

Reference

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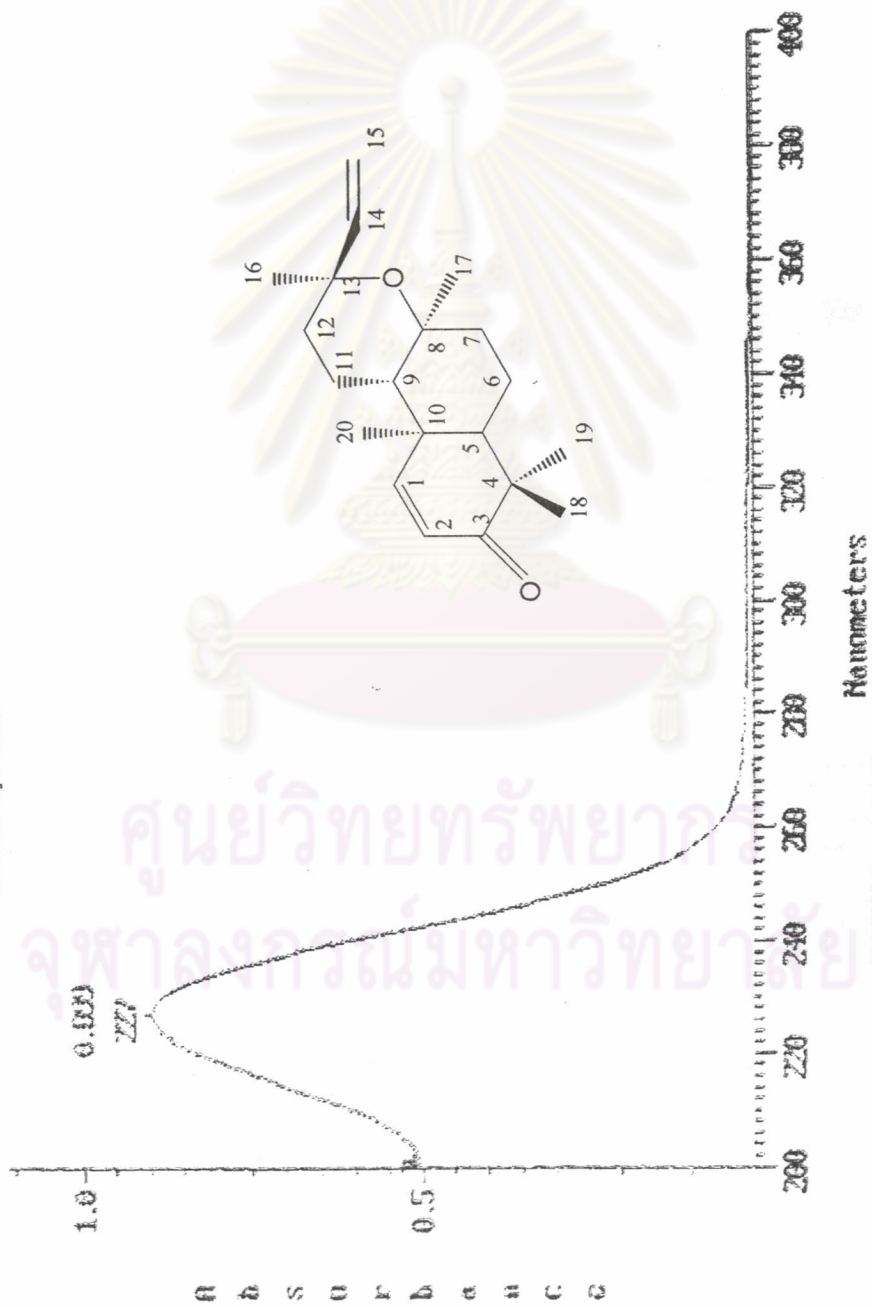


Figure 10: The UV spectrum of compound C-1 (in MeOH)

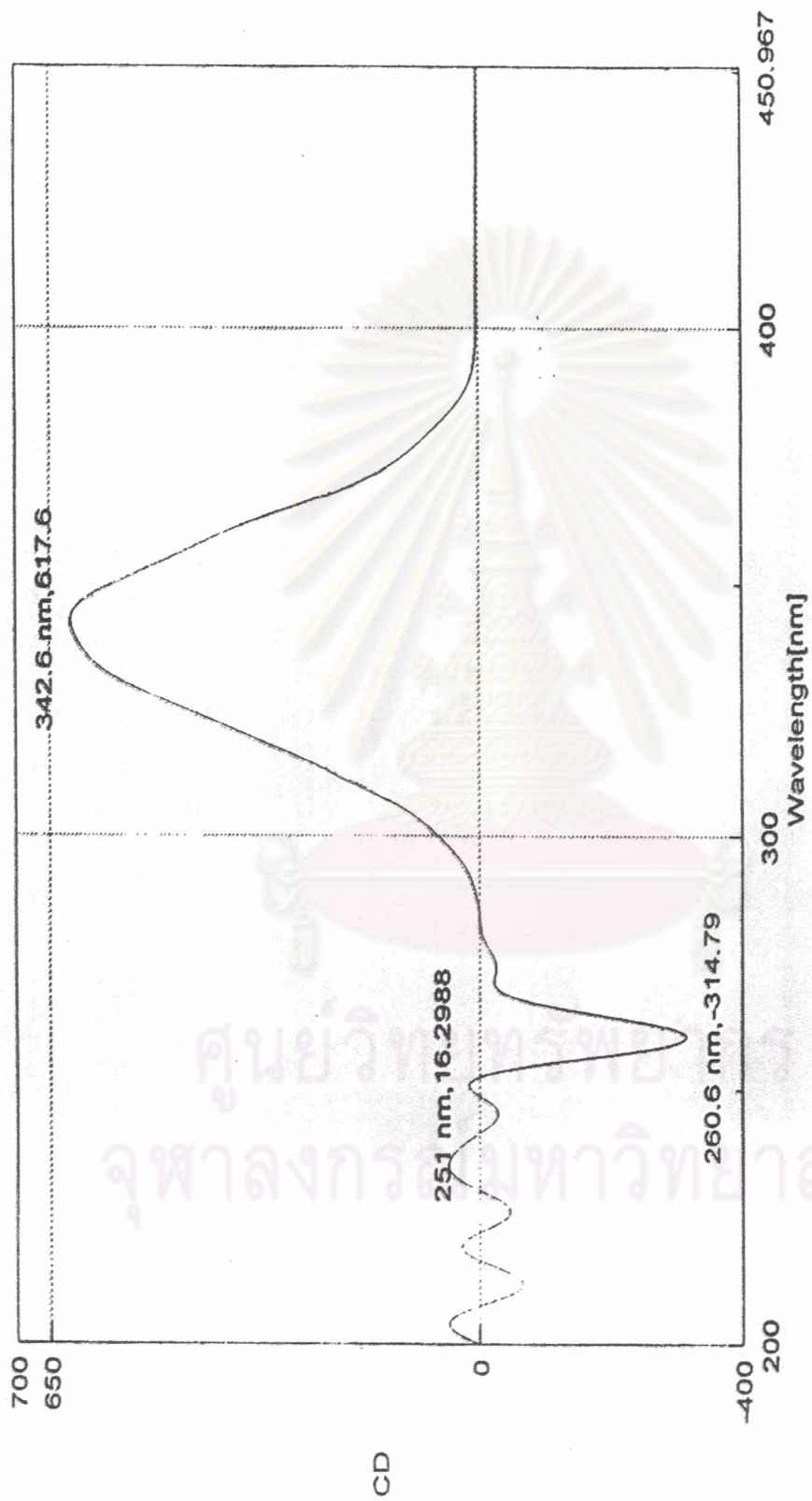


Figure 11: The CD spectrum of compound C-1

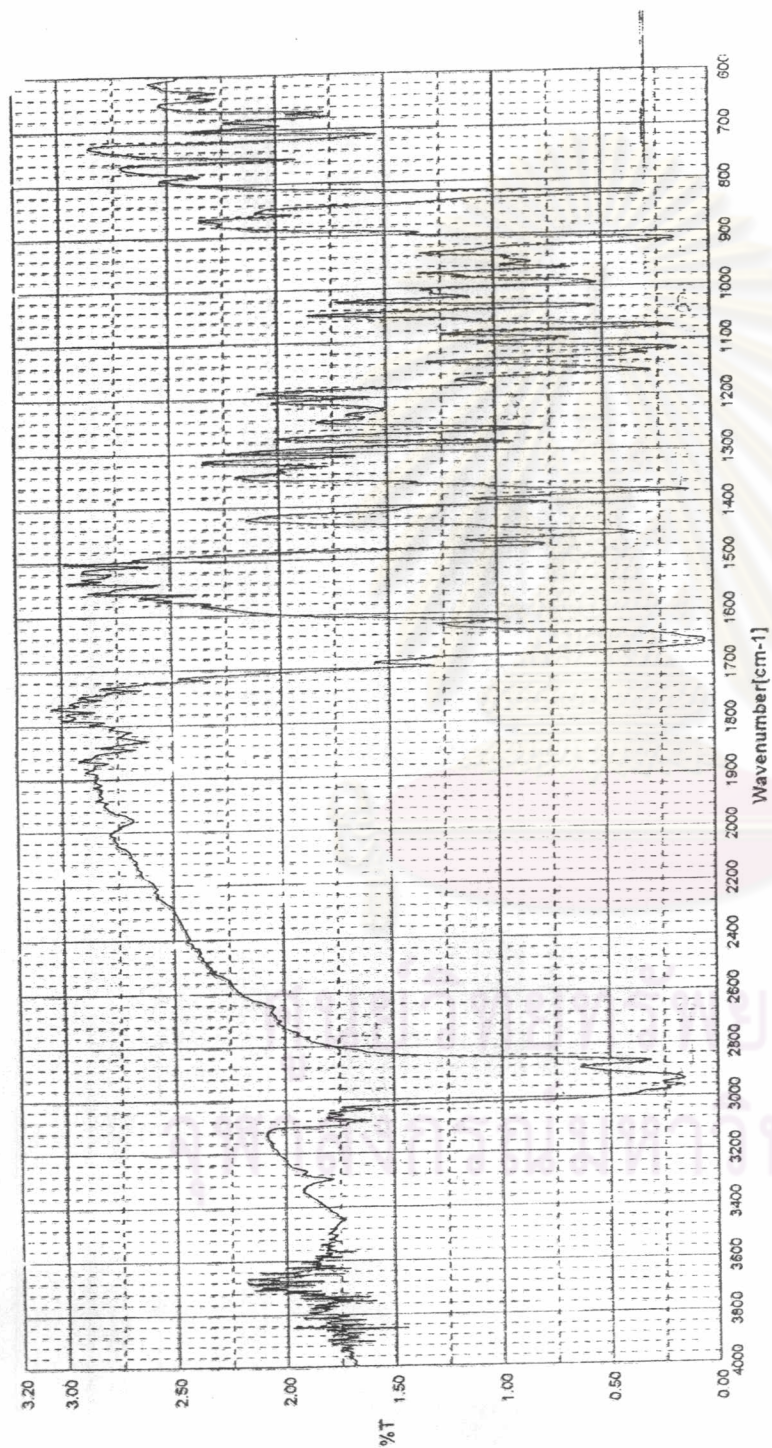


Figure 12: The IR spectrum of compound C-1 (KBr disc)

