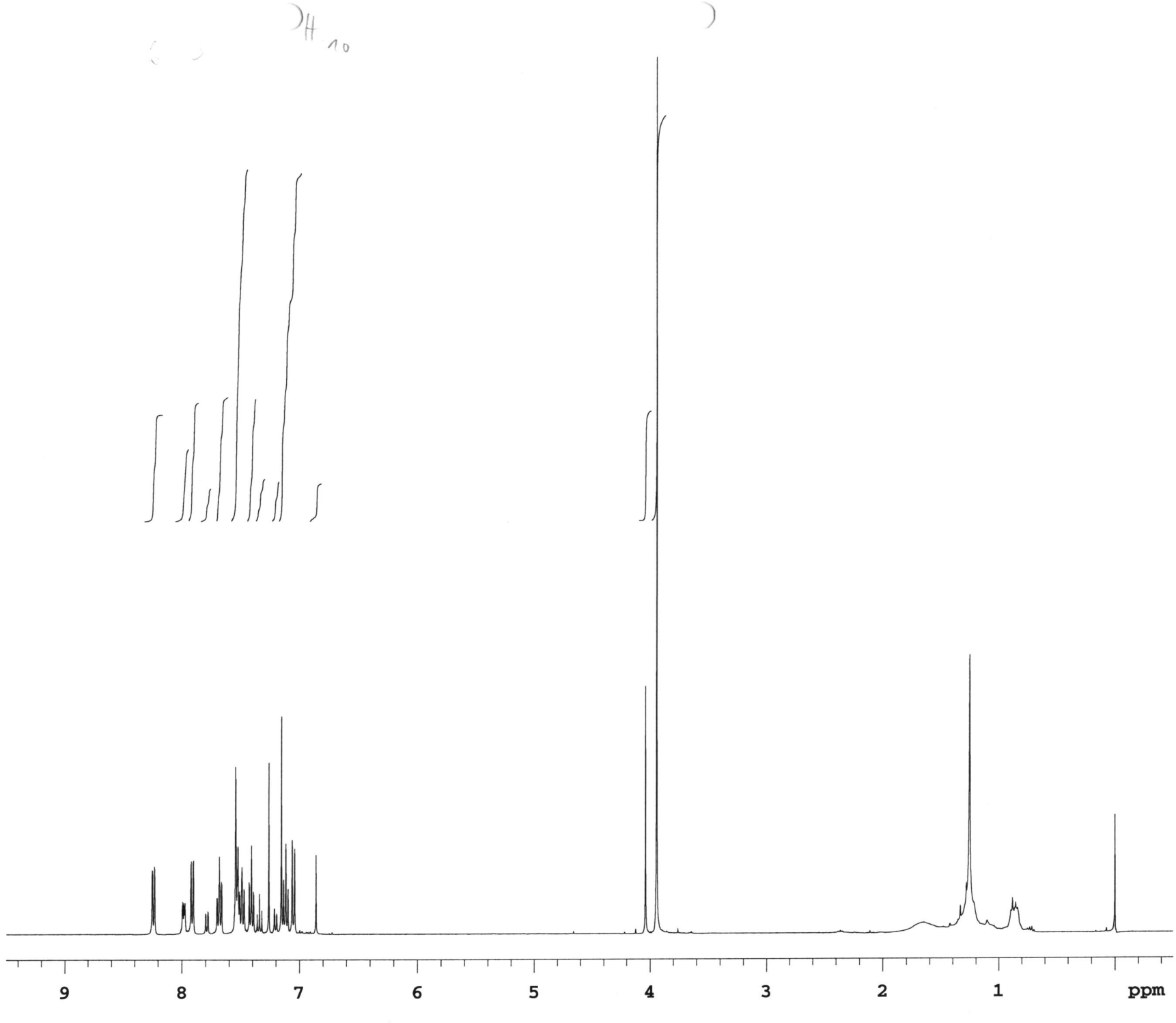
WEB100_A/CDCl3/1H
Stark 20120418

Wed Apr 18 18:24 2012
duration: 0h 2min

exp1 Proton

SAMPLE	
date	Apr 18 2012
samplename	WEB100_A
solvent	cdcl3
file	exp
ACQUISITION	
instrum	m400
probe_	autoX
seqfil	s2pul
sfrq	399.918
tn	H1
at	2.561
np	32768
sw	6398.0
bs	4
tpwr	59
pw	5.5
d1	0.439
d2	0
tof	368.7
nt	40
ct	40
alock	n
gain	not used
FLAGS	
il	n
in	n
dp	y
DEC. & VT	
dn	C13
dfrq	100.568
homo	n
dpwr	45
dof	0
dm	nnn
dmm	c
dmf	17100
PROCESSING	
lb	0.40
wtfile	
proc	ft
fn	not used
DISPLAY	
sp	-200.3
wp	3999.1
vs	170
sc	0
wc	225
hzmm	17.77
is	2500.00
rfl	798.2
rfp	0
th	20.0
ins	100.000
rp	25.0
lp	-102.4
nm cdc ph	



Halle/Saale, 18-04-12 18 Uhr 29

WEB100_A/CDCl3/1H
Stark 20120418

Apr 18 2012 H1 399.915 MHz Proton
9.50 bis -0.50 ppm, vs= 170.0
th= 1.0, rfp=0.00 ppm, rfl=798.18

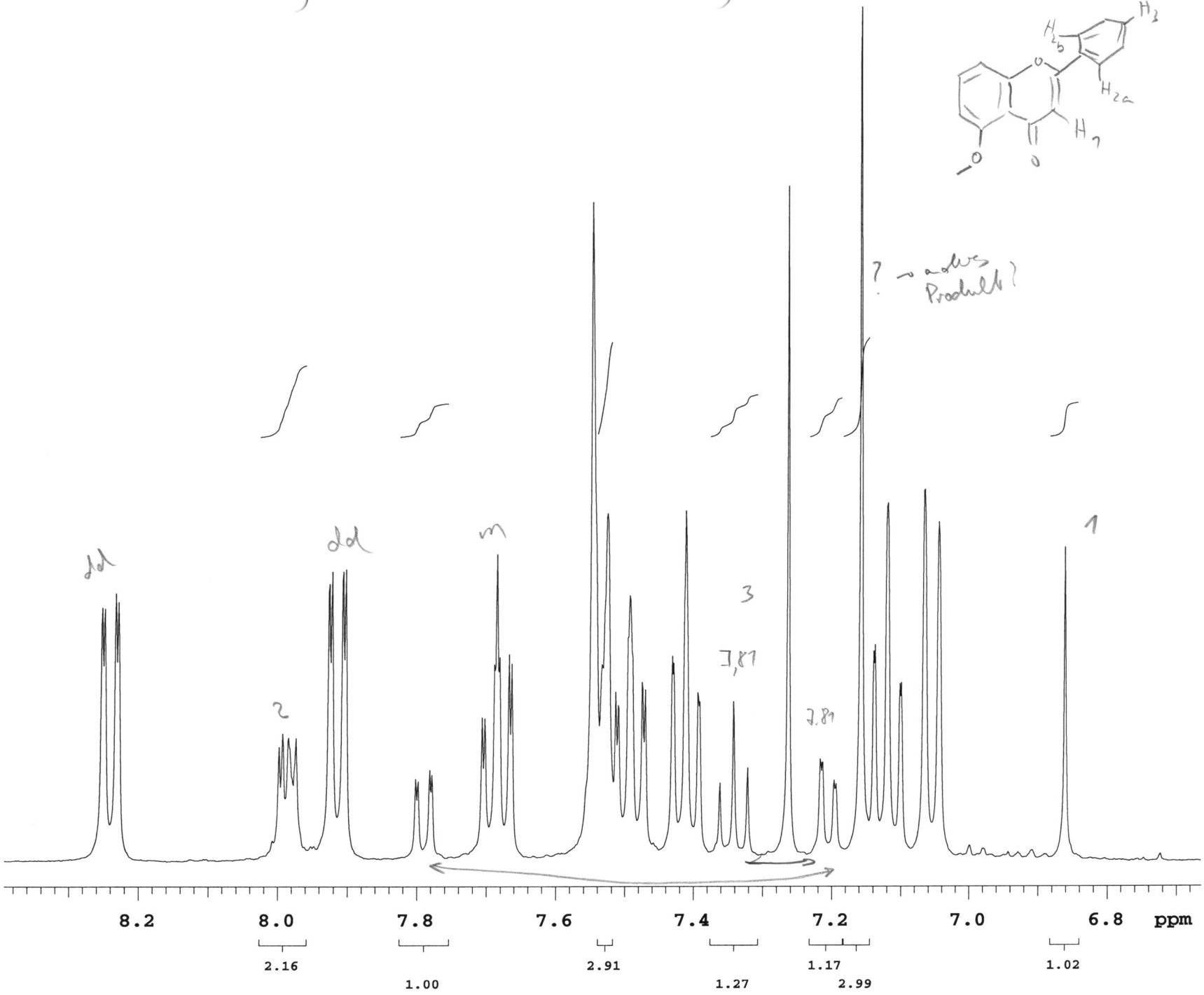
Nr.	Hz	ppm	Hoehe	Nr.	Hz	ppm	Hoehe
1	3300.12	8.252	12.5	51	2825.27	7.065	18.3
2	3298.55	8.248	12.4	52	2817.07	7.044	16.7
3	3292.31	8.233	13.2	53	2743.65	6.861	15.4
4	3290.74	8.229	12.7	54	1615.50	4.040	47.9
5	3198.59	7.998	5.6	55	1577.23	3.944	170.0
6	3196.63	7.993	6.3	56	659.95	1.650	2.0
7	3193.12	7.984	6.1	57	591.22	1.478	1.2
8	3188.82	7.974	6.0	58	586.92	1.468	1.1
9	3169.69	7.926	13.6	59	569.35	1.424	1.8
10	3168.13	7.922	14.2	60	564.66	1.412	1.4
11	3161.88	7.906	14.2	61	533.42	1.334	5.3
12	3160.32	7.902	14.3	62	513.51	1.284	9.7
13	3120.10	7.802	4.0	63	501.40	1.254	53.8
14	3118.53	7.798	3.9	64	461.96	1.155	1.8
15	3111.89	7.781	4.5	65	457.28	1.143	1.7
16	3110.72	7.778	4.2	66	441.27	1.103	2.4
17	3081.83	7.706	7.0	67	415.49	1.039	1.3
18	3080.26	7.702	7.0	68	357.70	0.894	4.3
19	3074.80	7.689	9.7	69	355.36	0.889	4.3
20	3073.24	7.685	15.1	70	351.84	0.880	6.7
21	3071.67	7.681	10.0	71	347.55	0.869	4.3
22	3066.21	7.667	10.2	72	344.81	0.862	4.8
23	3064.64	7.663	9.7	73	340.91	0.852	5.8
24	3018.17	7.547	32.5	74	334.27	0.836	4.8
25	3012.71	7.533	9.7	75	285.07	0.713	1.1
26	3009.58	7.526	17.1	76	-0.00	-0.000	22.8
27	3004.90	7.514	8.3				
28	3003.34	7.510	7.7				
29	2996.31	7.492	13.1				
30	2989.28	7.475	8.8				
31	2987.33	7.470	8.4				
32	2971.71	7.431	10.1				
33	2970.92	7.429	9.7				
34	2963.90	7.411	17.3				
35	2956.87	7.394	8.3				
36	2955.69	7.391	7.8				
37	2943.98	7.362	3.8				
38	2936.17	7.342	7.8				
39	2927.97	7.321	4.6				
40	2904.54	7.263	33.3				
41	2886.19	7.217	5.0				
42	2884.62	7.213	4.8				
43	2877.99	7.196	4.0				
44	2876.81	7.194	3.8				
45	2861.97	7.156	42.2				
46	2854.95	7.139	10.3				
47	2854.16	7.137	10.6				
48	2846.75	7.118	17.6				
49	2839.72	7.101	8.7				
50	2838.94	7.099	8.8				

