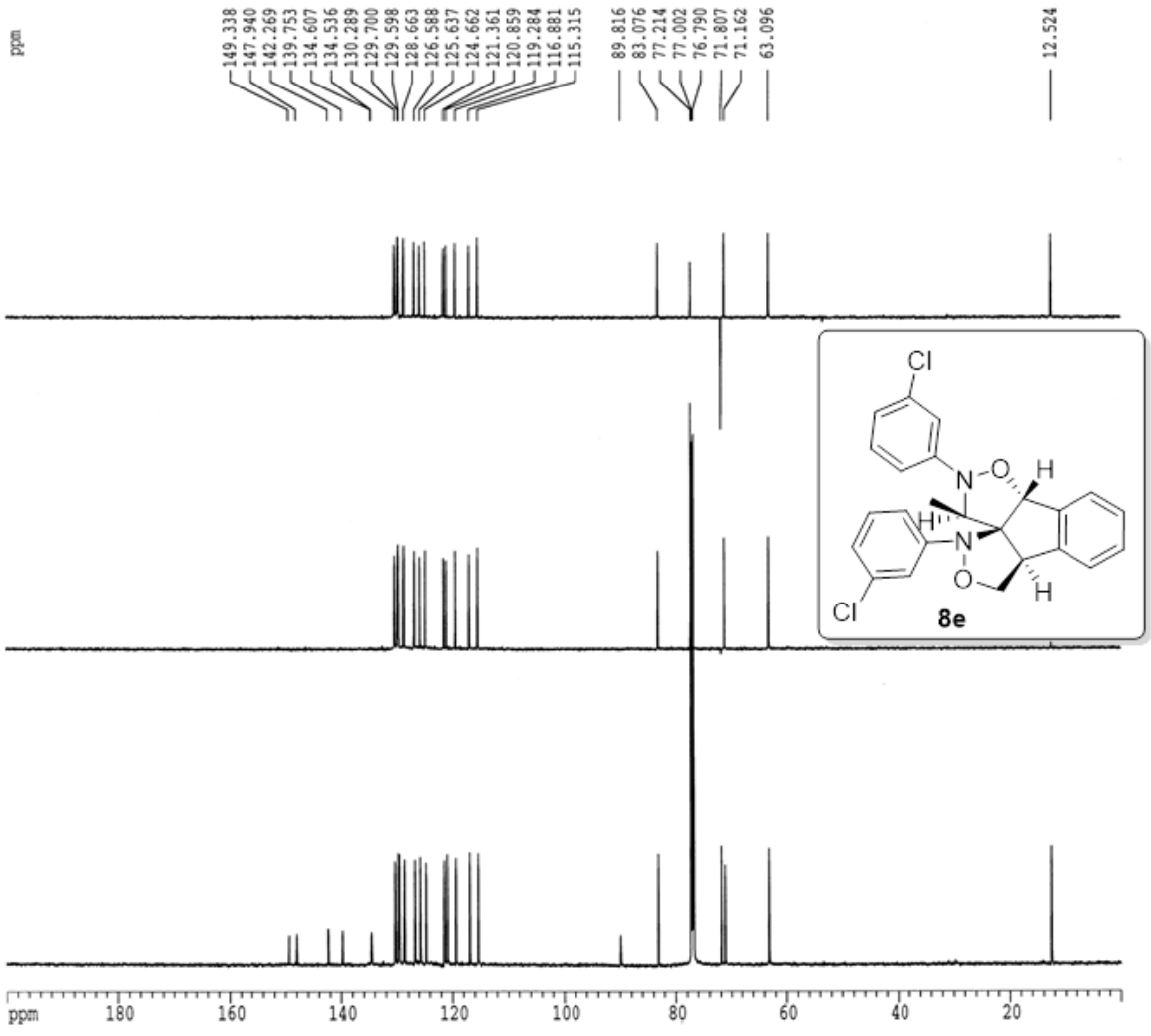
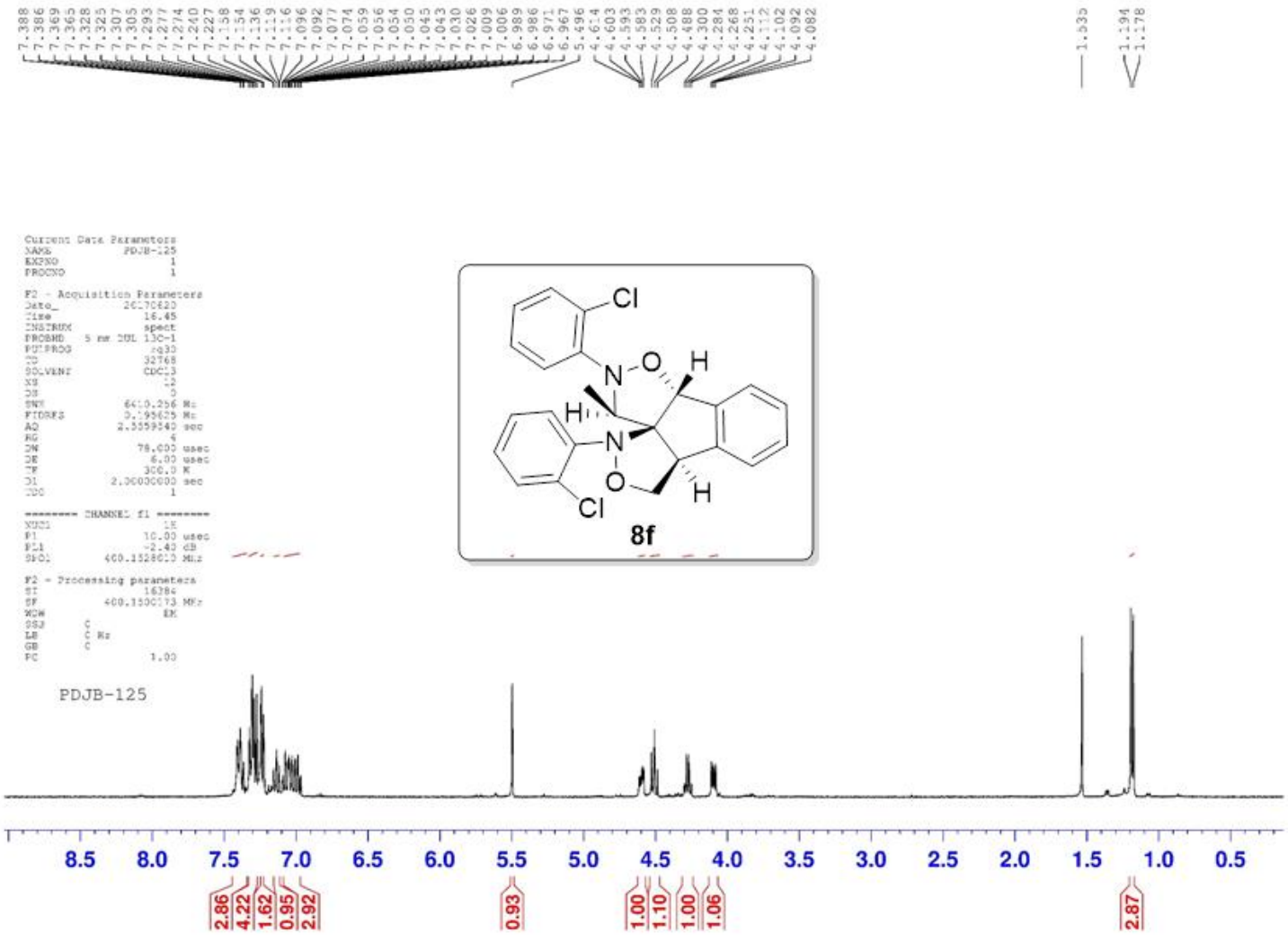



7.388
7.386
7.369
7.365
7.328
7.325
7.307
7.305
7.293
7.277
7.274
7.240
7.227
7.158
7.154
7.136
7.119
7.116
7.096
7.092
7.077
7.074
7.059
7.056
7.054
7.050
7.045
7.043
7.030
7.026
7.009
7.006
6.989
6.986
6.971
6.967
5.496
4.614
4.603
4.593
4.583
4.529
4.508
4.488
4.300
4.284
4.268
4.251
4.102
4.092
4.082
1.535
1.194
1.178
Current Data Parameters
NAME PDJB-125
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170620
Time 16.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559240 sec
RG 6
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1328013 MHz
F2 - Processing parameters
SI 16384
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
PDJB-125
Cl
N
O
H
H
N
O
H
Cl
8f
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
2.86
4.22
1.62
0.95
2.92
0.93
1.00
1.10
1.00
1.06
2.87

```
Current Data Parameters
NAME                  PDJ-B-125
EXPNO                         2
PROCNO                        1

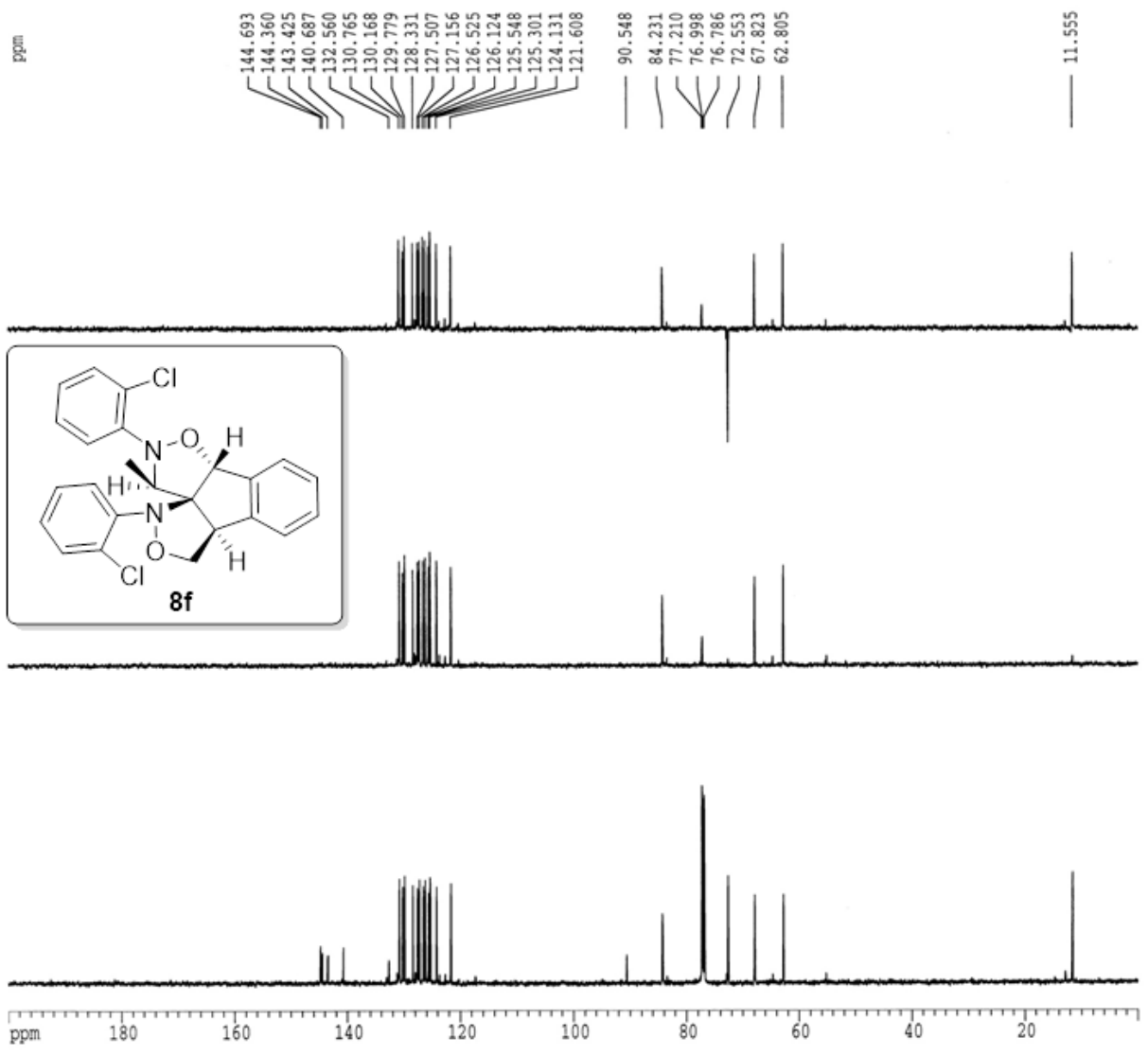
F2 - Acquisition Parameters
Date_                  20161121
Time                       8.48
INSTRUM                   spect
PROBHD    5 mm QNP  1H/1
PULPROG                   zgpg
TD                        32768
SOLVENT                   CDCl3
NS                          232
DS                            0
SWH                   45045.047 Hz
FIDRES                 1.374666 Hz
AQ                    0.3637748 sec
RG                         4096
DW                       11.100 usec
DE                        6.50 usec
TE                       296.8 K
D1                   3.50000000 sec
d11                  0.03000000 sec
DELTA                3.40000010 sec
MCREST               0.00000000 sec
MCWRK                0.01500000 sec

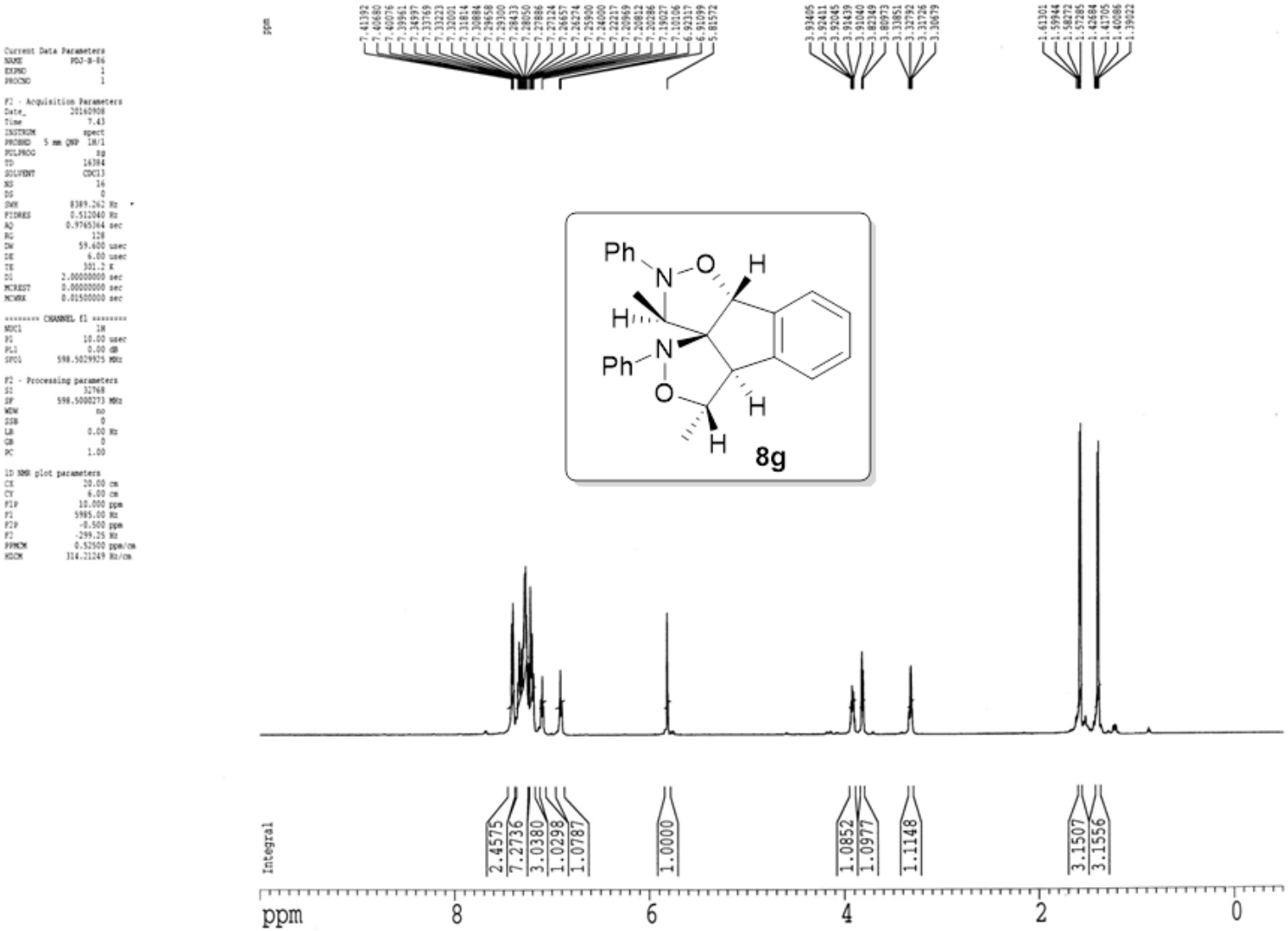
======== CHANNEL f1 ========
NUC1                        13C
P1                        4.80 usec
PL1                       0.00 dB
SFO1                150.4843515 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    92.00 usec
PL2                      120.00 dB
PL12                       9.00 dB
PL13                      14.00 dB
SFO2                598.4029920 MHz

F2 - Processing parameters
SI                         65536
SF                  150.4678070 MHz
WDW                           EM
SSB                           0
LB                         3.00 Hz
GB                            0
PC                         1.00

1D NMR plot parameters
CX                        20.00 cm
CY                         3.50 cm
F1P                      200.000 ppm
F1                     30093.56 Hz
F2P                        0.000 ppm
F2                         0.00 Hz
PPMCM                  10.00000 ppm/cm
HZCM                1504.67798 Hz/cm
```




