Appendix 1. Chemical constituents of the *Artemisia ciniformis* aerial parts grown in the Northeast of Iran and their chemotaxonomic significance

Contents

1. Compound (1): Hydroxydavanone 3

Table 1. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR data of compound (**1**), hydroxydavanone, in CDCl3. 4

Figure 1. ^{1}H-NMR (400 MHz) spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$ 5

Figure 2. ^{13}C-NMR (100 MHz) spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$ 6

Figure 3. DEPT 90˚ (100 MHz) spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$ 7

Figure 4. DEPT 135˚ (100 MHz) spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$ 7

Figure 5. COSY spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$ 8

Figure 6. HSQC spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$ 9

Figure 7. HMBC spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$ 10

2. Compound (2): Arteincultone 11

Figure 8. ^{1}H-NMR (400 MHz) spectrum of compound (**2**), arteincultone, in $CDCl_3$ 12

3. Compound (3): Xanthoxylin 13

Figure 9. ^{1}H-NMR (400 MHz) spectrum of compound (**3**), xanthoxylin, in $CDCl_3$ 14

Figure 10. HSQC spectrum of compound (**3**), xanthoxylin, in $CDCl_3$ 15

Figure 11. COSY spectrum of compound (**3**), xanthoxylin, in $CDCl_3$ 16

Figure 12. HMBC spectrum of compound (**3**), xanthoxylin, in $CDCl_3$ 17

4. Compound (4): 2,4-dihydroxy-6-methoxyacetophenone 18

Table 3. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR data of compound **4**, 2,4-dihydroxy-6-methoxyacetophenone, in CDCl3 18

Figure 13. ^{1}H-NMR spectrum of compound (**4**), 2,4-dihydroxy-6-methoxyacetophenone, in $CDCl_3$ 19

Figure 14. HSQC spectrum of compound (**4**), 2,4-dihydroxy-6-methoxyacetophenone, in $CDCl_3$ 20

Figure 15. COSY spectrum of compound (**4**), 2,4-dihydroxy-6-methoxyacetophenone, in $CDCl_3$ 21

5. Compound (5): Jaceosidin 22

Figure 16. ^{1}H-NMR (400 MHz) spectrum of compound (**5**), jaceosidin, in $CDCl_3$ 23

6. Compound (6): Ciniformon 24

Table 4. UV spectrophotometric results of tentatively identified compound (**6**), ciniformon in methanol 24

Figure 17. ^{1}H-NMR (400 MHz) spectrum of compound (**6**), ciniformon, in CH3OD 25

Figure 18. EI-MS spectrum of compound (**6**); ciniformon 26

Figure 19. UV absorption spectrum of compound (**6**), ciniformon in methanol, λ_{max} I: 335 nm & λ_{max} II: 275 nm 26

Figure 20. UV absorption spectrum of compound (**6**), ciniformon in methanol after adding CH_3ONa, λ_{max} I: 370 nm & λ_{max} II: 275 nm. 27

Figure 21. UV absorption spectrum of compound (**6**), ciniformon in methanol, 5 minutes after adding CH_3ONa, λ_{max} I: 370 nm & λ_{max} II: 275 nm. 27

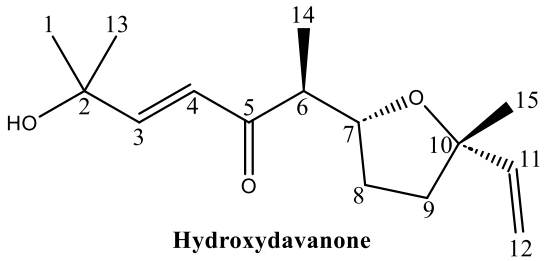
Figure 22. UV absorption spectrum of compound (**6**), ciniformon in methanol after adding $AlCl_3$, λ_{max} I: 357 nm & λ_{max} II: 280 nm. 28

Figure 23. UV absorption spectrum of compound (**6**), ciniformon in methanol after adding $AlCl_3$ and HCl, λ_{max} I: 350 nm & λ_{max} II: 275 nm. 28

Figure 24. UV absorption spectrum of compound (**6**), ciniformon in methanol after adding CH_3COONa, λ_{max} I: 375 nm & λ_{max} II: 275 nm. 29

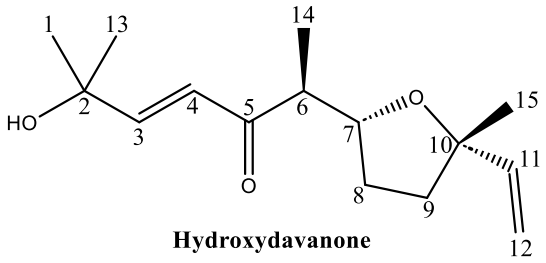
Figure 25. UV absorption spectrum of compound (**6**), ciniformon in methanol after adding CH_3COONa and $B(OH)_3$, λ_{max} I: 340 nm & λ_{max} II: 275 nm. 29

1. Compound (1): Hydroxydavanone



Hydroxydavanone

$C_{15}H_{24}O_3$; MW 252.35 g/mol; ^{1}H-NMR ($CDCl_3$, 400 MHz, *J* in Hz): δ_H 1.39 (*s*, 3H, H-1), 6.90 (*d*, *J* = 16, 1H, H-3), 6.43 (*d*, *J* = 16, 1H, H-4), 2.91 (*m*, 1H, H-6), 4.19 (*dt*, *J* = 8, 6, 1H, H-7), 1.59 (*m*, 1H, H-8_a), 1.84 (*m*, 1H, H-8_b), 1.69 (*m*, 1H, H-9_a), 1.94 (*m*, 1H, H-9_b), 5.87 (*dd*, *J* = 17.3, 10.5, 1H, H-11), 4.94 (*dd*, *J* = 16, 10.5, 1H, H-12_a), 5.17 (*dd*, *J* = 17.3, 16, 1H, H-12_b), 1.39 (*s*, 3H, H-13), 1.04 (*d*, *J* = 7, 3H, H-14), 1.26 (*s*, 3H, H-15). ^{13}C-NMR ($CDCl_3$, 100 MHz): δ_C 29.2 (*q*, C-1), 70.9 (*s*, C-2), 152.6 (*d*, C-3), 125.2 (*d*, C-4), 203.0 (*s*, C-5), 49.8 (*d*, C-6), 80.4 (*d*, C-7), 29.3 (*t*, C-8), 37.5 (*t*, C-9), 82.9 (*s*, C-10), 144.6 (*d*, C-11), 111.4 (*t*, C-12), 29.3 (*q*, C-13), 13.0 (*q*, C-14), 26.5 (*q*, C-15).



Hydroxydavanone

Table 1. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR data of compound (**1**), hydroxydavanone, in CDCl3.

Pos.	**δ_H, Mult., *J* in Hz**	**δ_C**	**COSY**	**HSQC**	**HMBC**
1	1.39 *s*	29.2	-	C_1	C_2, C_3, C_{13}
2	-	70.9	-	-	-
3	6.90 *d* (16)	152.6	4	C_3	C_1, C_2, C_4, C_5, C_{13}
4	6.43 *d* (16)	125.2	3	C_4	C_2, C_3, C_5, C_6
5	-	203.0	-	-	-
6	2.91 *m*	49.8	7, 14	C_6	C_4, C_5, C_7, C_8, C_{14}
7	4.19 *dt* (8, 6)	80.4	6, 8_a, 8_b	C_7	C_5, C_6, C_8, C_9, C_{14}
8_a	1.59 *m*	29.3	7, 9	C_8	C_6, C_7, C_9, C_{10}
8_b	1.84 *m*	29.3	7, 9	C_8	C_6, C_7, C_9, C_{10}
9_a	1.69 *m*	37.5	8_a, 8_b, 9_b	C_9	C_7, C_8, C_{10}, C_{11}, C_{15}
9_b	1.94 *m*	37.5	8_a, 8_b, 9_a	C_9	C_7, C_8, C_{10}, C_{11}, C_{15}
10	-	82.9	-	-	-
11	5.87 *dd* (17.3, 10.5)	144.6	12_a, 12_b	C_{11}	C_9, C_{12}, C_{15}
12_a	4.94 *dd* (16, 10.5)	111.4	11, 12_b	C_{12}	C_9, C_{11}, C_{15}
12_b	5.17 *dd* (17.3, 16)	111.4	11, 12_a	C_{12}	C_9, C_{11}, C_{15}
13	1.39 *s*	29.3	-	C_{13}	C_1, C_2, C_3
14	1.04 *d* (7)	13.0	6	C_{14}	C_5, C_6, C_7
15	1.26 *s*	26.5	-	C_{15}	C_9, C_{10}, C_{11}

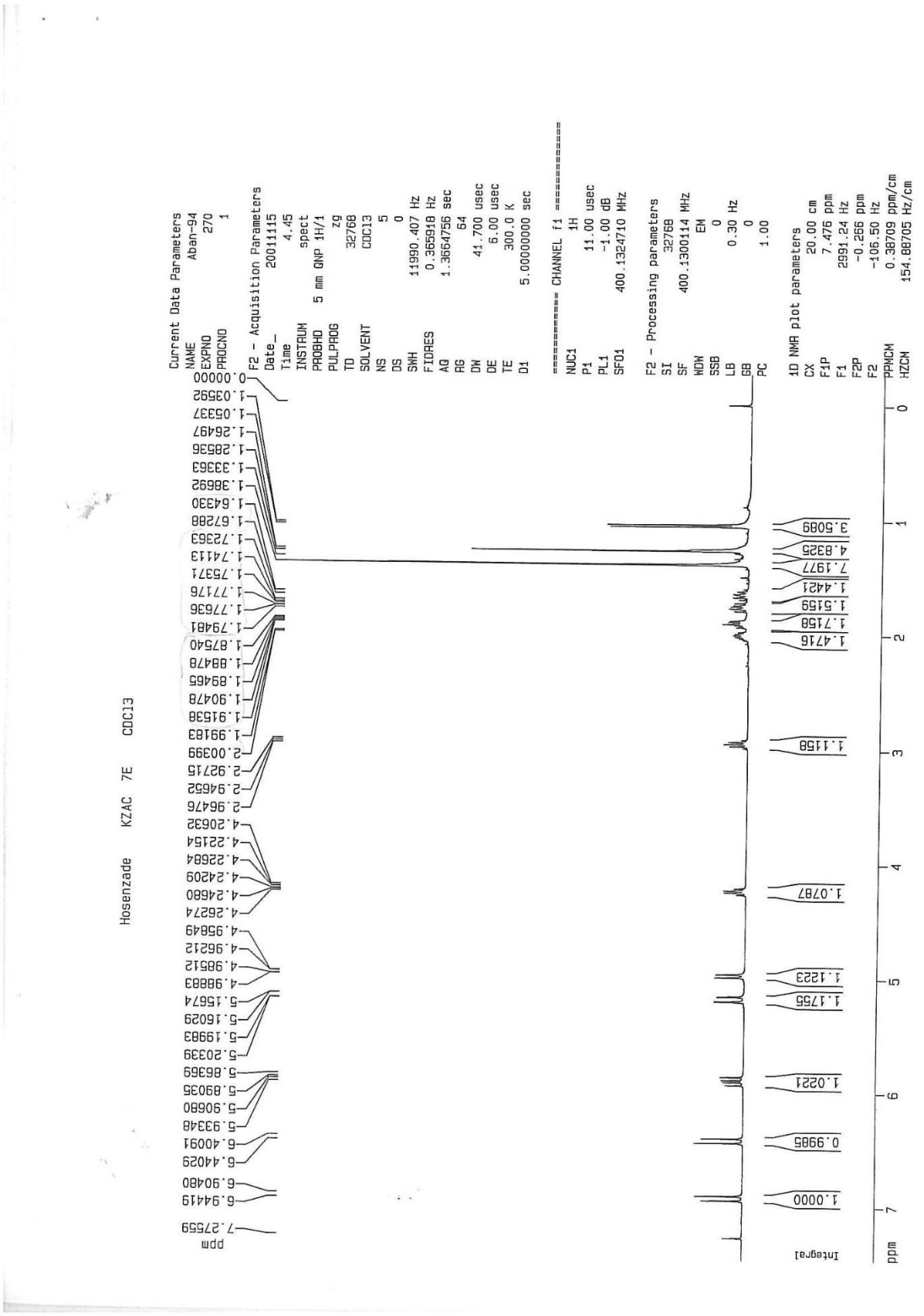


Figure 1. ^{1}H-NMR (400 MHz) spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$

