Selective mono- to perarylations of tetrabromothiophene by a cyclobutene-1,2-diyl-bisimidazolium preligand

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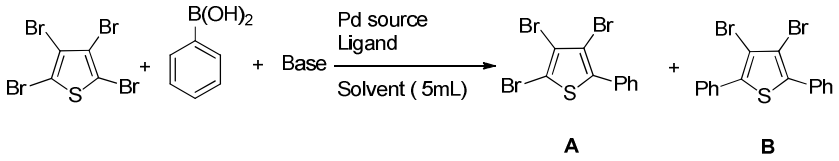
Contents

1. Reaction Optimization:

For optimizing the reaction conditions we selected tetrabromothiophene and phenylboronic acid as a reference reaction.



A B

Initially, the effects of catalyst systems (Pd + Ligands) were investigated. The following table summarizes our results.

Table S1. Optimization of the reaction conditions.

Entry	Catalyst (mol %)	equiv. of boronic acid	Solvent	H_2O (mL)	Base	T (^oC)	T (h)	Yield(%) A/B
1	$PdCl_2(PPh_3)_2$ (10 mol %)	1.2	toluene	1	K_3PO_4	90	12	0
2	$Pd(PPh_3)_4$ (6 mol%)	2.4	toluene	1	K_3PO_4	90	12	42/55
3	$Pd(PPh_3)_4$ (6 mol%)	1.2	toluene	0.1	K_3PO_4	reflux	10	48/23
4	$Pd(PPh_3)_4$ (6 mol%)	2.4	toluene	0.1	K_3PO_4	reflux	12	28/56
5	$Pd(OAc)_2$ (5mol %) + XPhos(10 mol%)	1.2	toluene	0.1	K_3PO_4	reflux	10	31/7
6	$Pd(OAc)_2$ (5mol %) + XPhos(10 mol%)+	2.4	toluene	0.2	K_3PO_4	100	10	11/41
7	$Pd(OAc)_2$ (5mol %) + XPhos(10 mol%)+	1.2	dioxane	1	K_3PO_4	reflux	12	23/5
8	$Pd(OAc)_2$ (4 mol %) + **3** (4mol %)	1.2	dioxane	0	K_3PO_4	80	12	18/32

9	$Pd(OAc)_2$ (4 mol %) + **3** (4mol %)	1.2	toluene	0	NaOtBu	70	7	39/31
10	$Pd(OAc)_2$ (4 mol %) + **3** (4mol %)	1.2	Toluene	0	K_3PO_4	75	8	72/11
11	$Pd(OAc)_2$ (4 mol %) + **3** (4mol %)	2.4	Toluene	0	K_3PO_4	75	12	9/69

2. Crystal Structure Determination of 11

The single-crystal X-ray diffraction study was carried out on a Nonius Kappa-CCD diffractometer at 123(2) K using MoKα radiation (λ = 0.71073 Å). The structure was solved by Patterson Methods (SHELXS-97)[a] and refinement was carried out using SHELXL-97[a] (full-matrix least-squares on F^2). Hydrogen atoms were localized by difference electron density determination and refined using a riding model. A semi-empirical absorption correction was applied.

11: colorless crystals, $C_{32}H_{28}O_2S$, M = 476.60, crystal size 0.35 x 0.15 x 0.10 mm, monoclinic, space group $P2_1/c$ (No. 14), a = 11.985(1) Å, b = 9.940(1) Å, c = 21.337(2) Å, β = 97.10(1)°, V = 2522.4(4) Å^3, Z = 4, ρ(calc) = 1.255 Mg m^{-3}, F(000) = 1008, μ = 0.156 mm^{-1}, 36097 reflections ($2\theta_{max}$ = 55°), 5771 unique [R_{int} = 0.053], 320 parameters, *R1* ($I > 2\sigma(I)$) = 0.047, *wR2 (all data)* = 0.109, S = 1.04, largest diff. peak and hole 0.266 and -0.330 e Å^{-3}. Crystallographic data (excluding structure factors) for the structures reported in this work have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 828244 (**xy**). Copies of the data can be obtained free of charge on application to The Director, CCDC, 12 Union Road, Cambridge DB2 1EZ, UK (Fax: int.code+(1223)336-033; e-mail: deposit@ccdc.cam.ac.uk).

Reference:

a) G. M. Sheldrick, *Acta Crystallogr*. **2008**, *A64*, 112 - 122.

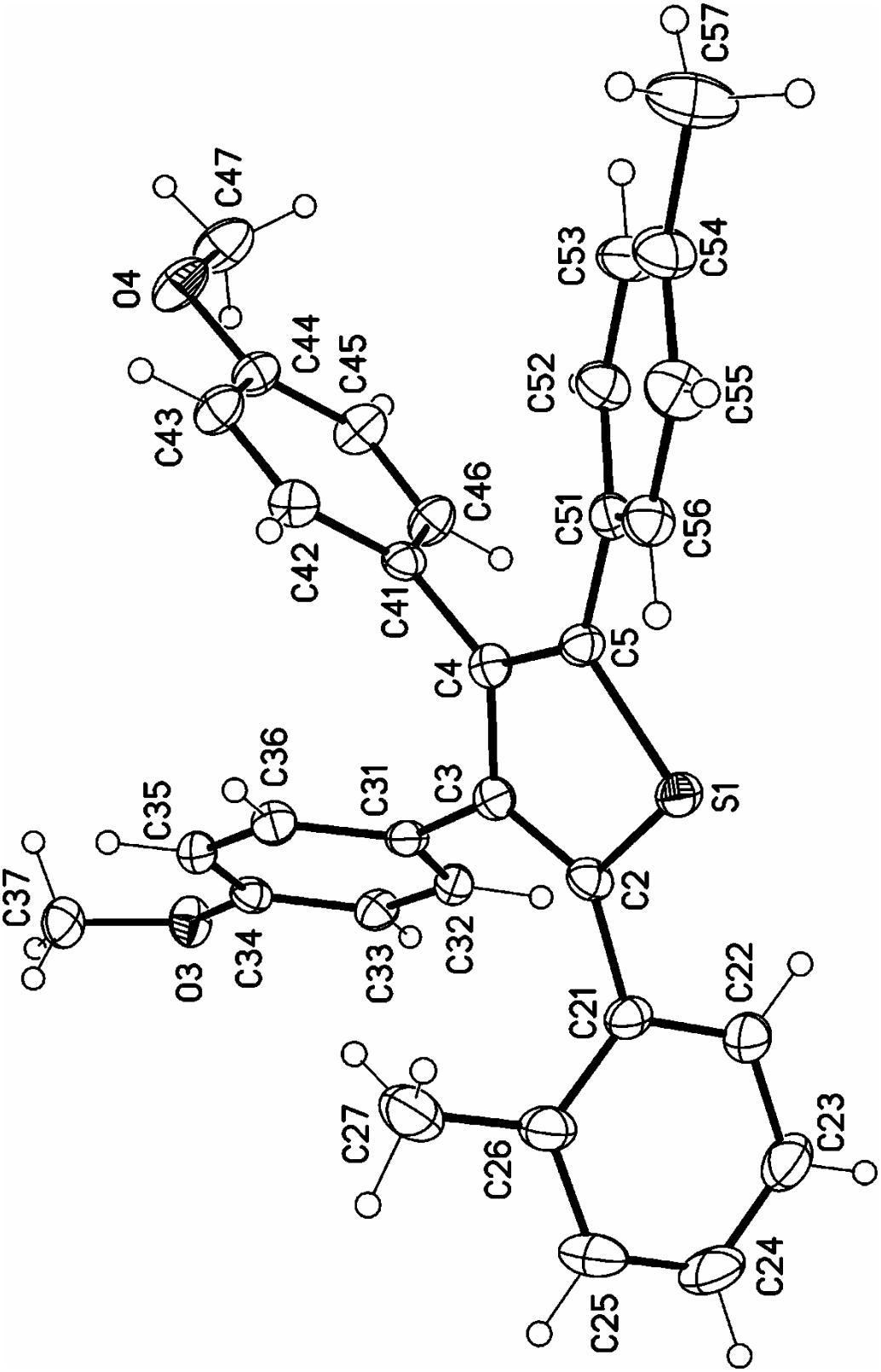


Fig. S1. Molecular structure of **11** (displacement parameters are drawn at 50% probability level).

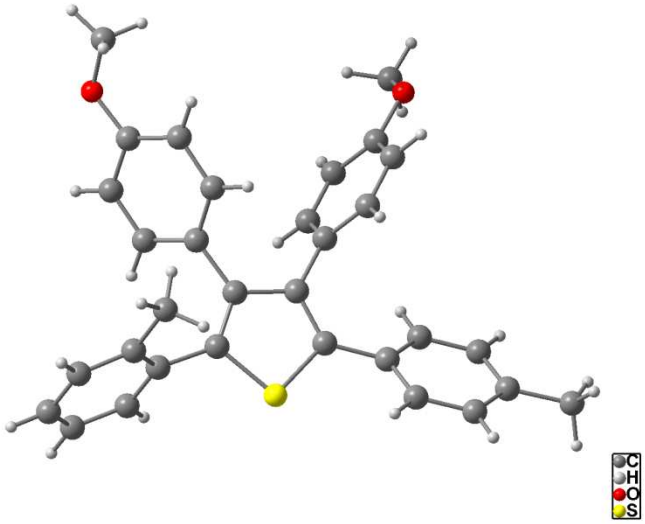


Fig. S2. Molecular structure of **11**.

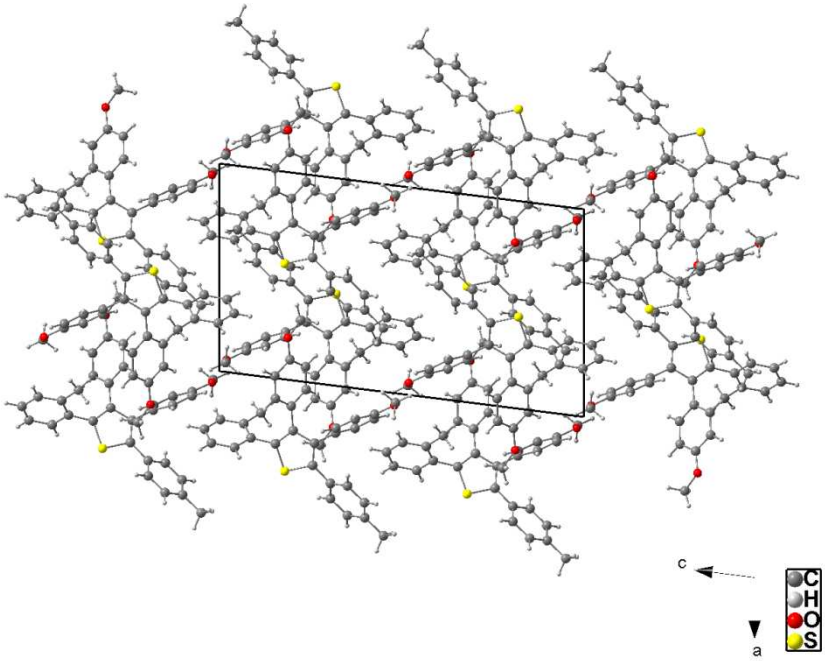


Fig. S3. Unit cell of **11** (view along the b-axis).

Table S2. Crystal data and structure refinement for schm46.

Identification code	schm46
Empirical formula	C32 H28 O2 S
Formula weight	476.60
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c (No.14)
Unit cell dimensions	a = 11.985(1) A alpha = 90 deg. b = 9.940(1) A beta = 97.10(1) deg. c = 21.337(2) A gamma = 90 deg.
Volume	2522.4(4) A^3
Z, Calculated density	4, 1.255 Mg/m^3
Absorption coefficient	0.156 mm^-1
F(000)	1008
Crystal size	0.35 x 0.15 x 0.10 mm
Theta range for data collection	3.17 to 27.48 deg.
Limiting indices	-15<=h<=15, -12<=k<=12, -27<=l<=27
Reflections collected / unique	36097 / 5771 [R(int) = 0.0525]
Completeness to theta = 27.48	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9803 and 0.8502
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5771 / 0 / 320
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0468, wR2 = 0.0991
R indices (all data)	R1 = 0.0686, wR2 = 0.1086
Largest diff. peak and hole	0.266 and -0.330 e.A^-3

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for schm46.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	4420(1)	6093(1)	3205(1)	21(1)
C(2)	3153(1)	5695(2)	3461(1)	20(1)
C(3)	2414(1)	5213(2)	2975(1)	19(1)
C(4)	2891(1)	5146(2)	2392(1)	18(1)
C(5)	3969(1)	5607(2)	2439(1)	18(1)
C(21)	3020(1)	5901(2)	4133(1)	22(1)
C(22)	3583(2)	5049(2)	4583(1)	29(1)
C(23)	3504(2)	5219(2)	5217(1)	38(1)
C(24)	2879(2)	6248(3)	5408(1)	44(1)
C(25)	2320(2)	7097(2)	4968(1)	43(1)
C(26)	2372(2)	6947(2)	4326(1)	29(1)
C(27)	1754(2)	7892(2)	3859(1)	41(1)
C(31)	1243(1)	4809(2)	3027(1)	18(1)
C(32)	977(1)	3853(2)	3459(1)	21(1)
C(33)	-110(1)	3437(2)	3475(1)	22(1)
C(34)	-974(1)	3987(2)	3062(1)	19(1)
C(35)	-736(1)	4957(2)	2635(1)	20(1)
C(36)	364(1)	5350(2)	2620(1)	21(1)
O(3)	-2021(1)	3500(1)	3117(1)	26(1)
C(37)	-2951(1)	4144(2)	2765(1)	29(1)
C(41)	2276(1)	4547(2)	1812(1)	18(1)
C(42)	1924(1)	5301(2)	1278(1)	22(1)
C(43)	1353(2)	4706(2)	750(1)	24(1)
C(44)	1145(1)	3343(2)	744(1)	23(1)
C(45)	1488(2)	2575(2)	1270(1)	26(1)
C(46)	2041(2)	3189(2)	1801(1)	24(1)
O(4)	582(1)	2843(1)	197(1)	31(1)
C(47)	452(2)	1426(2)	172(1)	36(1)
C(51)	4734(1)	5719(2)	1952(1)	20(1)
C(52)	4746(2)	4753(2)	1481(1)	25(1)
C(53)	5454(2)	4889(2)	1019(1)	30(1)
C(54)	6173(2)	5974(2)	1011(1)	30(1)
C(55)	6172(2)	6917(2)	1488(1)	28(1)
C(56)	5469(1)	6800(2)	1950(1)	22(1)
C(57)	6924(2)	6122(2)	498(1)	44(1)

Table S4. Bond lengths [A] and angles [deg] for schm46.

S(1)-C(2)	1.7221(17)
S(1)-C(5)	1.7262(16)
C(2)-C(3)	1.364(2)
C(2)-C(21)	1.477(2)
C(3)-C(4)	1.435(2)
C(3)-C(31)	1.476(2)
C(4)-C(5)	1.362(2)
C(4)-C(41)	1.484(2)
C(5)-C(51)	1.472(2)
C(21)-C(26)	1.390(3)
C(21)-C(22)	1.390(3)
C(22)-C(23)	1.379(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.360(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.374(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.388(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.497(3)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(31)-C(32)	1.388(2)
C(31)-C(36)	1.388(2)
C(32)-C(33)	1.372(2)
C(32)-H(32)	0.9500
C(33)-C(34)	1.385(2)
C(33)-H(33)	0.9500
C(34)-O(3)	1.3634(19)
C(34)-C(35)	1.381(2)
C(35)-C(36)	1.379(2)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
O(3)-C(37)	1.417(2)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(41)-C(46)	1.379(2)
C(41)-C(42)	1.385(2)
C(42)-C(43)	1.378(2)
C(42)-H(42)	0.9500
C(43)-C(44)	1.377(3)
C(43)-H(43)	0.9500
C(44)-O(4)	1.3668(19)
C(44)-C(45)	1.378(2)
C(45)-C(46)	1.381(2)
C(45)-H(45)	0.9500
C(46)-H(46)	0.9500
O(4)-C(47)	1.418(2)
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(51)-C(56)	1.390(2)
C(51)-C(52)	1.392(2)
C(52)-C(53)	1.385(2)
C(52)-H(52)	0.9500
C(53)-C(54)	1.382(3)
C(53)-H(53)	0.9500
C(54)-C(55)	1.385(3)
C(54)-C(57)	1.508(2)
C(55)-C(56)	1.377(2)
C(55)-H(55)	0.9500
C(56)-H(56)	0.9500
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800
C(57)-H(57C)	0.9800

C(2)-S(1)-C(5)	92.89(8)
C(3)-C(2)-C(21)	130.42(15)
C(3)-C(2)-S(1)	110.81(12)
C(21)-C(2)-S(1)	118.77(12)
C(2)-C(3)-C(4)	112.59(15)
C(2)-C(3)-C(31)	124.98(14)
C(4)-C(3)-C(31)	122.43(14)
C(5)-C(4)-C(3)	113.34(14)
C(5)-C(4)-C(41)	124.44(15)
C(3)-C(4)-C(41)	122.11(14)
C(4)-C(5)-C(51)	129.87(15)
C(4)-C(5)-S(1)	110.35(12)
C(51)-C(5)-S(1)	119.78(12)
C(26)-C(21)-C(22)	119.56(16)
C(26)-C(21)-C(2)	121.47(16)
C(22)-C(21)-C(2)	118.95(16)
C(23)-C(22)-C(21)	121.05(18)
C(23)-C(22)-H(22)	119.5
C(21)-C(22)-H(22)	119.5
C(24)-C(23)-C(22)	119.61(19)
C(24)-C(23)-H(23)	120.2
C(22)-C(23)-H(23)	120.2
C(23)-C(24)-C(25)	119.83(18)
C(23)-C(24)-H(24)	120.1
C(25)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	122.1(2)
C(24)-C(25)-H(25)	119.0
C(26)-C(25)-H(25)	119.0
C(25)-C(26)-C(21)	117.86(18)
C(25)-C(26)-C(27)	120.66(18)
C(21)-C(26)-C(27)	121.48(16)
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(32)-C(31)-C(36)	117.48(15)
C(32)-C(31)-C(3)	122.26(15)
C(36)-C(31)-C(3)	120.22(15)
C(33)-C(32)-C(31)	121.34(15)
C(33)-C(32)-H(32)	119.3
C(31)-C(32)-H(32)	119.3
C(32)-C(33)-C(34)	120.17(16)
C(32)-C(33)-H(33)	119.9
C(34)-C(33)-H(33)	119.9
O(3)-C(34)-C(35)	124.88(15)
O(3)-C(34)-C(33)	115.42(15)
C(35)-C(34)-C(33)	119.70(15)
C(36)-C(35)-C(34)	119.33(15)
C(36)-C(35)-H(35)	120.3
C(34)-C(35)-H(35)	120.3
C(35)-C(36)-C(31)	121.96(15)
C(35)-C(36)-H(36)	119.0
C(31)-C(36)-H(36)	119.0
C(34)-O(3)-C(37)	117.84(13)
O(3)-C(37)-H(37A)	109.5
O(3)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
O(3)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(46)-C(41)-C(42)	118.33(15)
C(46)-C(41)-C(4)	119.14(15)
C(42)-C(41)-C(4)	122.53(15)
C(43)-C(42)-C(41)	120.69(16)
C(43)-C(42)-H(42)	119.7
C(41)-C(42)-H(42)	119.7
C(44)-C(43)-C(42)	120.07(16)
C(44)-C(43)-H(43)	120.0
C(42)-C(43)-H(43)	120.0
O(4)-C(44)-C(43)	115.79(15)

O(4)-C(44)-C(45)	124.08(16)
C(43)-C(44)-C(45)	120.13(16)
C(44)-C(45)-C(46)	119.19(16)
C(44)-C(45)-H(45)	120.4
C(46)-C(45)-H(45)	120.4
C(41)-C(46)-C(45)	121.57(16)
C(41)-C(46)-H(46)	119.2
C(45)-C(46)-H(46)	119.2
C(44)-O(4)-C(47)	115.69(14)
O(4)-C(47)-H(47A)	109.5
O(4)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
O(4)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(56)-C(51)-C(52)	117.85(15)
C(56)-C(51)-C(5)	120.78(15)
C(52)-C(51)-C(5)	121.37(15)
C(53)-C(52)-C(51)	120.61(17)
C(53)-C(52)-H(52)	119.7
C(51)-C(52)-H(52)	119.7
C(54)-C(53)-C(52)	121.57(17)
C(54)-C(53)-H(53)	119.2
C(52)-C(53)-H(53)	119.2
C(53)-C(54)-C(55)	117.46(16)
C(53)-C(54)-C(57)	120.97(18)
C(55)-C(54)-C(57)	121.57(18)
C(56)-C(55)-C(54)	121.70(17)
C(56)-C(55)-H(55)	119.1
C(54)-C(55)-H(55)	119.1
C(55)-C(56)-C(51)	120.79(16)
C(55)-C(56)-H(56)	119.6
C(51)-C(56)-H(56)	119.6
C(54)-C(57)-H(57A)	109.5
C(54)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(54)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5

Table S5. Anisotropic displacement parameters (A^2 x 10^3) for schm46.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	16(1)	27(1)	19(1)	-3(1)	2(1)	-3(1)
C(2)	17(1)	22(1)	22(1)	-2(1)	6(1)	-1(1)
C(3)	18(1)	19(1)	20(1)	0(1)	3(1)	0(1)
C(4)	19(1)	17(1)	19(1)	2(1)	2(1)	0(1)
C(5)	19(1)	18(1)	17(1)	-2(1)	2(1)	-1(1)
C(21)	18(1)	29(1)	19(1)	-4(1)	3(1)	-4(1)
C(22)	23(1)	40(1)	25(1)	-2(1)	2(1)	2(1)
C(23)	31(1)	59(1)	21(1)	3(1)	-1(1)	2(1)
C(24)	45(1)	70(2)	19(1)	-9(1)	7(1)	1(1)
C(25)	46(1)	51(1)	33(1)	-16(1)	13(1)	8(1)
C(26)	29(1)	34(1)	26(1)	-7(1)	8(1)	0(1)
C(27)	46(1)	36(1)	41(1)	-3(1)	12(1)	13(1)
C(31)	18(1)	21(1)	16(1)	-4(1)	4(1)	-1(1)
C(32)	19(1)	27(1)	18(1)	1(1)	2(1)	2(1)
C(33)	23(1)	23(1)	19(1)	3(1)	5(1)	-2(1)
C(34)	16(1)	21(1)	21(1)	-4(1)	5(1)	-2(1)
C(35)	18(1)	23(1)	20(1)	0(1)	1(1)	1(1)
C(36)	22(1)	22(1)	20(1)	3(1)	5(1)	-1(1)
O(3)	16(1)	31(1)	31(1)	5(1)	3(1)	-4(1)
C(37)	16(1)	39(1)	31(1)	3(1)	2(1)	-2(1)
C(41)	16(1)	22(1)	18(1)	-2(1)	5(1)	-1(1)
C(42)	25(1)	17(1)	23(1)	0(1)	5(1)	-2(1)
C(43)	32(1)	22(1)	19(1)	4(1)	1(1)	-2(1)
C(44)	24(1)	24(1)	19(1)	-3(1)	0(1)	-5(1)
C(45)	36(1)	17(1)	25(1)	1(1)	0(1)	-6(1)
C(46)	29(1)	22(1)	20(1)	4(1)	0(1)	-3(1)
O(4)	44(1)	25(1)	21(1)	0(1)	-5(1)	-10(1)
C(47)	52(1)	26(1)	26(1)	-6(1)	-4(1)	-10(1)
C(51)	17(1)	23(1)	19(1)	2(1)	2(1)	2(1)
C(52)	22(1)	25(1)	27(1)	-3(1)	7(1)	-1(1)
C(53)	31(1)	34(1)	26(1)	-8(1)	10(1)	0(1)
C(54)	28(1)	36(1)	28(1)	2(1)	12(1)	1(1)
C(55)	24(1)	27(1)	33(1)	1(1)	9(1)	-6(1)
C(56)	21(1)	23(1)	23(1)	-1(1)	4(1)	-1(1)
C(57)	48(1)	49(1)	42(1)	-4(1)	30(1)	-7(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for schm46.

	x	y	z	U(eq)
H(22)	4029	4337	4451	35
H(23)	3884	4622	5519	45
H(24)	2829	6380	5845	53
H(25)	1884	7810	5108	51
H(27A)	2291	8349	3621	61
H(27B)	1353	8562	4084	61
H(27C)	1213	7386	3568	61
H(32)	1560	3480	3749	25
H(33)	-272	2770	3769	26
H(35)	-1323	5349	2354	24
H(36)	525	6012	2323	25
H(37A)	-2936	5107	2866	43
H(37B)	-3651	3748	2874	43
H(37C)	-2910	4023	2313	43
H(42)	2079	6238	1276	26
H(43)	1101	5236	390	29
H(45)	1345	1635	1268	31
H(46)	2266	2662	2166	29
H(47A)	1194	998	214	53
H(47B)	28	1170	-233	53
H(47C)	43	1130	518	53
H(52)	4264	3994	1476	29
H(53)	5446	4221	700	35
H(55)	6668	7664	1498	33
H(56)	5487	7466	2270	27
H(57A)	6786	5377	197	67
H(57B)	7713	6108	686	67
H(57C)	6762	6977	277	67

Table S7. Torsion angles [deg] for schm46.

C(5)-S(1)-C(2)-C(3)	-0.23(14)
C(5)-S(1)-C(2)-C(21)	179.55(14)
C(21)-C(2)-C(3)-C(4)	-178.73(17)
S(1)-C(2)-C(3)-C(4)	1.01(19)
C(21)-C(2)-C(3)-C(31)	1.9(3)
S(1)-C(2)-C(3)-C(31)	-178.36(13)
C(2)-C(3)-C(4)-C(5)	-1.6(2)
C(31)-C(3)-C(4)-C(5)	177.83(15)
C(2)-C(3)-C(4)-C(41)	174.78(15)
C(31)-C(3)-C(4)-C(41)	-5.8(2)
C(3)-C(4)-C(5)-C(51)	-179.18(16)
C(41)-C(4)-C(5)-C(51)	4.6(3)
C(3)-C(4)-C(5)-S(1)	1.34(19)
C(41)-C(4)-C(5)-S(1)	-174.89(13)
C(2)-S(1)-C(5)-C(4)	-0.65(14)
C(2)-S(1)-C(5)-C(51)	179.81(14)
C(3)-C(2)-C(21)-C(26)	-73.4(3)
S(1)-C(2)-C(21)-C(26)	106.92(18)
C(3)-C(2)-C(21)-C(22)	108.4(2)
S(1)-C(2)-C(21)-C(22)	-71.4(2)
C(26)-C(21)-C(22)-C(23)	0.3(3)
C(2)-C(21)-C(22)-C(23)	178.61(17)
C(21)-C(22)-C(23)-C(24)	-0.9(3)
C(22)-C(23)-C(24)-C(25)	0.9(3)
C(23)-C(24)-C(25)-C(26)	-0.3(4)
C(24)-C(25)-C(26)-C(21)	-0.4(3)
C(24)-C(25)-C(26)-C(27)	-179.9(2)
C(22)-C(21)-C(26)-C(25)	0.3(3)
C(2)-C(21)-C(26)-C(25)	-177.94(18)
C(22)-C(21)-C(26)-C(27)	179.82(18)
C(2)-C(21)-C(26)-C(27)	1.6(3)
C(2)-C(3)-C(31)-C(32)	-55.9(2)
C(4)-C(3)-C(31)-C(32)	124.81(18)
C(2)-C(3)-C(31)-C(36)	126.53(19)
C(4)-C(3)-C(31)-C(36)	-52.8(2)
C(36)-C(31)-C(32)-C(33)	1.4(2)
C(3)-C(31)-C(32)-C(33)	-176.26(16)
C(31)-C(32)-C(33)-C(34)	-1.1(3)
C(32)-C(33)-C(34)-O(3)	179.88(15)
C(32)-C(33)-C(34)-C(35)	-0.1(3)
O(3)-C(34)-C(35)-C(36)	-179.04(15)
C(33)-C(34)-C(35)-C(36)	0.9(2)
C(34)-C(35)-C(36)-C(31)	-0.6(3)
C(32)-C(31)-C(36)-C(35)	-0.5(2)
C(3)-C(31)-C(36)-C(35)	177.16(15)
C(35)-C(34)-O(3)-C(37)	-8.0(2)
C(33)-C(34)-O(3)-C(37)	172.05(15)
C(5)-C(4)-C(41)-C(46)	109.9(2)
C(3)-C(4)-C(41)-C(46)	-66.0(2)
C(5)-C(4)-C(41)-C(42)	-70.2(2)
C(3)-C(4)-C(41)-C(42)	113.92(19)
C(46)-C(41)-C(42)-C(43)	0.1(3)
C(4)-C(41)-C(42)-C(43)	-179.85(16)
C(41)-C(42)-C(43)-C(44)	-1.3(3)
C(42)-C(43)-C(44)-O(4)	-179.37(16)
C(42)-C(43)-C(44)-C(45)	1.3(3)
O(4)-C(44)-C(45)-C(46)	-179.35(17)
C(43)-C(44)-C(45)-C(46)	-0.1(3)
C(42)-C(41)-C(46)-C(45)	1.1(3)
C(4)-C(41)-C(46)-C(45)	-178.90(16)
C(44)-C(45)-C(46)-C(41)	-1.1(3)
C(43)-C(44)-O(4)-C(47)	174.95(17)
C(45)-C(44)-O(4)-C(47)	-5.8(3)
C(4)-C(5)-C(51)-C(56)	143.09(19)
S(1)-C(5)-C(51)-C(56)	-37.5(2)
C(4)-C(5)-C(51)-C(52)	-36.8(3)
S(1)-C(5)-C(51)-C(52)	142.64(14)
C(56)-C(51)-C(52)-C(53)	-1.3(3)

C(5)-C(51)-C(52)-C(53)	178.60(16)
C(51)-C(52)-C(53)-C(54)	0.4(3)
C(52)-C(53)-C(54)-C(55)	0.9(3)
C(52)-C(53)-C(54)-C(57)	-178.85(19)
C(53)-C(54)-C(55)-C(56)	-1.2(3)
C(57)-C(54)-C(55)-C(56)	178.55(19)
C(54)-C(55)-C(56)-C(51)	0.2(3)
C(52)-C(51)-C(56)-C(55)	1.0(3)
C(5)-C(51)-C(56)-C(55)	-178.89(16)

Table S8. Hydrogen bonds for schm46 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(24)-H(24)...O(3)#1	0.95	2.53	3.439(2)	160.6

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z+1

3. Calculations

All calculations were performed applying these conditions: basis set: LACVP*; 6-31G*, for large atoms ECP (effective core potential), hybride: B3LYP, level of theory: DFT, number of D functions: 5

3.1. Calculations of thiophene 8

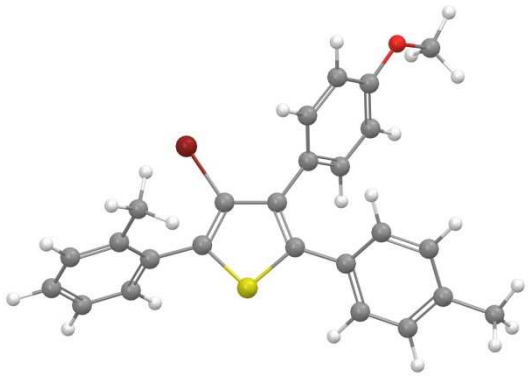


Figure S4: Most stable conformation

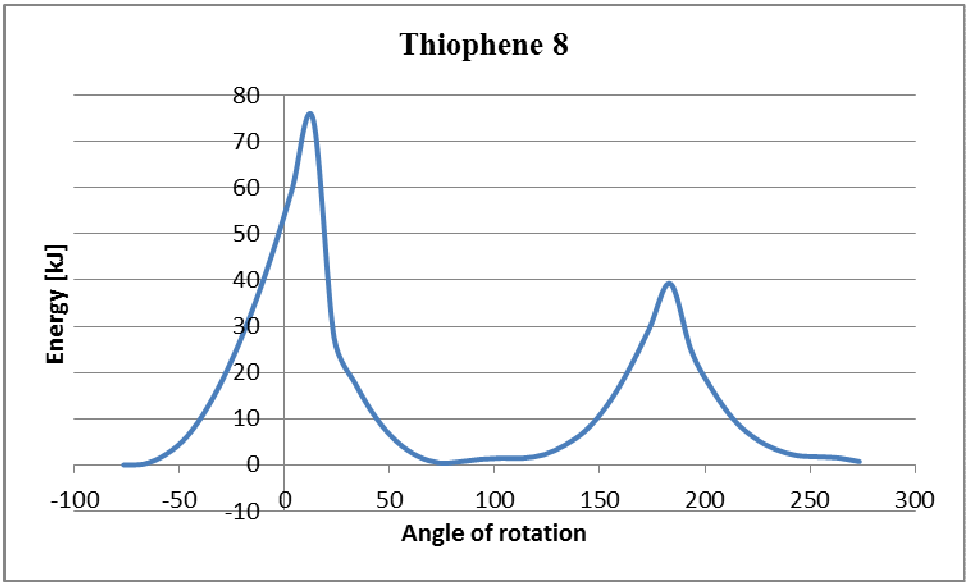


Figure S5: Calculated rotational barrier of thiophene **8** (rotation of *o*-tolyl ring).

3.2. Calculations of thiophene 8´

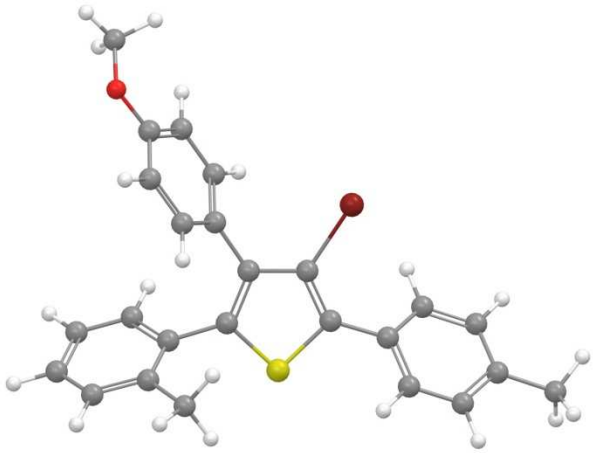


Figure S6: Most stable conformation of **8´**

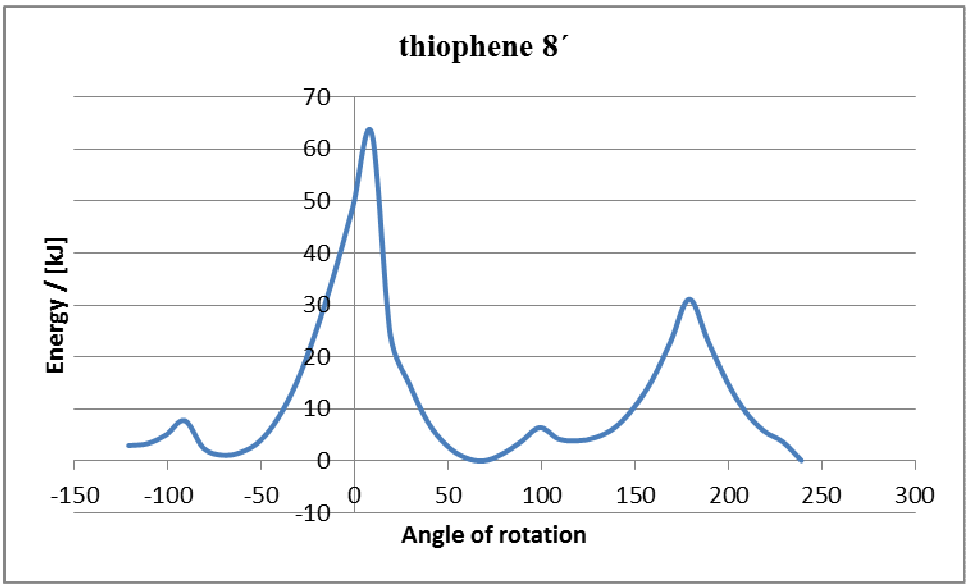


Figure S7: Calculated rotational barrier of thiophene **8´** (rotation of 4-methoxyphenyl ring).

3.3. Calculations of thiophene 13

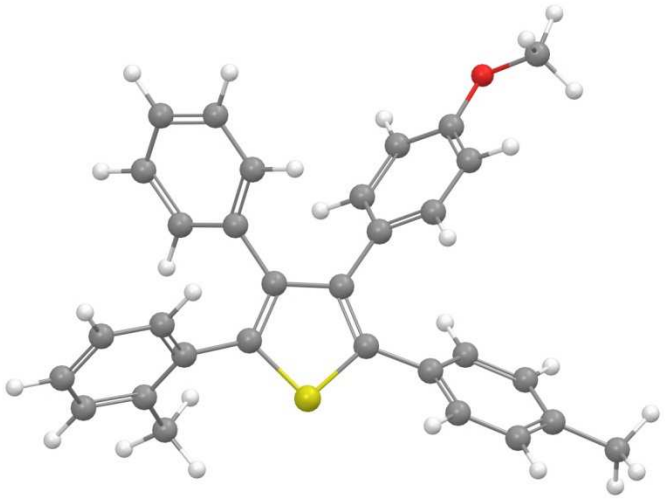


Figure S8: Most stable conformation of thiophene **13**

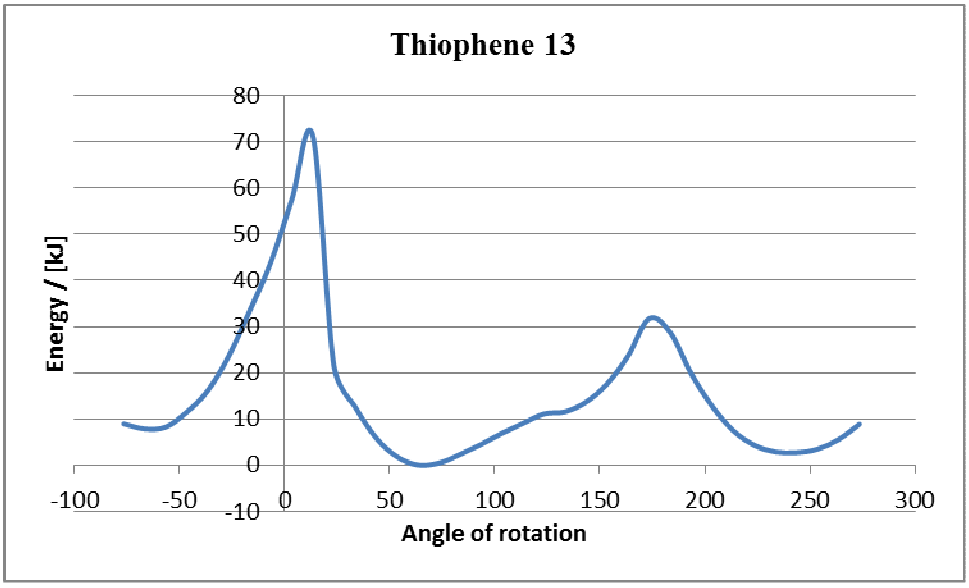


Figure S9: Calculated rotational barrier of thiophene **13**: Rotation of the $C_{thiophene}$-$C_{o\text{-}tolyl}$ bond

Molecule 8:

Total energy: -1451.85935424695 H

# of imaginary frequencies: 0

Z-matrix:

```
 C1
 C2     C1   r2
 C3     C2   r3     C1   a3
 C4     C3   r4     C2   a4     C1   d4
 S5     C3   r5     C2   a5     C1   d5
 Br6    C4   r6     C3   a6     C2   d6
 C7     C4   r7     C3   a7     C2   d7
 C8     S5   r8     C3   a8     C2   d8
 C9     C4   r9     C3   a9     C2   d9
 C10    C7   r10    C4   a10    C3   d10
 C11    C10  r11    C7   a11    C4   d11
 C12    C11  r12    C10  a12    C7   d12
 C13    C12  r13    C11  a13    C10  d13
 C14    C13  r14    C12  a14    C11  d14
 C15    C8   r15    S5   a15    C3   d15
 C16    C15  r16    C8   a16    S5   d16
 C17    C16  r17    C15  a17    C8   d17
 C18    C17  r18    C16  a18    C15  d18
 C19    C18  r19    C17  a19    C16  d19
 C20    C2   r20    C1   a20    C3   d20
 C21    C20  r21    C2   a21    C1   d21
 C22    C21  r22    C20  a22    C2   d22
 C23    C22  r23    C21  a23    C20  d23
 C24    C9   r24    C4   a24    C3   d24
 O25    C12  r25    C11  a25    C10  d25
 C26    O25  r26    C12  a26    C11  d26
 C27    C17  r27    C16  a27    C15  d27
 C28    C1   r28    C2   a28    C3   d28
 H29    C10  r29    C7   a29    C4   d29
 H30    C11  r30    C10  a30    C7   d30
 H31    C13  r31    C12  a31    C11  d31
 H32    C14  r32    C13  a32    C12  d32
 H33    C15  r33    C8   a33    S5   d33
 H34    C16  r34    C15  a34    C8   d34
 H35    C18  r35    C17  a35    C16  d35
 H36    C19  r36    C18  a36    C17  d36
 H37    C20  r37    C2   a37    C1   d37
 H38    C21  r38    C20  a38    C2   d38
 H39    C22  r39    C21  a39    C20  d39
 H40    C23  r40    C22  a40    C21  d40
 H41    C26  r41    O25  a41    C12  d41
 H42    C26  r42    O25  a42    C12  d42
 H43    C26  r43    O25  a43    C12  d43
 H44    C27  r44    C17  a44    C16  d44
 H45    C27  r45    C17  a45    C16  d45
 H46    C27  r46    C17  a46    C16  d46
 H47    C28  r47    C1   a47    C2   d47
 H48    C28  r48    C1   a48    C2   d48
 H49    C28  r49    C1   a49    C2   d49

 r2 =     1.4129236294
 r3 =     1.4814549824
 a3 =   121.4407508593
 r4 =     1.3681416112
 a4 =   131.354988348
 d4 =   -76.5155015668
 r5 =     1.7469225382
 a5 =   119.9227845575
 d5 =   105.8933748786
 r6 =     1.9548227767
 a6 =   121.3481965897
 d6 =    -0.9197876653
 r7 =     2.5921523035
```

a7 = 144.3725687953
d7 = -174.6921576516
r8 = 2.7772610655
a8 = 120.7829654584
d8 = 179.0135694131
r9 = 1.4380295422
a9 = 116.4155656928
d9 = -177.2321170038
r10 = 1.3988210779
a10 = 129.8135901929
d10 = 75.3408800082
r11 = 1.3959911562
a11 = 121.6284917953
d11 = 149.3143837763
r12 = 1.3990672651
a12 = 119.5608248315
d12 = 0.0072748219
r13 = 1.4026055885
a13 = 119.5670285257
d13 = -0.1847053476
r14 = 1.3876798741
a14 = 120.1652869826
d14 = 0.0576013717
r15 = 1.4069074339
a15 = 93.8195015181
d15 = -148.3204338689
r16 = 1.3913956365
a16 = 121.023902318
d16 = -156.6293949319
r17 = 1.4016339283
a17 = 121.2089304424
d17 = -0.2361277498
r18 = 1.399954791
a18 = 117.6913323954
d18 = 0.1274717354
r19 = 1.3929450668
a19 = 121.5097834857
d19 = 0.1722300927
r20 = 1.4025025965
a20 = 119.8371950724
d20 = 178.3378845014
r21 = 1.3930824936
a21 = 121.0231143232
d21 = 0.8955570832
r22 = 1.3937274126
a22 = 119.3961691154
d22 = -0.3064741722
r23 = 1.3946874876
a23 = 119.8765712913
d23 = -0.2792909703
r24 = 1.3843907396
a24 = 110.7108999918
d24 = -0.5208994207
r25 = 1.3644376286
a25 = 124.7737070739
d25 = 179.7869069725
r26 = 1.4179071565
a26 = 118.2519227477
d26 = -0.0398425635
r27 = 1.5114021703
a27 = 120.8764678085
d27 = 179.9400102156
r28 = 1.5109662255
a28 = 121.65846679
d28 = 0.3823843959
r29 = 1.0861213358
a29 = 119.3080081496
d29 = -30.5635847868
r30 = 1.0841954572
a30 = 119.3032569303
d30 = -179.8249165373

r31 = 1.0858054572
a31 = 118.5958301549
d31 = -179.9950764186
r32 = 1.0862903847
a32 = 119.3371330808
d32 = 179.8705788053
r33 = 1.0872789854
a33 = 119.4668594572
d33 = 24.2577100539
r34 = 1.0882980871
a34 = 119.2346995505
d34 = -179.8159309883
r35 = 1.0879379282
a35 = 119.3848704533
d35 = 179.565973268
r36 = 1.0849413506
a36 = 119.6503428684
d36 = 179.0383056064
r37 = 1.0867758134
a37 = 118.8862663402
d37 = -179.7447161735
r38 = 1.0867587932
a38 = 120.043134623
d38 = 179.6093915283
r39 = 1.0871979169
a39 = 120.2692367353
d39 = -179.9329456789
r40 = 1.0877883261
a40 = 119.5159852496
d40 = -179.2939720872
r41 = 1.0918420408
a41 = 105.9378270962
d41 = -179.8107631424
r42 = 1.0983866963
a42 = 111.6018593063
d42 = -60.9788646605
r43 = 1.0982610129
a43 = 111.6104825707
d43 = 61.3593111409
r44 = 1.0947475699
a44 = 111.4256331601
d44 = 178.850977906
r45 = 1.0975764116
a45 = 111.3791165775
d45 = -60.8701729858
r46 = 1.0974333465
a46 = 111.4198265071
d46 = 58.4869519414
r47 = 1.0966337519
a47 = 111.3125731854
d47 = 70.7833545032
r48 = 1.0947082067
a48 = 110.7529234778
d48 = -169.2187663458
r49 = 1.095953551
a49 = 111.5710558165
d49 = -48.7240067151