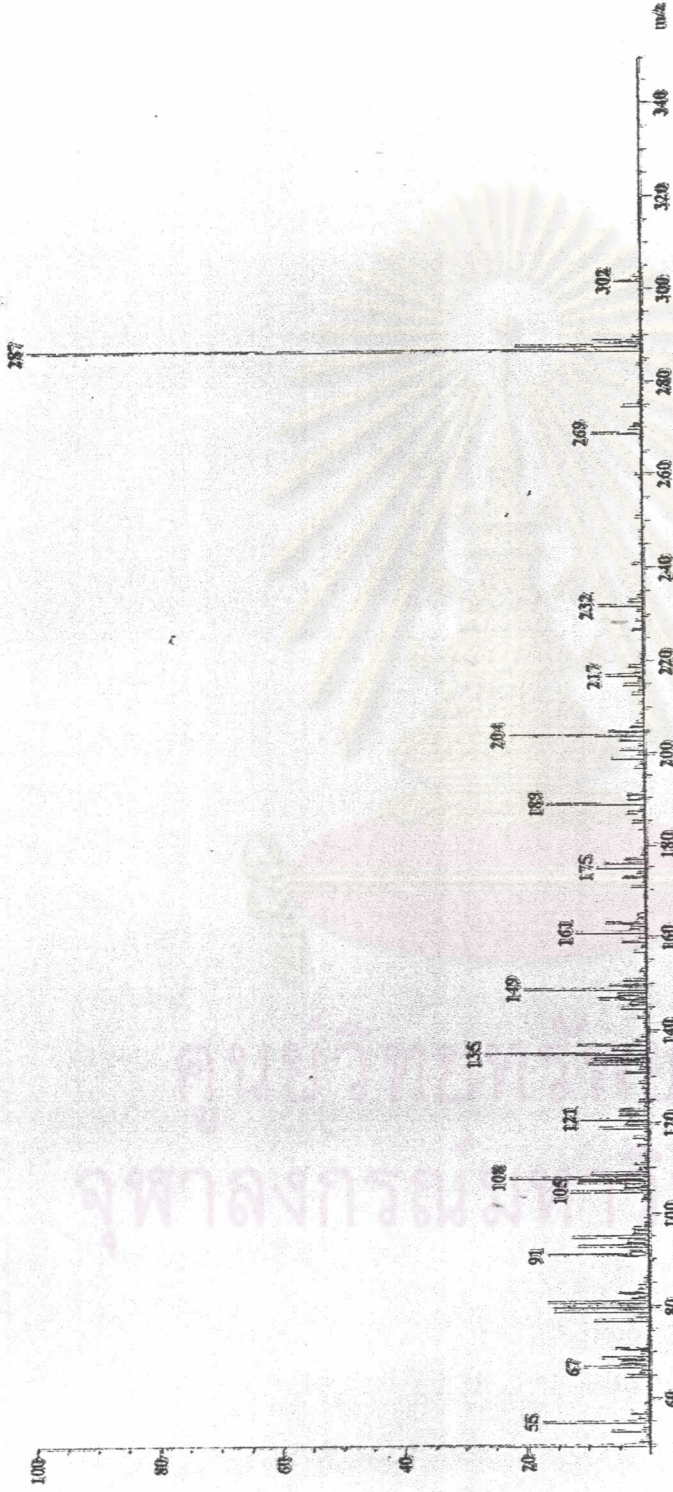


Figure 13: The EIMS spectrum of compound C-1

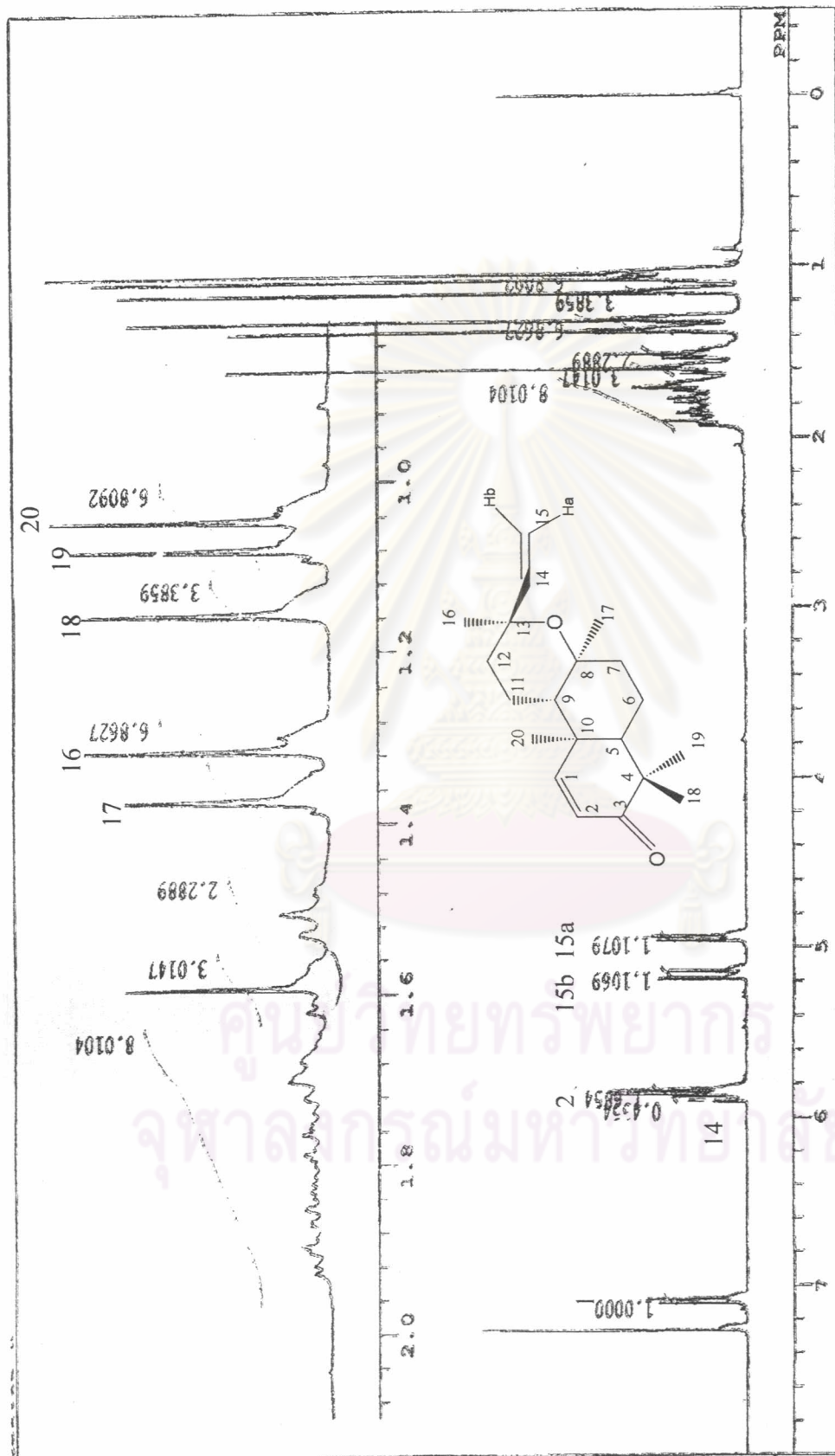


Figure 14: The 400MHz $^1\text{H-NMR}$ spectrum of compound C- 1 (in CDCl_3)

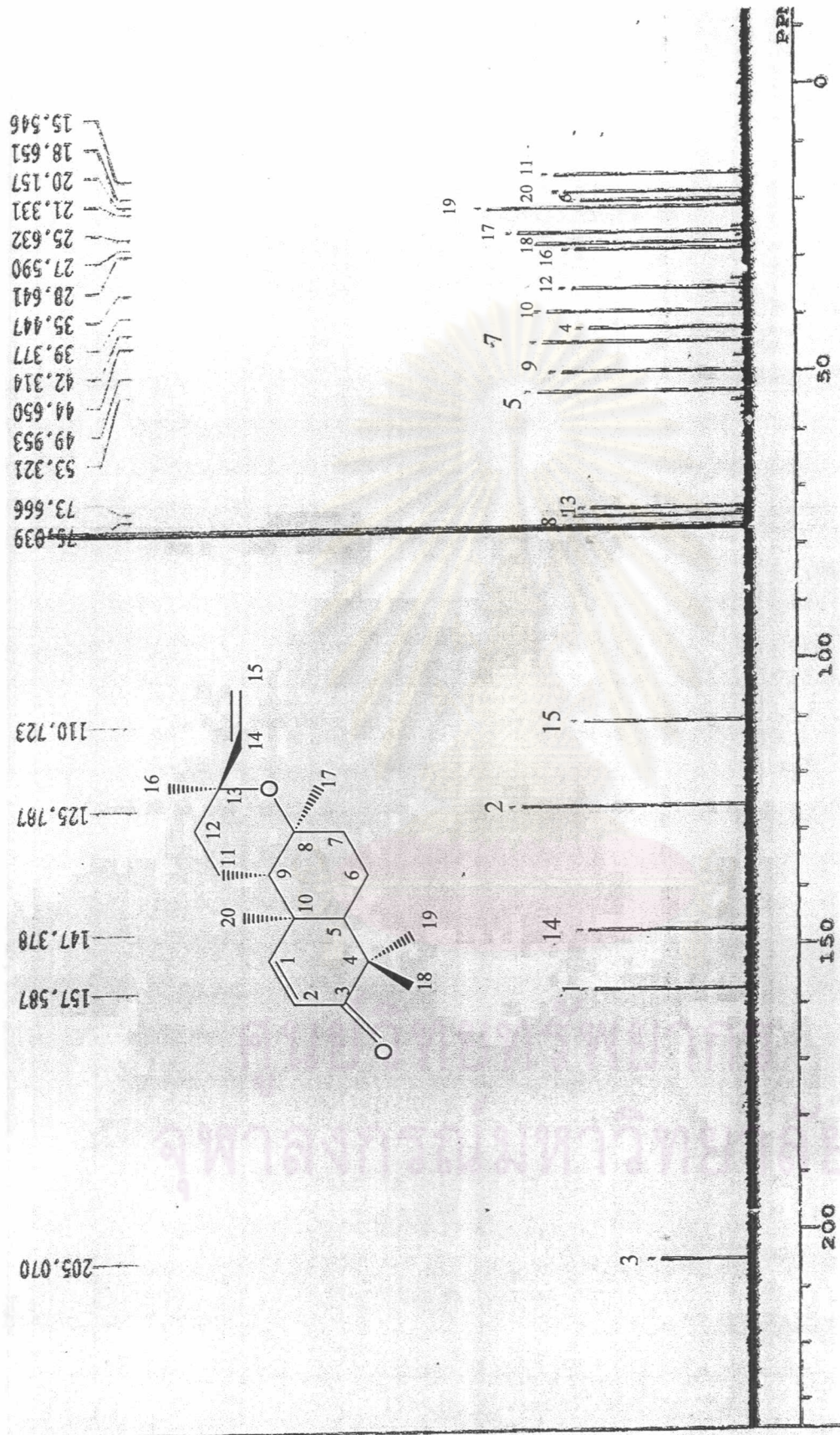


Figure 15: The 100MHz ^{13}C -NMR spectrum of compound C-1 (in CDCl_3)