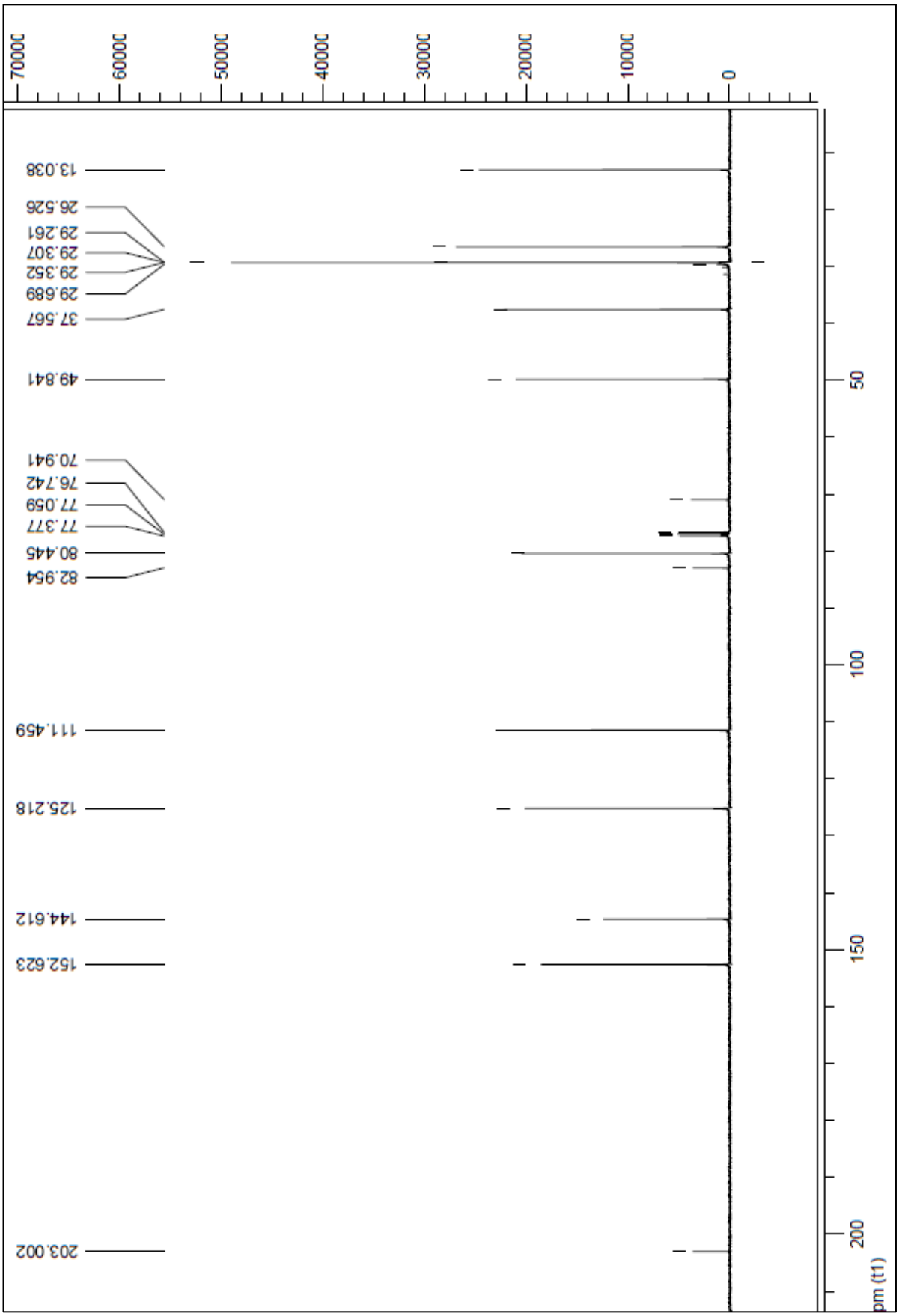


Figure 2. ^{13}C-NMR (100 MHz) spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$

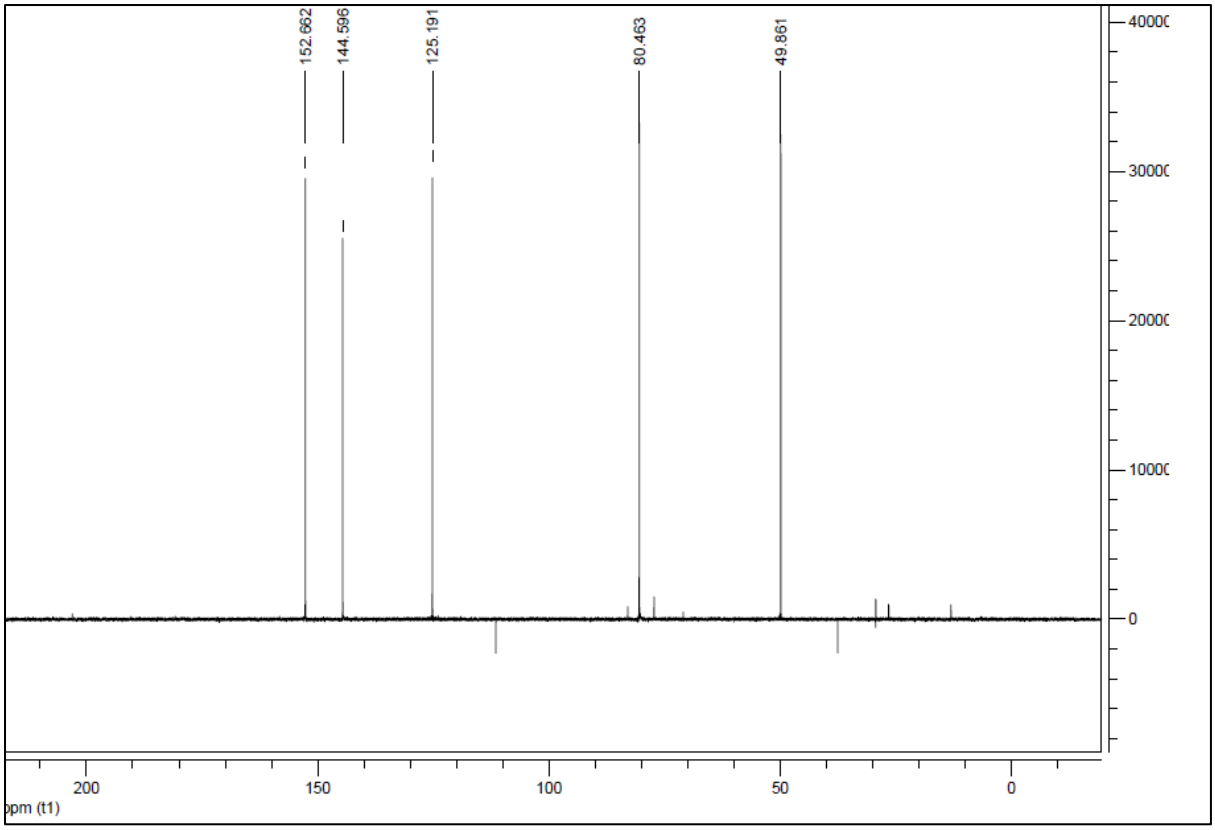


Figure 3. DEPT 90˚ (100 MHz) spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$

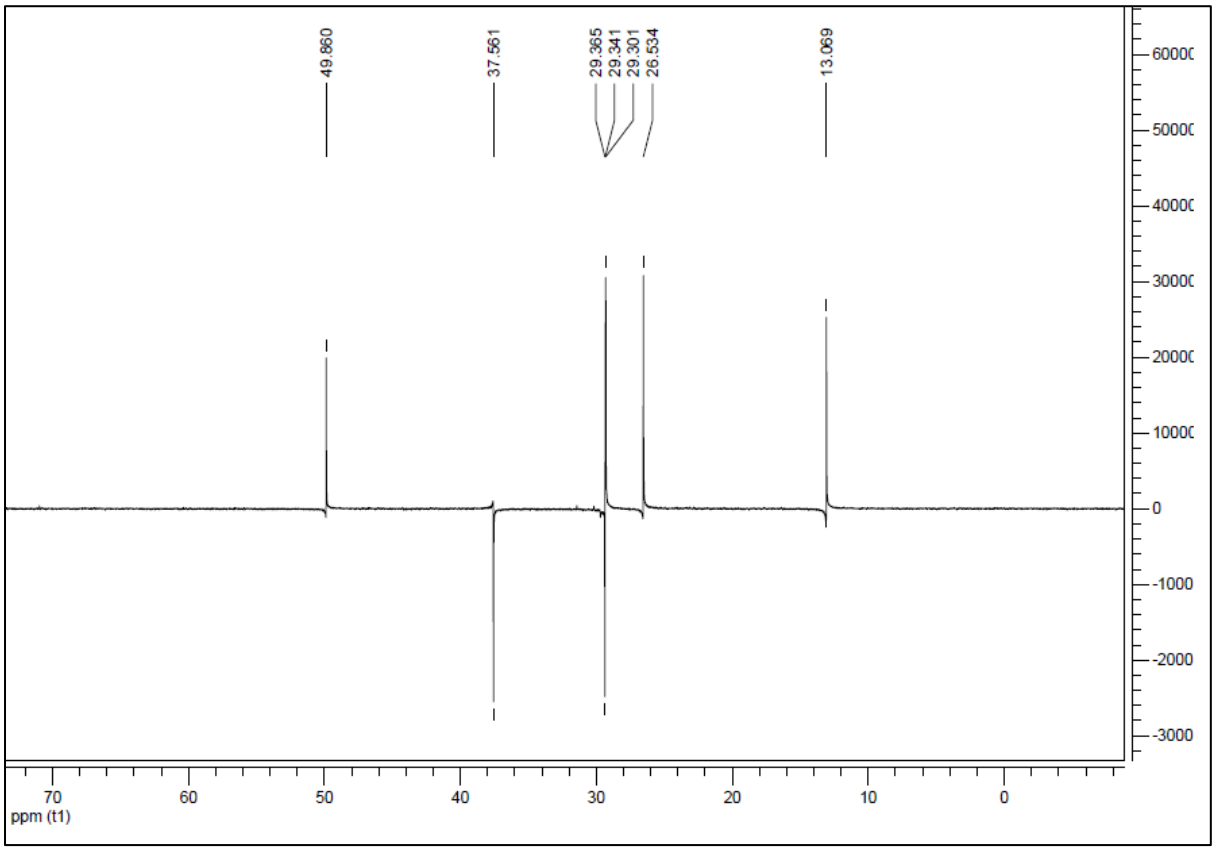


Figure 4. DEPT 135˚ (100 MHz) spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$