Molecule 8':

Total energy: -1451.85784700082 H
# of imaginary frequencies: 0

Z-matrix:
C1
C2 C1 r2
C3 C2 r3 C1 a3
C4 C3 r4 C2 a4 C1 d4
C5 C4 r5 C3 a5 C2 d5
S6 C3 r6 C2 a6 C1 d6
C7 C5 r7 C4 a7 C3 d7

Br8 C5 r8 C4 a8 C3 d8
C9 C7 r9 C5 a9 C4 d9
C10 C9 r10 C7 a10 C5 d10
C11 C10 r11 C9 a11 C7 d11
C12 C11 r12 C10 a12 C9 d12
C13 C12 r13 C11 a13 C10 d13
C14 C13 r14 C12 a14 C11 d14
C15 C2 r15 C1 a15 C3 d15
C16 C15 r16 C2 a16 C1 d16
C17 C16 r17 C15 a17 C2 d17
C18 C17 r18 C16 a18 C15 d18
C19 C1 r19 C2 a19 C3 d19
C20 C12 r20 C11 a20 C10 d20
C21 C4 r21 C3 a21 C2 d21
C22 C21 r22 C4 a22 C3 d22
C23 C22 r23 C21 a23 C4 d23
C24 C23 r24 C22 a24 C21 d24
C25 C24 r25 C23 a25 C22 d25
C26 C25 r26 C24 a26 C23 d26
O27 C24 r27 C23 a27 C22 d27
C28 O27 r28 C24 a28 C23 d28
H29 C10 r29 C9 a29 C7 d29
H30 C11 r30 C10 a30 C9 d30
H31 C13 r31 C12 a31 C11 d31
H32 C14 r32 C13 a32 C12 d32
H33 C15 r33 C2 a33 C1 d33
H34 C16 r34 C15 a34 C2 d34
H35 C17 r35 C16 a35 C15 d35
H36 C18 r36 C17 a36 C16 d36
H37 C20 r37 C12 a37 C11 d37
H38 C20 r38 C12 a38 C11 d38
H39 C20 r39 C12 a39 C11 d39
H40 C19 r40 C1 a40 C2 d40
H41 C19 r41 C1 a41 C2 d41
H42 C19 r42 C1 a42 C2 d42
H43 C22 r43 C21 a43 C4 d43
H44 C23 r44 C22 a44 C21 d44
H45 C25 r45 C24 a45 C23 d45
H46 C26 r46 C25 a46 C24 d46
H47 C28 r47 O27 a47 C24 d47
H48 C28 r48 O27 a48 C24 d48
H49 C28 r49 O27 a49 C24 d49

r2 = 1.4144496662
r3 = 1.4832417271
a3 = 122.2918678107
r4 = 1.3833053521
a4 = 128.7992640514
d4 = -120.9000004499
r5 = 1.4392915945
a5 = 110.8641751238
d5 = -175.3869903058
r6 = 1.7452670735
a6 = 119.7505303337
d6 = 64.974752159
r7 = 1.3725621858
a7 = 116.2089365052
d7 = 0.0429941352
r8 = 1.9572824176
a8 = 121.3490870694
d8 = -174.3995276089
r9 = 1.472732302
a9 = 132.5189696569
d9 = -178.2019965384
r10 = 1.4055112581
a10 = 120.2987942151
d10 = 136.193191718
r11 = 1.3918993573
a11 = 120.9314921637
d11 = 178.4415067398
r12 = 1.4004045084

a12 = 121.2052004519
d12 = 0.0069415095
r13 = 1.400981295
a13 = 117.7561157287
d13 = 0.0602744387
r14 = 1.3920299093
a14 = 121.440611712
d14 = -0.3543621567
r15 = 1.4046043344
a15 = 119.4165072826
d15 = 179.6397504754
r16 = 1.3918520041
a16 = 121.2488976316
d16 = -0.3565975988
r17 = 1.3942254018
a17 = 119.4947804385
d17 = -0.0716525122
r18 = 1.3936964435
a18 = 119.7050093026
d18 = 0.4285577692
r19 = 1.5135572909
a19 = 122.2793845202
d19 = 1.656498683
r20 = 1.5110510717
a20 = 121.0788319729
d20 = -178.7754923642
r21 = 1.4849407896
a21 = 123.4786365059
d21 = 5.963626569
r22 = 1.3995835379
a22 = 121.5767961723
d22 = -124.20778931
r23 = 1.3961153603
a23 = 121.5905151043
d23 = 178.9091316052
r24 = 1.399278257
a24 = 119.6301810681
d24 = 0.0564439399
r25 = 1.4019639325
a25 = 119.5402228136
d25 = -0.091683222
r26 = 1.3871220524
a26 = 120.1167354134
d26 = 0.0593541151
r27 = 1.3645187352
a27 = 124.8006530192
d27 = 179.8912763438
r28 = 1.4175462444
a28 = 118.3356477173
d28 = -0.69378665
r29 = 1.086772119
a29 = 119.4683227688
d29 = -2.7995891581
r30 = 1.0880265676
a30 = 119.2621161328
d30 = 179.4443716482
r31 = 1.0880253256
a31 = 119.4297996143
d31 = -179.9127432615
r32 = 1.0844970301
a32 = 119.6867384016
d32 = -178.9076803266
r33 = 1.0860415183
a33 = 118.7294704465
d33 = 179.6636838617
r34 = 1.0868215366
a34 = 119.9837630834
d34 = -179.9739063309
r35 = 1.0871438717
a35 = 120.3689224756
d35 = -179.9771799988

r36 = 1.0879384507
a36 = 119.4912260884
d36 = 179.1067003711
r37 = 1.0952896405
a37 = 111.4804228084
d37 = -152.6001228615
r38 = 1.095556867
a38 = 111.4629904002
d38 = -31.7741027005
r39 = 1.0987459257
a39 = 111.2095398059
d39 = 87.7641976128
r40 = 1.0953806904
a40 = 111.746813546
d40 = 41.1476812529
r41 = 1.0947678702
a41 = 110.4982085578
d41 = 161.7030625793
r42 = 1.0970827182
a42 = 111.9913939113
d42 = -78.6349107583
r43 = 1.0861548605
a43 = 119.5858023531
d43 = -0.712605067
r44 = 1.0842946992
a44 = 119.3004959497
d44 = -179.8315436827
r45 = 1.0858091818
a45 = 118.6208601988
d45 = 179.8129806538
r46 = 1.0860997846
a46 = 119.3366108684
d46 = 179.6722061905
r47 = 1.0919372253
a47 = 105.9165706859
d47 = -179.5660438933
r48 = 1.098276243
a48 = 111.6009132823
d48 = -60.7438124698
r49 = 1.0983632854
a49 = 111.6382508146
d49 = 61.6414039731

Molecule 13:

Total energy: -1670.35171121826 H
# of imaginary frequencies: 0

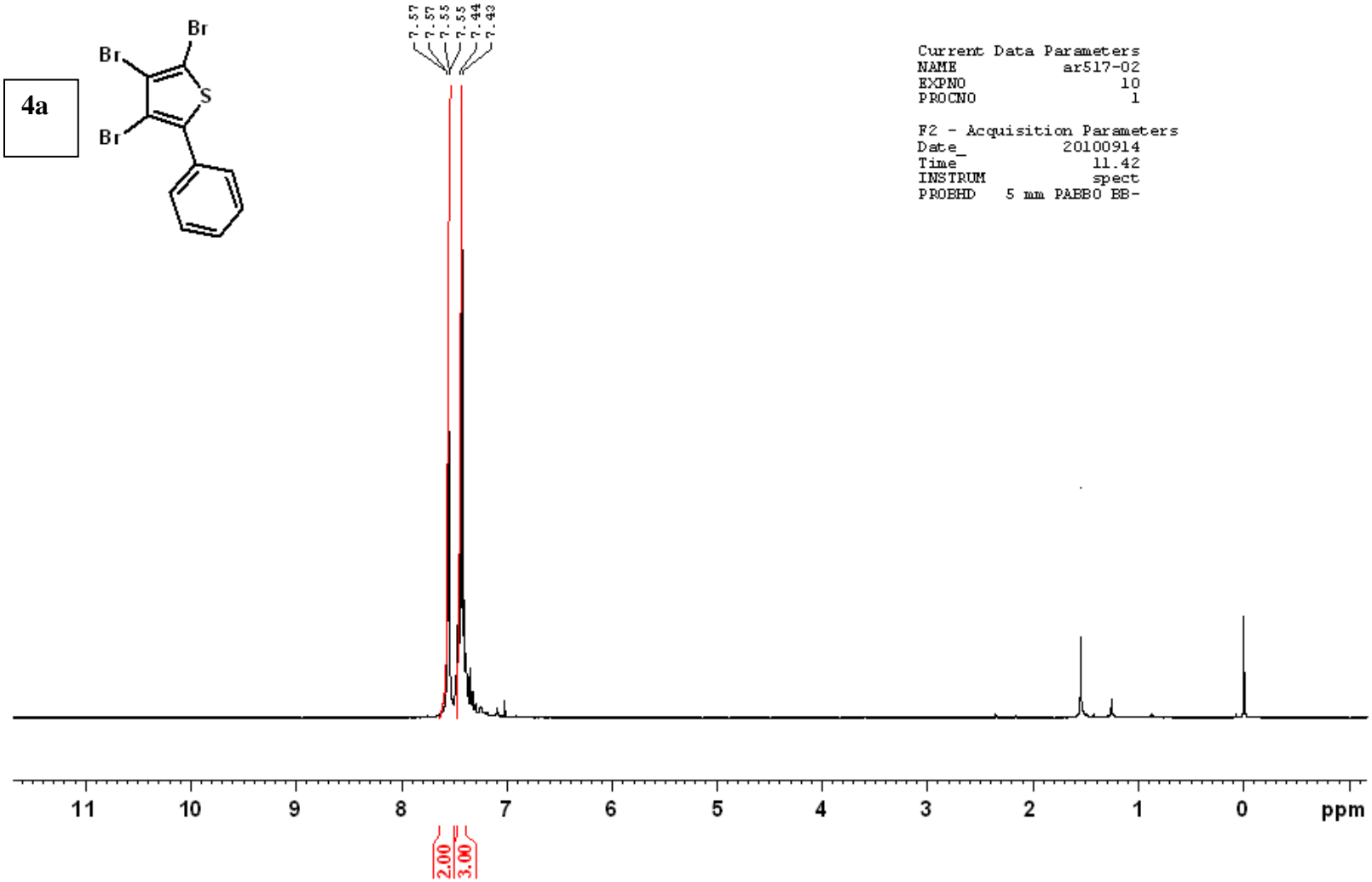
Z-matrix:
C1
C2 C1 r2
C3 C2 r3 C1 a3
C4 C3 r4 C2 a4 C1 d4
S5 C3 r5 C2 a5 C1 d5
C7 C4 r6 C3 a6 C2 d6
C8 S5 r7 C3 a7 C2 d7
C9 C4 r8 C3 a8 C2 d8
C10 C7 r9 C4 a9 C3 d9
C11 C10 r10 C7 a10 C4 d10
C12 C11 r11 C10 a11 C7 d11
C13 C12 r12 C11 a12 C10 d12
C14 C13 r13 C12 a13 C11 d13
C15 C8 r14 S5 a14 C3 d14
C16 C15 r15 C8 a15 S5 d15
C17 C16 r16 C15 a16 C8 d16
C18 C17 r17 C16 a17 C15 d17
C19 C18 r18 C17 a18 C16 d18
C20 C2 r19 C1 a19 C3 d19
C21 C20 r20 C2 a20 C1 d20
C22 C21 r21 C20 a21 C2 d21
C23 C22 r22 C21 a22 C20 d22

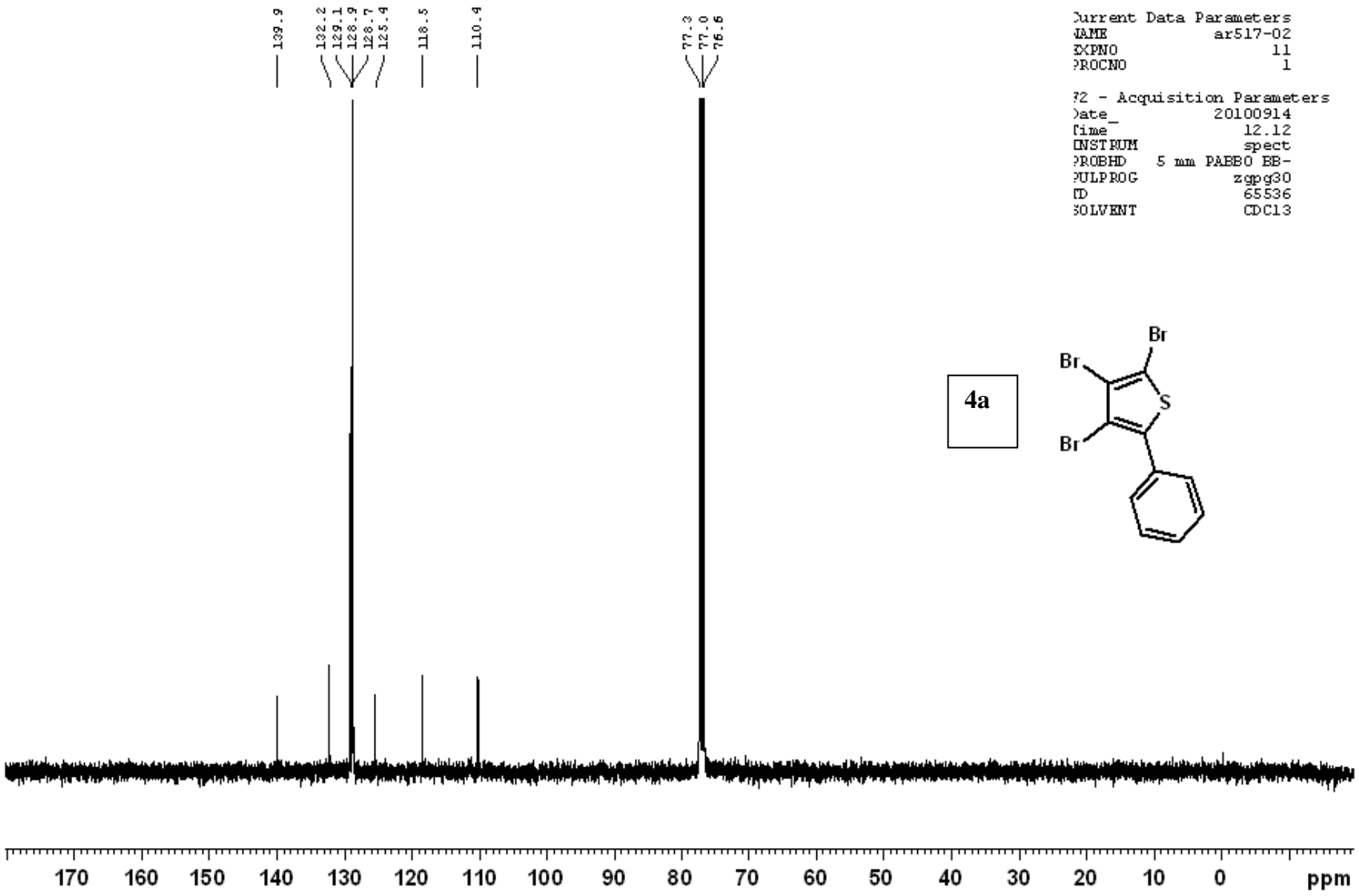
C24 C9 r23 C4 a23 C3 d23
O25 C12 r24 C11 a24 C10 d24
C26 O25 r25 C12 a25 C11 d25
C27 C17 r26 C16 a26 C15 d26
C28 C1 r27 C2 a27 C3 d27
H29 C10 r28 C7 a28 C4 d28
H30 C11 r29 C10 a29 C7 d29
H31 C13 r30 C12 a30 C11 d30
H32 C14 r31 C13 a31 C12 d31
H33 C15 r32 C8 a32 S5 d32
H34 C16 r33 C15 a33 C8 d33
H35 C18 r34 C17 a34 C16 d34
H36 C19 r35 C18 a35 C17 d35
H37 C20 r36 C2 a36 C1 d36
H38 C21 r37 C20 a37 C2 d37
H39 C22 r38 C21 a38 C20 d38
H40 C23 r39 C22 a39 C21 d39
H41 C26 r40 O25 a40 C12 d40
H42 C26 r41 O25 a41 C12 d41
H43 C26 r42 O25 a42 C12 d42
H44 C27 r43 C17 a43 C16 d43
H45 C27 r44 C17 a44 C16 d44
H46 C27 r45 C17 a45 C16 d45
H47 C28 r46 C1 a46 C2 d46
H48 C28 r47 C1 a47 C2 d47
H49 C28 r48 C1 a48 C2 d48
C49 C4 r49 C3 a49 C2 d49
C50 C49 r50 C4 a50 C3 d50
C51 C50 r51 C49 a51 C4 d51
C52 C51 r52 C50 a52 C49 d52
C53 C52 r53 C51 a53 C50 d53
C54 C49 r54 C4 a54 C3 d54
H55 C49 r55 C4 a55 C3 d55
H56 C50 r56 C49 a56 C4 d56
H57 C51 r57 C50 a57 C49 d57
H58 C53 r58 C52 a58 C51 d58
H59 C54 r59 C49 a59 C4 d59

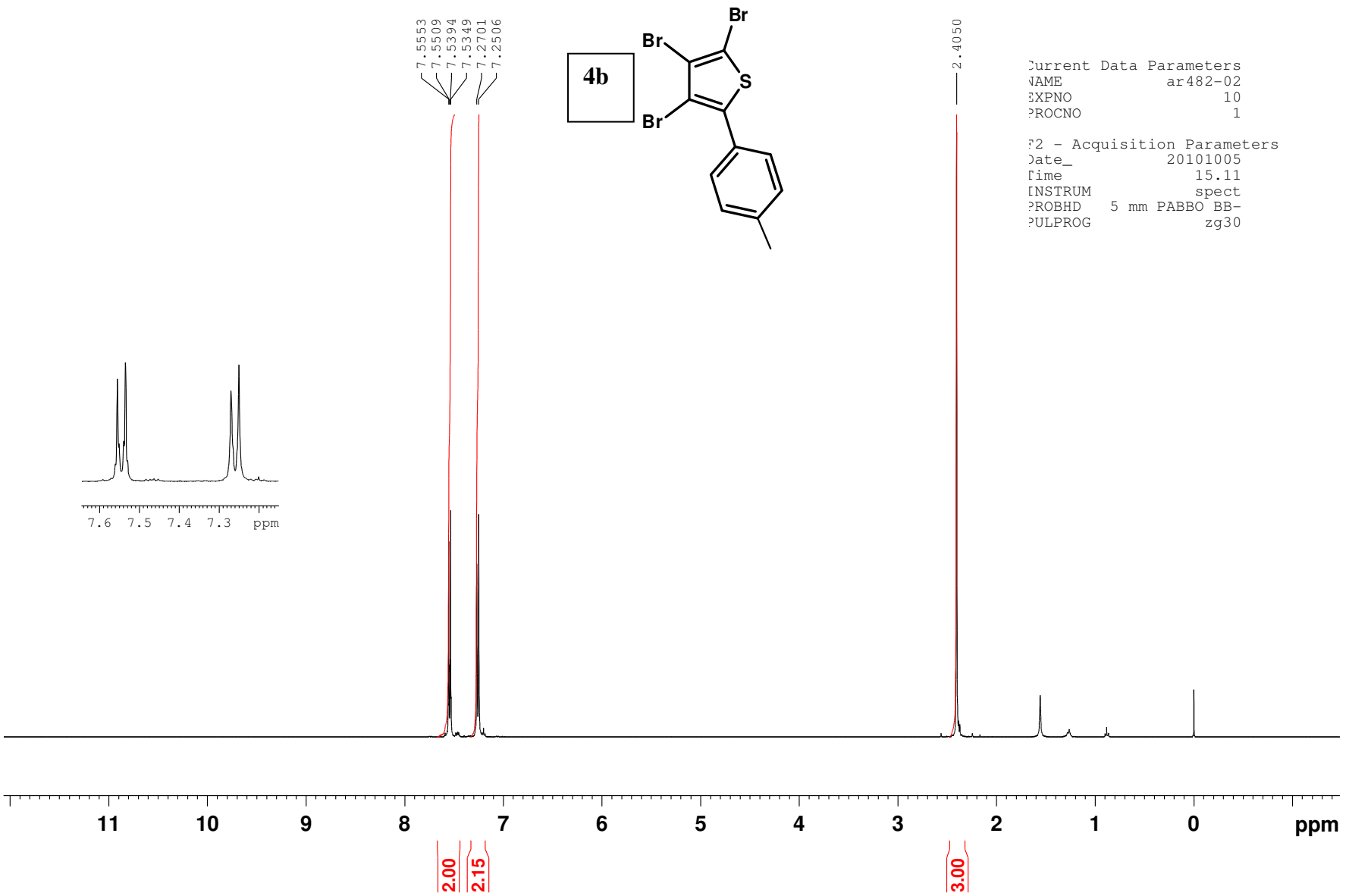
r2 = 1.4144114884
r3 = 1.484100648
a3 = 122.0613313169
r4 = 1.3815241379
a4 = 130.6644696654
d4 = 66.0587781765
r5 = 1.7437443053
a5 = 118.3920738877
d5 = -113.7589333785
r6 = 2.5913102869
a6 = 141.3748567941
d6 = -177.5551762611
r7 = 2.7734360944
a7 = 120.3421325462
d7 = -178.3131146987
r8 = 1.4497673515
a8 = 112.8738784496
d8 = -179.0496730433
r9 = 1.3999072686
a9 = 131.255743721
d9 = 75.2423106654
r10 = 1.3969797955
a10 = 121.741555632
d10 = 147.3527253549
r11 = 1.3989855957
a11 = 119.5889748305
d11 = 0.1092859904
r12 = 1.4023688968
a12 = 119.4832075961
d12 = 0.1136684847
r13 = 1.3879533435
a13 = 120.215346028
d13 = -0.3301279518

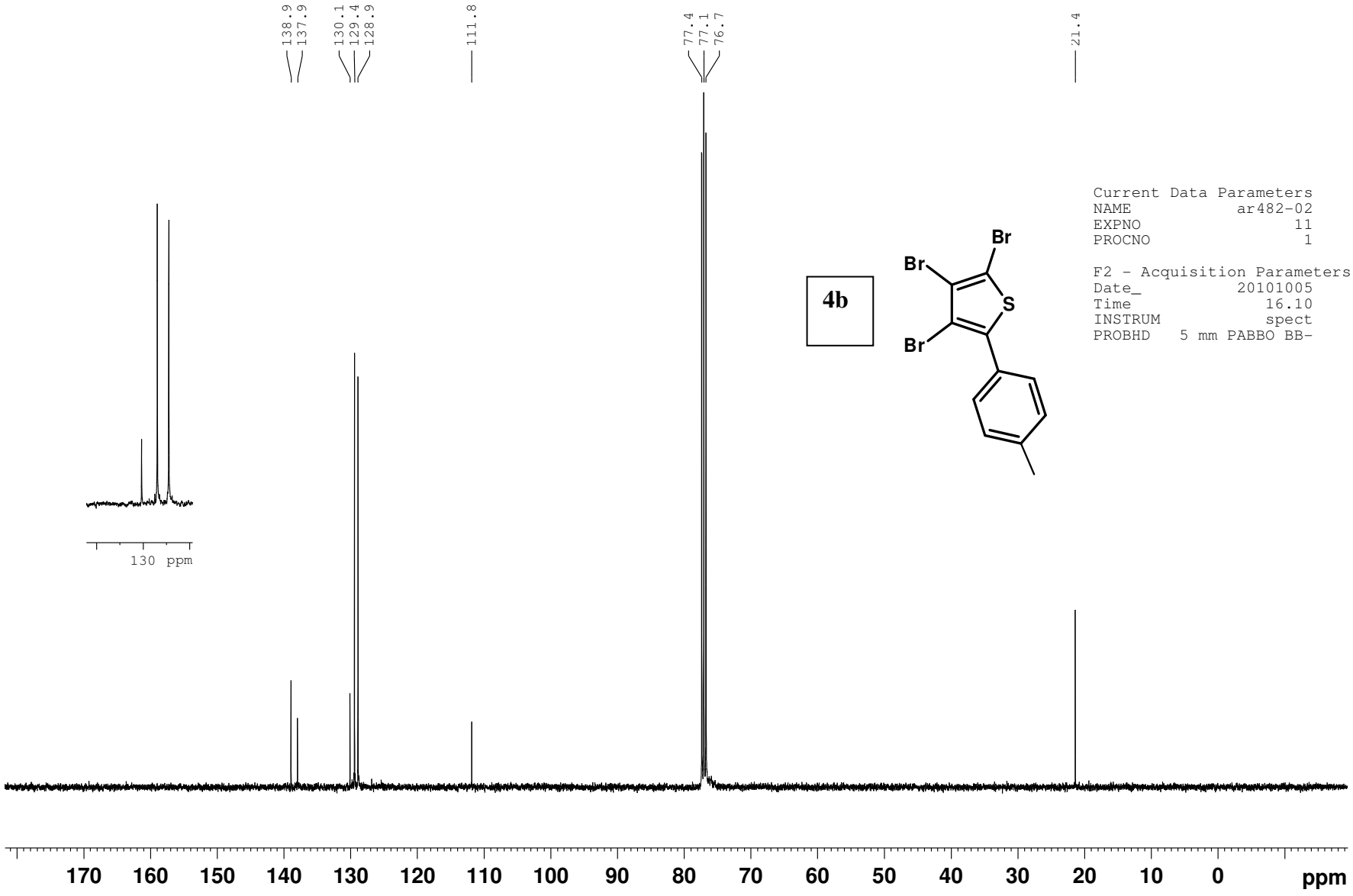
r14 = 1.4044818504
a14 = 93.9771860792
d14 = -150.2917759598
r15 = 1.3936261729
a15 = 121.0427280367
d15 = -155.9232938035
r16 = 1.3990794686
a16 = 121.2400053091
d16 = -0.4020206641
r17 = 1.4020094257
a17 = 117.6909974277
d17 = 0.4444790744
r18 = 1.3905414954
a18 = 121.4425795357
d18 = -0.0861748709
r19 = 1.4050743122
a19 = 119.3654635264
d19 = -178.0782304528
r20 = 1.3929104791
a20 = 121.3417616826
d20 = -1.4715283611
r21 = 1.3937604211
a21 = 119.3871224321
d21 = 0.3456428775
r22 = 1.3940661991
a22 = 119.7143458229
d22 = 0.6509999326
r23 = 1.3832425625
a23 = 112.816093059
d23 = -1.0539633098
r24 = 1.3655991655
a24 = 124.8436112588
d24 = -179.7601250693
r25 = 1.4172998815
a25 = 118.262271032
d25 = 1.0309043642
r26 = 1.5109134611
a26 = 121.4124324933
d26 = -178.851999921
r27 = 1.5106309321
a27 = 121.9716334331
d27 = 0.4166751164
r28 = 1.0864643349
a28 = 119.2230103584
d28 = -32.4260941096
r29 = 1.0842882572
a29 = 119.3116437373
d29 = -179.6877763308
r30 = 1.0858291883
a30 = 118.5855119419
d30 = 179.9543813087
r31 = 1.0858983673
a31 = 119.2616009014
d31 = -179.5214750472
r32 = 1.0871574647
a32 = 119.5090339589
d32 = 24.4821189136
r33 = 1.0880259274
a33 = 119.2430729024
d33 = 179.8009270833
r34 = 1.0882726898
a34 = 119.4246585558
d34 = 179.0613182493
r35 = 1.0848652404
a35 = 119.6418061239
d35 = 178.6931128946
r36 = 1.0870483297
a36 = 118.7425187204
d36 = 179.3107748078
r37 = 1.0868384133
a37 = 120.0388304678

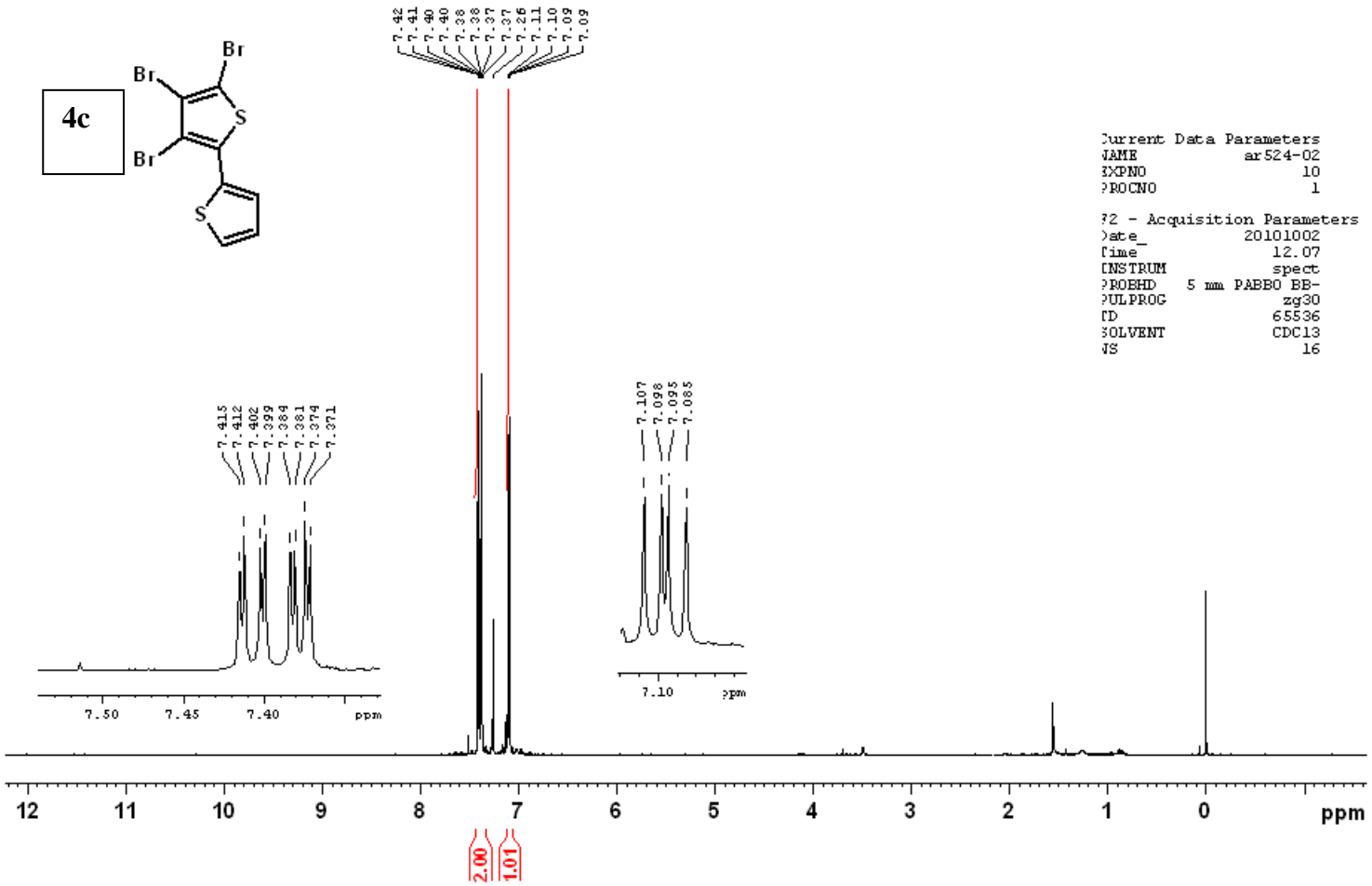
d37 = -179.5187189049
r38 = 1.0871283772
a38 = 120.356361102
d38 = -179.9185447869
r39 = 1.0878334618
a39 = 119.4507171721
d39 = 178.8562445046
r40 = 1.0919825793
a40 = 105.9602020543
d40 = 179.4095055075
r41 = 1.0983940943
a41 = 111.6710462912
d41 = -61.7498483982
r42 = 1.0984806831
a42 = 111.6051461442
d42 = 60.5988907049
r43 = 1.0961616097
a43 = 111.4288748224
d43 = -140.4160918739
r44 = 1.0949589479
a44 = 111.4628666374
d44 = -19.7126056358
r45 = 1.0984982494
a45 = 111.3112886125
d45 = 100.1602704716
r46 = 1.0954655474
a46 = 111.4630252716
d46 = 43.2862087678
r47 = 1.0948245761
a47 = 110.6457942658
d47 = 163.8377707904
r48 = 1.0963420686
a48 = 111.481970778
d48 = -76.1493651834
r49 = 4.3050226009
a49 = 122.5647127729
d49 = 2.265750045
r50 = 1.3953511262
a50 = 59.5821252474
d50 = 50.8529719028
r51 = 1.3944081678
a51 = 120.2332743397
d51 = 0.1400769771
r52 = 1.4045340234
a52 = 120.8951966764
d52 = -0.1047667064
r53 = 1.4053265227
a53 = 118.279639282
d53 = 0.1882794903
r54 = 1.3961276186
a54 = 59.9143145224
d54 = -129.291529498
r55 = 1.0871410362
a55 = 179.8375034997
d55 = 50.67663405
r56 = 1.0872027095
a56 = 120.1431575876
d56 = 179.8730028018
r57 = 1.0856674401
a57 = 119.7701378604
d57 = 179.5912808437
r58 = 1.085734791
a58 = 119.4778905997
d58 = 179.7534551706
r59 = 1.0871289702
a59 = 120.0886061954
d59 = 179.8891775298

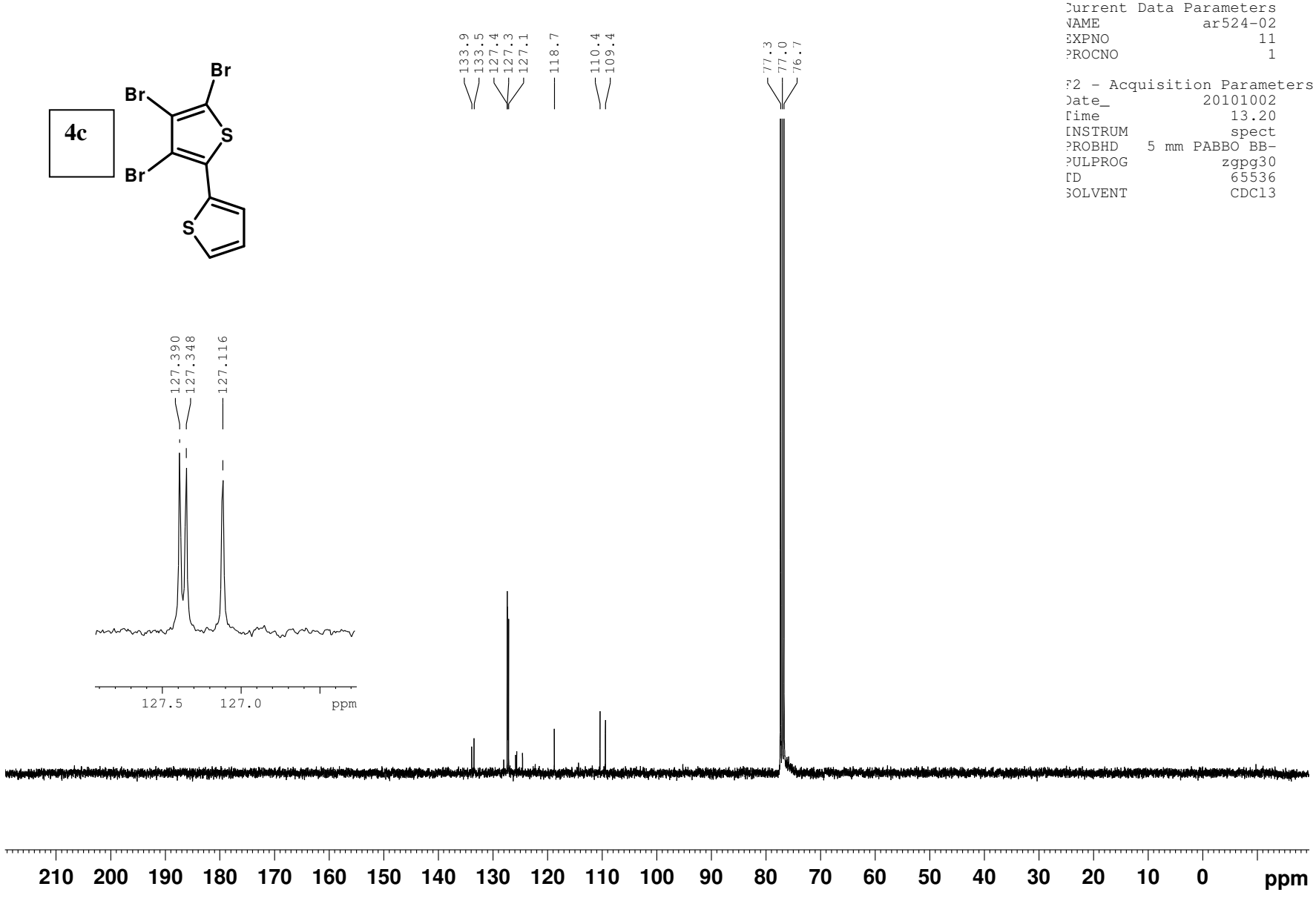

4a
Br
Br
Br
S
7.57
7.57
7.55
7.55
7.44
7.43
Current Data Parameters
NAME ar517-02
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100914
Time 11.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.00

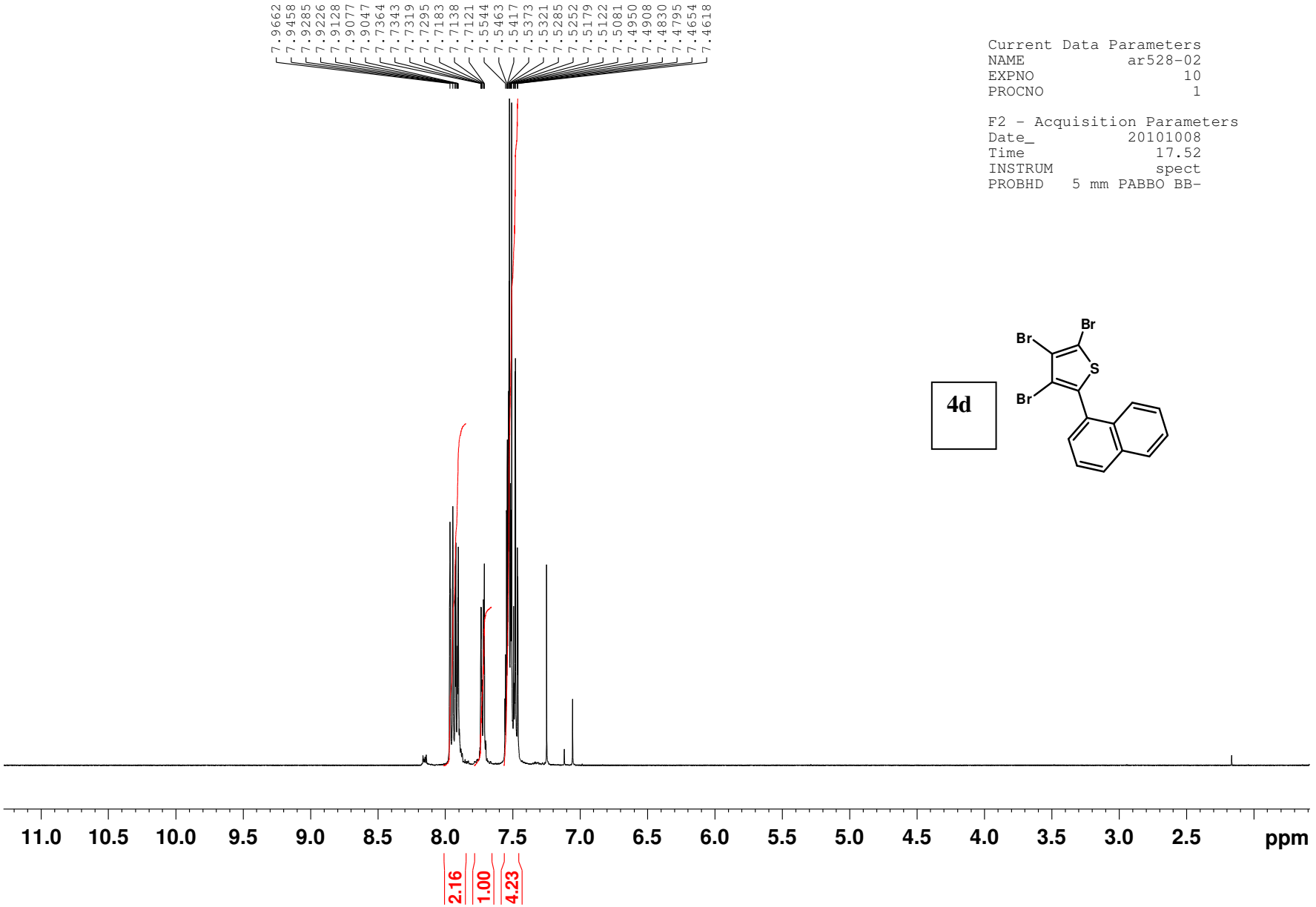

139.9
132.2
129.1
128.9
128.7
125.4
118.5
110.4
77.3
77.0
76.6
Current Data Parameters
NAME ar517-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100914
Time 12.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
4a
Br
Br
Br
S
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