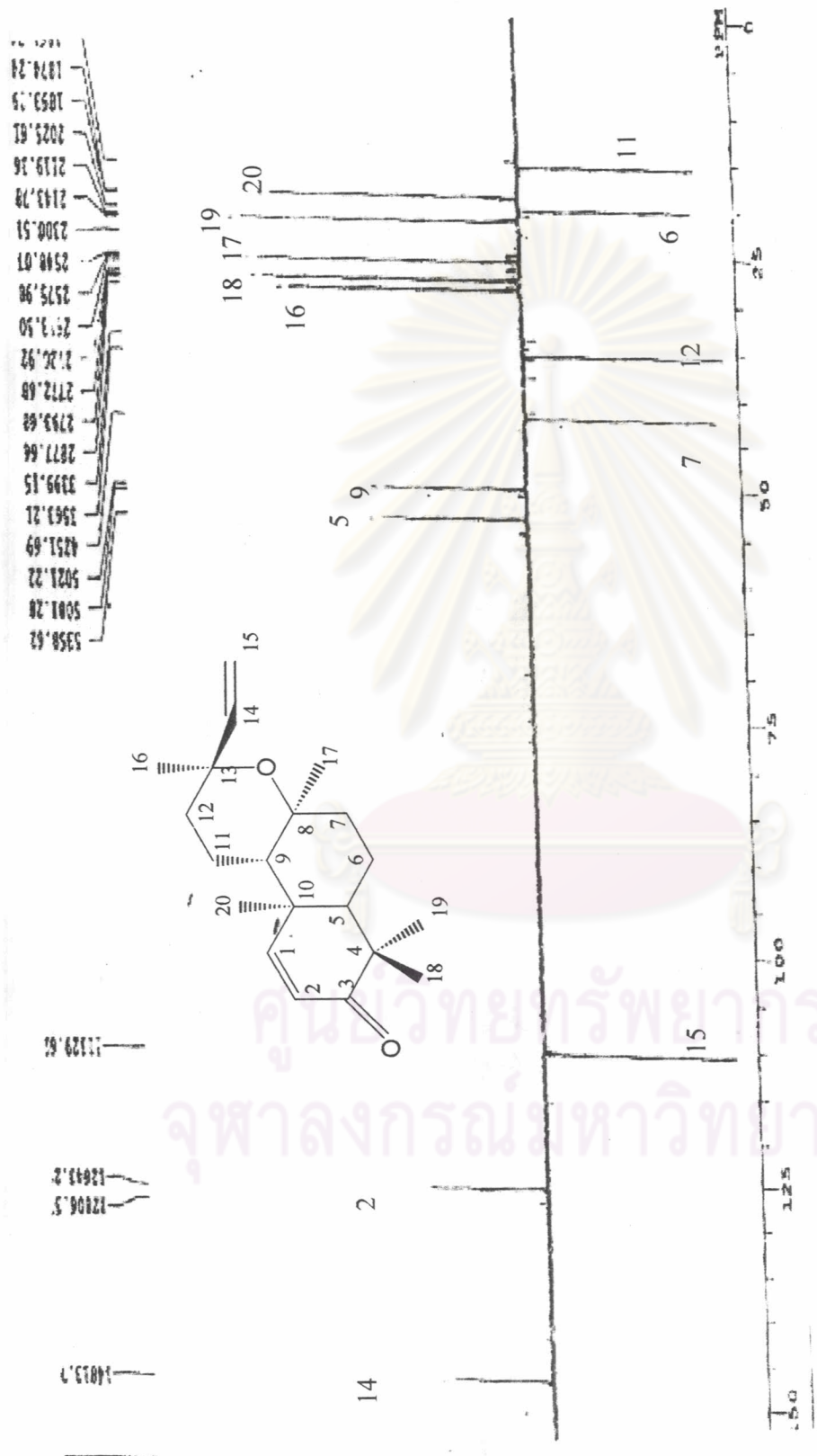


Figure 16: The DEPT-135 spectrum of compound C- 1 (in CDCl₃)

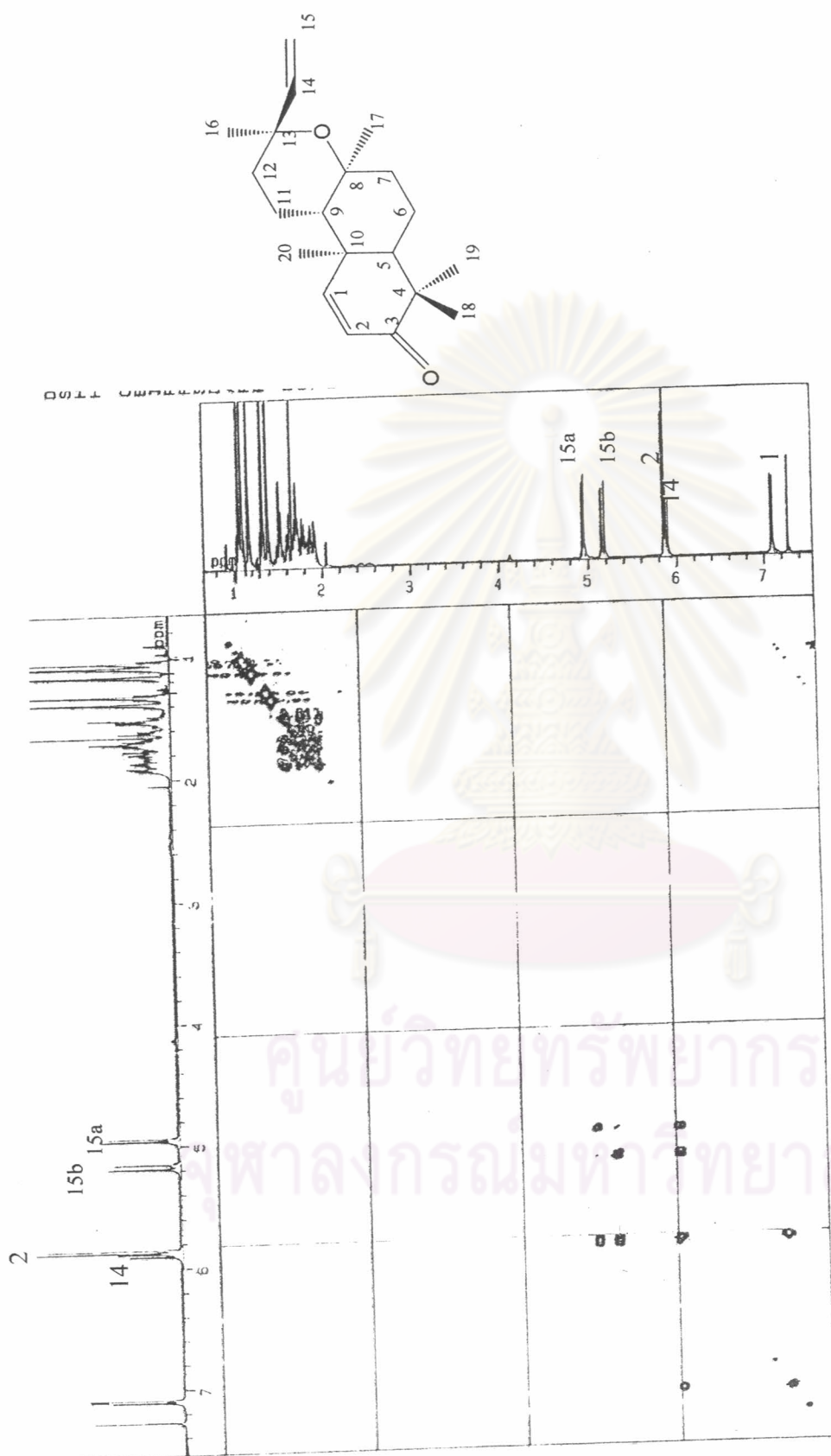


Figure 17: The 500MHz ^1H - ^1H COSY spectrum of compound C-1 (in CDCl_3)

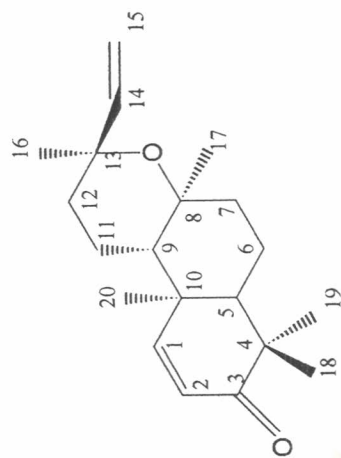
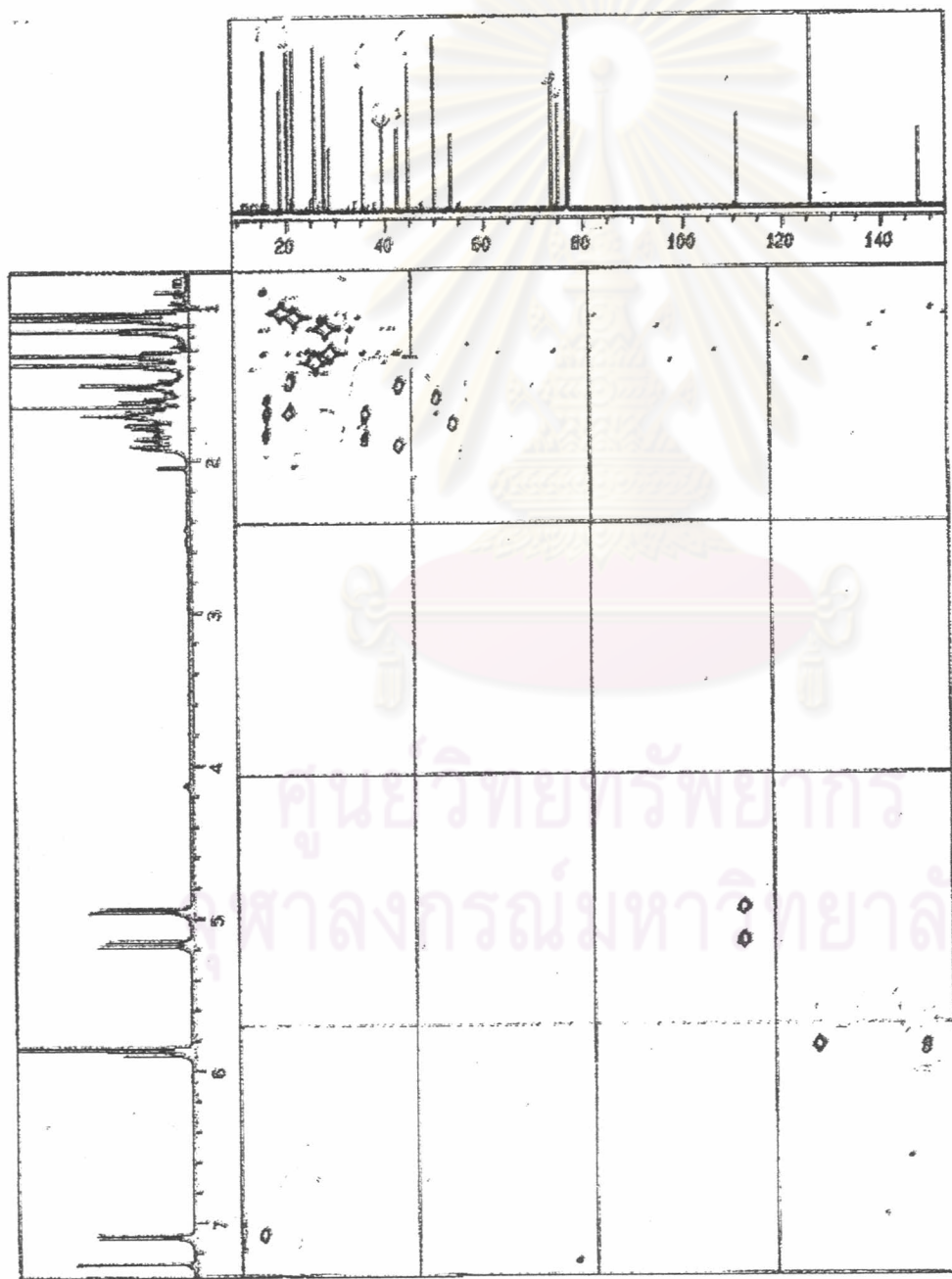


