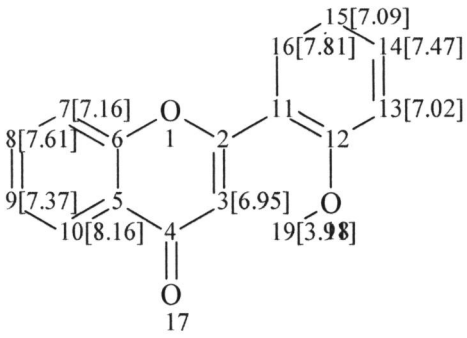
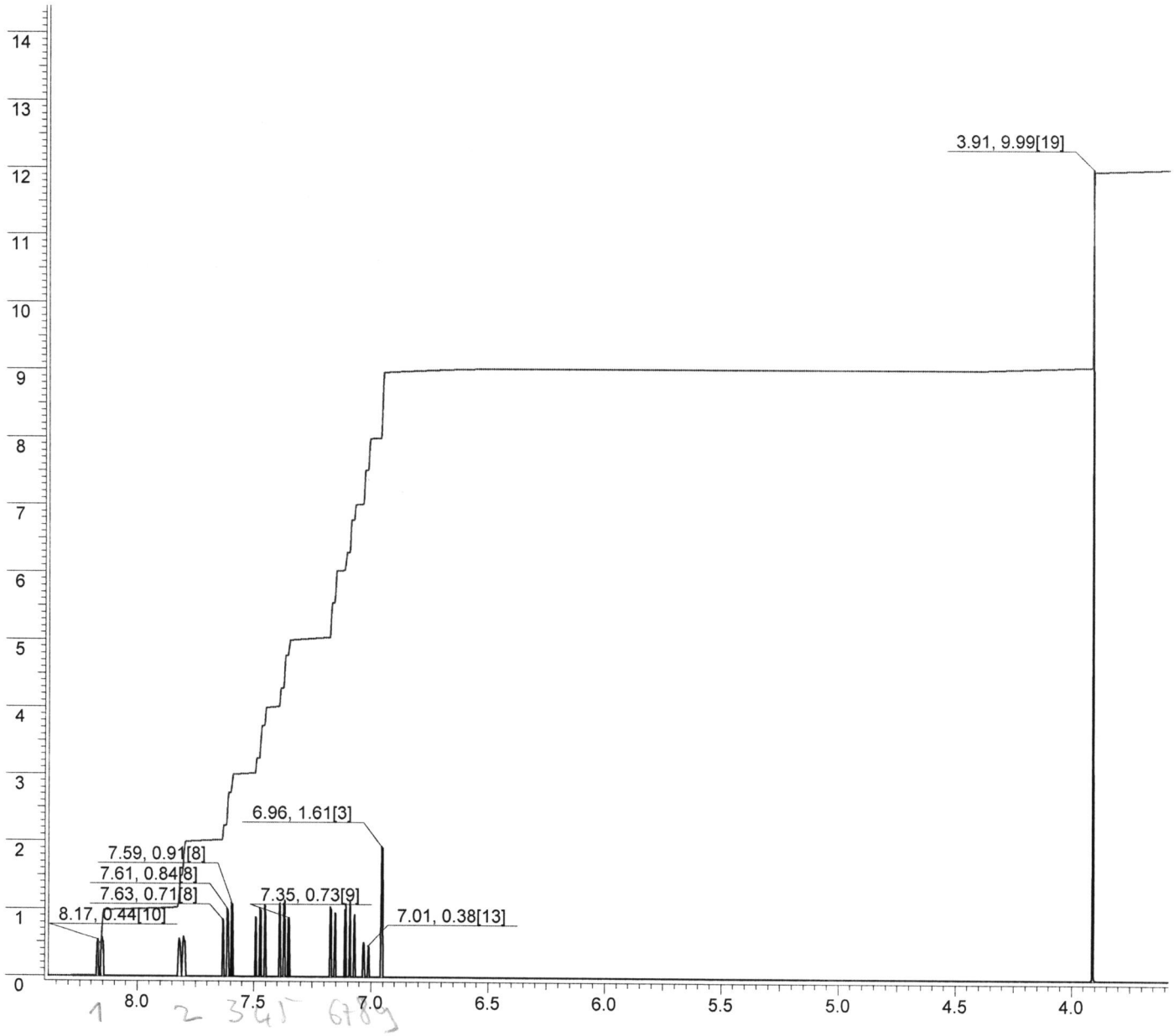
24/Apr/2012 15:27:05 ACD/C+H NMR Predictors and DB (v.12.01)