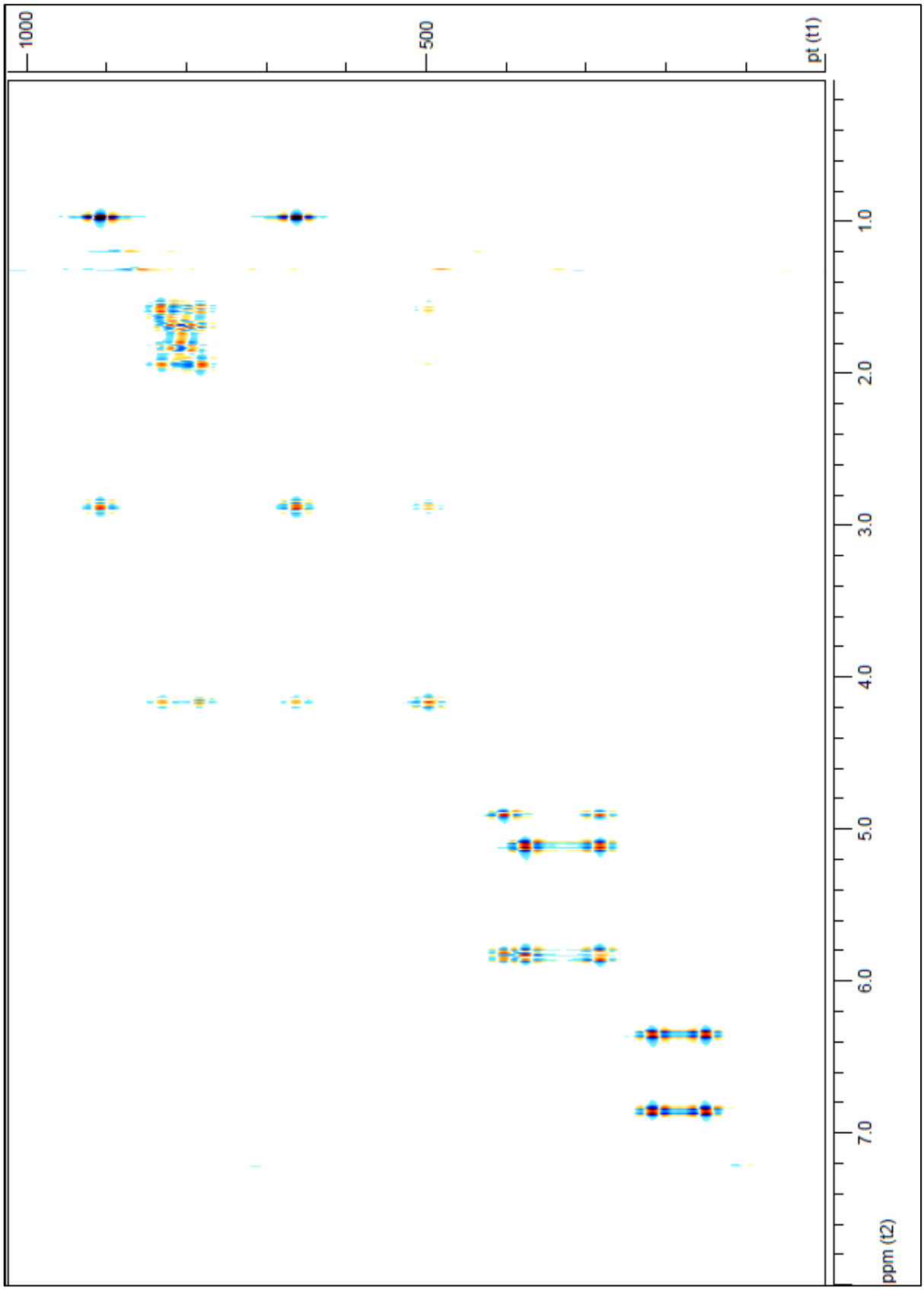


Figure 5. COSY spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$

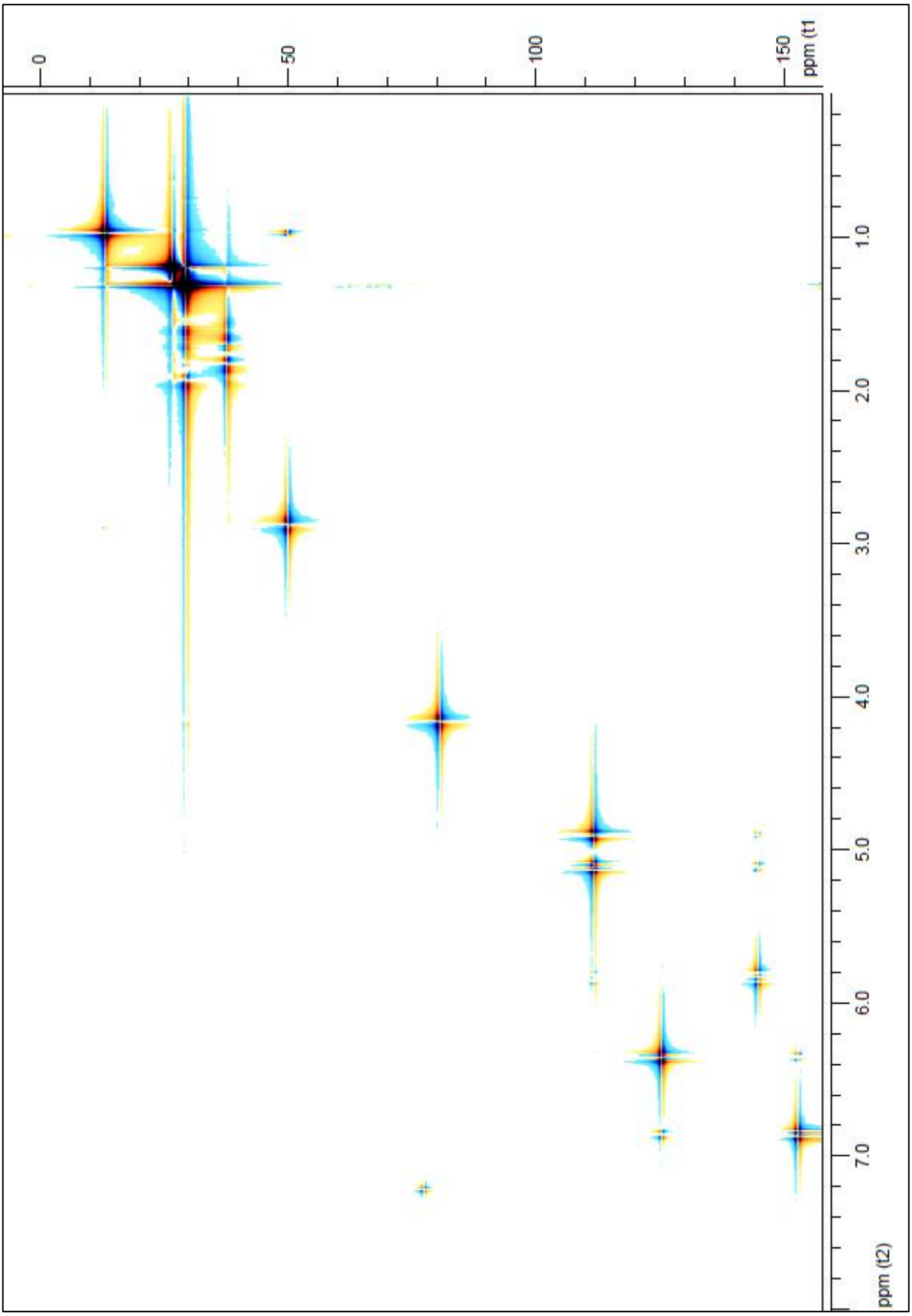


Figure 6. HSQC spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$

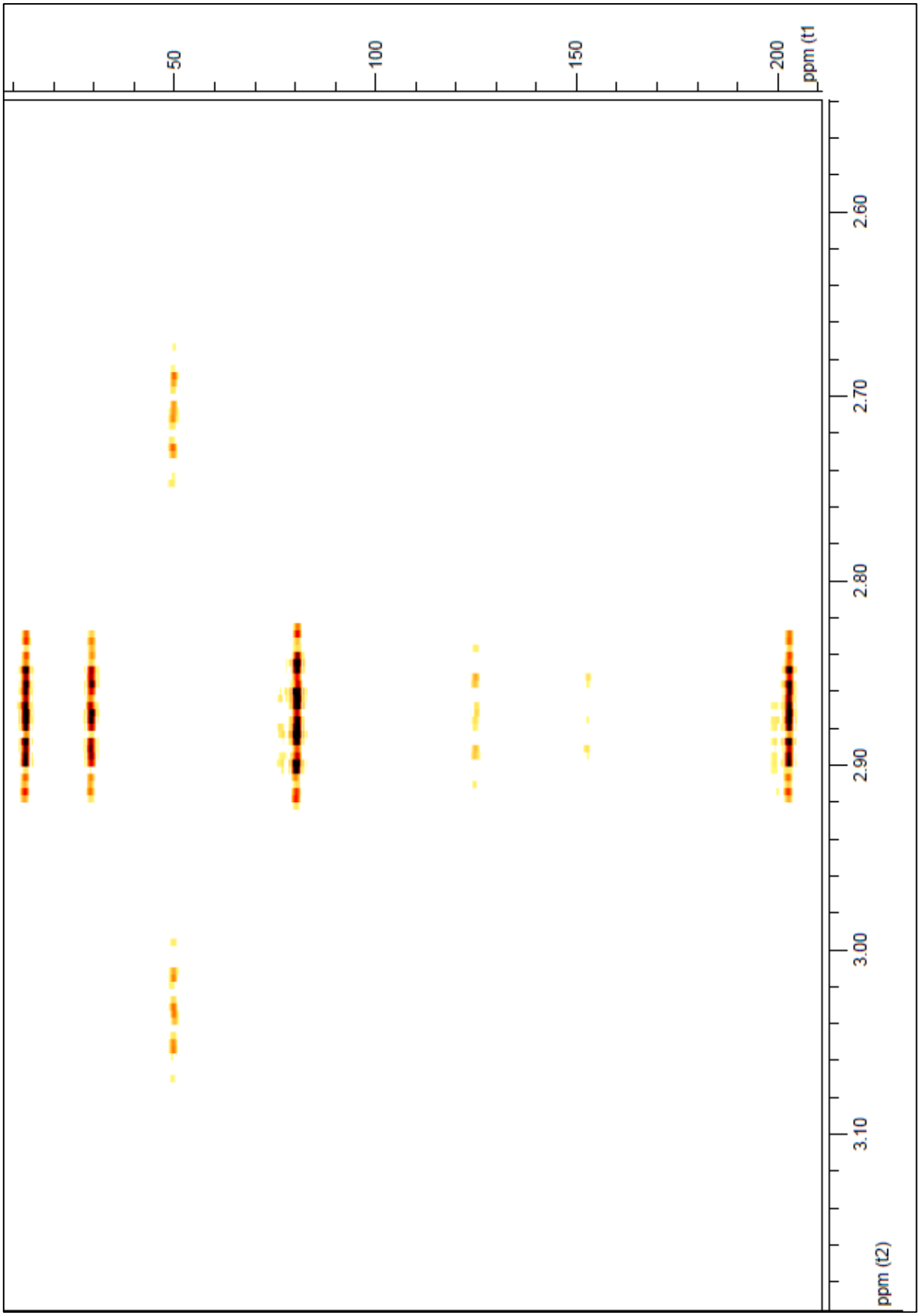
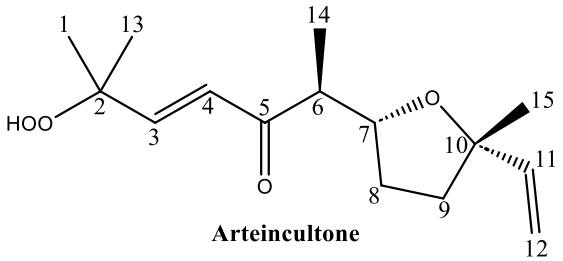


Figure 7. HMBC spectrum of compound (**1**), hydroxydavanone, in $CDCl_3$

2. Compound (2): Arteincultone



Arteincultone

$C_{15}H_{24}O_4$; MW 268.35 g/mol; ^{1}H-NMR ($CDCl_3$, 400 MHz, *J* in Hz): δ_H 1.39 (*s*, 3H, H-1), 6.86 (*d*, *J*= 16, 1H, H-3), 6.39 (*d*, *J* = 16, 1H, H-4), 2.99 (*m*, 1H, H-6), 4.15 (*dt*, *J* = 8, 6, 1H, H-7), 1.54-2.06 (*overlapped*, H-8_a & H-8_b, H-9_a & H-9_b), 5.88 (*dd*, *J* = 10.5, 17.3, 1H, H-11), 5.16 (*dd*, *J* = 16, 17.3, 1H, H-12_a), 4.97 (*dd*, *J* = 10.5, 16, 1H, H-12_b), 1.39 (*s*, 3H, H-13), 1.03 (*d*, *J* = 7, 3H, H-14), 1.24 (*s*, 3H, H-15), 8.29 (*s*, 1H, OH).

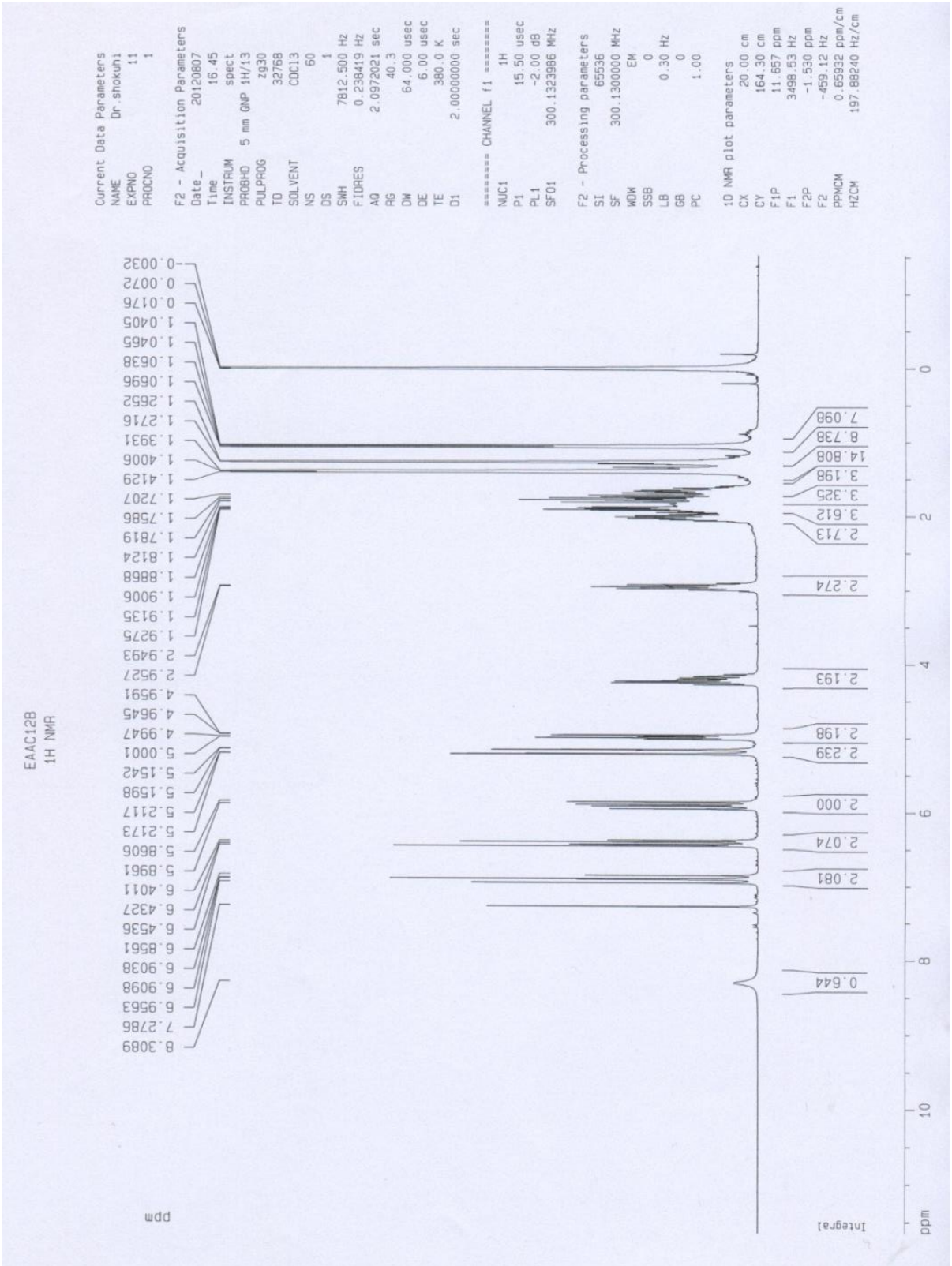
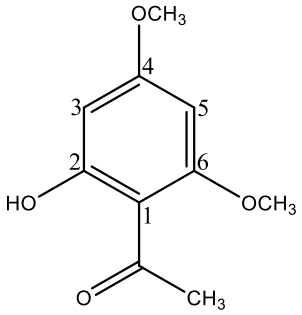


Figure 8. ^{1}H-NMR (400 MHz) spectrum of compound (**2**), arteincultone, in $CDCl_3$

3. Compound (3): Xanthoxylin



Xanthoxylin

$C_{10}H_{12}O_4$; MW 196.20 g/mol; ^{1}H-NMR ($CDCl_3$, 400 MHz, *J* in Hz): δ_H 5.92 (*d*, *J* = 2.4, 1H, H-3), 6.06 (*d*, *J* = 2.4, 1H, H-5), 3.85 (*s*, 3H, 4-Methoxy), 3.82 (*s*, 3H, 6-Methoxy), 2.61 (*s*, 3H, MeCO). ^{13}C-NMR ($CDCl_3$, 100 MHz): δ_C 105.9 (*s*, C-1), 162.9 (*s*, C-2), 93.5 (*d*, C-3), 167.6 (*s*, C-4), 90.7 (*d*, C-5), 166.1 (*d*, C-6), 203.2 (*s*, C=O), 32.8 (*q*, Ac), 55.5 (*q*, 4-Methoxy), 54.7 (*q*, 6-Methoxy).