Figure 18: The 500MHz HMQC spectrum of compound C-1 (in CDCl₃)

LASTACQU.NRD (200.0 - 400.0)

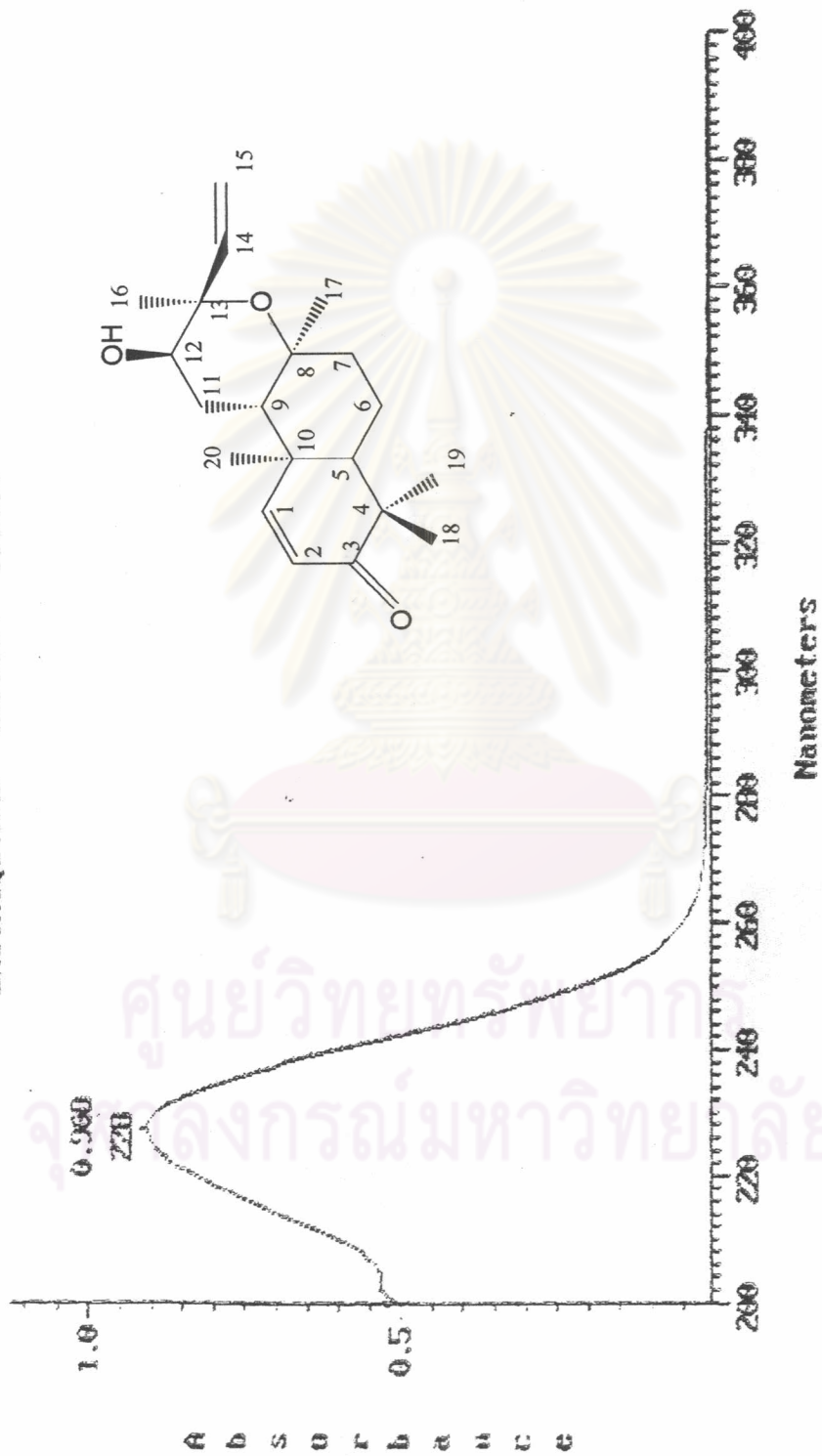


Figure 20: The UV spectrum of compound C-2 (in MeOH)