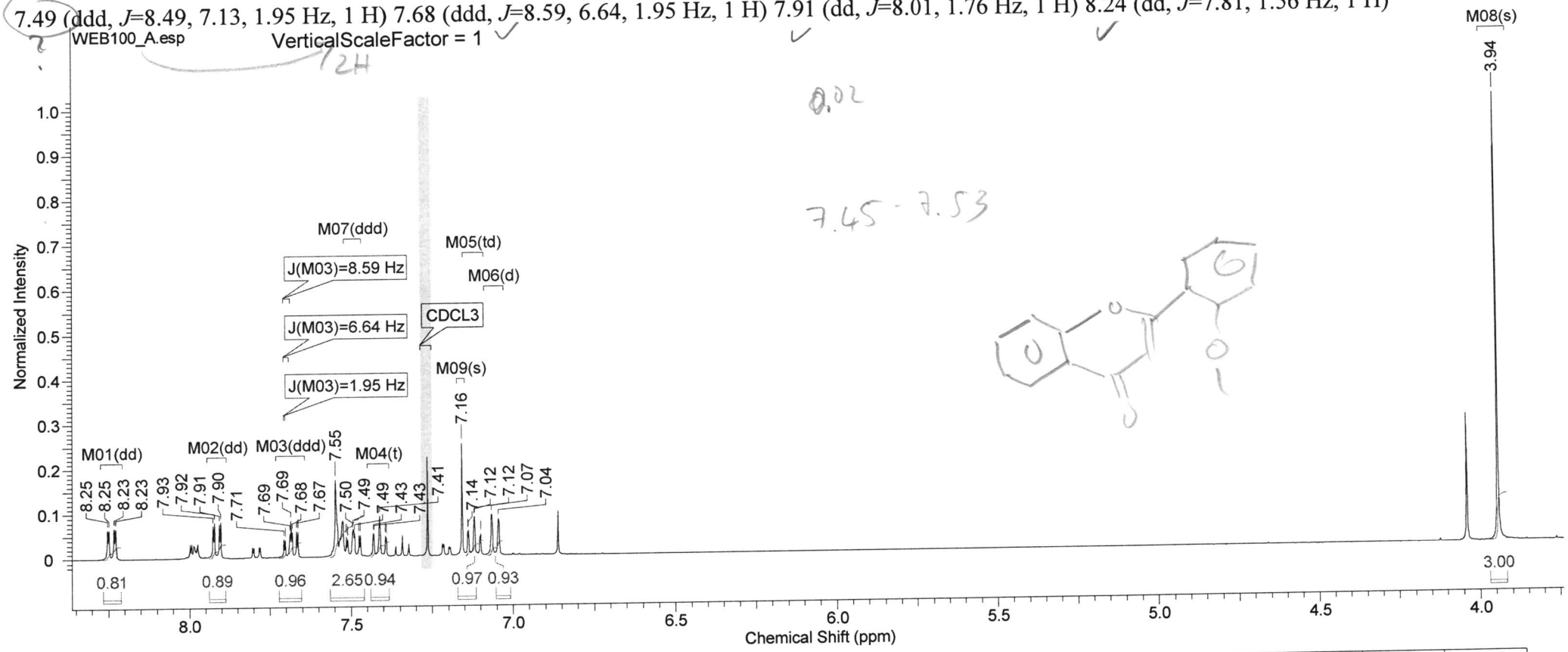
File Name \\nas1-ipb\nwc_ed\bweigel\Eigene Dateien\Projekte\Flavonoids\Primula\2'-methoxy-flavone_CDCL3.HSP (modified on 24 APR 2012)