Current Data Parameters
NAME PDJ-B-86
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160908
Time 7.43
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.512040 Hz
AQ 0.9765364 sec
RG 128
DW 59.600 usec
DE 6.00 usec
TE 301.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000273 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5985.00 Hz
F2P -0.500 ppm
F2 -299.25 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.21249 Hz/cm
ppm
7.41392
7.40880
7.40076
7.39961
7.34997
7.33769
7.33223
7.32001
7.31814
7.30884
7.29658
7.29300
7.28433
7.28050
7.27886
7.27124
7.26657
7.26274
7.25900
7.24000
7.22217
7.20969
7.20812
7.20286
7.19027
7.10106
6.92317
6.91099
5.81572
3.93405
3.92411
3.92045
3.91439
3.91040
3.82149
3.80973
3.33851
3.32792
3.31726
3.30879
1.61301
1.59944
1.58272
1.57285
1.42684
1.41705
1.40086
1.39022
Ph
N
O
H
H
N
Ph
O
H
H
8g
Integral
2.4575
7.2736
3.0380
1.0298
1.0787
1.0000
1.0852
1.0977
1.1148
3.1507
3.1556
ppm
8
6
4
2
0

```
Current Data Parameters
NAME                  PDJ-B-86
EXPNO                        2
PROCNO                       1

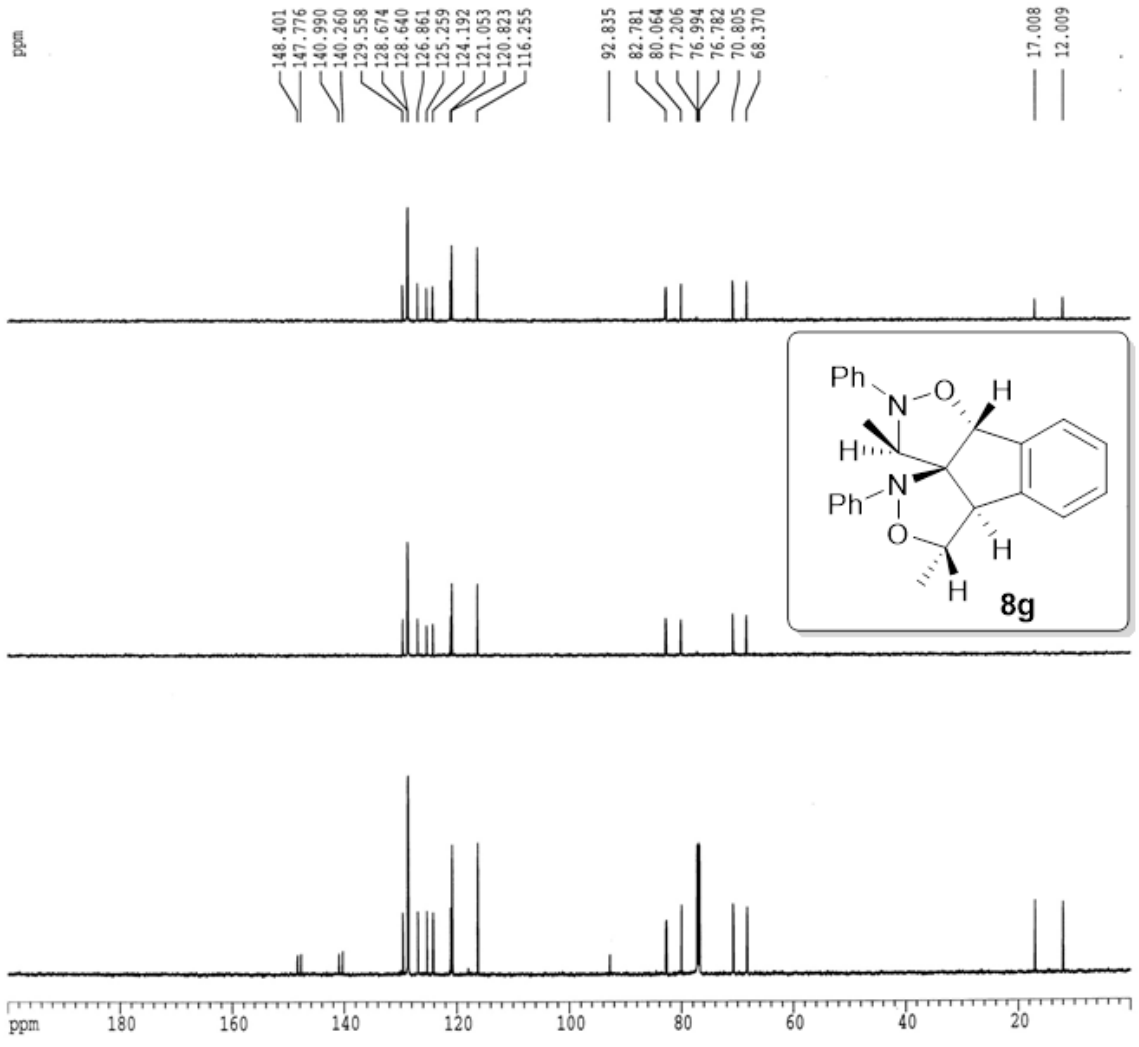
F2 - Acquisition Parameters
Date_              20160908
Time                    7.47
INSTRUM                spect
PROBHD   5 mm QNP  1H/1
PULPROG                 zgpg
TD                     32768
SOLVENT                CDCl3
NS                       273
DS                         0
SWH                45045.047 Hz
FIDRES                 1.374666 Hz
AQ                  0.3637748 sec
RG                        4096
DW                     11.100 usec
DE                      6.50 usec
TE                     301.3 K
D1                  3.50000000 sec
d11                 0.03000000 sec
DELTA               3.40000010 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

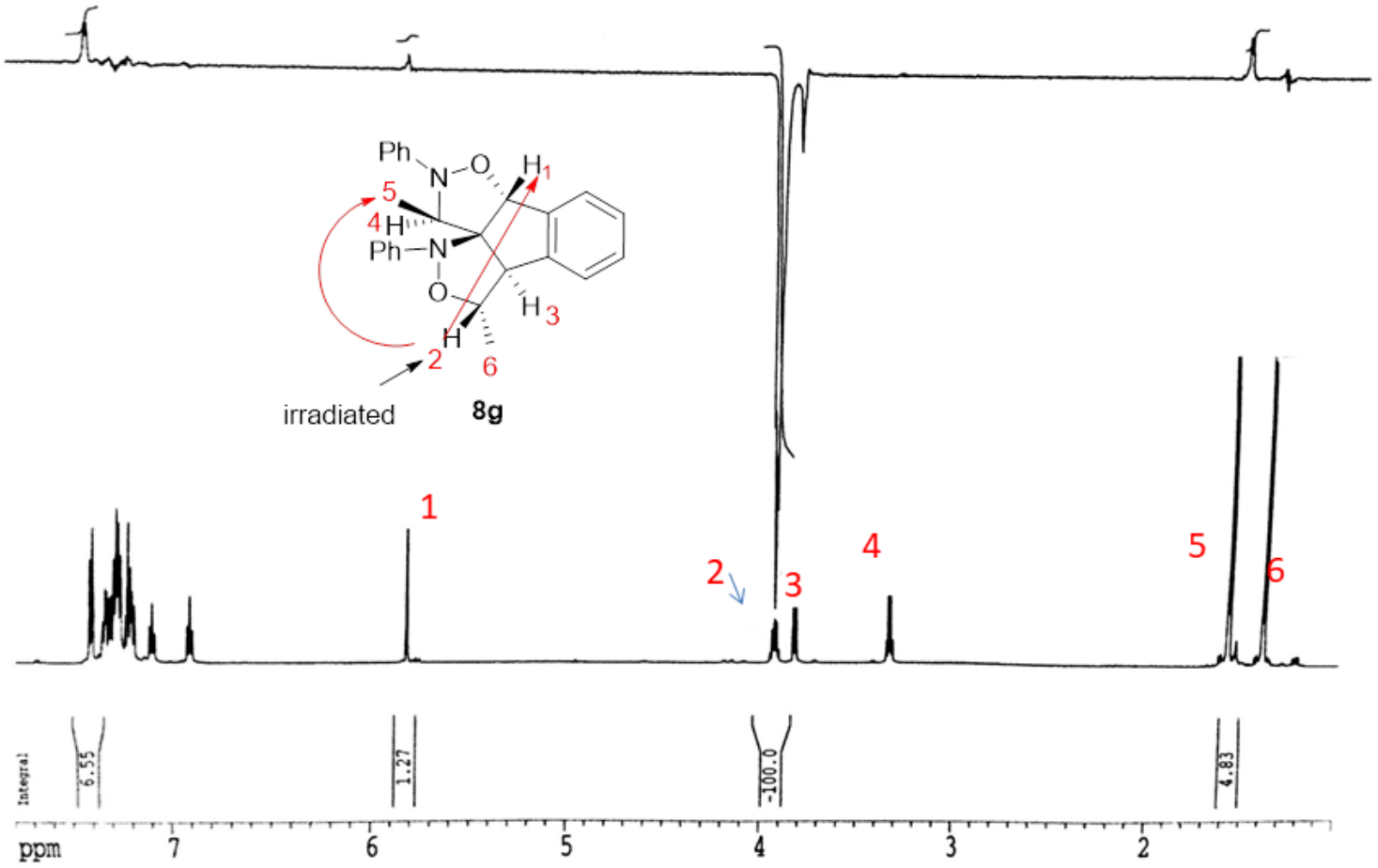
======== CHANNEL f1 ========
NUC1                      13C
P1                       4.80 usec
PL1                      0.00 dB
SFO1               150.5094992 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   92.00 usec
PL2                     120.00 dB
PL12                      9.00 dB
PL13                     14.00 dB
SFO2               598.5029925 MHz

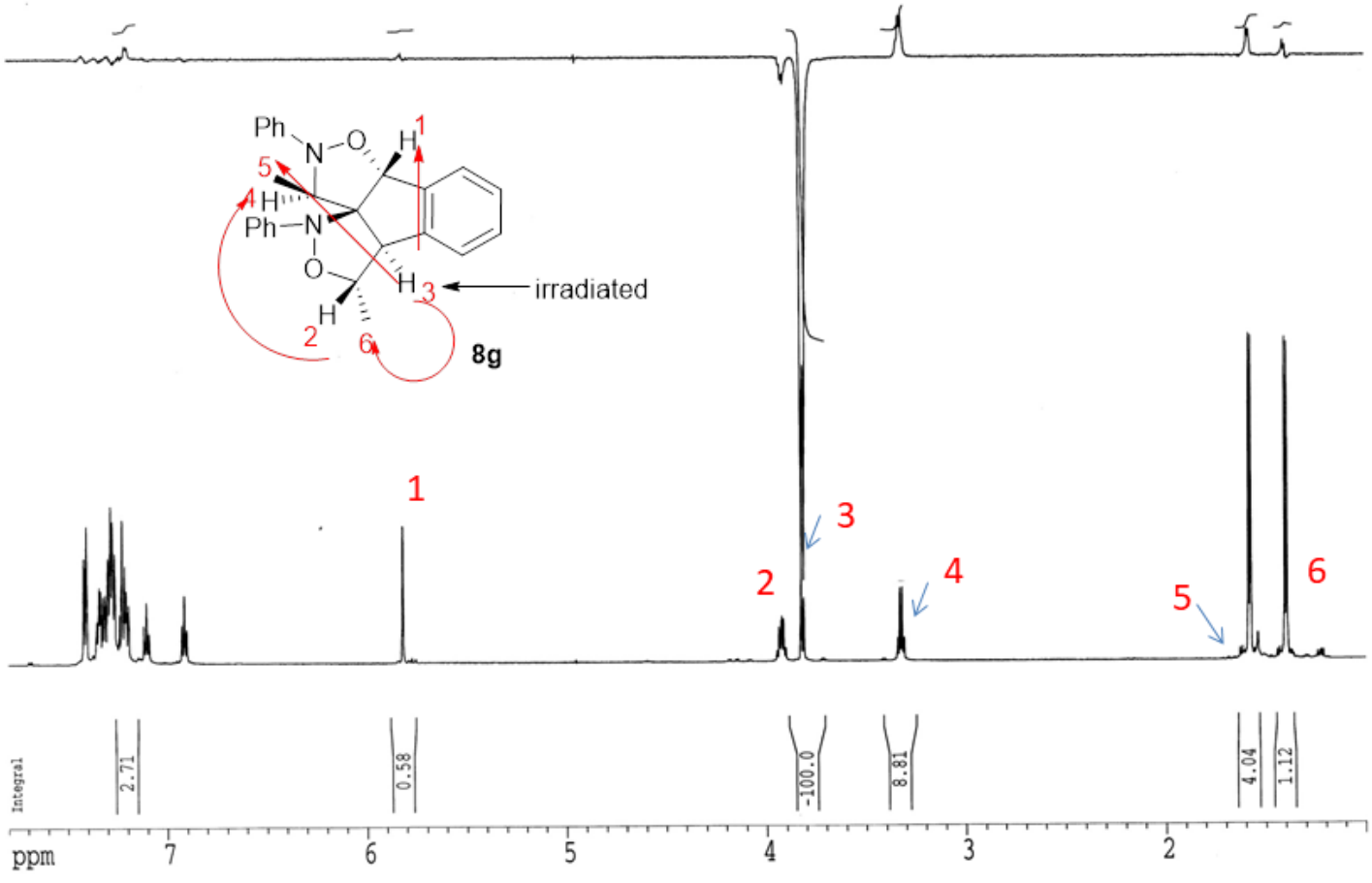
F2 - Processing parameters
SI                        65536
SF                 150.4929501 MHz
WDW                          EM
SSB                           0
LB                       3.00 Hz
GB                            0
PC                         1.00

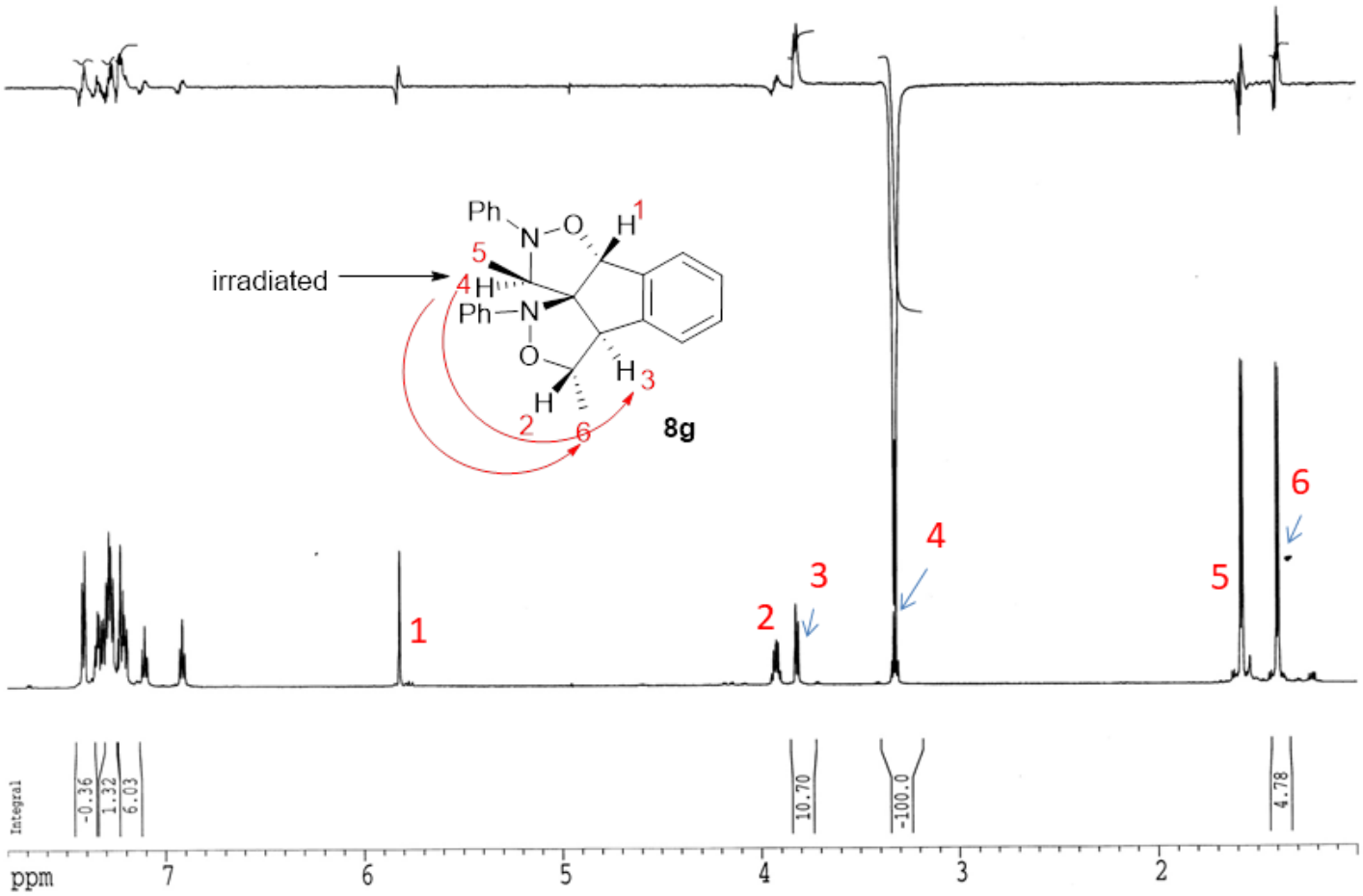
1D NMR plot parameters
CX                       20.00 cm
CY                        3.50 cm
F1P                     200.000 ppm
F1                    30098.59 Hz
F2P                       0.000 ppm
F2                        0.00 Hz
PPMCM                10.00000 ppm/cm
HZCM                 1504.92944 Hz/cm
```

