exp7   PROTON

SAMPLE
date   Apr 18 2012
samplename WEB097_D
solvent   cdcl3
file   exp
ACQUISITION
instrum   g400
probe_   g1nmr
seqfil   s2pul
sfrq   399.815
tn   H1
at   2.281
np   32768
sw   7183.9
bs   4
tpwr   61
pw   2.1
d1   0.719
d2   0
tof   799.6
nt   40
ct   40
alock   n
gain   44
FLAGS
il   n
in   n
dp   y
DEC. & VT
dn   C13
dfrq   100.542
homo   n
dpwr   36
dof   0
dm   nnn
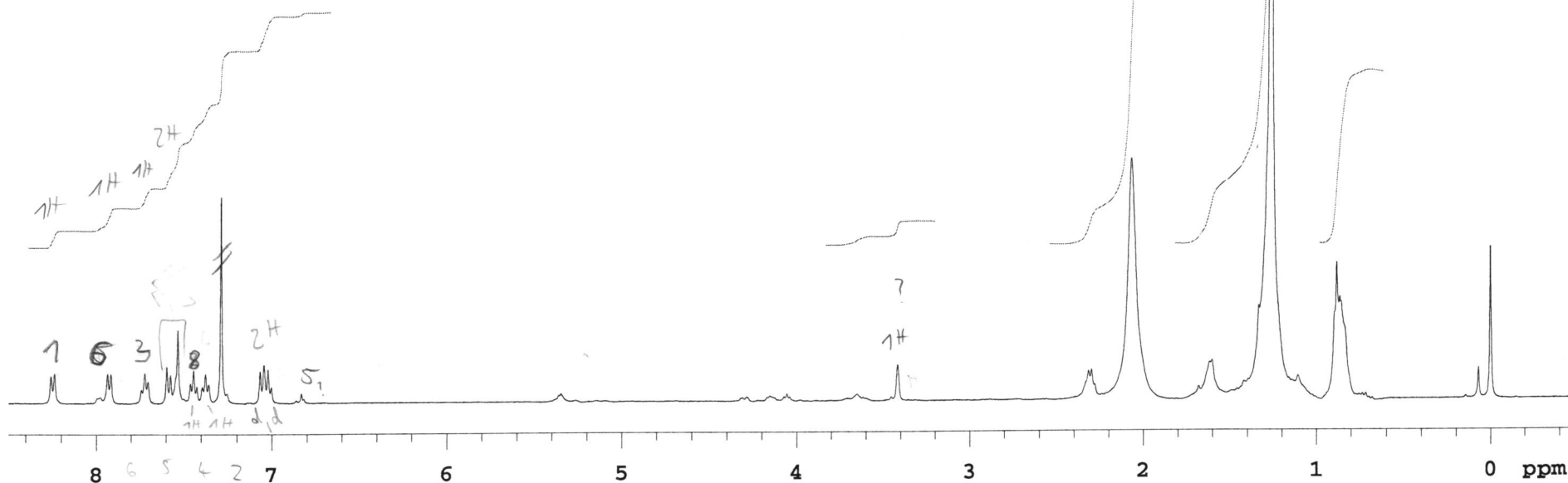dmm   c
dmf   29412
pplvl   55
pp   15.0
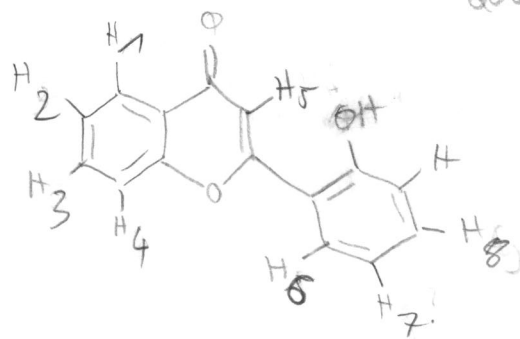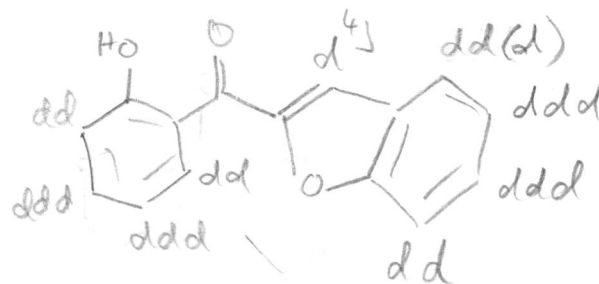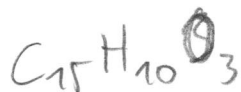temp   25.0
PROCESSING
lb   0.40
wtfile
proc   ft
fn   32768