Group	nH	Shift	Conf. Limits	Av.Exp	Neural Net
3	1	**6.95**	0.33	6.97..7.35	6.72
7	1	**7.16**	0.41	6.88..7.42	7.49
8	1	**7.61**	0.41	7.52..7.67	7.60
9	1	**7.37**	0.41	7.34..7.40	7.34
10	1	**8.16**	0.41	8.16	8.14
13	1	**7.02**	0.41	7.02	7.02
14	1	**7.47**	0.41	7.47	7.38
15	1	**7.09**	0.41	7.09	7.15
16	1	**7.81**	0.41	7.83	7.81
19	3	**3.91**	0.28	3.91	3.74



25.04.2012 14:02:27

^{1}H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 3.94 (s, 3 H) 7.06 (d, *J*=8.59 Hz, 1 H) 7.12 (td, *J*=7.40, 0.80 Hz, 1 H) 7.16 (s, 1 H) 7.41 (t, *J*=8.00 Hz, 1 H) 7.49 (ddd, *J*=8.49, 7.13, 1.95 Hz, 1 H) 7.68 (ddd, *J*=8.59, 6.64, 1.95 Hz, 1 H) 7.91 (dd, *J*=8.01, 1.76 Hz, 1 H) 8.24 (dd, *J*=7.81, 1.56 Hz, 1 H)



No.	(ppm)	(Hz)	Height
1	3.94	1577.4	1.0000
2	7.04	2817.3	0.0831
3	7.07	2825.9	0.0930
4	7.10	2839.2	0.0487
5	7.10	2839.9	0.0453
6	7.12	2847.0	0.0877
7	7.12	2847.7	0.0854
8	7.14	2854.4	0.0573

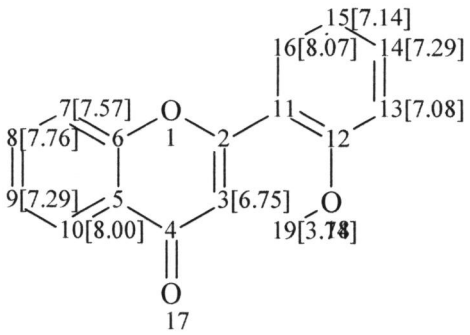
No.	(ppm)	(Hz)	Height
9	7.14	2855.2	0.0541
10	7.16	2862.2	0.2519
11	7.39	2955.9	0.0439
12	7.39	2957.1	0.0465
13	7.41	2964.1	0.0917
14	7.43	2971.2	0.0512
15	7.43	2971.9	0.0535
16	7.47	2987.6	0.0491

No.	(ppm)	(Hz)	Height
17	7.48	2989.5	0.0491
18	7.49	2995.0	0.0531
19	7.49	2996.5	0.0631
20	7.50	2997.7	0.0576
21	7.51	3003.2	0.0402
22	7.51	3005.1	0.0458
23	7.55	3018.4	0.1726
24	7.66	3064.9	0.0580