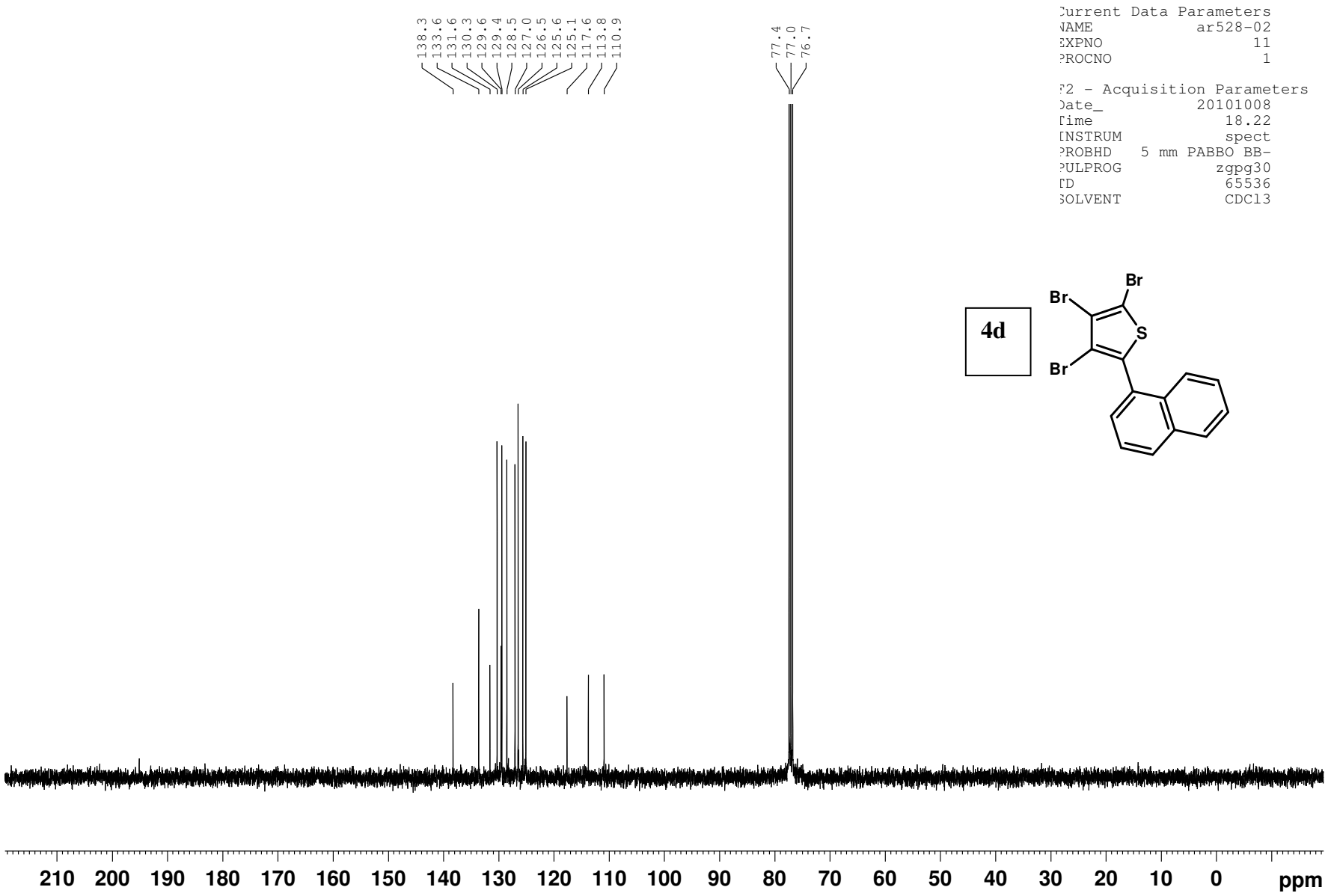

7.5553
7.5509
7.5394
7.5349
7.2701
7.2506
2.4050
4b
Br
Br
Br
S
Current Data Parameters
NAME ar482-02
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101005
Time 15.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
7.6 7.5 7.4 7.3 ppm
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.15
3.00

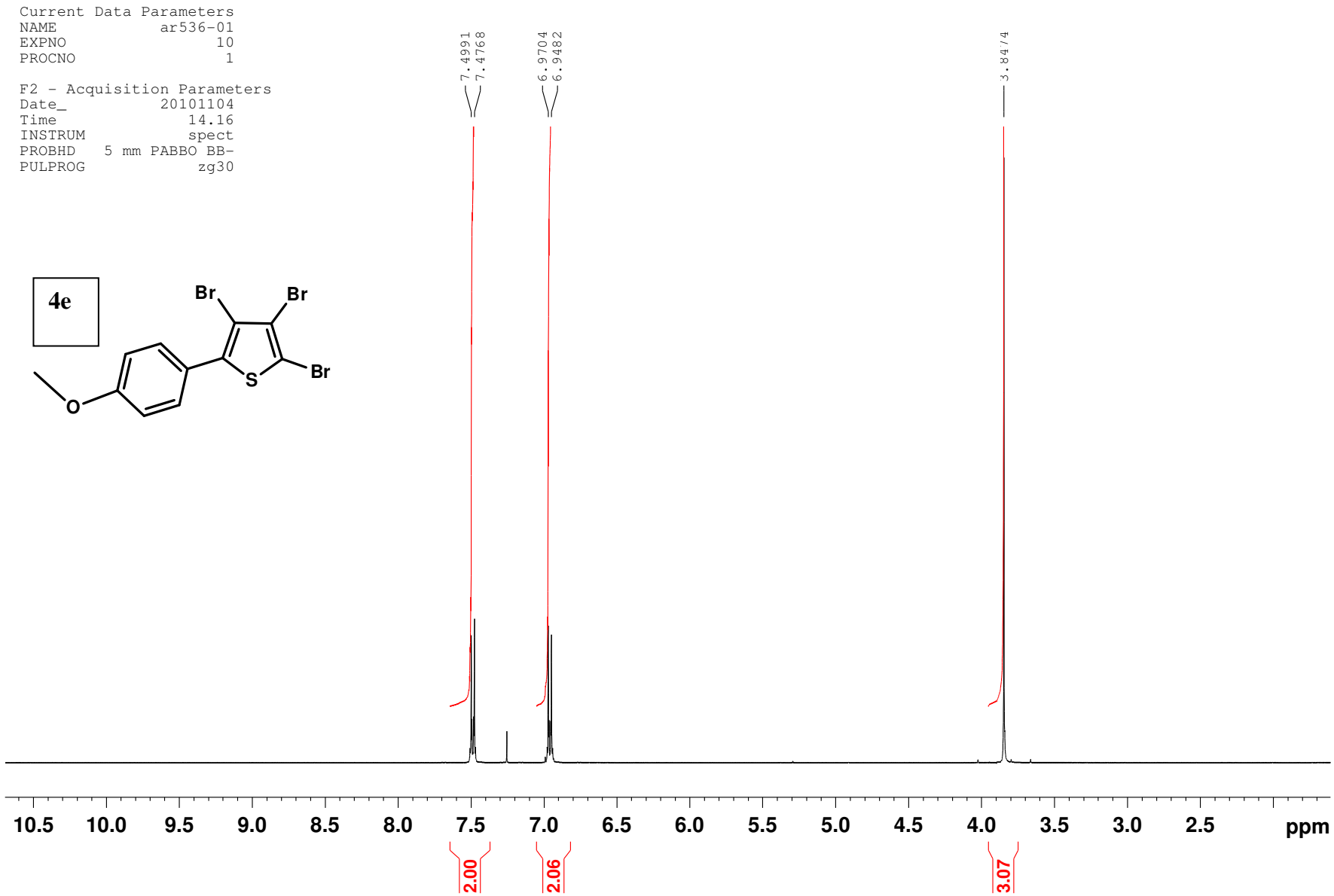

138.9
137.9
130.1
129.4
128.9
111.8
77.4
77.1
76.7
21.4
130 ppm
4b
Br
Br
Br
S
Current Data Parameters
NAME ar482-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101005
Time 16.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

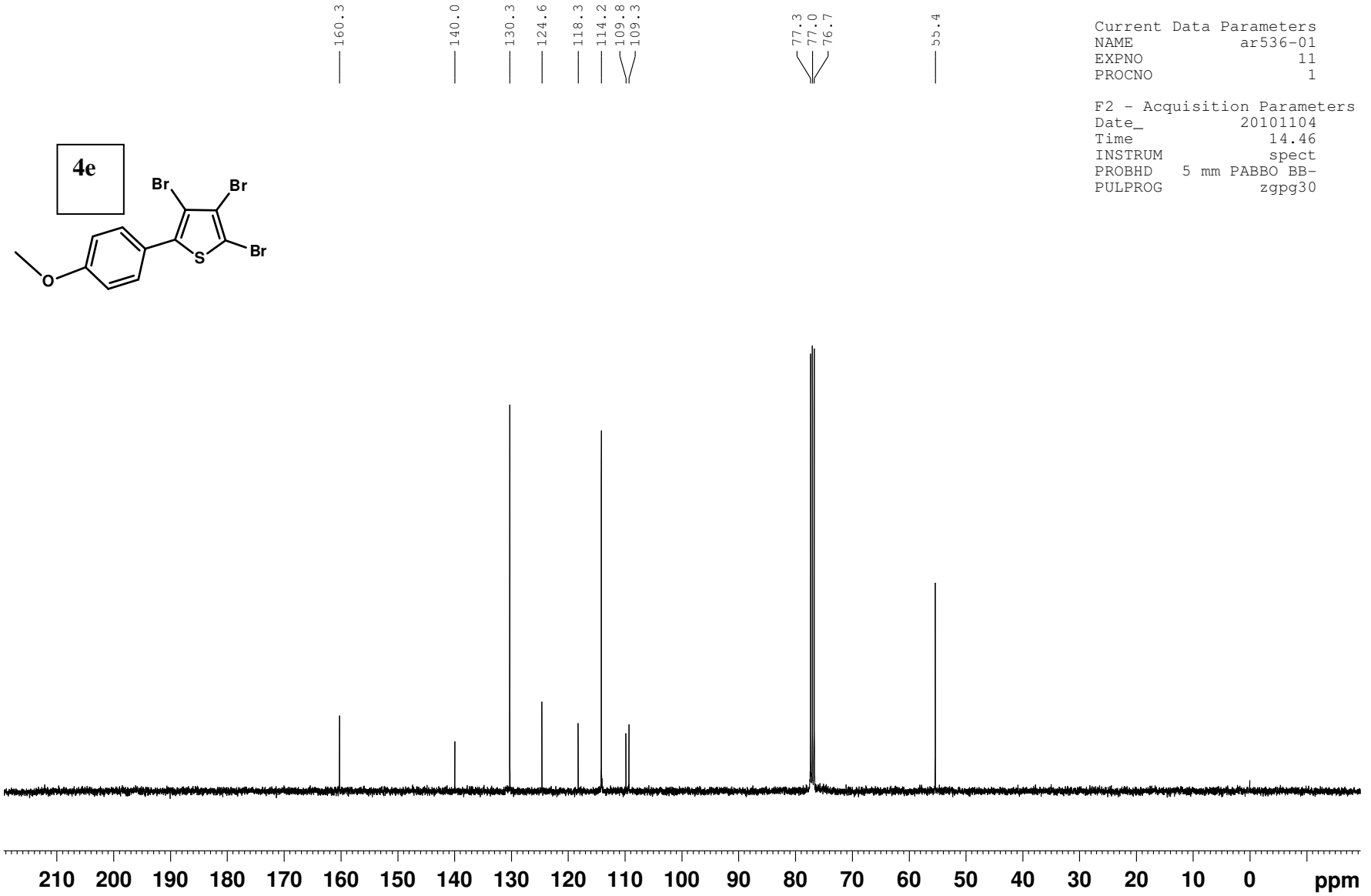

4c
Br
Br
Br
S
S
7.42
7.41
7.40
7.40
7.38
7.38
7.37
7.37
7.26
7.11
7.10
7.09
7.09
7.415
7.412
7.402
7.399
7.389
7.381
7.374
7.371
7.50
7.45
7.40
ppm
7.107
7.098
7.095
7.085
7.10
ppm
Current Data Parameters
NAME ar524-02
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101002
Time 12.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.01

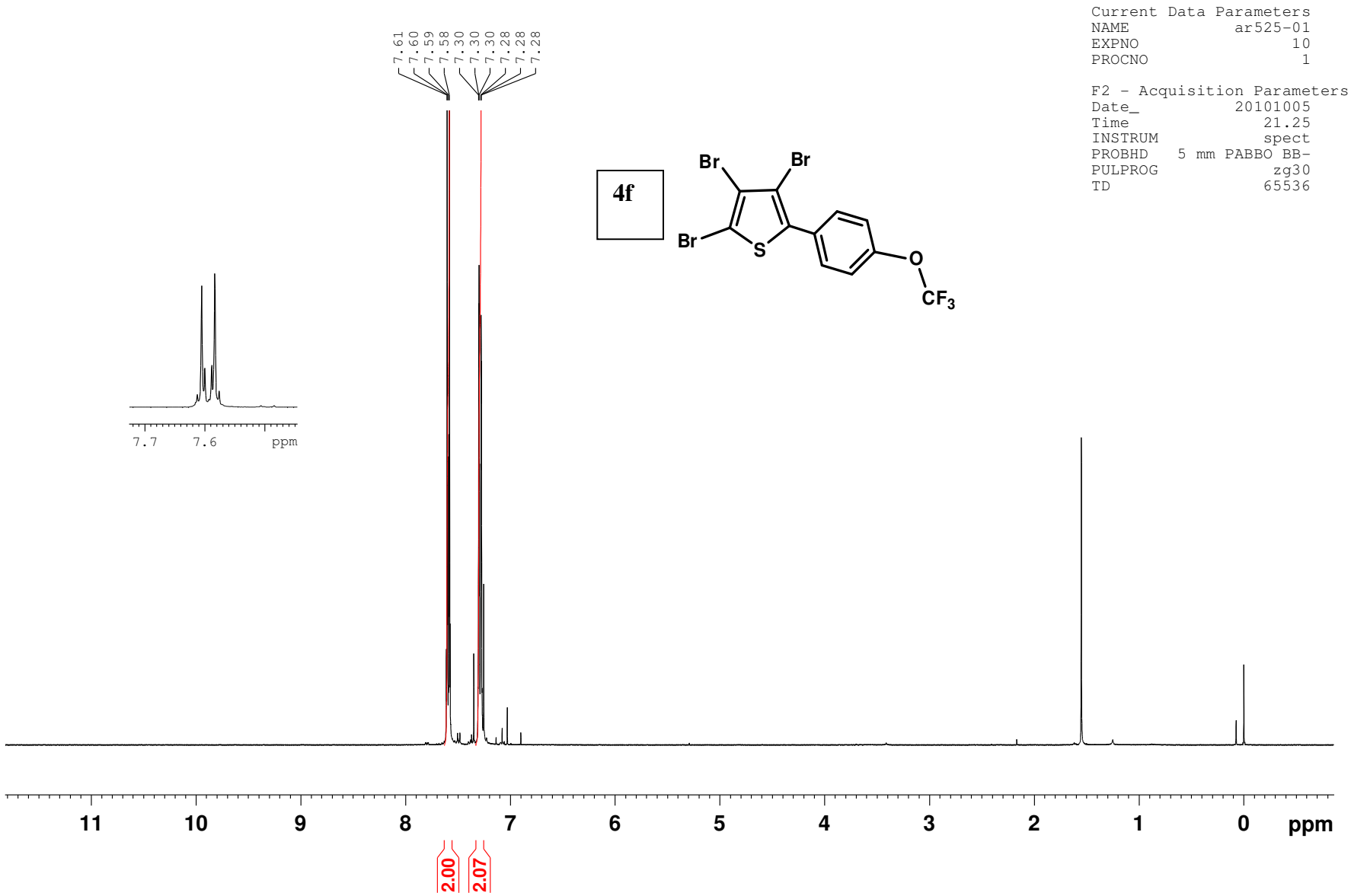

4c
Br
Br
Br
S
S
133.9
133.5
127.4
127.3
127.1
118.7
110.4
109.4
77.3
77.0
76.7
127.390
127.348
127.116
127.5
127.0
ppm
Current Data Parameters
NAME ar524-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101002
Time 13.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

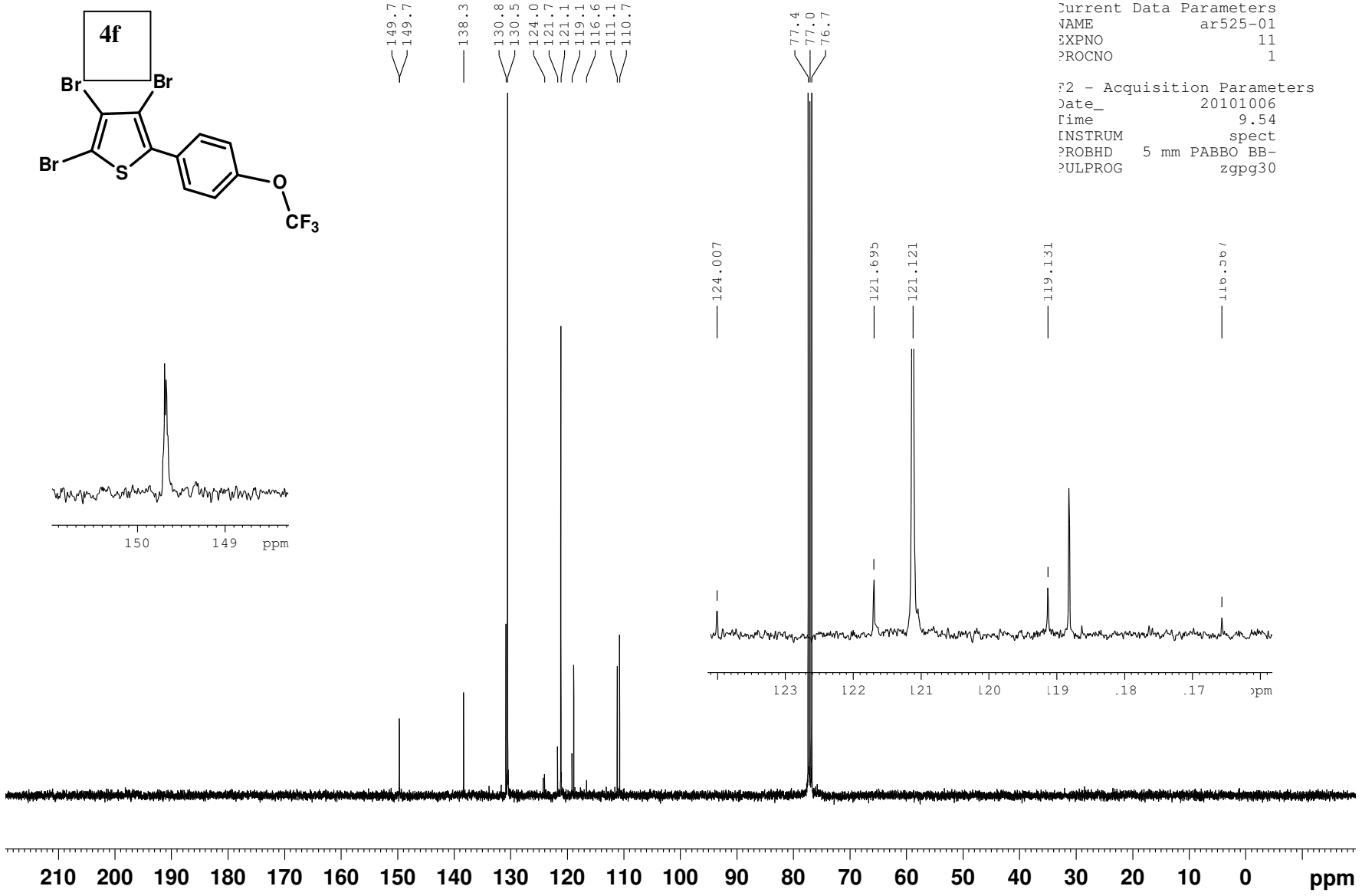

7.9662
7.9458
7.9285
7.9226
7.9128
7.9077
7.9047
7.7364
7.7343
7.7319
7.7295
7.7183
7.7138
7.7121
7.5544
7.5463
7.5417
7.5373
7.5321
7.5285
7.5252
7.5179
7.5122
7.5081
7.4950
7.4908
7.4830
7.4795
7.4654
7.4618
Current Data Parameters
NAME ar528-02
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101008
Time 17.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
4d
Br
Br
Br
S
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
2.16
1.00
4.23

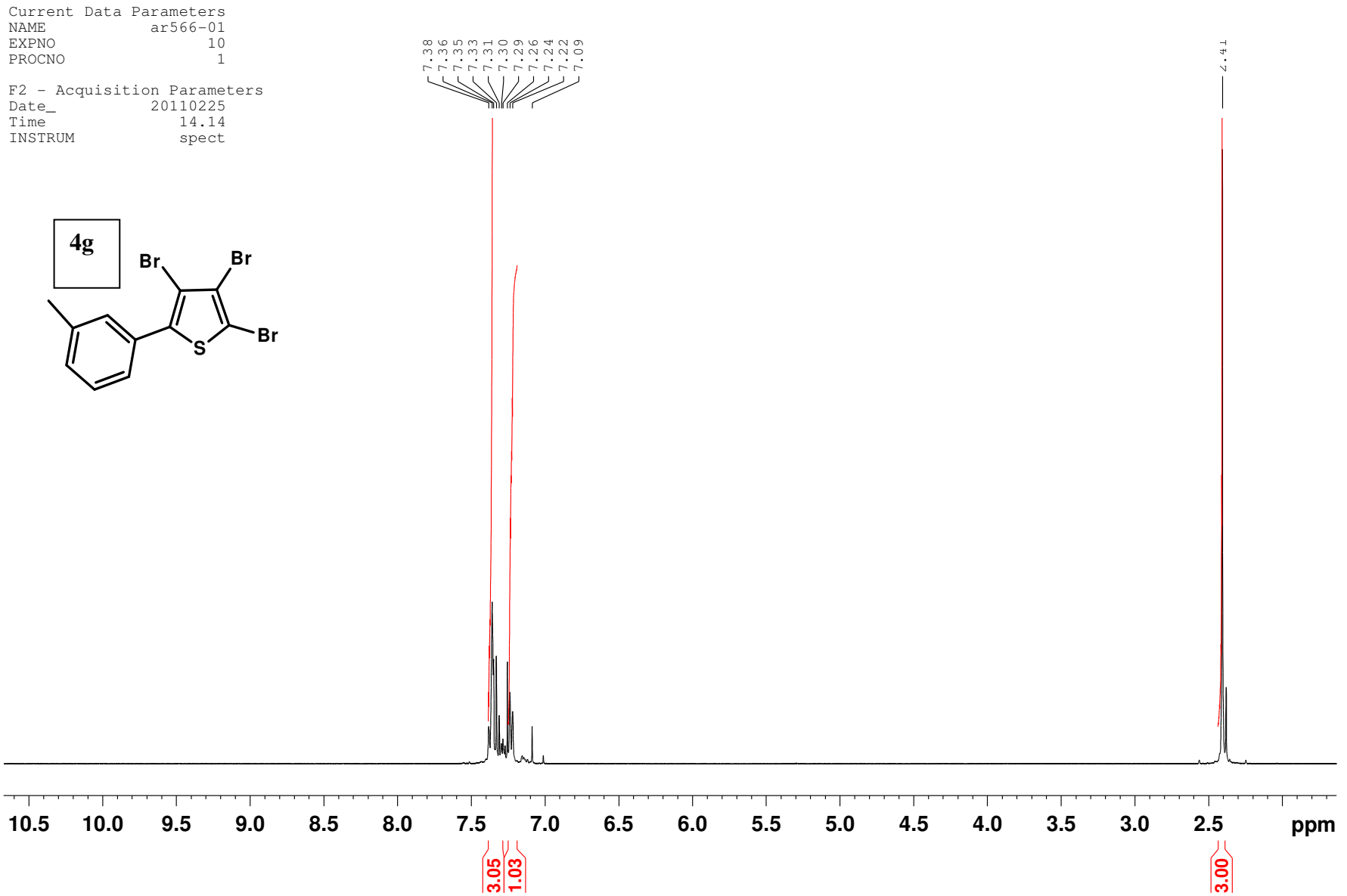

138.3
133.6
131.6
130.3
129.6
129.4
128.5
127.0
126.5
125.6
125.1
117.6
113.8
110.9
77.4
77.0
76.7
Current Data Parameters
NAME ar528-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101008
Time 18.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
4d
Br
Br
Br
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

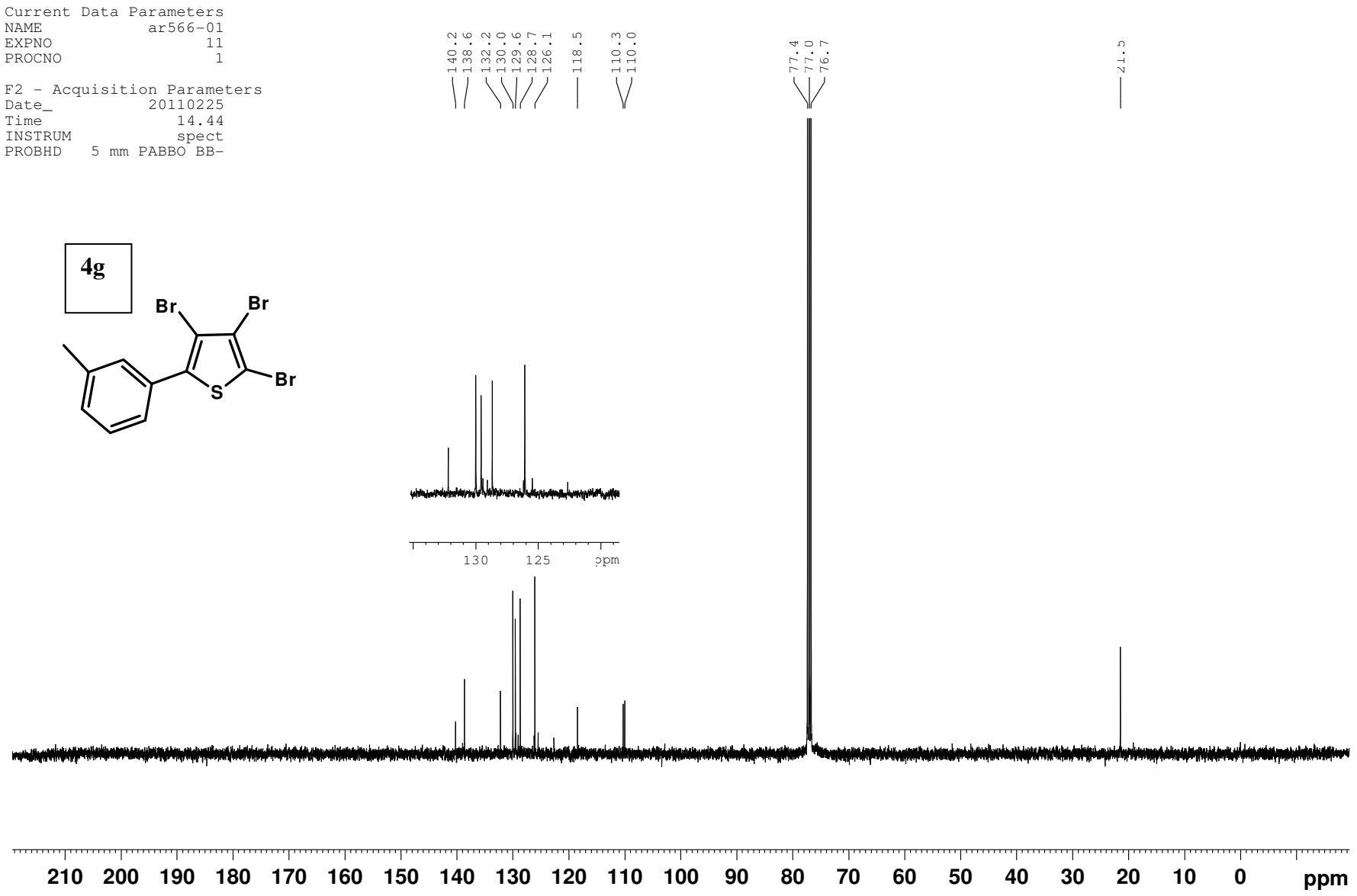

Current Data Parameters
NAME ar536-01
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101104
Time 14.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
4e
Br
Br
Br
S
O
7.4991
7.4768
6.9704
6.9482
3.8474
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
2.00
2.06
3.07

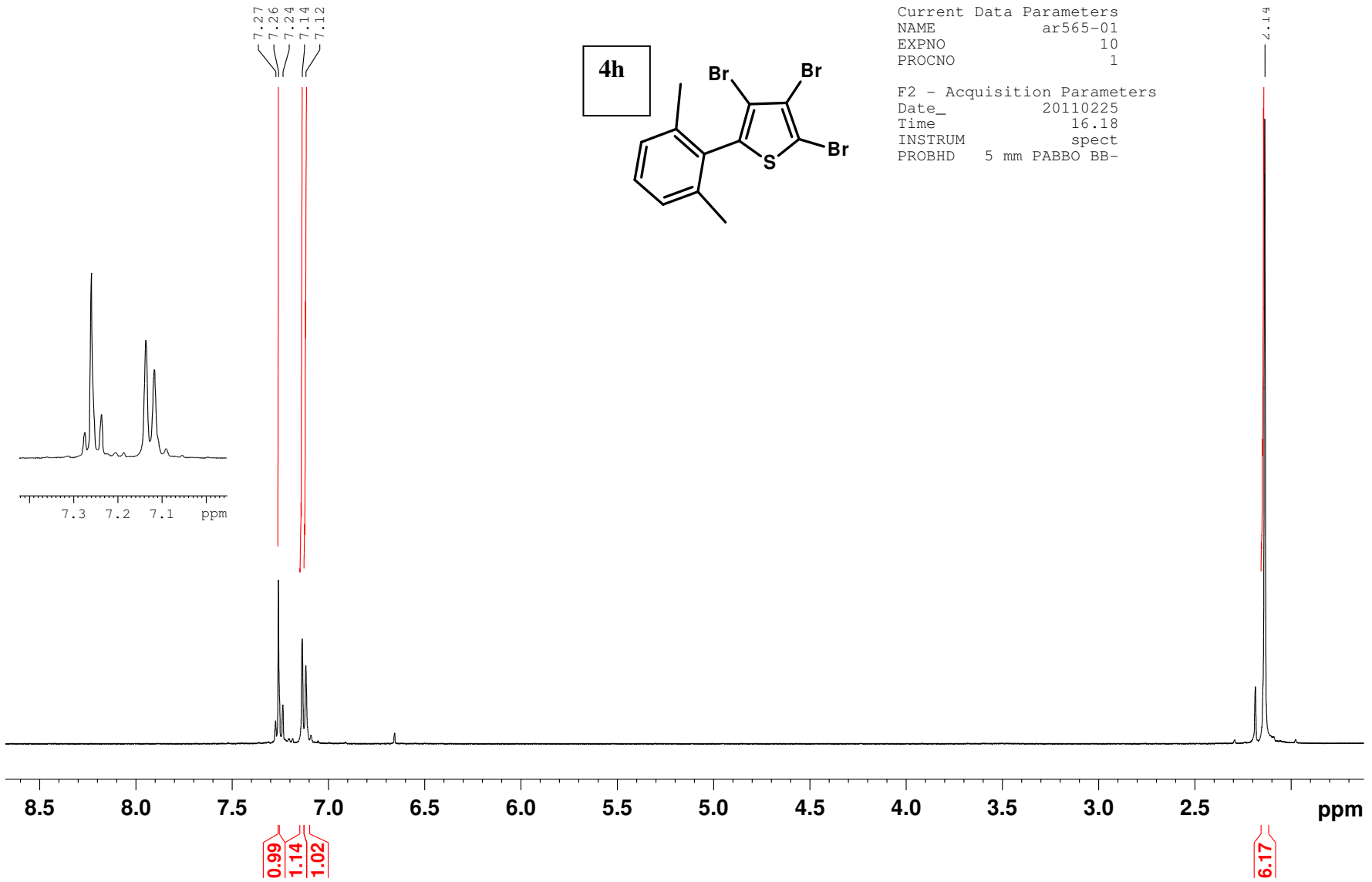

160.3
140.0
130.3
124.6
118.3
114.2
109.8
109.3
77.3
77.0
76.7
55.4
Current Data Parameters
NAME ar536-01
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101104
Time 14.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
4e
Br
Br
Br
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

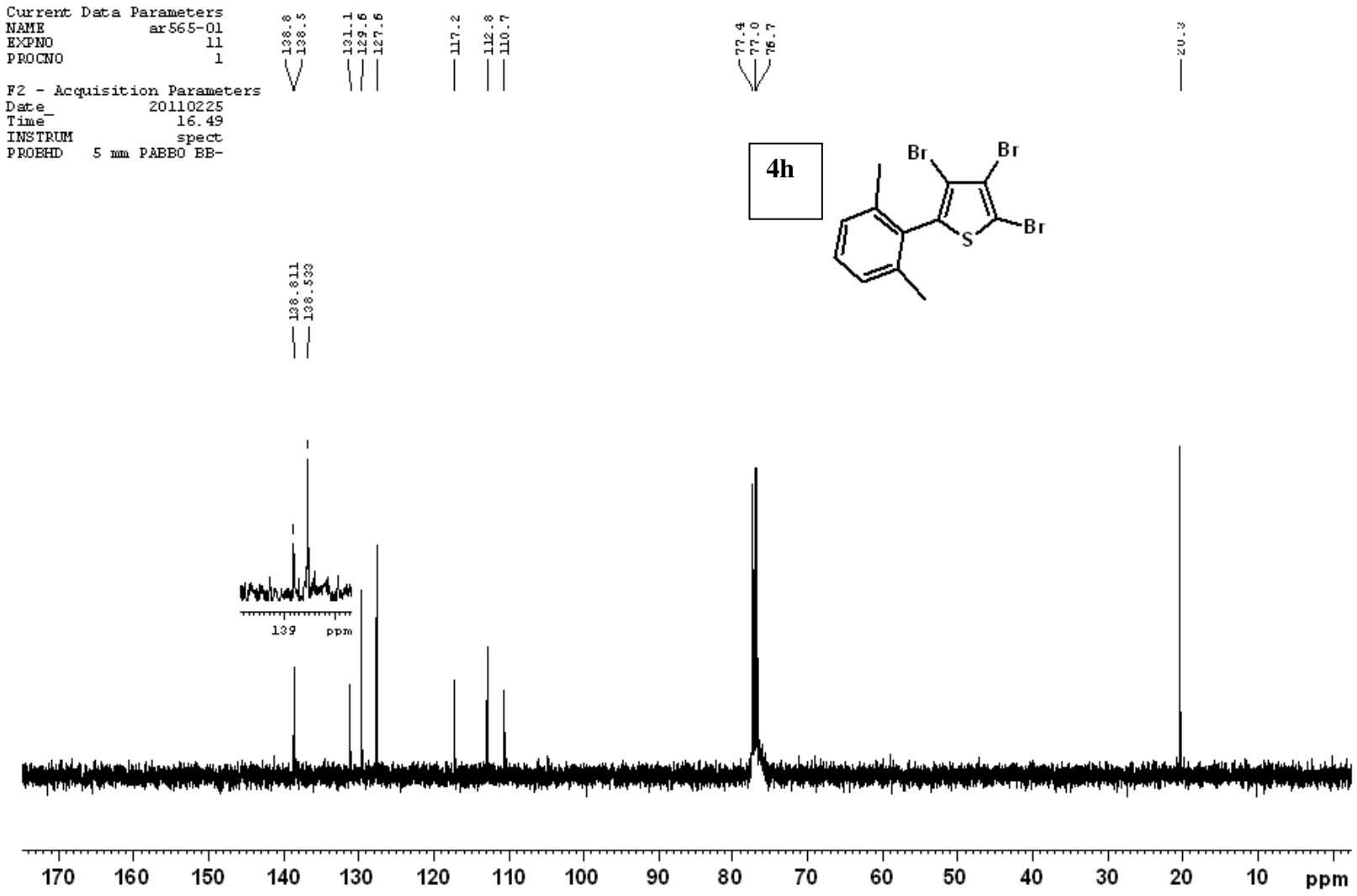

7.61
7.60
7.59
7.58
7.30
7.30
7.28
7.28
7.28
4f
Br
Br
Br
S
O
CF3
7.7
7.6
ppm
Current Data Parameters
NAME ar525-01
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101005
Time 21.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.07

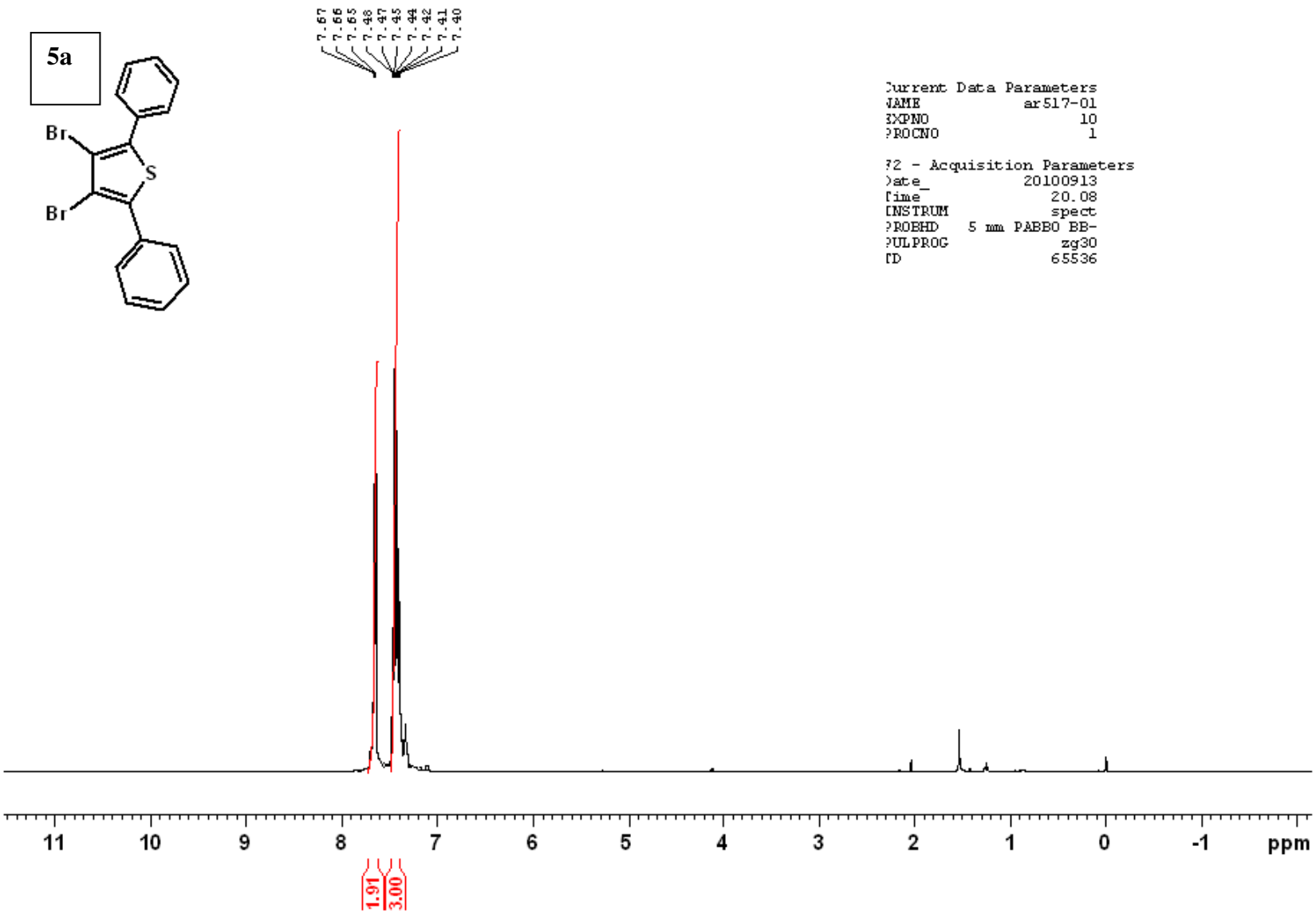

4f
Br
Br
Br
S
O
CF3
149.7
149.7
138.3
130.8
130.5
124.0
121.7
121.1
119.1
116.6
111.1
110.7
77.4
77.0
76.7
Current Data Parameters
NAME ar525-01
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101006
Time 9.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
124.007
121.695
121.121
119.131
150
149
ppm
123
122
121
120
119
118
117
ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