WEB100_A/CDCl3/1H
Stark 20120418

Wed Apr 18 18:24 2012

exp1 Proton

SAMPLE	
date	Apr 18 2012
samplename	WEB100_A
solvent	cdcl3
file	exp
ACQUISITION	
instrum	m400
probe_	autoX
seqfil	s2pul
sfrq	399.918
tn	H1
at	2.561
np	32768
sw	6398.0
bs	4
tpwr	59
pw	5.5
d1	0.439
d2	0
tof	368.7
nt	40
ct	40
alock	n
gain	not used
FLAGS	
il	n
in	n
dp	y
DEC. & VT	
dn	C13
dfrq	100.568
homo	n
dpwr	45
dof	0
dm	nnn
dmm	c
dmf	17100
PROCESSING	
lb	0.40
wtfile	
proc	ft
fn	not used
DISPLAY	
sp	2665.2
wp	691.2
vs	650
sc	0
wc	225
hzmm	3.07
is	2500.00
rfl	798.2
rfp	0
th	1.0
ins	1.000
rp	25.0
lp	-102.4
nm cdc ph	

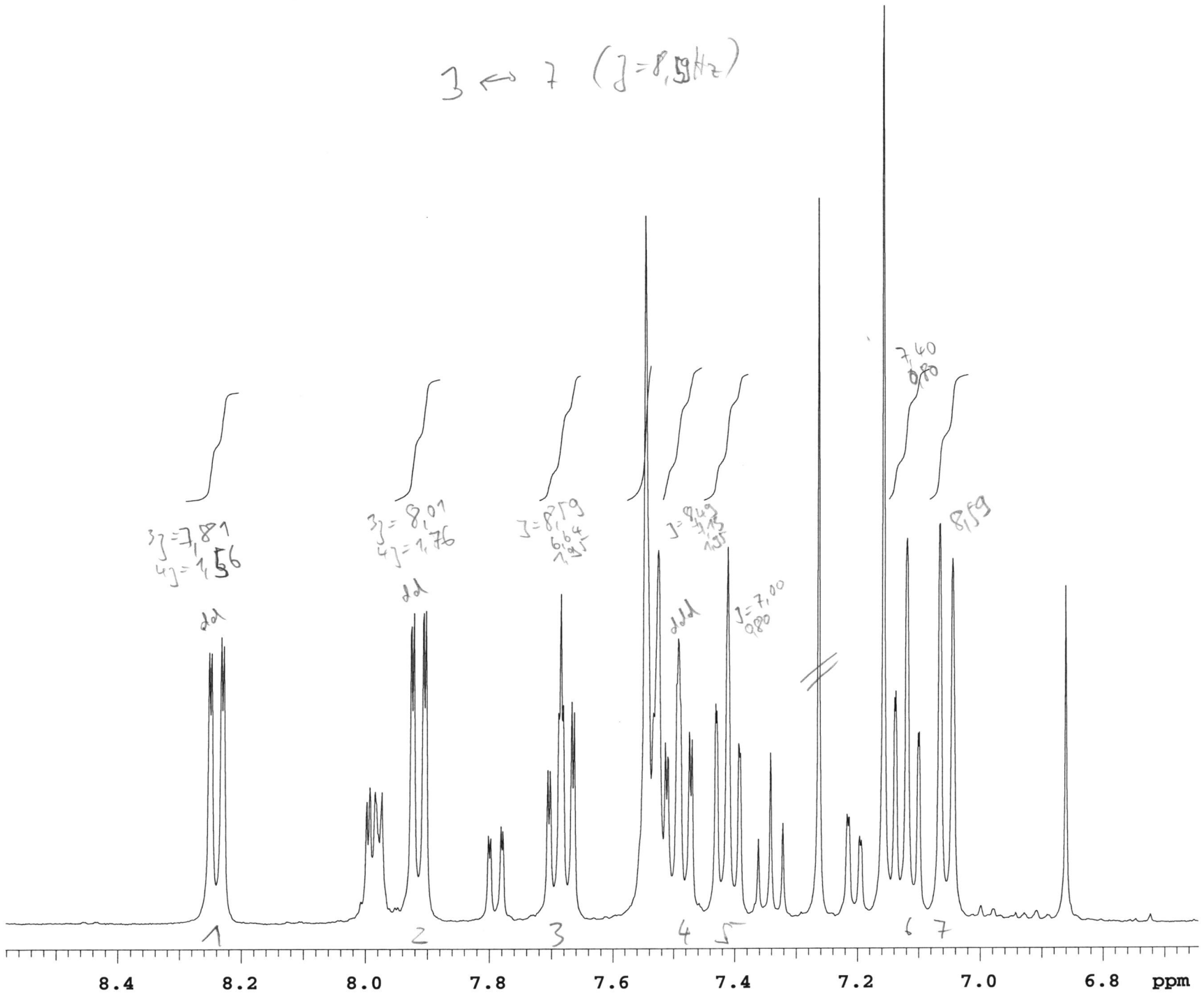


WEB100_A/CDCl3/1H
Stark 20120418

Wed Apr 18 18:24 2012
duration: 0h 2min

exp1 Proton

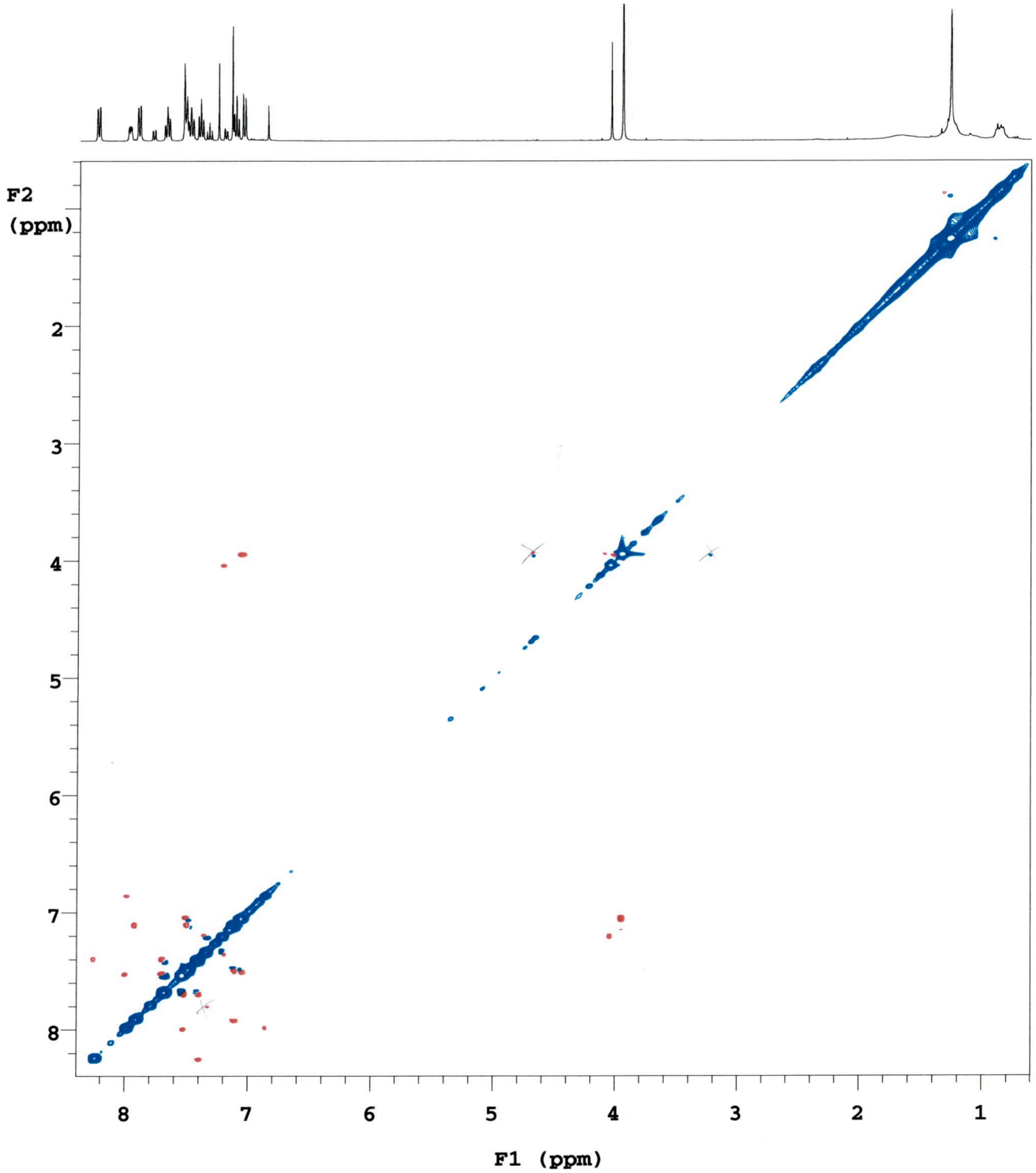
SAMPLE	
date	Apr 18 2012
samplename	WEB100_A
solvent	cdcl3
file	exp
ACQUISITION	
instrum	m400
probe_	autoX
seqfil	s2pul
sfrq	399.918
tn	H1
at	2.561
np	32768
sw	6398.0
bs	4
tpwr	59
pw	5.5
d1	0.439
d2	0
tof	368.7
nt	40
ct	40
alock	n
gain	not used
FLAGS	
il	n
in	n
dp	y
DEC. & VT	
dn	C13
dfrq	100.568
homo	n
dpwr	45
dof	0
dm	nnn
dmm	c
dmf	17100
PROCESSING	
lb	0.40
wtfile	
proc	ft
fn	not used
DISPLAY	
sp	2657.4
wp	774.4
vs	700
sc	0
wc	225
hzmm	3.44
is	2500.00
rfl	798.2
rfp	0
th	1.0
ins	100.000
rp	25.0
lp	-102.4
nm cdc ph	