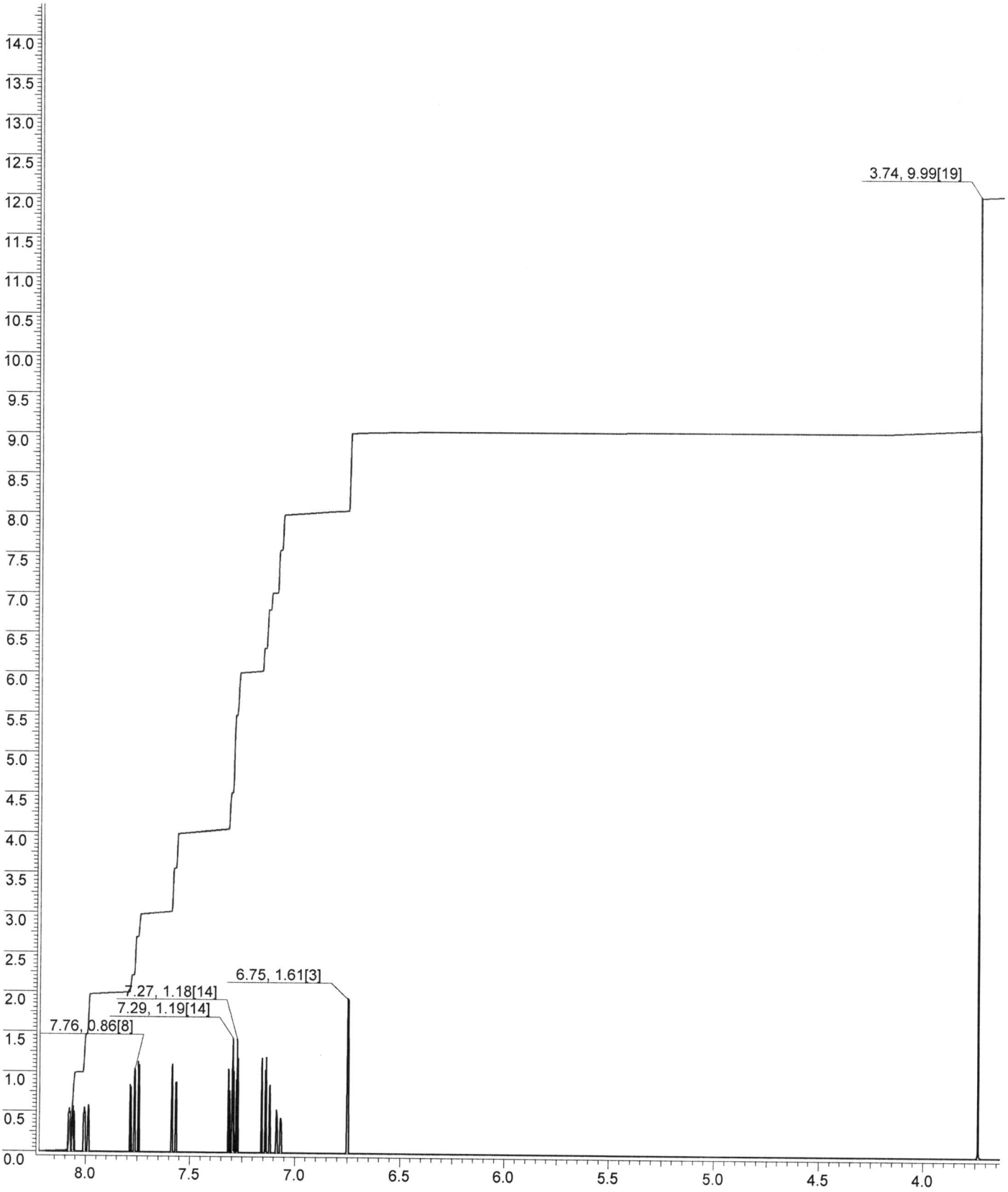
No.	(ppm)	(Hz)	Height
25	7.67	3066.4	0.0592
26	7.68	3071.9	0.0566
27	7.69	3073.5	0.0824
28	7.69	3075.0	0.0533
29	7.70	3080.5	0.0399
30	7.71	3082.1	0.0419
31	7.90	3160.6	0.0807
32	7.91	3162.1	0.0762

No.	(ppm)	(Hz)	Height
33	7.92	3168.4	0.0795
34	7.93	3170.3	0.0724
35	8.23	3291.0	0.0673
36	8.23	3292.6	0.0690
37	8.25	3298.8	0.0653
38	8.25	3300.4	0.0656

24/Apr/2012 15:25:37 ACD/C+H NMR Predictors and DB (v.12.01)