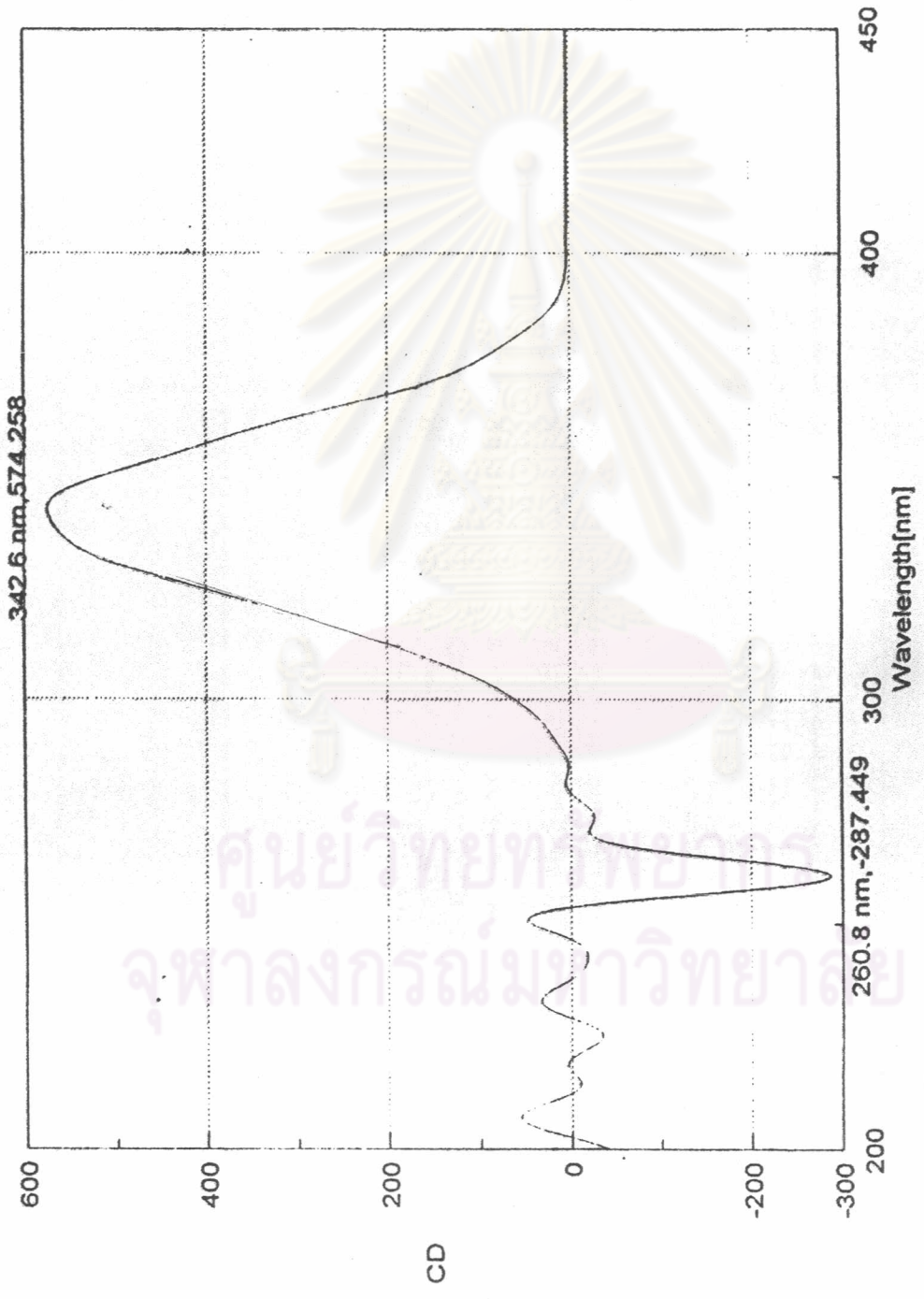


Figure 21: The CD spectrum of compound C-2

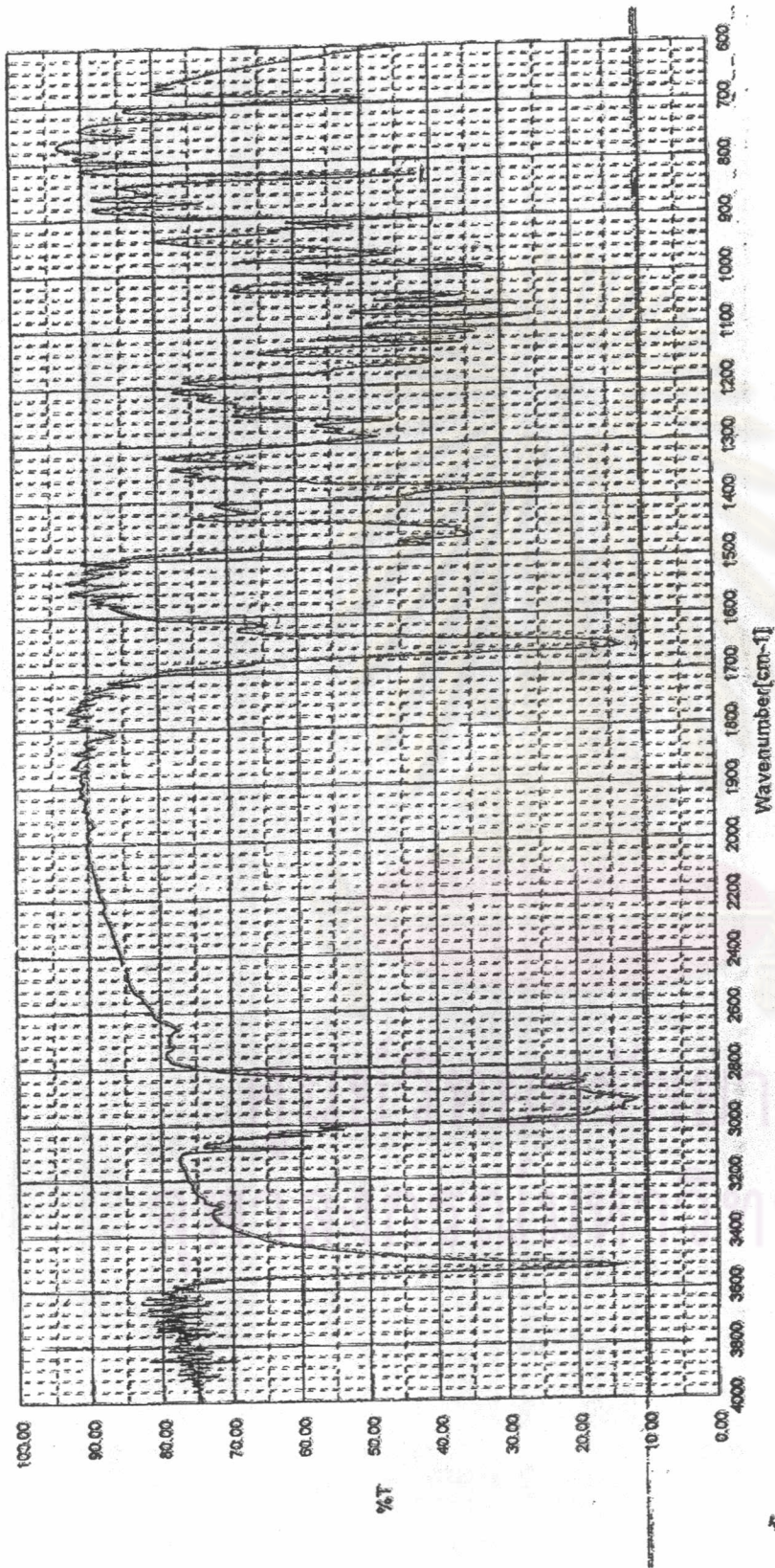


Figure 22: The IR spectrum of compound C-2 (KBr disc)

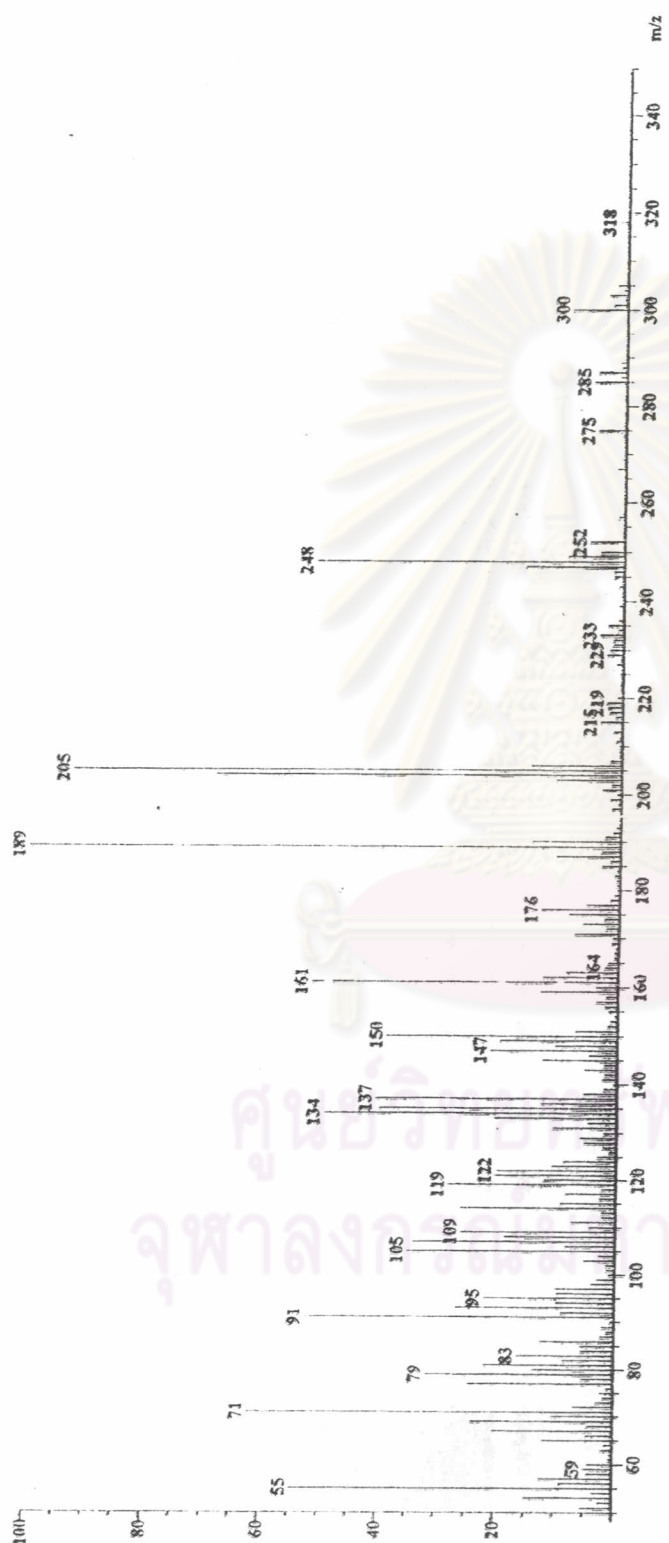


Figure 23: The EIMS spectrum of compound C-2

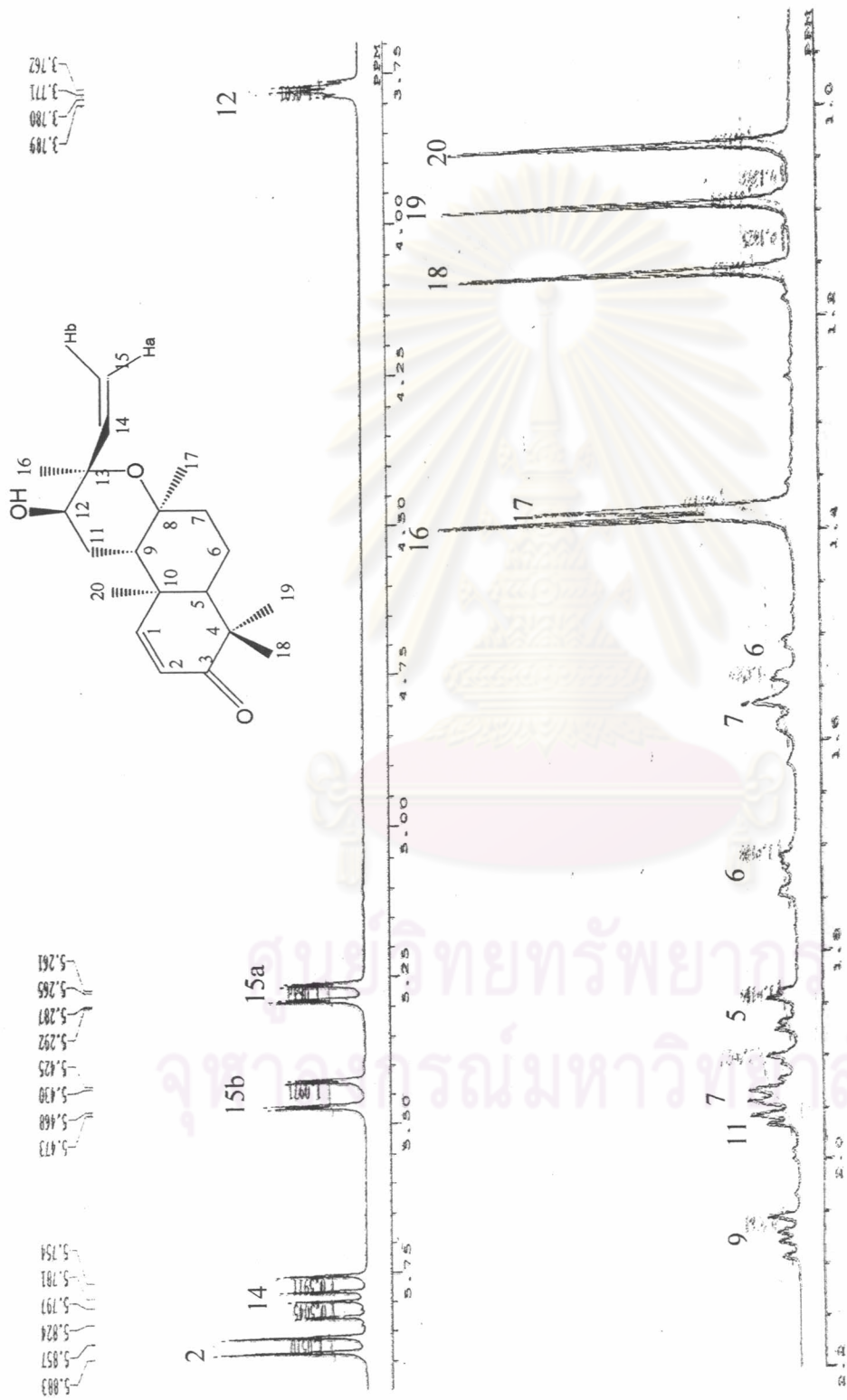


Figure 24b : The expanded 400MHz ¹H-NMR spectrum of compound C-2 (in CDCl₃)

