

474

<sup>1</sup>H nuclear magnetic resonance

Fig. 10.3 Chrysin (1).

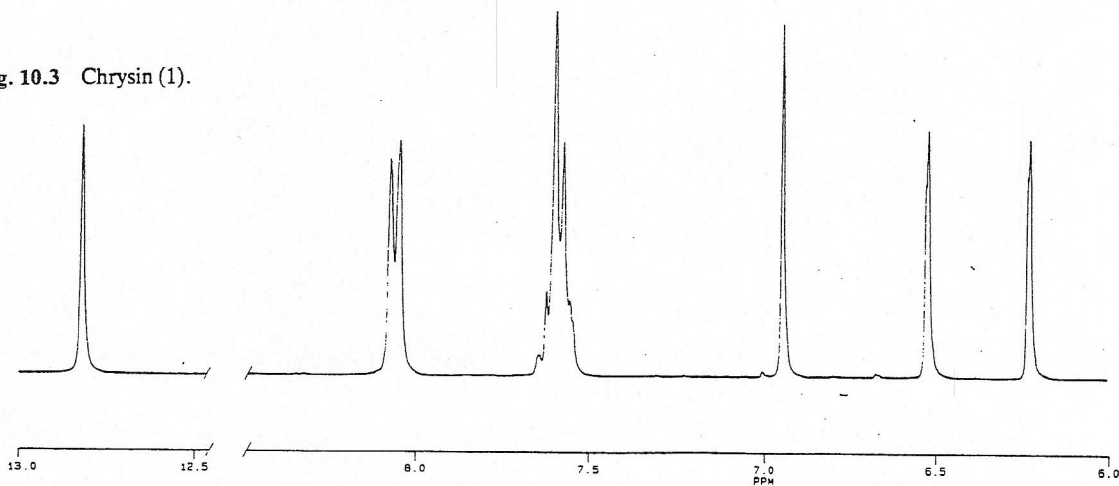


Fig.

Fig. 10.4 5,7,2'-Trihydroxyflavone (6).

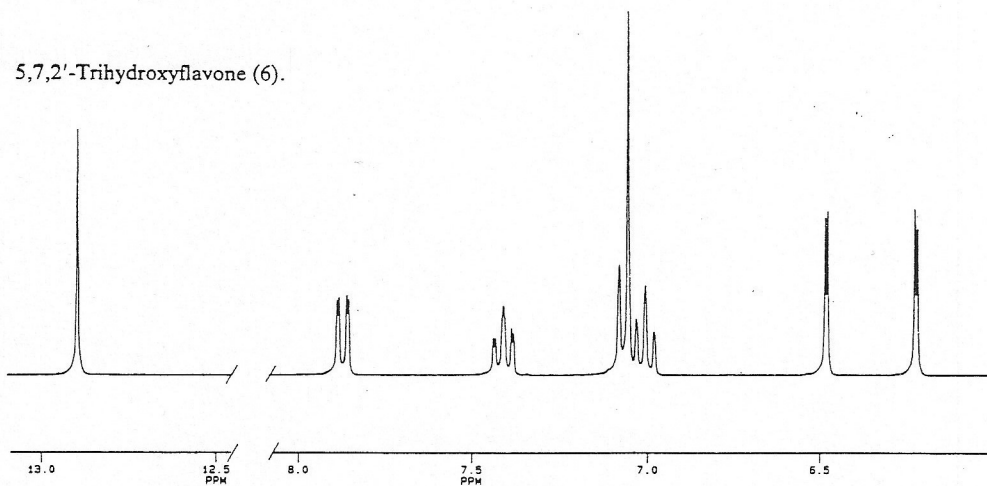


Fig.

Fig. 10.5 5,4'-Dihydroxyflavone (7).

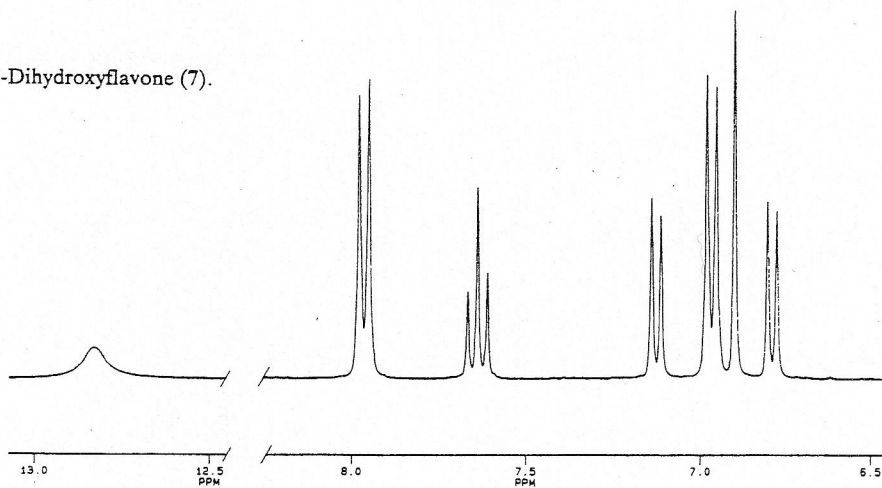


Fig.

Fig. 10.60 Naringenin (136).

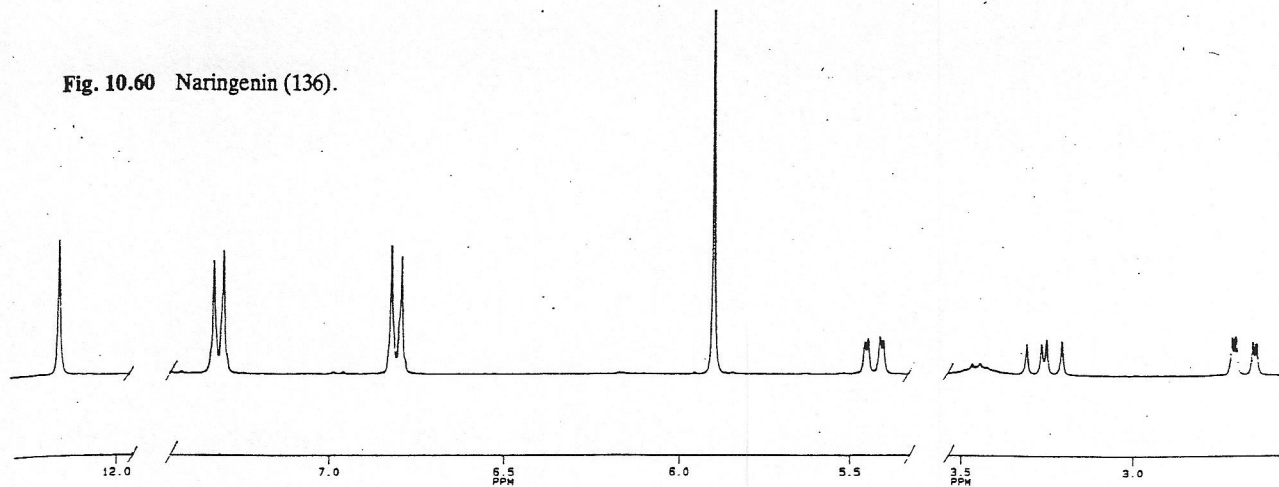


Fig. 10.61 Naringenin 7-glucoside (137).