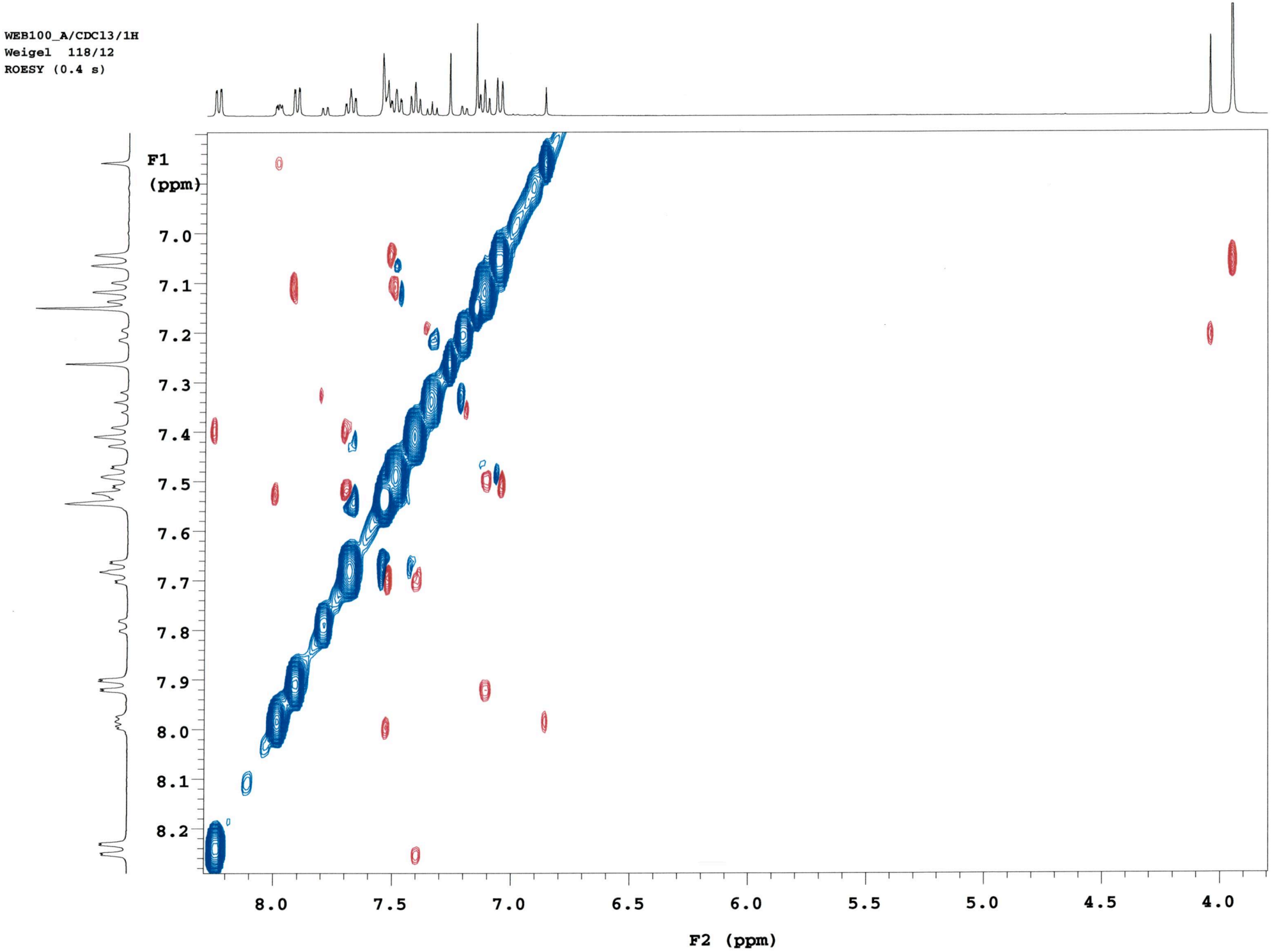
WEB100_A/CDCl3/1H
Weigel 118/12
ROESY (0.4 s)

exp122 ROESY

SAMPLE		FLAGS	
date	Apr 26 2012	hs	nn
solvent	cdcl3	sspul	y
sample	WEB100_A	PFGflg	y
ACQUISITION		hsglvl	6216
sw	3434.1	SPECIAL	
at	0.149	temp	25.0
np	1024	gain	44
fb	4000	spin	not used
ss	32	F2 PROCESSING	
d1	1.351	gf	0.069
nt	12	gfs	not used
2D ACQUISITION		fn	2048
sw1	3434.1	F1 PROCESSING	
ni	256	gf1	0.043
TRANSMITTER		gfs1	not used
tn	H1	proc1	lp
sfrq	399.814	fn1	2048
tof	-121.4	DISPLAY	
tpwr	61	sp	239.2
pw	6.400	wp	3115.5
TOCSY		sp1	239.2
mixR	0.400	wp1	3115.5
slpwrR	44	rf1	-162.0
slpwR	47.438	rfp	0
trim	0.0020	rf11	-162.0
PRESATURATION		rfp1	0
satmode	n	PLOT	
wet	n	wc	160.0
DECOUPLER		sc	0
dn	C13	wc2	153.5
dm	nnn	sc2	0
		vs	916
		th	2
		ai cdc ph	

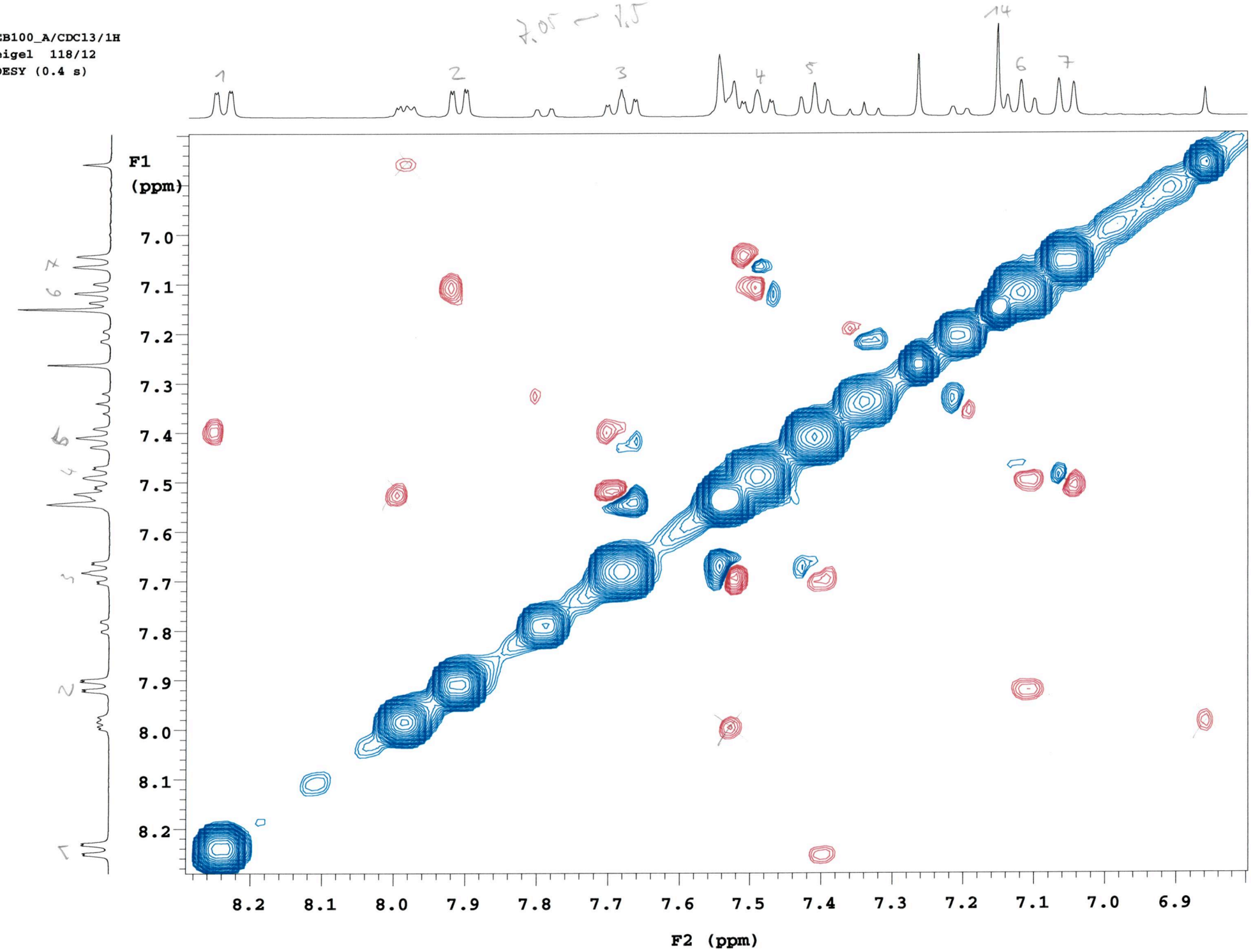


Plotname: WEB100_A.ROESY_01_plot01



Plotname: WEB100_A.ROESY_01_plot02

WEB100_A/CDC13/1H
Weigel 118/12
ROESY (0.4 s)