Table 2. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR data of compound (**3**), xanthoxylin, in CDCl3.

Pos.	**δ_H, Mult., *J* in Hz**	**δ_C**	**COSY**	**HSQC**	**HMBC**
1	-	105.9	-	-	-
2	-	162.9	-	-	-
3	5.92 *d* (2.4)	93.5	-	C_3	C_1, C_5
4	-	167.6	-	-	-
5	6.06 *d* (2.4)	90.7	-	C_5	C_1, C_3
6	-	166.1	-	-	-
C=O	-	203.2	-	-	-
-Ac	2.61 *s*	32.8	-	C_{Ac}	-
4-Methoxy	3.85 *s*	55.5	-	$C_{4\text{-Methoxy}}$	-
6-Methoxy	3.82 *s*	54.7	-	$C_{6\text{-Methoxy}}$	-

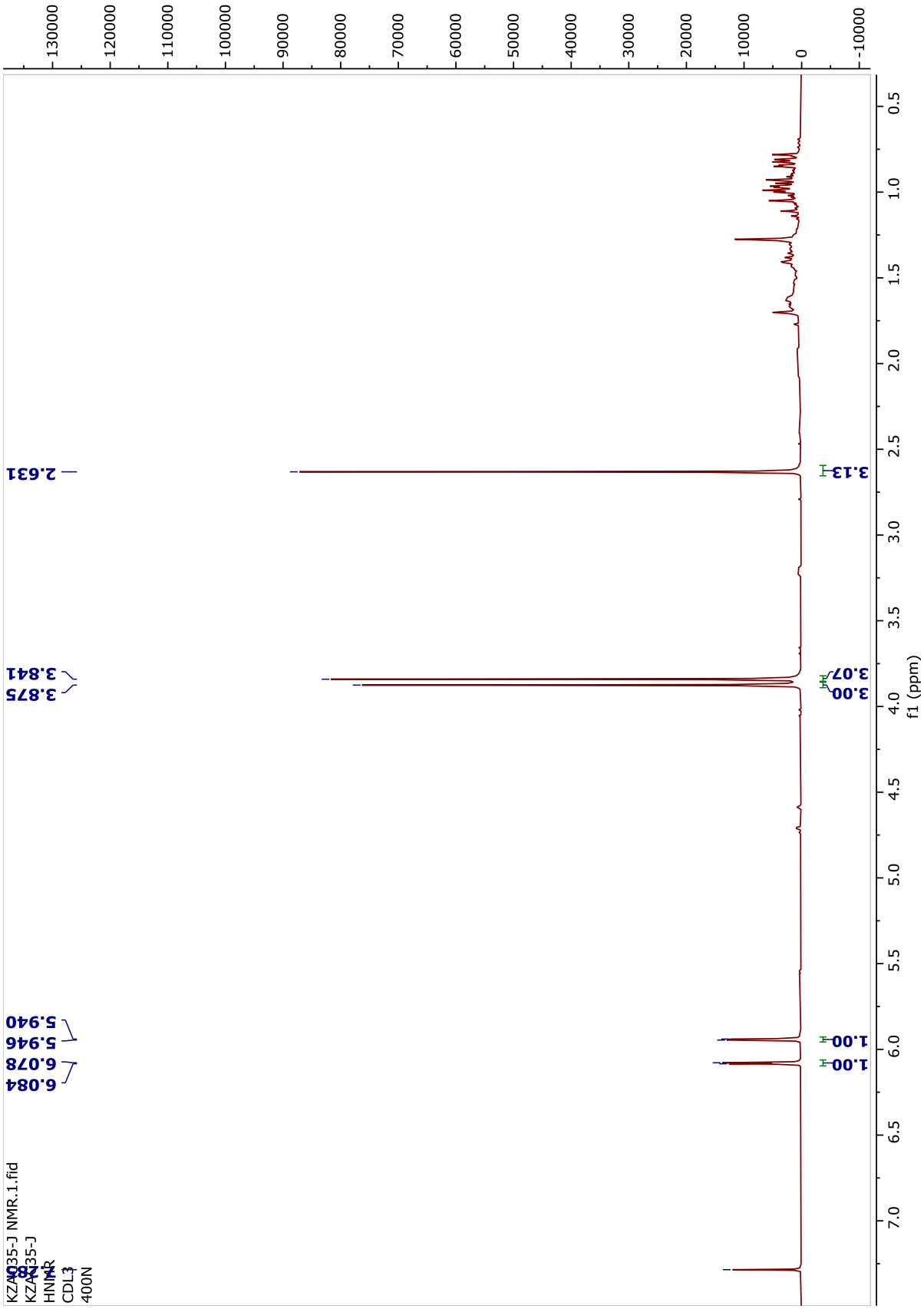


Figure 9. ^{1}H-NMR (400 MHz) spectrum of compound (**3**), xanthoxylin, in $CDCl_3$