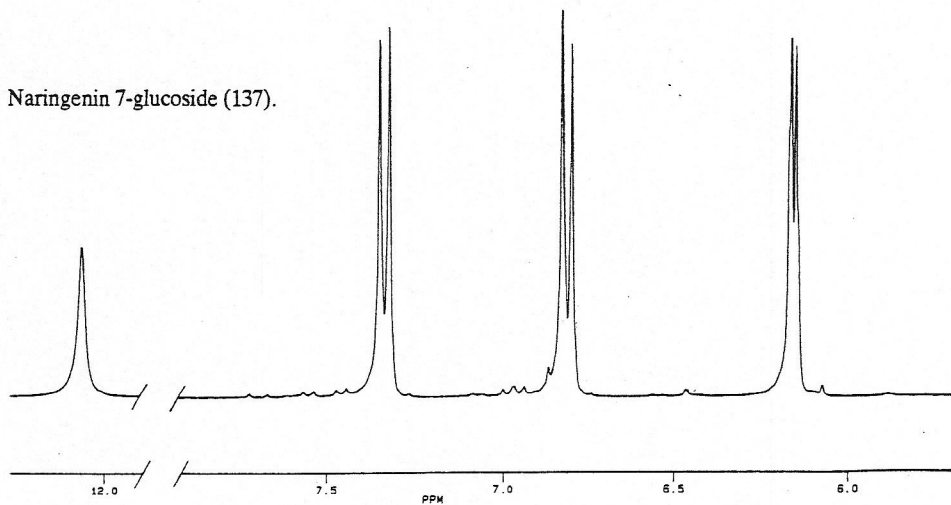
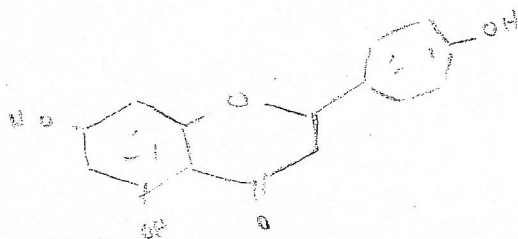
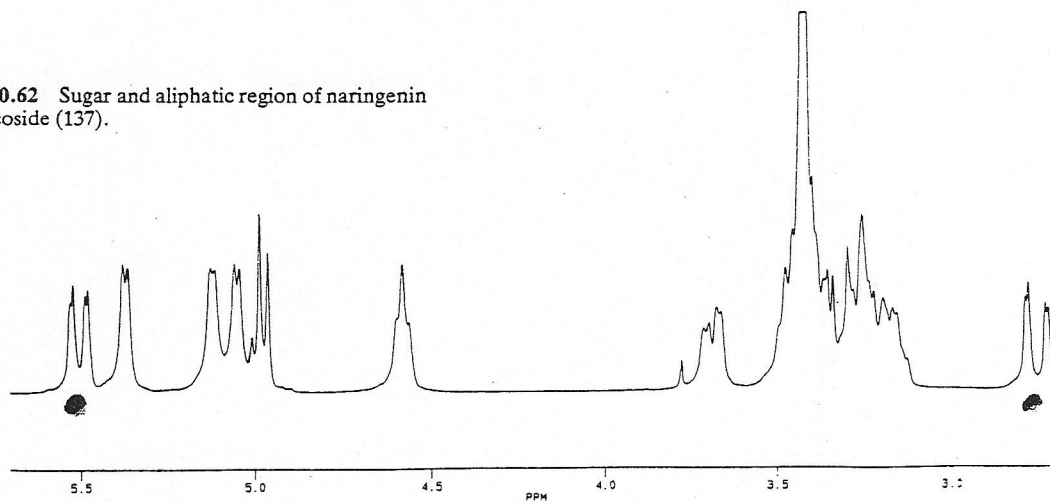
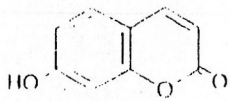
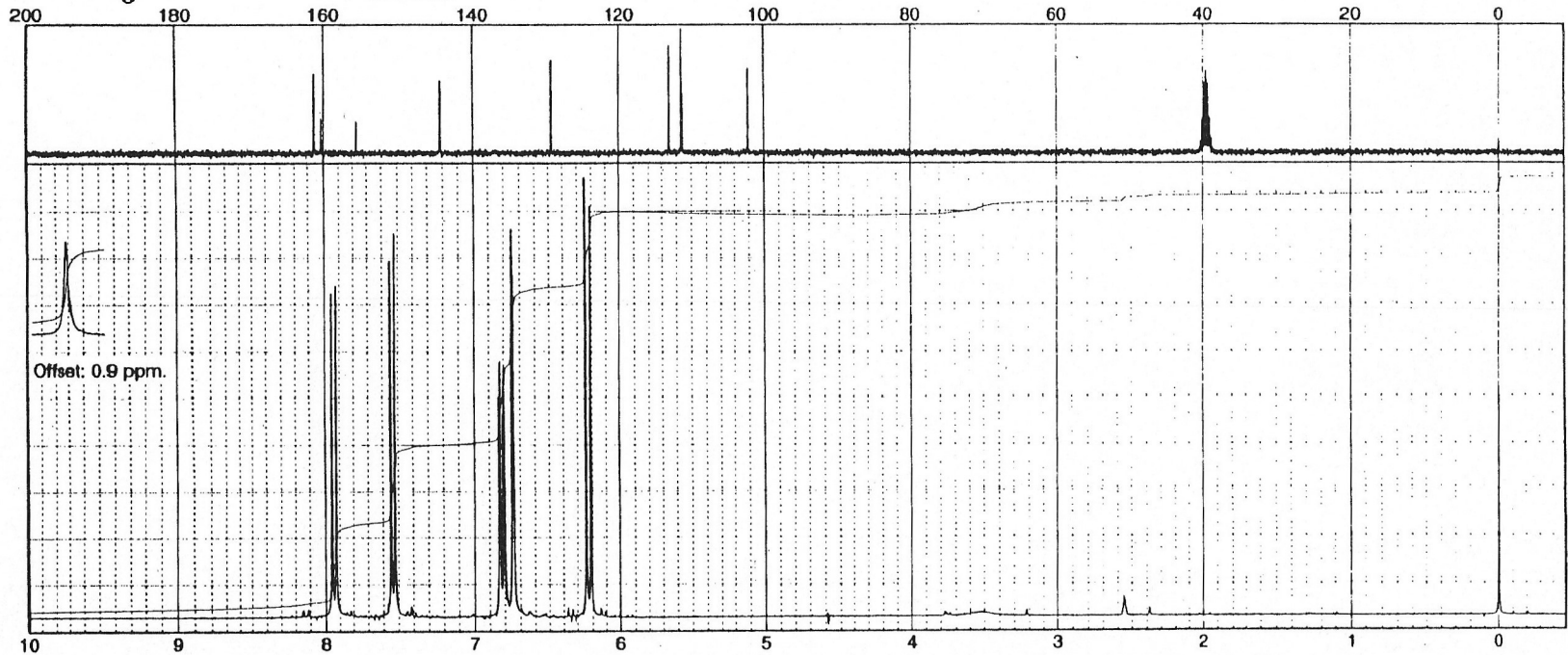


Fig. 10.62 Sugar and aliphatic region of naringenin 7-glucoside (137).



DMSO- $d_6$

QE-300



# Aromatic Esters and Lactones

Aldrich 27,572-7

CAS [484-20-8]

$C_{12}H_8O_4$

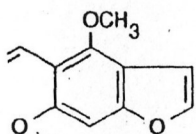
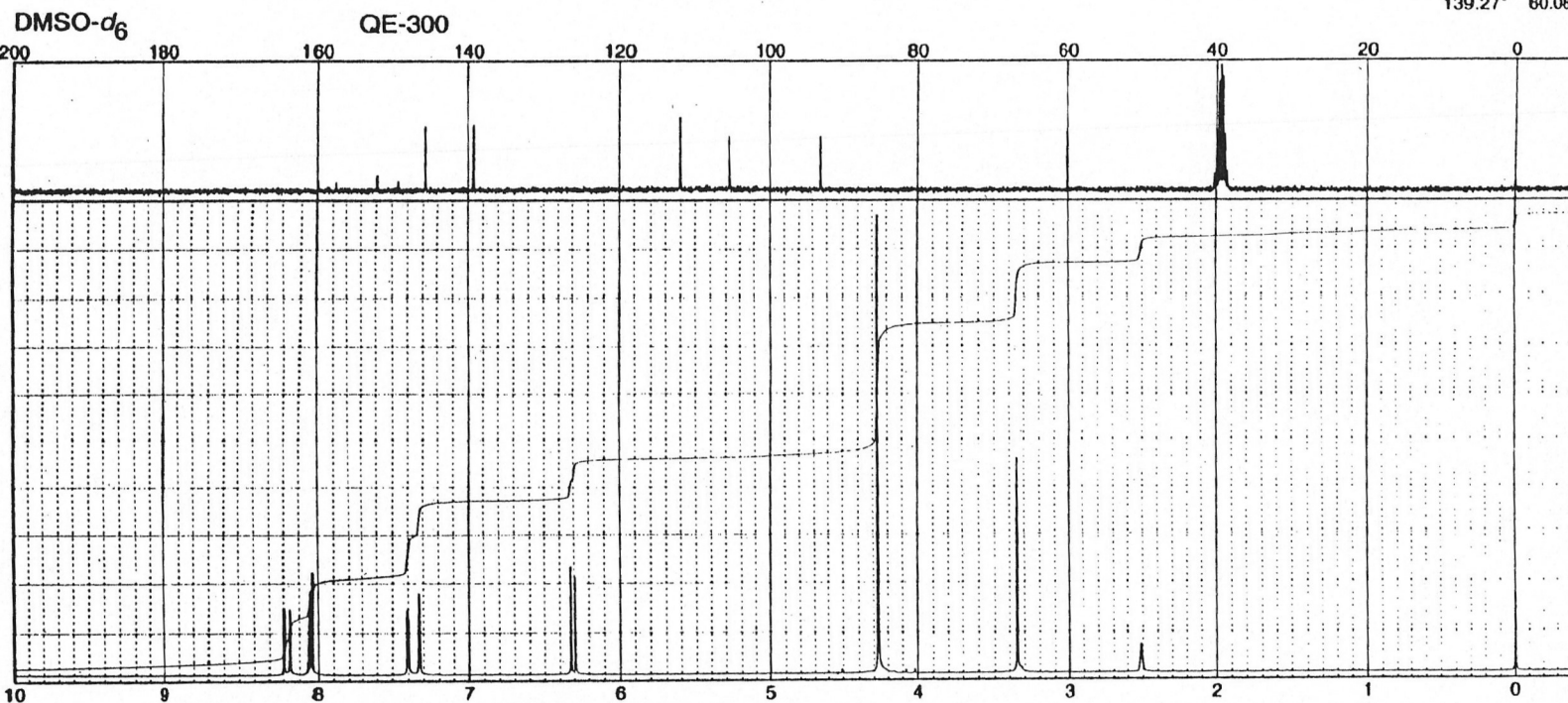
5-Methoxypsoralen, 99%

FW 216.20

mp 192°C

159.93	112.14
157.60	112.08*
151.94	105.52*
149.26	105.41
145.67*	92.92*
139.27*	60.08*

A



B

# Aromatic Ketones

920

Aldrich 14,563-7

CAS [491-80-5]