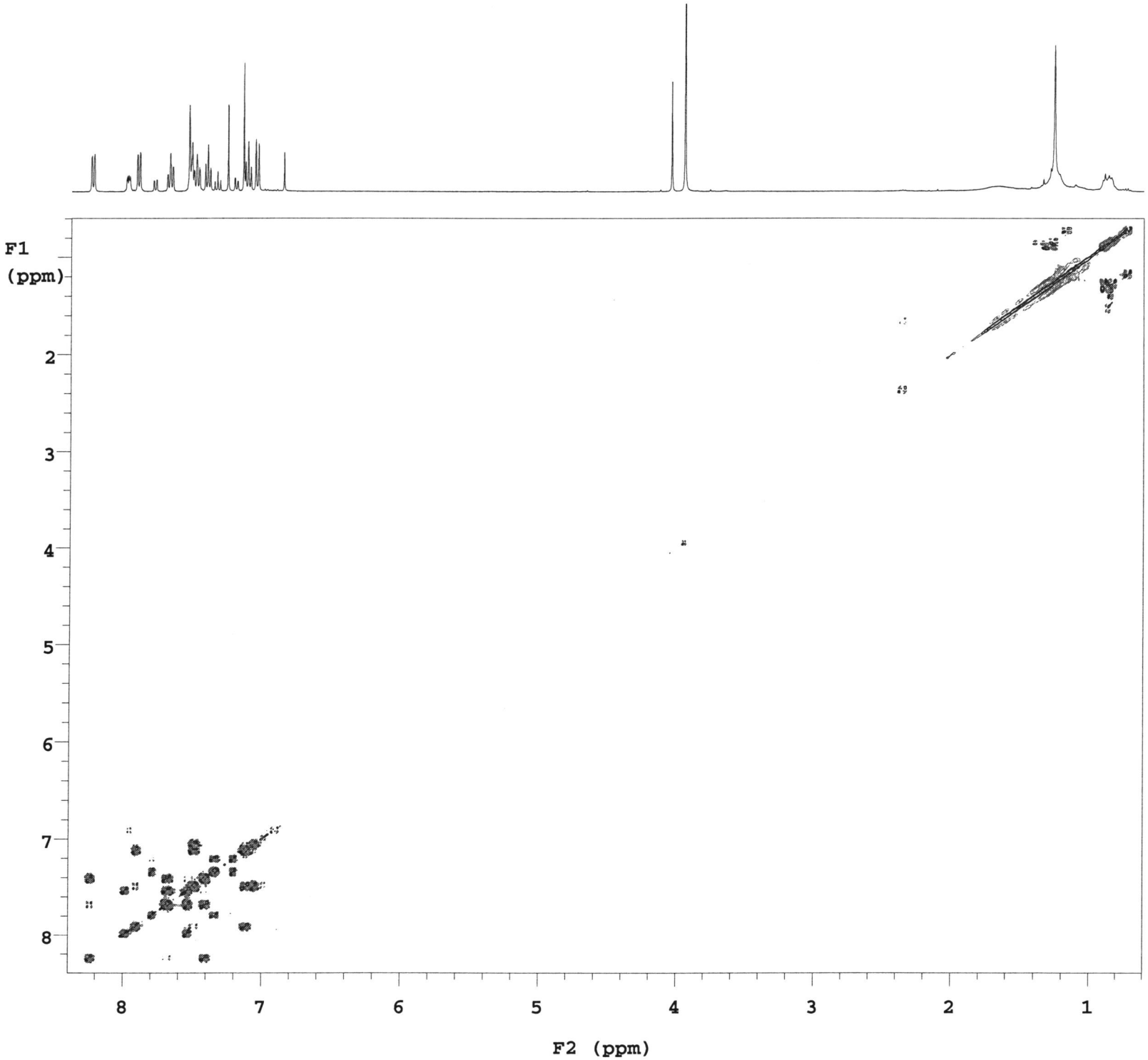


Plotname: WEB100_A.ROESY_01_plot03

WEB100_A/CDCl3/1H
Weigel 118/12
gDQCOSY

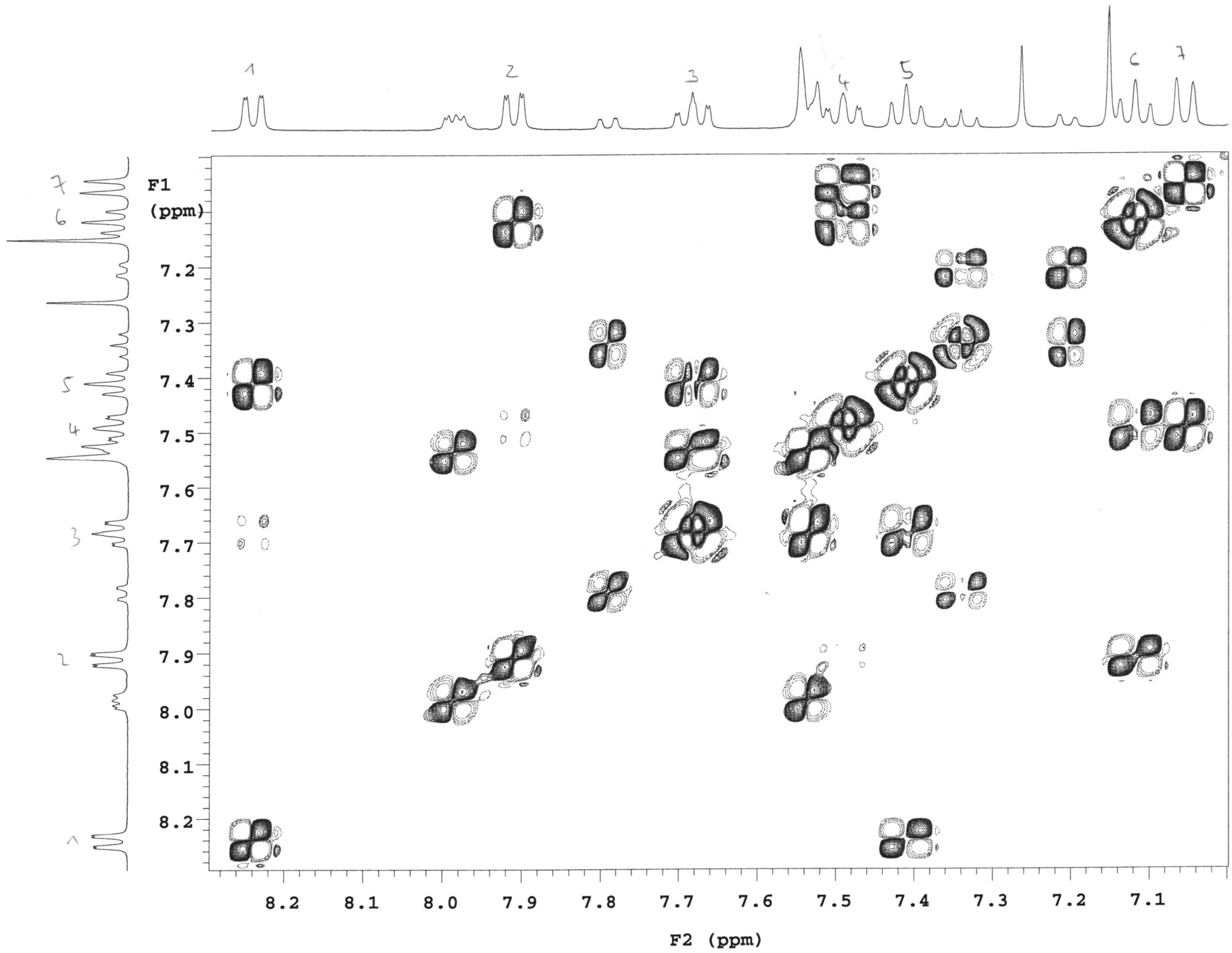
exp3 gDQCOSY

SAMPLE		FLAGS	
date	Apr 26 2012	hs	nn
solvent	cdcl3	sspul	y
sample	WEB100_A	hsglvl	6216
ACQUISITION		SPECIAL	
sw	3434.1	temp	25.0
at	0.149	gain	44
np	1024	spin	not used
fb	4000	F2 PROCESSING	
ss	32	sb	-0.125
d1	1.351	sbs	-0.100
nt	8	lsfid	-6
2D ACQUISITION		fn	4096
sw1	3434.1	F1 PROCESSING	
ni	256	sb1	-0.081
PRESATURATION		sbs1	-0.078
satmode	n	proc1	lp
wet	n	fn1	4096
TRANSMITTER		DISPLAY	
tn	H1	sp	239.2
sfrq	399.814	wp	3117.2
tof	-121.4	sp1	239.2
tpwr	61	wp1	3117.2
pw	6.400	rfl	-162.0
GRADIENTS		rfp	0
gzlvlE	4149	rfl1	-162.0
gtE	0.001000	rfp1	0
gstab	0.000500	PLOT	
DECOUPLER		wc	200.0
dn	C13	sc	0
dm	nnn	wc2	140.0
		sc2	0
		vs	380
		th	2
		ai cdc ph	



Plotname: WEB100_A_gDQCOSY_01_plot01

WEB100_A/CDCl3/1H
Weigel 118/12
gDQCOSY

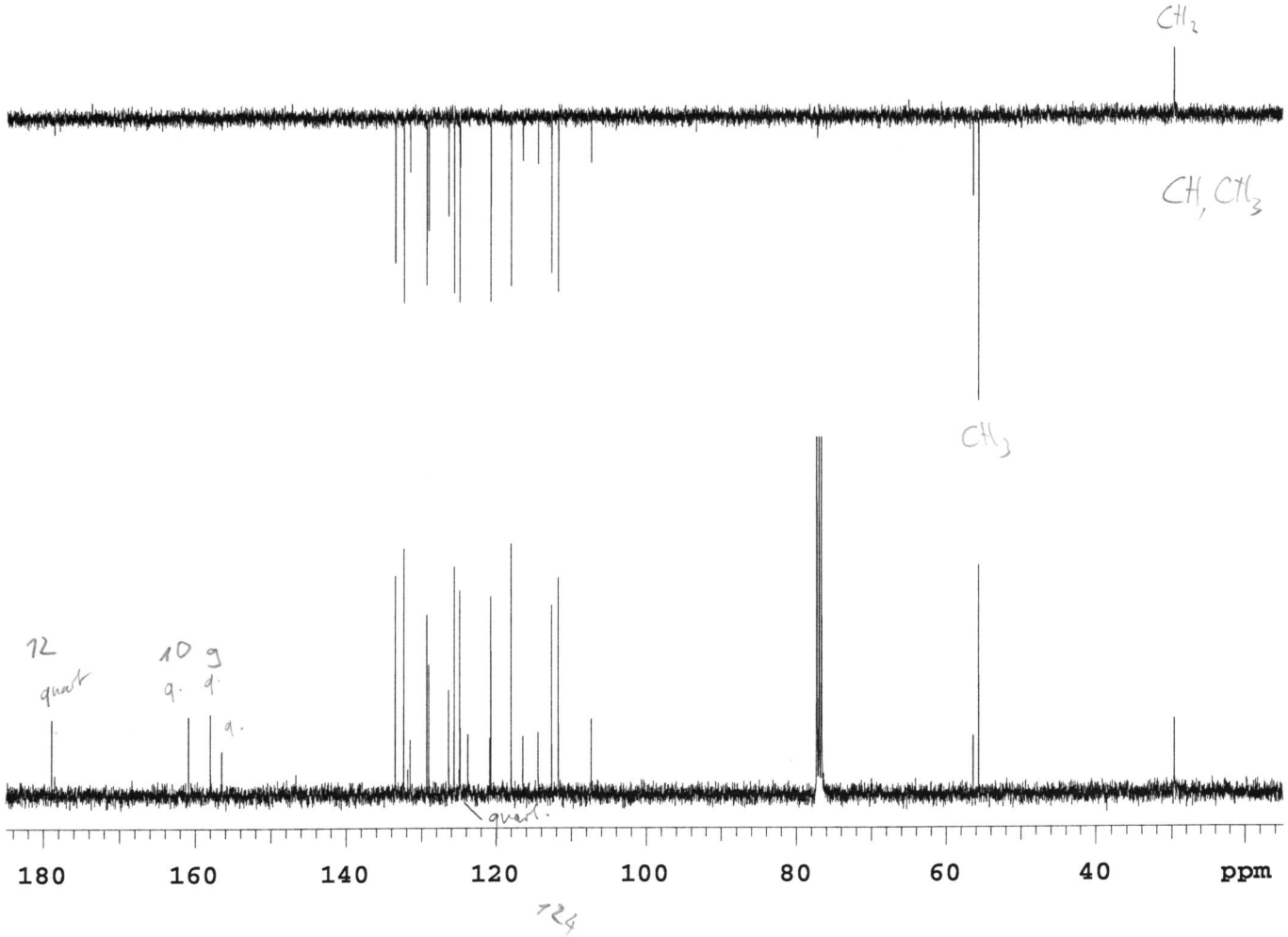


Plotname: WEB100_A_gDQCOSY_01_plot02

WEB100_A/CDCl3/1H
Weigel 118/12

exp8 DEPT

SAMPLE		DEPT	
date	Apr 26 2012	j1xh	146.0
solvent	cdcl3	mult	1.5
sample	WEB100_A	SPECIAL	
ACQUISITION		temp	25.0
sw	25000.0	gain	44
at	1.311	spin	not used
np	65536	PROCESSING	
bs	16	lb	0.80
ss	4	fn	65536
d1	2.189	SPECTRUM	
nt	600	wp	17092.1
ct	600	sp	1507.8
TRANSMITTER		rp	144.9
tn	C13	lp	0
tof	1530.8	nm	cdc ph
tpwr	59	REFERENCE	
pw	6.700	rfl	1441.7
DECOUPLER		rfp	0
dn	H1	PLOT	
dof	0	wc	180
dpwr	38	sc	0
dm	nny	vs	40
decwave	w	hzmm	94.96
dmf	9804	th	6
pplvl	61		
pp	7.000		



Plotname: WEB100_A_DEPT_01_plot01

Halle/Saale, 27-04-12 08 Uhr 39

WEB100_A/CDCl3/1H
Weigel 118/12

Apr 26 2012 C13 100.533 MHz DEPT
185.0 bis 15.0 ppm, vs= 40.0
th= 6.5, rfp= 0.0 ppm, rfl=1441.7

Nr.	ppm	Hoehe
1	133.54	-20.5
2	132.41	-26.2
3	131.56	-7.7
4	129.30	-23.6
5	129.04	-16.0
6	126.38	-13.9
7	125.64	-24.8
8	124.90	-26.0
9	124.83	-7.0
10	120.73	-26.0
11	118.02	-23.8
12	114.45	-6.6
13	112.65	-22.0
14	111.77	-24.6
15	56.39	-11.3
16	55.68	-40.0
17	29.69	9.4