File Name \\nas1-ipb\nwc_ed\bweigel\Eigene Dateien\Projekte\Flavonoids\Primula\2'-methoxy-flavone.HSP (modified on 24 APR 2012)



WEB100_A/CDCl3/1H
Weigel 118/12
Thu Apr 26 17:55 2012
duration: 0h 2min

exp1 PROTON

```
      SAMPLE          lp              0
date    Apr 26 2012   nm  cdc  ph
samplename WEB100_A
sample     WEB100_A
solvent       cdcl3
file /home/vnmr1/n-
wcnwc/WEB100_A/WEB-
100_A.PROTON_01.fi-
                  d
   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

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wp            3598.1
vs               170
sc                 0
wc               250
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is           1500.00
rfl            791.9
rfp                0
th               7.0
ins          100.000
rp              82.5
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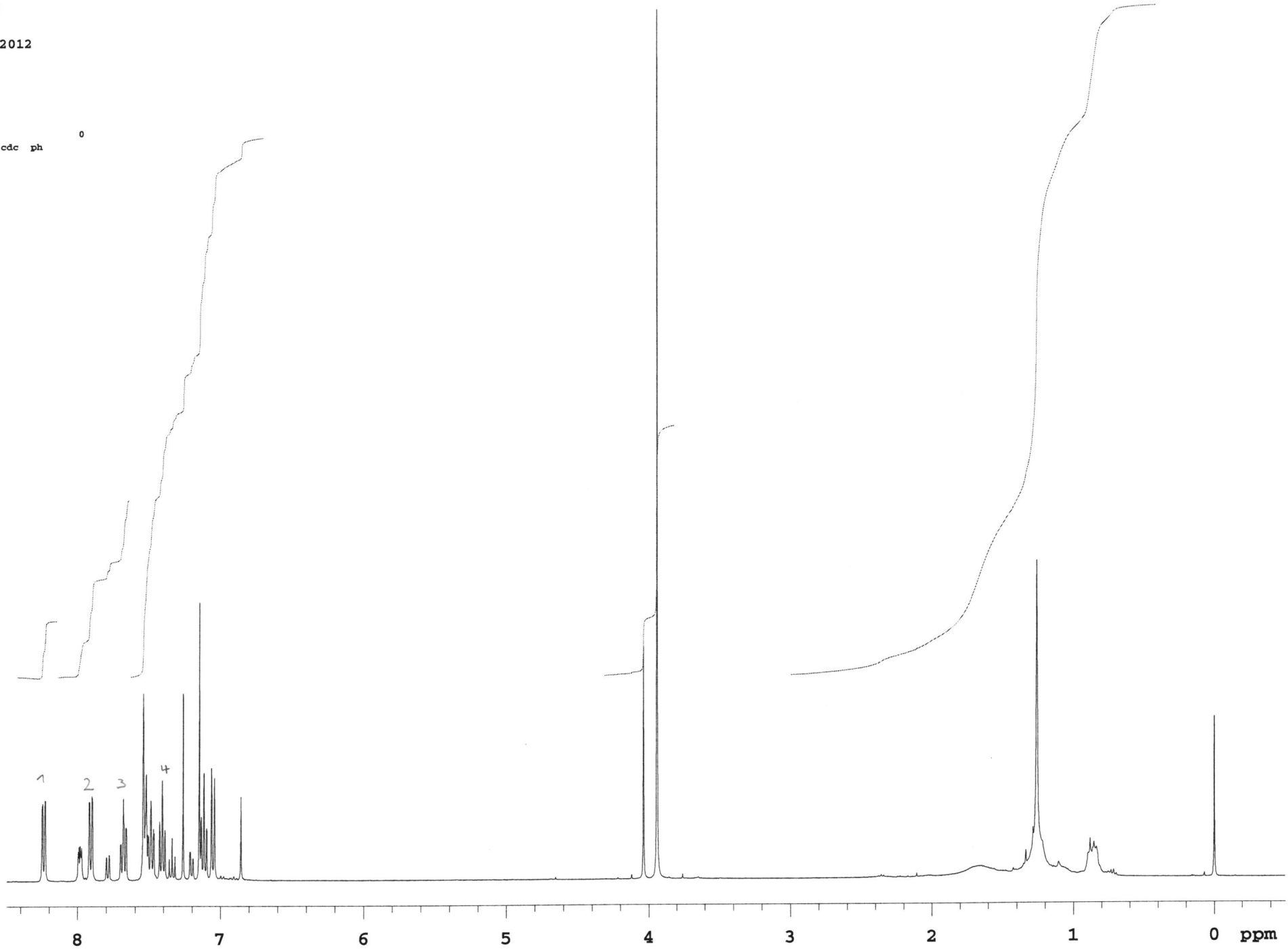
