# APPENDIX

**Table 56** Crystal data and structure refinement for compound XC1

| | |
|---|---|
| Identification code | XC1 |
| Empirical formula | $C_{26}H_{30}O_6$ |
| Formula weight | 438.50 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Monoclinic, P2(1) |
| Unit cell dimensions | a = 7.6623(12) Å alpha = 90° |
| | b = 11.1298(18) Å beta = 100.547° (3) |
| | c = 13.350(2) Å gamma = 90° |
| Volume | 1119.2(3) $Å^3$ |
| Z, Calculated density | 2, 1.301 $mg/m^3$ |
| Absorption coefficient | 0.092 $mm^{-1}$ |
| F(000) | 468 |
| Theta range for data collection | 1.55 to 26.00° |
| Limiting indices | -9<=h<=9, -13<=k<=13, -16<=l<=16 |
| Reflections collected / unique | 8802 / 2330 [R(int) = 0.0311] |
| Completeness to theta = 26.00 | 99.8 % |
| Max. and min. transmission | 0.9926 and 0.9770 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 2330 / 1 / 294 |
| Goodness-of-fit on $F^2$ | 1.112 |
| Final R indices [I>2sigma(I)] | R1 = 0.0473, wR2 = 0.1067 |
| R indices (all data) | R1 = 0.0551, wR2 = 0.1102 |
| Absolute structure parameter | 0(10) |

**Table 56** (Continued)

| | |
|---|---|
| Largest diff. peak and hole | 0.192 and -0.217 e. $Å^{-3}$ |

**Table 57** Bond lengths [Å] and angles [°] for compound XC1

| | | | |
|---|---|---|---|
| O(1)-C(4) | 1.210(4) | C(5)-C(23) | 1.535(6) |
| O(2)-C(8) | 1.211(4) | C(5)-C(22) | 1.538(5) |
| O(5)-C(16) | 1.195(4) | C(5)-C(6) | 1.552(4) |
| O(3)-C(15) | 1.431(4) | C(6)-C(7) | 1.540(5) |
| O(3)-C(14) | 1.453(4) | C(6)-H(6A) | 0.9800 |
| O(4)-C(16) | 1.340(4) | C(7)-C(8) | 1.507(5) |
| O(4)-C(17) | 1.464(4) | C(7)-H(7A) | 0.9700 |
| O(6)-C(20) | 1.349(6) | C(7)-H(7B) | 0.9700 |
| O(6)-C(21) | 1.357(5) | C(8)-C(9) | 1.517(5) |
| C(1)-C(2) | 1.522(4) | C(9)-C(25) | 1.542(5) |
| C(1)-C(6) | 1.548(4) | C(9)-C(14) | 1.552(4) |
| C(1)-C(10) | 1.548(4) | C(9)-C(10) | 1.579(4) |
| C(1)-C(24) | 1.550(5) | C(10)-C(11) | 1.525(4) |
| C(2)-C(3) | 1.318(5) | C(10)-H(10A) | 0.9800 |
| C(2)-H(2A) | 0.9300 | C(11)-C(12) | 1.530(5) |
| C(3)-C(4) | 1.462(5) | C(11)-H(11A) | 0.9700 |
| C(3)-H(3A) | 0.9300 | C(11)-H(11B) | 0.9700 |
| C(4)-C(5) | 1.529(5) | C(12)-C(13) | 1.556(4) |