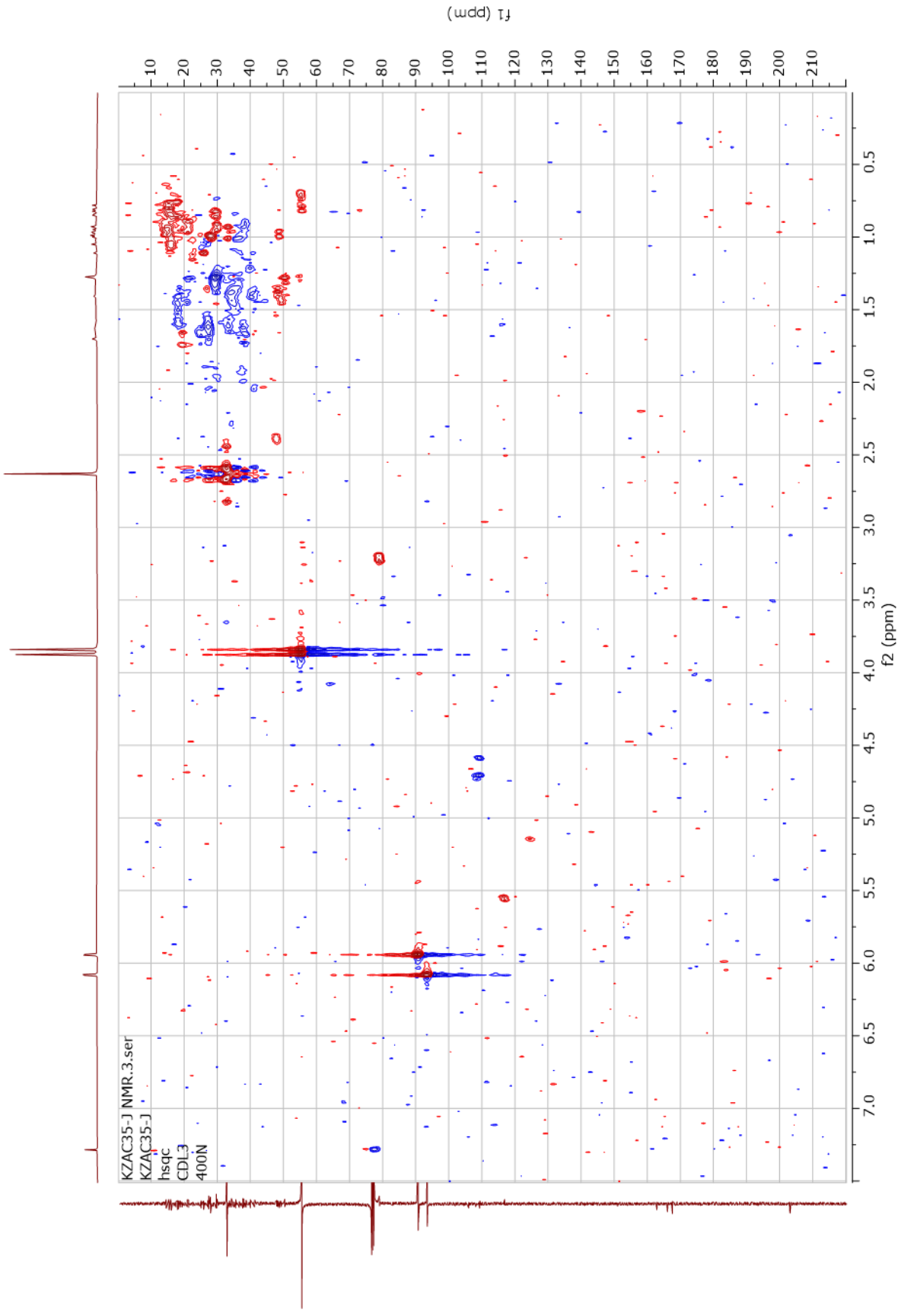


Figure 10. HSQC spectrum of compound (**3**), xanthoxylin, in $CDCl_3$

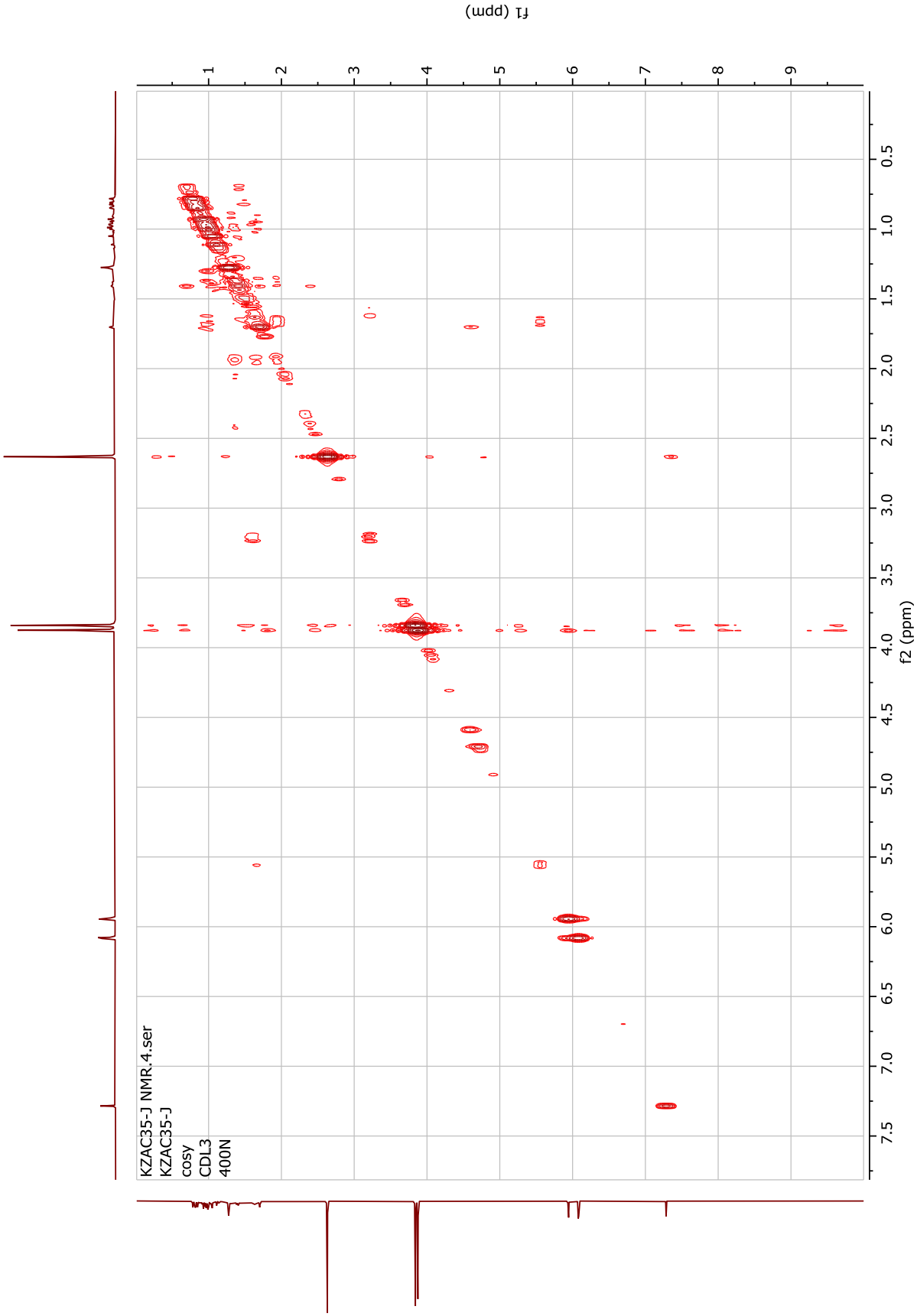


Figure 11. COSY spectrum of compound (**3**), xanthoxylin, in $CDCl_3$

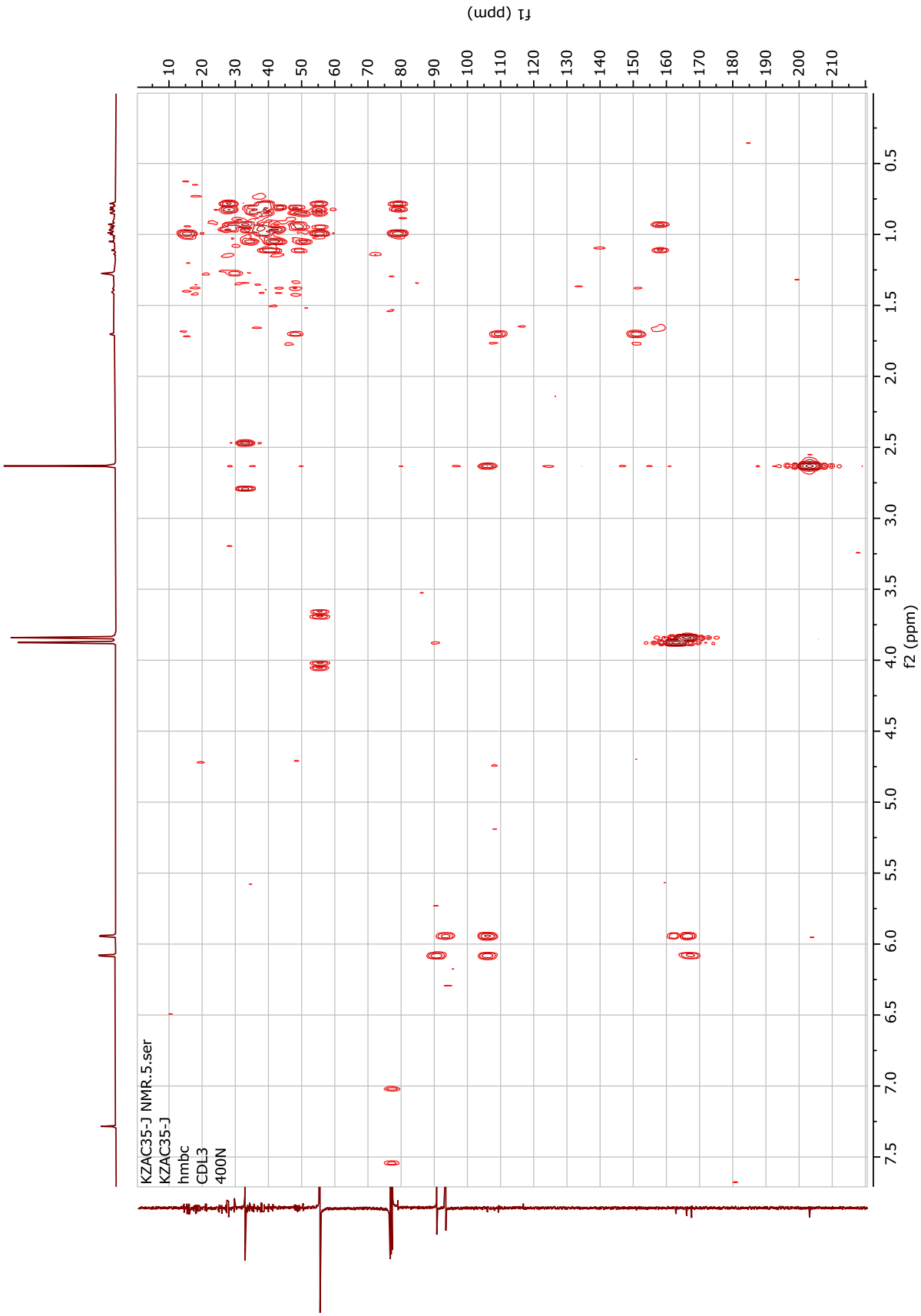
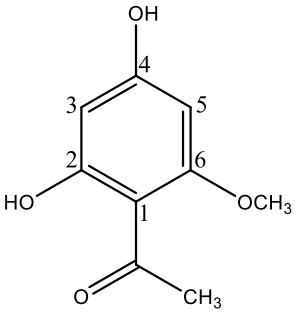


Figure 12. HMBC spectrum of compound (**3**), xanthoxylin, in $CDCl_3$

4. Compound (4): 2,4-dihydroxy-6-methoxyacetophenone



2,4-Dihydroxy-6-methoxy acetophenone

$C_9H_{10}O_4$; MW 182.18 g/mol; ^{1}H-NMR ($CDCl_3$, 400 MHz, *J* in Hz): δ_H 5.91 (*s*, 1H, H-3), 5.98 (*s*, 1H, H-5), 3.87 (*s*, 3H, 6-Methoxy), 2.61 (*s*, 3H, MeCO). ^{13}C-NMR ($CDCl_3$, 100 MHz): δ_C 106.3 (*s*, C-1), 166.1 (*s*, C-2), 96.4 (*d*, C-3), 165.3 (*s*, C-4), 91.9 (*d*, C-5), 167.2 (*d*, C-6), 203.4 (*s*, C=O), 33.0 (*q*, Ac), 55.7 (*q*, 6-Methoxy).

Table 3. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR data of compound **4**, 2,4-dihydroxy-6-methoxyacetophenone, in CDCl3.

Pos.	**δ_H, Mult., *J* in Hz**	**δ_C**	**COSY**	**HSQC**
1	-	106.3	-	
2	-	166.1	-	
3	5.91 *s*	96.4	-	C_3
4	-	165.3	-	
5	5.98 *s*	91.9	-	C_5
6	-	167.2	-	-
C=O	-	203.4	-	-
-Ac	2.61 *s*	33.0	-	C_{Ac}
6-Methoxy	3.87 *s*	55.7	-	$C_{6\text{-Methoxy}}$

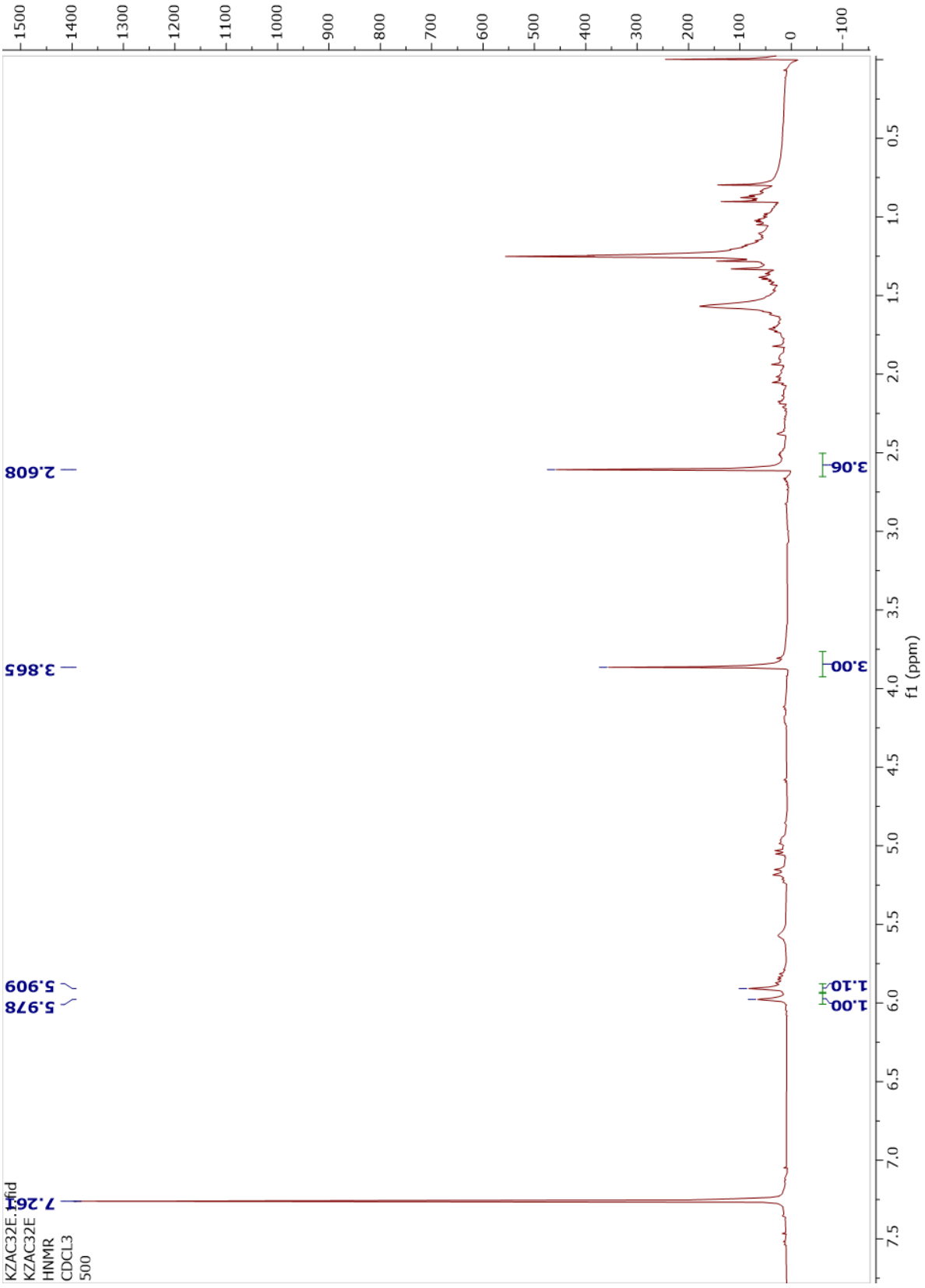


Figure 13. ^{1}H-NMR spectrum of compound (**4**), 2,4-dihydroxy-6-methoxyacetophenone, in $CDCl_3$

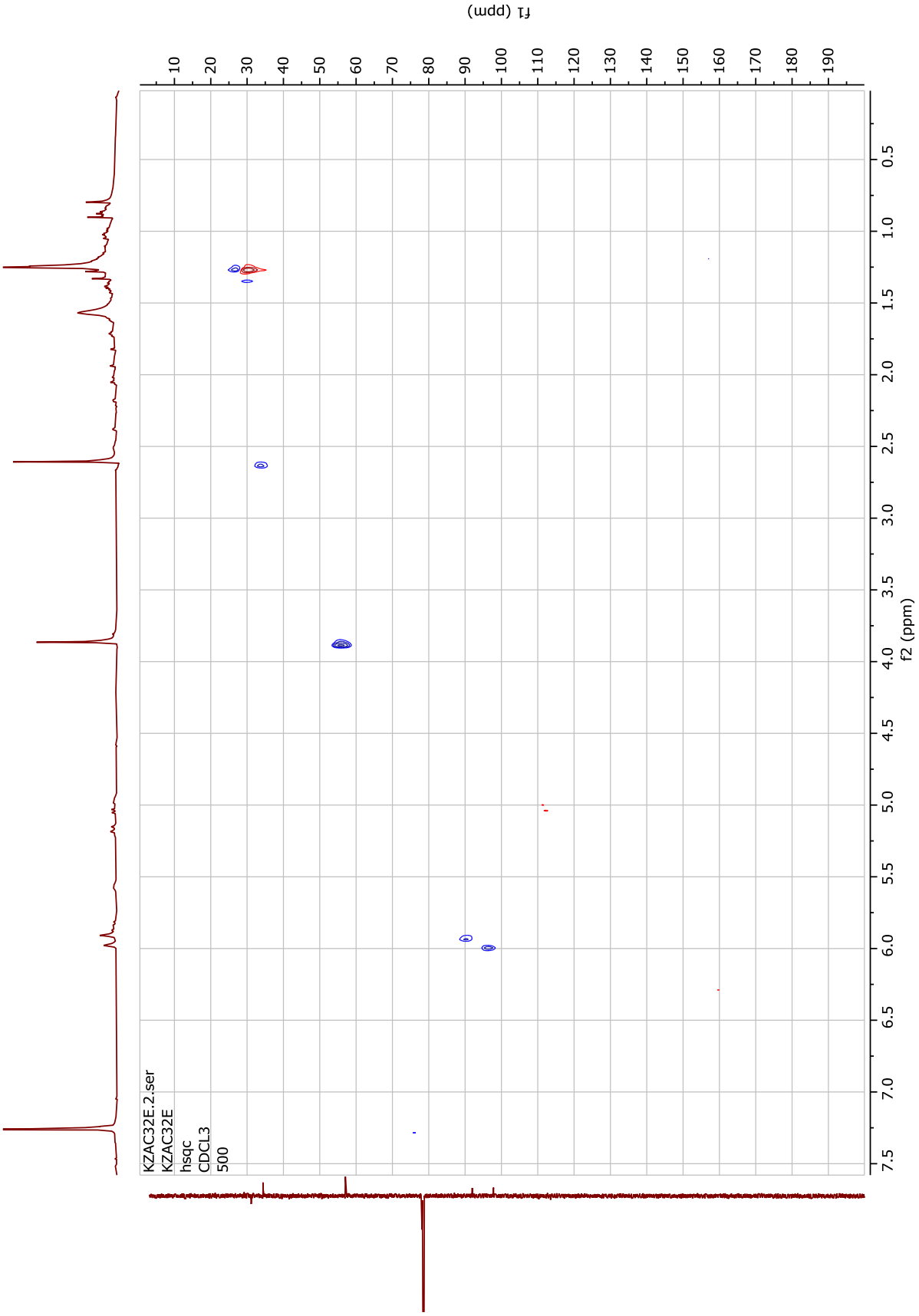


Figure 14. HSQC spectrum of compound (**4**), 2,4-dihydroxy-6-methoxyacetophenone, in $CDCl_3$