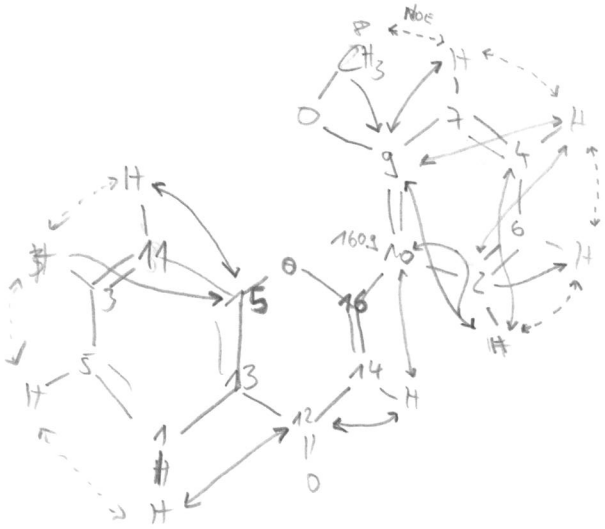
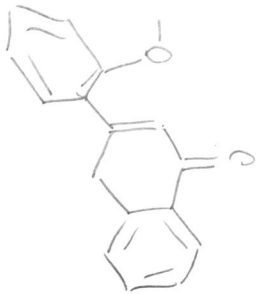




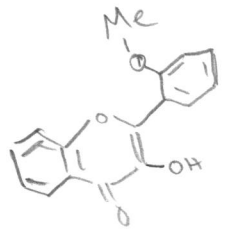
4 ↔ 9

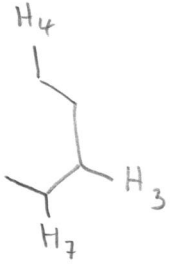
7.15 / 112.6

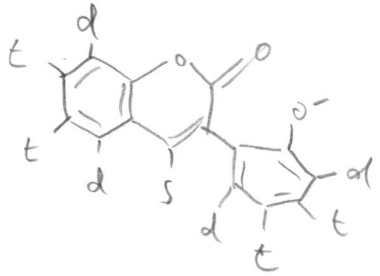
8



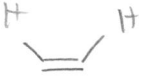
3 ↔ 7 (8,59 Hz)
3 ↔ 4 (1,95 Hz)



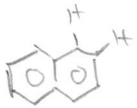




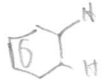
3J ortho 0-20 Hz



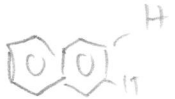
3J = 11,6



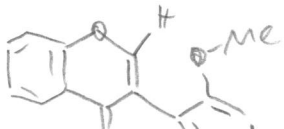
8,3



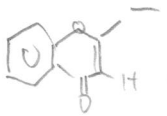
7,5



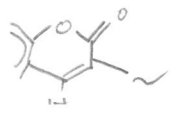
6,8 Hz



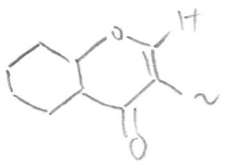
4) meta-Kopp. ~ 0-3 Hz
5) para-Kopp. ~ 0-2 Hz



6,8 ppm



7,74 ppm



8 ppm

HMBC

$9^{(H)} \rightarrow 9^{(C)}$ (158.0 ppm)

$9^{(C)} \rightarrow 2^{(H)}$ $6^{(H)}$

$2^{(H)} \rightarrow 9^{(C)}$ $10^{(C)}$ (160.9 ppm) ; $4^{(C)}$