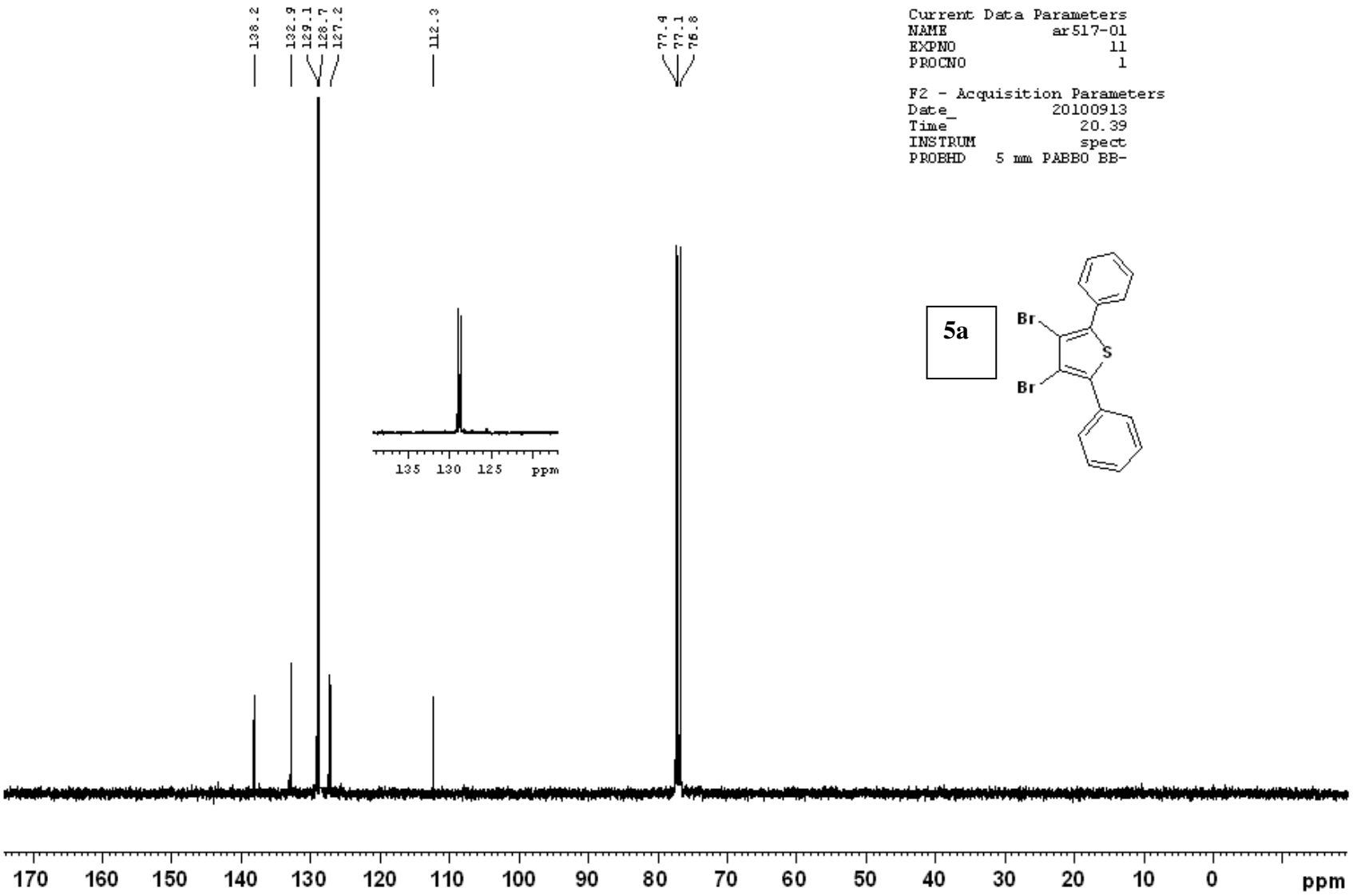

Current Data Parameters
NAME ar566-01
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110225
Time 14.14
INSTRUM spect
4g
Br
Br
Br
S
7.38
7.36
7.35
7.33
7.31
7.30
7.29
7.26
7.24
7.22
7.09
7.41
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
3.05
1.03
3.00

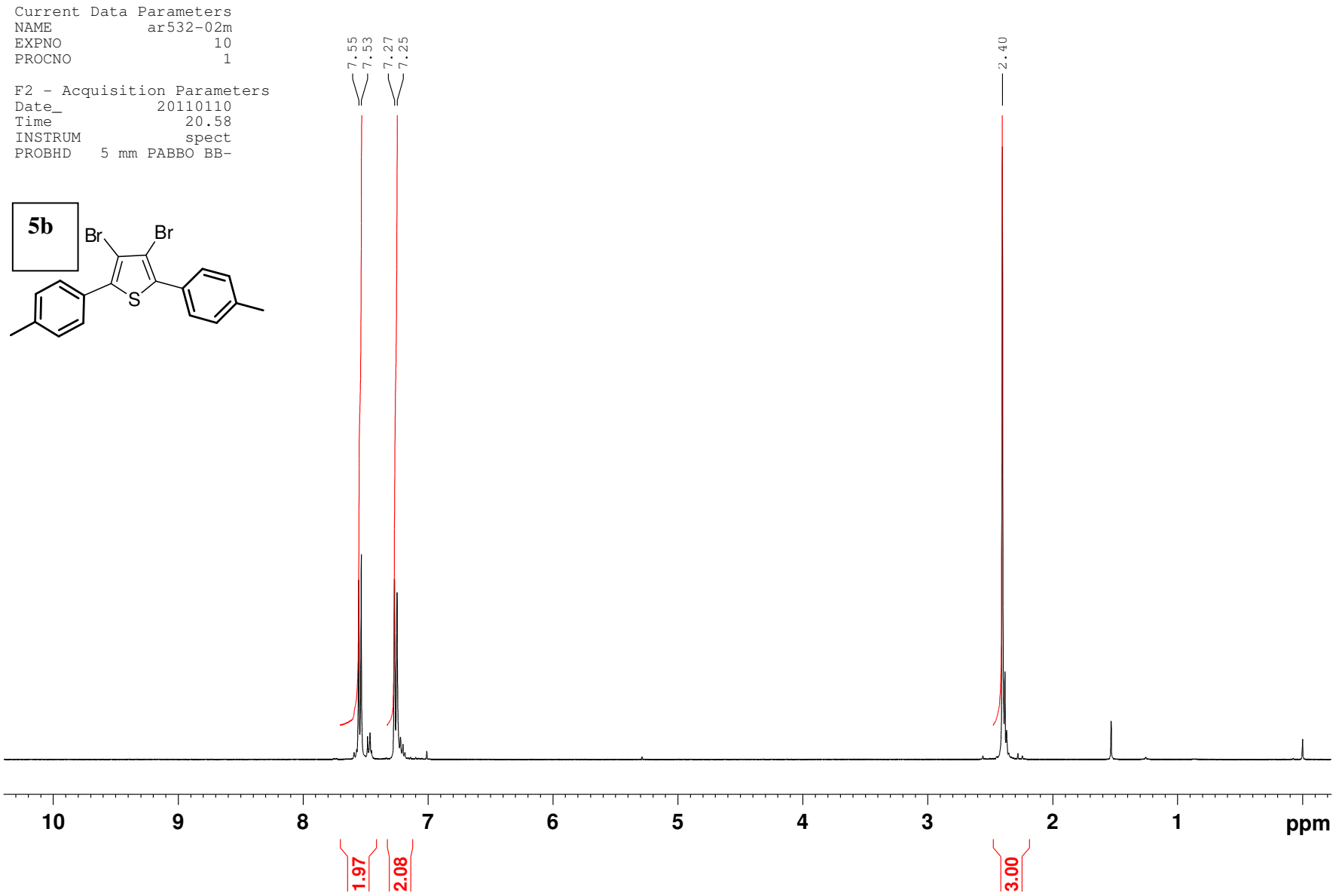

Current Data Parameters
NAME ar566-01
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110225
Time 14.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
140.2
138.6
132.2
130.0
129.6
128.7
126.1
118.5
110.3
110.0
77.4
77.0
76.7
21.5
4g
Br
Br
Br
S
130
125
ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

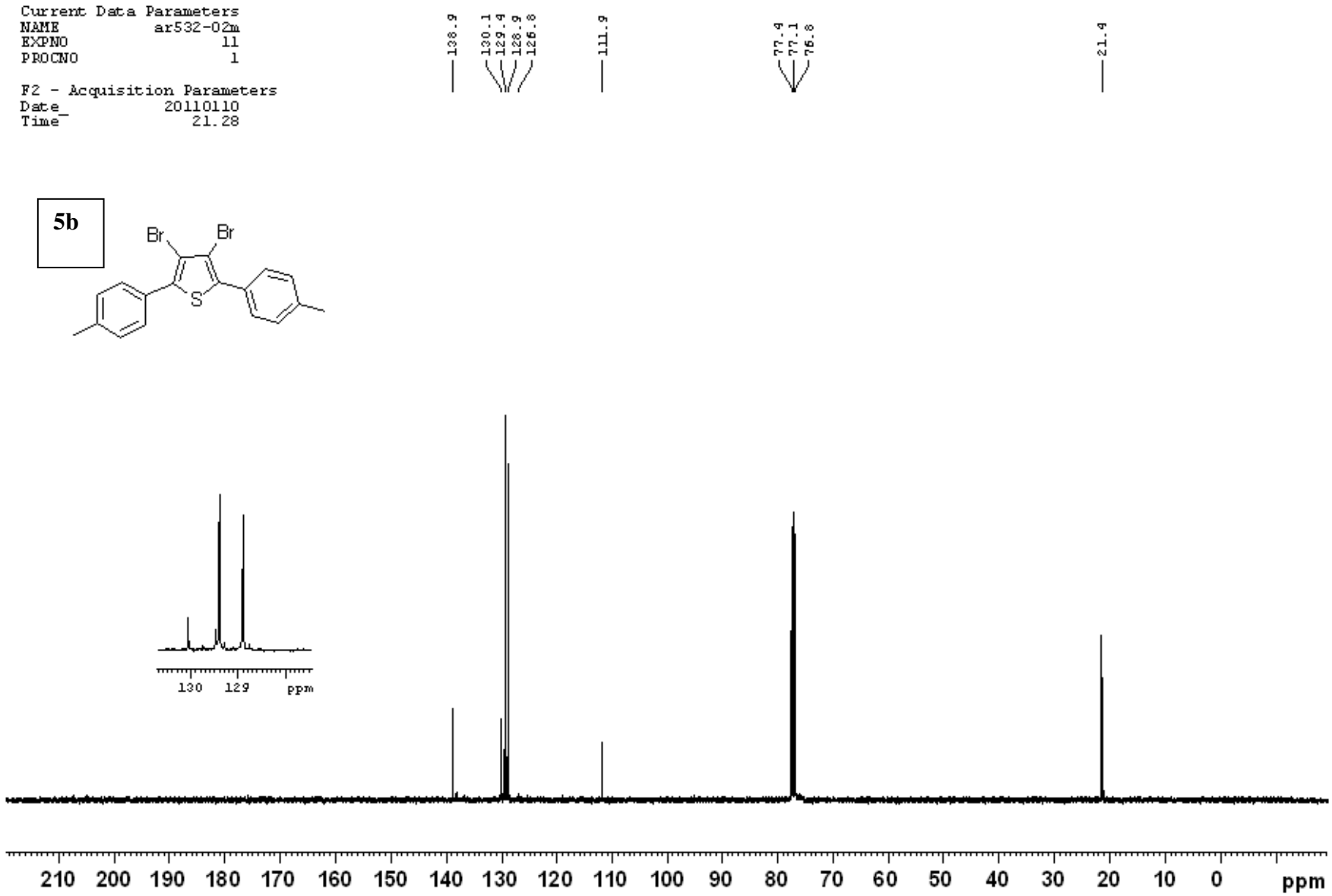

7.27
7.26
7.24
7.14
7.12
4h
Br
Br
Br
S
Current Data Parameters
NAME ar565-01
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110225
Time 16.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
7.14
7.3 7.2 7.1 ppm
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
0.99
1.14
1.02
6.17

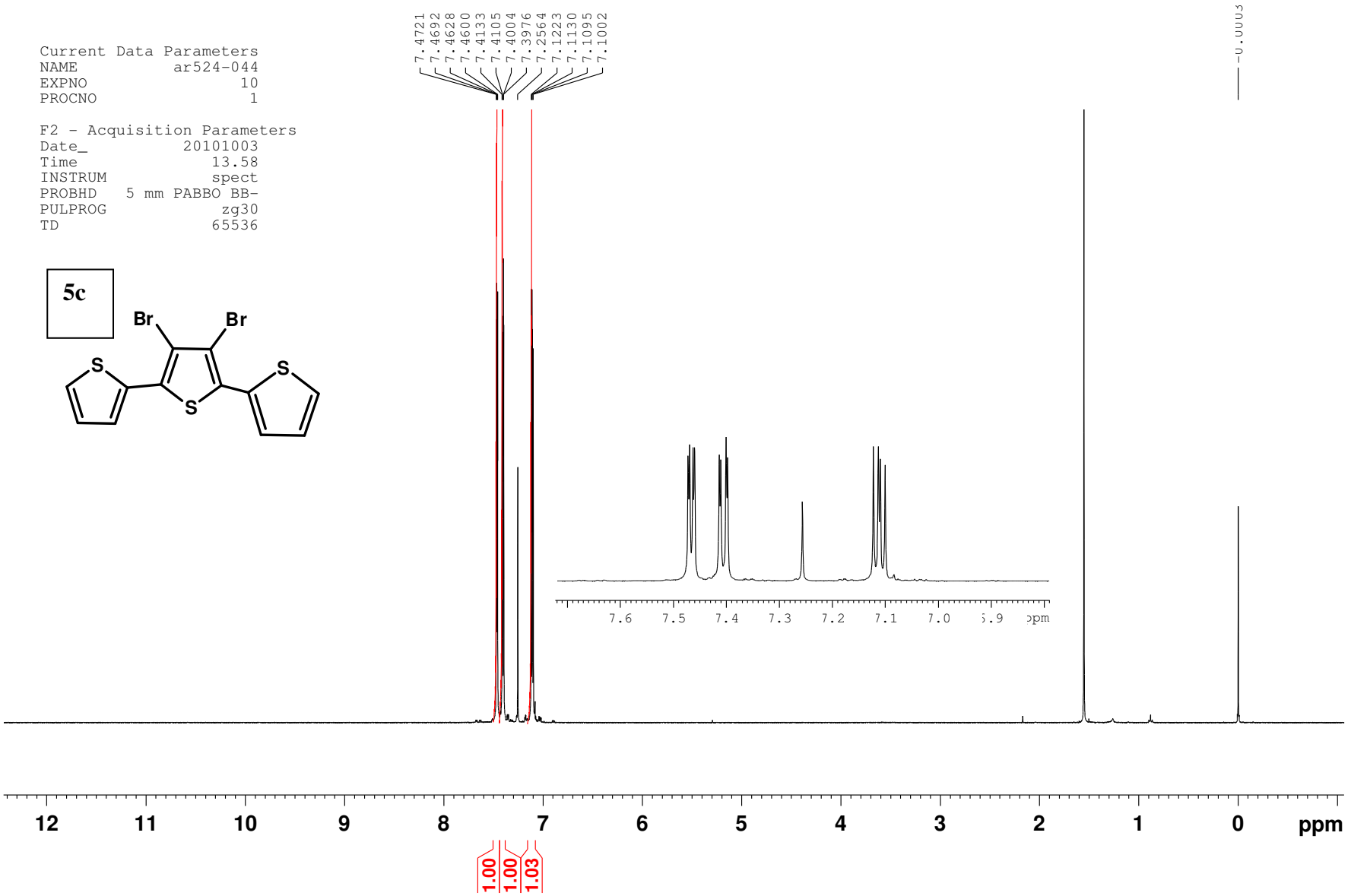

Current Data Parameters
NAME ar565-01
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110225
Time 16.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
138.8
138.5
131.1
129.6
127.6
117.2
112.8
110.7
77.4
77.0
76.7
20.3
4h
Br
Br
Br
S
138.811
138.533
139 ppm
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

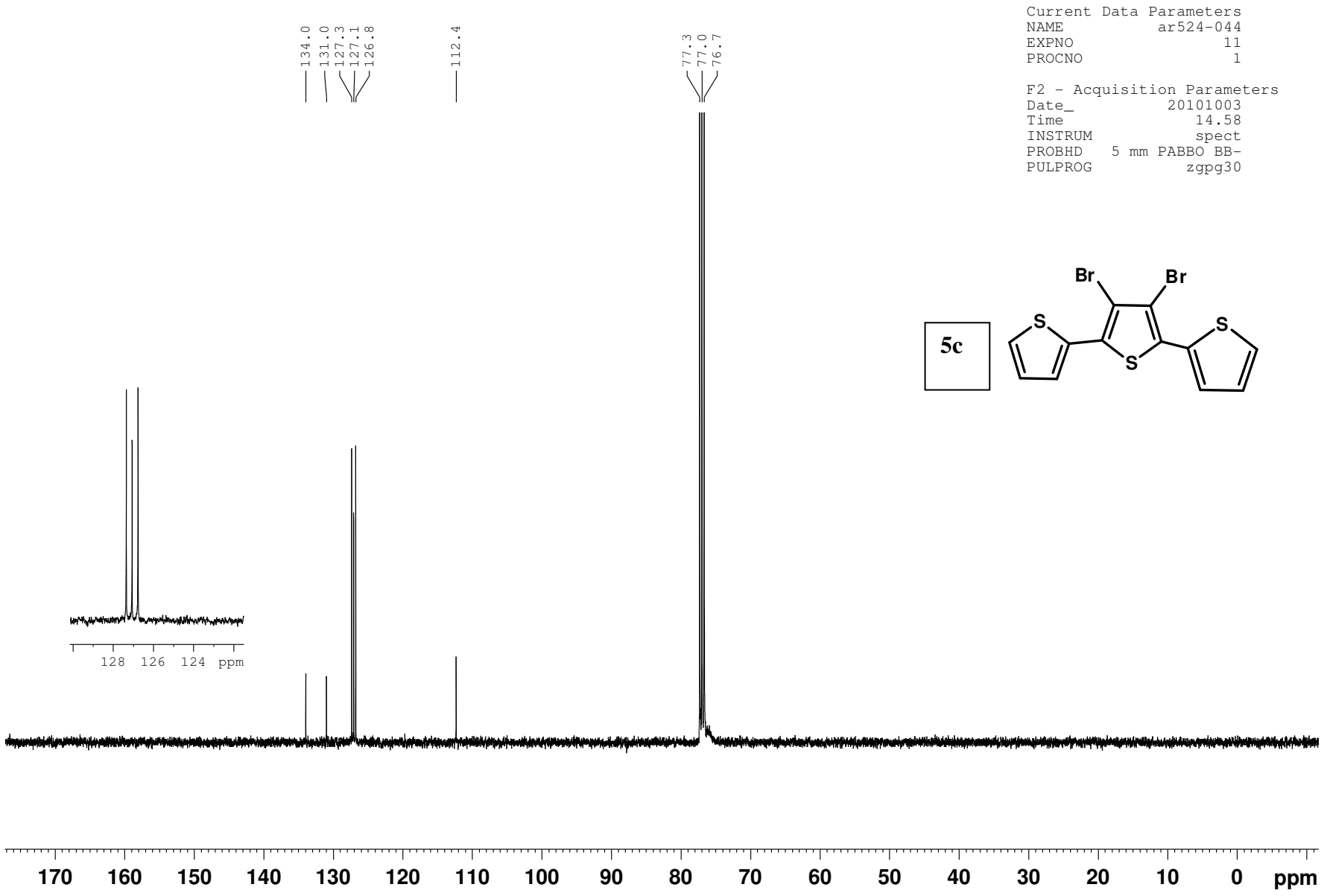

5a
Br
Br
S
7.67
7.66
7.65
7.46
7.47
7.45
7.44
7.42
7.41
7.40
Current Data Parameters
NAME ar517-01
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100913
Time 20.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
1.91
3.00

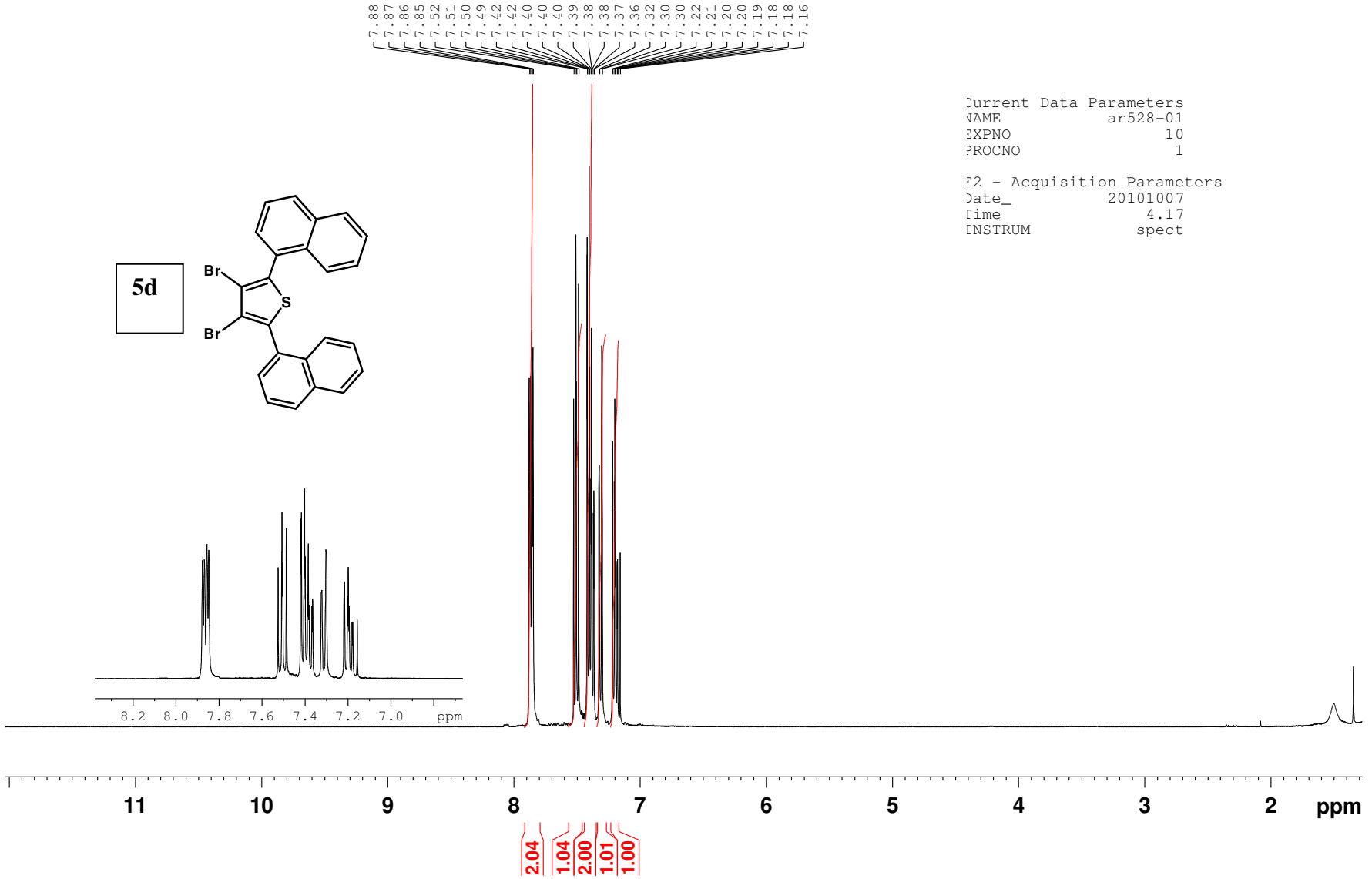

138.2
132.9
129.1
128.7
127.2
112.3
77.4
77.1
76.8
Current Data Parameters
NAME ar517-01
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100913
Time 20.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
135 130 125 ppm
5a
Br
Br
S
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

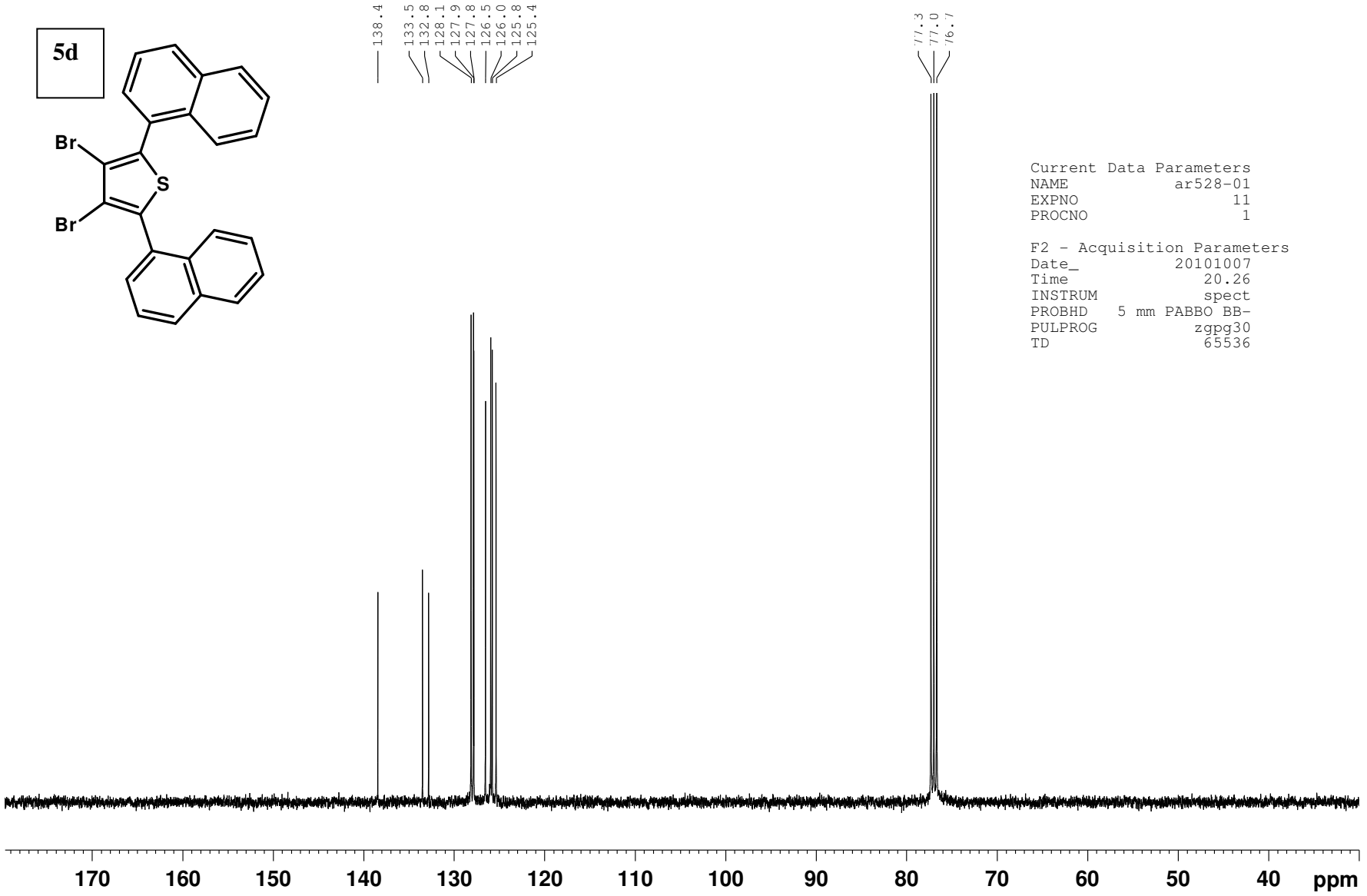

Current Data Parameters
NAME ar532-02m
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110110
Time 20.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
5b
Br
Br
S
7.55
7.53
7.27
7.25
2.40
10
9
8
7
6
5
4
3
2
1
ppm
1.97
2.08
3.00

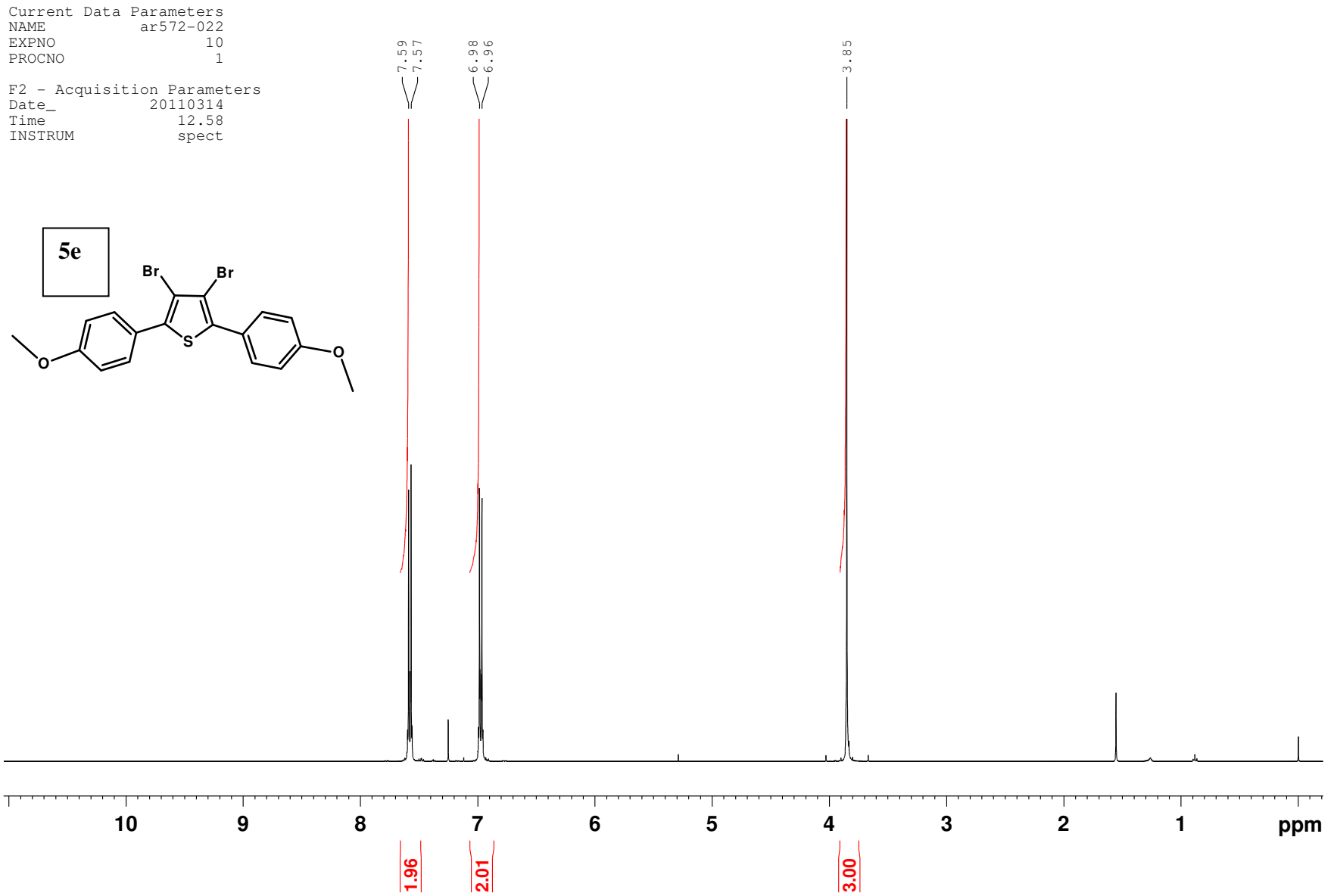

Current Data Parameters
NAME ar532-02m
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110110
Time 21.28
138.9
130.1
129.4
128.9
126.8
111.9
77.4
77.1
76.8
21.4
5b
Br
Br
S
130
129
ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

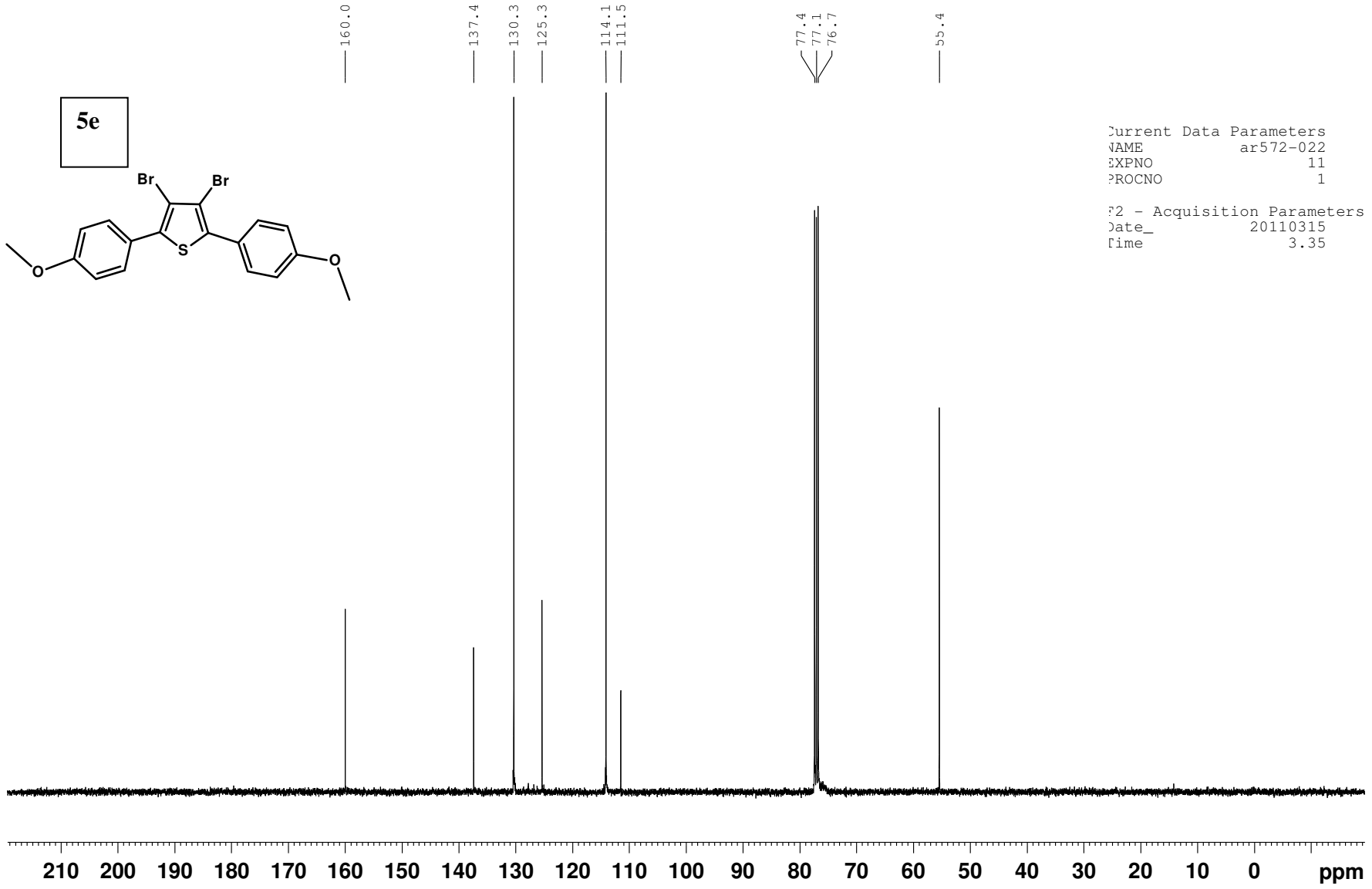

Current Data Parameters
NAME ar524-044
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101003
Time 13.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
5c
Br
Br
S
S
S
7.4721
7.4692
7.4628
7.4600
7.4133
7.4105
7.4004
7.3976
7.2564
7.1223
7.1130
7.1095
7.1002
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.03

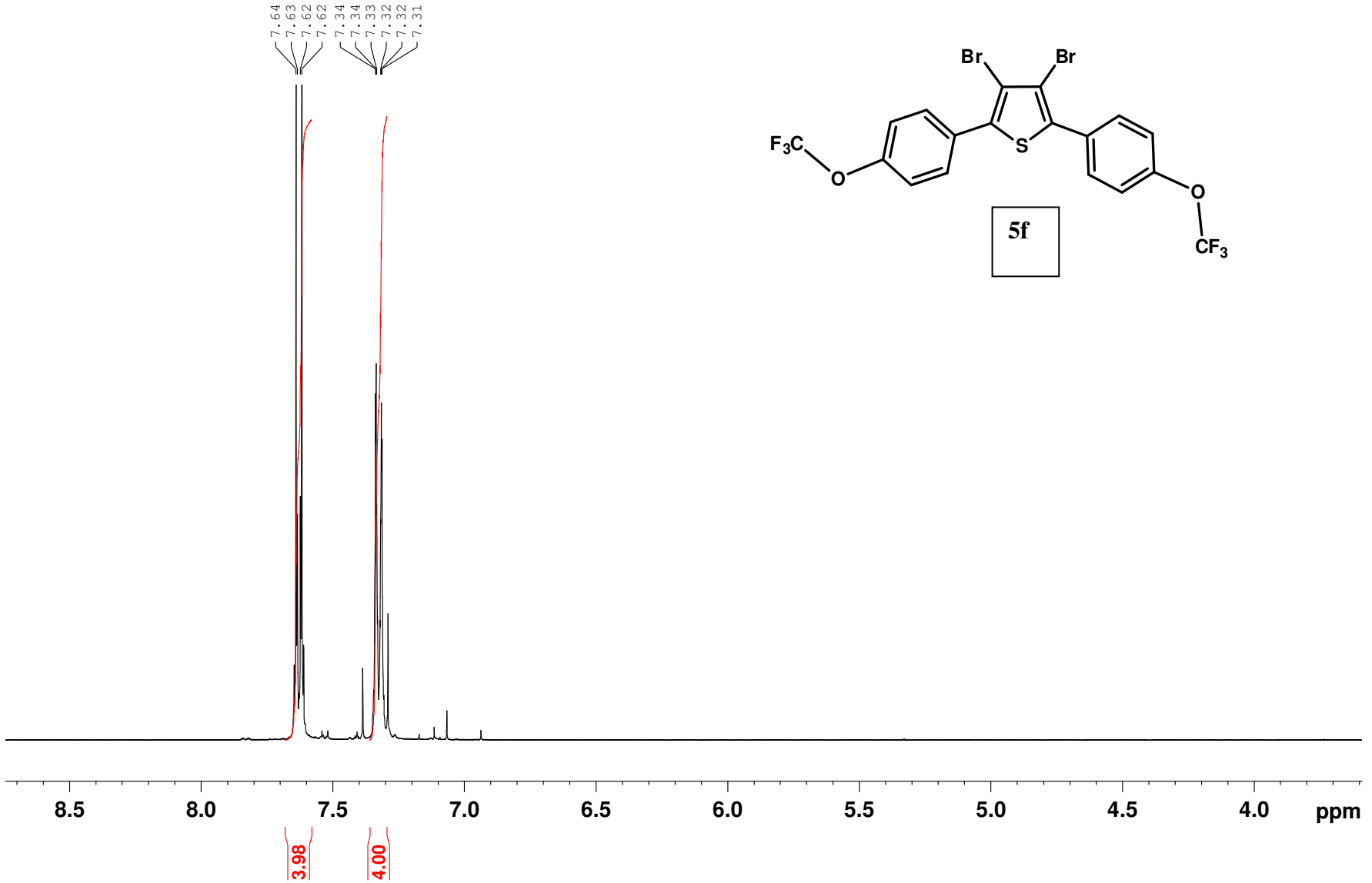

134.0
131.0
127.3
127.1
126.8
112.4
77.3
77.0
76.7
Current Data Parameters
NAME ar524-044
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101003
Time 14.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
5c
Br
Br
S
S
S
128 126 124 ppm
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

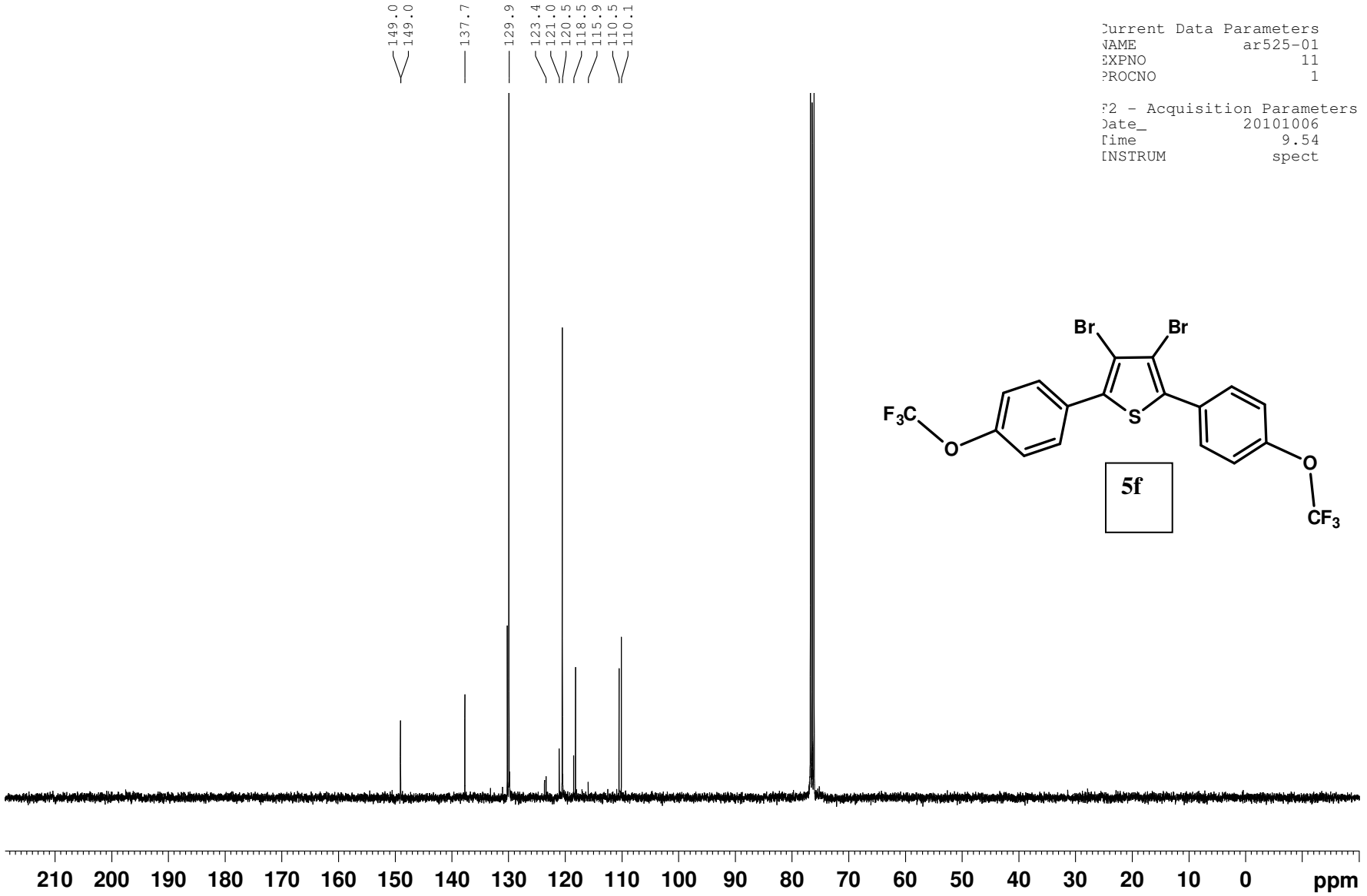

7.88
7.87
7.86
7.85
7.52
7.51
7.50
7.49
7.42
7.42
7.40
7.40
7.40
7.39
7.38
7.38
7.37
7.36
7.32
7.30
7.30
7.22
7.21
7.20
7.20
7.19
7.18
7.18
7.16
Current Data Parameters
NAME ar528-01
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101007
Time 4.17
INSTRUM spect
5d
Br
Br
S
8.2 8.0 7.8 7.6 7.4 7.2 7.0 ppm
11 10 9 8 7 6 5 4 3 2 ppm
2.04
1.04
2.00
1.01
1.00