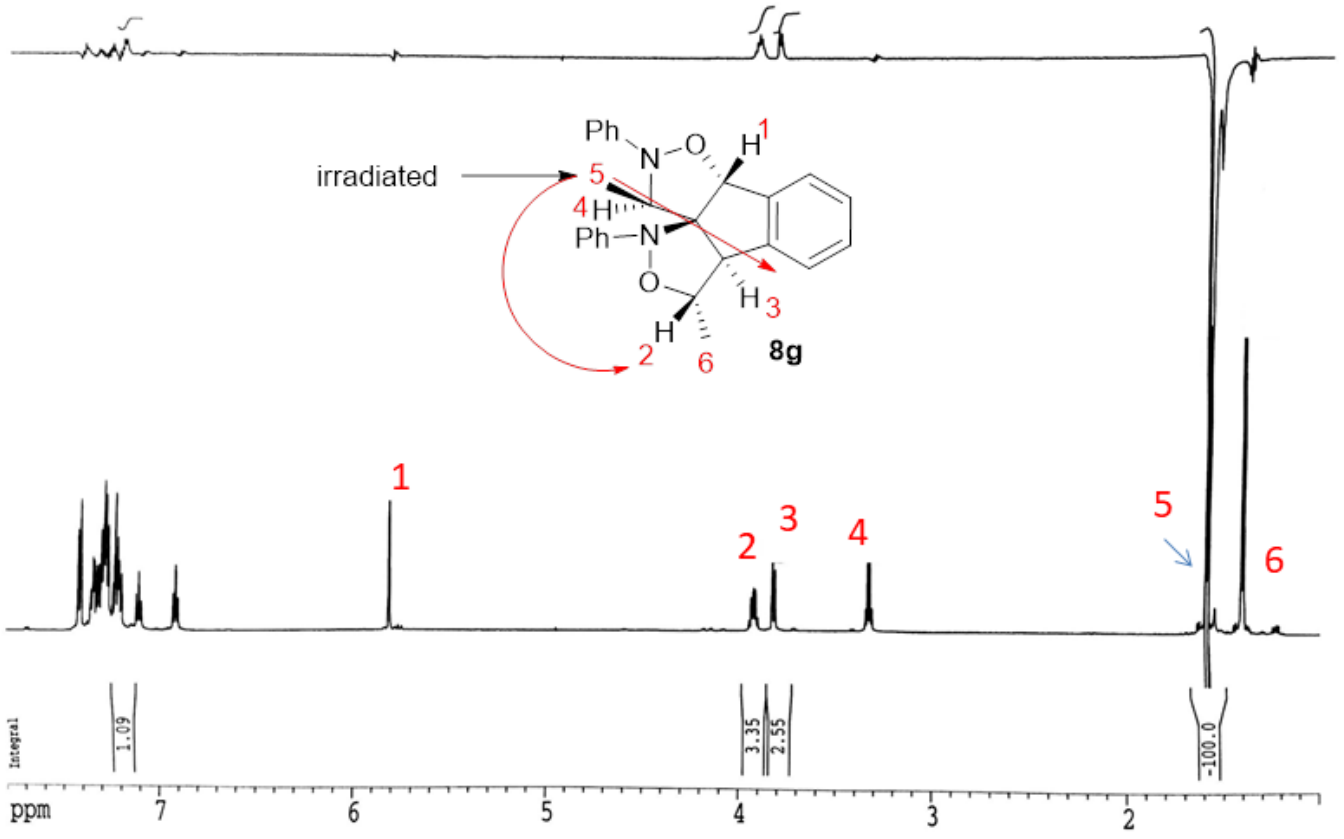


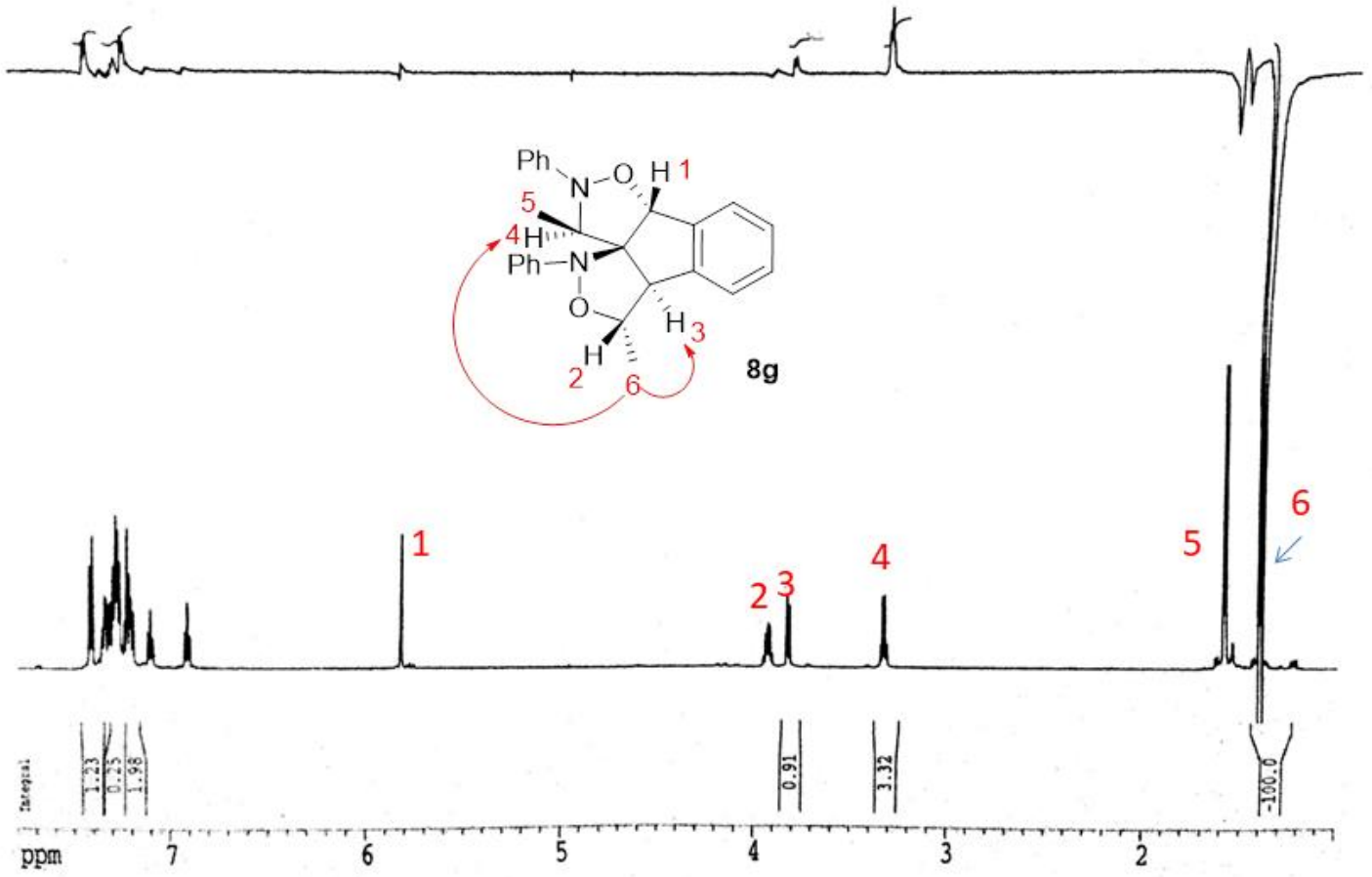

Ph
N
O
H1
5
4
H
Ph
N
O
H3
H
2
6
irradiated
8g
1
2
3
4
5
6
Integral
6.55
1.27
100.0
4.83
ppm
7
6
5
4
3
2

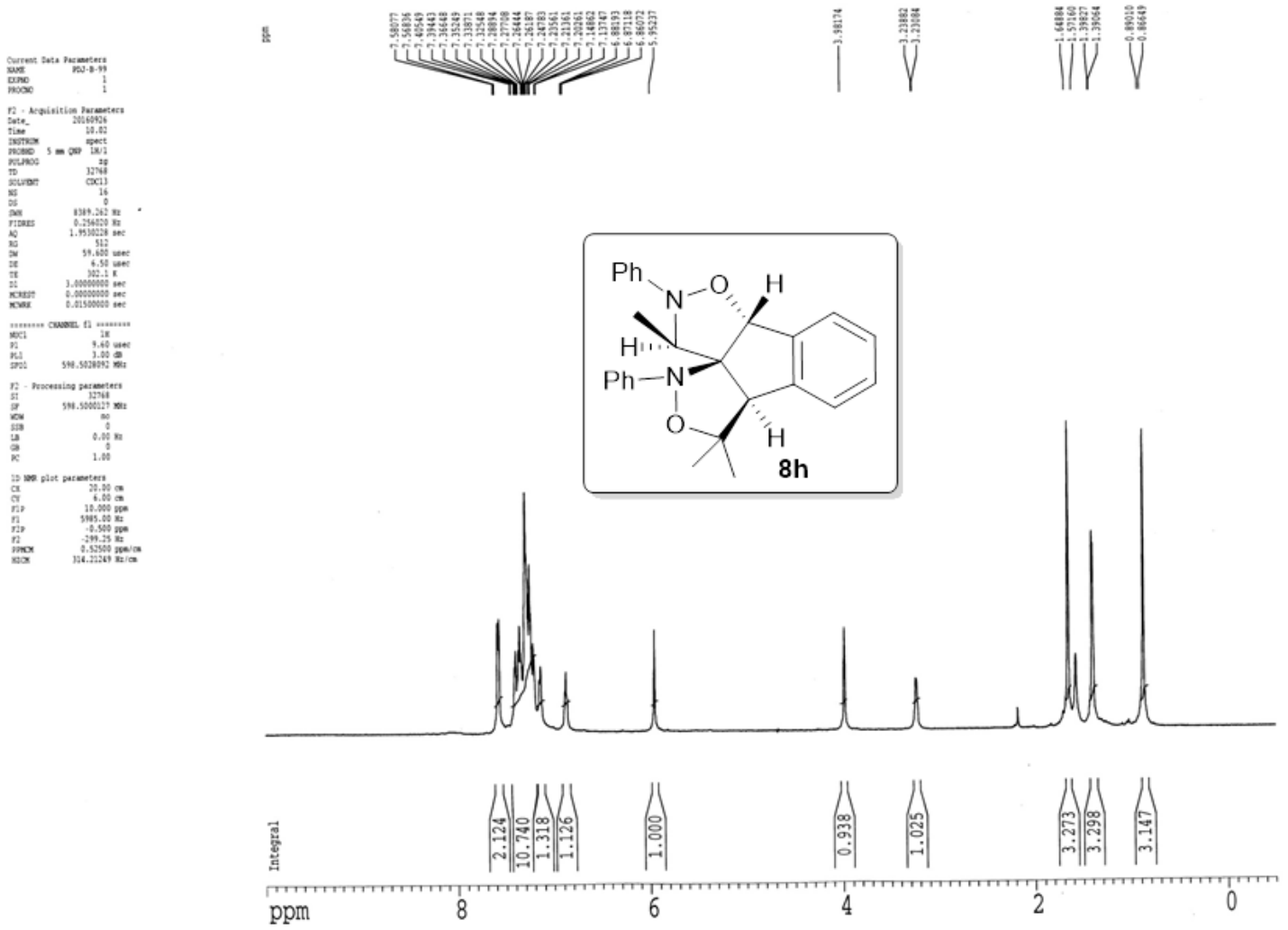
NOE

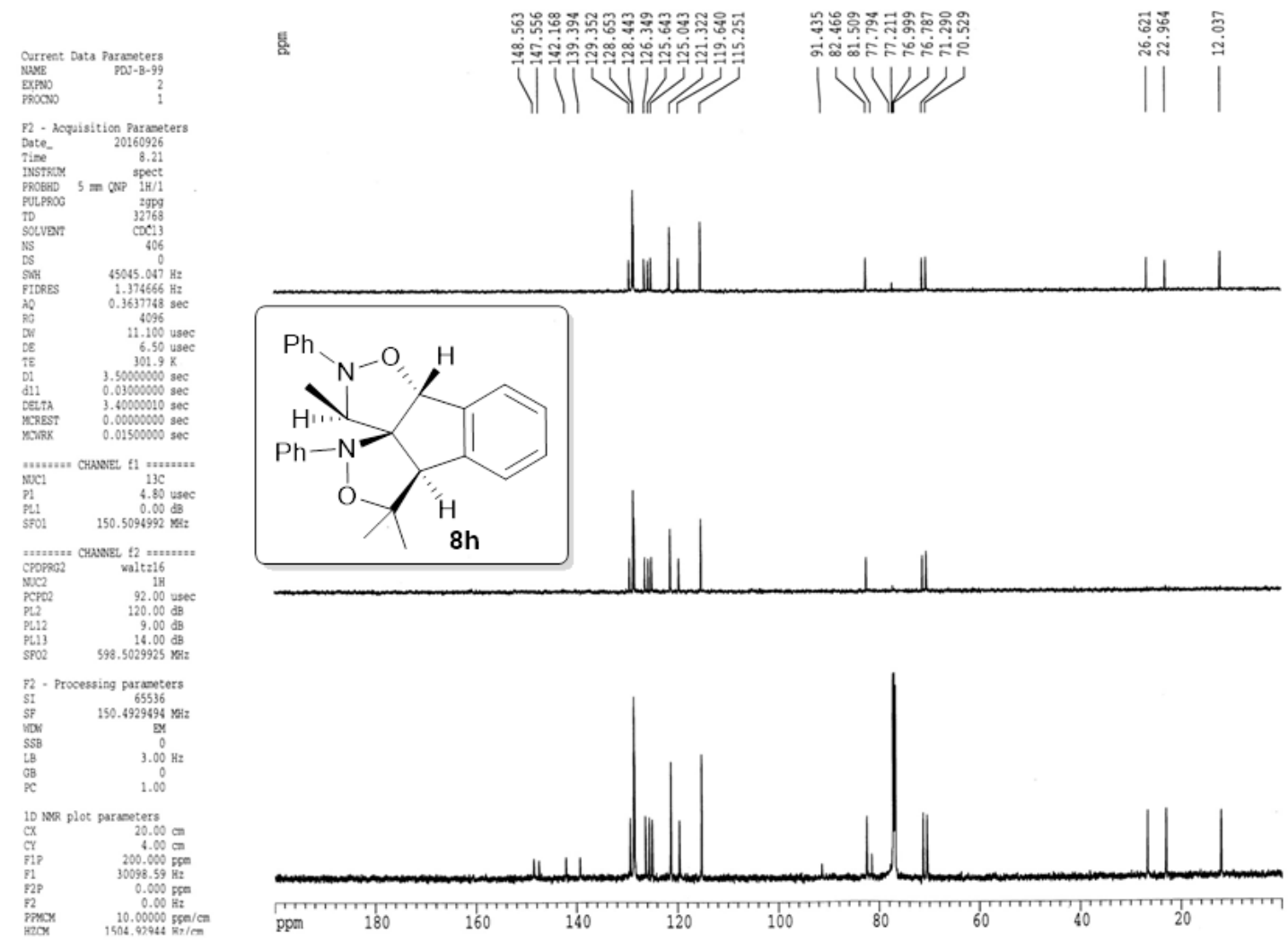

Ph
N
O
H
1
5
4
H
Ph
N
O
H
3
irradiated
H
2
6
8g
1
2
3
4
5
6
Integral
2.71
0.58
100.0
8.81
4.04
1.12
ppm
7
6
5
4
3
2

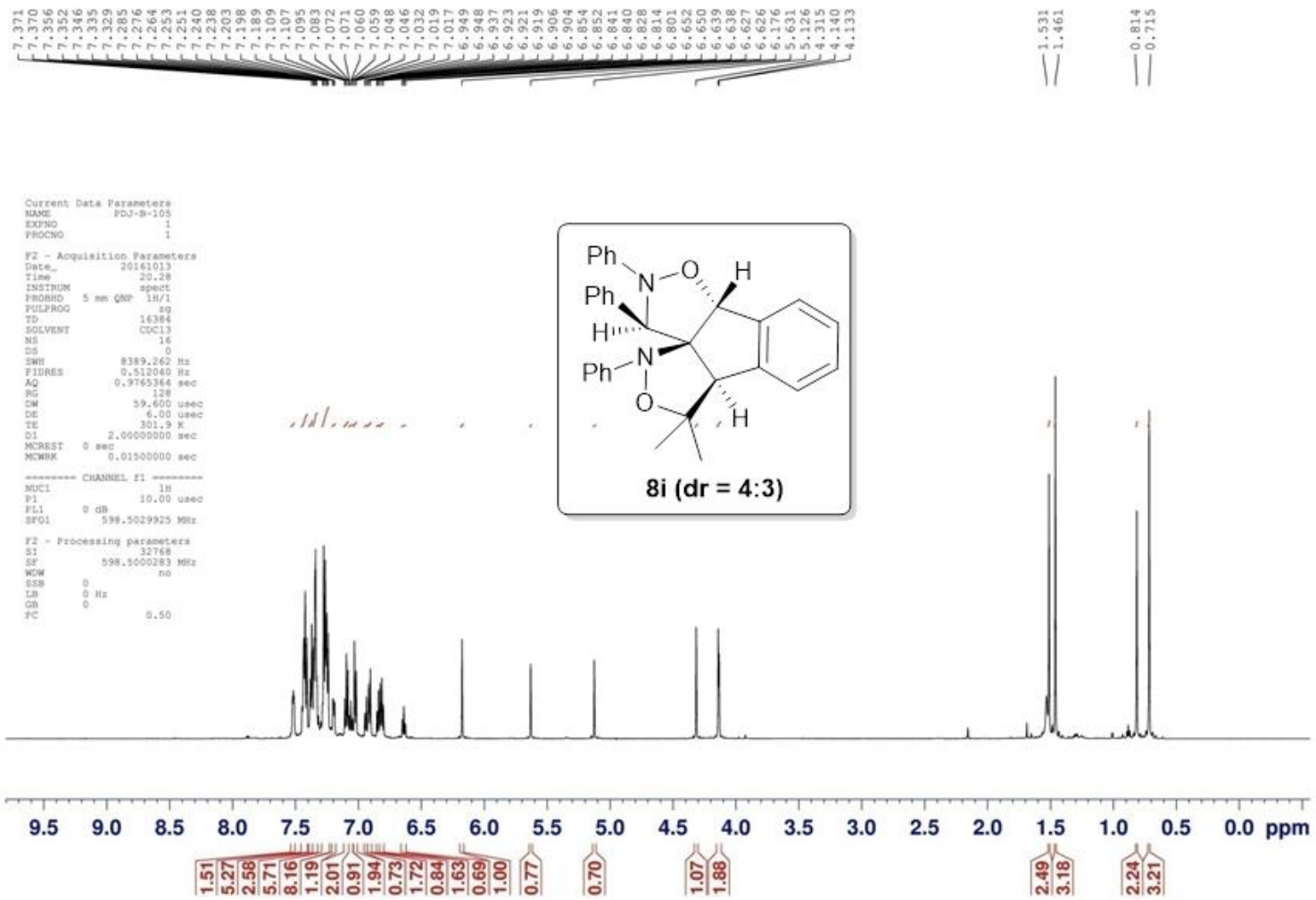

irradiated
Ph
N
O
H
1
5
4
H
Ph
N
O
H
3
H
2
6
8g
1
2
3
4
5
6
Integral
-0.36
1.32
6.03
10.70
-100.0
4.78
ppm
7
6
5
4
3
2