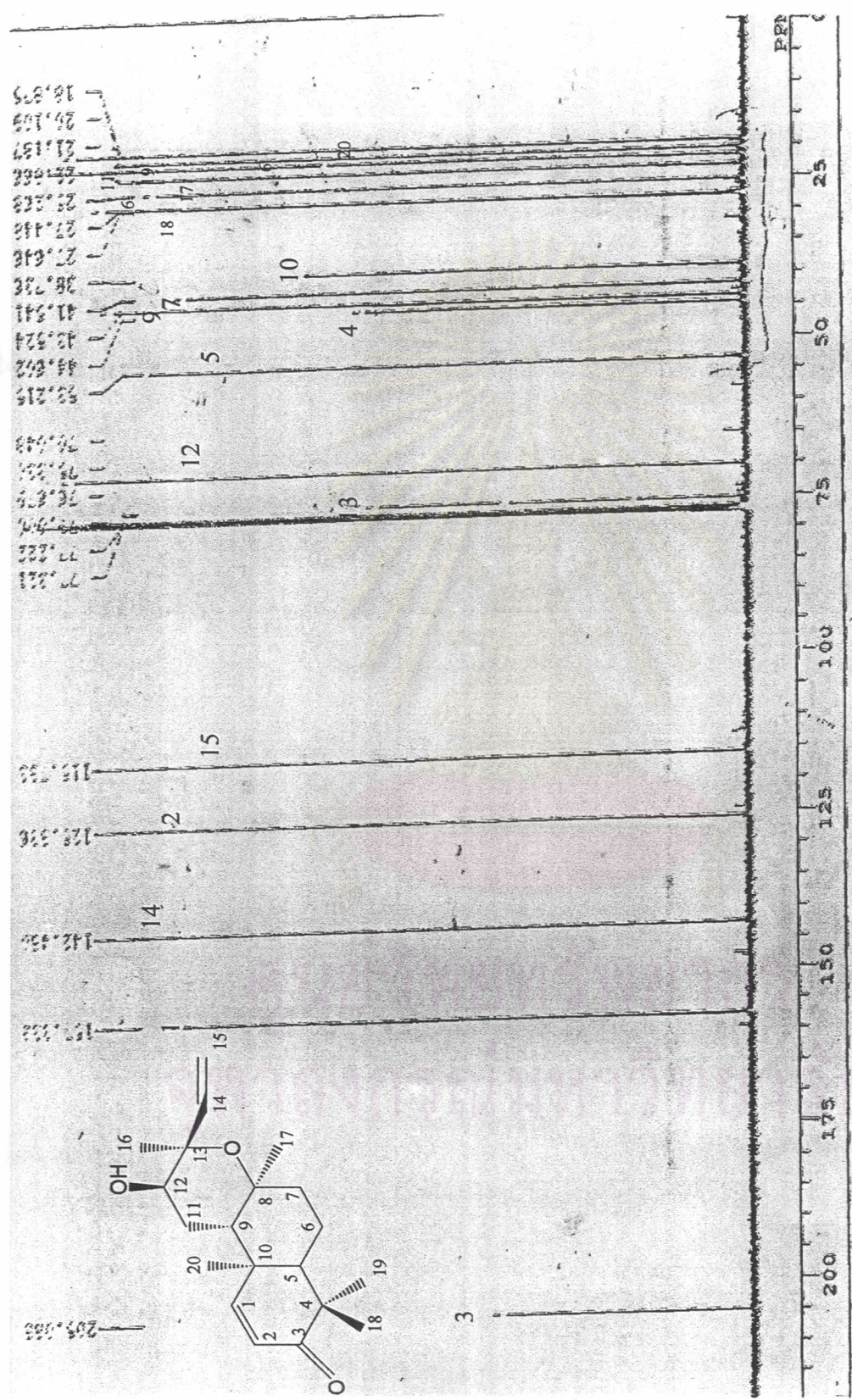


Figure 25: The 400MHz ¹³C-NMR spectrum of compound C-2 (in CDCl₃)

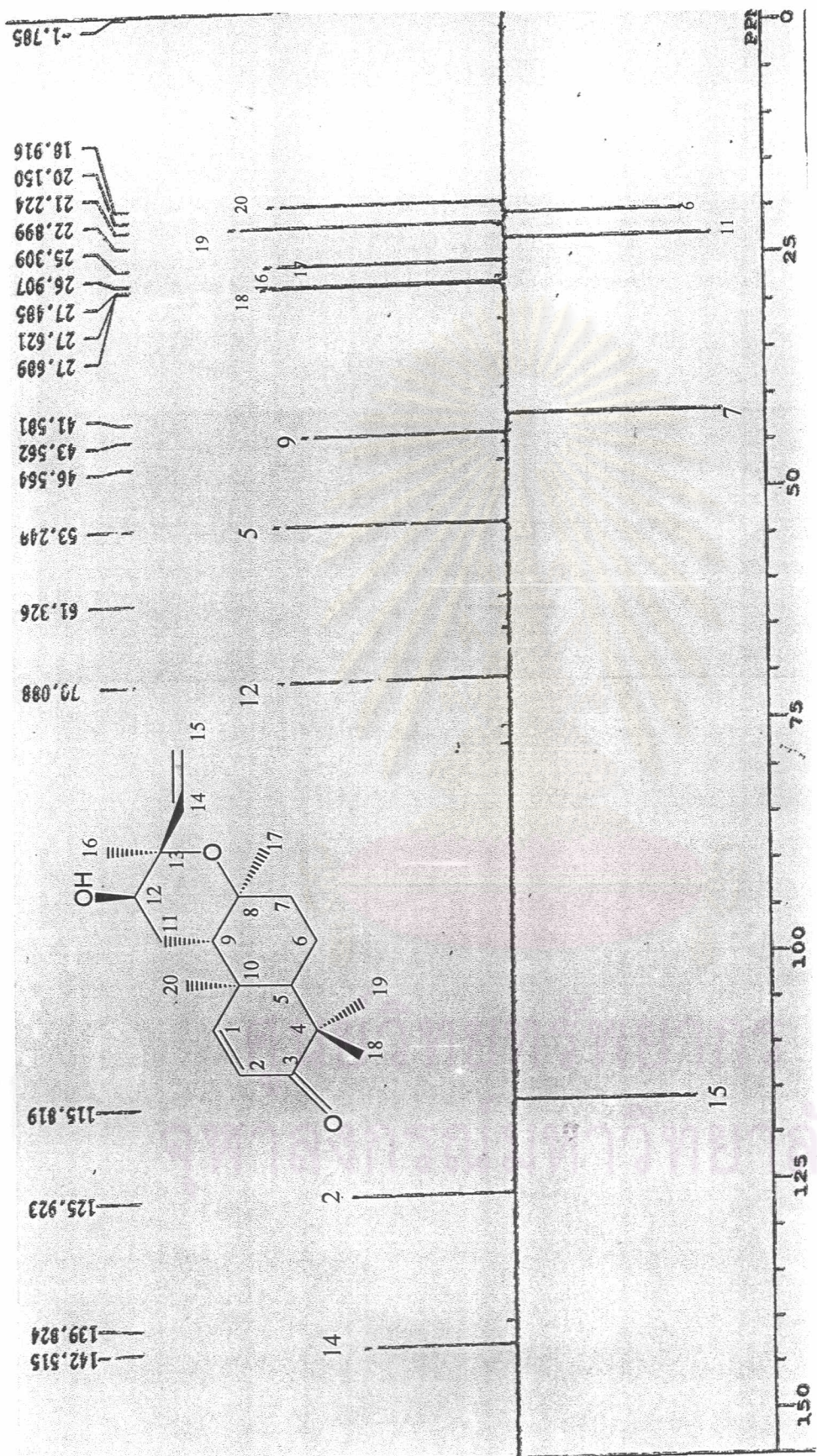


Figure 26: The DEPT-135 spectrum of compound C-2 (in CDCl₃)

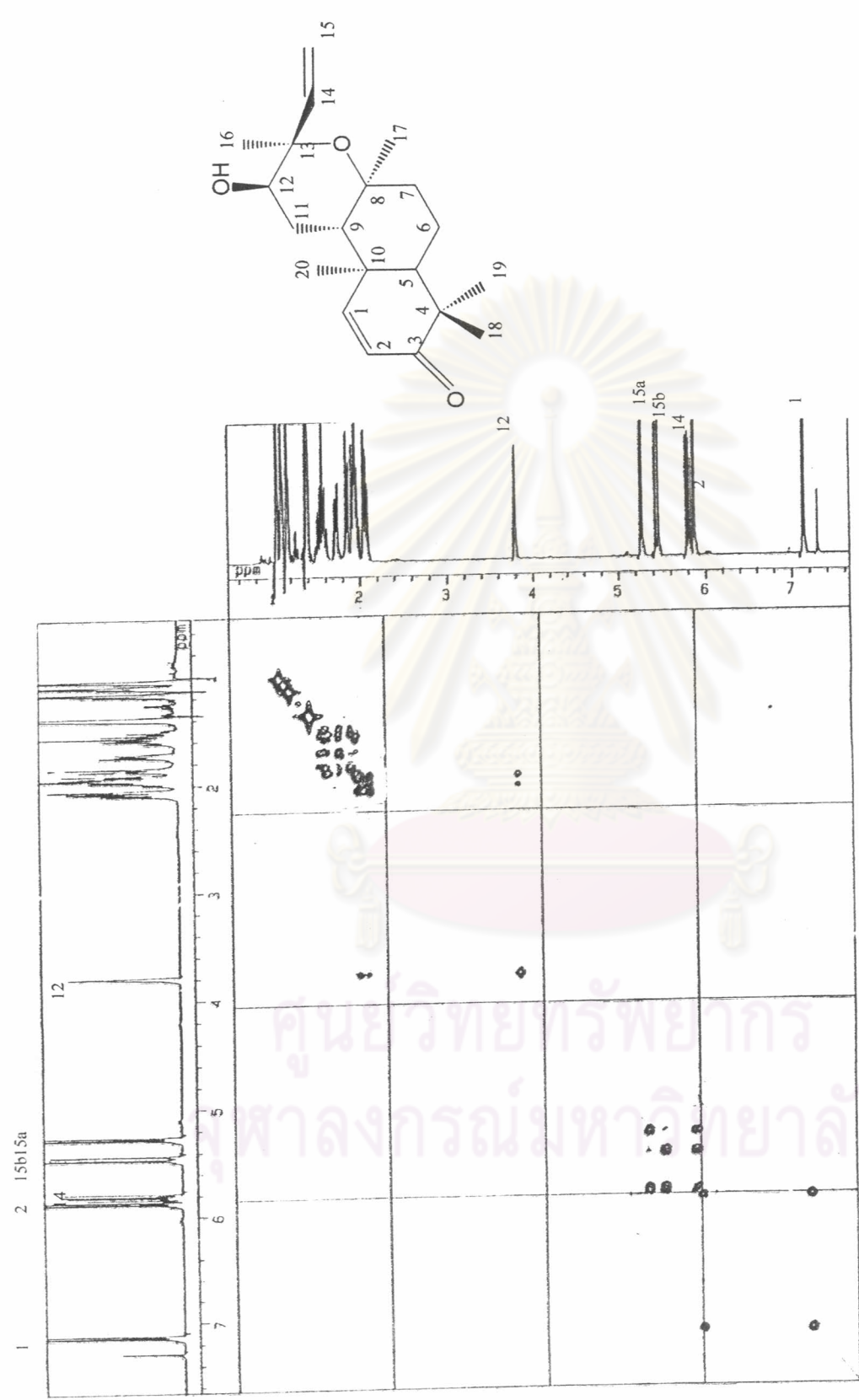


Figure 27: The 500MHz ¹H-¹H COSY spectrum of compound C-2 (in CDCl₃)