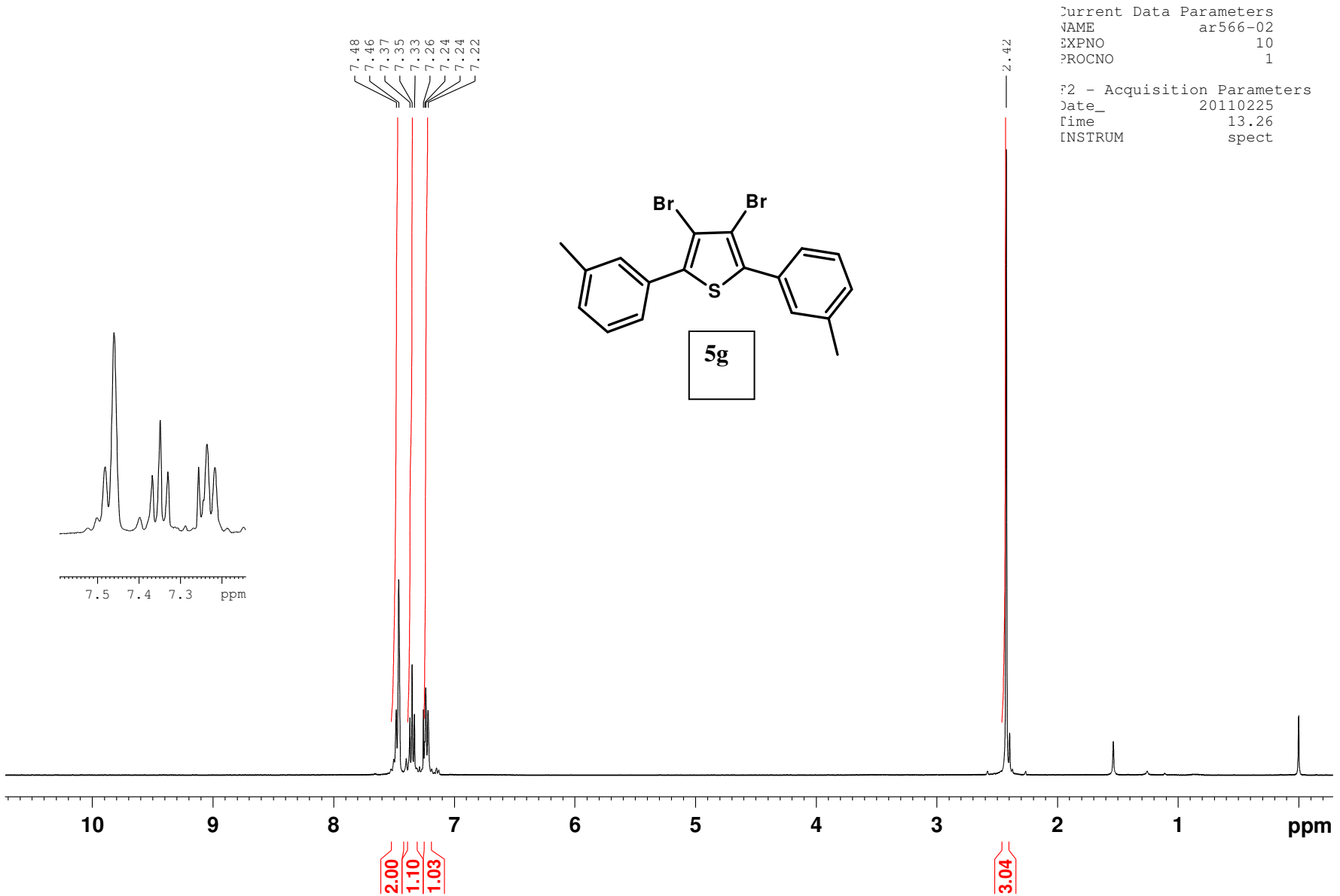

5d
Br
Br
S
138.4
133.5
132.8
128.1
127.9
127.8
126.5
126.0
125.8
125.4
77.3
77.0
76.7
Current Data Parameters
NAME ar528-01
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101007
Time 20.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

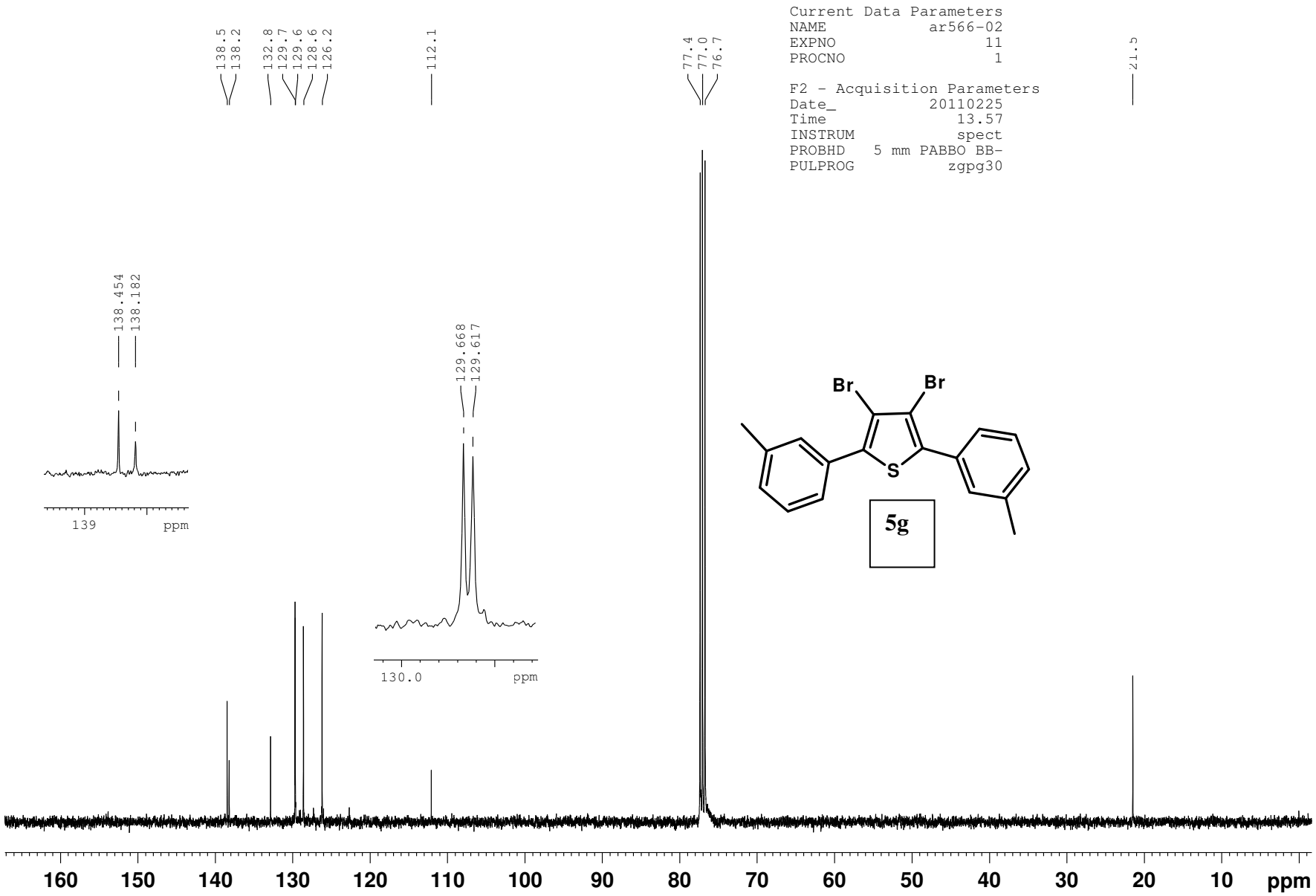

Current Data Parameters
NAME ar572-022
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110314
Time 12.58
INSTRUM spect
5e
Br
Br
S
O
O
7.59
7.57
6.98
6.96
3.85
10
9
8
7
6
5
4
3
2
1
ppm
1.96
2.01
3.00

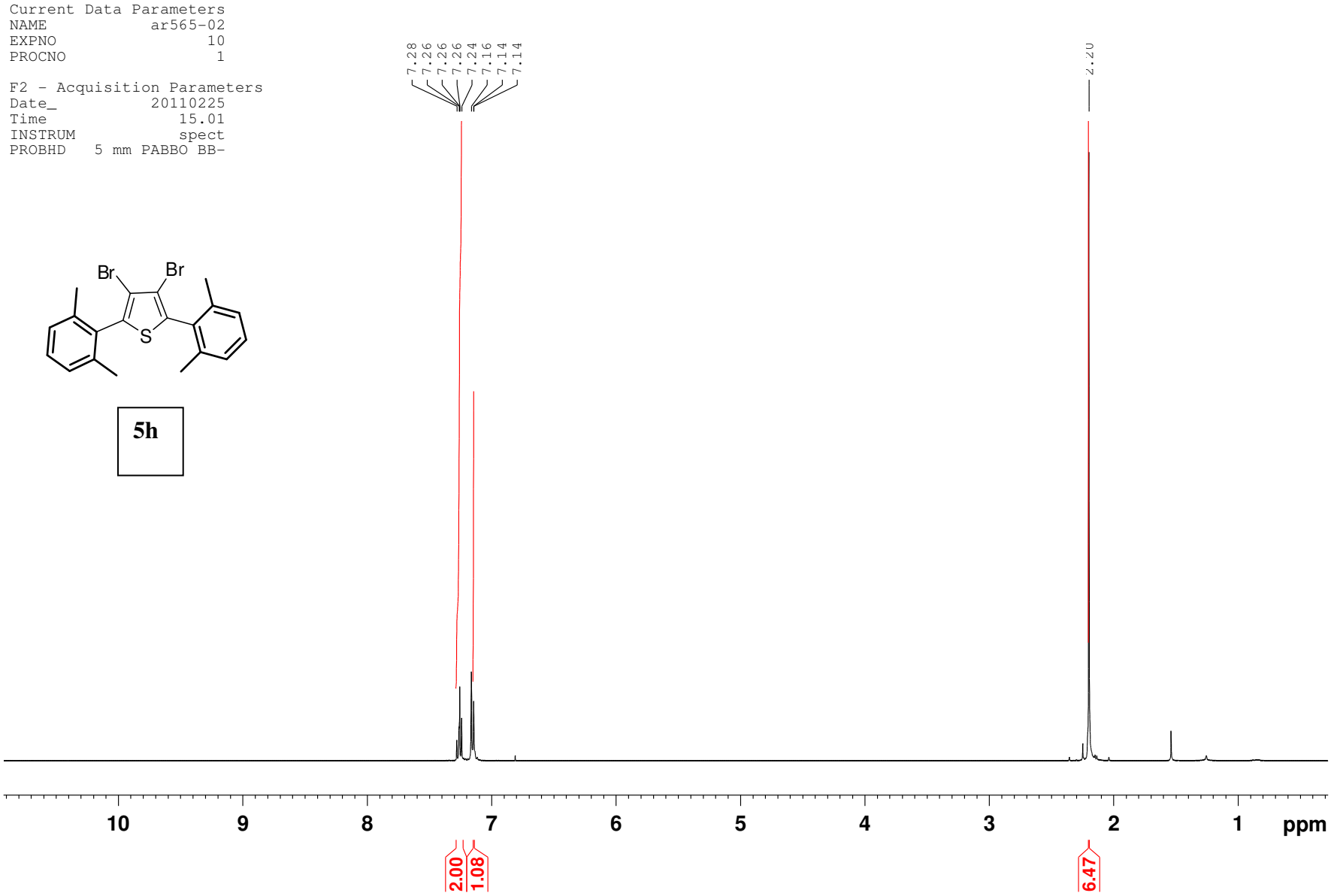

160.0
137.4
130.3
125.3
114.1
111.5
77.4
77.1
76.7
55.4
5e
Br
Br
S
O
O
Current Data Parameters
NAME ar572-022
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110315
Time 3.35
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

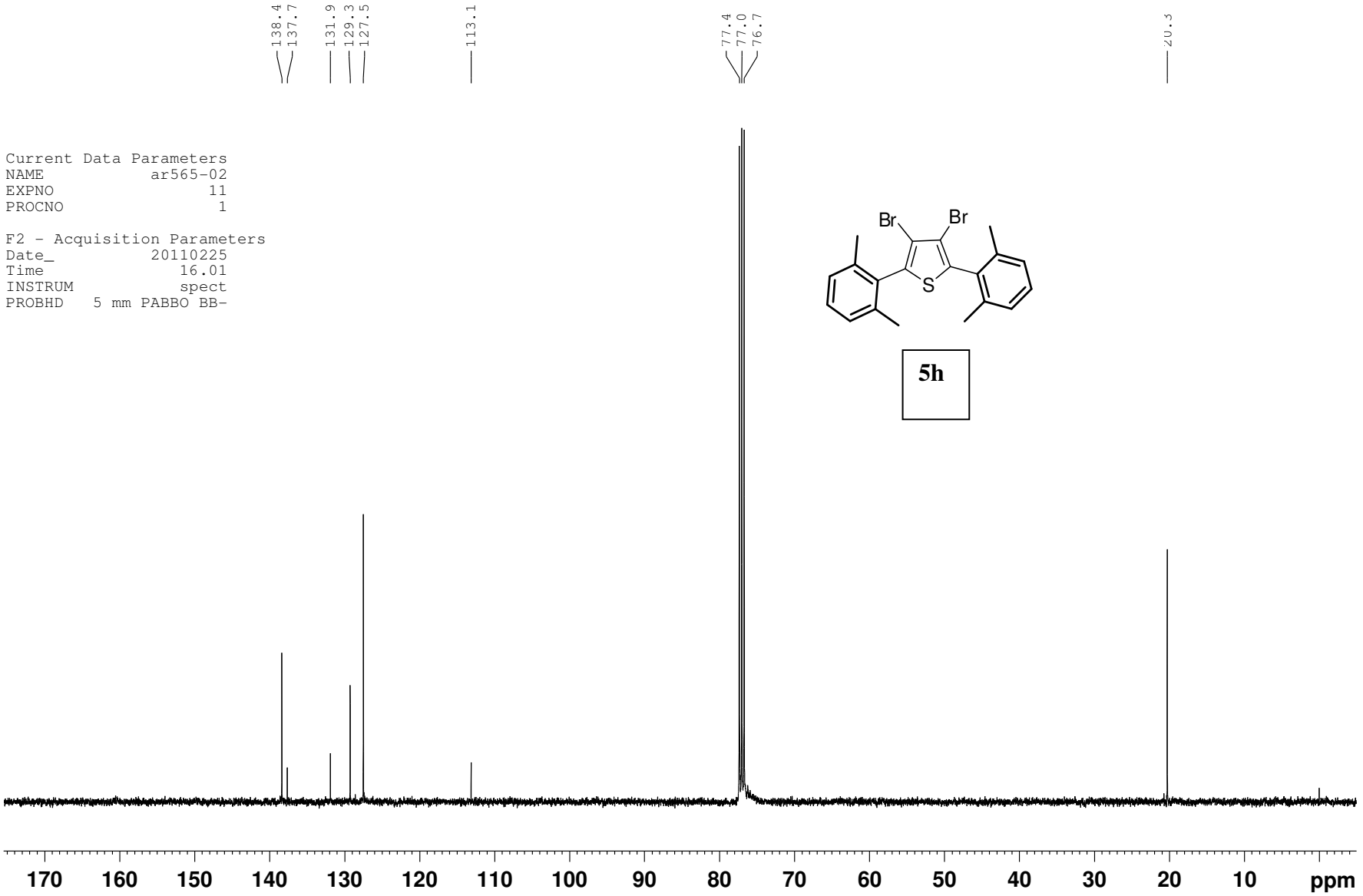

7.64
7.63
7.62
7.62
7.34
7.34
7.33
7.32
7.32
7.31
Br
Br
S
F3C
O
O
CF3
5f
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
ppm
3.98
4.00

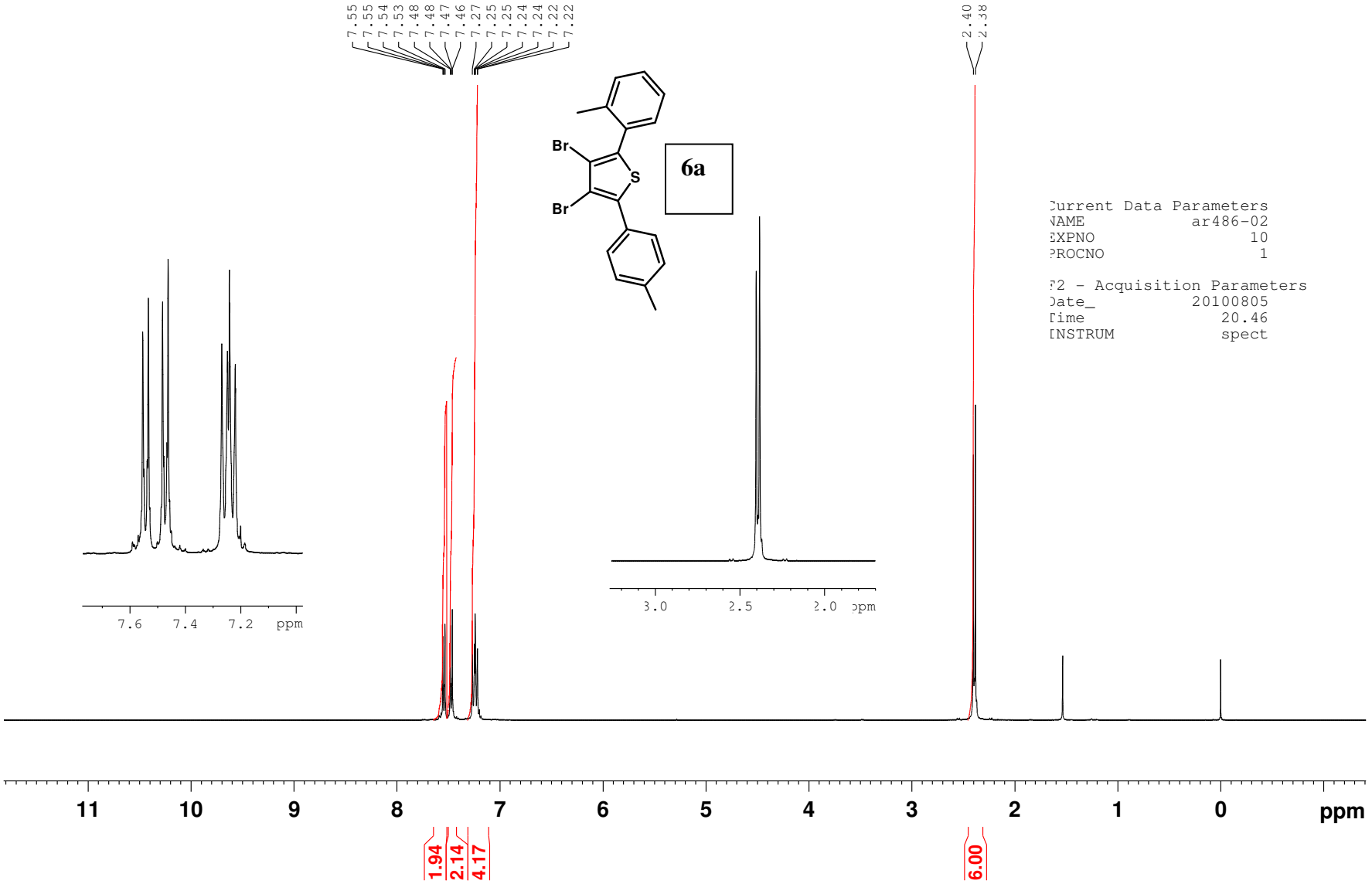

149.0
149.0
137.7
129.9
123.4
121.0
120.5
118.5
115.9
110.5
110.1
Current Data Parameters
NAME ar525-01
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101006
Time 9.54
INSTRUM spect
Br
Br
F3C
O
S
O
CF3
5f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

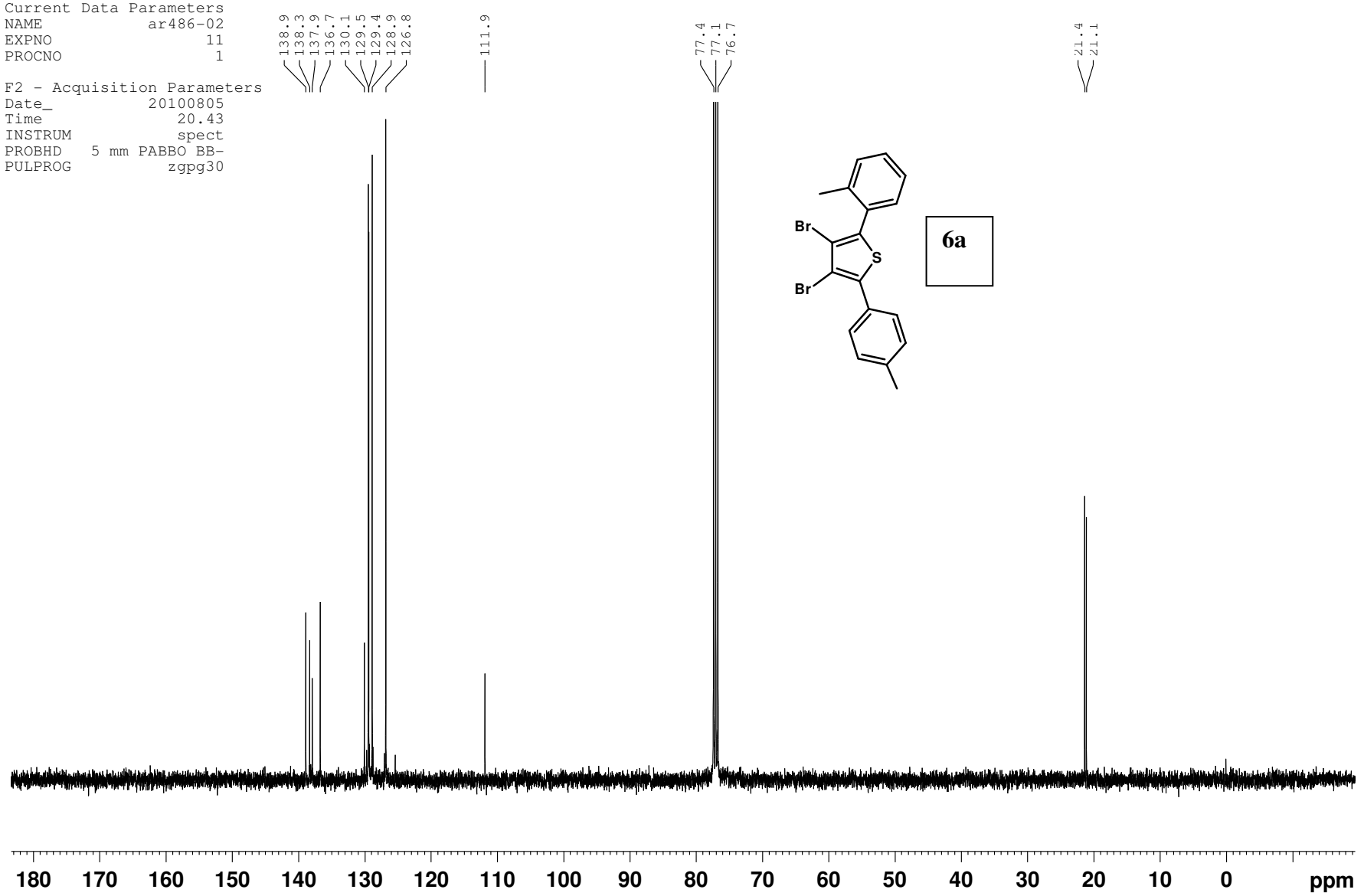

Current Data Parameters
NAME ar566-02
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110225
Time 13.26
INSTRUM spect
7.48
7.46
7.37
7.35
7.33
7.26
7.24
7.24
7.22
2.42
Br
Br
S
5g
7.5 7.4 7.3 ppm
10 9 8 7 6 5 4 3 2 1 ppm
2.00
1.10
1.03
3.04

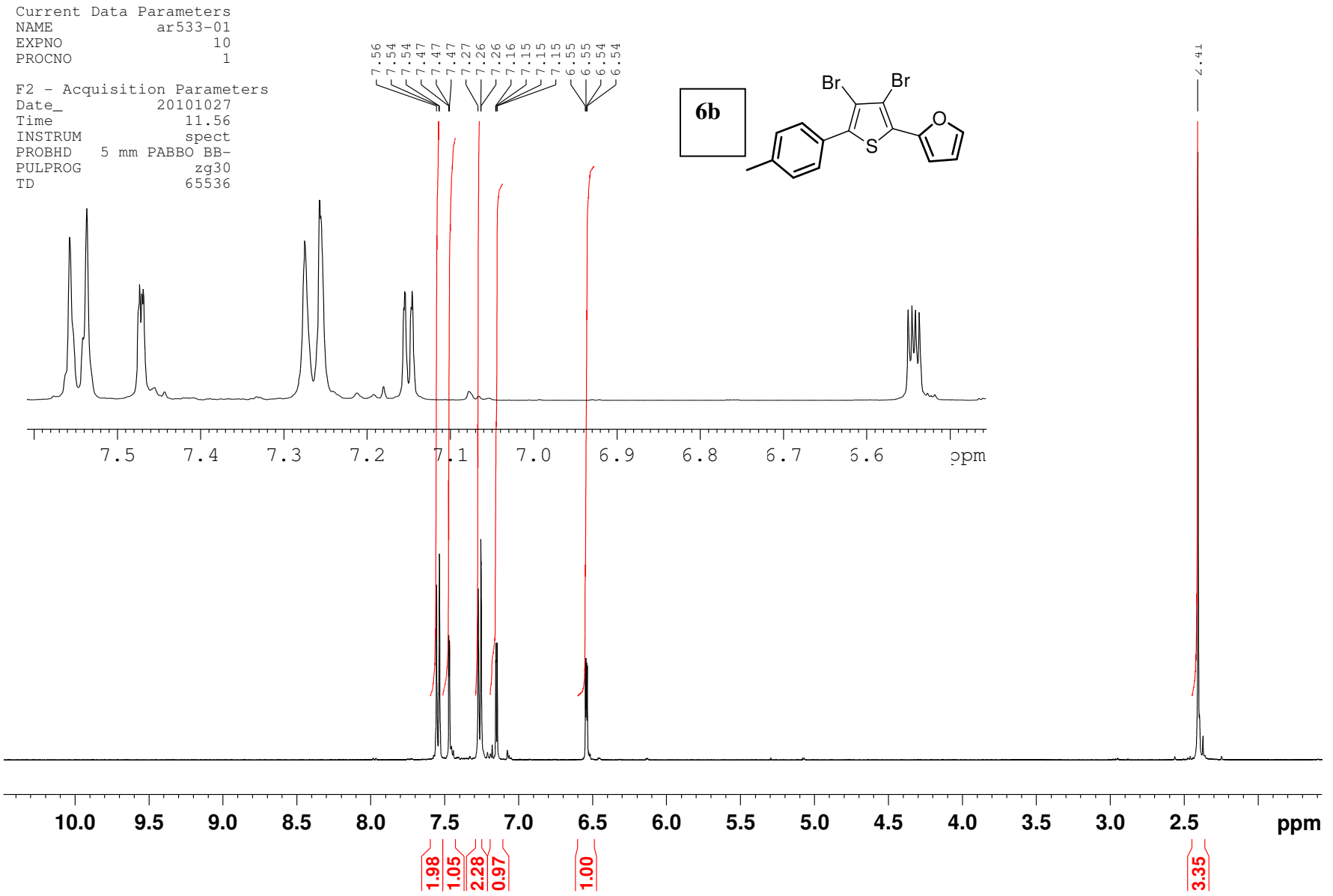

Current Data Parameters
NAME ar566-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110225
Time 13.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
138.5
138.2
132.8
129.7
129.6
128.6
126.2
112.1
77.4
77.0
76.7
21.5
138.454
138.182
139
ppm
129.668
129.617
130.0
ppm
Br
Br
S
5g
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

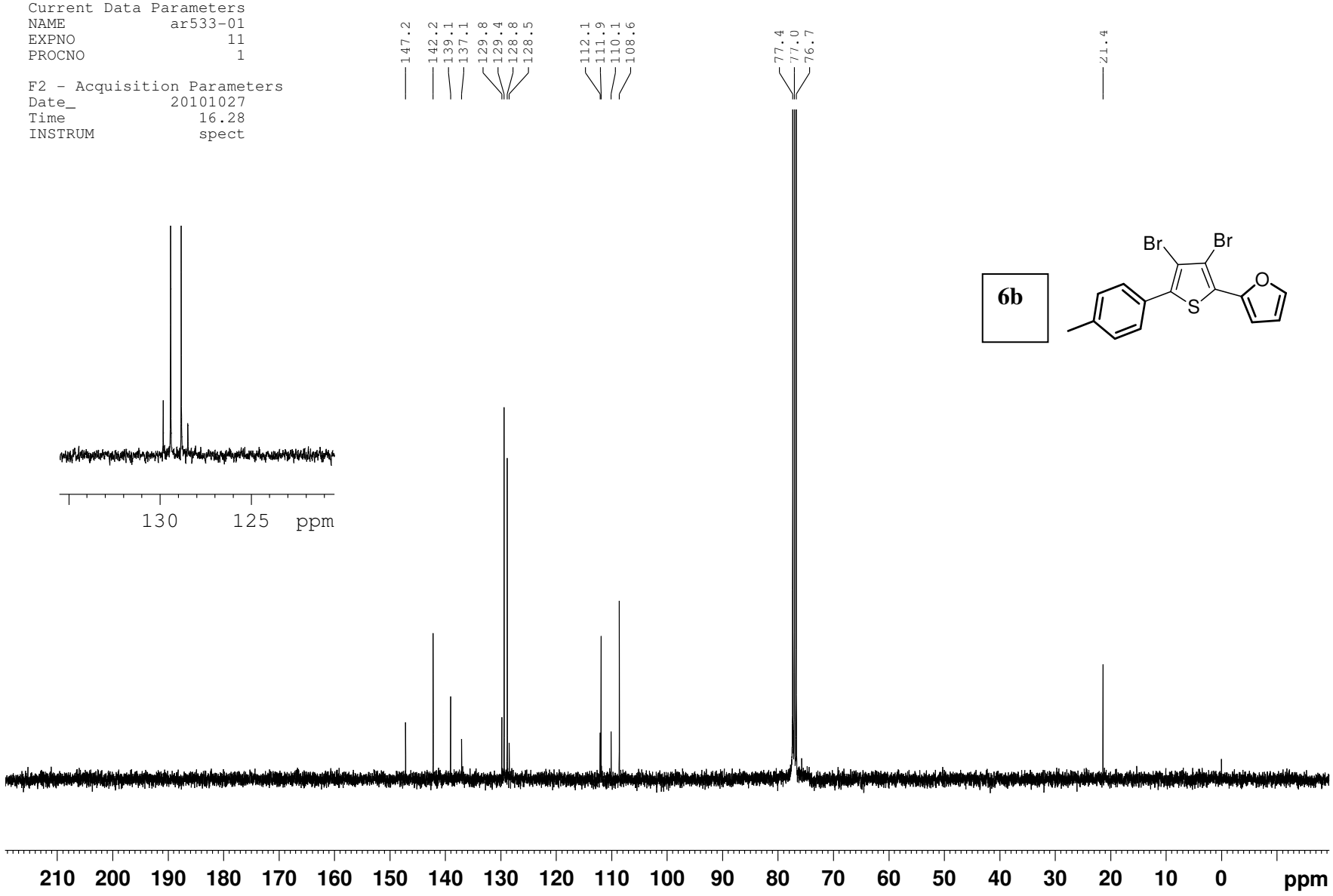

Current Data Parameters
NAME ar565-02
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110225
Time 15.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
Br
Br
S
5h
7.28
7.26
7.26
7.26
7.24
7.16
7.14
7.14
2.20
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.08
6.47

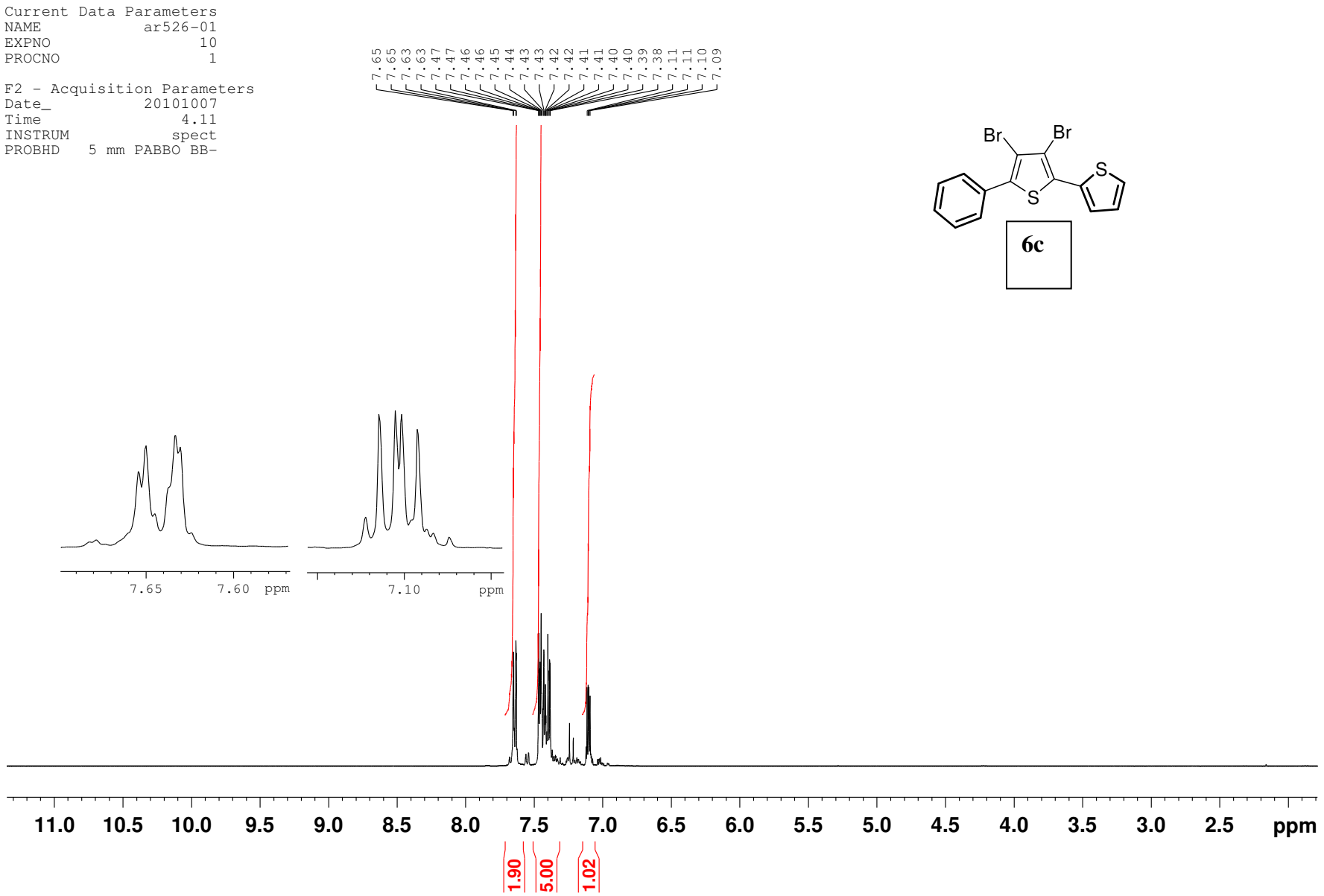

138.4
137.7
131.9
129.3
127.5
113.1
77.4
77.0
76.7
20.3
Current Data Parameters
NAME ar565-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110225
Time 16.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
Br
Br
S
5h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

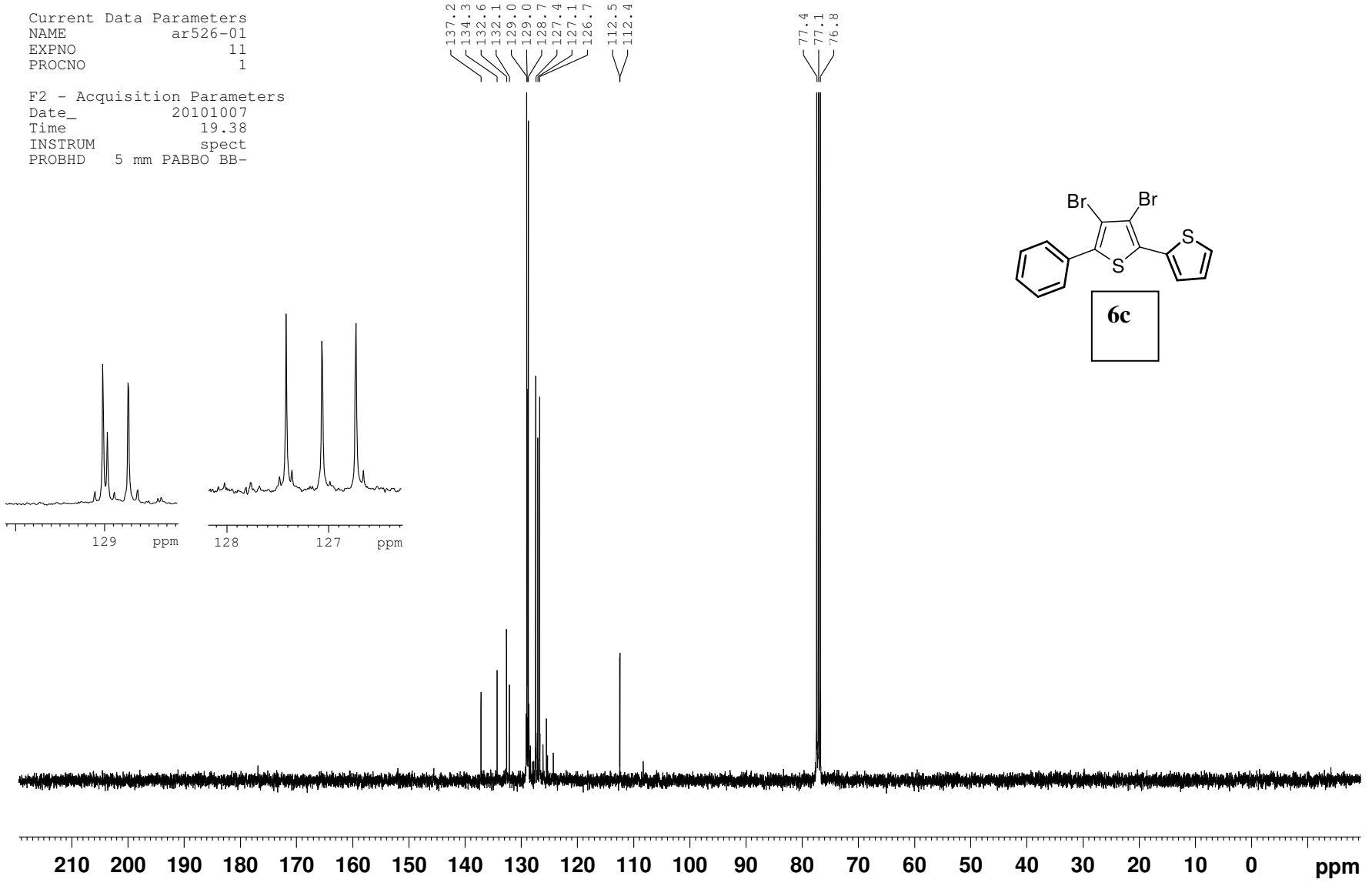

7.55
7.55
7.54
7.53
7.48
7.48
7.47
7.46
7.27
7.25
7.25
7.24
7.24
7.22
7.22
2.40
2.38
Br
Br
S
6a
Current Data Parameters
NAME ar486-02
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100805
Time 20.46
INSTRUM spect
7.6
7.4
7.2
ppm
3.0
2.5
2.0
ppm
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.94
2.14
4.17
6.00

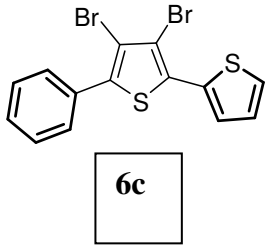

Current Data Parameters
NAME ar486-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100805
Time 20.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
138.9
138.3
137.9
136.7
130.1
129.5
129.4
128.9
126.8
111.9
77.4
77.1
76.7
21.4
21.1
Br
Br
S
6a
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Current Data Parameters
NAME ar533-01
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101027
Time 11.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
7.56 7.54 7.54 7.47 7.47 7.47 7.27 7.26 7.26 7.16 7.15 7.15 7.15 6.55 6.55 6.54 6.54
7.41
6b
Br
Br
S
O
7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 ppm
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
1.98
1.05
2.28
0.97
1.00
3.35


Current Data Parameters
NAME ar533-01
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101027
Time 16.28
INSTRUM spect
147.2
142.2
139.1
137.1
129.8
129.4
128.8
128.5
112.1
111.9
110.1
108.6
77.4
77.0
76.7
21.4
130
125
ppm
6b
Br
Br
O
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Current Data Parameters
NAME ar526-01
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101007
Time 4.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
7.65 7.65 7.63 7.63 7.47 7.47 7.46 7.46 7.45 7.44 7.43 7.43 7.42 7.42 7.41 7.41 7.40 7.40 7.39 7.38 7.11 7.11 7.10 7.09
Br
Br
S
S
6c
7.65 7.60 ppm
7.10 ppm
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
1.90
5.00
1.02


Current Data Parameters
NAME ar526-01
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101007
Time 19.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
137.2
134.3
132.6
132.1
129.0
129.0
128.7
127.4
127.1
126.7
112.5
112.4
77.4
77.1
76.8
Br
Br
S
S
6c
129
ppm
128
127
ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