wexp   process
DISPLAY
sp   -200.2
wp   3598.1
vs   170
sc   0
wc   250
hzmm   14.39
is   1900.00
rfl   781.1
rfp   0
th   7.0
ins   100.000
rp   74.2
lp   0
nm cdc ph

$C_{15}H_{10}O_3$

8 6 5 4 2 7   6   5   4   3   2   1   0   ppm

WEB097_D/CDC13/13C
Weigel 20120418_04
Thu Apr 19 17:25 2012
duration: 15h 28min

exp1 CARBON

         SAMPLE
date   Apr 19 2012
samplename WEB097_D
solvent   cdc13
file   exp
     ACQUISITION
instrum   g400
probe_   g1nmr
seqfil   s2pul
sfrq   100.544
tn   C13
at   1.311
np   65536
sw   25000.0
bs   16
tpwr   59
pw   3.4
d1   2.189
d2   0
tof   1530.8
nt   20000
ct   15920
alock   n
gain   30
        FLAGS
il   n
in   n
dp   y
     DEC. & VT
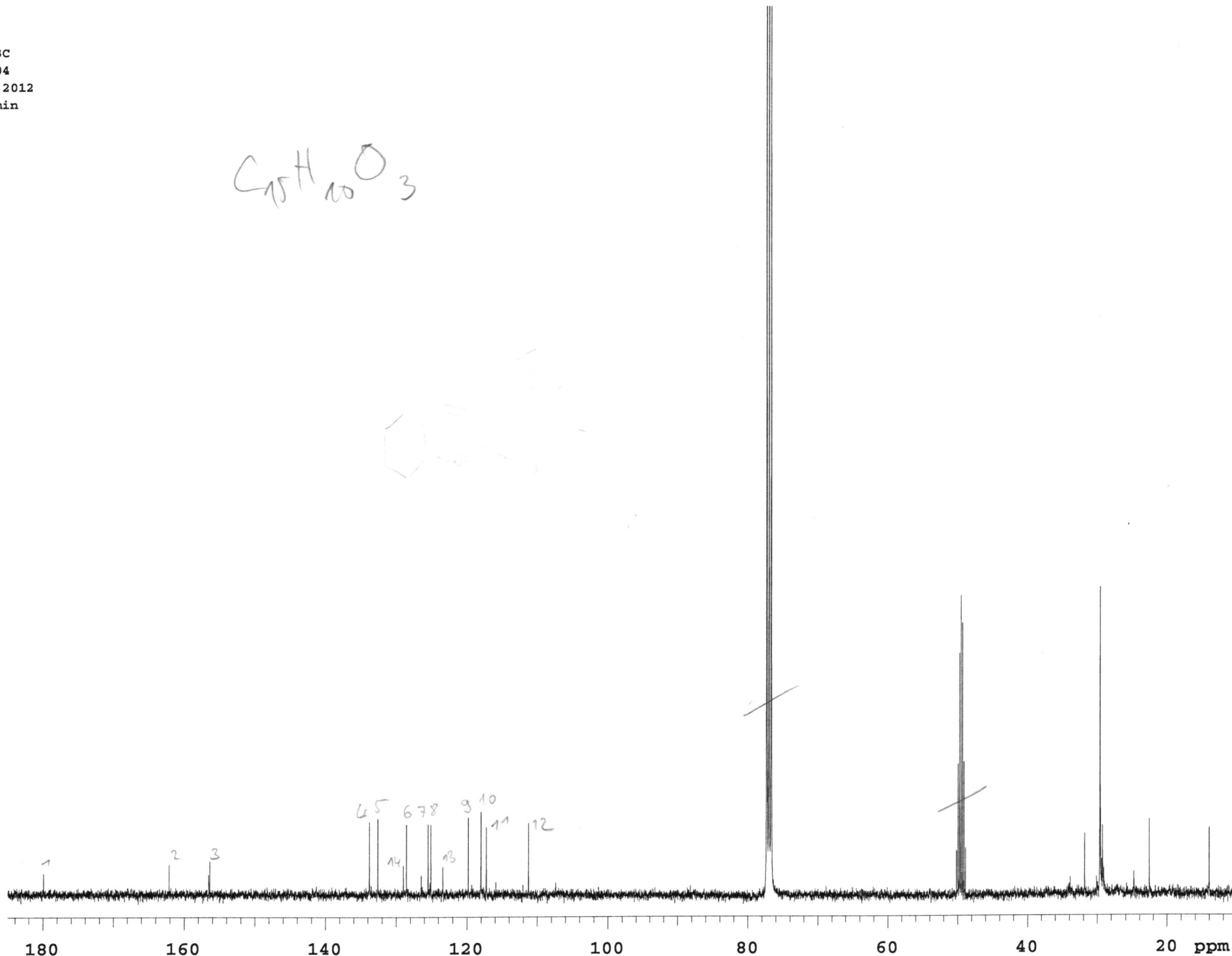dn   H1
dfrq   399.814
homo   n
dpwr   38
dof   0
dm   yyy
dmm   w
dmf   9804
pplvl   61
pp   7.0
temp   25.0
      PROCESSING
lb   0.80
wtfile
proc   ft
fn   65536