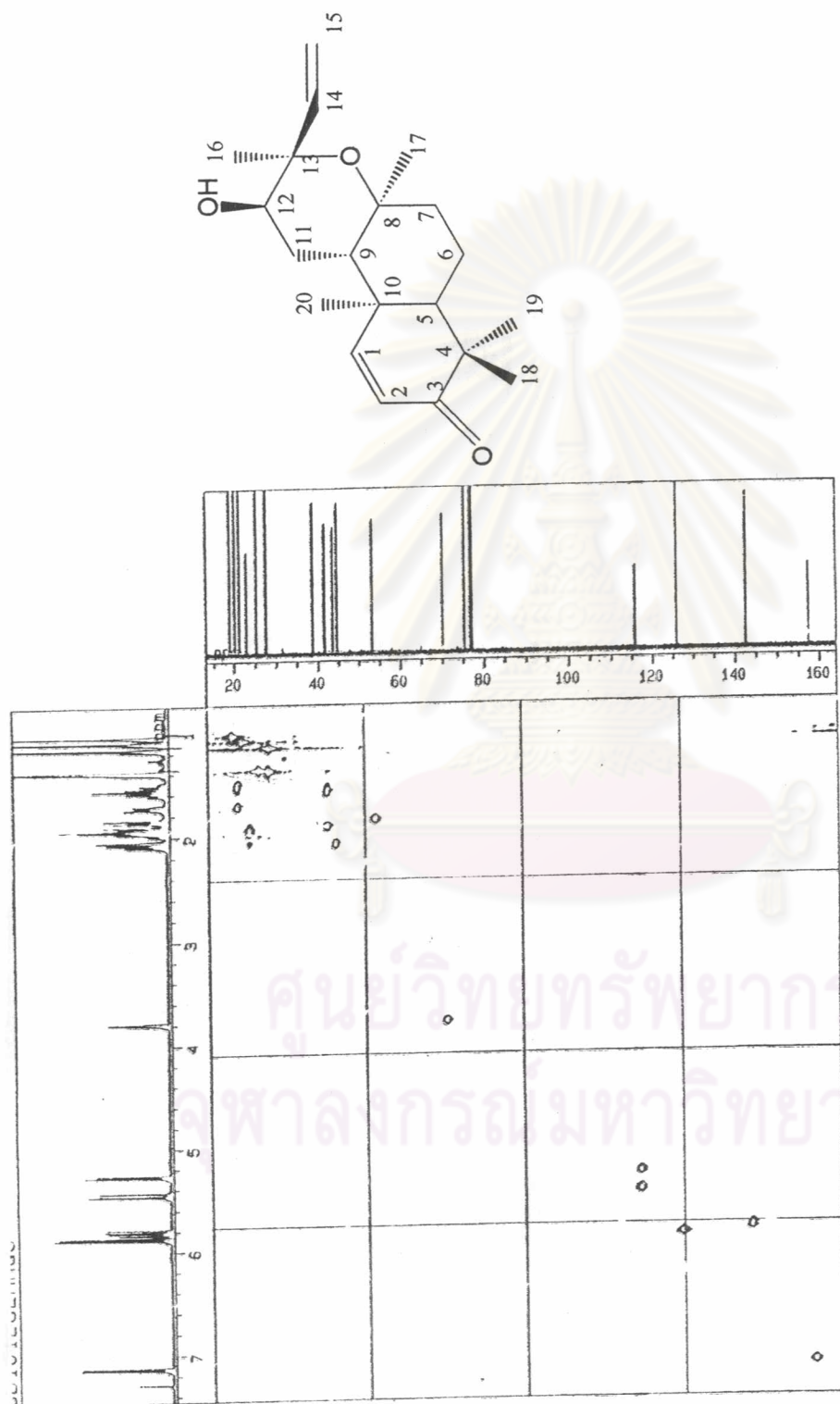


Figure 28: The 500MHz HMQC spectrum of compound C-2 (in CDCl₃)

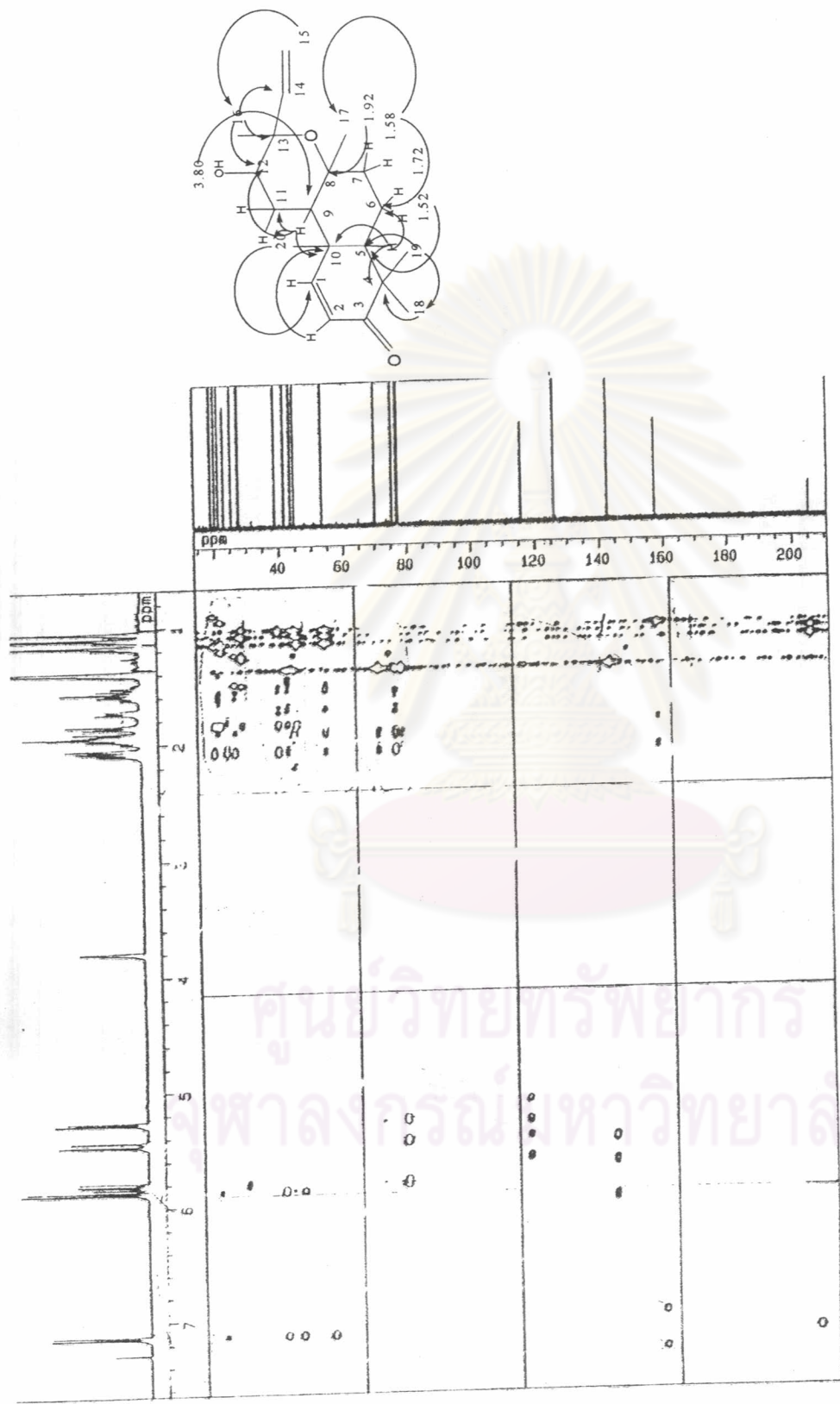


Figure 29: The 500MHz HMBC spectrum of compound C-2 (in CDCl₃)

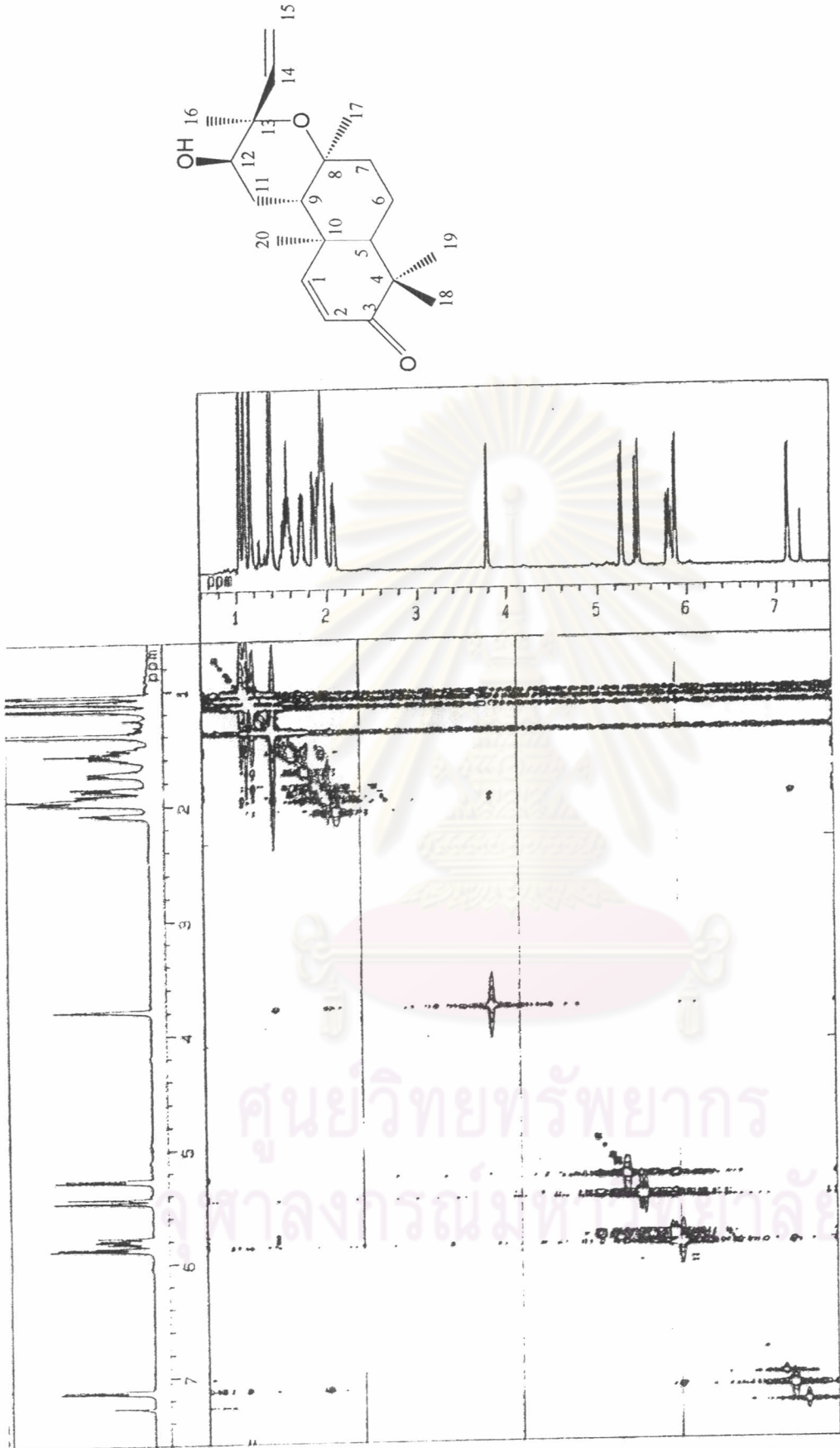


Figure 30: The 500MHz NOESY spectrum of compound C-2 (in CDCl₃)