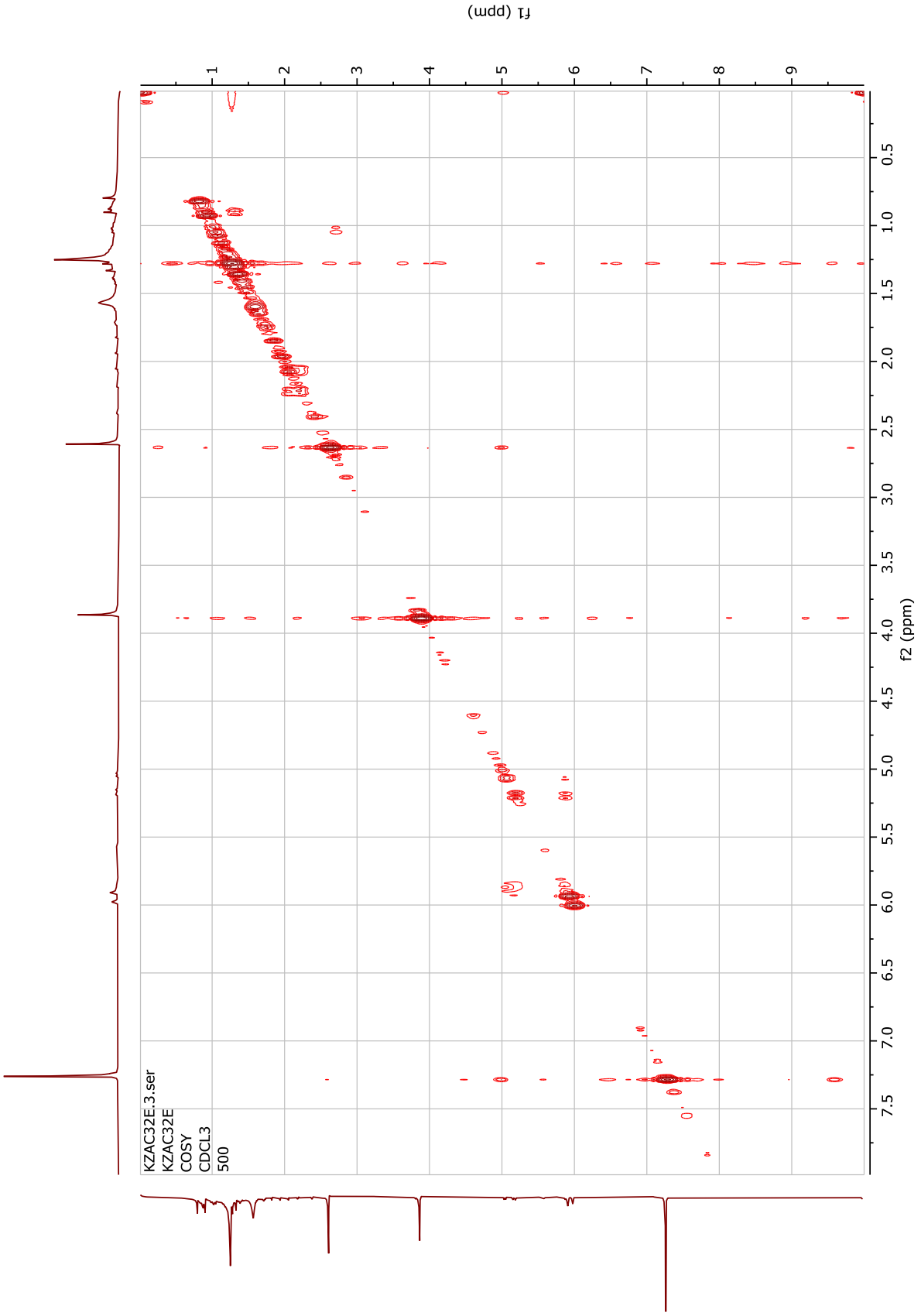
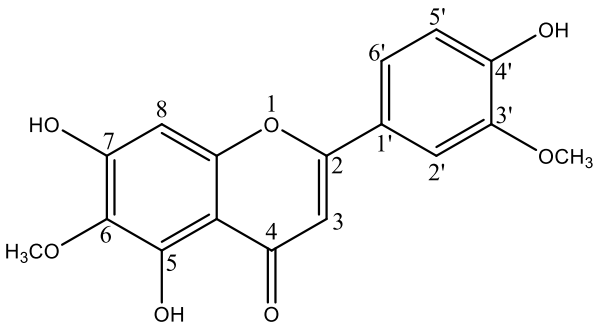


Figure 15. COSY spectrum of compound (**4**), 2,4-dihydroxy-6-methoxyacetophenone, in $CDCl_3$

5. Compound (5): Jaceosidin



Jaceosidin

$C_{17}H_{14}O_7$; MW 330.29 g/mol; ^{1}H-NMR (CH_3OD, 400 MHz, *J* in Hz): δ_H 6.66 (*s*, 1H, H-3), 6.61 (*s*, 1H, H-8), 7.52 (*s*, 1H, H-2′), 6.96 (*d*, *J* = 8.3,1H, H-5′), 7.54 (*d*, *J* = 8.3, 1H, H-6′), 3.99 (*s*, 3H, 6-Methoxy), 3.91 (*s*, 3H, 3′-Methoxy); EI-MS *m/z* (rel. int.): 51 (16.8), 63 (8.7), 69 (100), 77 (15.9), 83 (4.8), 89 (7.7), 95 (5.3), 105 (21.2), 115 (6.7), 122 (18.8), 133 (15.4), 139 (29.7), 149 (32.7), 156 (8.7), 167 (15.4), 175 (3.4), 183 (4.8), 189 (3.4), 217 (2.9), 229 (4.8), 237 (2.9), 243 (2.4), 257 (8.7), 272 (7.2), 278 (2.4), 287 (60.6), 301 (29.8), 312 (64.4), 318 (5.8), 330 (91.8).

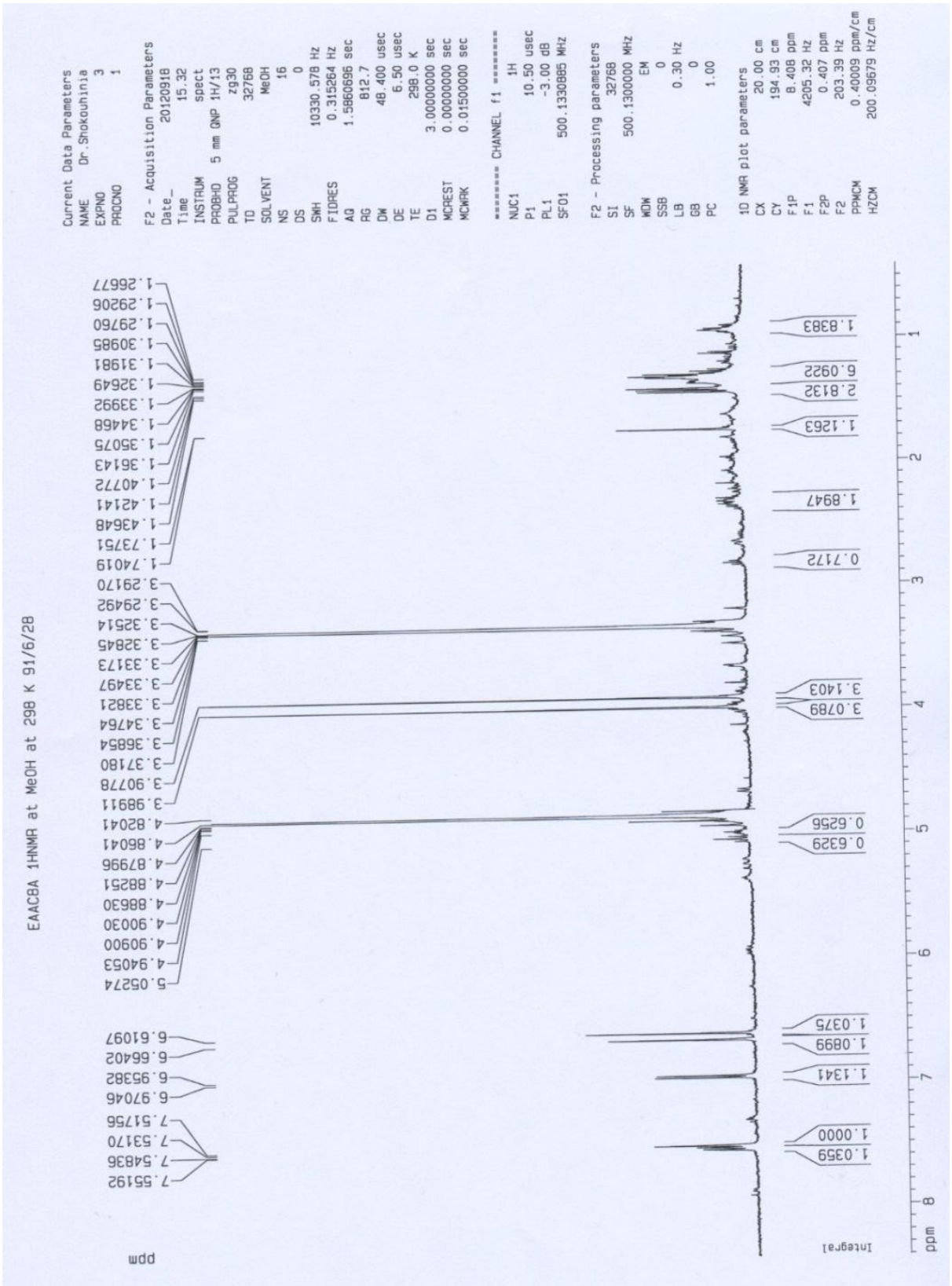
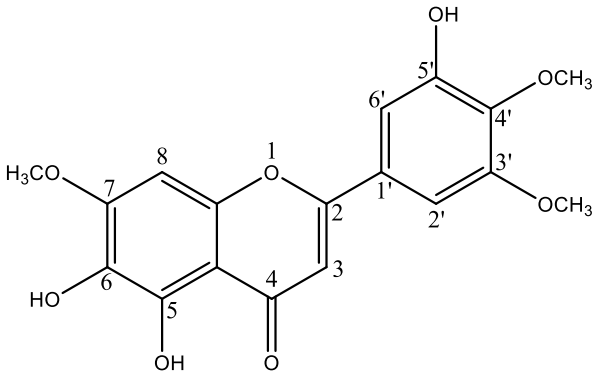


Figure 16. ^{1}H-NMR (400 MHz) spectrum of compound (**5**), jaceosidin, in $CDCl_3$

6. Compound (6): Ciniformon



Ciniformon

$C_{18}H_{16}O_8$; MW 360.32 g/mol; ^{1}H-NMR (CH_3OD, 400 MHz, *J* in Hz): δ_H 6.67 (*s*, 1H, H-3), 6.61 (*s*, 1H, H-8), 7.15 (*d*, *J* = 2, 1H, H-2′), 7.12 (*d*, *J* = 2, 1H, H-6′), 3.89 (*s*, 3H, 3′-Methoxy), 3.91 (*s*, 3H, 4′-Methoxy), 3.96 (*s*, 3H, 7-Methoxy). EI-MS *m/z* (rel. int.): 55 (22.0), 69 (100), 76 (5.1), 83 (20.3), 90 (5.9), 97 (14.4), 105 (12.3), 112 (5.9), 119 (16.1), 129 (10.2), 139 (36.4), 146 (5.1), 153 (19.5), 164 (36.4), 171 (23.7), 179 (26.7), 189 (5.5), 202 (5.1), 217 (7.2), 225 (3.8), 236 (4.2), 259 (12.3), 273 (11.0), 287 (5.9), 301 (10.6), 317 (46.2), 326 (5.9), 333 (28.8), 342 (62.3), 360 (86.4s).

Table 4. UV spectrophotometric results of tentatively identified compound (**6**), ciniformon in methanol.