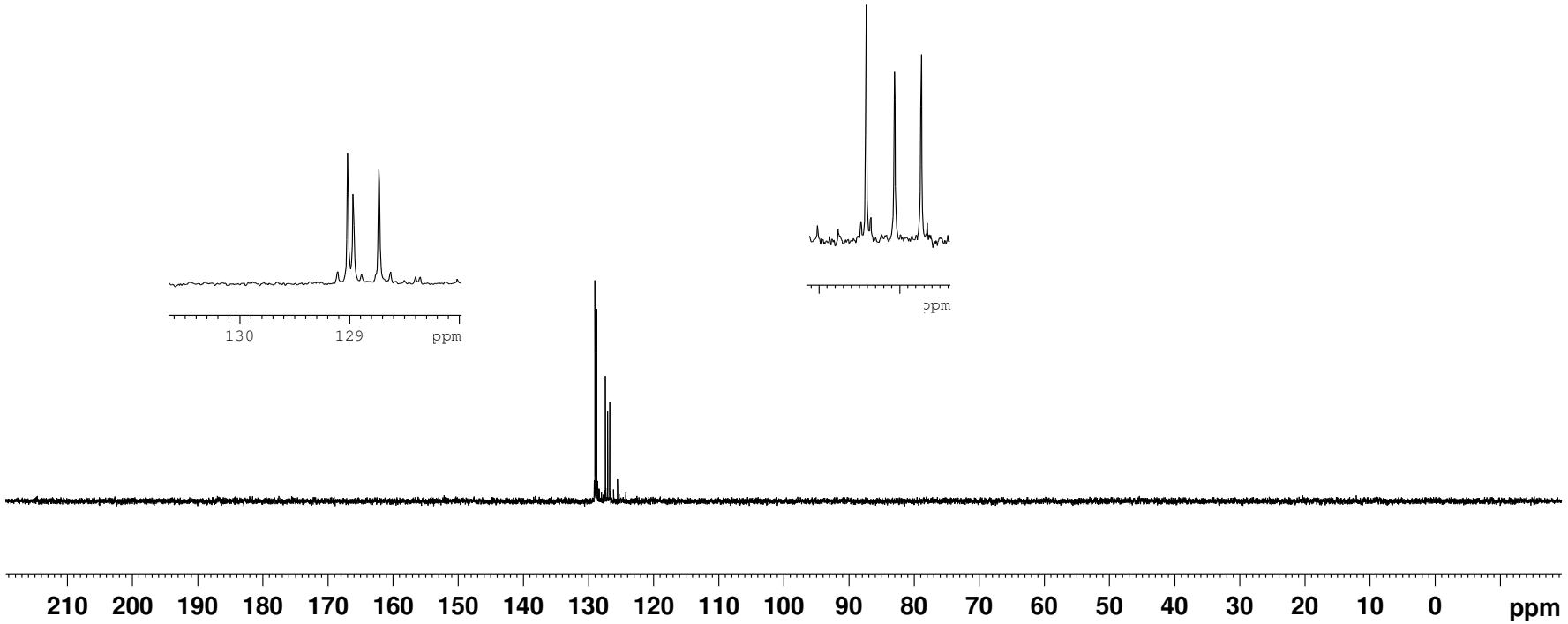


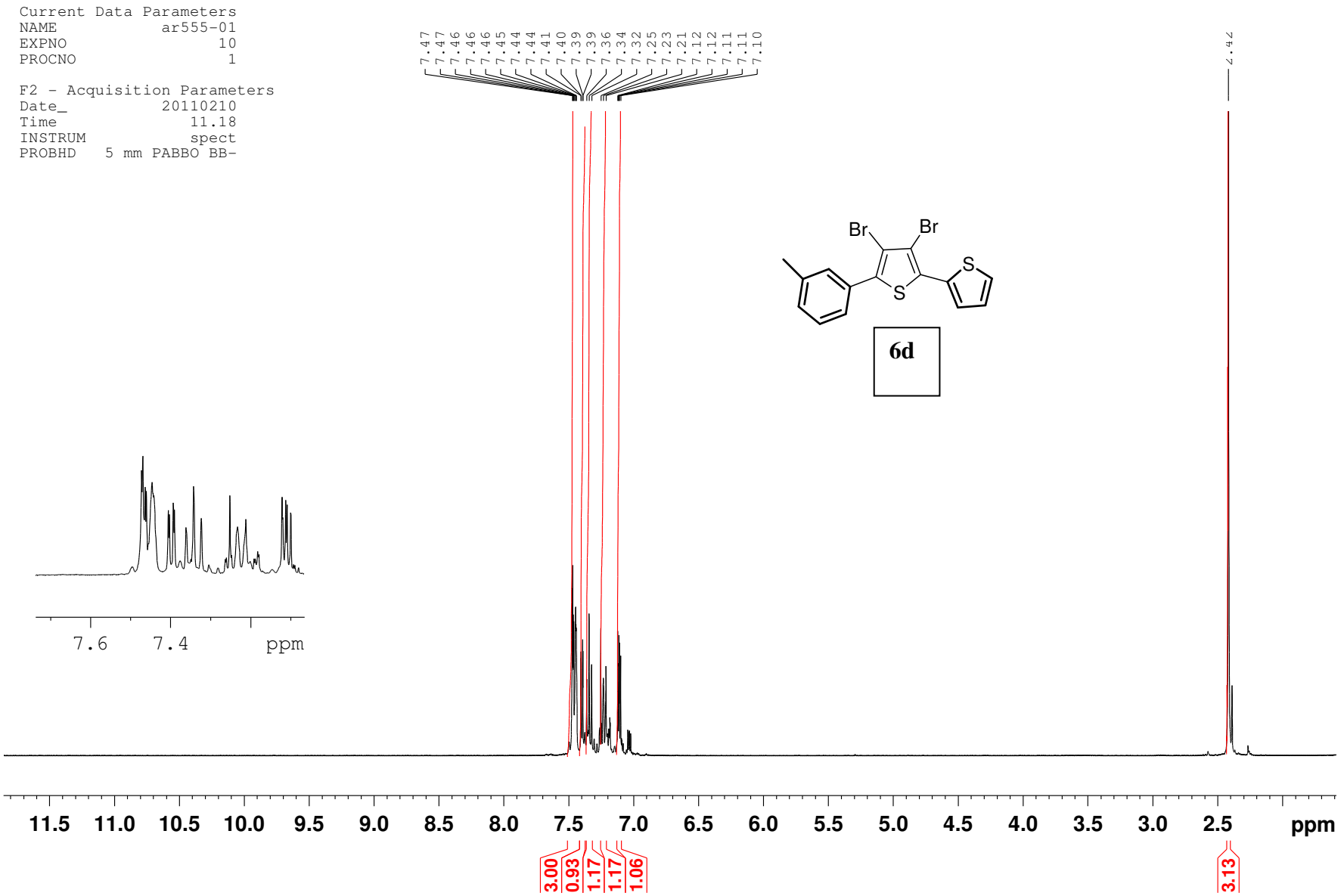
6c

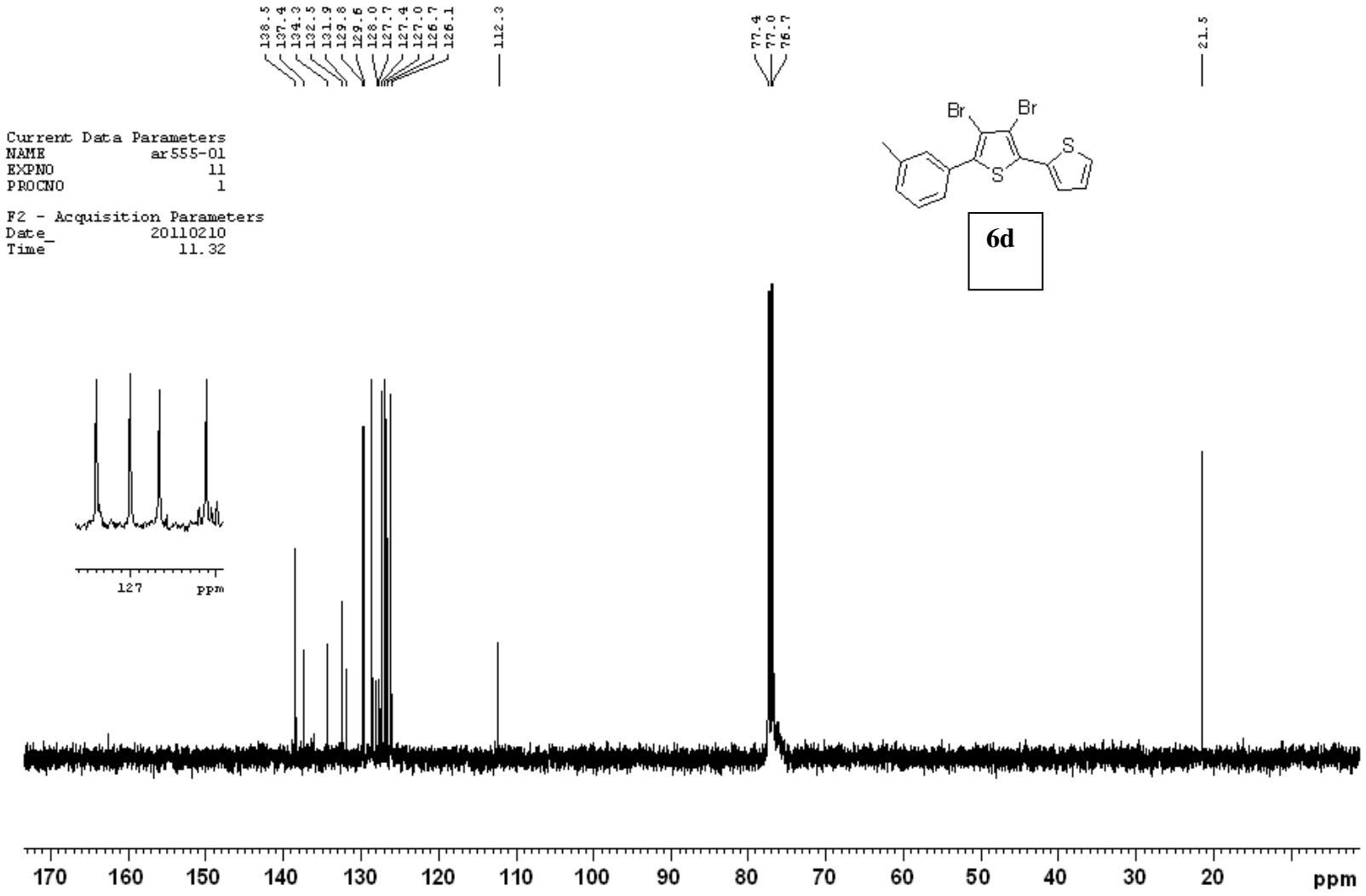
129.0
129.0
128.7
127.4
127.1
126.7

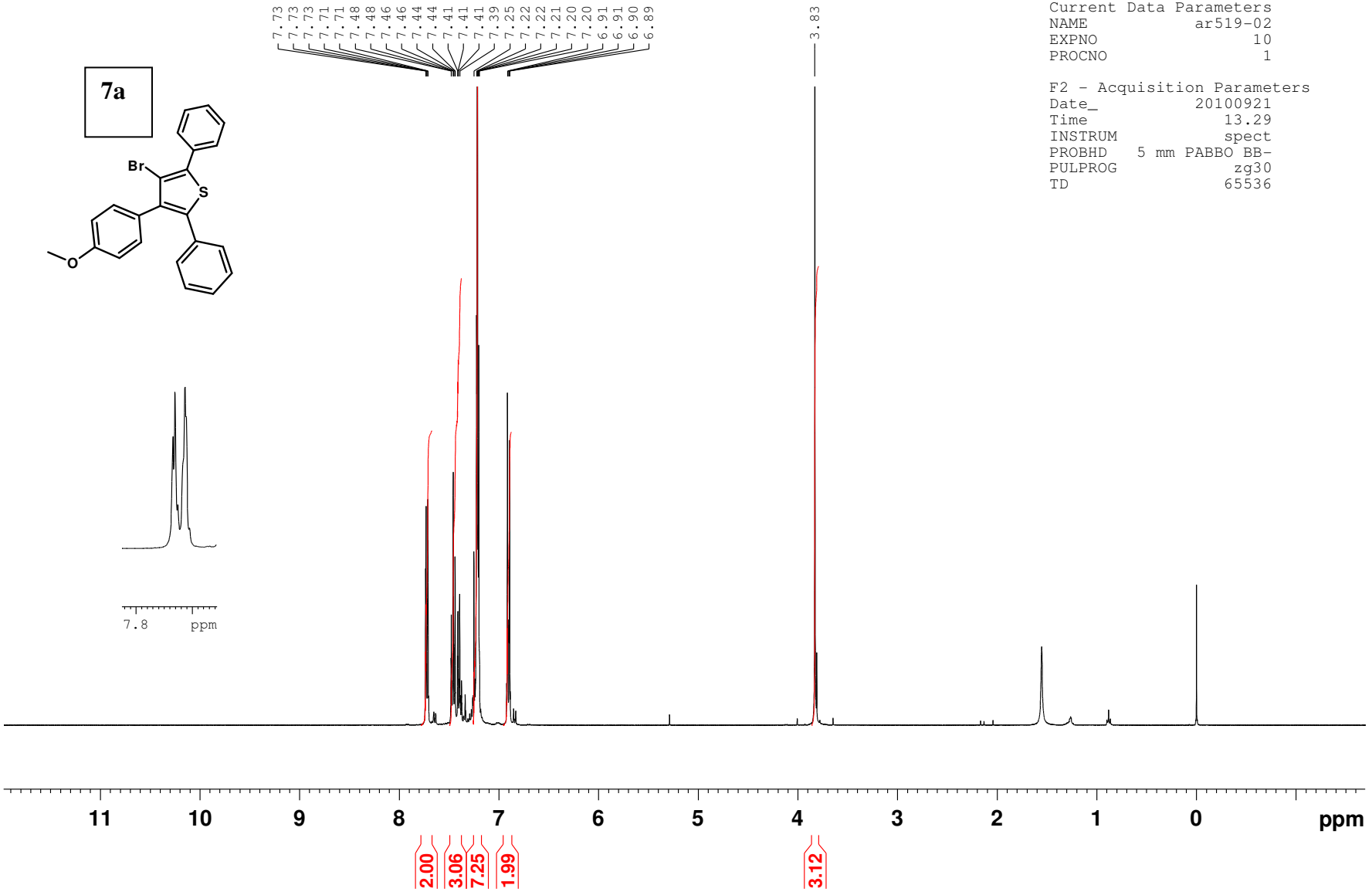
```
Current Data Parameters
NAME            ar526-01
EXPNO                 12
PROCNO                 1

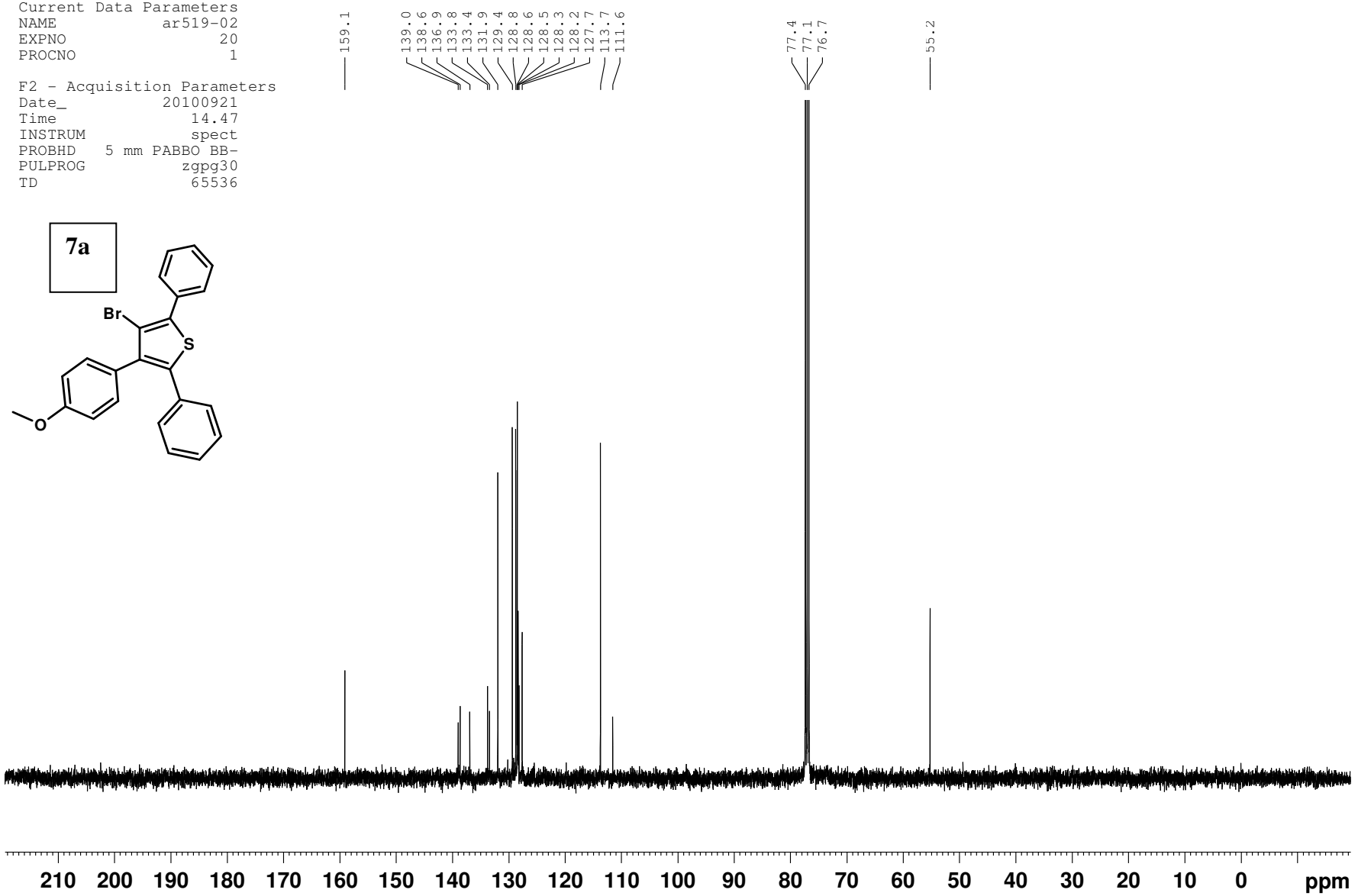
F2 - Acquisition Parameters
Date_           20101007
Time               19.50
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          dept135
TD                 65536
SOLVENT            CDCl3
NS                   256
```




Current Data Parameters
NAME ar555-01
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110210
Time 11.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
7.47 7.47 7.46 7.46 7.46 7.45 7.44 7.44 7.41 7.40 7.39 7.39 7.36 7.34 7.32 7.25 7.23 7.21 7.12 7.11 7.11 7.10
7.44
Br
Br
S
S
6d
7.6
7.4
ppm
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
3.00
0.93
1.17
1.17
1.06
3.13


138.5
137.4
134.3
132.5
131.9
129.8
129.6
128.0
127.7
127.4
127.0
126.7
126.1
112.3
77.4
77.0
76.7
21.5
Current Data Parameters
NAME ar555-01
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110210
Time 11.32
Br
Br
S
S
6d
127
ppm
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7a
Br
S
O
7.8
ppm
7.73
7.73
7.73
7.71
7.71
7.48
7.48
7.46
7.46
7.44
7.44
7.41
7.41
7.41
7.39
7.25
7.22
7.22
7.21
7.20
7.20
6.91
6.91
6.90
6.89
3.83
Current Data Parameters
NAME ar519-02
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100921
Time 13.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.06
7.25
1.99
3.12

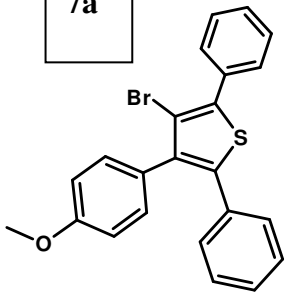

Current Data Parameters
NAME ar519-02
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100921
Time 14.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
159.1
139.0
138.6
136.9
133.8
133.4
131.9
129.4
128.8
128.6
128.5
128.3
128.2
127.7
113.7
111.6
77.4
77.1
76.7
55.2
7a
Br
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

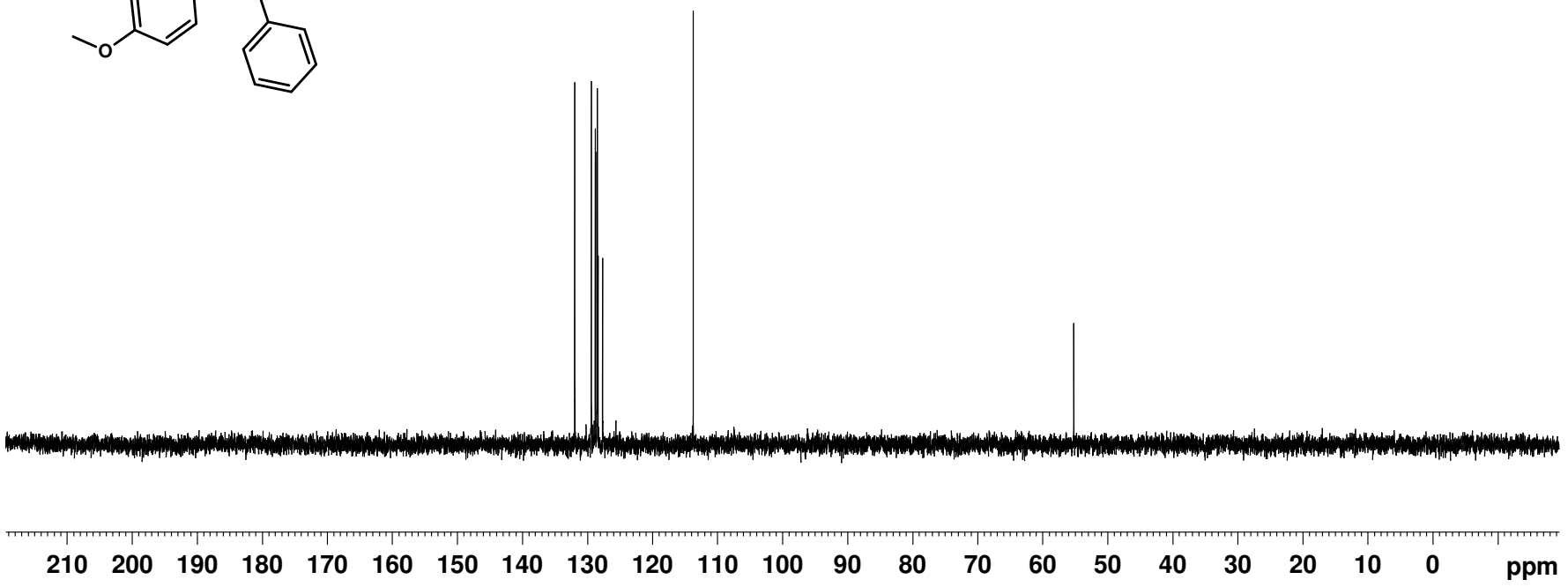
```
Current Data Parameters
NAME           ar519-02
EXPNO                21
PROCNO                1

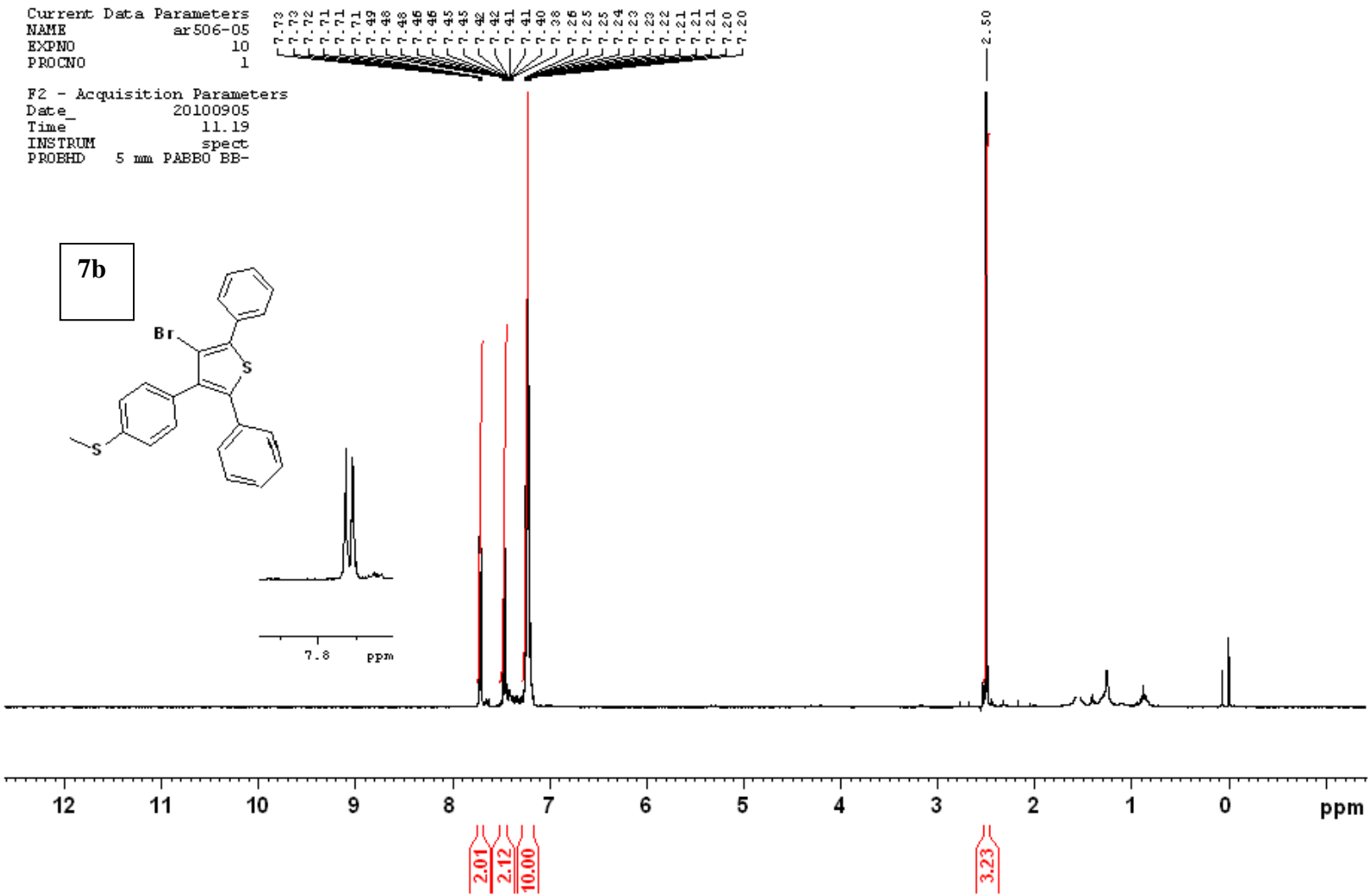
F2 - Acquisition Parameters
Date_          20100921
Time              14.58
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         dept135
TD                65536
```

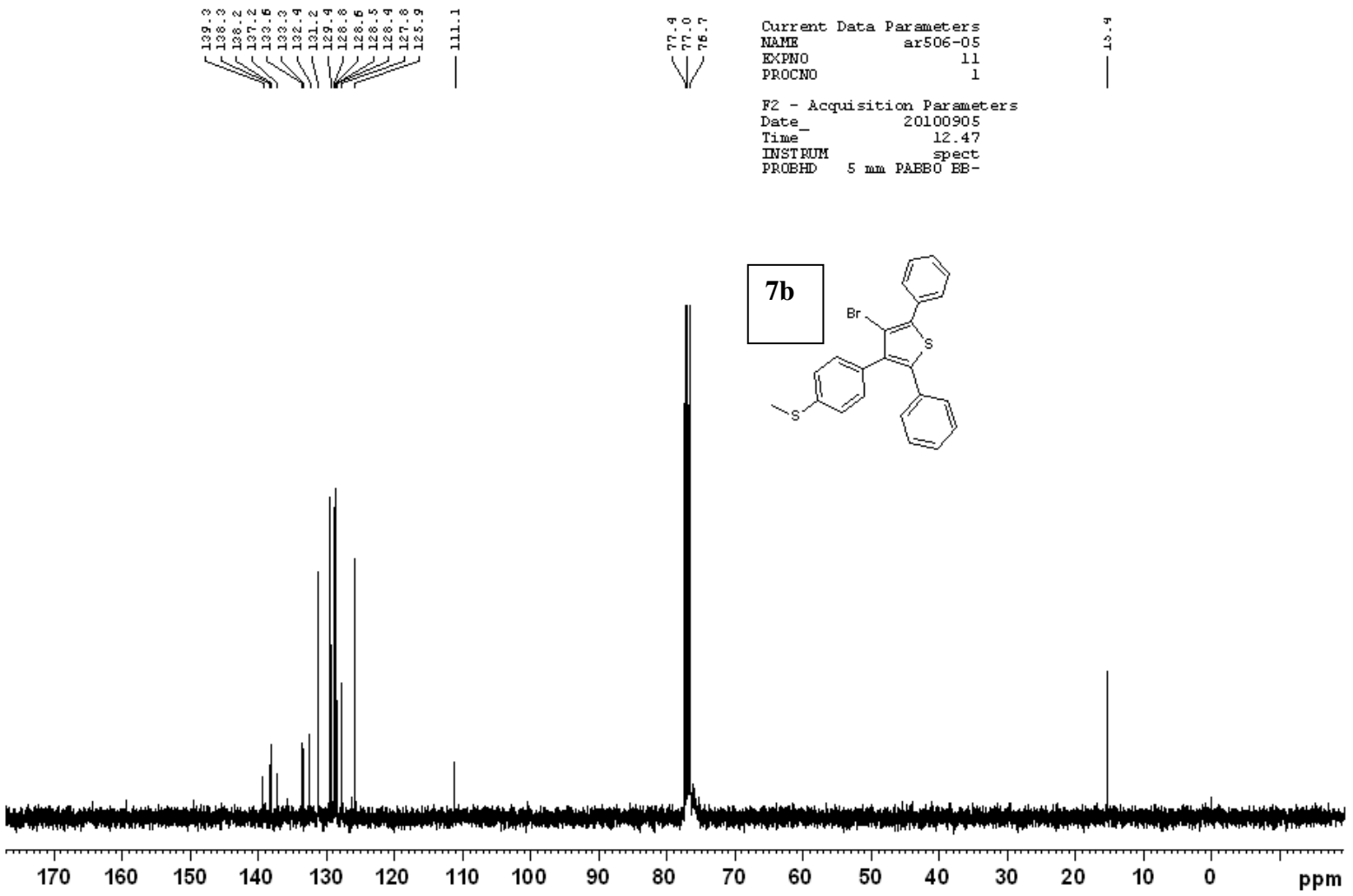
131.9
129.4
128.8
128.6
128.5
128.3
127.7
113.7
55.2

7a






Current Data Parameters
NAME ar506-05
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100905
Time 11.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
7b
Br
S
S
7.8
ppm
2.50
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.12
10.00
3.23


139.3
138.3
138.2
137.2
133.6
133.3
132.4
131.2
129.4
128.8
128.6
128.5
128.4
127.8
125.9
111.1
77.4
77.0
76.7
15.4
Current Data Parameters
NAME ar506-05
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100905
Time 12.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
7b
Br
S
S
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

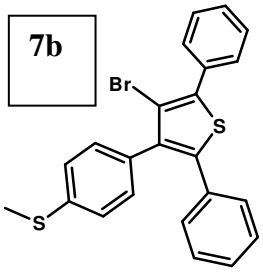
```
Current Data Parameters
NAME           ar506-05
EXPNO                12
PROCNO                1

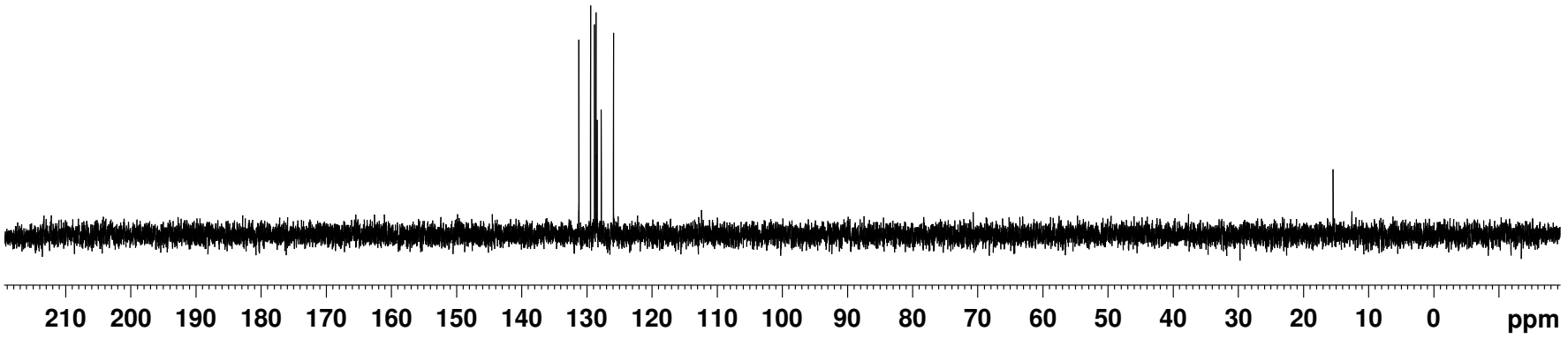
F2 - Acquisition Parameters
Date_          20100905
Time              12.58
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         dept135
TD                65536
SOLVENT           CDCl3
NS                  256
```

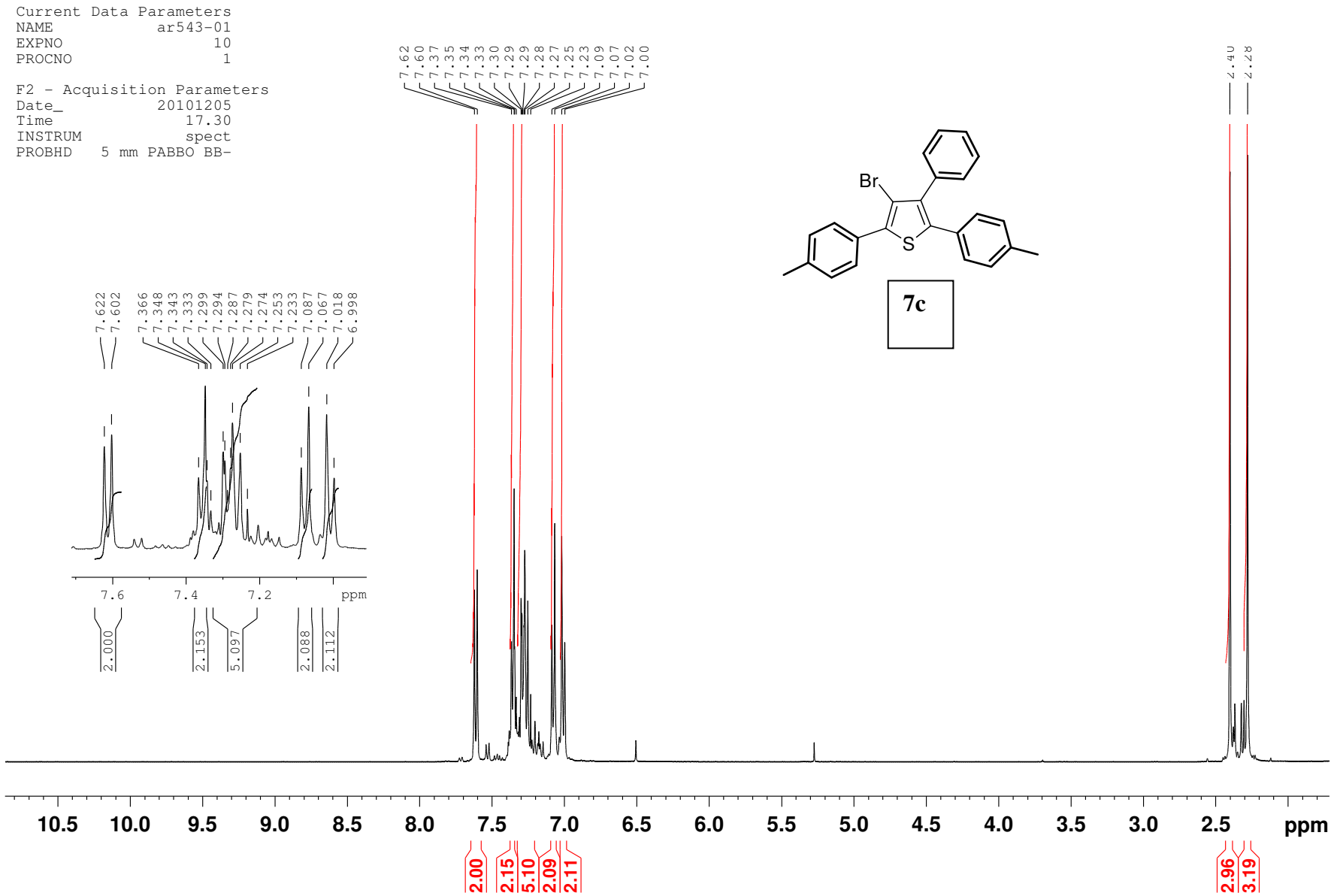
131.2
129.4
128.8
128.6
128.5
128.4
127.8
125.9