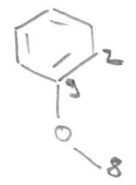
$1^{H} \rightarrow$ [178.9] $12^{(C)}$

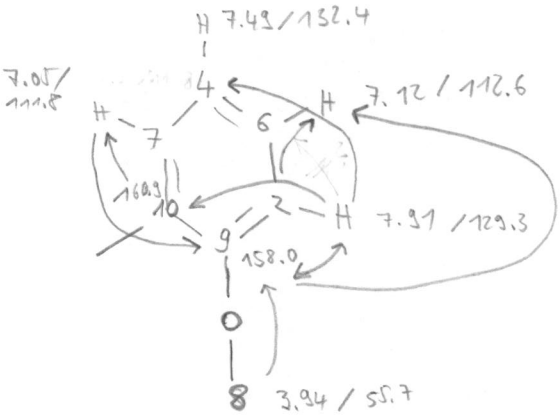
($12^{C} \rightarrow$ 7.15 $^{(H)}$) (S)

$12^{C} \rightarrow$ 7.54 $^{(H)}$ 11

$13^{C} \rightarrow 5^{H}$

$5^{H} \rightarrow 13^{C}$, 123.8 ppm





2 → 6

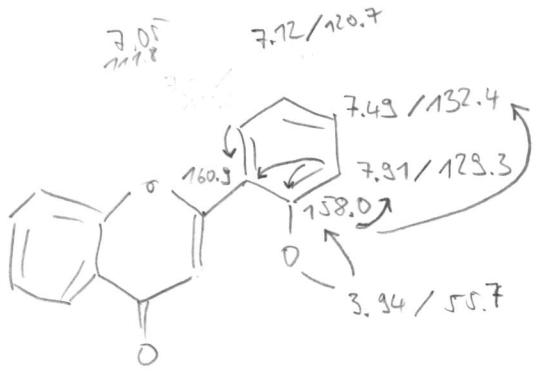
6 → 7, 2

(10 → 7.15 ?)

10 → 2, 7

ROESY ???

$H_8 \leftrightarrow H_7$ . . .

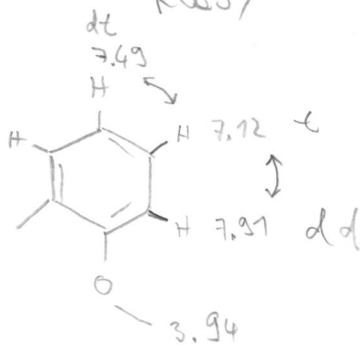


7.15 / 112.6

1	8.24	d	125.6	
2	7.91	d	129.3	
3	7.68	t	133.5	
4	7.49	t	132.4	
5	7.41	t	124.9	
6	7.12	t	120.7	
7	7.05	d	111.8	
8	3.94	s	55.7	

9 158 ppm
10 160.9 ppm
11 7.54 / 129.0 ppm (zuordnung bei HMBC signale)
12 178.9
13 118.0 / 7.54
14 7.15 / 112.6

ROESY



3.94 ↔ 7.05 (d)

COSY

1 ↔ 5
(1 ↔ 3 Schwach))
2 ↔ 6
3 ↔ 5 (x) ~11
4 ↔ 7,6 ; 2 (schwach)
5 ↔ 3,1
6 ↔ 4,2
7 ↔ 4

7.05 → 7,49 (t)

ROESY

8 ↔ 7
2 ↔ 6
1 ↔ 5
3 ↔ 11
3 ↔ 5

$C_{16}H_{10}O_3$