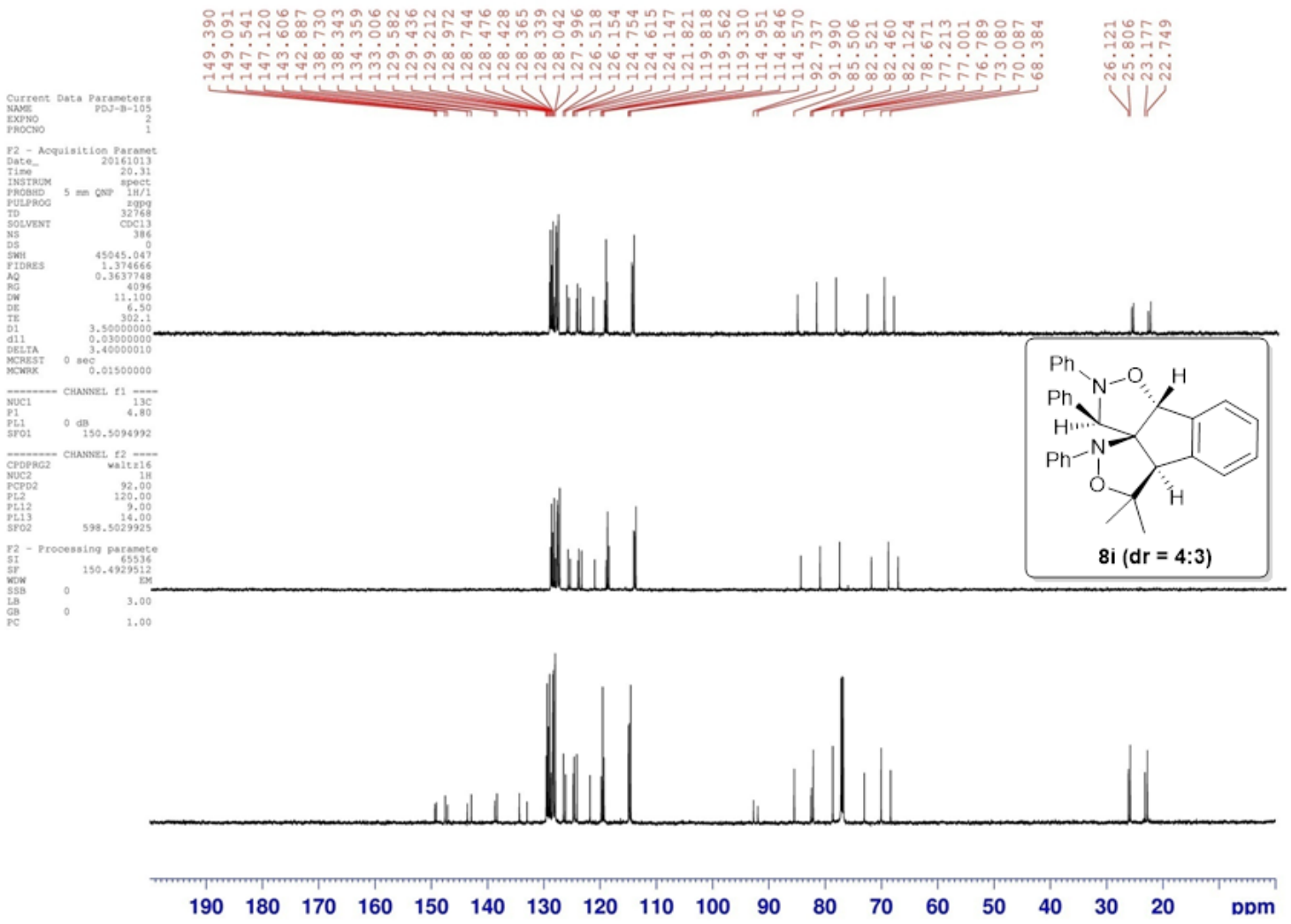

irradiated
Ph
N
O
H
1
5
4
H
Ph
N
O
H
3
H
2
6
8g
1
2
3
4
5
6
Integral
1.09
3.35
2.55
100.0
ppm
7
6
5
4
3
2


Ph
N
O
H
1
5
4
H
Ph
N
O
H
3
H
2
6
8g
1
2
3
4
5
6
1.23
0.25
1.98
0.91
3.32
100.0
ppm
7
6
5
4
3
2


Current Data Parameters
NAME PDJ-B-99
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160926
Time 10.02
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 302.1 K
D1 3.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.40 usec
PL1 3.00 dB
SFO1 598.5028092 MHz
F2 - Processing parameters
SI 32768
SF 598.5000127 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5985.00 Hz
F2P -0.500 ppm
F2 -299.25 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.21249 Hz/cm
ppm
7.58077
7.56896
7.40549
7.39443
7.36648
7.35249
7.33871
7.32548
7.28894
7.27708
7.26444
7.26187
7.24783
7.23561
7.21361
7.20261
7.14862
7.13747
6.88193
6.87118
6.86072
5.95237
3.38174
3.23882
3.23084
1.64884
1.57160
1.39827
1.39064
0.89010
0.86649
Ph
N
O
H
H
Ph
N
O
H
8h
Integral
2.124
10.740
1.318
1.126
1.000
0.938
1.025
3.273
3.298
3.147
ppm
8
6
4
2
0


Current Data Parameters
NAME PDJ-B-99
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160926
Time 8.21
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 406
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5094992 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.5029925 MHz
F2 - Processing parameters
SI 65536
SF 150.4929494 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30098.59 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.92944 Hz/cm
ppm
148.563
147.556
142.168
139.394
129.352
128.653
128.443
126.349
125.643
125.043
121.322
119.640
115.251
91.435
82.466
81.509
77.794
77.211
76.999
76.787
71.290
70.529
26.621
22.964
12.037
Ph
N
O
H
H
Ph
N
O
H
8h
ppm
180
160
140
120
100
80
60
40
20


7.371
7.370
7.356
7.352
7.346
7.335
7.329
7.285
7.276
7.264
7.253
7.251
7.240
7.238
7.203
7.198
7.189
7.109
7.107
7.095
7.083
7.072
7.071
7.060
7.059
7.048
7.046
7.032
7.019
7.017
6.949
6.948
6.937
6.923
6.921
6.919
6.906
6.904
6.854
6.852
6.841
6.840
6.828
6.814
6.801
6.652
6.650
6.639
6.638
6.627
6.626
6.176
5.631
5.126
4.315
4.140
4.133
1.531
1.461
0.814
0.715
Current Data Parameters
NAME PDJ-B-105
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161013
Time 20.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.512040 Hz
AQ 0.9765364 sec
RG 128
DW 59.600 usec
DE 6.00 usec
TE 301.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.5029925 MHz
F2 - Processing parameters
SI 32768
SF 598.5000283 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.50
Ph
N
O
H
Ph
H
Ph
N
O
H
8i (dr = 4:3)
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 ppm
1.51
5.27
2.58
5.71
8.16
1.19
2.01
0.91
1.94
0.73
1.72
0.84
1.63
0.69
1.00
0.77
0.70
1.07
1.88
2.49
3.18
2.24
3.21

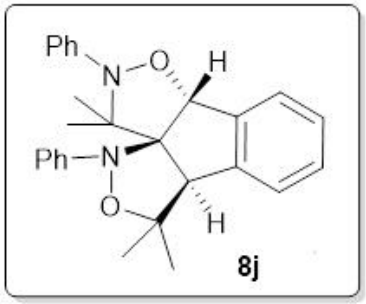

149.390
149.091
147.541
147.120
143.606
142.887
138.730
138.343
134.359
133.006
129.582
129.436
129.212
128.972
128.744
128.476
128.428
128.365
128.339
128.042
127.996
126.518
126.154
124.754
124.615
124.147
121.821
119.818
119.562
119.310
114.951
114.846
114.570
92.737
91.990
85.506
82.521
82.460
82.124
78.671
77.213
77.001
76.789
73.080
70.087
68.384
26.121
25.806
23.177
22.749
Current Data Parameters
NAME PDJ-B-105
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20161013
Time 20.31
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 386
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 302.1
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.5094992
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 9.00
PL13 14.00
SFO2 598.5029925
F2 - Processing paramete
SI 65536
SF 150.4929512
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
Ph
N
O
H
Ph
H
Ph
N
O
H
8i (dr = 4:3)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