werr   cpreact
wexp   process
      DISPLAY
sp   1004.7
wp   17594.9
vs   800
sc   0
wc   250
hzmm   70.38
rf1   9184.6
rfp   7741.0
th   3.0
rp   40.9
lp   0
nm cdc ph

$C_{15}H_{10}O_3$

Halle/Saale, 20-04-12 08 Uhr 55

WEB097_D/CDCl3/13C
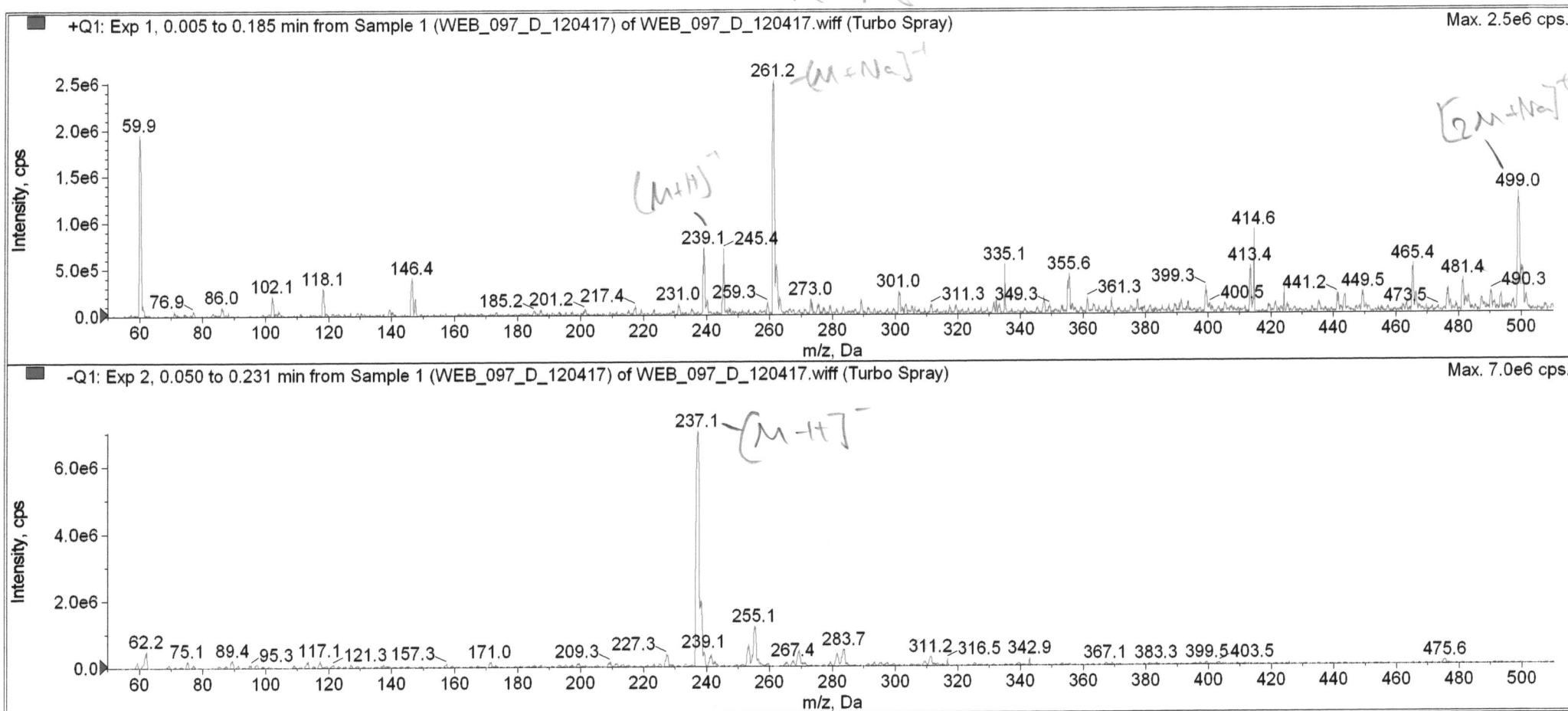Weigel 20120418_04

Apr 19 2012   C13 100.533 MHz CARBON
185.0 bis 10.0 ppm, vs= 800.0
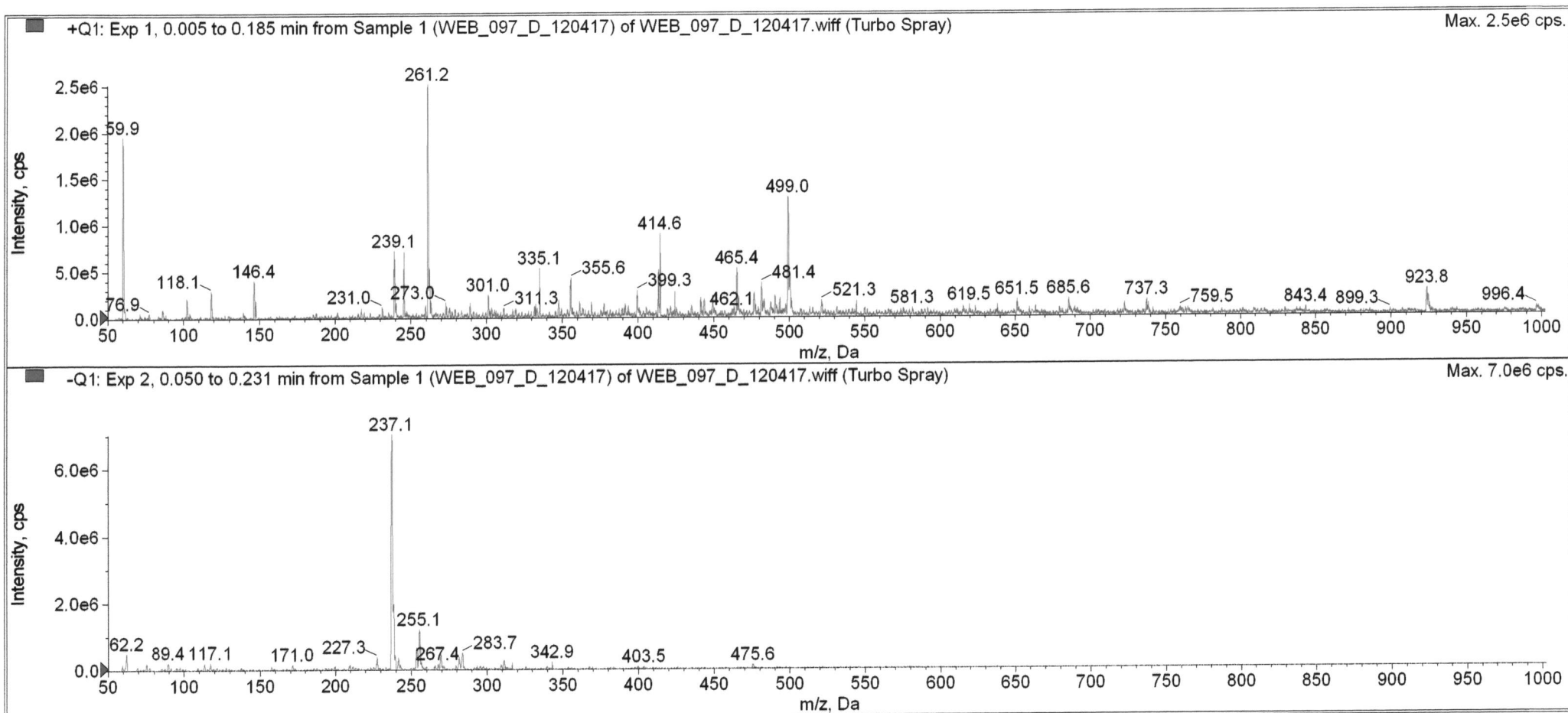th=   3.0, rfp=77.0 ppm, rfl=9184.6