Halle/Saale, 27-04-12 08 Uhr 37

WEB100_A/CDCl3/1H
Weigel 118/12

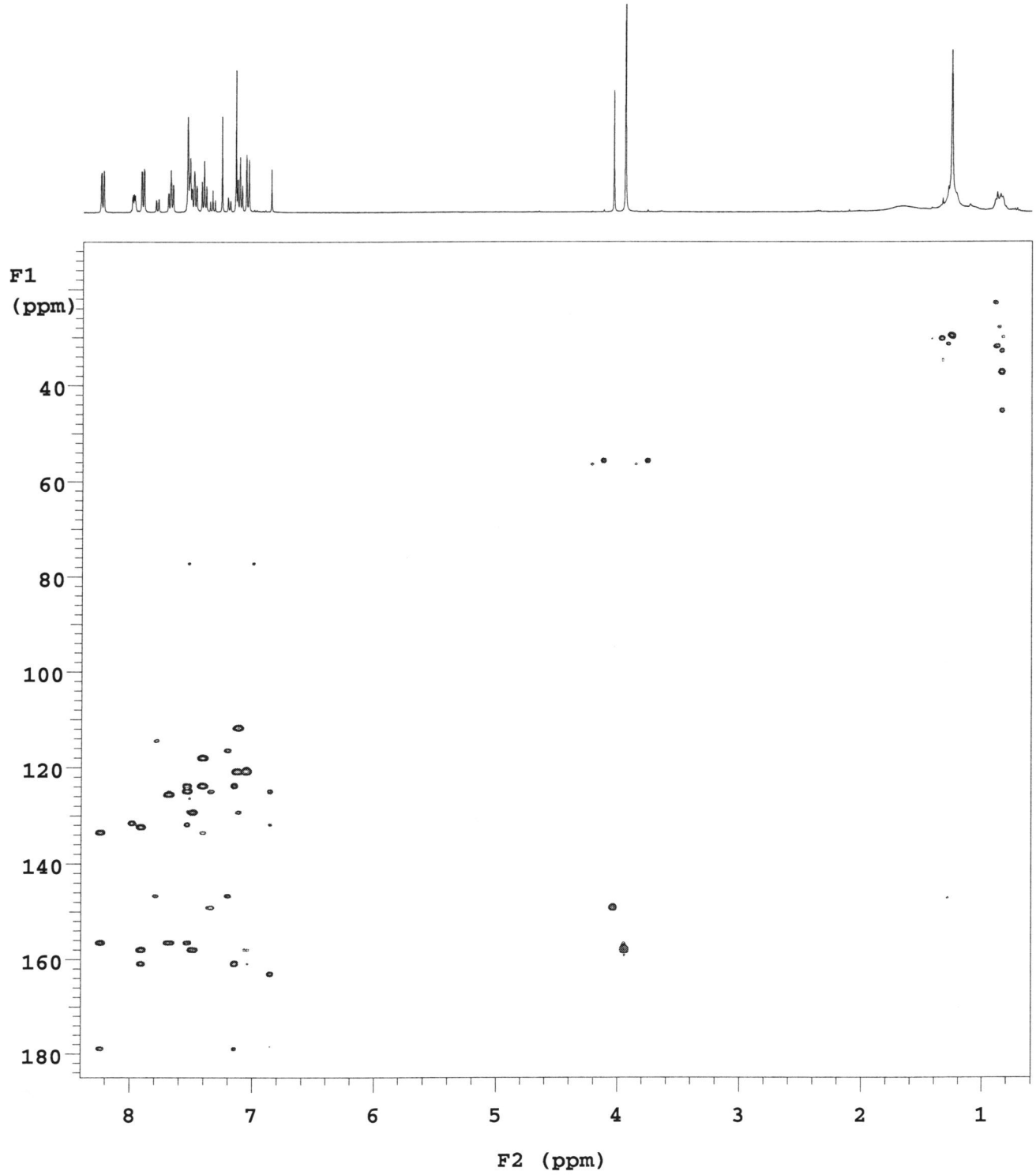
Apr 26 2012 C13 100.533 MHz CARBON
185.0 bis 15.0 ppm, vs= 300.0
th= 4.3, rfp= 0.0 ppm, rfl=1441.7

Nr.	ppm	Hoehe	
1	178.93	10.5	12
2	160.92	10.9	10
3	158.00	11.3	9
4	156.51	6.0	15
5	133.53	30.7	3
6	132.41	34.5	4
7	131.56	7.6	
8	129.29	25.2	2
9	129.04	18.2	11
10	126.38	14.6	
11	125.64	32.0	1
12	124.90	28.7	5
13	124.83	9.2	
14	123.81	8.4	
15	120.87	7.8	
16	120.73	27.8	14
17	118.02	35.2	
18	116.47	8.1	
19	114.45	8.6	
20	112.65	26.6	6
21	111.77	30.5	7
22	107.38	10.5	
23	77.32	294.4	
24	77.00	300.0	
25	76.68	295.0	
26	56.39	8.1	
27	55.68	32.1	8
28	29.69	10.4	

WEB100_A/CDCl3/1H
Weigel 118/12
gHMBCAD

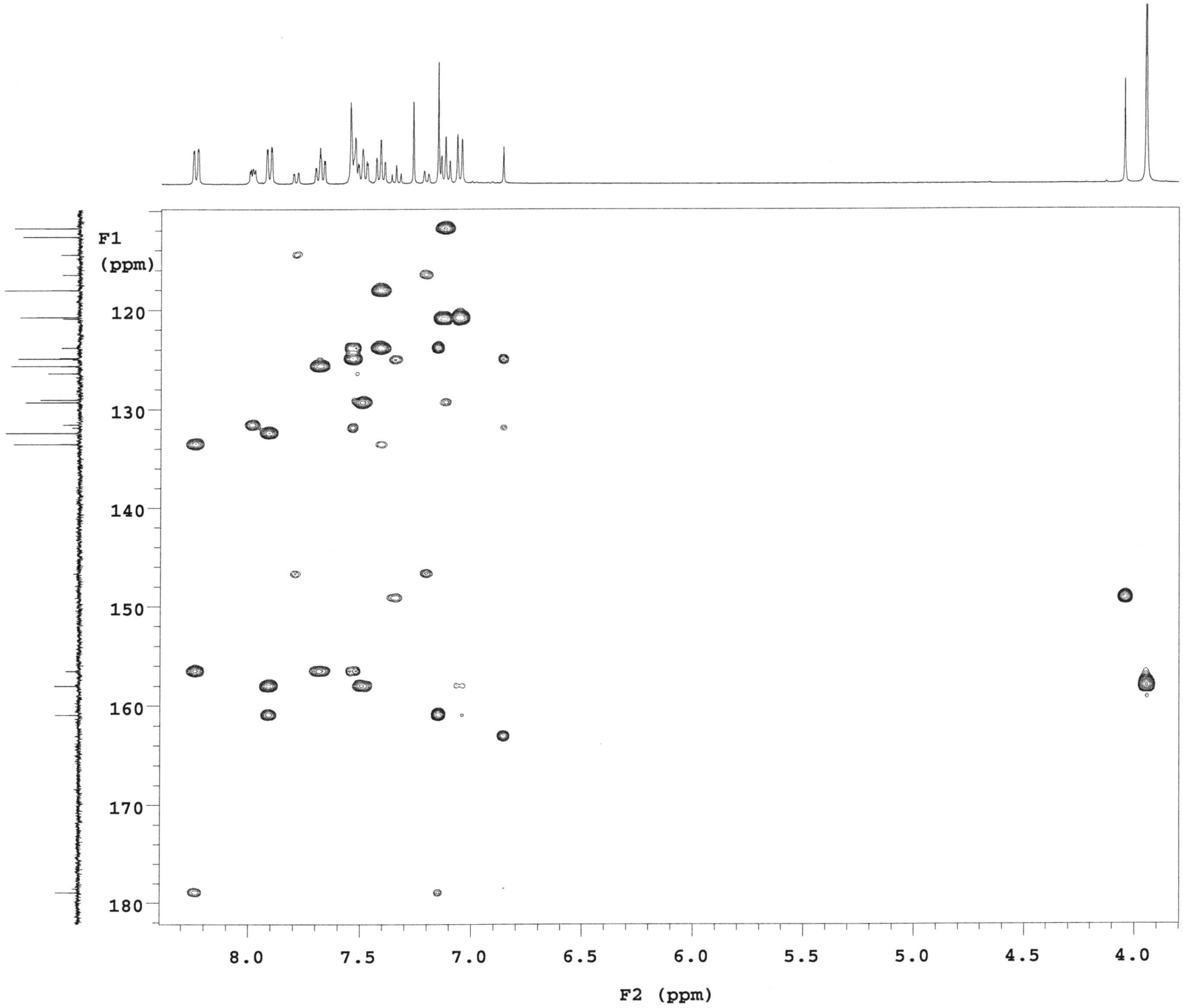
exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Apr 26 2012	hs	nn	array	phase
solvent	cdcl3	sspul	y	arraydim	512
sample	WEB100_A	PFGflg	y		
ACQUISITION		hsglvl	6216	i	phase
sw	3434.1	SPECIAL		1	1
at	0.149	temp	25.0	2	2
np	1024	gain	56		
fb	4000	spin	not used		
ss	32	GRADIENTS			
d1	1.351	gzlvl1	518		
nt	8	gt1	0.001000		
2D ACQUISITION		gzlvl3	1554		
sw1	18115.9	gt3	0.001000		
ni	256	gstab	0.000500		
phase	arrayed	F2 PROCESSING			
PRESATURATION		sb	-0.075		
satmode	n	sbs	not used		
wet	n	fn	4096		
TRANSMITTER		F1 PROCESSING			
tn	H1	gf1	0.008		
sfrq	399.814	gfs1	not used		
tof	-121.4	proc1	lp		
tpwr	61	fn1	2048		
pw	6.400	DISPLAY			
DECOUPLER		sp	239.2		
dn	C13	wp	3117.2		
dof	525.5	sp1	1013.0		
dm	nnn	wp1	17585.2		
decwave	W40_g1nmr	rf1	-162.0		
dmf	29412	rfp	0		
dpwr	36	rf11	-995.3		
pwxlvl	60	rfp1	0		
pwx	6.400	PLOT			
HMBC		wc	160.0		
j1xh	146.0	sc	0		
jnxh	8.0	wc2	140.0		
ADIABATCIC		sc2	0		
pwx180ad	g1nmr_ad3~00	vs	380		
		th	2		
pwxlvl180	49	ai cdc av			
pwx180	570.6				