PDJ-B-108 / 1H

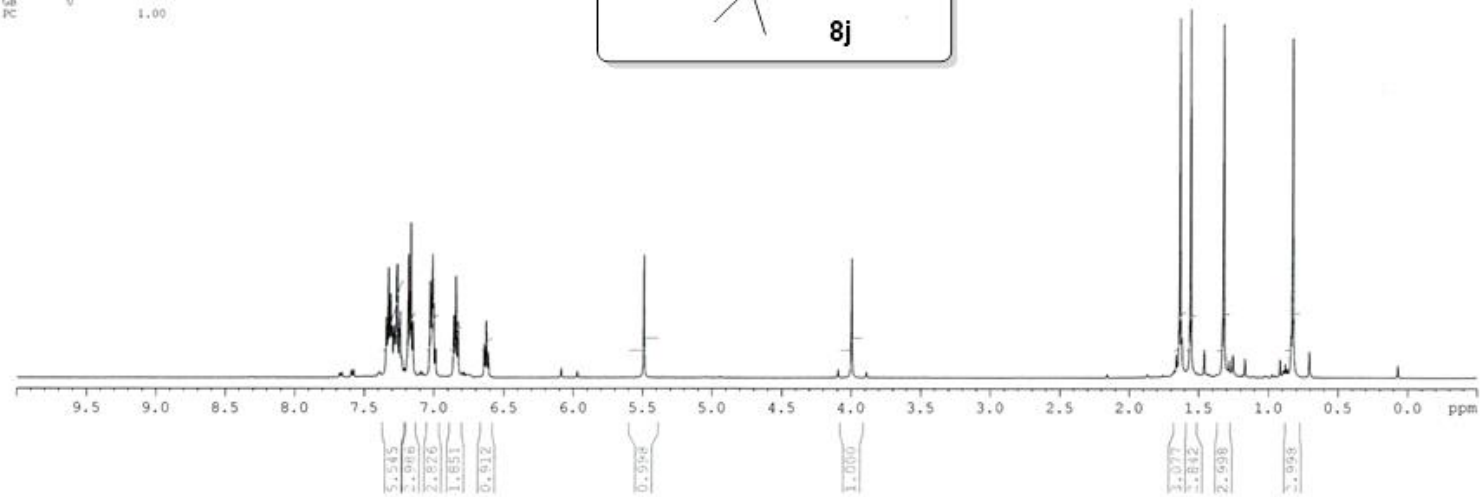

```
Current Data Parameters
NAME        liou1020.001
EXPNO                  1
PROCNO                 1

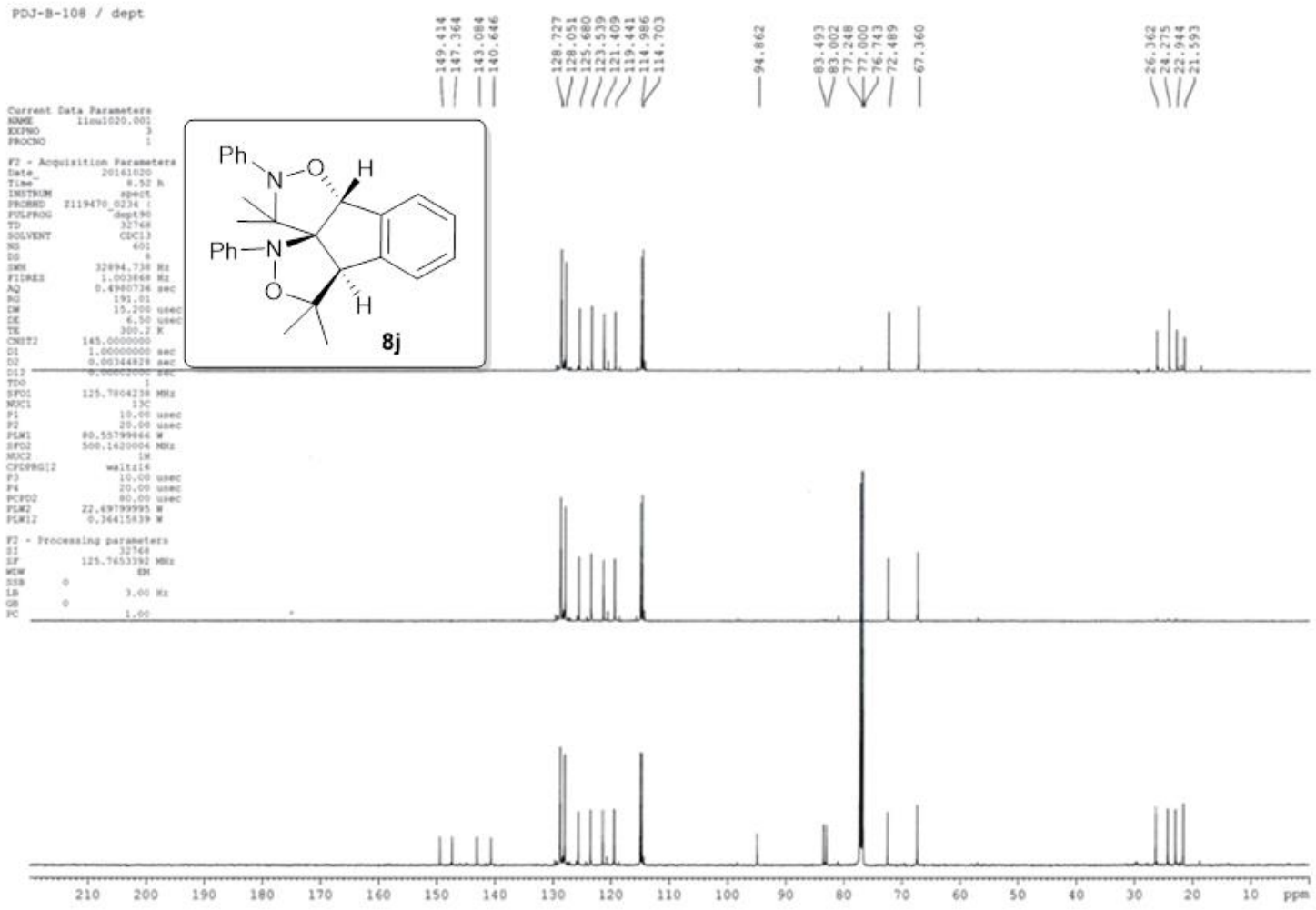
F2 - Acquisition Parameters
Date_           20161020
Time                8.02 h
INSTRUM            spect
PROBHD   Z119470_0234 (
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    0
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             1.6384000 sec
RG                 55.6
DW                50.000 usec
DE                13.50 usec
TE                299.7 K
D1             2.00000000 sec
TD0                    1
SFO1          500.1640013 MHz
NUC1                1H
P1                10.00 usec
PLW1          22.69799995 W

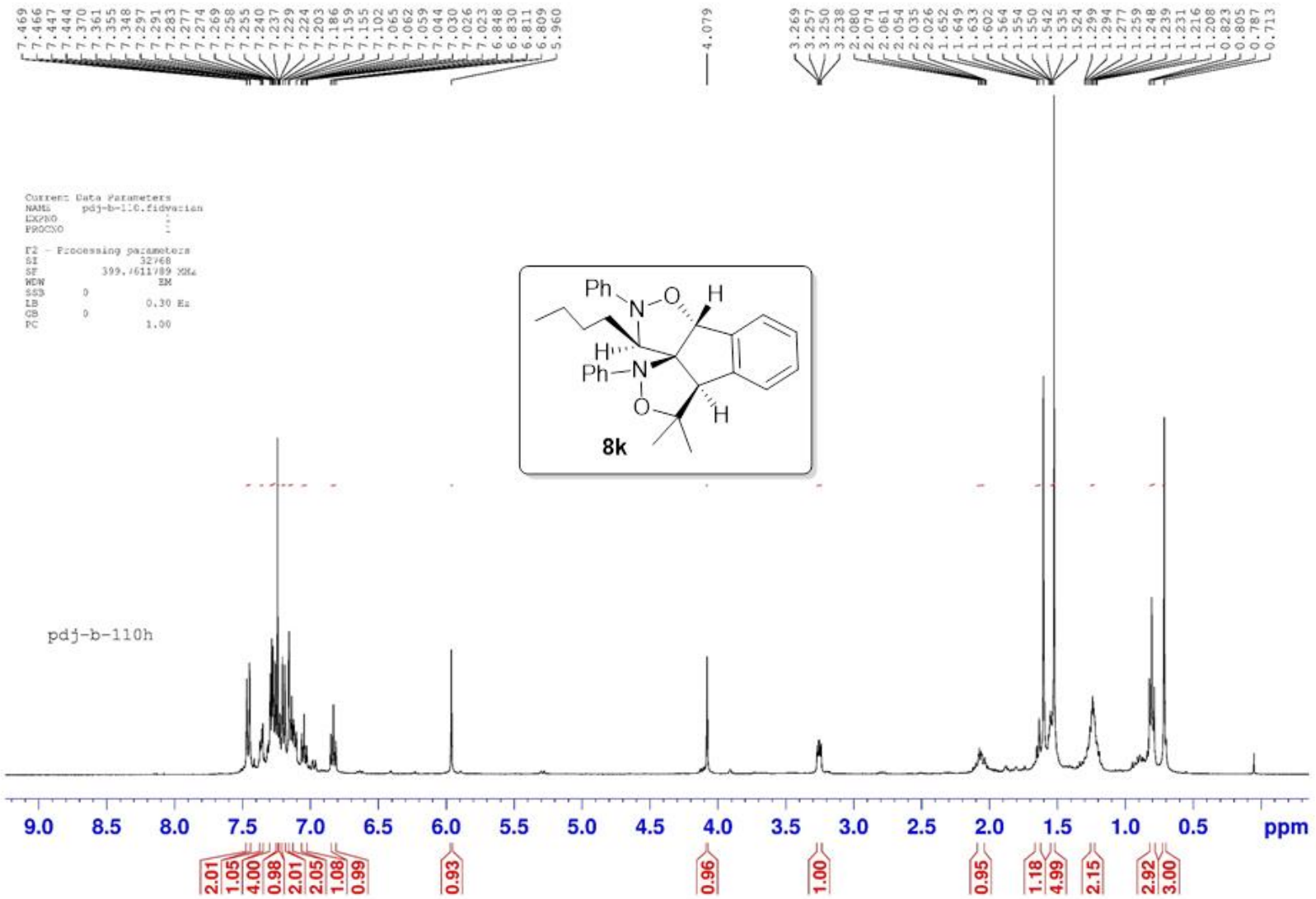
F2 - Processing parameters
SI                 16384
SF            500.1600206 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

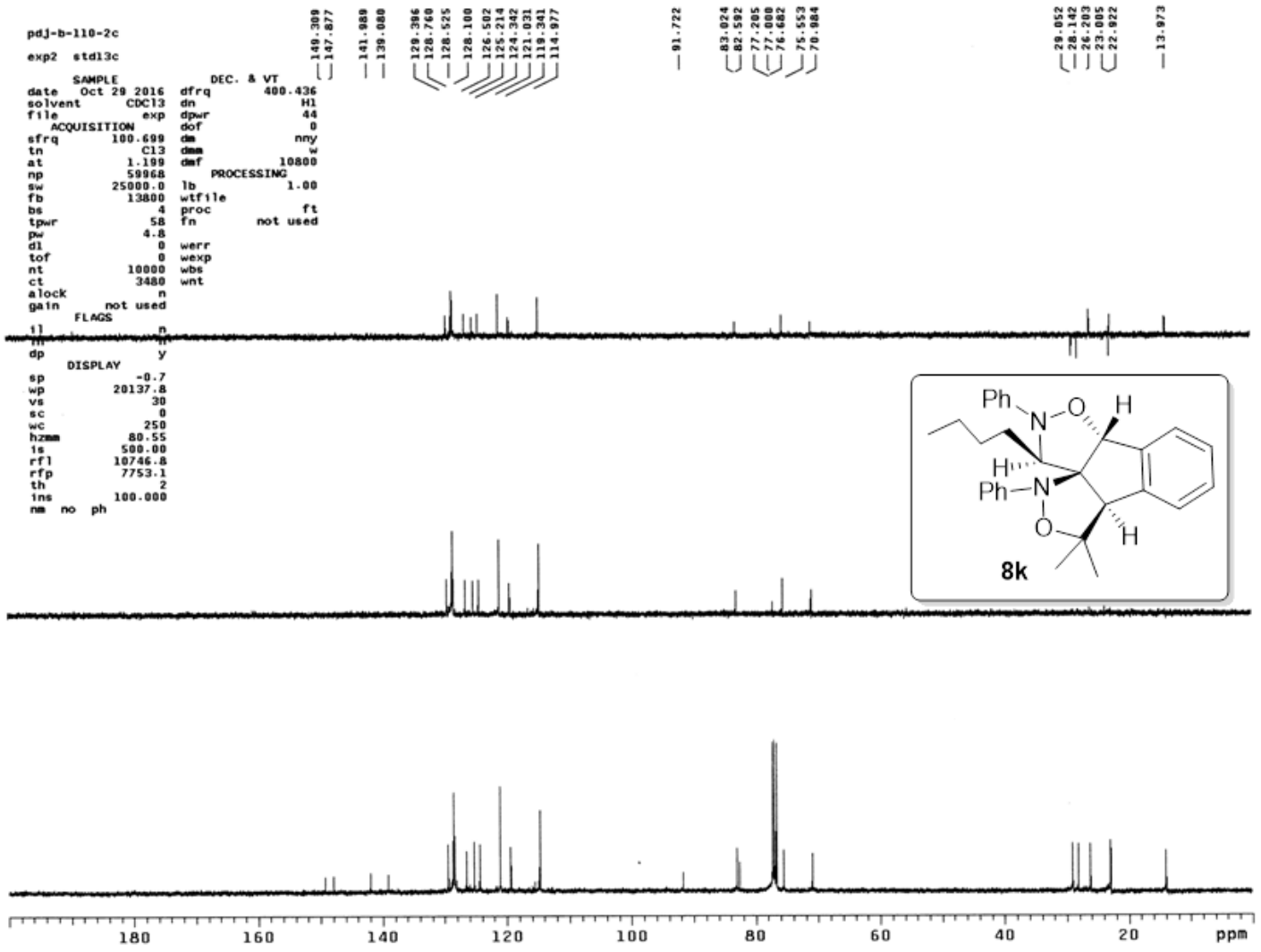


8j




PDJ-B-108 / dept
149.414
147.364
143.084
140.646
128.727
128.051
125.680
123.539
121.409
119.441
114.986
114.703
94.862
83.493
83.002
77.248
77.000
76.743
72.489
67.360
26.362
24.275
22.944
21.593
Ph
N
O
H
Ph
N
O
H
8j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.469
7.466
7.447
7.444
7.370
7.361
7.355
7.348
7.297
7.291
7.283
7.277
7.274
7.269
7.258
7.255
7.240
7.237
7.229
7.224
7.203
7.186
7.159
7.155
7.102
7.065
7.062
7.059
7.044
7.030
7.026
7.023
6.848
6.830
6.811
6.809
5.960
4.079
3.269
3.257
3.250
3.238
2.080
2.074
2.061
2.054
2.035
2.026
1.652
1.649
1.633
1.602
1.564
1.554
1.550
1.542
1.535
1.524
1.299
1.294
1.277
1.259
1.248
1.239
1.231
1.216
1.208
0.823
0.805
0.787
0.713
Current Data Parameters
NAME pdj-b-110.fidvarian
EXPNO
PROCNO
F2 - Processing parameters
SI 32768
SF 399.7611789 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