$C_{16}H_{12}O_5$

60 MHz: 2, 98C

Blochanin A

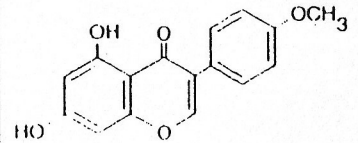
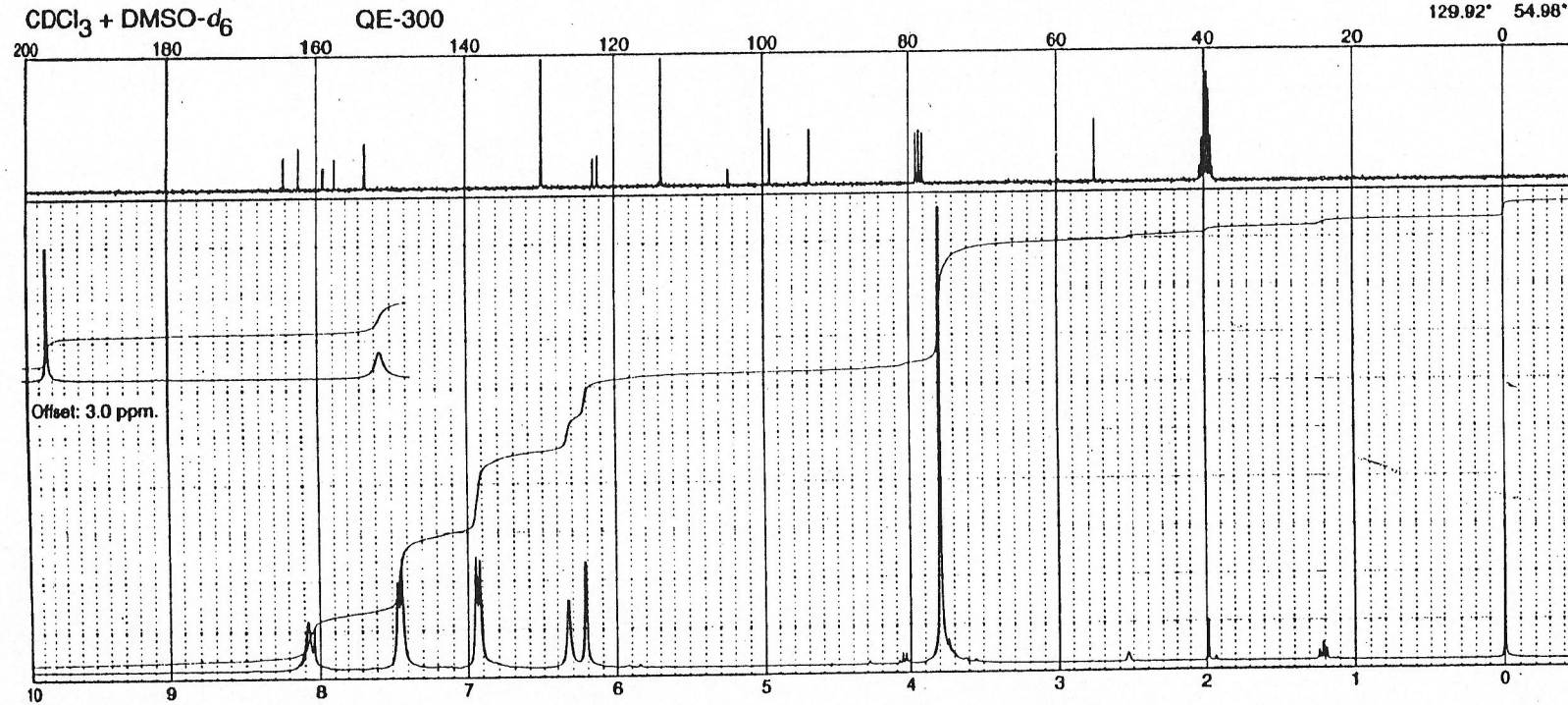
FW 284.27

FT-IR: 2, 95D

mp 212°C

180.07	122.95
164.28	122.27
162.14	113.52*
159.14	104.65
157.61	99.08*
153.19*	93.66*
129.92*	54.98*

A



B

Apigenin, 98%

FW 270.24

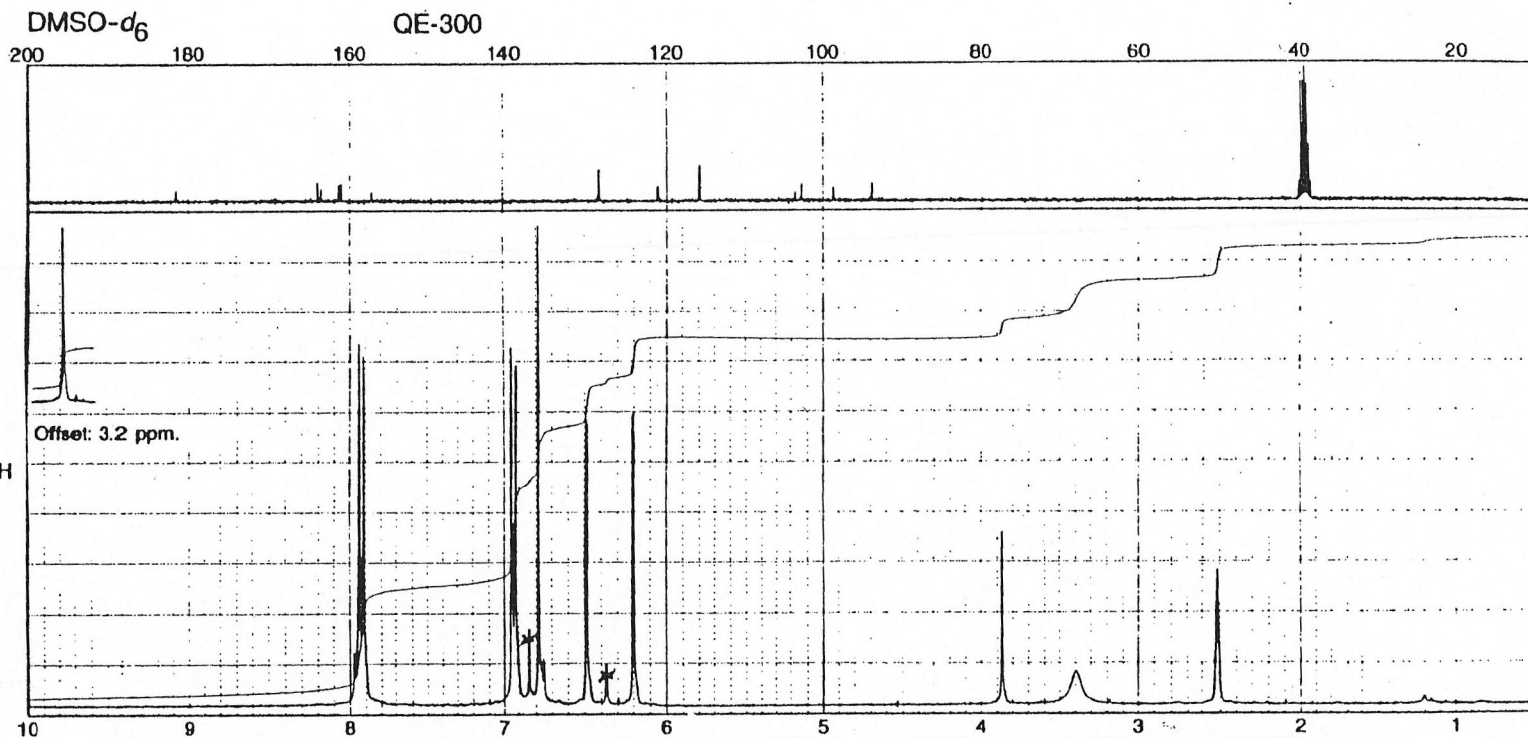
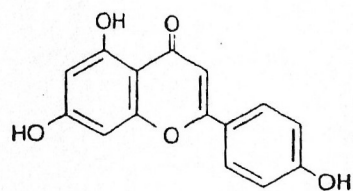


Fig. 10.18 Sugar region of luteolin 7-glucuronide (31).

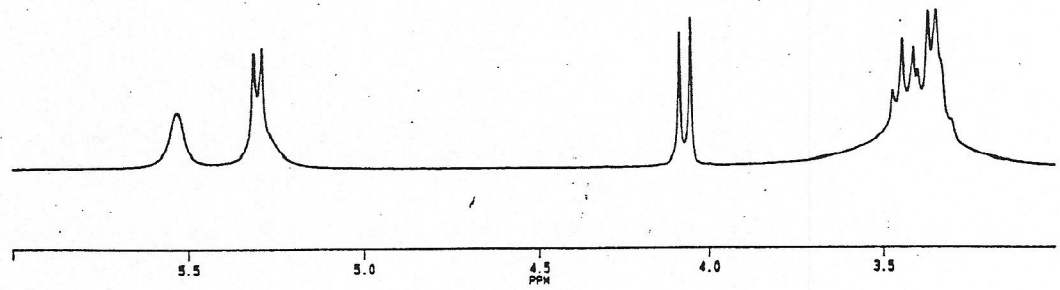


Fig. 10.19 Luteolin 7-glucoside (32).



Fig. 10.20 Sugar region of luteolin 7-glucoside (32).

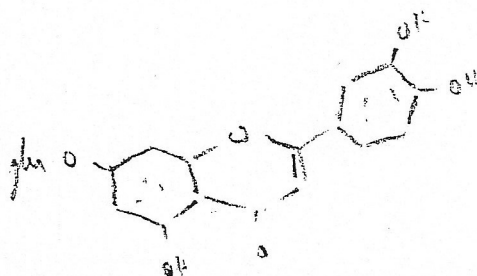
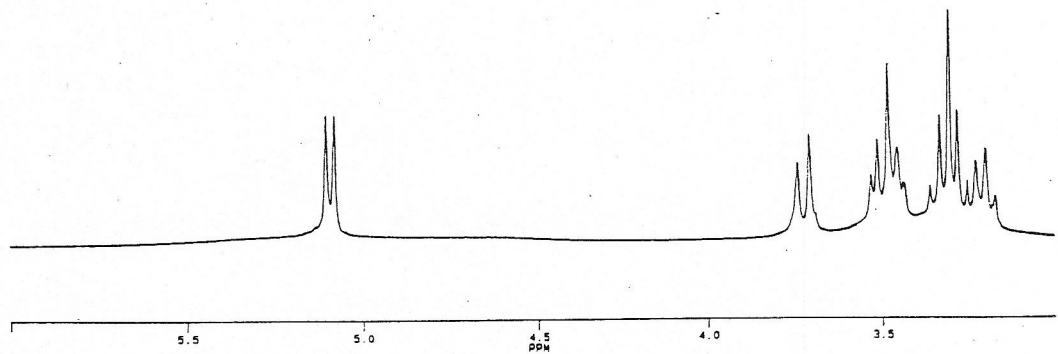


Fig. 10.30 Sugar region of datiscetin 3-rutinoside (56).