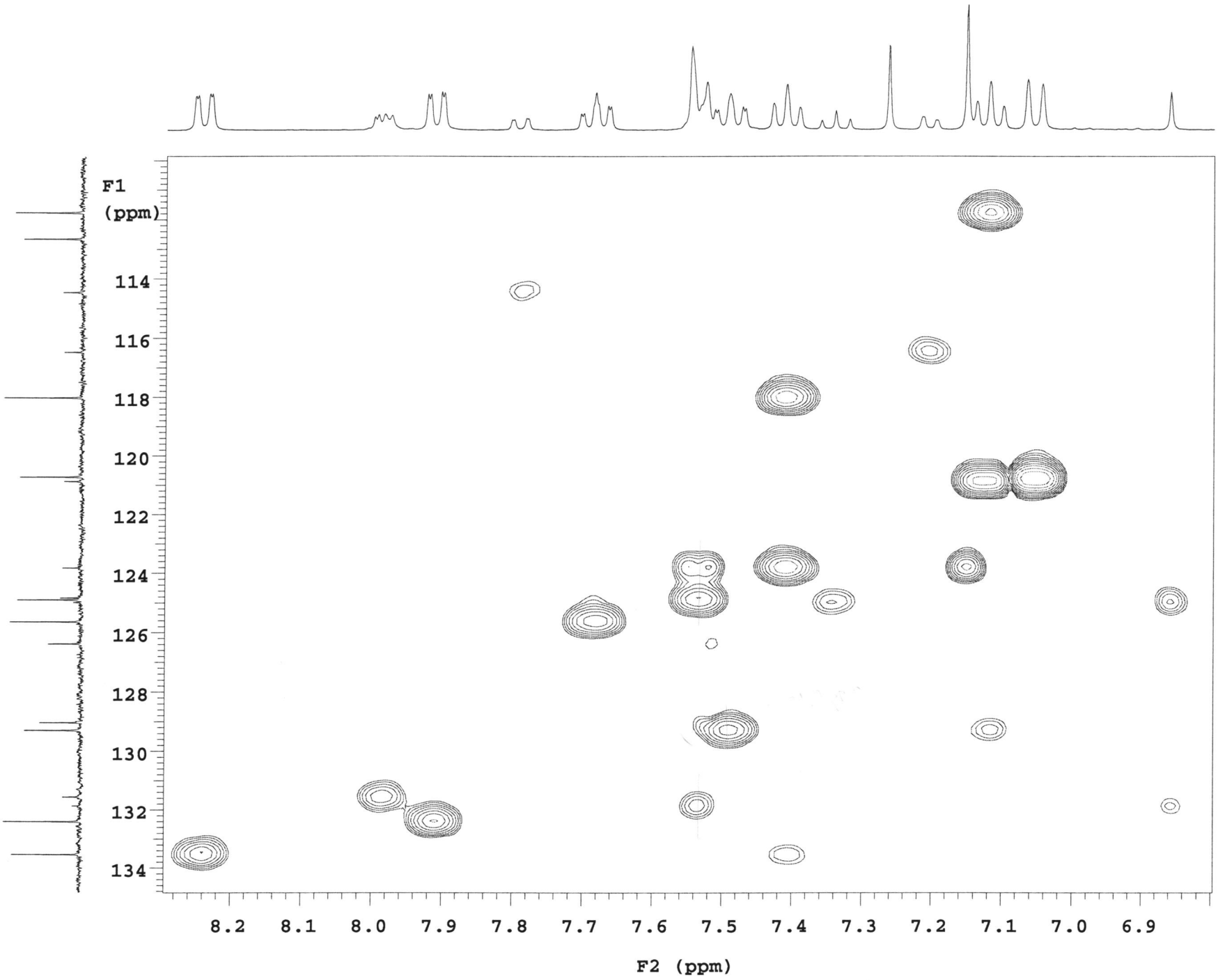
Plotname: WEB100_A_gHMBCAD_01_plot01

WEB100_A/CDCl3/1H
Weigel 118/12
gHMBCAD



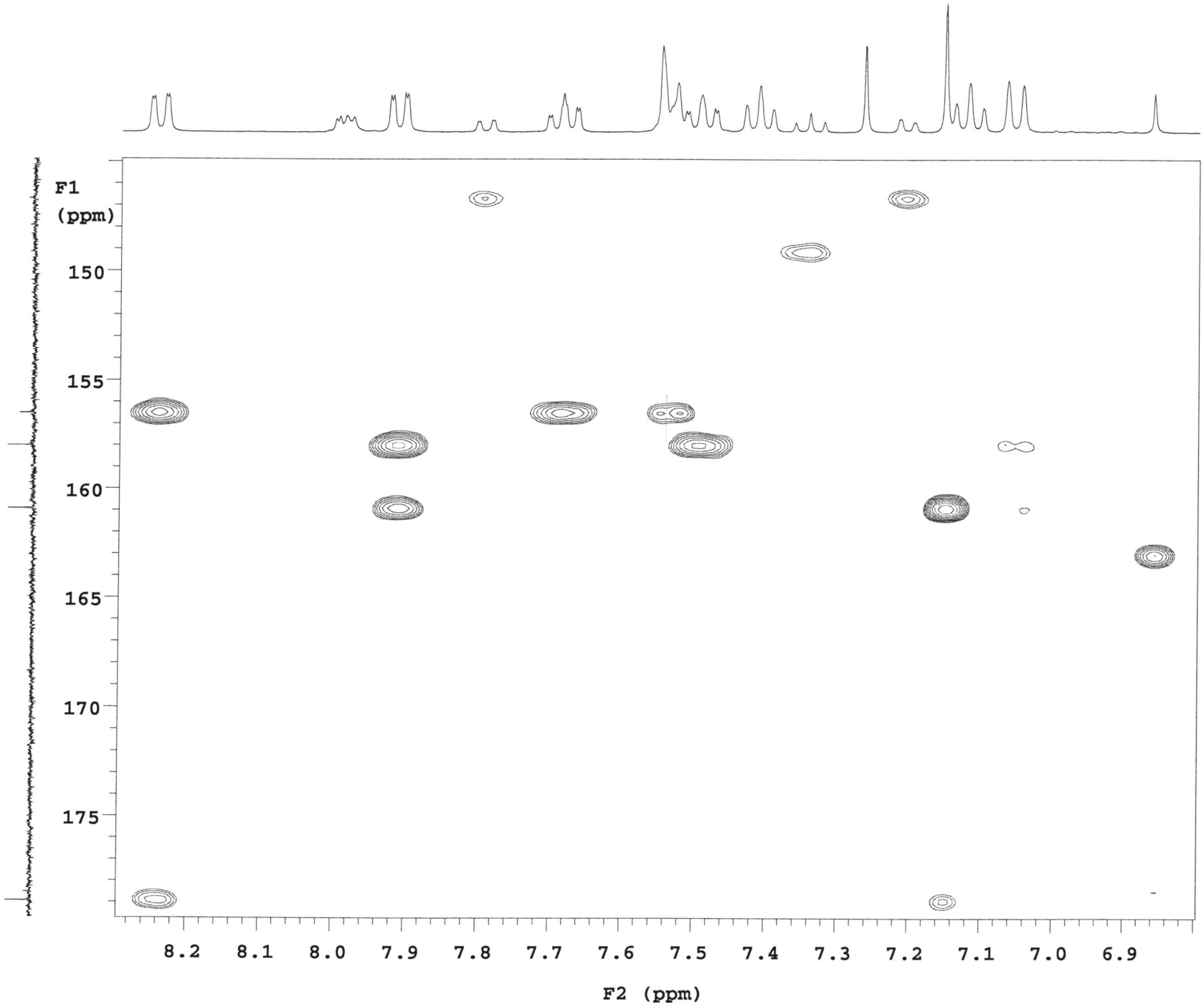
Plotname: WEB100_A_gHMBCAD_01_plot02

WEB100_A/CDC13/1H
Weigel 118/12
gHMBCAD



Plotname: WEB100_A_gHMBCAD_01_plot03

WEB100_A/CDCl3/1H
Weigel 118/12
gHMBCAD

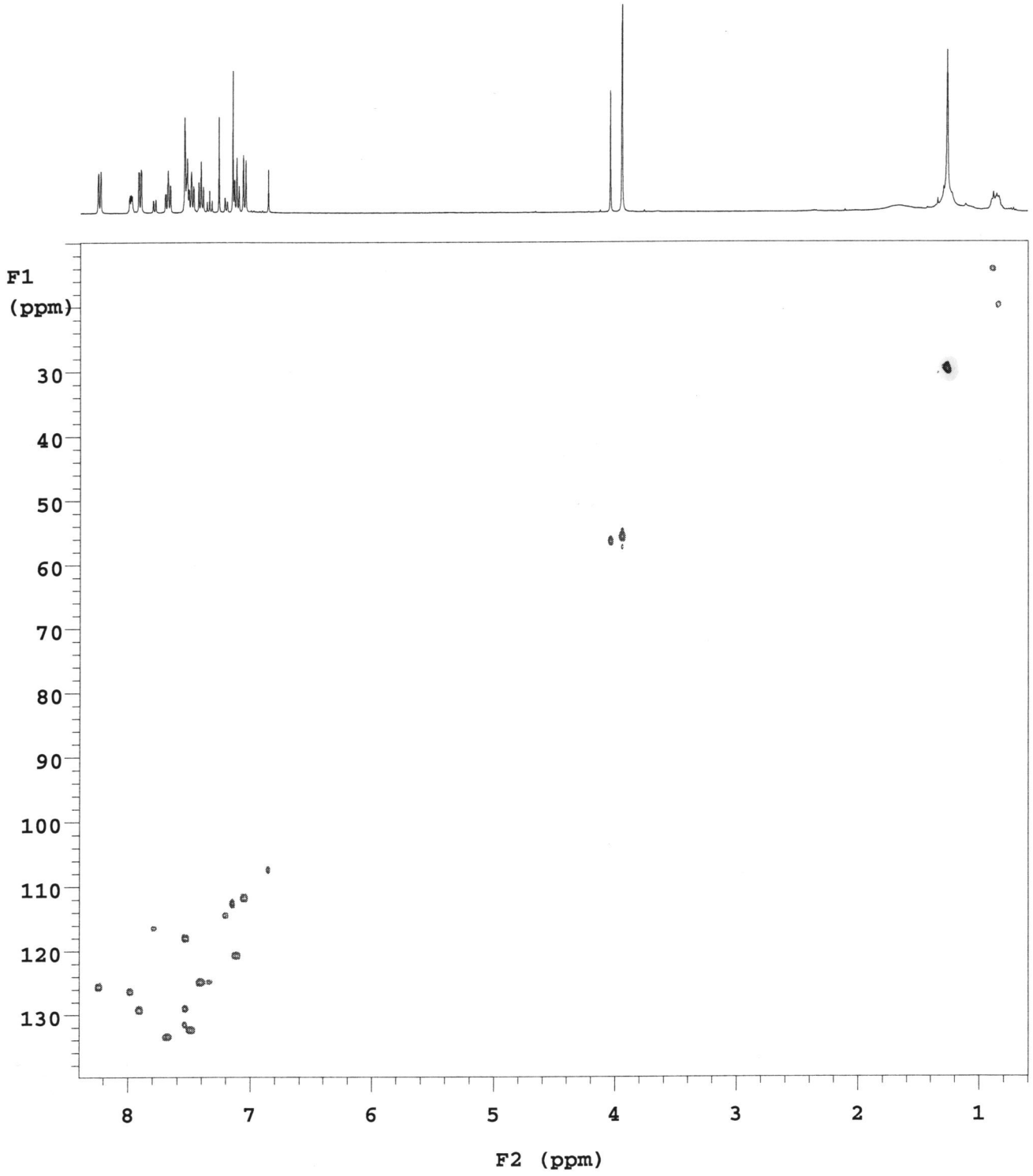


Plotname: WEB100_A_gHMBCAD_01_plot04

WEB100_A/CDCl3/1H
Weigel 118/12
gHSQCAD

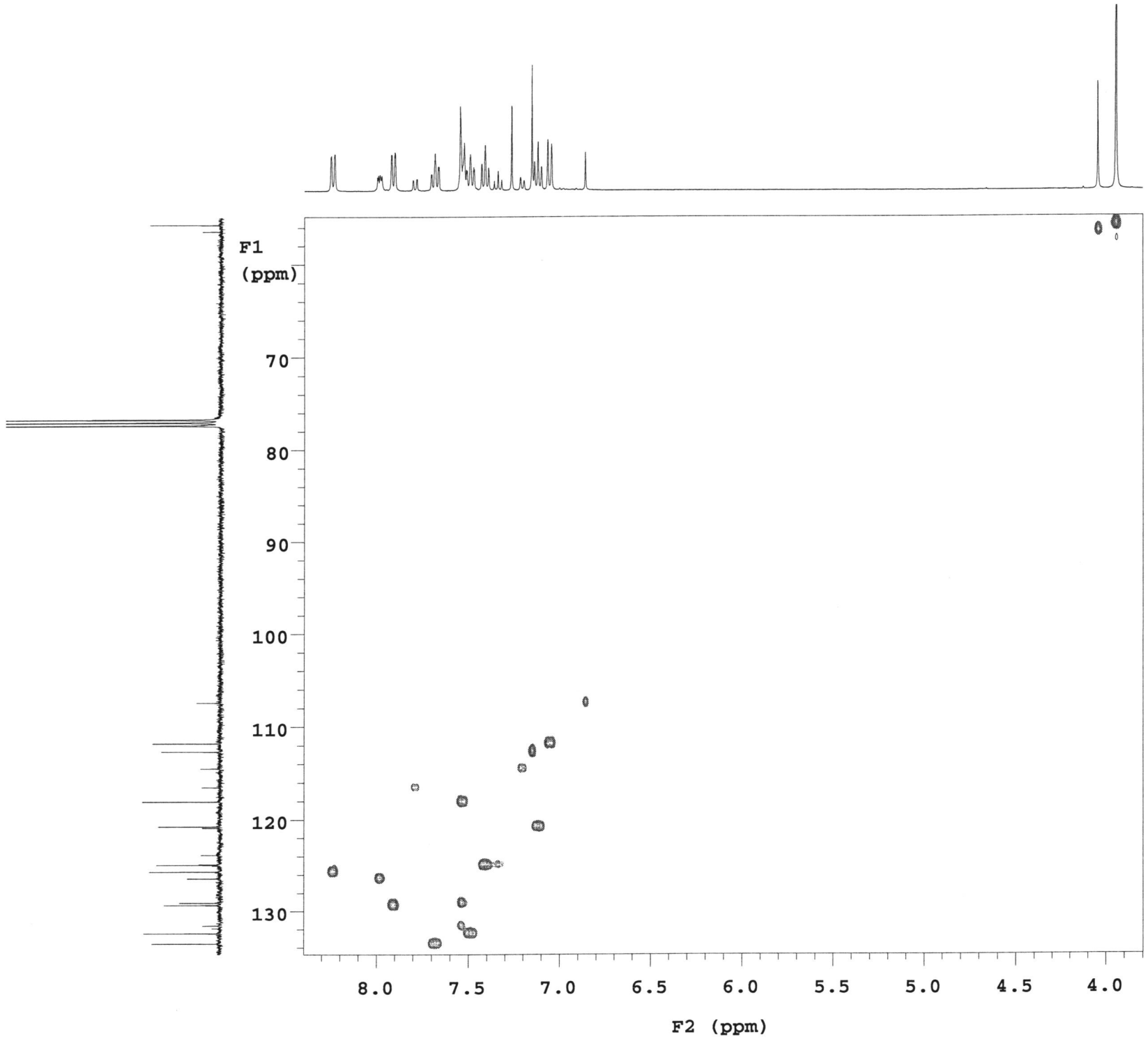
exp4 gHSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Apr 26 2012	hs	nn	array	phase
solvent	cdcl3	sspul	y	arraydim	512
sample	WEB100_A	PFGflg	y		
ACQUISITION		hsglvl	6216	i	phase
sw	3434.1	SPECIAL		1	1
at	0.149	temp	25.0	2	2
np	1024	gain	56		
fb	4000	spin	not used		
ss	32	GRADIENTS			
d1	1.351	gzlvlE	5186		
nt	4	gtE	0.002000		
2D ACQUISITION		EDratio	3.977		
sw1	20105.6	gstab	0.000500		
ni	256	F2 PROCESSING			
phase	arrayed	lb	0.40		