Crystal data and structure refinement for Compound C-1

| | | |
|-----------------------------------|-----------------------------------------------------------|--------------------|
| Empirical formula | $C_{20}H_{30}O_2$ | |
| Formula weight | 302.43 | |
| Temperature | 293(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system, space group | orthorhombic, P212121 | |
| Unit cell dimensions | $a = 6.3271(4)$ Å | $\alpha = 90$ deg. |
| | $b = 11.4575(7)$ Å | $\beta = 90$ deg. |
| | $c = 24.6115(15)$ Å | $\gamma = 90$ deg. |
| Volume | $1784.16(19)$ Å ³ | |
| Z, Calculated density | 4, 1.122 Mg/m ³ | |
| Absorption coefficient | 0.070 mm ⁻¹ | |
| F(000) | 660 | |
| Theta range for data collection | 8.20 to 24.71 deg. | |
| Limiting indices | $-7 \leq h \leq 7, -13 \leq k \leq 8, -28 \leq l \leq 28$ | |
| Reflection collected / unique | 8749/ 2920 [R(int) = 0.0348] | |
| Completeness to theta = 24.71 | 95.1% | |
| Refinement method | Full-matrix least squares on F ² | |
| Data / restraints / parameters | 2920/ 7/ 257 | |
| Goodness-of-fit on F ² | 1.063 | |
| Final R indices [I > 2 sigma (I)] | R1 = 0.0593, wR2 = 0.1354 | |
| R indices (all data) | R1 = 0.0774, wR2 = 0.1462 | |
| Absolute structure parameter | 0 (3) | |
| Largest diff. peak and hole | 0.171 and -0.127 e.Å ⁻³ | |

Table13. Atomic coordinates($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for compound C-1

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|--------|----------|----------|---------|--------|
| C(1) | 2182(5) | 8481(3) | 7817(1) | 67(1) |
| C(2) | 1135(6) | 9398(3) | 7632(2) | 73(1) |
| C(3) | 1431(5) | 10560(3) | 7858(2) | 80(1) |
| C(4) | 2482(5) | 10706(3) | 8411(1) | 68(1) |
| C(5) | 2984(5) | 9504(3) | 8668(1) | 58(1) |
| C(6) | 4357(7) | 9559(3) | 9182(1) | 70(1) |
| C(7) | 4413(7) | 8382(3) | 9471(1) | 72(1) |
| C(8) | 5196(5) | 7409(3) | 9108(1) | 62(1) |
| C(9) | 3838(5) | 7380(2) | 8588(1) | 55(1) |
| C(10) | 3793(4) | 8558(2) | 8267(1) | 53(1) |
| C(11) | 4317(7) | 6282(3) | 8261(2) | 71(1) |
| C(12) | 3755(8) | 5233(3) | 8610(2) | 87(1) |
| C(13) | 4899(7) | 5225(3) | 9158(2) | 84(1) |
| C(14) | 3732(12) | 4439(5) | 9545(3) | 143(2) |
| C(15) | 3890(40) | 3377(11) | 9800(7) | 194(8) |
| C(15a) | 3300(20) | 4180(20) | 9868(7) | 199(9) |
| C(16) | 7189(9) | 4809(4) | 9107(3) | 119(2) |
| C(17) | 7591(5) | 7529(3) | 9027(2) | 79(1) |
| C(18) | 841(8) | 11346(4) | 8769(2) | 106(1) |
| C(19) | 4407(6) | 11511(3) | 8348(2) | 85(1) |
| C(20) | 5917(5) | 8841(3) | 7992(1) | 63(1) |
| O(1) | 856(6) | 11411(3) | 7598(1) | 125(1) |
| O(2) | 4745(4) | 6347(2) | 9415(1) | 77(1) |

Table 14. Bond lengths [$^{\circ}$ A] for compound C-1

| | Bond lengths [A] |
|-------------|------------------|
| C(1)-C(2) | 1.323(5) |
| C(1)-C(10) | 1.507(4) |
| C(2)-C(3) | 1.456(5) |
| C(3)-O(1) | 1.222(4) |
| C(3)-C(4) | 1.523(5) |
| C(4)-C(19) | 1.536(5) |
| C(4)-C(18) | 1.547(5) |
| C(4)-C(5) | 1.548(4) |
| C(5)-C(6) | 1.535(5) |
| C(5)-C(10) | 1.553(4) |
| C(6)-C(7) | 1.526(5) |
| C(7)-C(8) | 1.513(5) |
| C(8)-O(2) | 1.460(4) |
| C(8)-C(17) | 1.535(5) |
| C(8)-C(9) | 1.542(4) |
| C(9)-C(11) | 1.523(4) |
| C(9)-C(10) | 1.563(4) |
| C(10)-C(20) | 1.539(4) |
| C(11)-C(12) | 1.520(5) |
| C(12)-C(13) | 1.529(6) |
| C(13)-O(2) | 1.436(4) |
| C(13)-C(14) | 1.506(9) |
| C(13)-C(16) | 1.530(7) |
| C(14)-C(15) | 1.378(12) |

Crystal data and structure refinement for Compound C-2

| | | |
|-------------------------------------|------------------------------------------------------------|--------------------|
| Empirical formula | $C_{20}H_{30}O_3$ | |
| Formula weight | 318.44 | |
| Temperature | 293(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system, space group | orthorhombic, P(21) (21) (21) | |
| Unit cell dimensions | $a = 6.1692(3)$ Å | $\alpha = 90$ deg. |
| | $b = 14.2262(2)$ Å | $\beta = 90$ deg. |
| | $c = 20.4812(3)$ Å | $\gamma = 90$ deg. |
| Volume | $1797.52(9)$ Å ³ | |
| Z, Calculated density | 4, 1.177 Mg/m ³ | |
| Absorption coefficient | 0.077 mm ⁻¹ | |
| F(000) | 696 | |
| Theta range for data collection | 1.74 to 30.51 deg. | |
| Limiting indices | $-8 \leq h \leq 8, -18 \leq K \leq 19, -28 \leq l \leq 24$ | |
| Reflection collected / unique | 13405/ 5107 [R(int) = 0.0221] | |
| Completeness to theta = 24.71 | 96.1% | |
| Refinement method | Full-matrix least squares on F ² | |
| Data / restraints / parameters | 5107/ 0/ 268 | |
| Goodness -of -fit on F ² | 1.100 | |
| Final R indices [I > 2 sigma (I)] | R1 = 0.0699, wR2 = 0.1998 | |
| R indices (all data) | R1 = 0.0823, wR2 = 0.2147 | |
| Absolute structure parameter | -0.1(16) | |
| Largest diff. peak and hole | 0.948 and -0.383e.Å ⁻³ | |

Table 15. Atomic coordinates($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for compound C-2

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|-------|----------|---------|----------|--------|
| C(1) | 8040(5) | 5720(3) | 12241(1) | 57(1) |
| C(2) | 8937(7) | 6303(3) | 12666(2) | 76(1) |
| C(3) | 8729(7) | 7325(3) | 12617(2) | 81(1) |
| C(4) | 7657(6) | 7768(2) | 12018(2) | 61(1) |
| C(5) | 7547(4) | 7030(2) | 11466(1) | 40(1) |
| C(6) | 6463(5) | 7376(2) | 10839(1) | 43(1) |
| C(7) | 7033(4) | 6718(2) | 10270(1) | 39(1) |
| C(8) | 6331(3) | 5709(1) | 10405(1) | 32(1) |
| C(9) | 6738(4) | 6036(2) | 11661(1) | 36(1) |
| C(10) | 7268(3) | 5382(1) | 11069(1) | 31(1) |
| C(11) | 6785(4) | 4326(2) | 11150(1) | 39(1) |
| C(12) | 8001(4) | 3787(2) | 10620(1) | 40(1) |
| C(13) | 7472(4) | 4160(1) | 9931(1) | 38(1) |
| C(14) | 9198(5) | 3885(2) | 9448(1) | 57(1) |
| C(15) | 9993(9) | 4342(4) | 8999(2) | 94(1) |
| C(16) | 5309(5) | 3724(2) | 9704(2) | 54(1) |
| C(17) | 3852(4) | 5642(2) | 10326(1) | 43(1) |
| C(18) | 9094(8) | 8600(3) | 11797(2) | 89(1) |
| C(19) | 5403(8) | 8166(4) | 12229(3) | 105(2) |
| C(20) | 4328(5) | 5977(2) | 11869(2) | 51(1) |
| O(1) | 7419(3) | 5177(1) | 9903(1) | 37(1) |
| O(2) | 9455(9) | 7811(3) | 13059(2) | 143(2) |
| O(3) | 10283(3) | 3837(1) | 10729(1) | 48(1) |

Table16. Bond lengths [°A] for compound C-2

| | Bond lengths [A] |
|-------------|------------------|
| C(1)-C(2) | 1.324(5) |
| C(1)-C(9) | 1.501(3) |
| C(2)-C(3) | 1.463(7) |
| C(3)-O(2) | 1.223(4) |
| C(3)-C(4) | 1.529(5) |
| C(4)-C(5) | 1.545(3) |
| C(4)-C(18) | 1.547(5) |
| C(4)-C(19) | 1.562(5) |
| C(5)-C(6) | 1.529(4) |
| C(5)-C(9) | 1.552(3) |
| C(6)-C(7) | 1.534(3) |
| C(7)-C(8) | 1.525(3) |
| C(8)-O(1) | 1.443(2) |
| C(8)-C(17) | 1.541(3) |
| C(8)-C(10) | 1.549(3) |
| C(9)-C(20) | 1.549(3) |
| C(9)-C(10) | 1.563(3) |
| C(10)-C(11) | 1.541(3) |
| C(11)-C(12) | 1.525(3) |
| C(12)-O(3) | 1.427(3) |
| C(12)-C(13) | 1.542(3) |
| C(13)-O(1) | 1.448(2) |
| C(13)-C(14) | 1.506(4) |
| C(13)-C(16) | 1.543(4) |
| C(14)-C(15) | 1.229(6) |

VITA

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