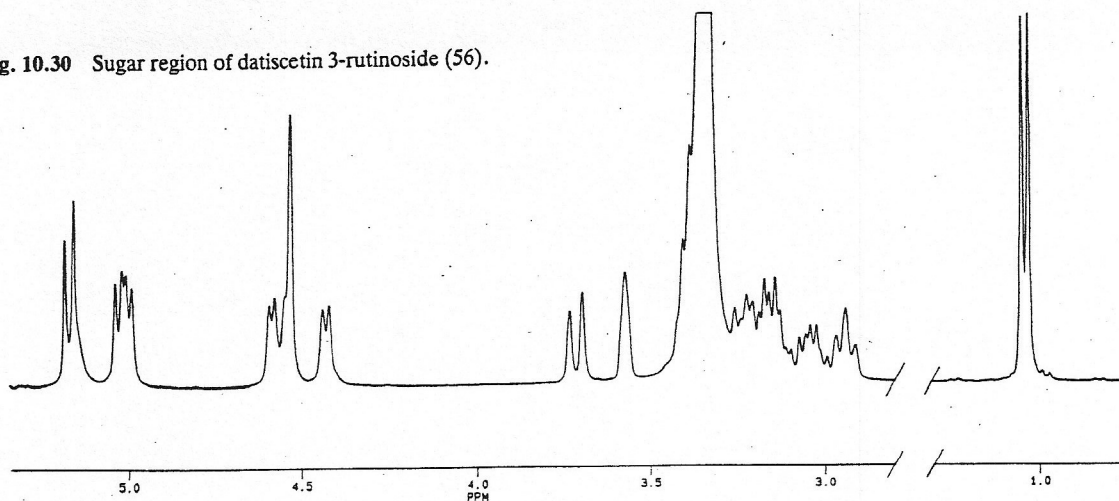


Fig. 10.31 Kaempferol (57).

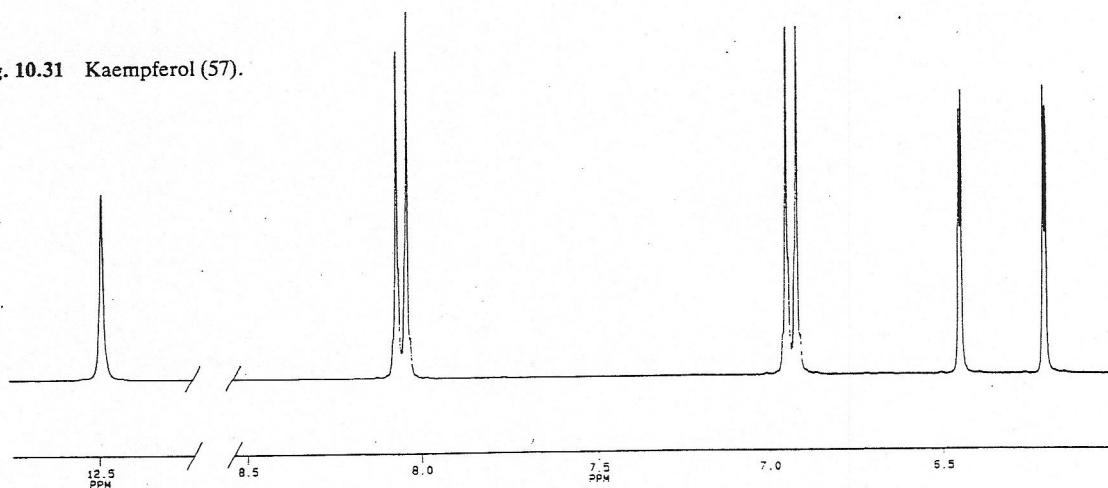
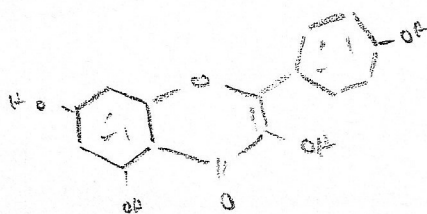
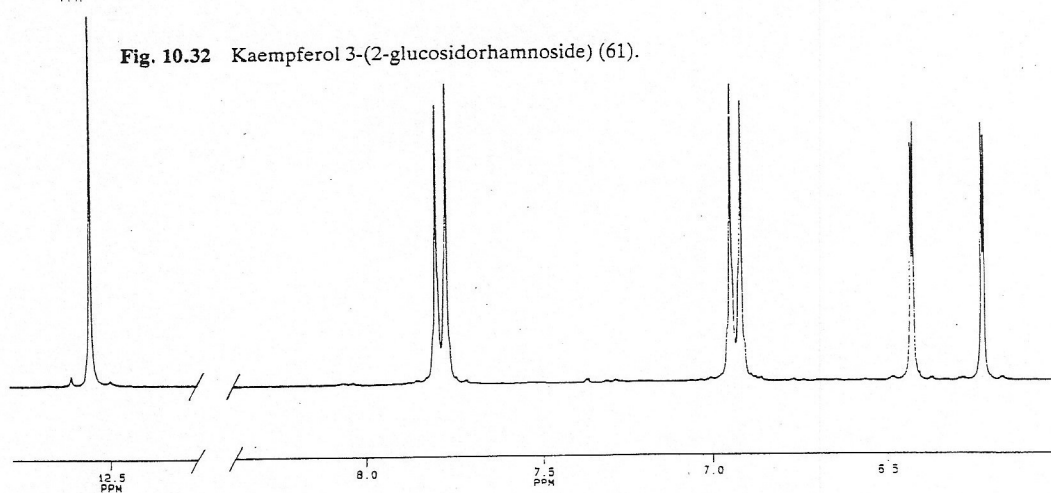


Fig. 10.32 Kaempferol 3-(2-glucosidorhamnoside) (61).

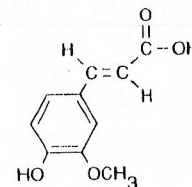
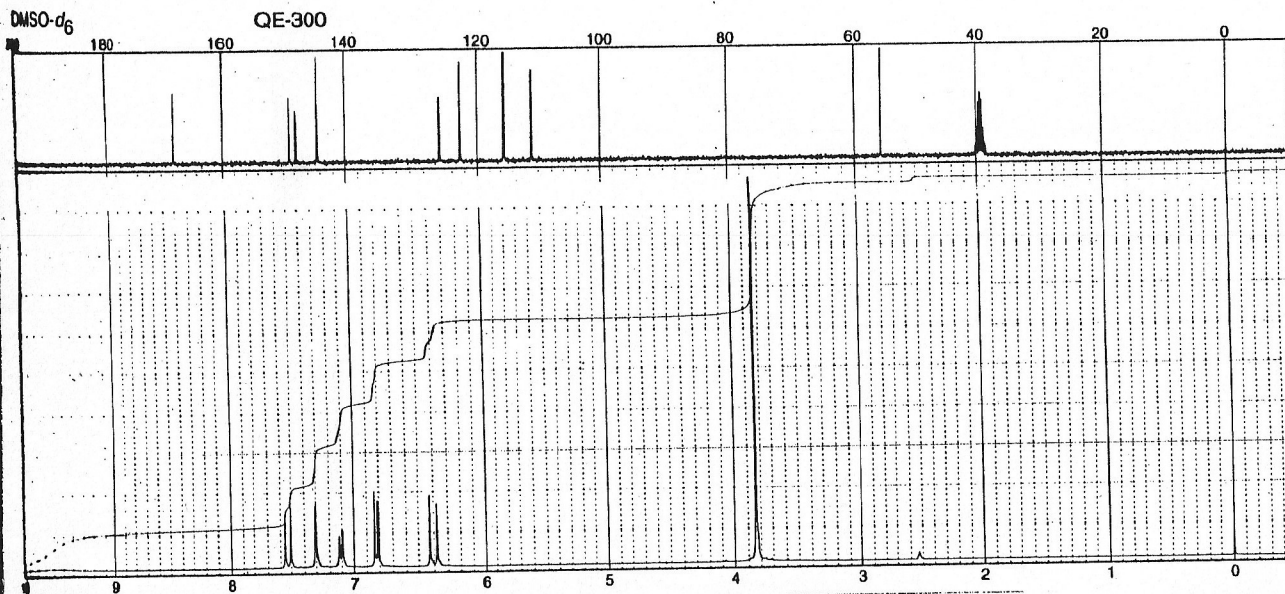




Aldrich 12,870-8 CAS [537-98-4]  
 trans-4-Hydroxy-3-methoxycinnamic acid,  
 99%

C<sub>10</sub>H<sub>10</sub>O<sub>4</sub> 60 MHz: 2, 180B  
 FW 194.19 FT-IR: 2, 184C  
 mp 170°C

167.89 122.69\*  
 148.95 115.52\*  
 147.78 115.42\*  
 144.39\* 111.02\*  
 125.67 55.58\*