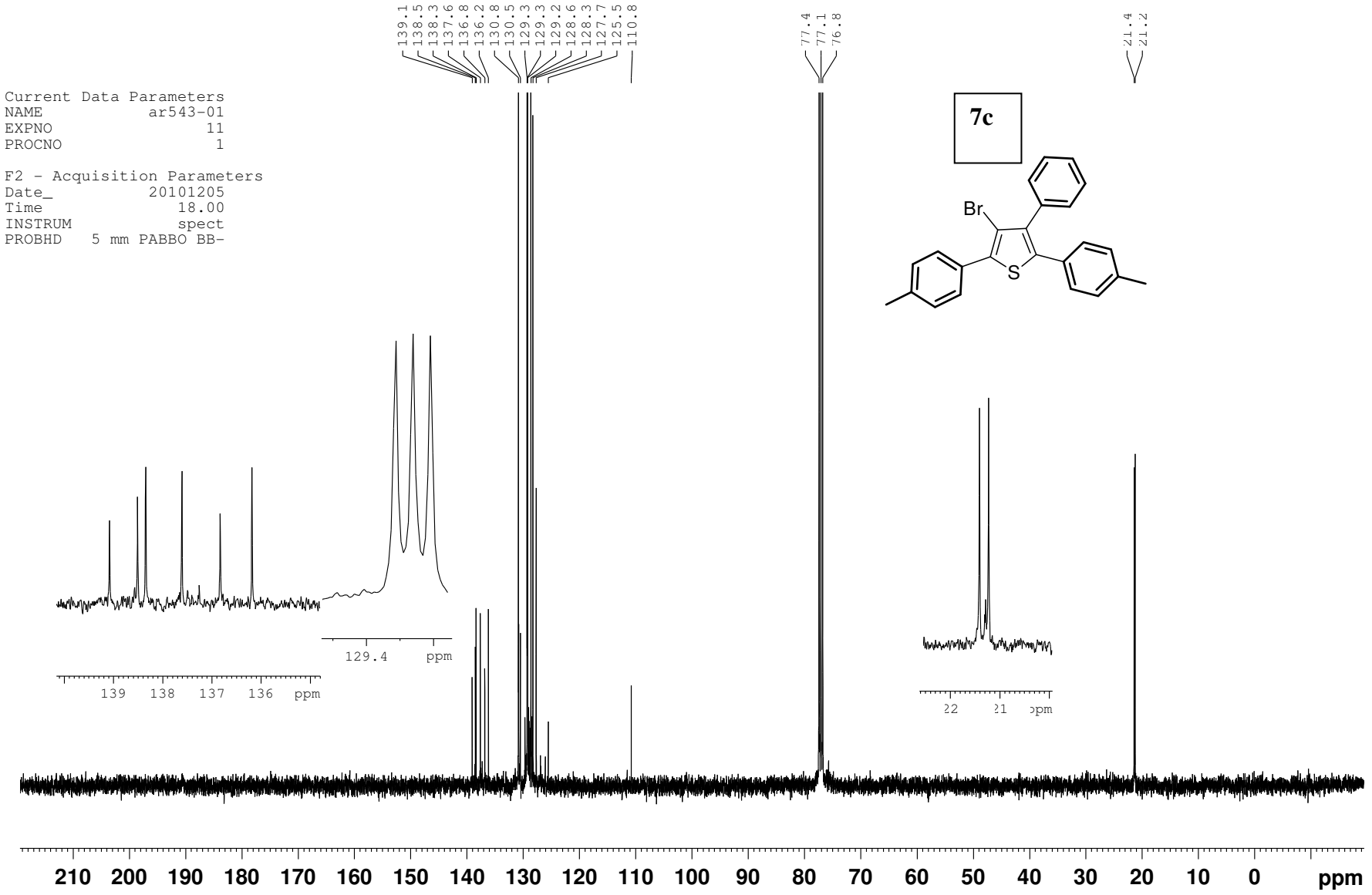
15.4

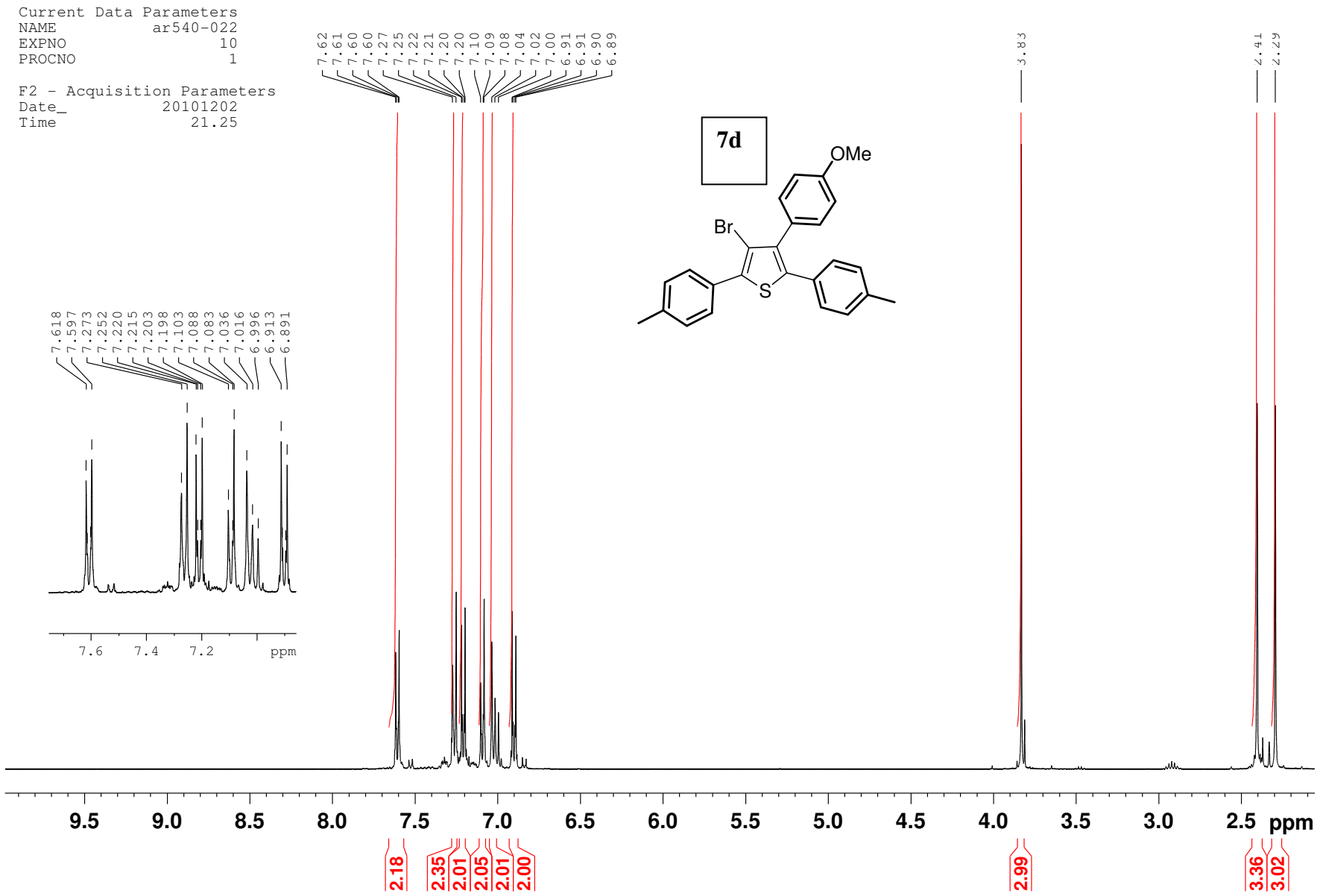
7b

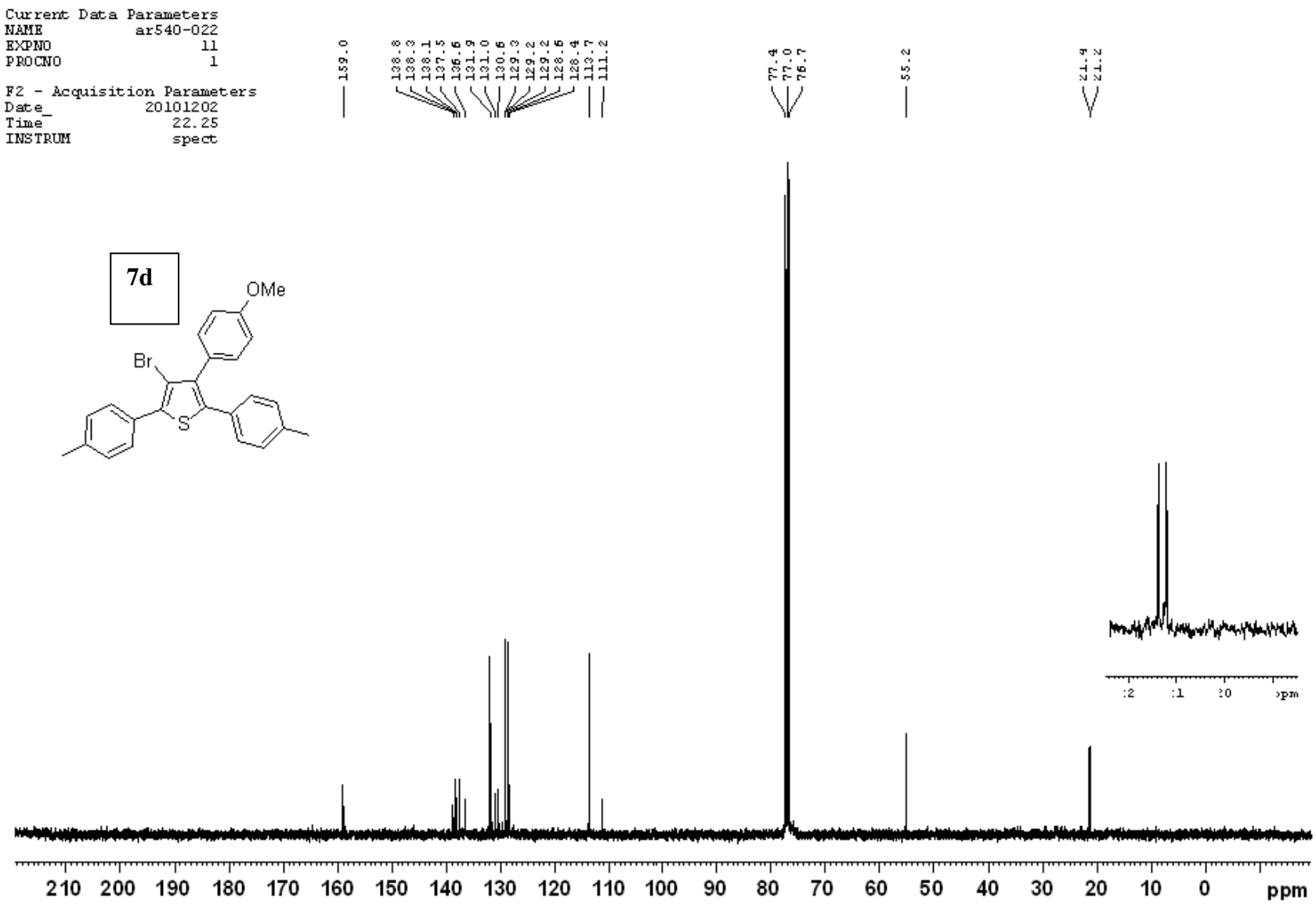




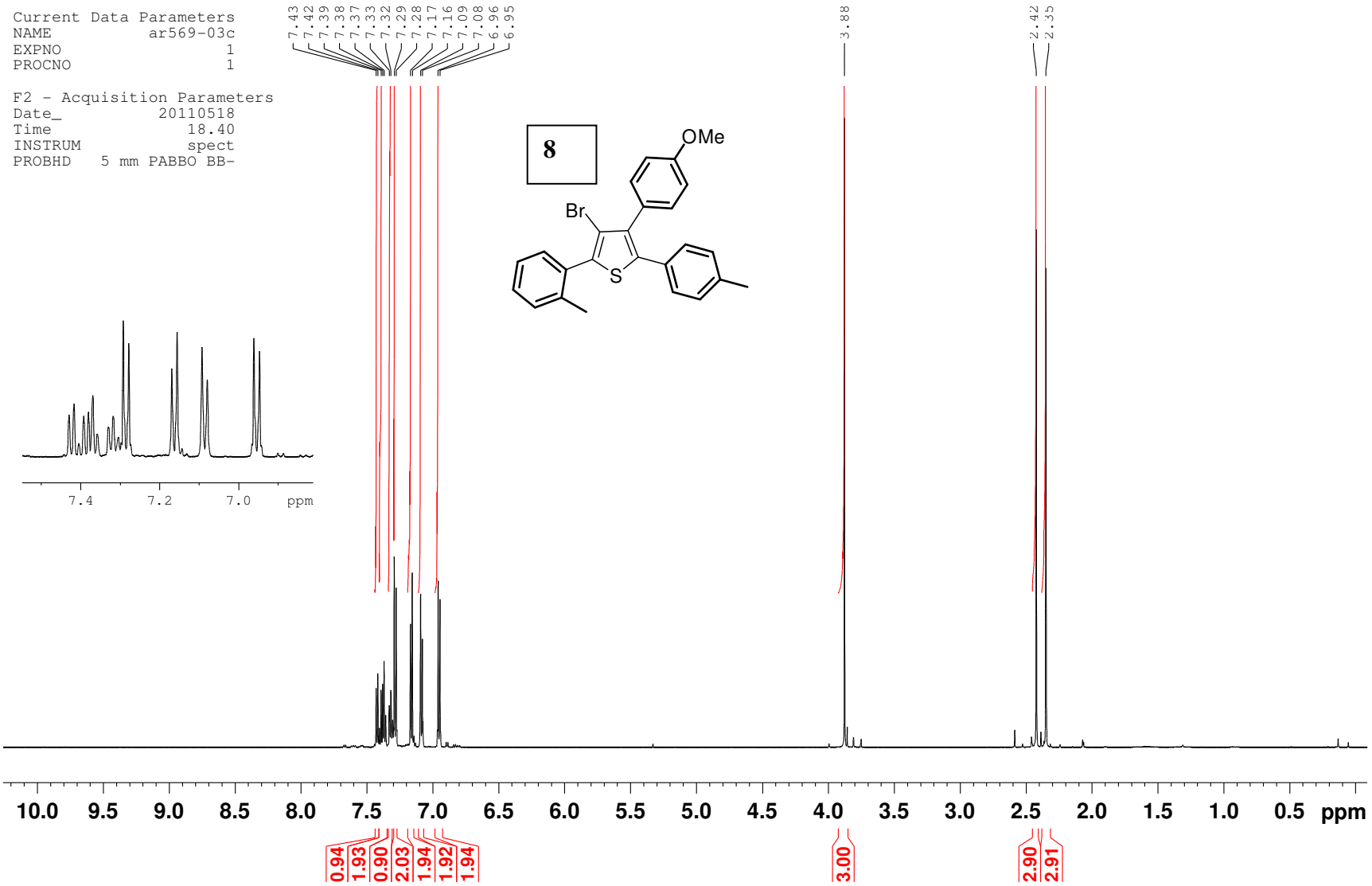

Current Data Parameters
NAME ar543-01
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101205
Time 17.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
7.62 7.60 7.37 7.35 7.34 7.33 7.30 7.29 7.29 7.28 7.27 7.25 7.23 7.09 7.07 7.02 7.00
2.40 2.28
Br
S
7c
7.622 7.602 7.366 7.348 7.343 7.333 7.299 7.294 7.287 7.279 7.274 7.253 7.233 7.087 7.067 7.018 6.998
7.6 7.4 7.2 ppm
2.000 2.153 5.097 2.088 2.112
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
2.00 2.15 5.10 2.09 2.11
2.96 3.19

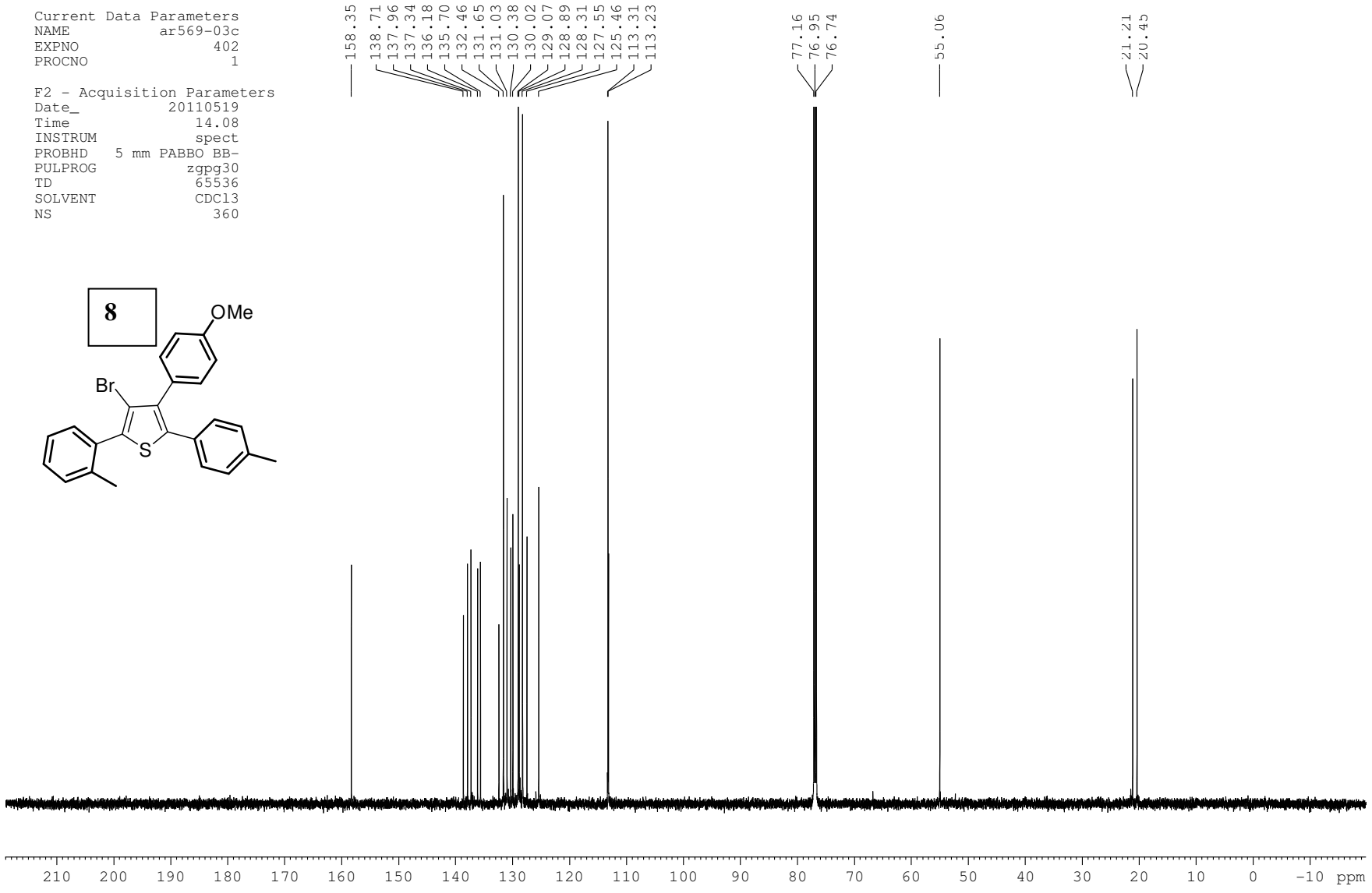

Current Data Parameters
NAME ar543-01
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101205
Time 18.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
139.1
138.5
138.3
137.6
136.8
136.2
130.8
130.5
129.3
129.3
129.2
128.6
128.3
127.7
125.5
110.8
77.4
77.1
76.8
21.4
21.2
7c
Br
S
129.4 ppm
139 138 137 136 ppm
22 21 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

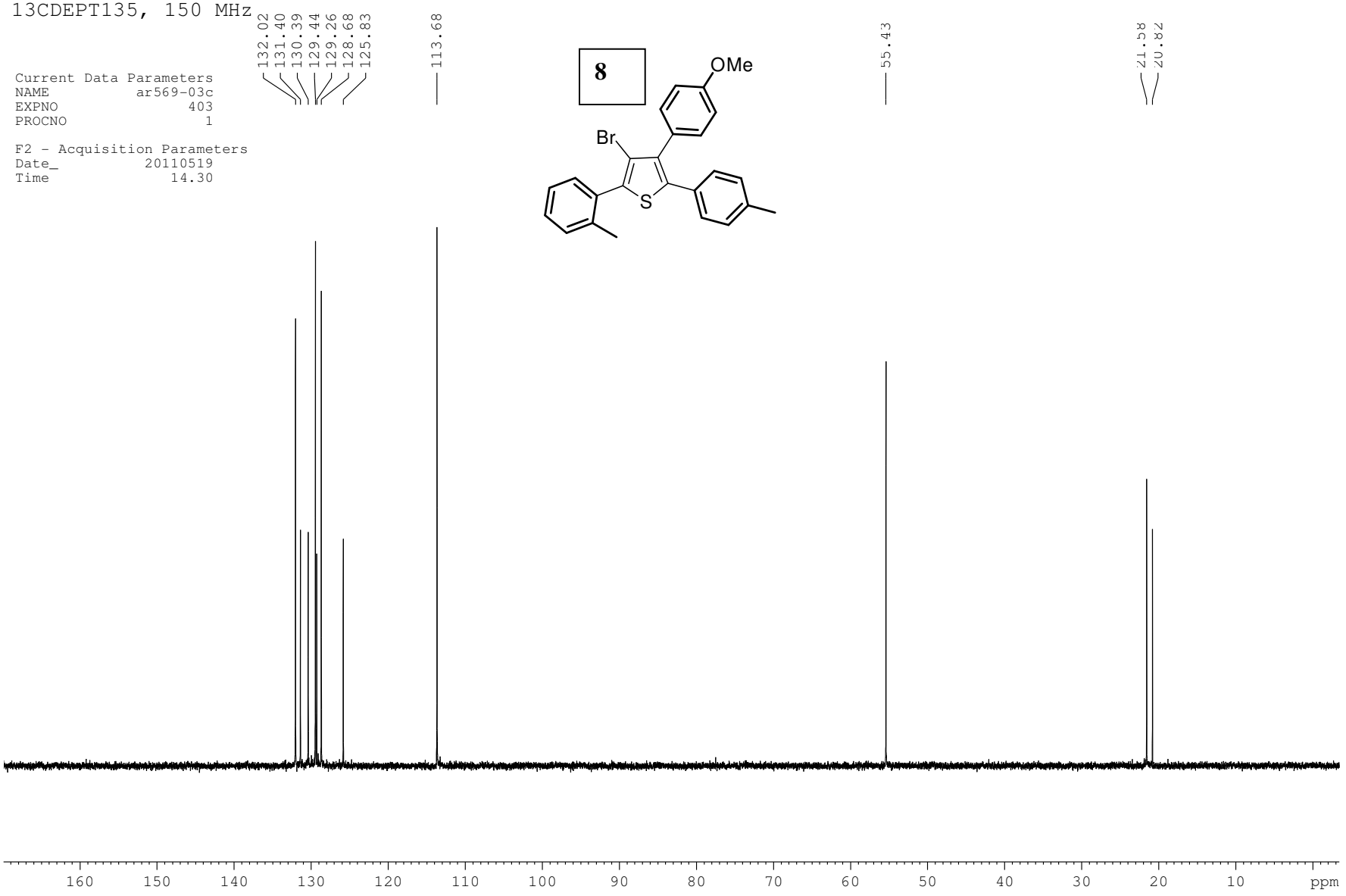

Current Data Parameters
NAME ar540-022
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101202
Time 21.25
7.62
7.61
7.60
7.60
7.27
7.25
7.22
7.21
7.20
7.20
7.10
7.09
7.08
7.04
7.02
7.00
6.91
6.91
6.90
6.89
3.83
2.41
2.29
7d
OMe
Br
S
7.618
7.597
7.273
7.252
7.220
7.215
7.203
7.198
7.103
7.088
7.083
7.036
7.016
6.996
6.913
6.891
7.6
7.4
7.2
ppm
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
ppm
2.18
2.35
2.01
2.05
2.01
2.00
2.99
3.36
3.02

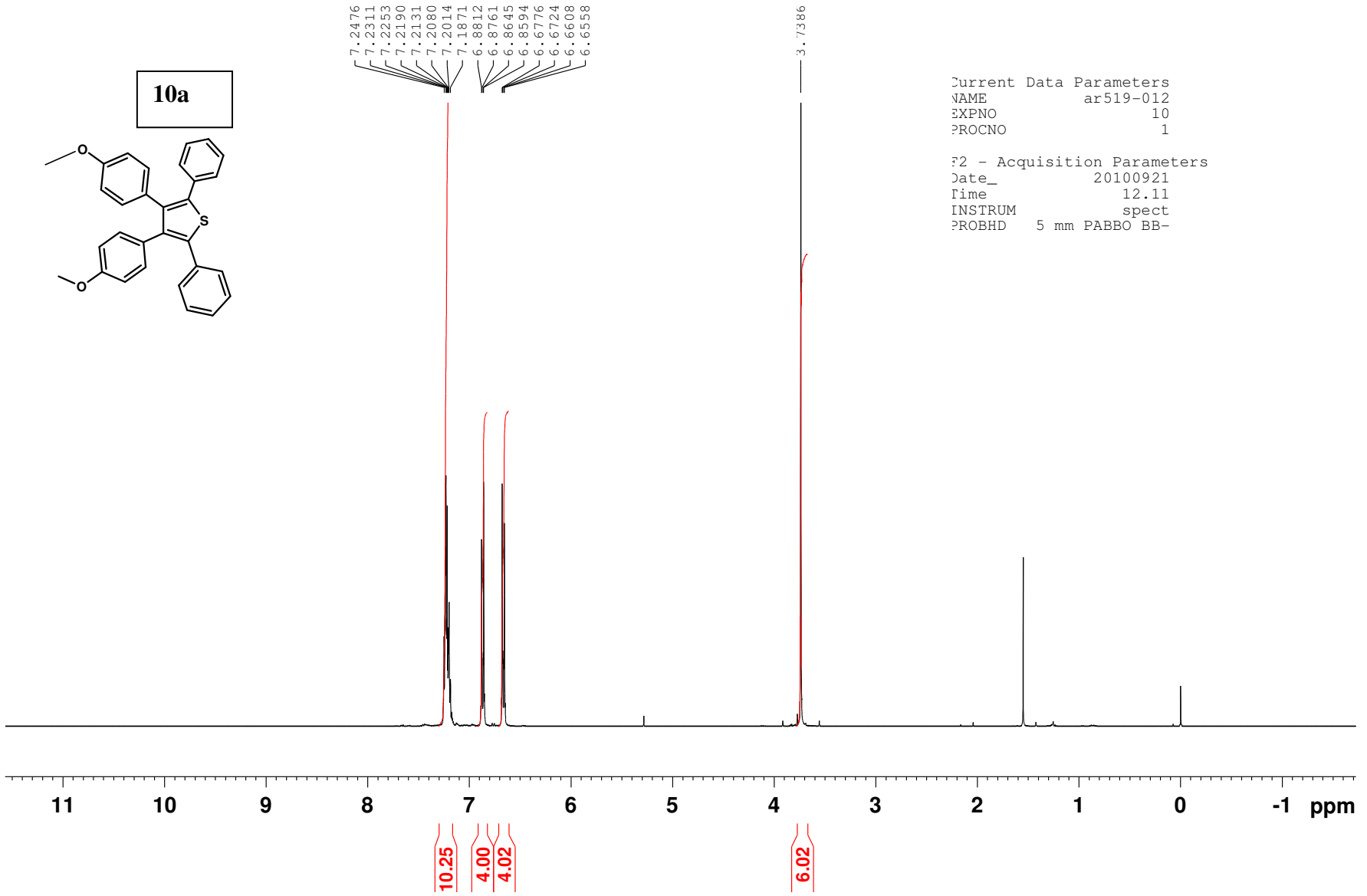

Current Data Parameters
NAME ar540-022
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101202
Time 22.25
INSTRUM spect
159.0
138.8
138.3
138.1
137.5
136.6
131.9
131.0
130.6
129.3
129.2
129.2
128.6
128.4
113.7
111.2
77.4
77.0
76.7
55.2
21.4
21.2
7d
OMe
Br
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

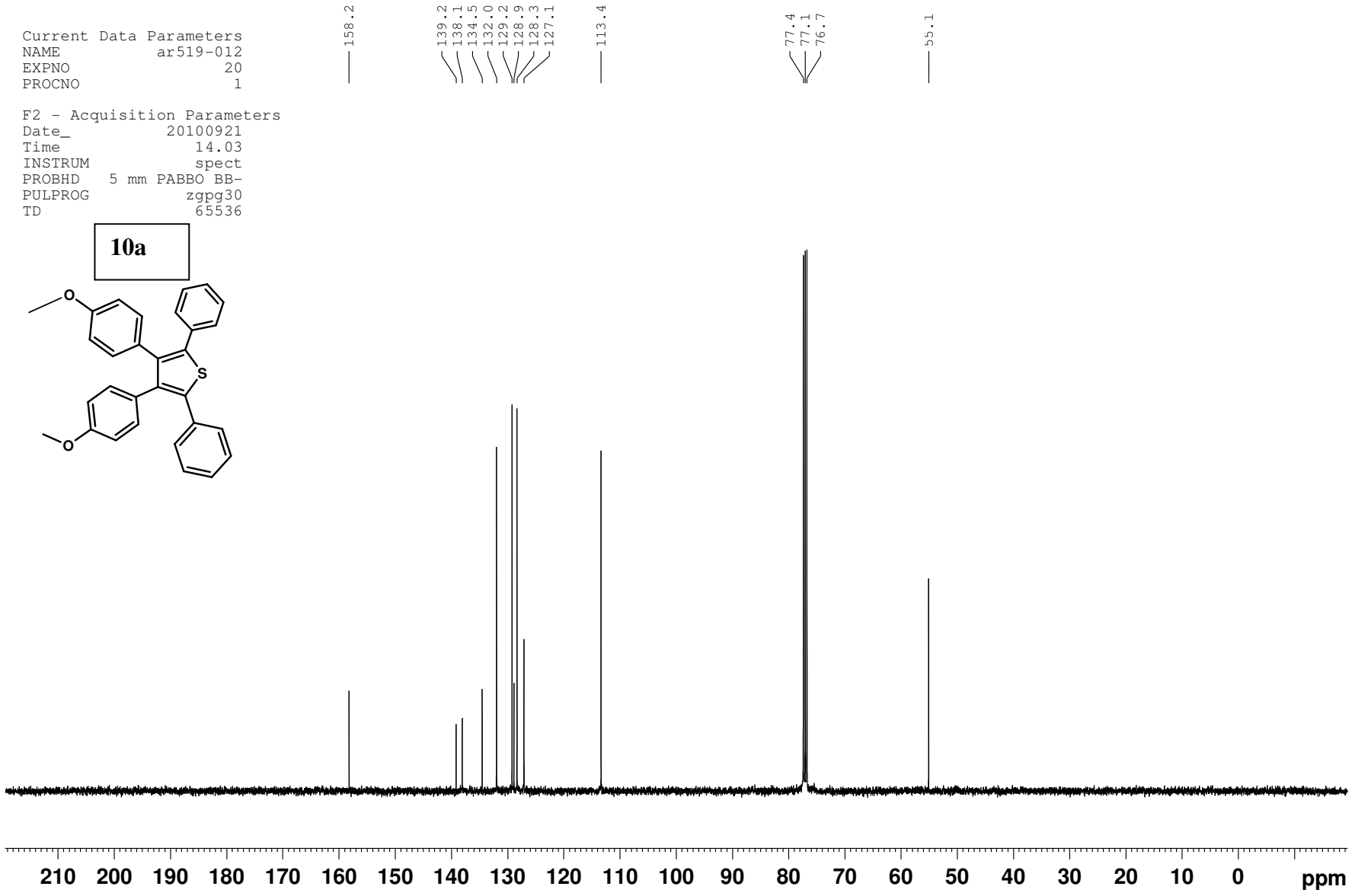
1H-NMR@23°C


Current Data Parameters
NAME ar569-03c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110518
Time 18.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
7.43
7.42
7.39
7.38
7.37
7.33
7.32
7.29
7.28
7.17
7.16
7.09
7.08
6.96
6.95
3.88
2.42
2.35
8
OMe
Br
S
7.4
7.2
7.0
ppm
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.94
1.93
0.90
2.03
1.94
1.92
1.94
3.00
2.90
2.91


Current Data Parameters
NAME ar569-03c
EXPNO 402
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110519
Time 14.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 360
158.35
138.71
137.96
137.34
136.18
135.70
132.46
131.65
131.03
130.38
130.02
129.07
128.89
128.31
127.55
125.46
113.31
113.23
77.16
76.95
76.74
55.06
21.21
20.45
8
OMe
Br
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


13CDEPT135, 150 MHz
132.02
131.40
130.39
129.44
129.26
128.68
125.83
113.68
55.43
21.58
20.82
Current Data Parameters
NAME ar569-03c
EXPNO 403
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110519
Time 14.30
8
OMe
Br
S
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

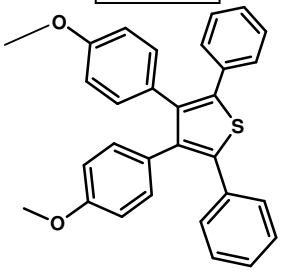

10a
7.2476
7.2311
7.2253
7.2190
7.2131
7.2080
7.2014
7.1871
6.8812
6.8761
6.8645
6.8594
6.6776
6.6724
6.6608
6.6558
3.7386
Current Data Parameters
NAME ar519-012
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100921
Time 12.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
10.25
4.00
4.02
6.02

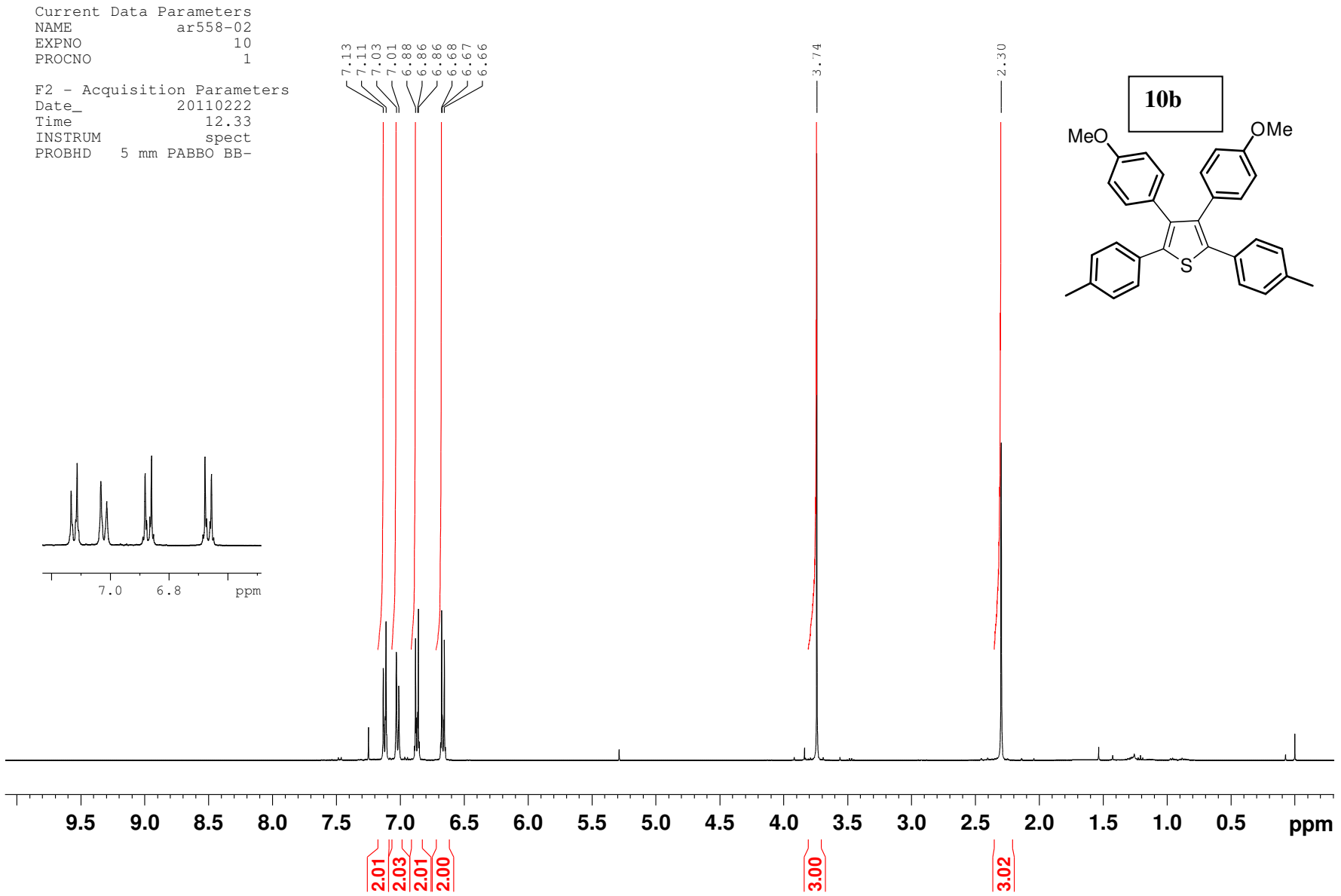

158.2
139.2
138.1
134.5
132.0
129.2
128.9
128.3
127.1
113.4
77.4
77.1
76.7
55.1
Current Data Parameters
NAME ar519-012
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100921
Time 14.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
10a
O
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

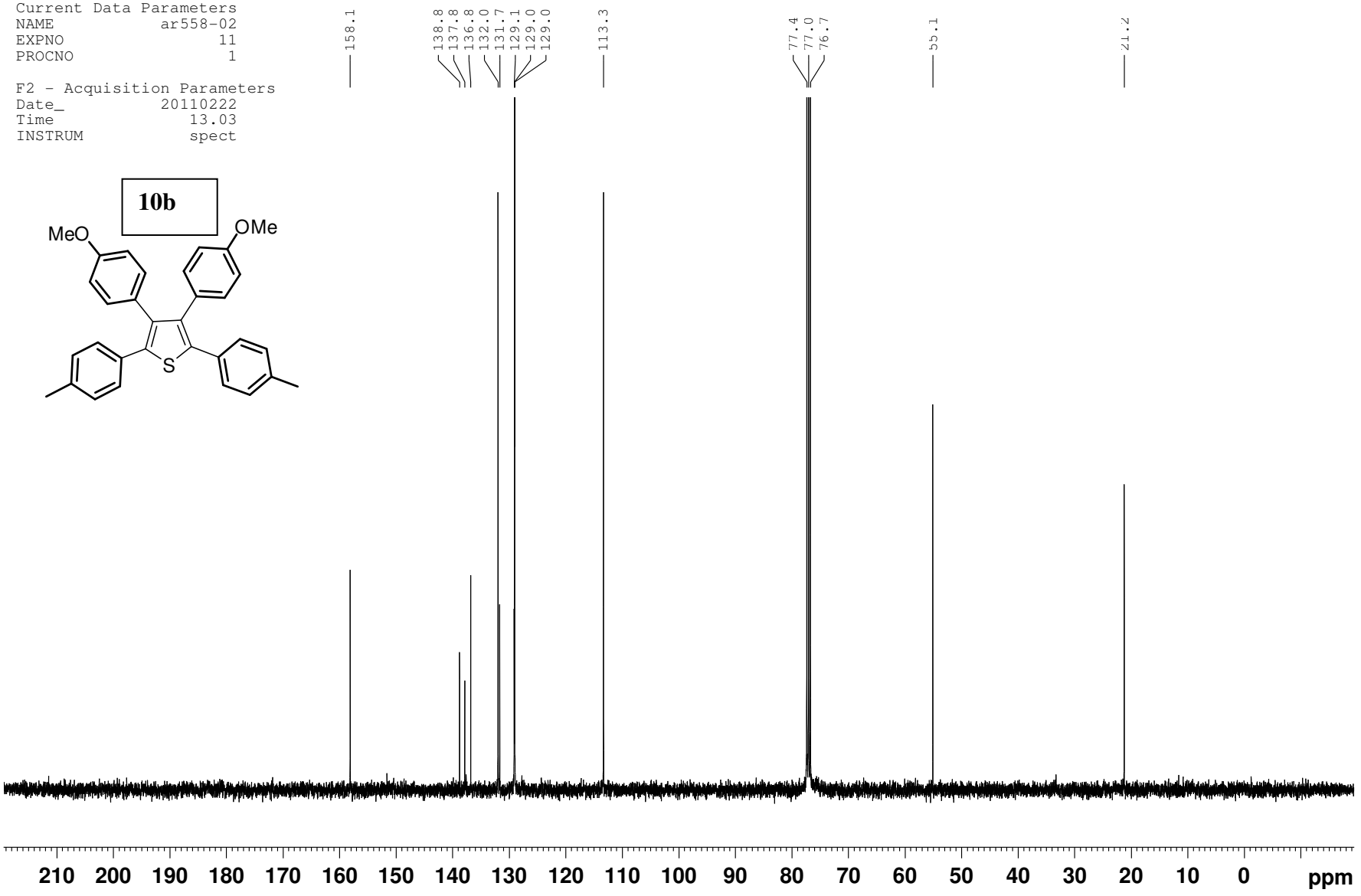
Current Data Parameters
NAME ar519-012
EXPNO 21
PROCNO 1

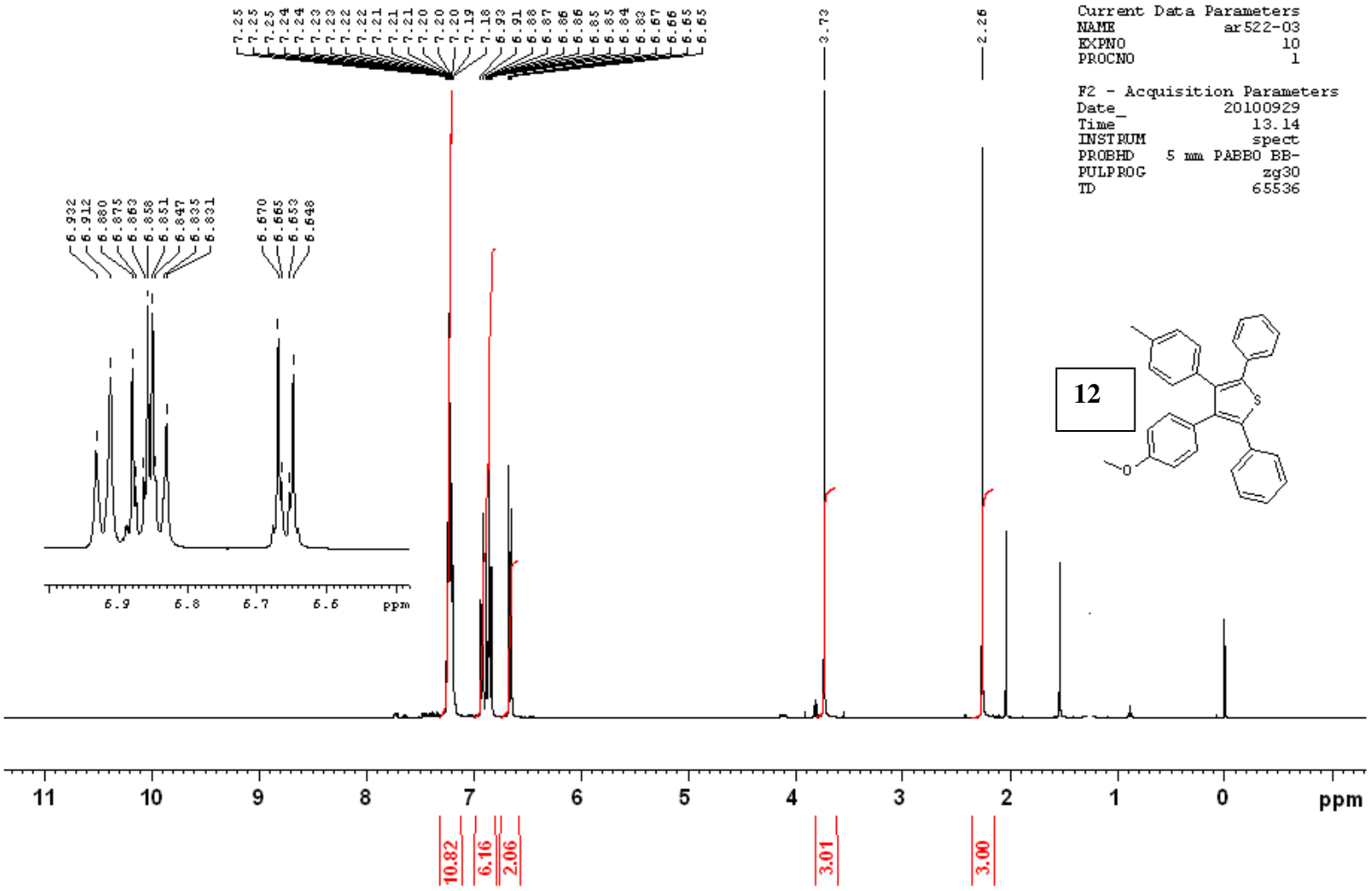
F2 - Acquisition Parameters
Date_ 20100921
Time 14.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135