N
O
H
H
Ph
N
O
H
8k
pdj-b-110h
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
ppm
2.01
1.05
4.00
0.98
2.01
2.05
1.08
0.99
0.93
0.96
1.00
0.95
1.18
4.99
2.15
2.92
3.00


pdj-b-110-2c
exp2 std13c
SAMPLE
date Oct 29 2016
solvent CDCl3
file exp
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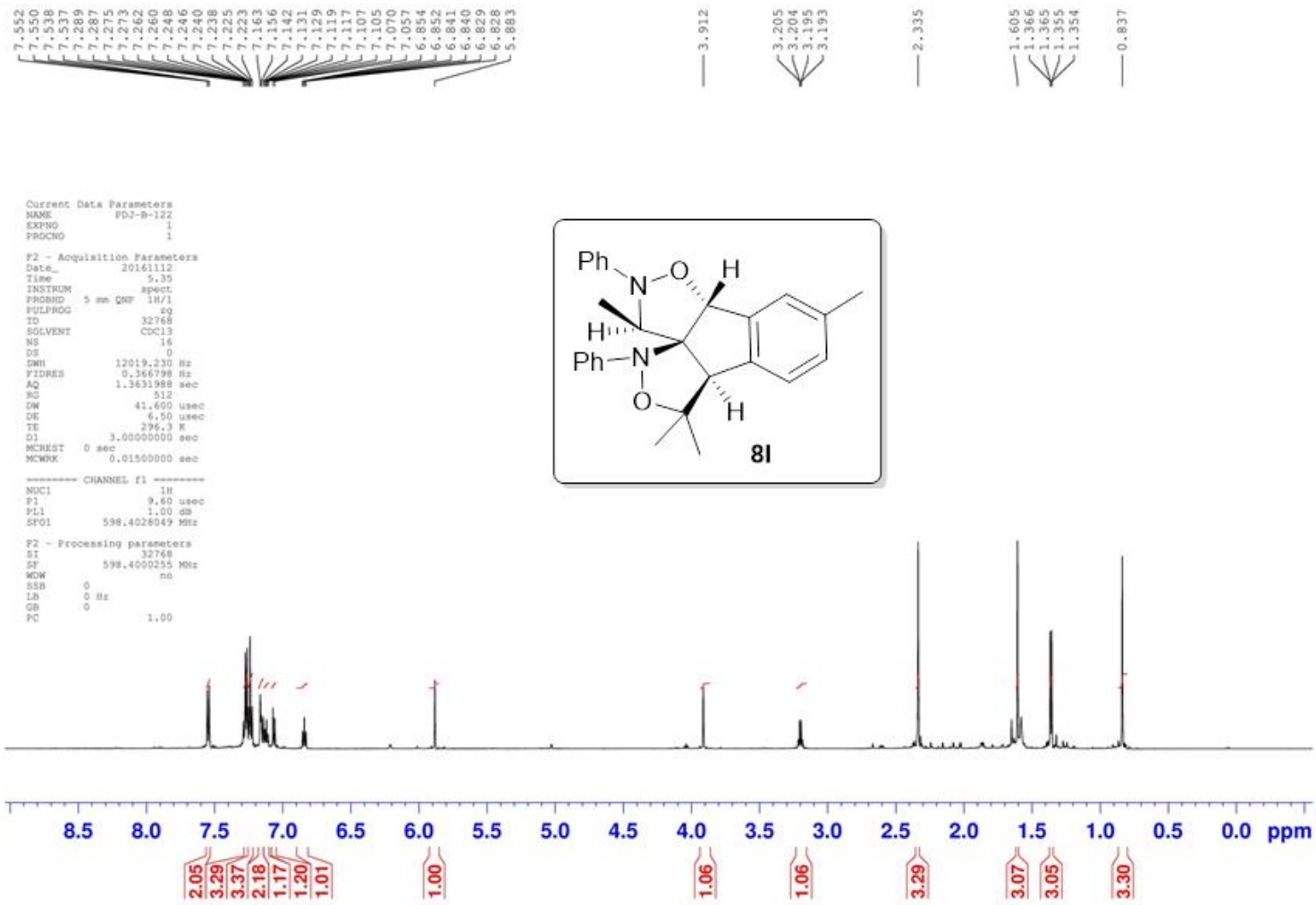
sfrq 100.699
tn C13
at 1.199
np 59968
sw 25000.0
fb 13800
bs 4
tpwr 58
pw 4.8
dl 0
tof 0
nt 10000
ct 3480
alock n
gain not used
FLAGS
il n
dp y
DISPLAY
sp -0.7
wp 20137.8
vs 30
sc 0
wc 250
hzmm 80.55
is 500.00
rfl 10746.8
rfp 7753.1
th 2
ins 100.000
nm no ph
DEC. & VT
dfrq 400.436
dn H1
dpwr 44
dof 0
dm nny
dmm w
dmf 10800
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
149.309
147.877
141.988
139.080
129.396
128.760
128.525
128.100
126.502
125.214
124.342
121.031
119.341
114.977
91.722
83.024
82.592
77.205
77.000
76.682
75.553
70.984
29.052
28.142
26.203
23.005
22.922
13.973
Ph
N
O
H
H
Ph
N
O
H
8k
180
160
140
120
100
80
60
40
20
ppm


7.552
7.550
7.538
7.537
7.289
7.287
7.275
7.273
7.262
7.260
7.248
7.246
7.240
7.238
7.225
7.223
7.163
7.156
7.142
7.131
7.129
7.119
7.117
7.107
7.105
7.070
7.057
6.854
6.852
6.841
6.840
6.829
6.828
5.883
3.912
3.205
3.204
3.195
3.193
2.335
1.605
1.366
1.365
1.355
1.354
0.837
Current Data Parameters
NAME PDJ-B-122
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161112
Time 5.35
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 296.3 K
D1 3.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 1.00 dB
SFO1 598.4028049 MHz
F2 - Processing parameters
SI 32768
SF 598.4000255 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
N
O
H
H
Ph
N
O
H
8l
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
ppm
2.05
3.29
3.37
2.18
1.17
1.20
1.01
1.00
1.06
1.06
3.29
3.07
3.05
3.30