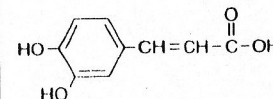
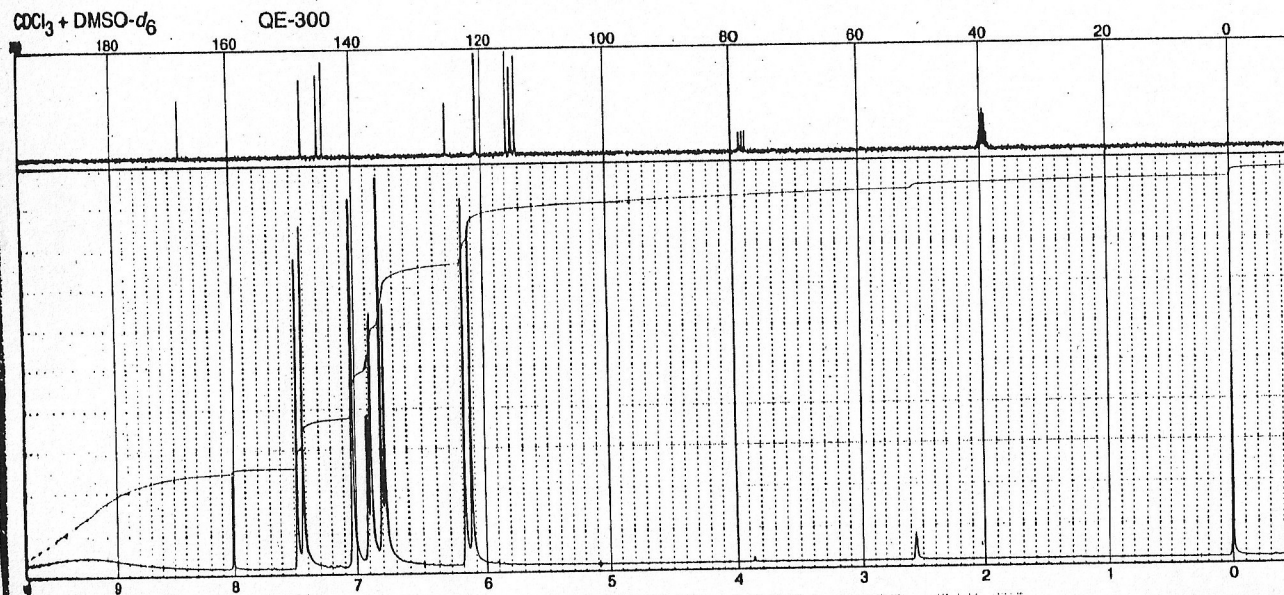


A

Aldrich D11,080-9 CAS [331-39-5]  
 3,4-Dihydroxycinnamic acid, 97%

C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> 60 MHz: 2, 181C  
 FW 180.16 FT-IR: 2, 184D  
 mp 196°C d.

168.14 121.01\*  
 147.89 115.66\*  
 145.39 115.01\*  
 144.54\* 114.32\*  
 125.84



B

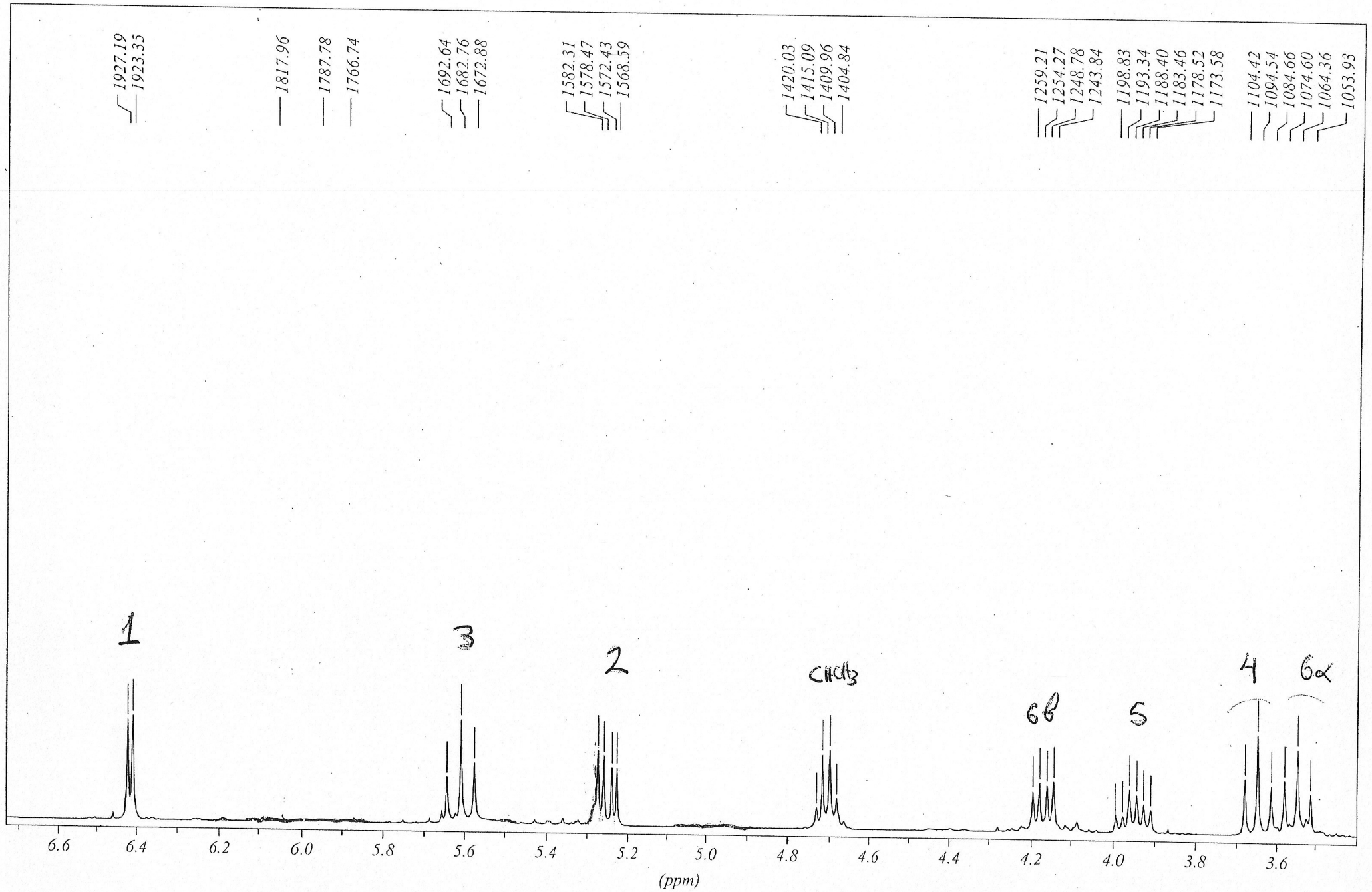
Aldrich 30,065-9 CAS [36015-19-7]  
 2-Chloro-5-nitrocinnamic acid, 98%,  
 predominantly trans

C<sub>9</sub>H<sub>6</sub>ClNO<sub>4</sub>  
 FW 227.61  
 mp 220°C

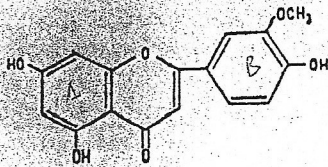
166.53 131.23\*  
 146.72 125.29\*  
 139.58 125.19\*  
 136.60\* 122.77\*  
 133.45

C

A



## CHRYSOERIOL



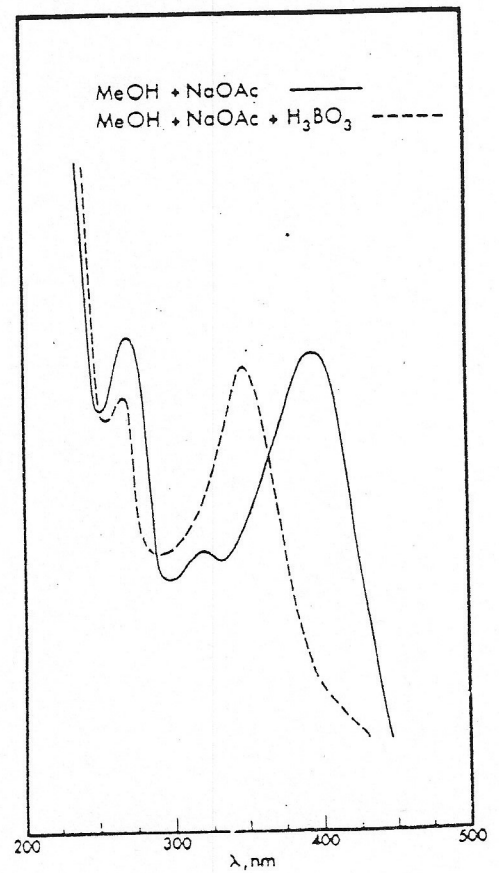
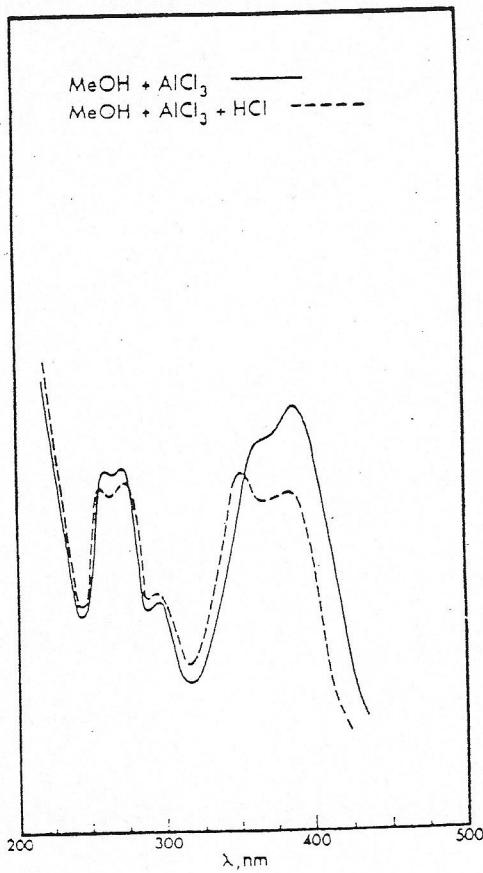
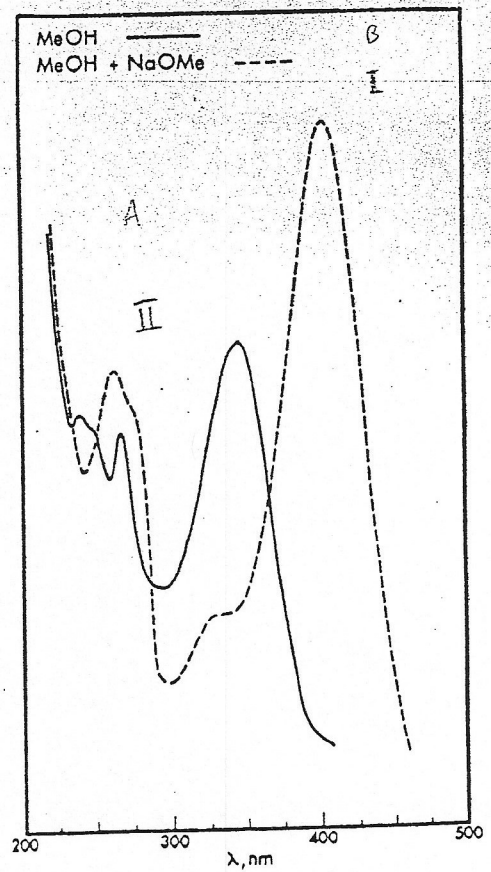
## CHROMATOGRAPHIC DATA