**Table 57** (Continued)

| | | | |
|---|---|---|---|
| C(12)-H(12A) | 0.9700 | C(24)-H(24C) | 0.9600 |
| C(12)-H(12B) | 0.9700 | C(25)-H(25A) | 0.9600 |
| C(13)-C(14) | 1.523(4) | C(25)-H(25B) | 0.9600 |
| C(13)-C(26) | 1.536(4) | C(25)-H(25C) | 0.9600 |
| C(13)-C(17) | 1.545(4) | C(26)-H(26A) | 0.9600 |
| C(14)-C(15) | 1.473(4) | C(26)-H(26B) | 0.9600 |
| C(15)-C(16) | 1.483(5) | C(26)-H(26C) | 0.9600 |
| C(15)-H(15A) | 0.9800 | C(15)-O(3)-C(14) | 61.4(2) |
| C(17)-C(18) | 1.495(5) | C(16)-O(4)-C(17) | 121.1(2) |
| C(17)-H(17A) | 0.9800 | C(20)-O(6)-C(21) | 106.0(3) |
| C(18)-C(21) | 1.341(5) | C(2)-C(1)-C(6) | 105.4(3) |
| C(18)-C(19) | 1.422(5) | C(2)-C(1)-C(10) | 108.9(2) |
| C(19)-C(20) | 1.330(6) | C(6)-C(1)-C(10) | 105.6(2) |
| C(19)-H(19A) | 0.9300 | C(2)-C(1)-C(24) | 105.2(2) |
| C(20)-H(20A) | 0.9300 | C(6)-C(1)-C(24) | 117.6(3) |
| C(21)-H(21A) | 0.9300 | C(10)-C(1)-C(24) | 113.7(3) |
| C(22)-H(22A) | 0.9600 | C(3)-C(2)-C(1) | 123.0(3) |
| C(22)-H(22B) | 0.9600 | C(3)-C(2)-H(2A) | 118.5 |
| C(22)-H(22C) | 0.9600 | C(1)-C(2)-H(2A) | 118.5 |
| C(23)-H(23A) | 0.9600 | C(2)-C(3)-C(4) | 123.4(3) |
| C(23)-H(23B) | 0.9600 | C(2)-C(3)-H(3A) | 118.3 |
| C(23)-H(23C) | 0.9600 | C(4)-C(3)-H(3A) | 118.3 |
| C(24)-H(24A) | 0.9600 | O(1)-C(4)-C(3) | 120.2(4) |
| C(24)-H(24B) | 0.9600 | O(1)-C(4)-C(5) | 120.2(4) |

**Table 57** (Continued)

| | | | |
|---|---|---|---|
| C(3)-C(4)-C(5) | 119.5(3) | C(25)-C(9)-C(14) | 107.8(3) |
| C(4)-C(5)-C(23) | 107.2(3) | C(8)-C(9)-C(10) | 105.1(2) |
| C(4)-C(5)-C(22) | 108.1(3) | C(25)-C(9)-C(10) | 114.9(3) |
| C(23)-C(5)-C(22) | 108.1(3) | C(14)-C(9)-C(10) | 107.0(2) |
| C(4)-C(5)-C(6) | 109.2(3) | C(11)-C(10)-C(1) | 120.2(2) |
| C(23)-C(5)-C(6) | 109.8(3) | C(11)-C(10)-C(9) | 107.2(3) |
| C(22)-C(5)-C(6) | 114.3(3) | C(1)-C(10)-C(9) | 115.1(2) |
| C(7)-C(6)-C(1) | 113.0(3) | C(11)-C(10)-H(10A) | 104.2 |
| C(7)-C(6)-C(5) | 113.4(3) | C(1)-C(10)-H(10A) | 104.2 |
| C(1)-C(6)-C(5) | 116.4(2) | C(9)-C(10)-H(10A) | 104.2 |
| C(7)-C(6)-H(6A) | 104.1 | C(10)-C(11)-C(12) | 108.8(3) |
| C(1)-C(6)-H(6A) | 104.1 | C(10)-C(11)-H(11A) | 109.9 |
| C(5)-C(6)-H(6A) | 104.1 | C(12)-C(11)-H(11A) | 109.9 |
| C(8)-C(7)-C(6) | 110.2(3) | C(10)-C(11)-H(11B) | 109.9 |
| C(8)-C(7)-H(7A) | 109.6 | C(12)-C(11)-H(11B) | 109.9 |
| C(6)-C(7)-H(7A) | 109.6 | H(11A)-C(11)-H(11B) | 108.3 |
| C(8)-C(7)-H(7B) | 109.6 | C(11)-C(12)-C(13) | 114.1(3) |
| C(6)-C(7)-H(7B) | 109.6 | C(11)-C(12)-H(12A) | 108.7 |
| H(7A)-C(7)-H(7B) | 108.1 | C(13)-C(12)-H(12A) | 108.7 |
| O(2)-C(8)-C(7) | 121.8(3) | C(11)-C(12)-H(12B) | 108.7 |
| O(2)-C(8)-C(9) | 123.4(3) | C(13)-C(12)-H(12B) | 108.7 |
| C(7)-C(8)-C(9) | 114.7(3) | H(12A)-C(12)-H(12B) | 107.6 |
| C(8)-C(9)-C(25) | 108.6(3) | C(14)-C(13)-C(26) | 109.7(2) |
| C(8)-C(9)-C(14) | 113.5(2) | C(14)-C(13)-C(17) | 108.2(2) |