Reagent	λ_{max} I (nm)	λ_{max} II (nm)
CH_3OH	335	275
CH_3ONa	370	275
CH_3ONa (after 5 min.)	370	275
$AlCl_3$	357	280
$AlCl_3$/HCl	350	275
CH_3COONa	375	275
$CH_3COONa/B(OH)_3$	340	275

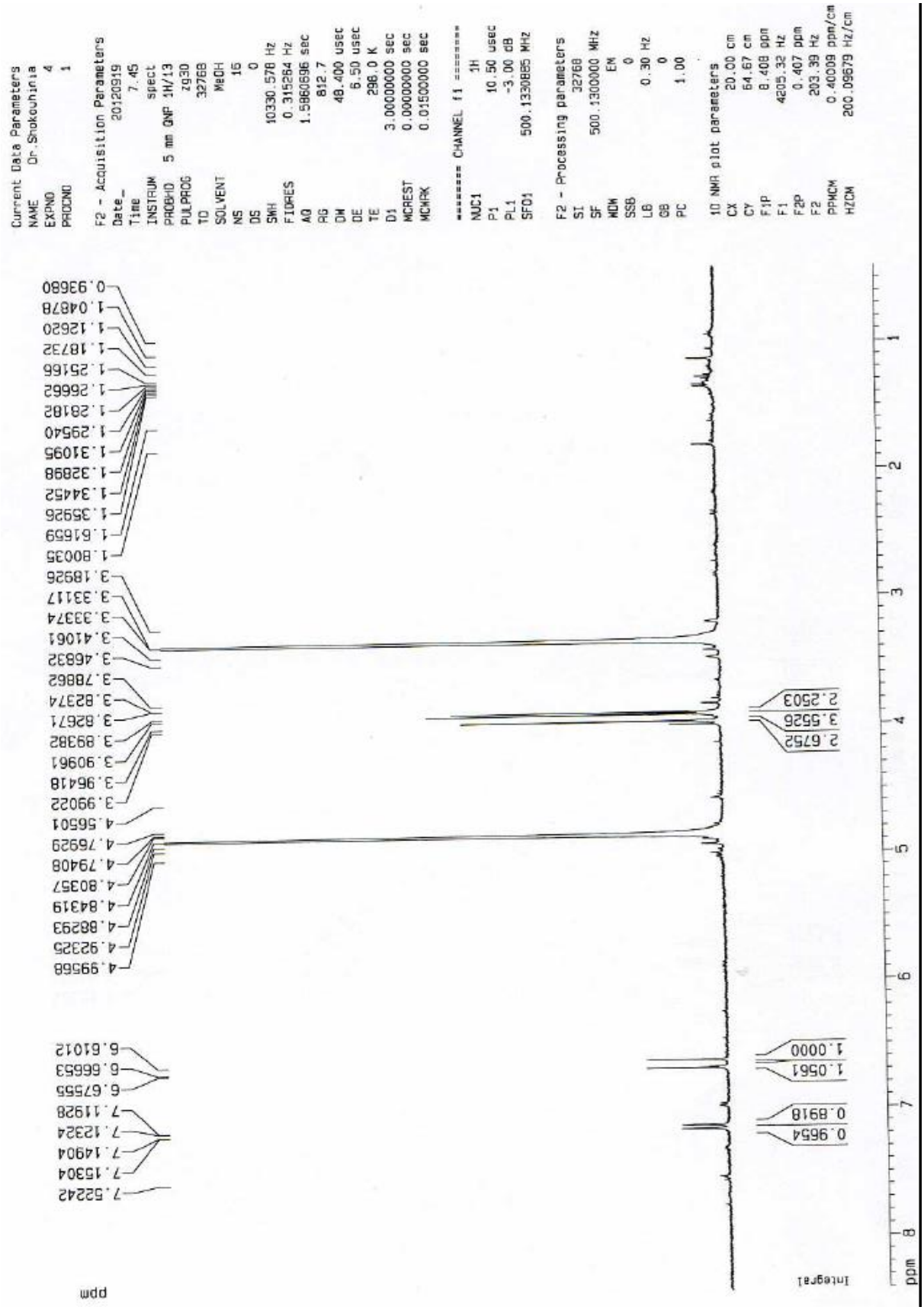


Figure 17. [1]H-NMR (400 MHz) spectrum of compound (**6**), ciniformon, in CH3OD

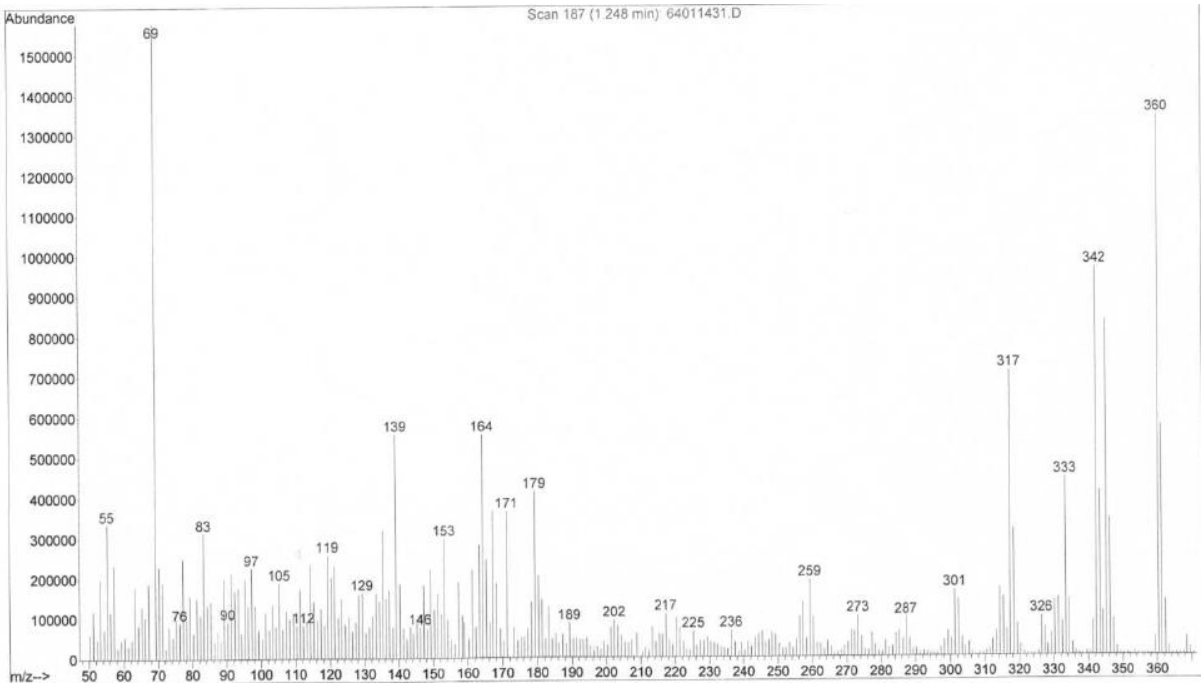


Figure 18. EI-MS spectrum of compound (**6**); ciniformon

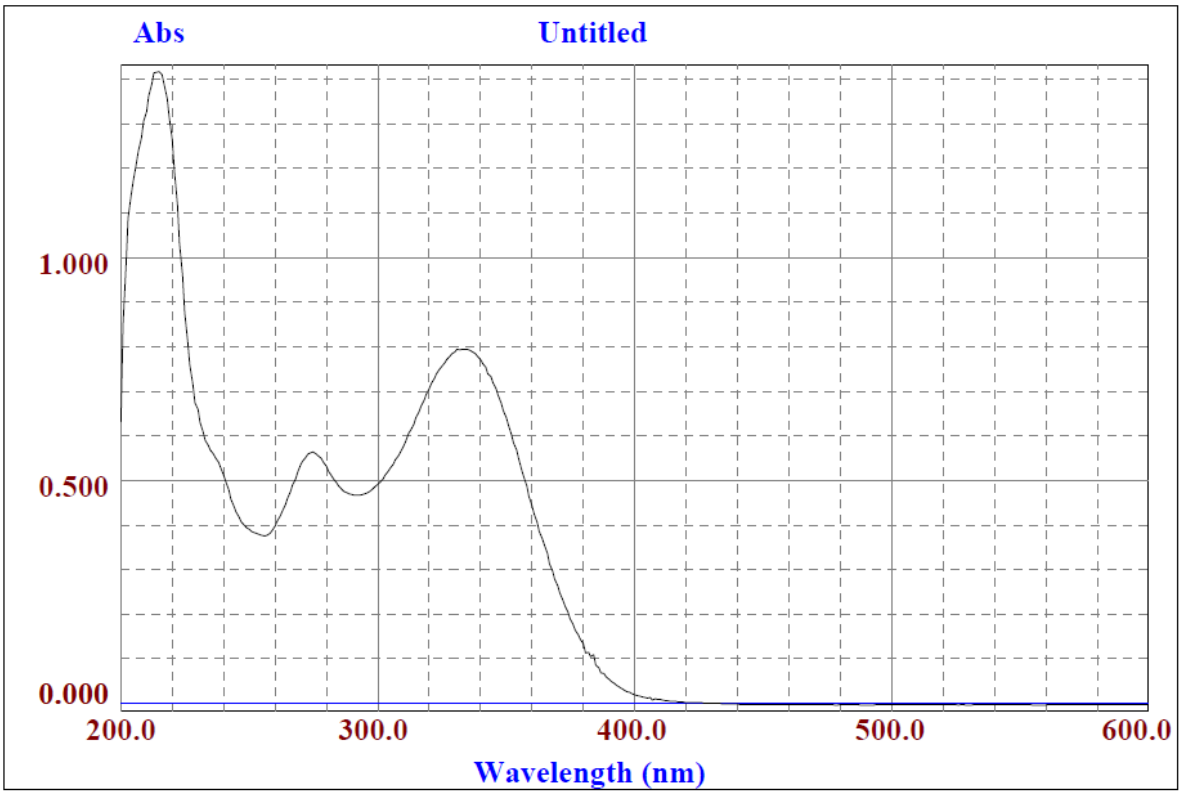


Figure 19. UV absorption spectrum of compound (**6**), ciniformon in methanol, λ_{max} I: 335 nm & λ_{max} II: 275 nm.

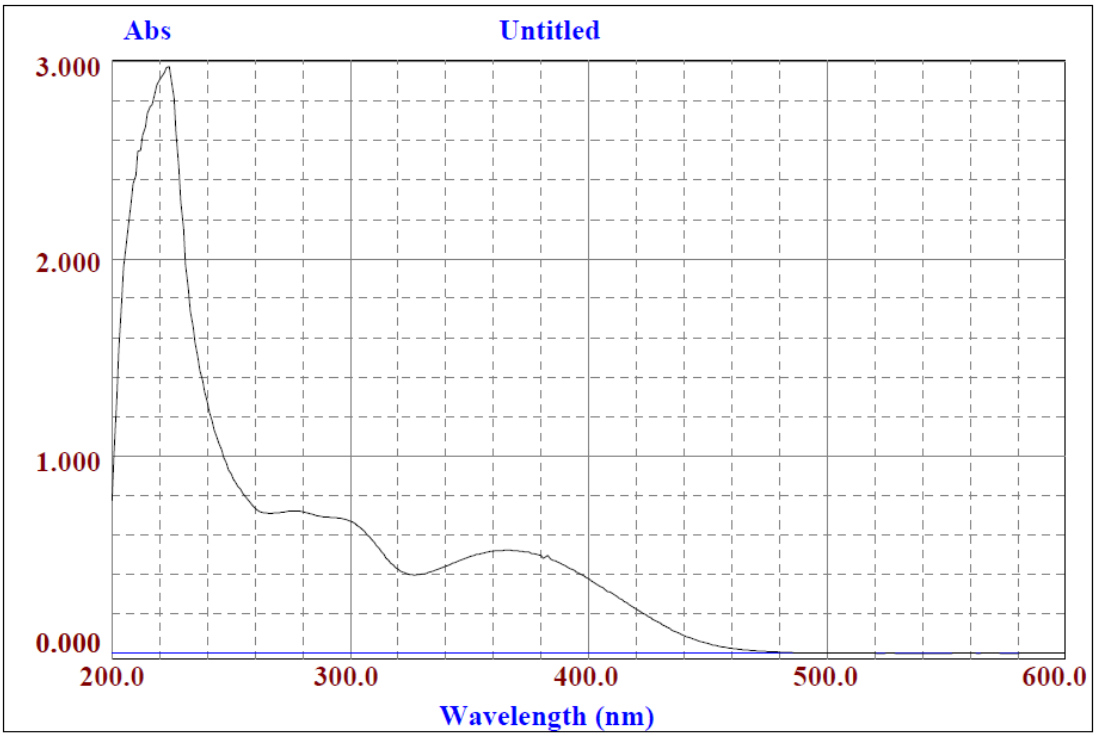


Figure 20. UV absorption spectrum of compound (**6**), ciniformon in methanol after adding CH_3ONa, λ_{max} I: 370 nm & λ_{max} II: 275 nm.