```
Current Data Parameters
NAME          PDJ-B-122
EXPNO                 2
PROCNO                1

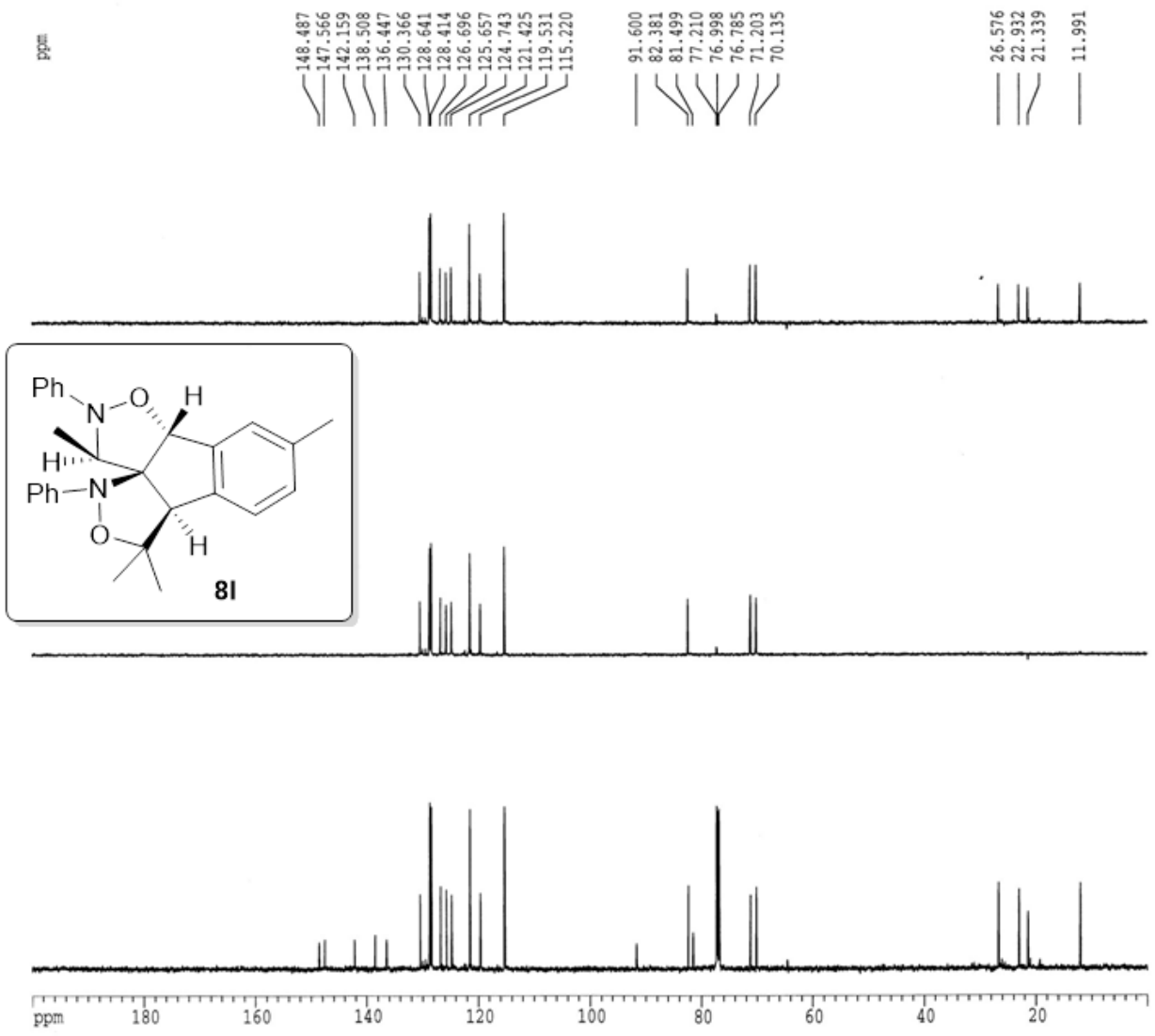
F2 - Acquisition Parameters
Date_          20161111
Time              13.36
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG           zgpg
TD               32768
SOLVENT           CDCl3
NS                  258
DS                    0
SWH           45045.047 Hz
FIDRES        1.374666 Hz
AQ            0.3637748 sec
RG                 4096
DW               11.100 usec
DE                6.50 usec
TE               296.3 K
D1            3.50000000 sec
d11           0.03000000 sec
DELTA         3.40000010 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 4.80 usec
PL1                0.00 dB
SFO1         150.4843515 MHz

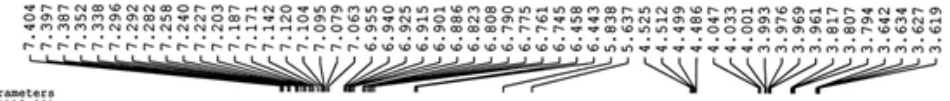
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             92.00 usec
PL2              120.00 dB
PL12               9.00 dB
PL13              14.00 dB
SFO2         598.4029920 MHz

F2 - Processing parameters
SI                 65536
SF           150.4678056 MHz
WDW                   EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                 3.00 cm
F1P              200.000 ppm
F1             30093.56 Hz
F2P              0.000 ppm
F2               0.00 Hz
PPMCM          10.00000 ppm/cm
HZCM         1504.67798 Hz/cm
```



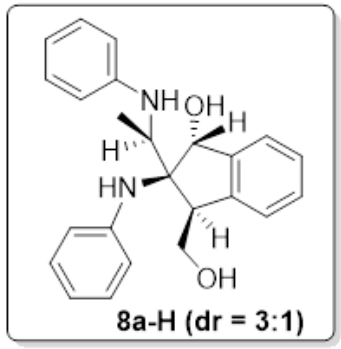
PDJ-B-123



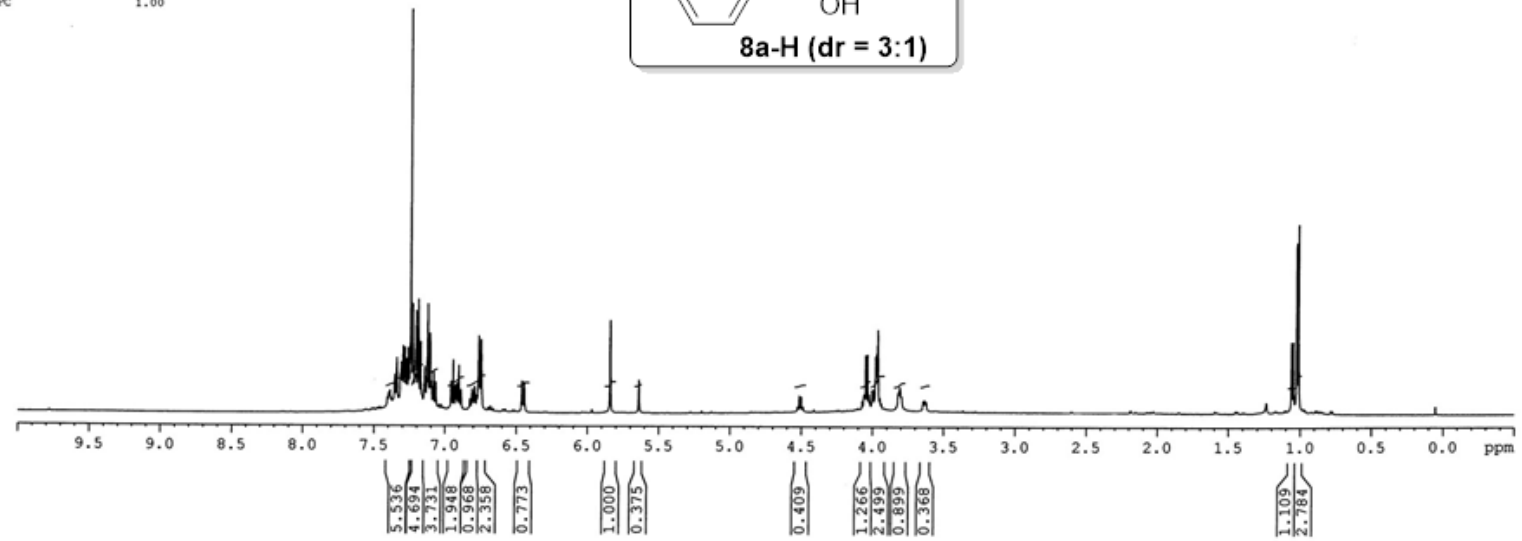

```
Current Data Parameters
NAME        liou1118.001
EXPNO                  1
PROCNO                 1