Nr.	ppm	Hoehe
1	179.95	4.0
2	162.12	5.8
3	156.57	3.7
4	156.41	6.5
5	133.82	14.5
6	132.62	15.2
7	129.00	5.6
8	128.58	14.0
9	126.45	3.5
10	125.48	14.0
11	125.09	14.0
12	123.40	5.3
13	119.83	15.4
14	118.02	16.6
15	117.26	13.5
16	111.27	14.3
17	77.32	791.7
18	77.20	25.1
19	77.00	800.0
20	76.68	777.4
21	50.16	8.4
22	49.95	26.1
23	49.74	48.4
24	49.52	60.1
25	49.30	54.5
26	49.09	26.6
27	48.88	8.9
28	31.85	11.8
29	29.63	61.7
30	29.41	6.6
31	29.29	13.5
32	29.22	5.6
33	29.09	4.7
34	24.85	4.0
35	22.61	14.7
36	14.02	13.0

$C_{17}H_{10}O_3$?

M = 238   Flavonol ?
XX hydroxylich flavon

+Q1: Exp 1, 0.005 to 0.185 min from Sample 1 (WEB_097_D_120417) of WEB_097_D_120417.wiff (Turbo Spray)   Max. 2.5e6 cps.

261.2 [M+Na]+

[M+H]+

[2M+Na]+

Intensity, cps

59.9
76.9 86.0 102.1 118.1 146.4 185.2 201.2 217.4 231.0 239.1 245.4 259.3 273.0 301.0 311.3 349.3 335.1 355.6 361.3 399.3 400.5 413.4 414.6 441.2 449.5 465.4 473.5 481.4 490.3 499.0

m/z, Da

-Q1: Exp 2, 0.050 to 0.231 min from Sample 1 (WEB_097_D_120417) of WEB_097_D_120417.wiff (Turbo Spray)   Max. 7.0e6 cps.

237.1 [M-H]-

Intensity, cps

62.2 75.1 89.4 95.3 117.1 121.3 157.3 171.0 209.3 227.3 239.1 255.1 267.4 283.7 311.2 316.5 342.9 367.1 383.3 399.5 403.5 475.6

m/z, Da

+Q1: Exp 1, 0.005 to 0.185 min from Sample 1 (WEB_097_D_120417) of WEB_097_D_120417.wiff (Turbo Spray)   Max. 2.5e6 cps.