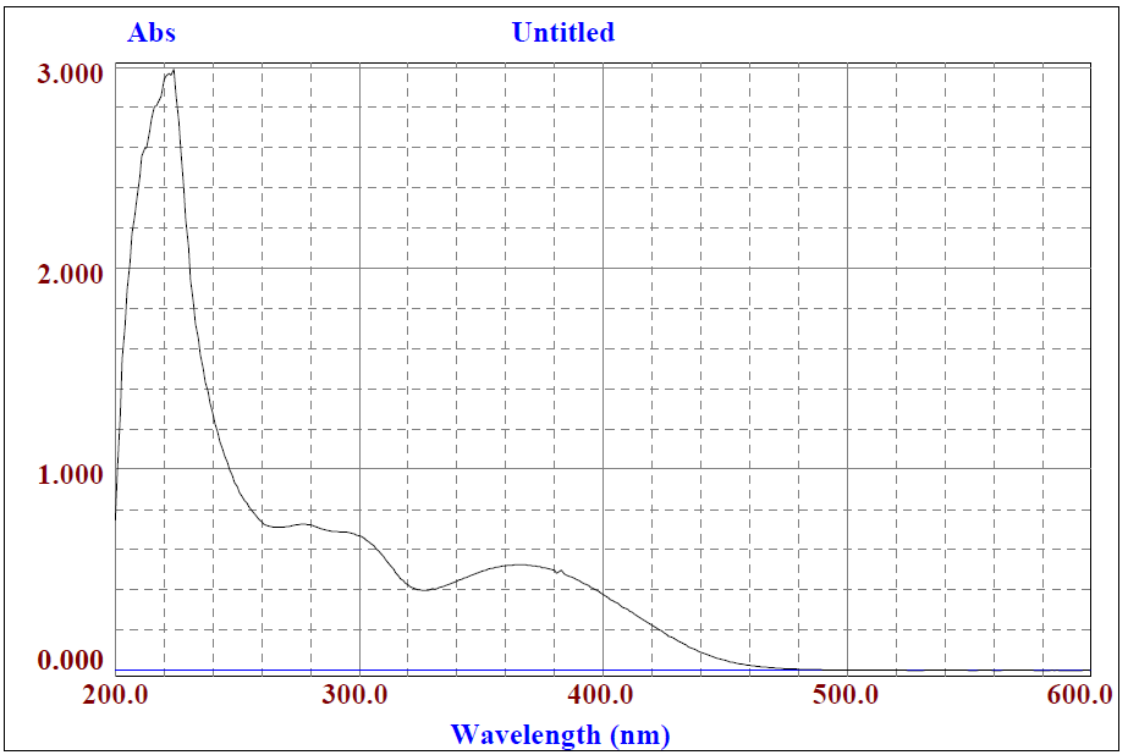


Figure 21. UV absorption spectrum of compound (**6**), ciniformon in methanol, 5 minutes after adding CH_3ONa, λ_{max} I: 370 nm & λ_{max} II: 275 nm.

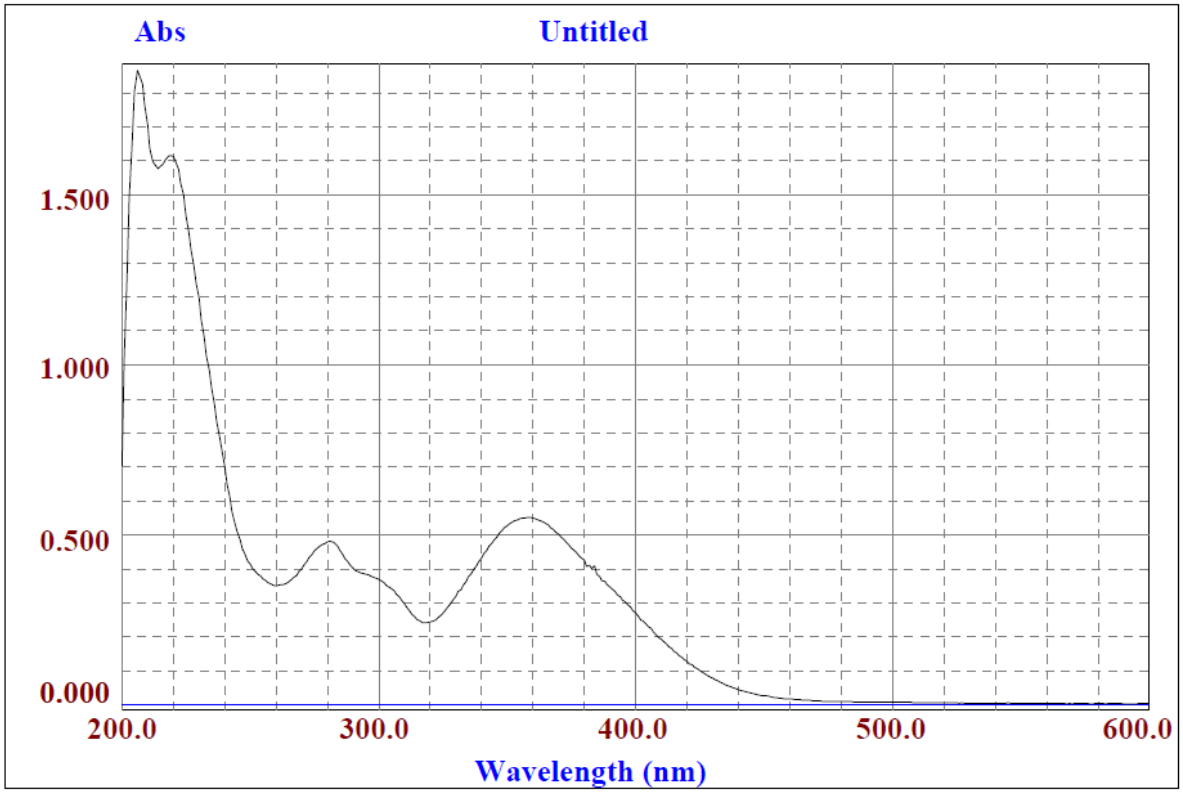


Figure 22. UV absorption spectrum of compound (**6**), ciniformon in methanol after adding $AlCl_3$, λ_{max} I: 357 nm & λ_{max} II: 280 nm.

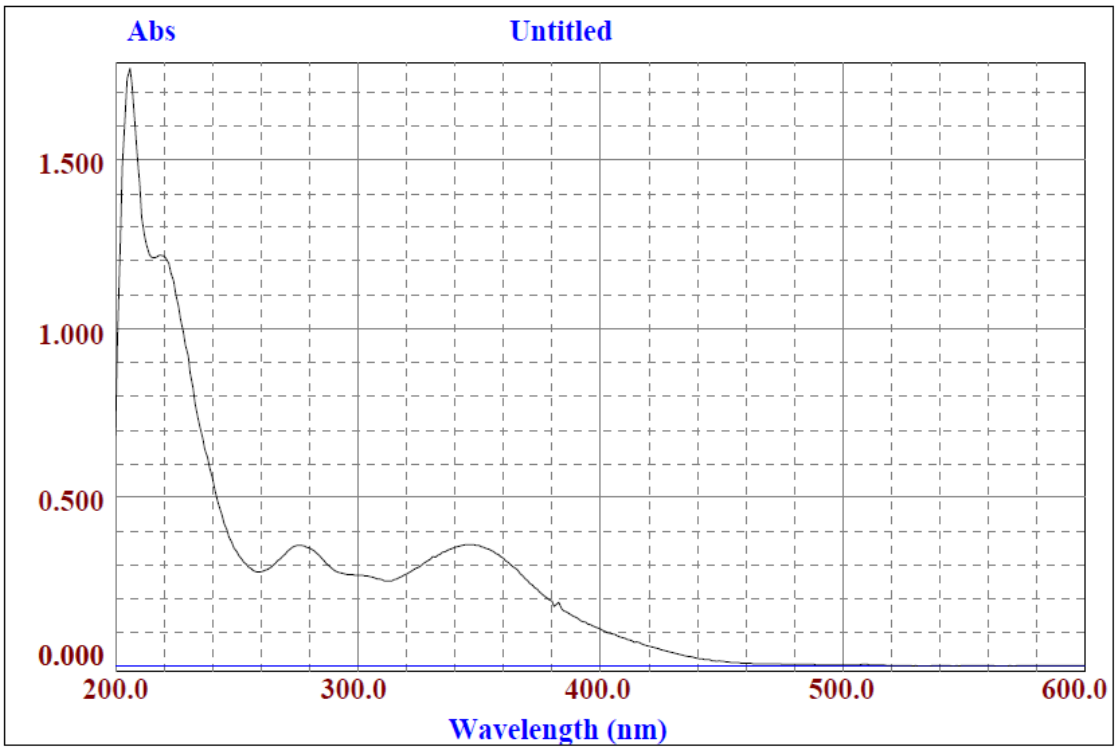


Figure 23. UV absorption spectrum of compound (**6**), ciniformon in methanol after adding $AlCl_3$ and HCl, λ_{max} I: 350 nm & λ_{max} II: 275 nm.

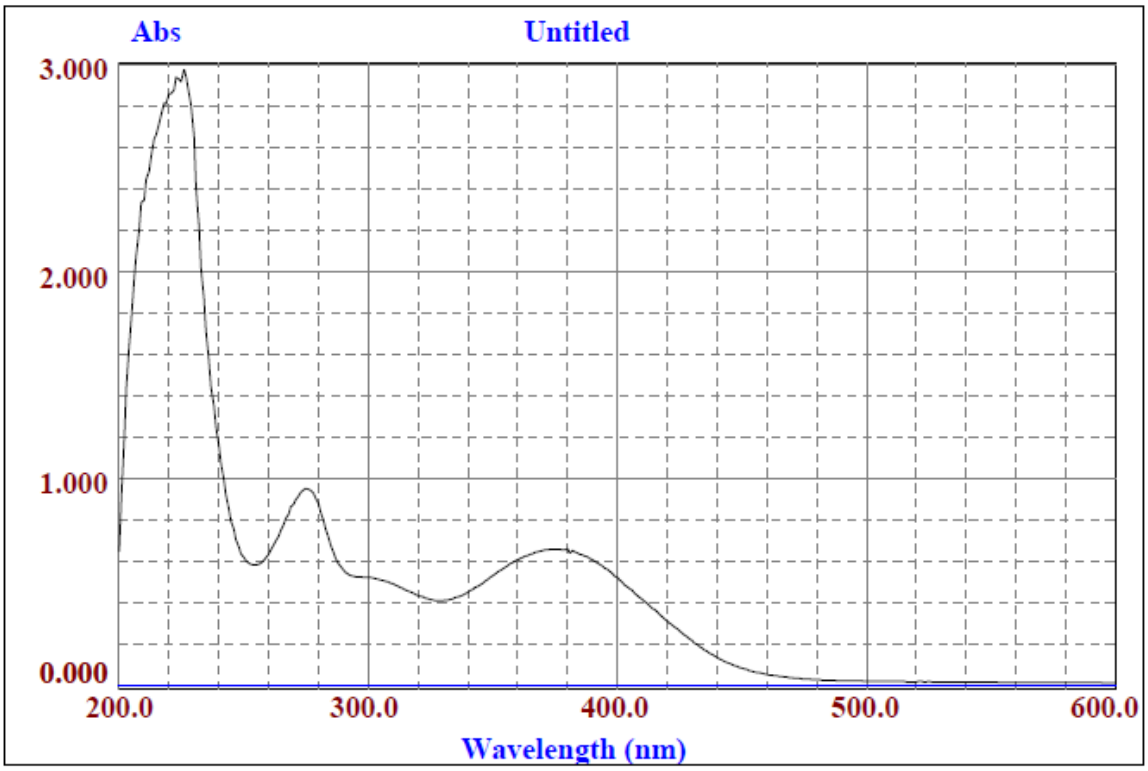


Figure 24. UV absorption spectrum of compound (**6**), ciniformon in methanol after adding CH_3COONa, λ_{max} I: 375 nm & λ_{max} II: 275 nm.

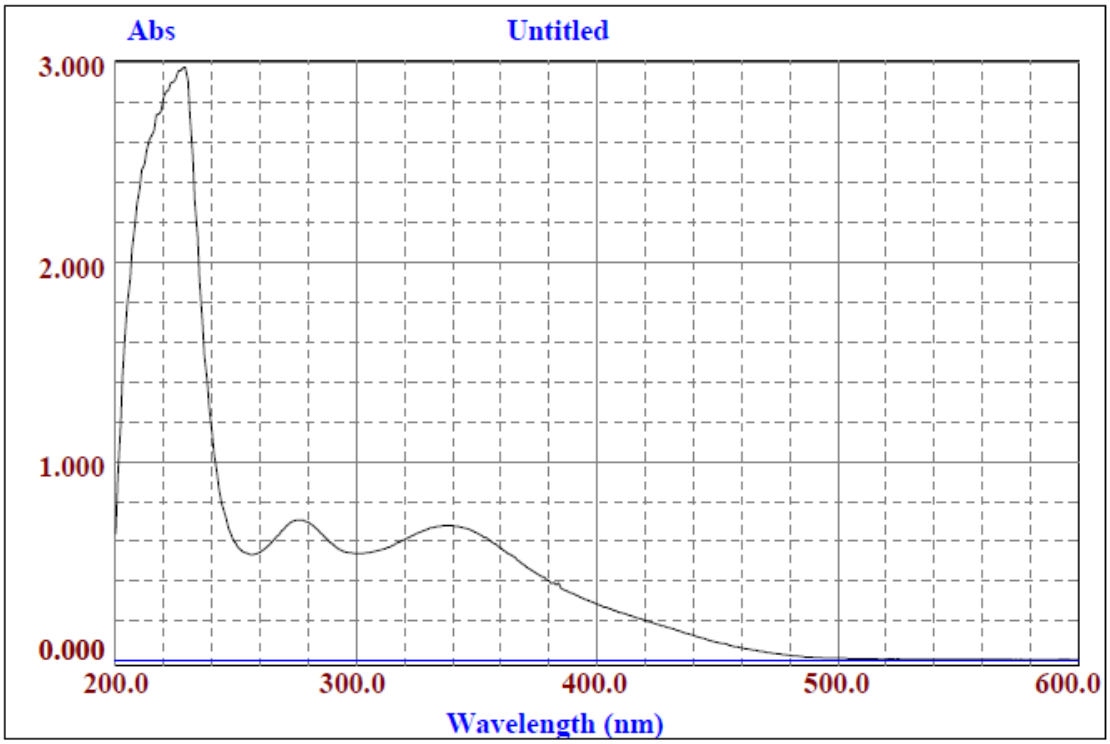


Figure 25. UV absorption spectrum of compound (**6**), ciniformon in methanol after adding CH_3COONa and $B(OH)_3$, λ_{max} I: 340 nm & λ_{max} II: 275 nm.