Spot Appearance: (UV) deep purple  
(UV/NH<sub>3</sub>) yellow-green

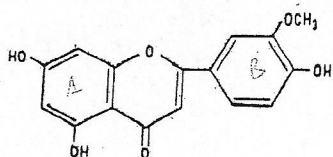
R<sub>f</sub> Values: 0.80 (TBA), 0.05 (HOAc)

UV SPECTRAL DATA ( $\lambda_{max}$ , nm)

MeOH	241, 249sh, 269, 347,
NaOMe	264, 275sh, 329sh, 405
AlCl <sub>3</sub>	262, 274, 296, 366sh, 390
AlCl <sub>3</sub> /HCl	259, 276, 294, 353, 386
NaOAc	271, 321, 396
NaOAc/H <sub>3</sub> BO <sub>3</sub>	268, 349
(Proc. I)	



## CHRYSOERIOL



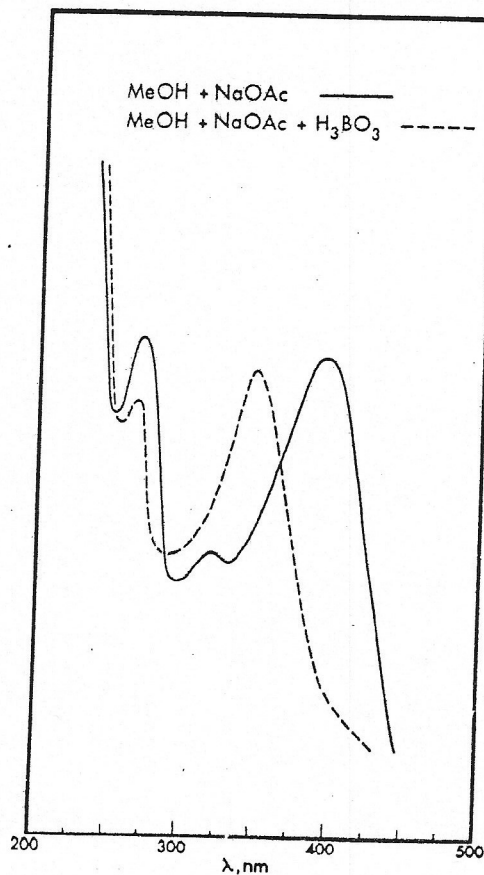
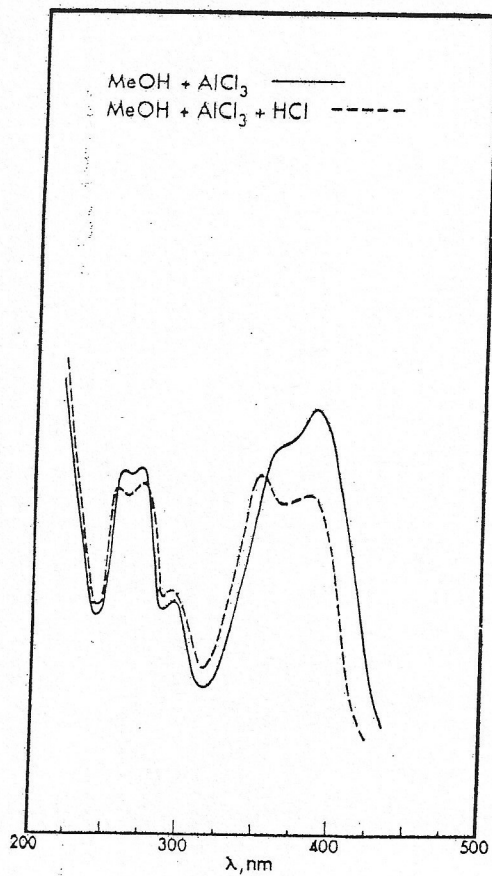
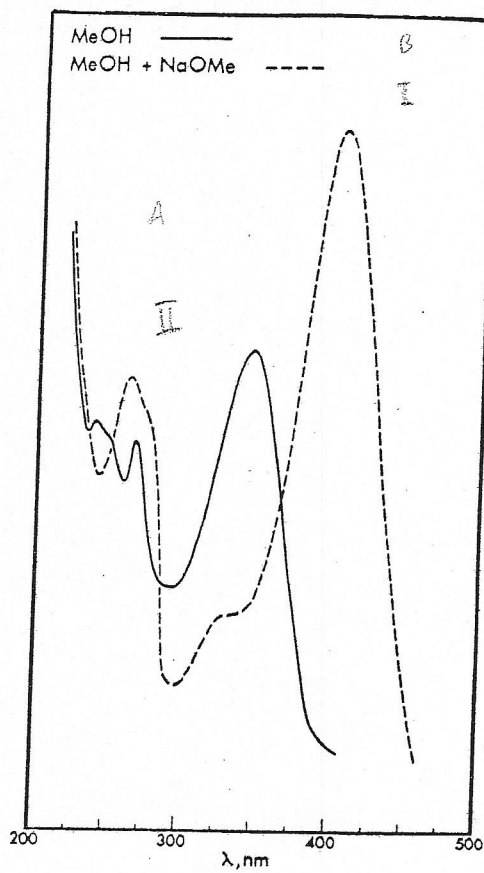
## CHROMATOGRAPHIC DATA

Spot Appearance: (UV) deep purple  
(UV/NH<sub>3</sub>) yellow-green

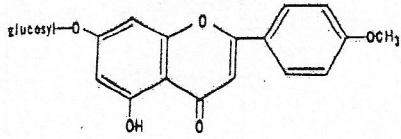
R<sub>f</sub> Values: 0.80 (TBA), 0.05 (HOAc)

UV SPECTRAL DATA ( $\lambda_{max}, nm$ )

MeOH	241, 249sh, 269, 347,
NaOMe	264, 275sh, 329sh, 405
AlCl <sub>3</sub>	262, 274, 296, 366sh, 390
AlCl <sub>3</sub> /HCl	259, 276, 294, 353, 386
NaOAc	271, 321, 396
NaOAc/H <sub>3</sub> BO <sub>3</sub>	268, 349
(Proc. I)	



## ACACETIN 7-O-GLUCOSIDE



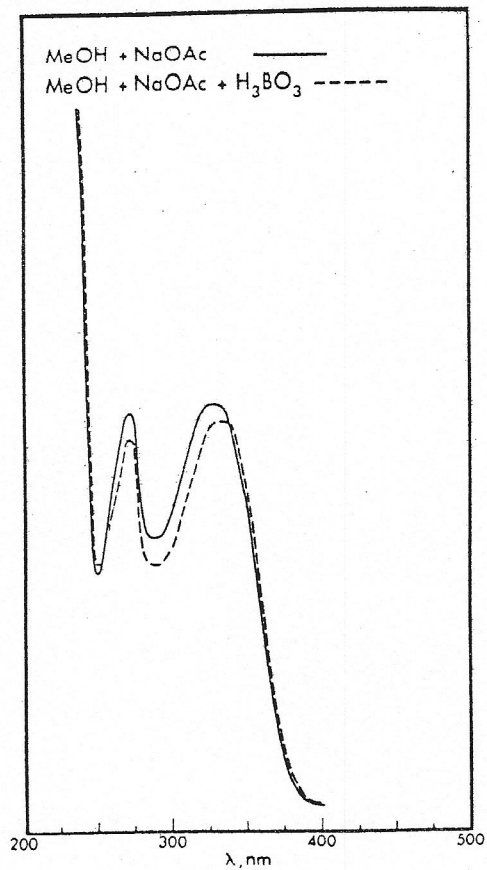
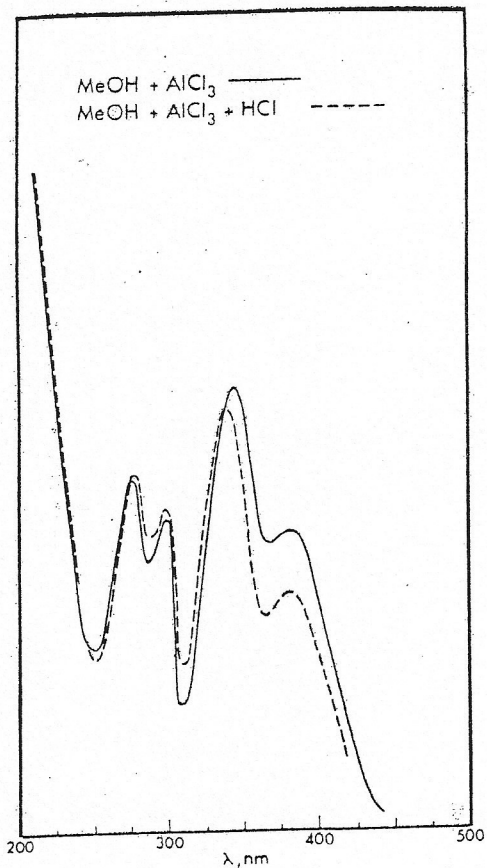
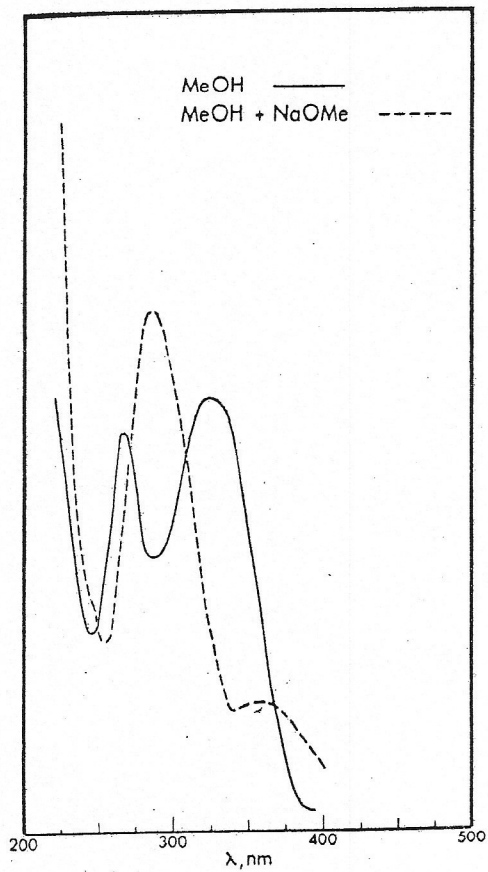
## CHROMATOGRAPHIC DATA