PRESATURATION		gf	0.069		
satmode	n	gfs	not used		
wet	n	fn	4096		
TRANSMITTER		F1 PROCESSING			
tn	H1	gf1	0.007		
sfrq	399.814	gfs1	not used		
tof	-121.4	proc1	lp		
tpwr	61	fn1	2048		
pw	6.400	DISPLAY			
DECOUPLER		sp	239.2		
dn	C13	wp	3117.2		
dof	-479.9	sp1	997.8		
dm	nny	wp1	13056.8		
decwave	W40_g1nmr	rf1	-162.0		
dmf	29412	rfp	0		
dpwr	36	rfl1	1004.9		
pwxlvl	60	rfp1	0		
pwx	6.400	PLOT			
HSQC		wc	160.0		
j1xh	146.0	sc	0		
nullflg	y	wc2	140.0		
mult	2	sc2	0		
ADIABATIC		vs	380		
pwx180ad	g1nmr_ad300	th	2		
		ai cdc ph			
pwx180adR	g1nmr_ad300R				
pwx180	570.6				
pwxlvl180	49				
pwx180ref	g1nmr_ref200				
pwx180r	1999.2				
pwxlvl180r	42				



Plotname: WEB100_A_gHSQCAD_01_plot01

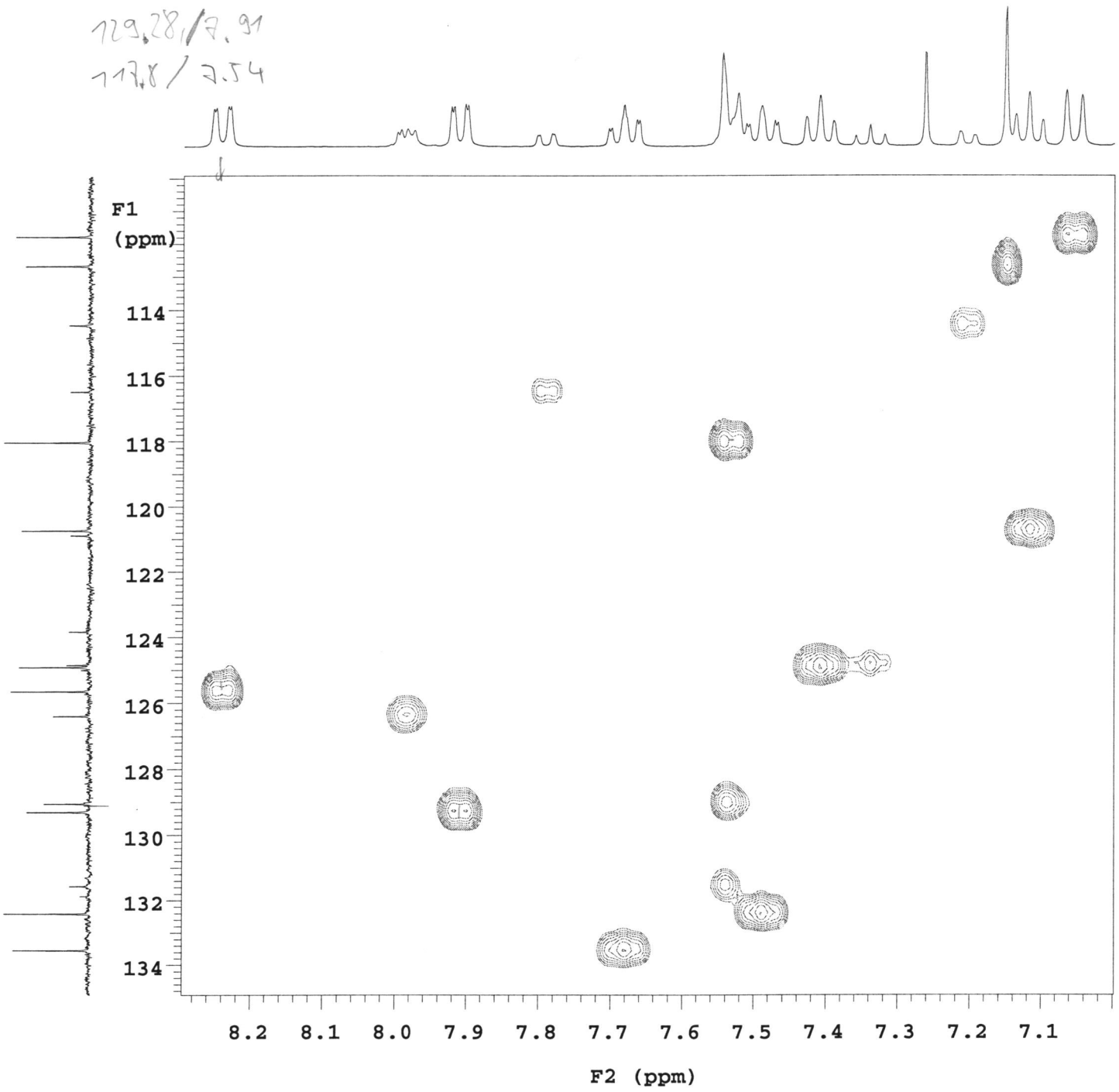
WEB100_A/CDCl3/1H
Weigel 118/12
gHSQCAD



Plotname: WEB100_A_gHSQCAD_01_plot02

WEB100_A/CDCl3/1H
Weigel 118/12
gHSQCAD

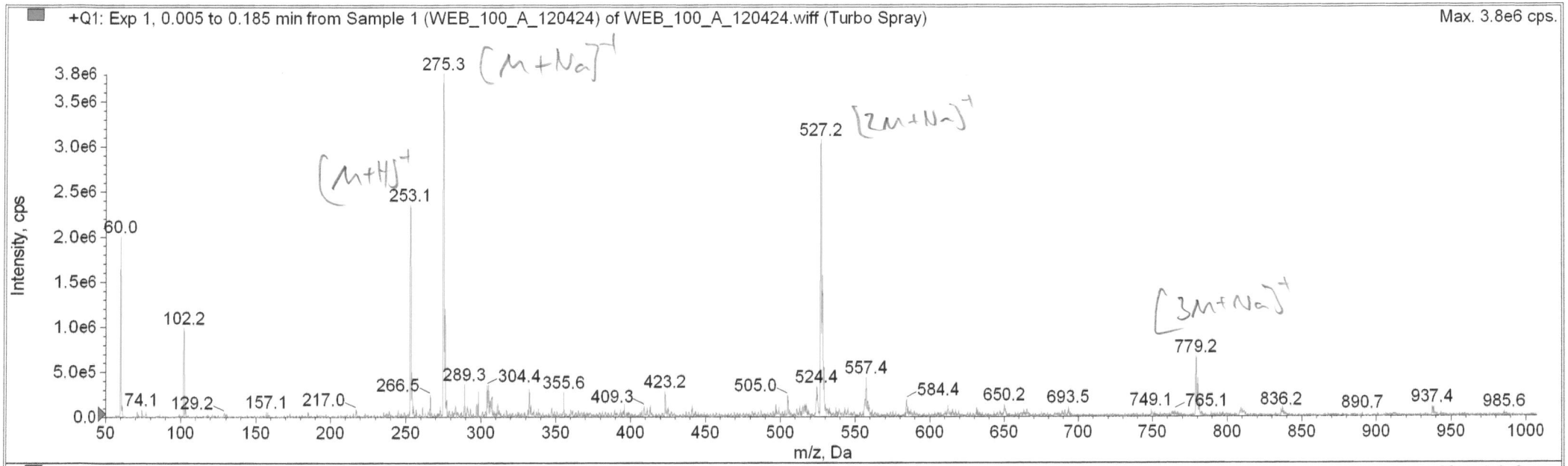
125.6 ppm / 8.23 ppm
129.28 / 7.91
117.8 / 7.54