-Q1: Exp 2, 0.050 to 0.231 min from Sample 1 (WEB_097_D_120417) of WEB_097_D_120417.wiff (Turbo Spray)   Max. 7.0e6 cps.

WEB 097D   ESI neg   Weigel   24/04/12

$C_{15}H_9O_3^-$ (0.7 ppm)

237.05554

238.05884

255.23282

283.26429

PULPROG se__curr_pp
TD   524288
NS   8
DS   0
SW   1907163.677 ppm

exp9 PROTON

SAMPLE
date   Apr 17 2012
samplename WEB097_A
solvent   cdcl3
file   exp
ACQUISITION
instrum   g400
probe_   g1nmr
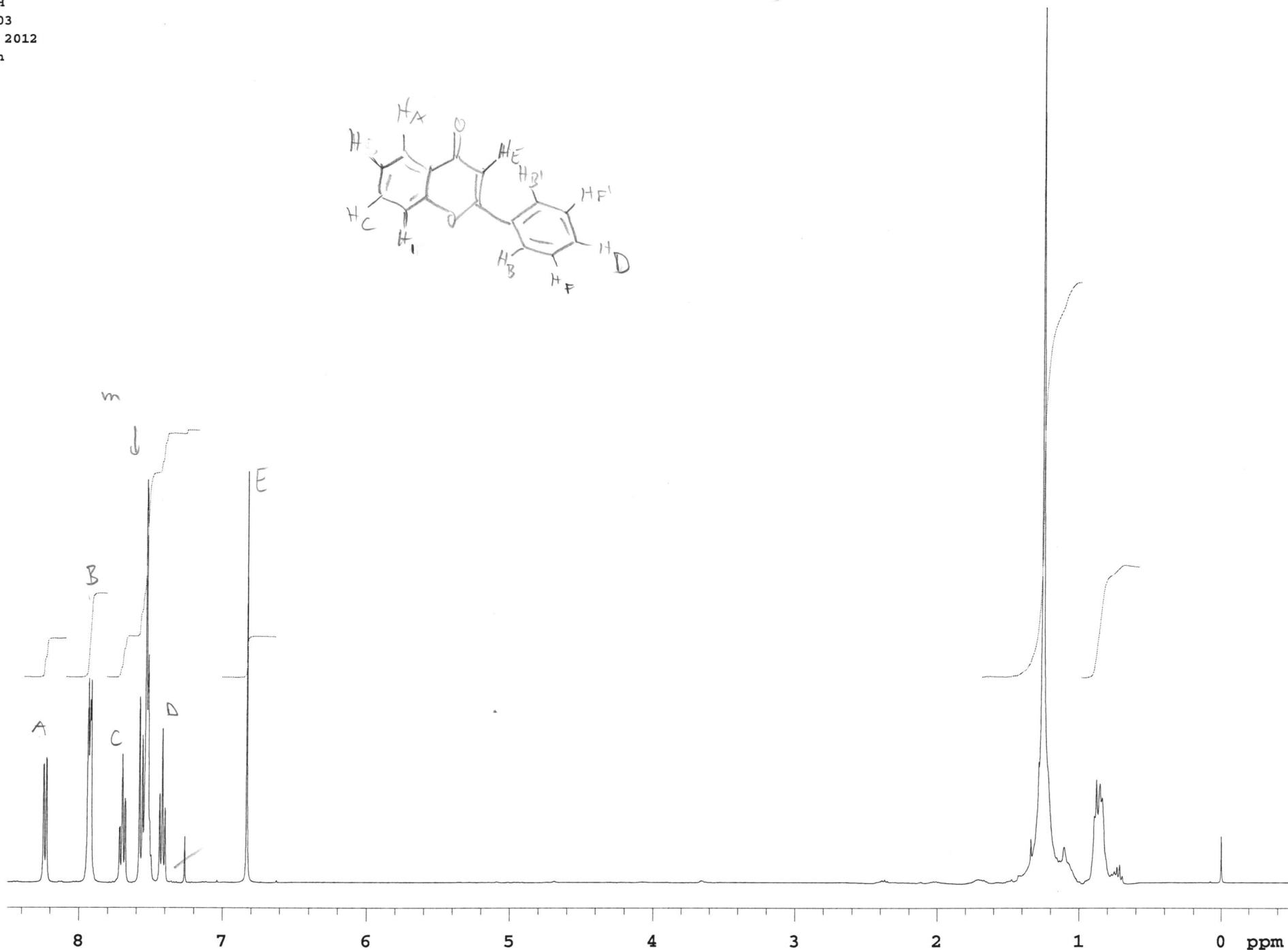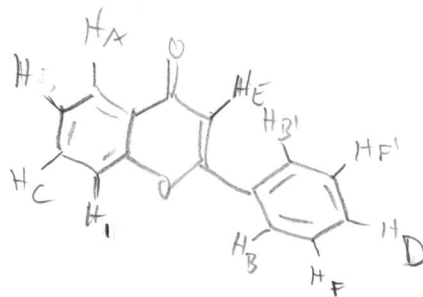seqfil   s2pul
sfrq   399.815
tn   H1
at   2.281
np   32768
sw   7183.9
bs   4
tpwr   61
pw   2.1
d1   0.719
d2   0
tof   799.6
nt   40
ct   40
alock   n
gain   34
FLAGS
il   n
in   n
dp   y
DEC. & VT
dn   C13
dfrq   100.542
homo   n
dpwr   36
dof   0
dm   nnn
dmm   c
dmf   29412
pplvl   55
pp   15.0
temp   25.0
PROCESSING
lb   0.40
wtfile
proc   ft
fn   32768