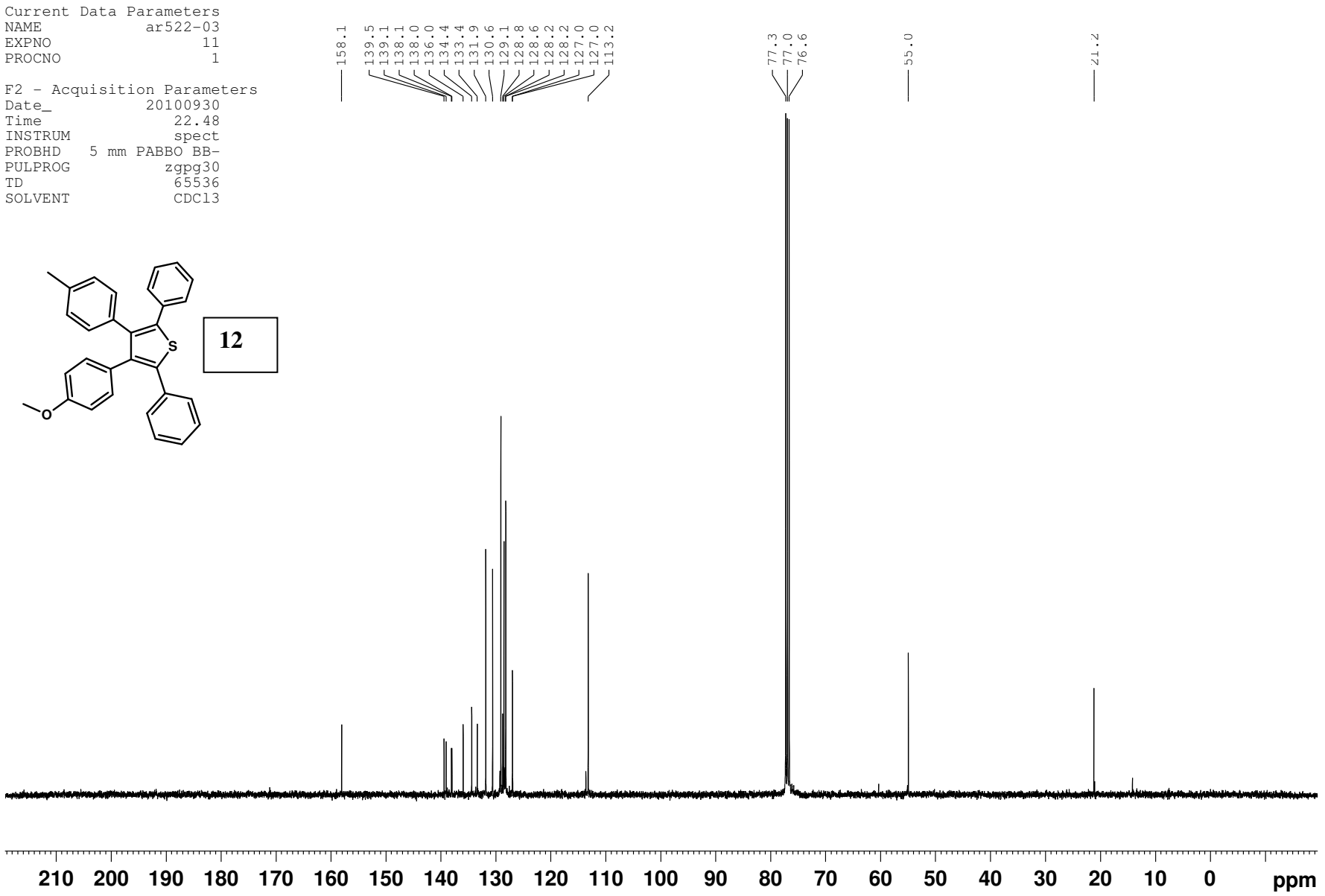
10a

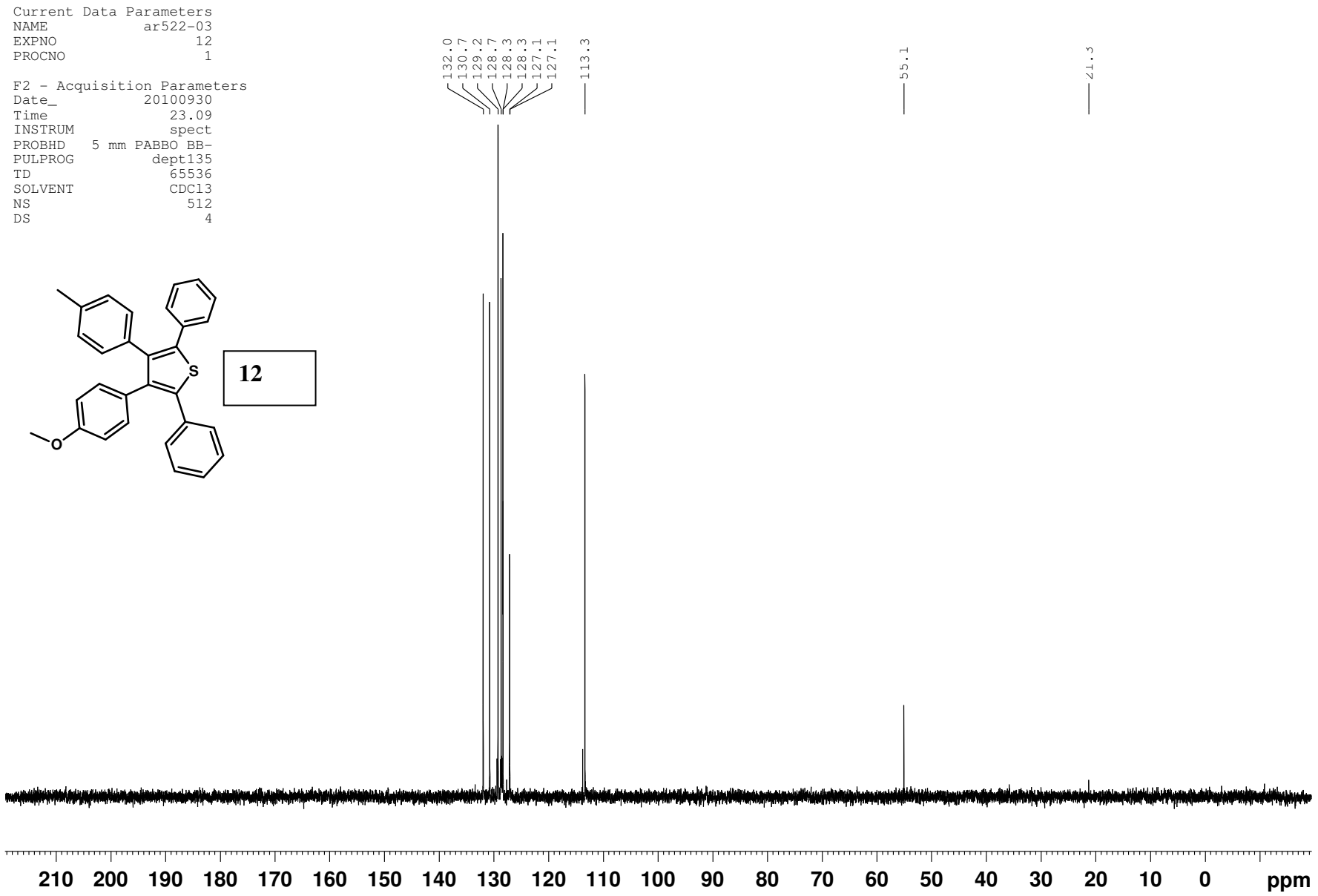


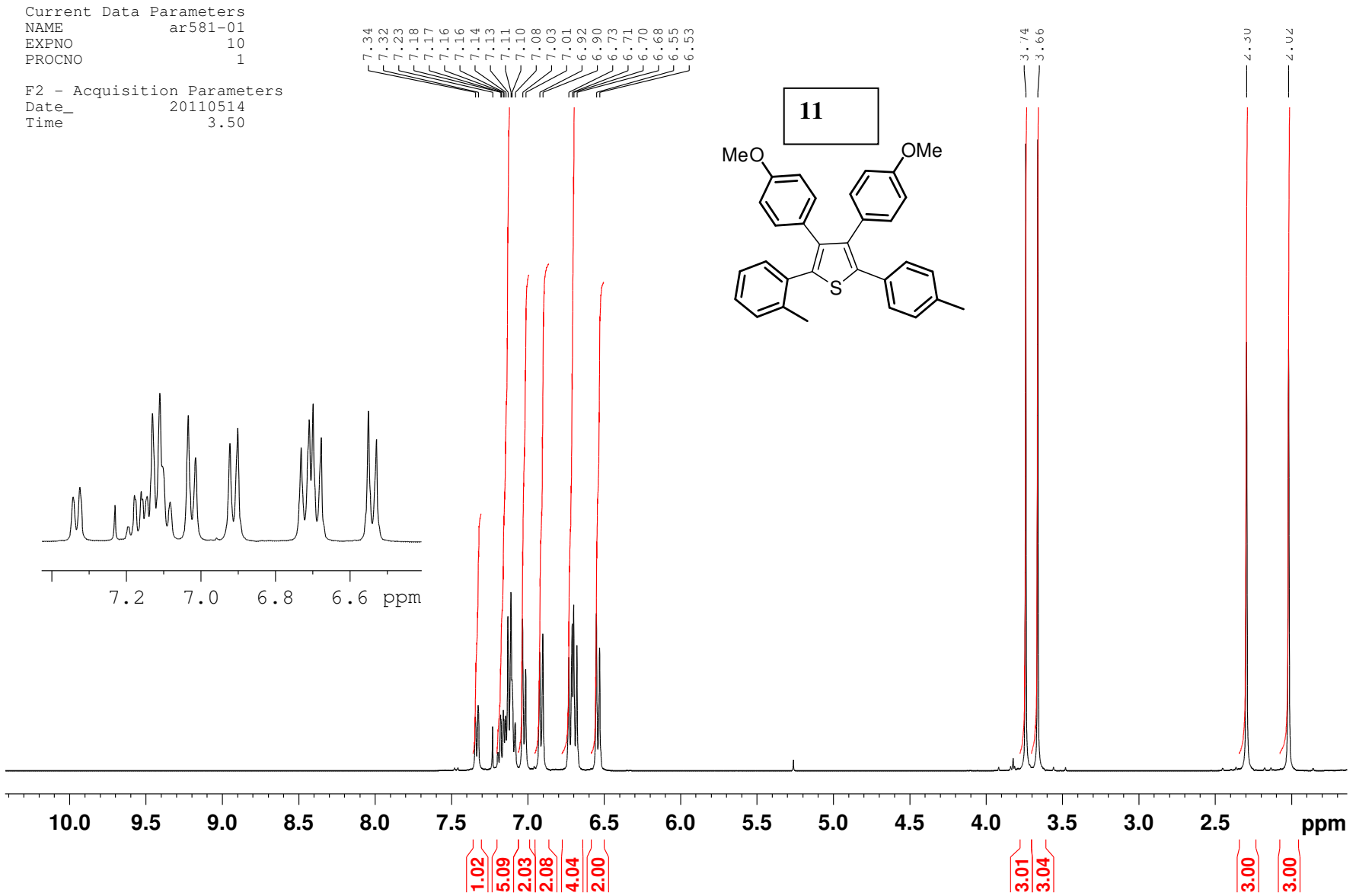

Current Data Parameters
NAME ar558-02
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110222
Time 12.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
7.13
7.11
7.03
7.01
6.88
6.86
6.86
6.68
6.67
6.66
3.74
2.30
10b
MeO
OMe
S
7.0
6.8
ppm
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.01
2.03
2.01
2.00
3.00
3.02

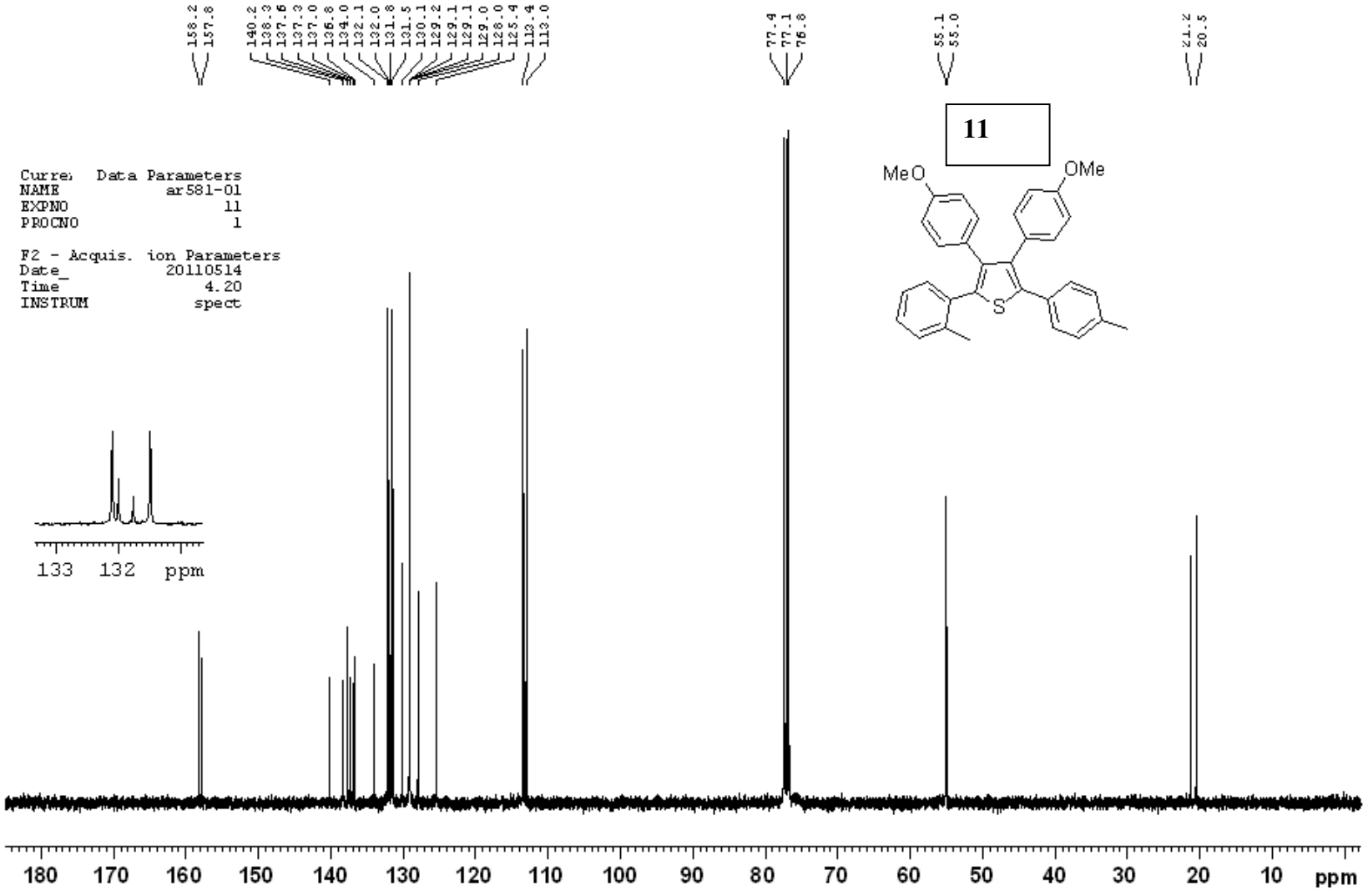

Current Data Parameters
NAME ar558-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110222
Time 13.03
INSTRUM spect
10b
MeO
OMe
S
158.1
138.8
137.8
136.8
132.0
131.7
129.1
129.0
129.0
113.3
77.4
77.0
76.7
55.1
21.2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

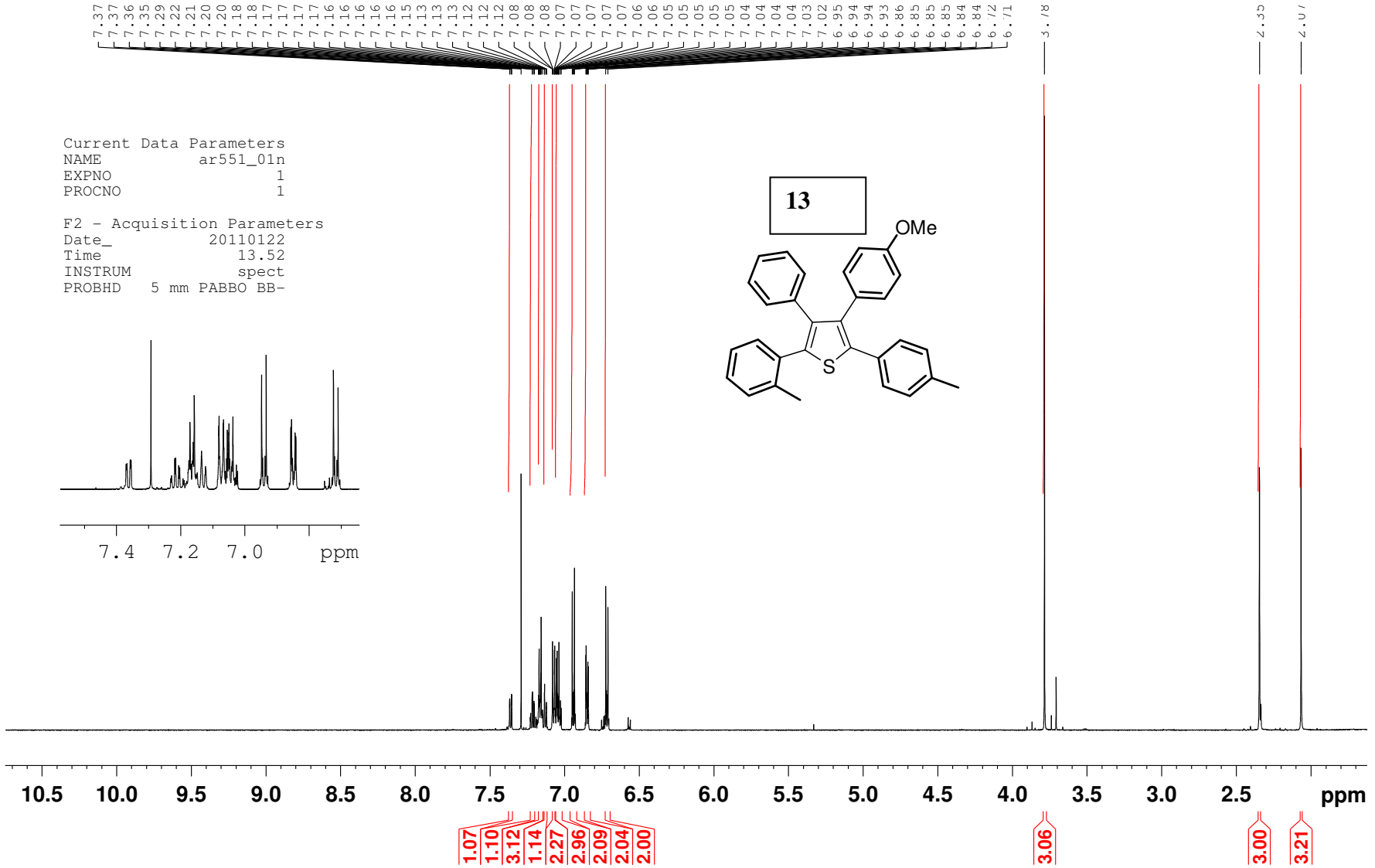

Current Data Parameters
NAME ar522-03
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100929
Time 13.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
12
ppm
10.82
6.16
2.06
3.01
3.00


Current Data Parameters
NAME ar522-03
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100930
Time 22.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
158.1
139.5
139.1
138.1
138.0
136.0
134.4
133.4
131.9
130.6
129.1
128.8
128.6
128.2
128.2
127.0
127.0
113.2
77.3
77.0
76.6
55.0
21.2
S
O
12
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

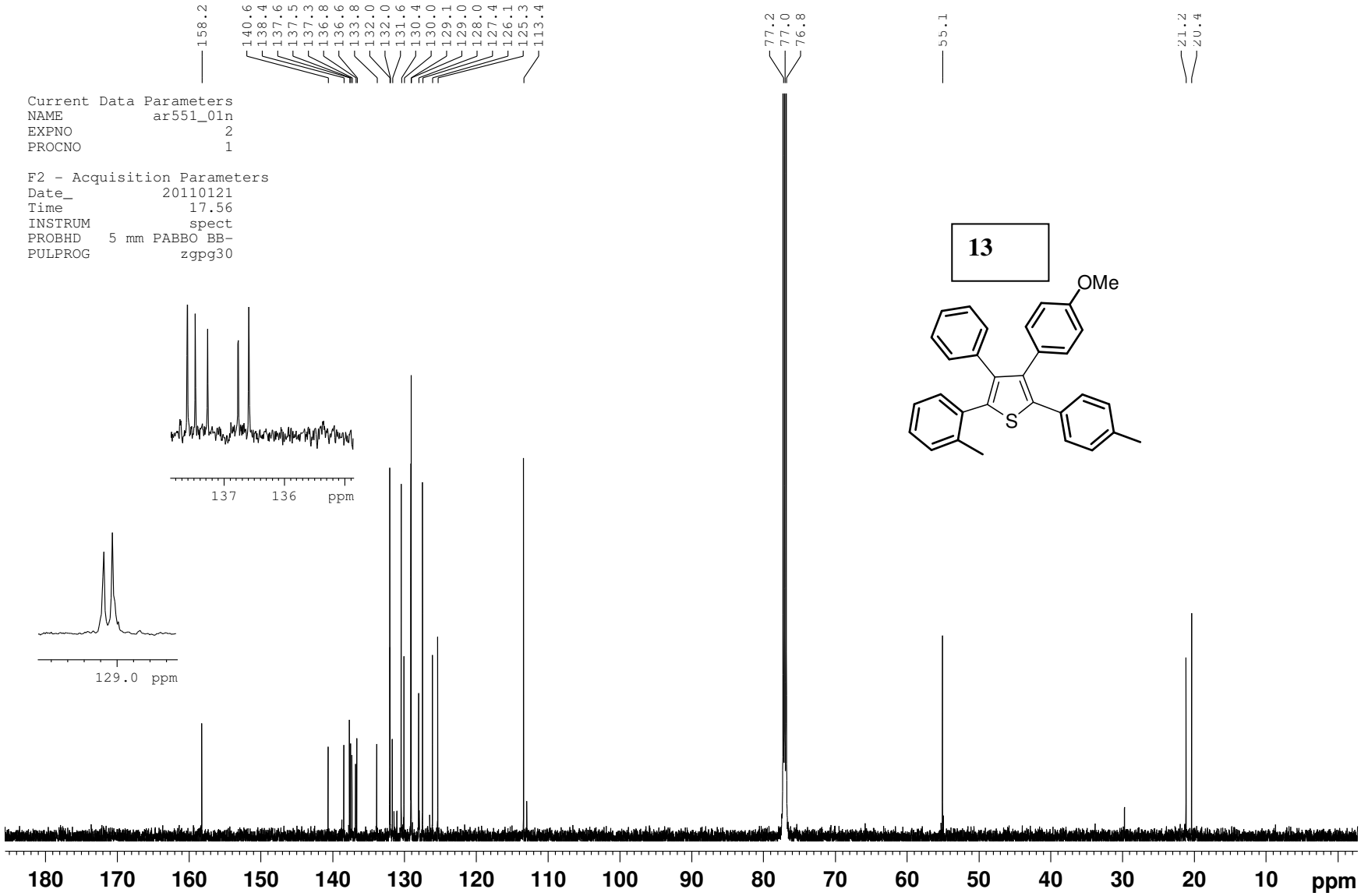

Current Data Parameters
NAME ar522-03
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100930
Time 23.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 512
DS 4
132.0
130.7
129.2
128.7
128.3
128.3
127.1
127.1
113.3
55.1
41.3
S
O
12
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Current Data Parameters
NAME ar581-01
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110514
Time 3.50
7.34
7.32
7.23
7.18
7.17
7.16
7.16
7.14
7.13
7.11
7.10
7.08
7.03
7.01
6.92
6.90
6.73
6.71
6.70
6.68
6.55
6.53
3.74
3.66
2.30
2.02
11
MeO
OMe
S
7.2
7.0
6.8
6.6 ppm
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
1.02
5.09
2.03
2.08
4.04
2.00
3.01
3.04
3.00
3.00


158.2
157.8
140.2
138.3
137.6
137.3
137.0
136.8
134.0
132.1
132.0
131.8
131.5
130.1
129.2
129.1
129.1
129.0
128.0
125.4
113.4
113.0
77.4
77.1
76.8
55.1
55.0
21.2
20.5
11
MeO
OMe
S
Curre: Data Parameters
NAME ar581-01
EXPNO 11
PROCNO 1
F2 - Acquis. ion Parameters
Date_ 20110514
Time 4.20
INSTRUM spect
133 132 ppm
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


Current Data Parameters
NAME ar551_01n
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110122
Time 13.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
7.4 7.2 7.0 ppm
13
OMe
S
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
1.07 1.10 3.12 1.14 2.27 2.96 2.09 2.04 2.00
3.06
3.00 3.21

13C{1H} 150 MHz



13CDEPT135, 150 MHz

```
Current Data Parameters
NAME          ar551_01n
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20110121
Time              18.12
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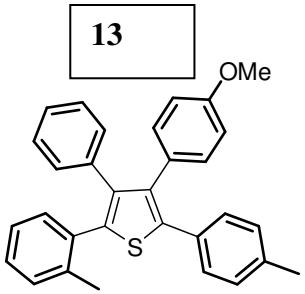
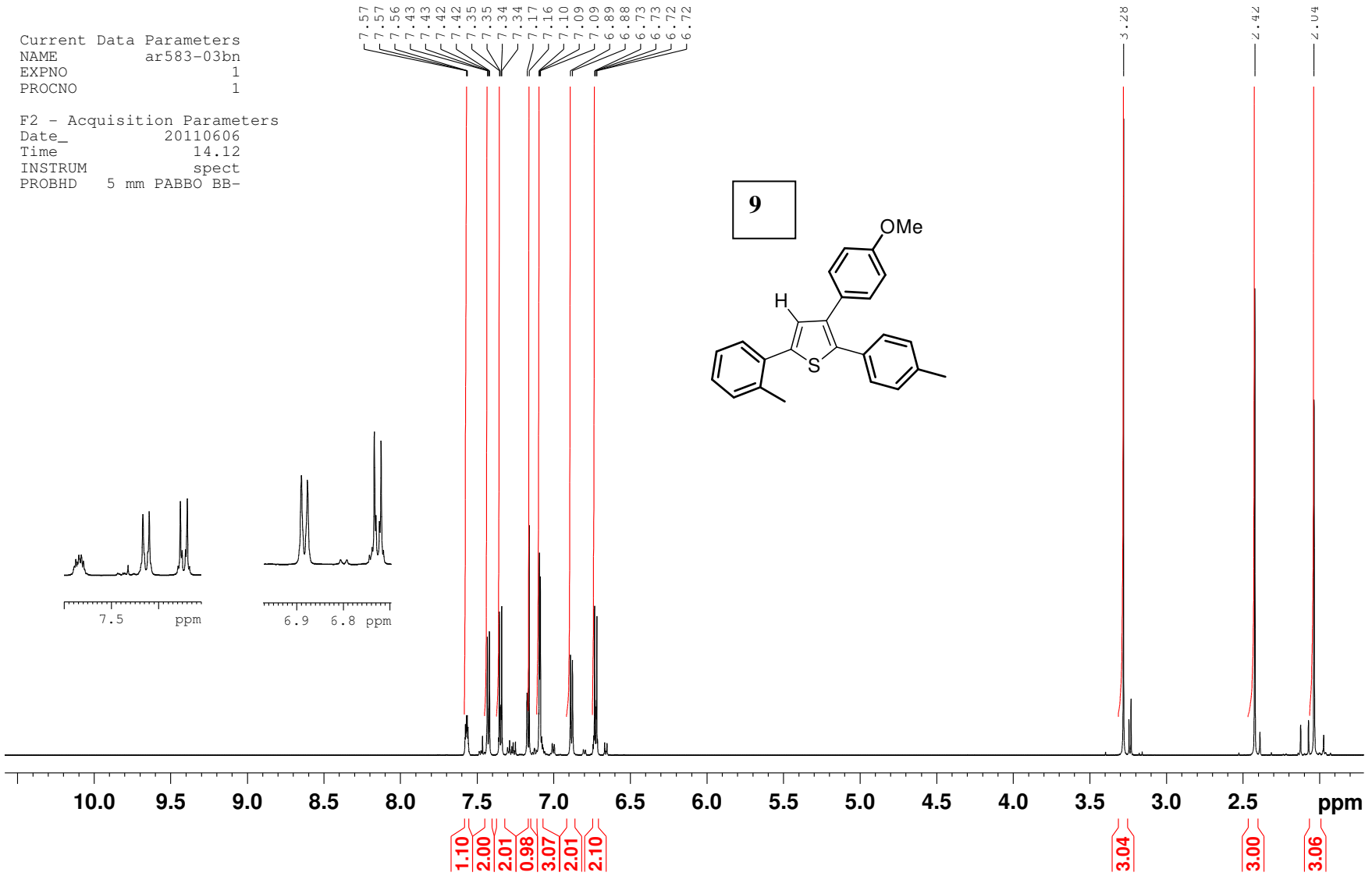
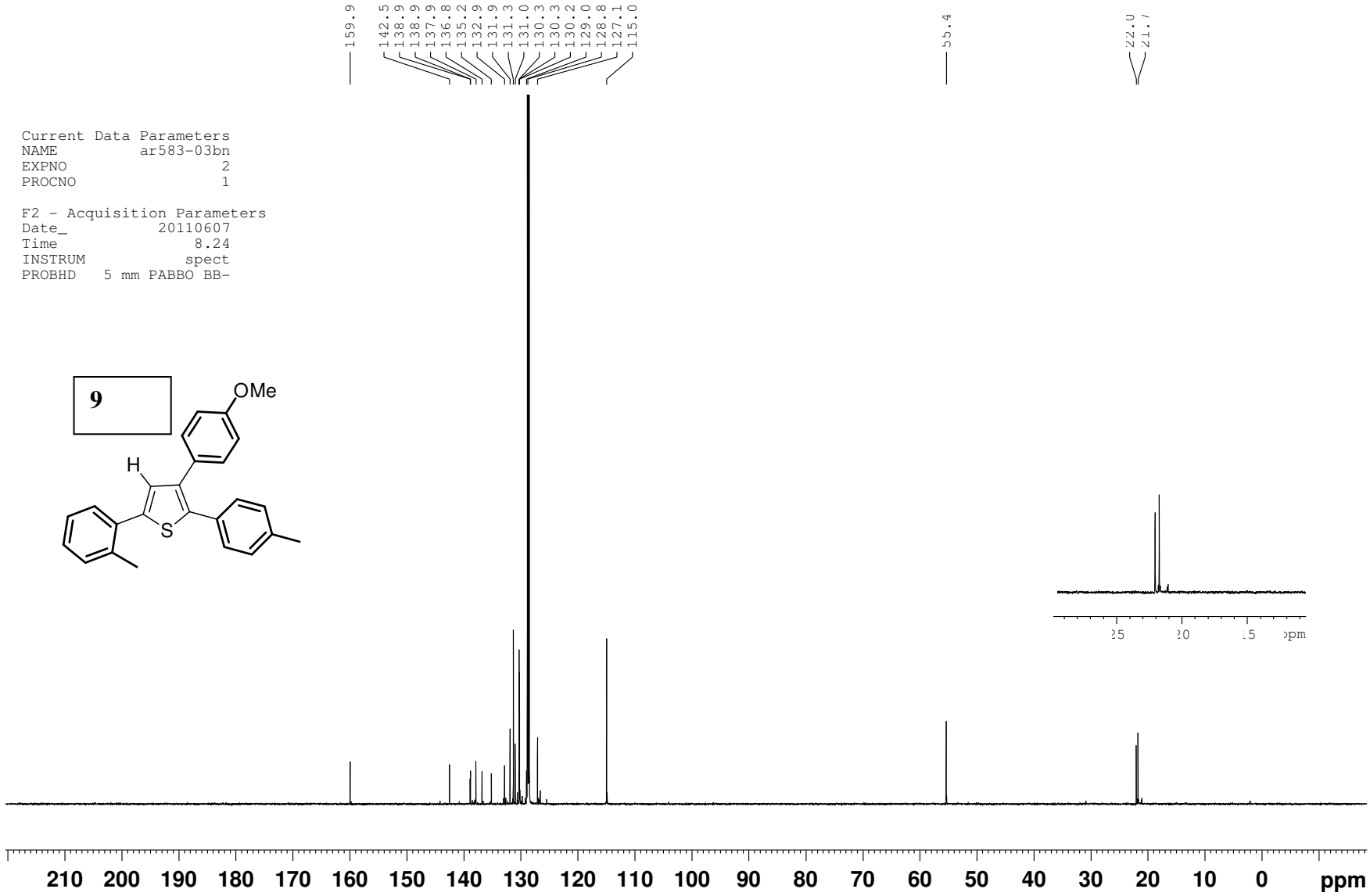


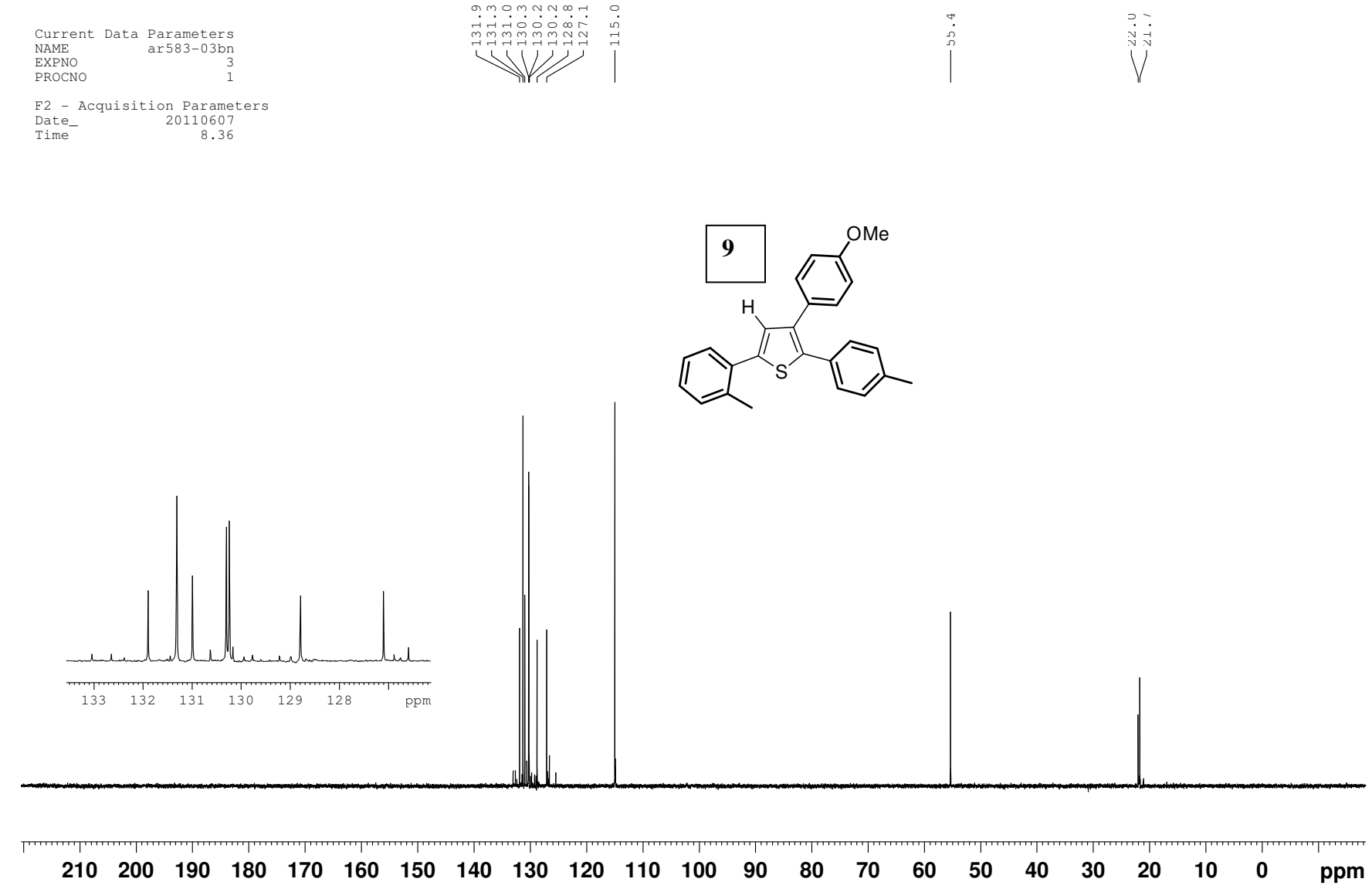
1H-NMR


Current Data Parameters
NAME ar583-03bn
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110606
Time 14.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
7.57 7.57 7.56 7.43 7.43 7.42 7.42 7.35 7.35 7.34 7.34 7.17 7.16 7.10 7.09 7.09 6.89 6.88 6.73 6.73 6.72 6.72
3.28
2.42
2.04
9
OMe
H
S
7.5 ppm
6.9 6.8 ppm
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
1.10 2.00 2.01 0.98 3.07 2.01 2.10
3.04
3.00
3.06

13C{1H} 150 MHz

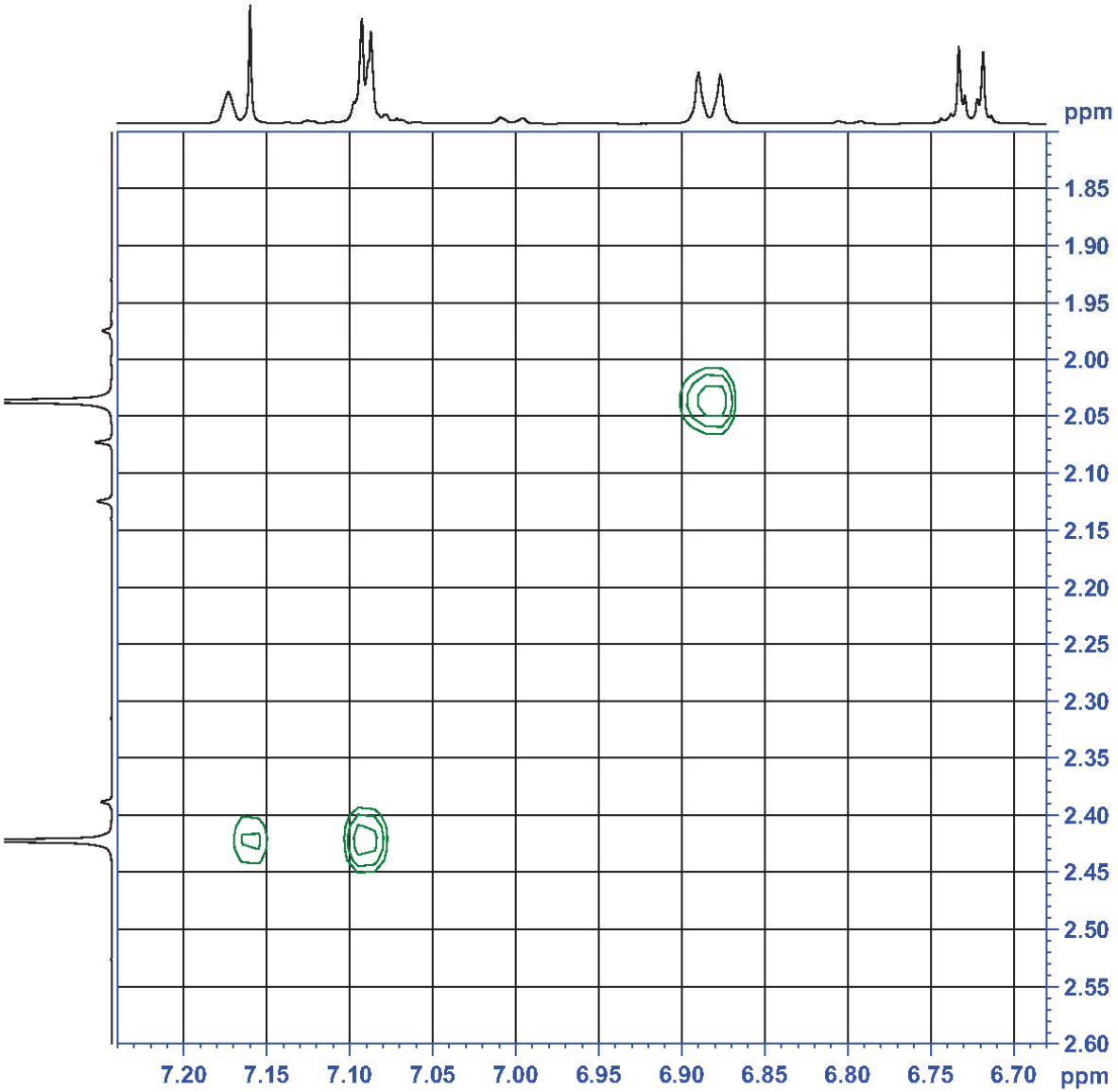


13CDEPT135, 150 MHz



9

NOESY



NMR-Abteilung

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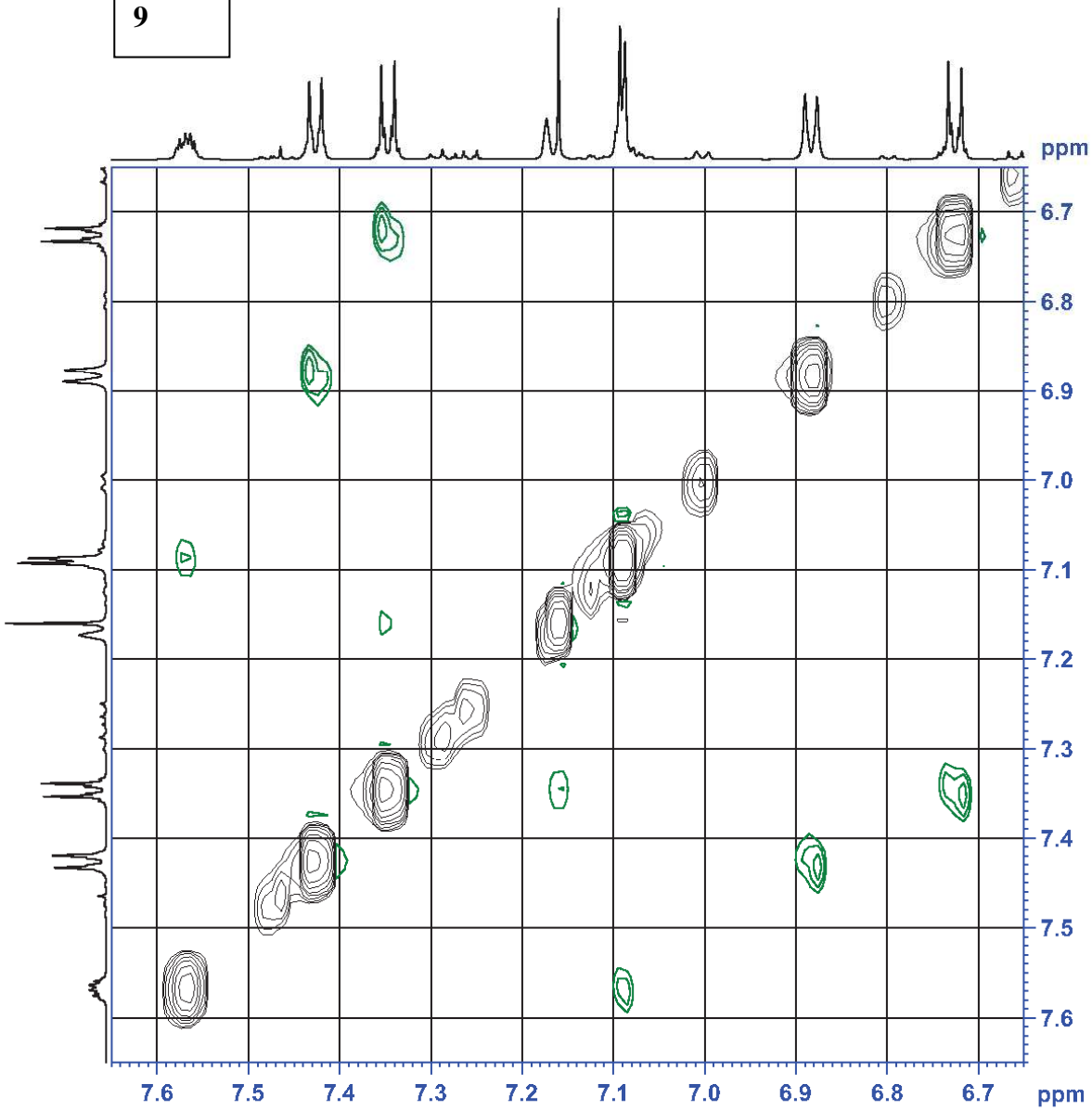
NAME	ar583-03bn	
EXPNO	1000	
PROCNO	1	
Date_	20110607	
Time	17.32	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	noesyph	
TD	4096	
SOLVENT	C6D6	
NS	16	
DS	16	
SWH	6127.451	Hz
FIDRES	1.495960	Hz
AQ	0.3342836	sec
RG	114	
DW	81.600	usec
DE	6.50	usec
TE	296.3	K
D0	0.00006808	sec
D1	5.00000000	sec
D8	0.75000000	sec
IN0	0.00016315	sec
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.60	usec
PL1	-4.00	dB
PL1W	32.36811066	W
SFO1	600.3527635	MHz
ND0	1	
TD	512	
SFO1	600.3528	MHz
FIDRES	11.970768	Hz
SW	10.209	ppm
FnMODE	States-TPPI	
SI	1024	
SF	600.3499851	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	
PC	1.00	
SI	1024	
MC2	States-TPPI	
SF	600.3499849	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	

NOESY

9



NMR-Abteilung

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```
NAME          ar583-03bn
EXPNO               1000
PROCNO                 1
Date_           20110607
Time               17.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG         noesyph
TD                 4096
SOLVENT            C6D6
NS                   16
DS                   16
SWH            6127.451 Hz
FIDRES         1.495960 Hz
AQ             0.3342836 sec
RG                   114
DW              81.600 usec
DE               6.50 usec
TE              296.3 K
D0             0.00006808 sec
D1             5.00000000 sec
D8             0.75000000 sec
IN0            0.00016315 sec

======== CHANNEL f1 ========
NUC1                  1H
P1              10.60 usec
PL1               -4.00 dB
PL1W        32.36811066 W
SFO1       600.3527635 MHz
ND0                    1
TD                   512
SFO1         600.3528 MHz
FIDRES       11.970768 Hz
SW             10.209 ppm
FnMODE      States-TPPI
SI                  1024
SF         600.3499851 MHz
WDW               QSINE
SSB                    2
LB              0.00 Hz
GB                     0
PC                  1.00
SI                  1024
MC2         States-TPPI
SF         600.3499849 MHz
WDW               QSINE
SSB                    2
LB              0.00 Hz
GB                     0
```