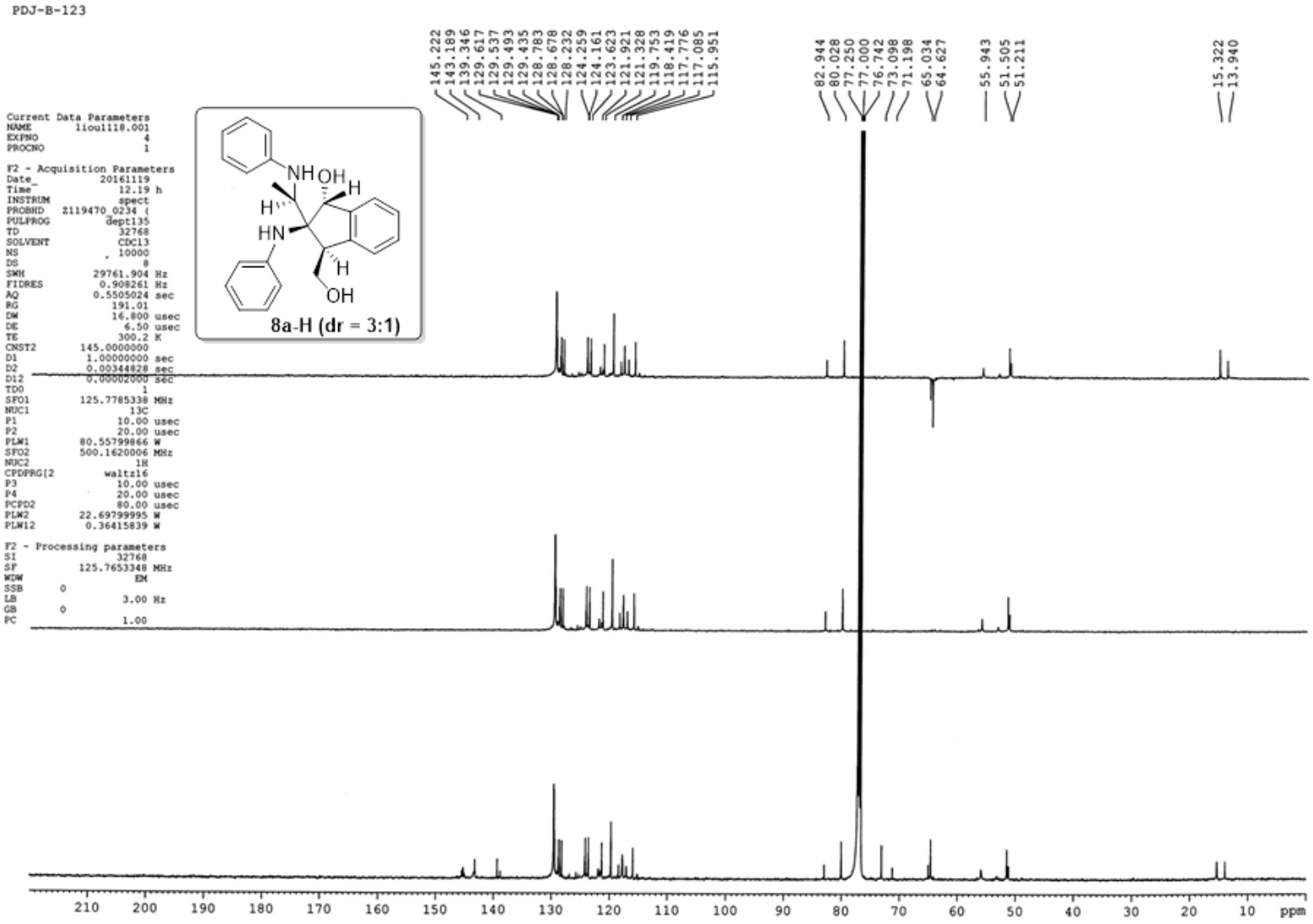
F2 - Acquisition Parameters
Date_           20161118
Time_              15.00 h
INSTRUM             spect
PROBHD   Z119470_0234 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH           10026.738 Hz
FIDRES        0.305992 Hz
AQ            1.6340309 sec
RG                  95.8
DW                49.867 usec
DE                 7.71 usec
TE                299.8 K
D1           2.00000000 sec
TD0                    1
SFO1        500.1630010 MHz
NUC1                1H
P1                10.00 usec
PLW1        22.69799995 W

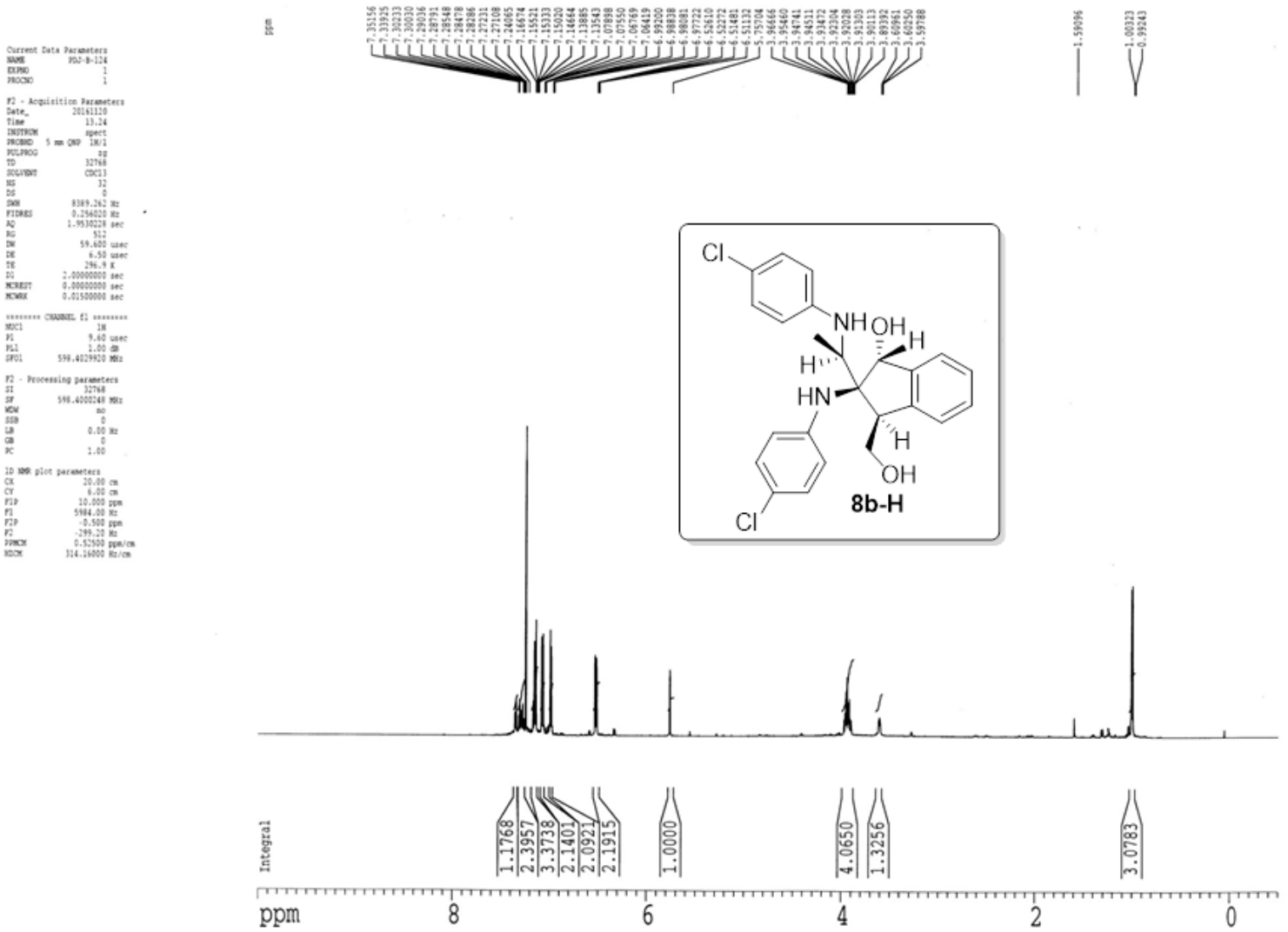
F2 - Processing parameters
SI                 16384
SF          500.1600211 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

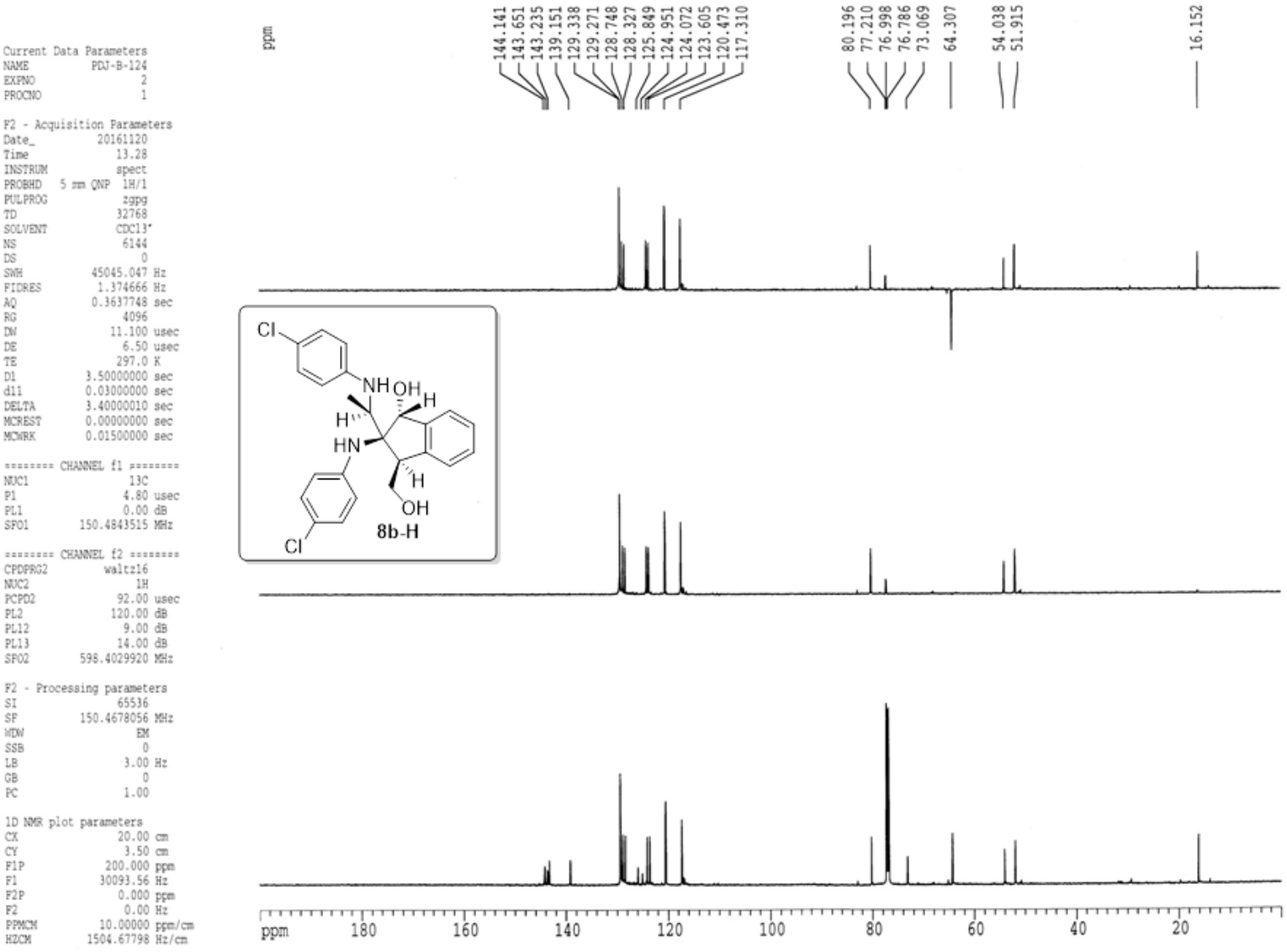


8a-H (dr = 3:1)




PDJ-B-123
145.222
143.189
139.346
129.617
129.537
129.493
129.435
128.783
128.678
128.232
124.259
124.161
123.623
121.921
121.328
119.753
118.419
117.776
117.085
115.951
82.944
80.028
77.250
77.000
76.742
73.098
71.198
65.034
64.627
55.943
51.505
51.211
15.322
13.940
Current Data Parameters
NAME liou1118.001
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161119
Time 12.19 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG dept135
TD 32768
SOLVENT CDCl3
NS 10000
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505024 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 300.2 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7785338 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 80.55799866 W
SFO2 500.1620006 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 22.69799995 W
PLW12 0.36415839 W
F2 - Processing parameters
SI 32768
SF 125.7653348 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
NH
OH
H
H
HN
H
OH
8a-H (dr = 3:1)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Current Data Parameters
NAME PDJ-B-124
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161120
Time 13.24
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9535220 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.60 usec
PL1 1.00 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000248 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5984.00 Hz
F2P -0.500 ppm
F2 -299.20 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.16000 Hz/cm
ppm
7.35156
7.33925
7.30233
7.30030
7.29036
7.28791
7.28548
7.28478
7.28286
7.27231
7.27108
7.24065
7.16674
7.15521
7.15333
7.15020
7.14664
7.13885
7.13543
7.07898
7.07550
7.06769
7.06419
6.99200
6.98838
6.98081
6.97722
6.52610
6.52272
6.51481
6.51133
5.75704
3.96666
3.95469
3.94741
3.94511
3.93472
3.92304
3.92028
3.91303
3.90113
3.89392
3.60961
3.60250
3.59788
1.59096
1.00323
0.99243
Cl
NH
OH
H
H
HN
H
OH
Cl
8b-H
Integral
1.1768
2.3957
3.3738
2.1401
2.0921
2.1915
1.0000
4.0650
1.3256
3.0783
ppm
8
6
4
2
0


Current Data Parameters
NAME PDJ-B-124
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161120
Time 13.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 297.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678056 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 3.50 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67798 Hz/cm
ppm
144.141
143.651
143.235
139.151
129.338
129.271
128.748
128.327
125.849
124.951
124.072
123.605
120.473
117.310
80.196
77.210
76.998
76.786
73.069
64.307
54.038
51.915
16.152
Cl
NH
OH
H
H
HN
H
OH
Cl
8b-H
ppm
180
160
140
120
100
80
60
40
20