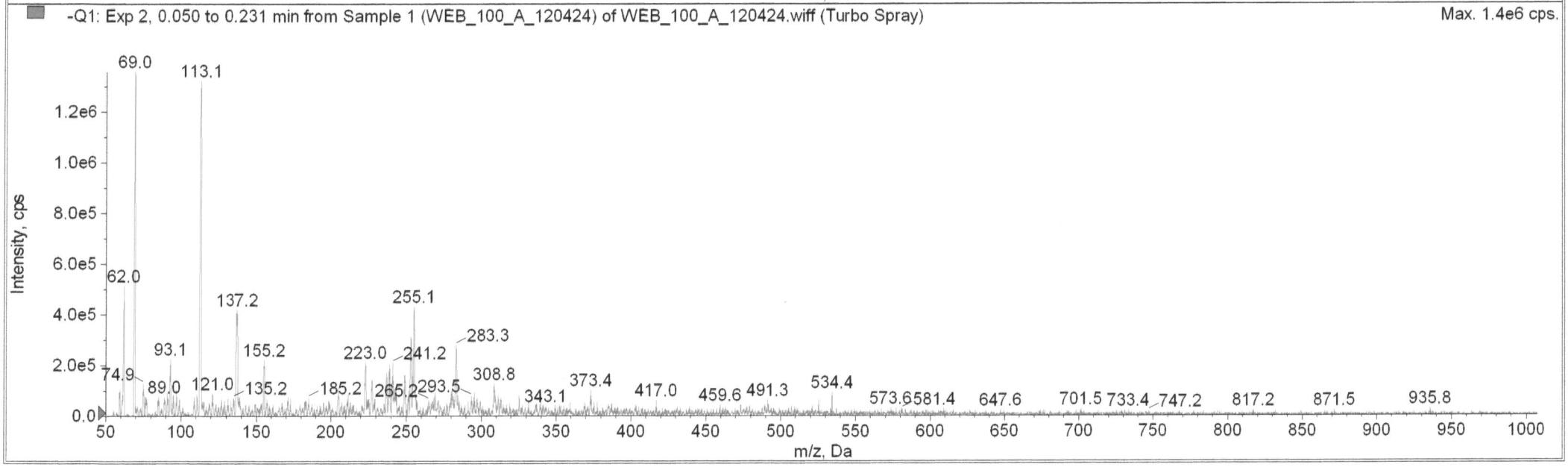


Plotname: WEB100_A_gHSQCAD_01_plot03

Acq. File: WEB_100_A_120424.wiff
Acq. Date: Tuesday, April 24, 2012
Acq. Time: 12:54

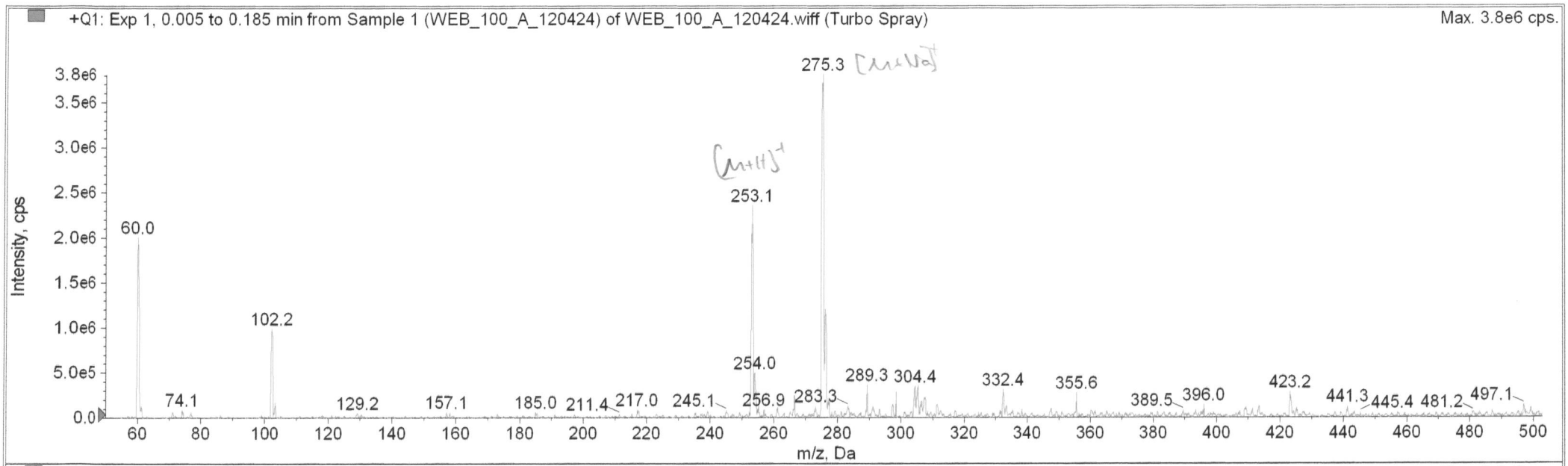
$C_{16}H_{12}O_3$?

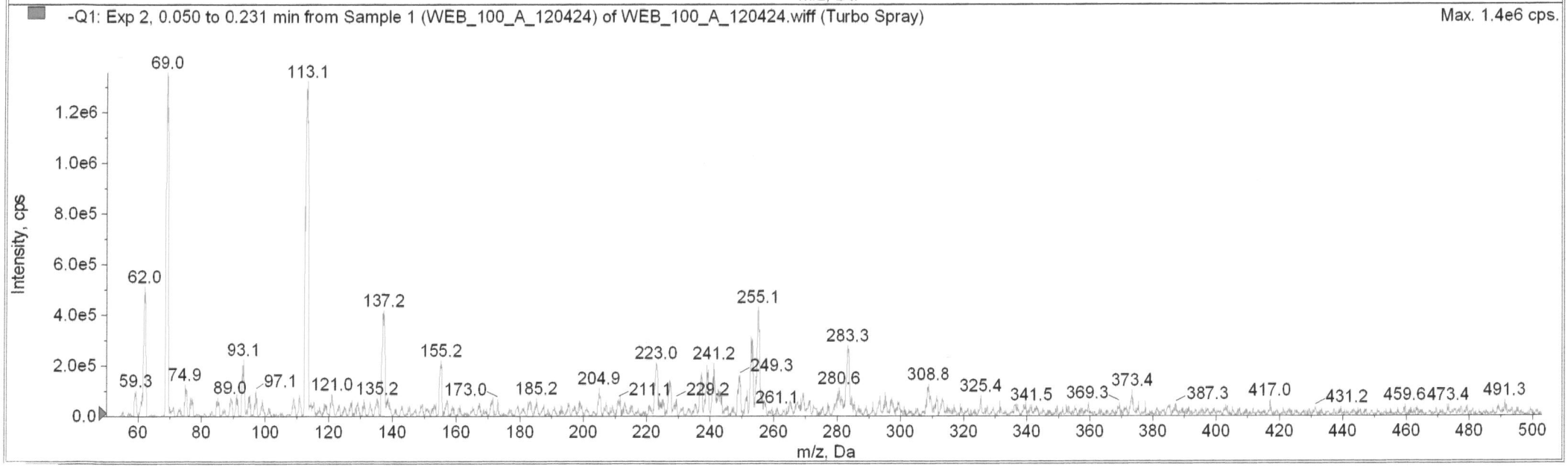


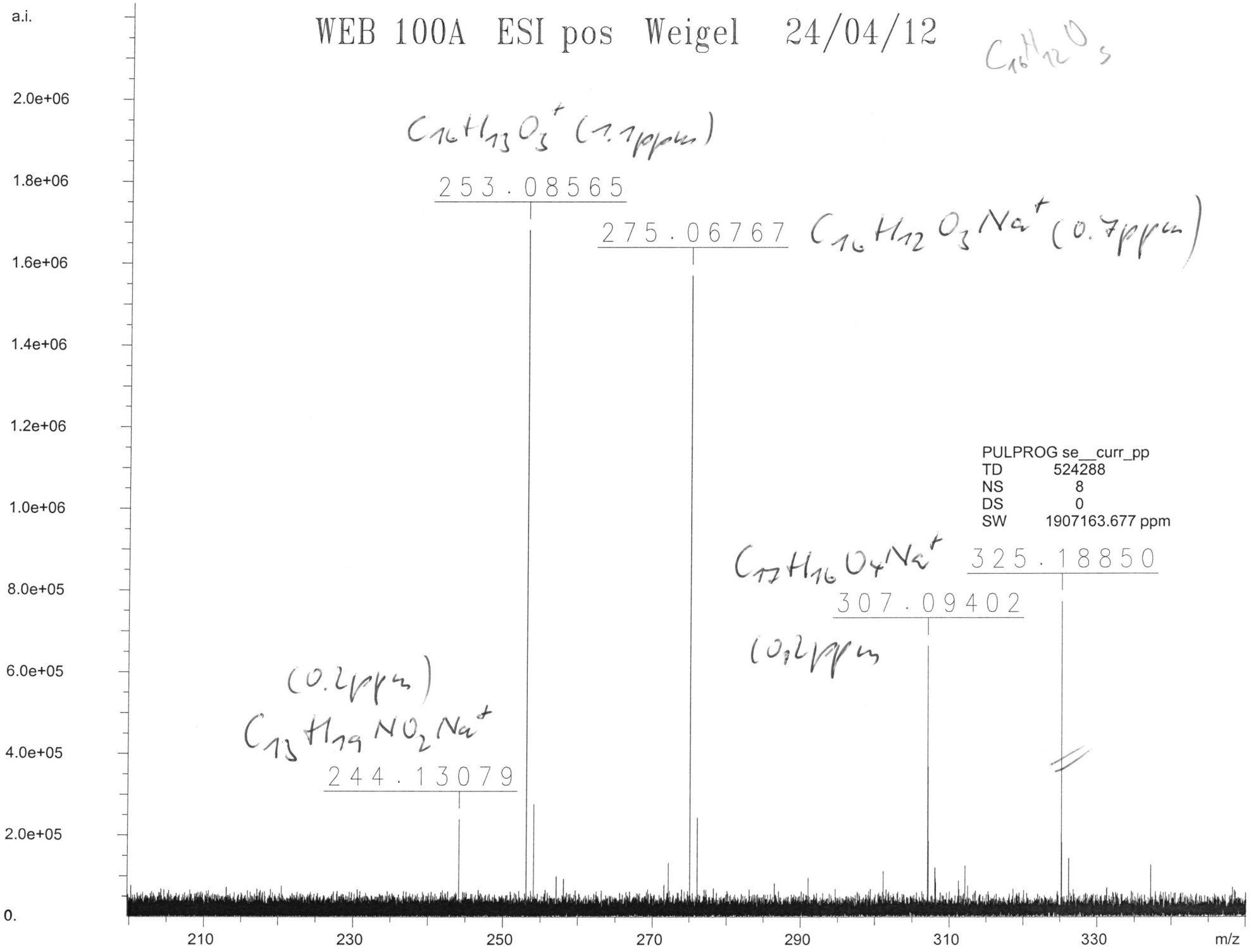


Acq. File: WEB_100_A_120424.wiff
Acq. Date: Tuesday, April 24, 2012

Acq. Time: 12:54






WEB 100A ESI pos Weigel 24/04/12
C16H12O3
C16H13O3+ (1.7ppm)
253.08565
275.06767 C16H12O3Na+ (0.7ppm)
C17H16O4Na+ 325.18850
307.09402
(0.2ppm)
(0.2ppm)
C13H19NO2Na+
244.13079
PULPROG se__curr_pp
TD 524288
NS 8
DS 0
SW 1907163.677 ppm
a.i.
2.0e+06
1.8e+06
1.6e+06
1.4e+06
1.2e+06
1.0e+06
8.0e+05
6.0e+05
4.0e+05
2.0e+05
0.
210
230
250
270
290
310
330
m/z