Spot Appearance: (UV) deep purple  
(UV/NH<sub>3</sub>) deep purple

R<sub>f</sub> Values: 0.58 (TBA), 0.27 (HOAc)

UV SPECTRAL DATA ( $\lambda_{max}$ , nm)

MeOH	268, 324
NaOMe	244sh, 287, 357
AlCl <sub>3</sub>	277, 300, 345, 383
AlCl <sub>3</sub> /HCl	278, 299, 338, 381
NaOAc	268, 324
NaOAc/H <sub>3</sub> BO <sub>3</sub>	269, 328
(Proc. I)	



Aldrich 24,658-1  
Scopoletin, 95%

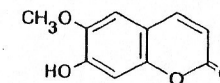
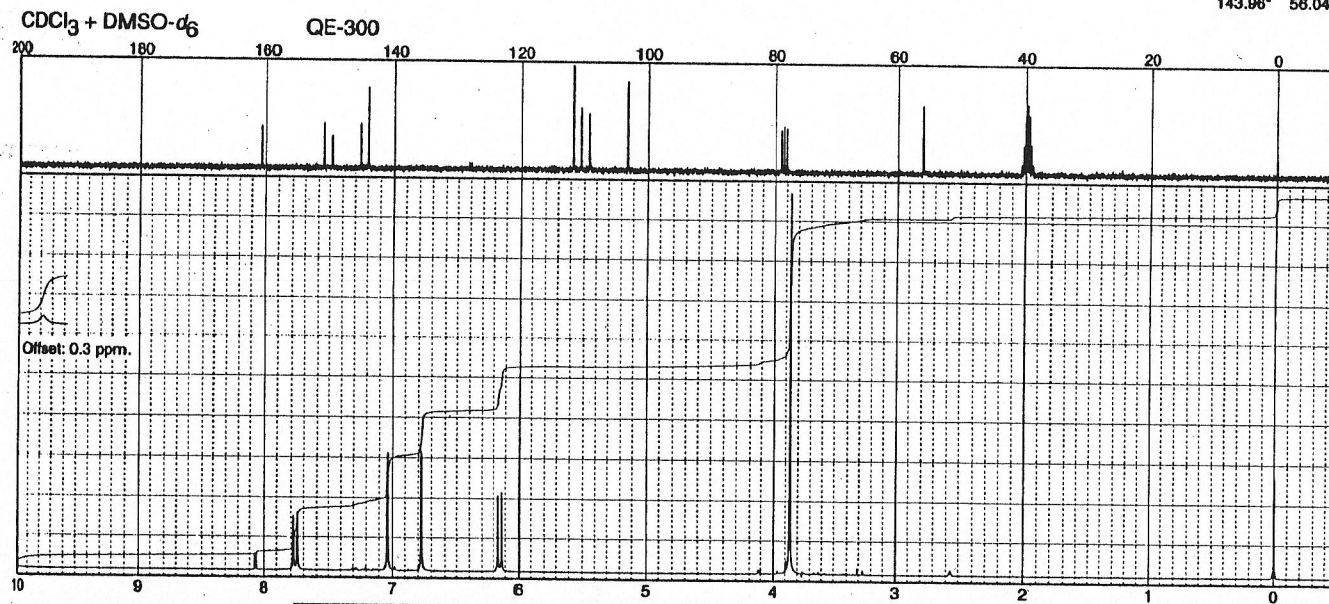
CAS [92-61-5]

$C_{10}H_8O_4$   
FW 192.17  
mp 204°C

60 MHz: 2, 311A  
FT-IR: 2, 324B

180.73 111.61\*  
151.21 110.53  
149.69 109.16\*  
145.22 102.93\*  
143.96\* 56.04\*

B



Aldrich 24,657-3  
Esculetin, 98%

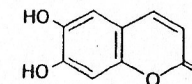
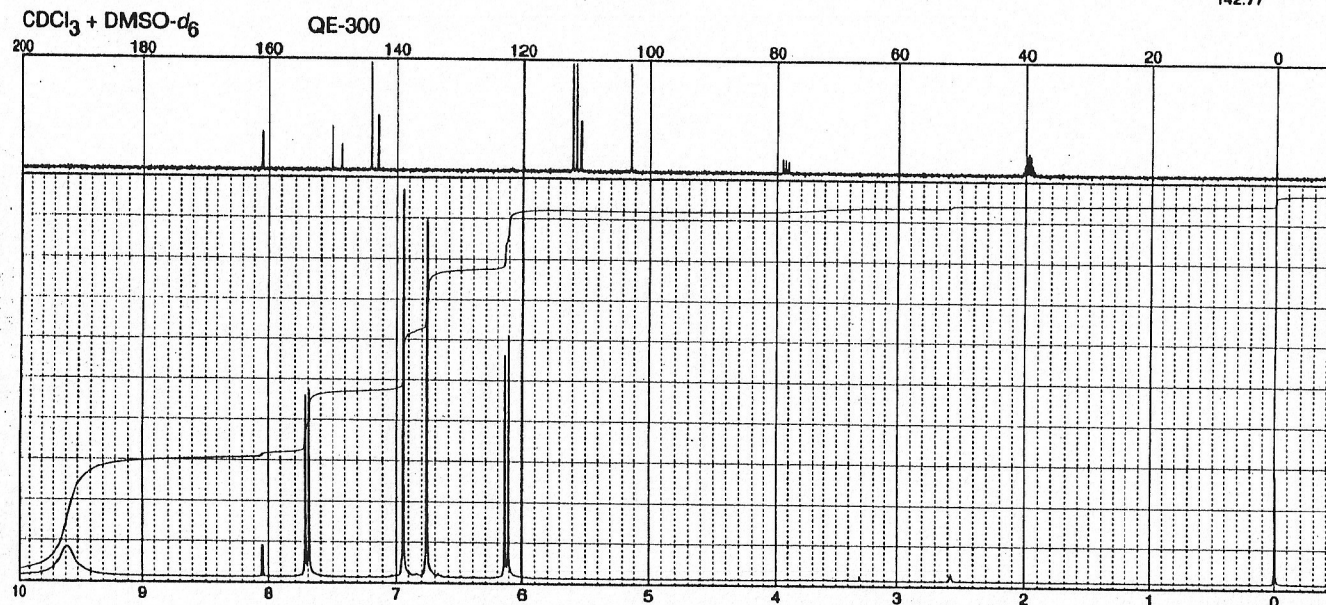
CAS [305-01-1]