wexp   process
DISPLAY
sp   -200.3
wp   3598.1
vs   170
sc   0
wc   250
hzmm   14.39
is   630.00
rfl   791.4
rfp   0
th   7.0
ins   100.000
rp   87.8
lp   3.9
nm cdc ph

Halle/Saale, 17-04-12 16 Uhr 12

WEB097_A/CDCl3/1H
Weigel 20120417_03

Apr 17 2012   H1 399.812 MHz   PROTON
8.50 bis -0.50 ppm, vs= 170.0
th=   2.2, rfp=0.00 ppm, rfl=791.35

Nr.	Hz	ppm	Hoehe
1	3297.83	8.248	23.0
2	3296.51	8.245	23.2
3	3289.94	8.229	24.4
4	3288.62	8.225	24.1
5	3175.06	7.941	33.7
6	3173.30	7.937	39.7
7	3168.04	7.924	35.6
8	3165.85	7.918	39.4
9	3086.92	7.721	10.7
10	3085.17	7.717	11.0
11	3078.15	7.699	25.1
12	3071.14	7.681	16.5
13	3069.82	7.678	15.9
14	3030.80	7.581	36.2
15	3022.47	7.560	28.7
16	3013.70	7.538	78.2
17	3012.38	7.535	76.6
18	3006.68	7.520	44.3
19	2997.91	7.498	5.3
20	2974.24	7.439	17.4
21	2966.78	7.420	30.1
22	2959.33	7.402	14.6
23	2903.64	7.263	9.0
24	2731.76	6.833	79.8
25	535.02	1.338	8.6
26	513.54	1.284	23.7
27	501.70	1.255	170.0
28	463.11	1.158	4.9
29	455.22	1.139	4.2
30	453.03	1.133	4.2
31	442.07	1.106	7.0
32	357.44	0.894	13.1
33	355.69	0.890	13.0
34	351.30	0.879	20.2
35	341.66	0.855	19.4
36	335.08	0.838	16.7
37	300.88	0.753	2.2
38	292.99	0.733	3.0
39	285.53	0.714	3.5
40	0.09	0.000	9.1