$C_9H_6O_4$   
FW 178.15  
mp 272°C

60 MHz: 2, 311B  
FT-IR: 2, 324C

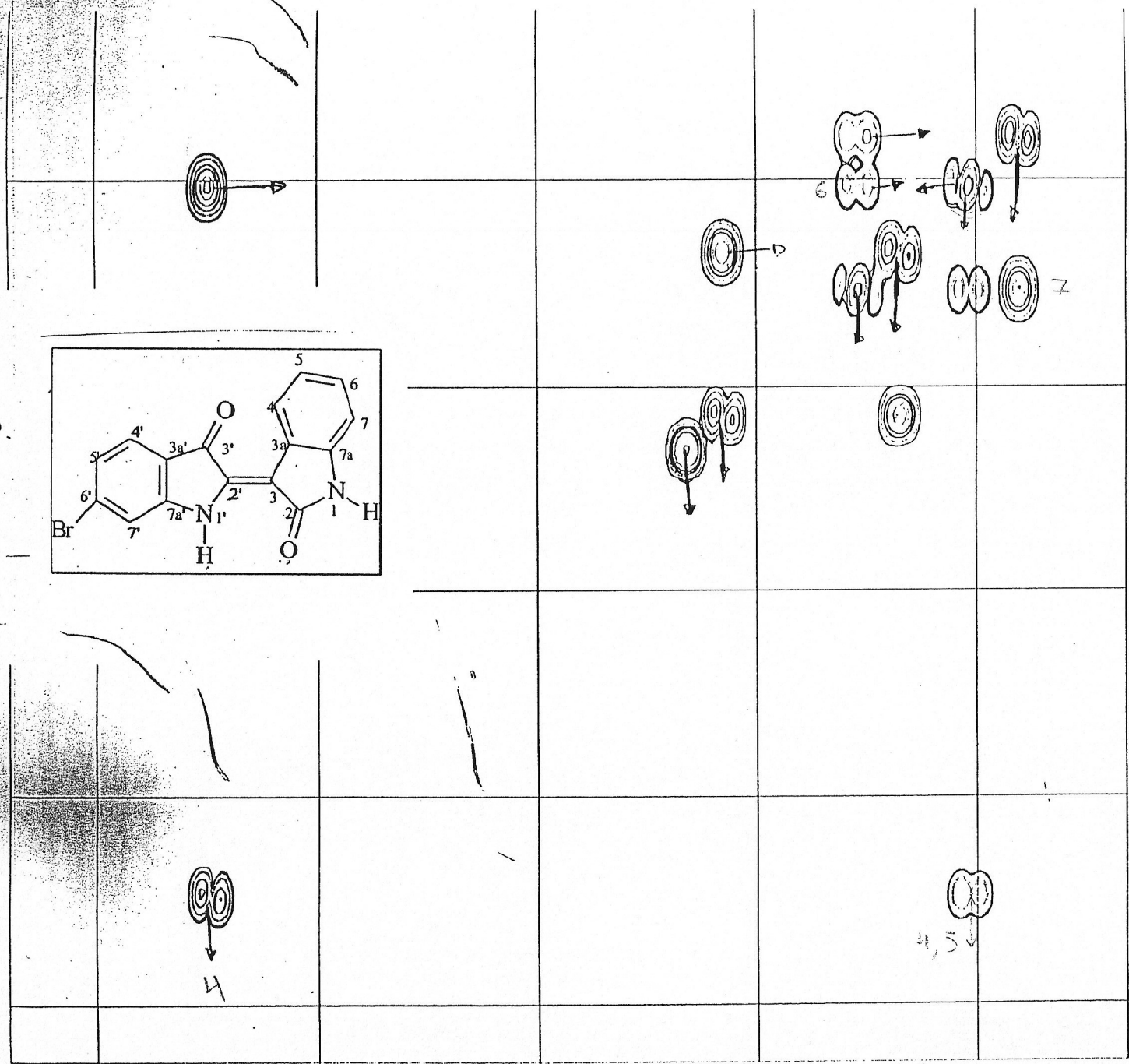
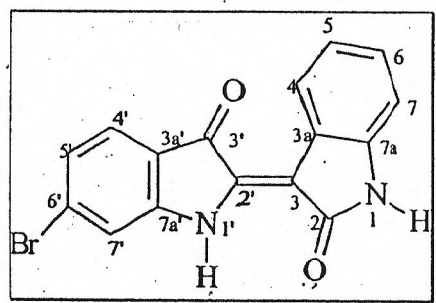
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150.24 111.44\*  
148.60 110.76  
143.93\* 102.68\*  
142.77

C



COSY

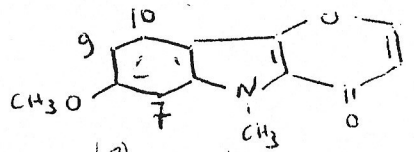
COSY  
DMSO



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7.5  
8.0  
8.5  
9.0  
ppm

9.0 8.5 8.0 7.5 7.0  
ppm

Ref 34



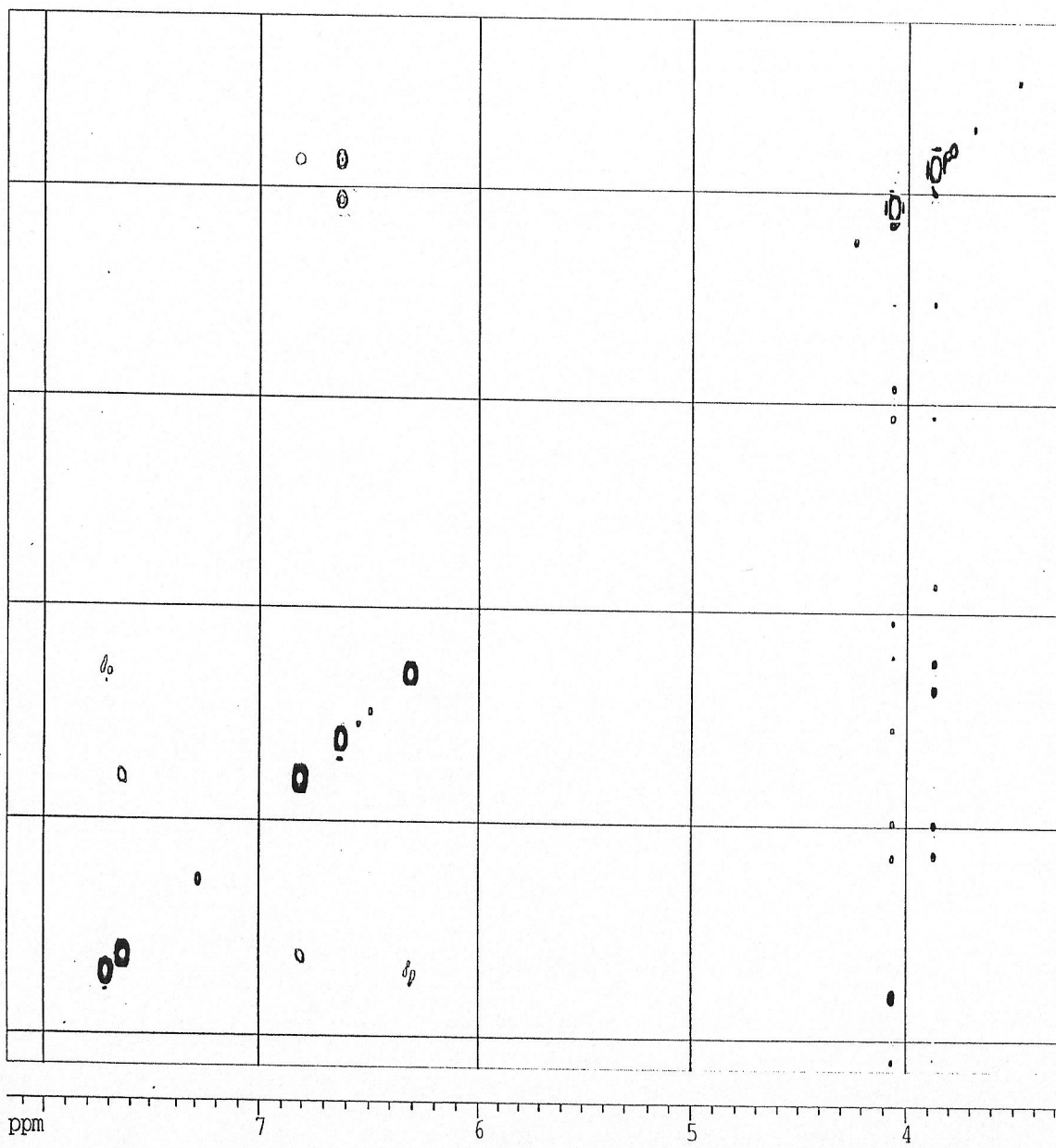
(6) (8)  
d d

(8) s  
d s

(6) d

NOESY

noesy



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 PROCNO 1

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 DE 3.50 MHz  
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 EI 2.0000000 sec  
 DE 1.0000000 sec  
 DRO 0.0012460 sec

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 NU1 1H  
 P1 10.00 MHz  
 PL1 2.70 dB  
 SFO1 400.1420007 MHz

F1 Acquisition parameters  
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 SW 10.011 ppm

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 SSB 0  
 LB 0.00 Hz  
 GB 0  
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F1 Processing parameters  
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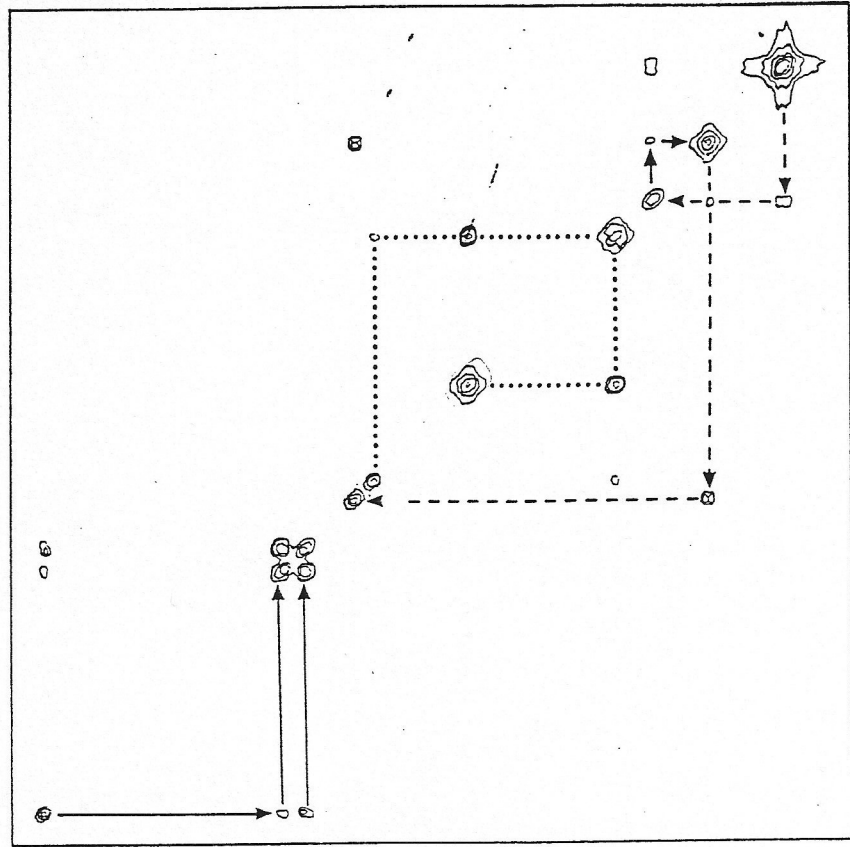
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 F2H1 0.294 ppm  
 F2H0 1314.01 Hz  
 F1PL0 4.145 ppm  
 F1L0 3269.48 Hz  
 F1H1 0.291 ppm  
 F1H0 1359.0 Hz  
 F2PRGM 9.4594 ppm/cm  
 F1PRGM 180.41701 Hz/cm  
 F2ORR 0.4295 ppm/cm  
 F1ORR 0.4295 ppm/cm

ppm

ppm



44 Interpretation of spectra



C11E AP01