**Table 57** (Continued)

| | | | |
|---|---|---|---|
| C(26)-C(13)-C(17) | 109.3(2) | C(13)-C(17)-H(17A) | 108.3 |
| C(14)-C(13)-C(12) | 108.5(2) | C(21)-C(18)-C(19) | 105.6(4) |
| C(26)-C(13)-C(12) | 113.4(3) | C(21)-C(18)-C(17) | 127.1(3) |
| C(17)-C(13)-C(12) | 107.7(2) | C(19)-C(18)-C(17) | 127.2(3) |
| O(3)-C(14)-C(15) | 58.6(2) | C(20)-C(19)-C(18) | 106.5(4) |
| O(3)-C(14)-C(13) | 111.5(2) | C(20)-C(19)-H(19A) | 126.8 |
| C(15)-C(14)-C(13) | 116.5(3) | C(18)-C(19)-H(19A) | 126.8 |
| O(3)-C(14)-C(9) | 114.5(2) | C(19)-C(20)-O(6) | 111.1(4) |
| C(15)-C(14)-C(9) | 119.5(3) | C(19)-C(20)-H(20A) | 124.5 |
| C(13)-C(14)-C(9) | 120.0(2) | O(6)-C(20)-H(20A) | 124.5 |
| O(3)-C(15)-C(14) | 60.0(19) | C(18)-C(21)-O(6) | 110.8(4) |
| O(3)-C(15)-C(16) | 116.7(3) | C(18)-C(21)-H(21A) | 124.6 |
| C(14)-C(15)-C(16) | 119.9(3) | O(6)-C(21)-H(21A) | 124.6 |
| O(3)-C(15)-H(15A) | 116.1 | C(5)-C(22)-H(22A) | 109.5 |
| C(14)-C(15)-H(15A) | 116.1 | C(5)-C(22)-H(22B) | 109.5 |
| C(16)-C(15)-H(15A) | 116.1 | H(22A)-C(22)-H(22B) | 109.5 |
| O(5)-C(16)-O(4) | 120.0(3) | C(5)-C(22)-H(22C) | 109.5 |
| O(5)-C(16)-C(15) | 122.6(3) | H(22A)-C(22)-H(22C) | 109.5 |
| O(4)-C(16)-C(15) | 117.4(3) | H(22B)-C(22)-H(22C) | 109.5 |
| O(4)-C(17)-C(18) | 104.4(2) | C(5)-C(23)-H(23A) | 109.5 |
| O(4)-C(17)-C(13) | 112.4(2) | C(5)-C(23)-H(23B) | 109.5 |
| C(18)-C(17)-C(13) | 114.8(3) | H(23A)-C(23)-H(23B) | 109.5 |
| O(4)-C(17)-H(17A) | 108.3 | C(5)-C(23)-H(23C) | 109.5 |
| C(18)-C(17)-H(17A) | 108.3 | H(23A)-C(23)-H(23C) | 109.5 |

**Table 57** (Continued)

| | | | |
|---|---|---|---|
| H(23B)-C(23)-H(23C) | 109.5 | C(9)-C(25)-H(25C) | 109.5 |
| C(1)-C(24)-H(24A) | 109.5 | H(25A)-C(25)-H(25C) | 109.5 |
| C(1)-C(24)-H(24B) | 109.5 | H(25B)-C(25)-H(25C) | 109.5 |
| H(24A)-C(24)-H(24B) | 109.5 | C(13)-C(26)-H(26A) | 109.5 |
| C(1)-C(24)-H(24C) | 109.5 | C(13)-C(26)-H(26B) | 109.5 |
| H(24A)-C(24)-H(24C) | 109.5 | H(26A)-C(26)-H(26B) | 109.5 |
| H(24B)-C(24)-H(24C) | 109.5 | C(13)-C(26)-H(26C) | 109.5 |
| C(9)-C(25)-H(25A) | 109.5 | H(26A)-C(26)-H(26C) | 109.5 |
| C(9)-C(25)-H(25B) | 109.5 | H(26B)-C(26)-H(26C) | 109.5 |
| H(25A)-C(25)-H(25B) | 109.5 | | |

Symmetry transformations used to generate equivalent atoms:

**Table 58** Torsion angles [°] for compound XC1.

| | | | |
|---|---|---|---|
| C(6)-C(1)-C(2)-C(3) | 32.8(4) | C(3)-C(4)-C(5)-C(22) | 114.7(4) |
| C(10)-C(1)-C(2)-C(3) | 145.7(3) | O(1)-C(4)-C(5)-C(6) | 171.5(4) |
| C(24)-C(1)-C(2)-C(3) | -92.1(4) | C(3)-C(4)-C(5)-C(6) | -10.2(4) |
| C(1)-C(2)-C(3)-C(4) | -1.0(5) | C(2)-C(1)-C(6)-C(7) | 170.8(3) |
| C(2)-C(3)-C(4)-O(1) | 166.4(4) | C(10)-C(1)-C(6)-C(7) | 55.6(3) |
| C(2)-C(3)-C(4)-C(5) | -11.9(5) | C(24)-C(1)-C(6)-C(7) | -72.4(3) |
| O(1)-C(4)-C(5)-C(23) | 52.6(5) | C(2)-C(1)-C(6)-C(5) | -55.4(3) |
| C(3)-C(4)-C(5)-C(23) | -129.0(4) | C(10)-C(1)-C(6)-C(5) | -170.6(3) |
| O(1)-C(4)-C(5)-C(22) | -63.7(5) | C(24)-C(1)-C(6)-C(5) | 61.3(4) |

**Table 58** (Continued)

| | | | |
|---|---|---|---|
| C(4)-C(5)-C(6)-C(7) | 178.8(3) | C(14)-C(9)-C(10)-C(11) | -43.8(3) |
| C(23)-C(5)-C(6)-C(7) | -64.0(4) | C(8)-C(9)-C(10)-C(1) | 58.6(3) |
| C(22)-C(5)-C(6)-C(7) | 57.7(4) | C(25)-C(9)-C(10)-C(1) | -60.7(4) |
| C(4)-C(5)-C(6)-C(1) | 45.2(4) | C(14)-C(9)-C(10)-C(1) | 179.6(2) |
| C(23)-C(5)-C(6)-C(1) | 162.4(3) | C(1)-C(10)-C(11)-C(12) | -150.9(3) |
| C(22)-C(5)-C(6)-C(1) | -75.9(4) | C(9)-C(10)-C(11)-C(12) | 75.1(3) |
| C(1)-C(6)-C(7)-C(8) | -56.3(4) | C(10)-C(11)-C(12)-C(13) | -38.9(4) |
| C(5)-C(6)-C(7)-C(8) | 168.5(3) | C(11)-C(12)-C(13)-C(14) | -21.1(4) |
| C(6)-C(7)-C(8)-O(2) | -119.2(4) | C(11)-C(12)-C(13)-C(26) | 101.0(3) |
| C(6)-C(7)-C(8)-C(9) | 57.6(4) | C(11)-C(12)-C(13)-C(17) | -138.0(3) |
| O(2)-C(8)-C(9)-C(25) | -116.2(4) | C(15)-O(3)-C(14)-C(13) | -108.7(3) |
| C(7)-C(8)-C(9)-C(25) | 67.0(4) | C(15)-O(3)-C(14)-C(9) | 110.9(3) |
| O(2)-C(8)-C(9)-C(14) | 3.7(5) | C(26)-C(13)-C(14)-O(3) | 151.2(2) |
| C(7)-C(8)-C(9)-C(14) | -173.0(3) | C(17)-C(13)-C(14)-O(3) | 32.0(3) |
| O(2)-C(8)-C(9)-C(10) | 120.4(4) | C(12)-C(13)-C(14)-O(3) | -84.5(3) |
| C(7)-C(8)-C(9)-C(10) | -56.4(4) | C(26)-C(13)-C(14)-C(15) | 86.6(3) |
| C(2)-C(1)-C(10)-C(11) | 58.0(4) | C(17)-C(13)-C(14)-C(15) | -32.6(4) |
| C(6)-C(1)-C(10)-C(11) | 170.8(3) | C(12)-C(13)-C(14)-C(15) | -149.1(3) |
| C(24)-C(1)-C(10)-C(11) | -58.9(4) | C(26)-C(13)-C(14)-C(9) | -70.9(3) |
| C(2)-C(1)-C(10)-C(9) | -171.4(2) | C(17)-C(13)-C(14)-C(9) | 169.9(2) |
| C(6)-C(1)-C(10)-C(9) | -58.6(3) | C(12)-C(13)-C(14)-C(9) | 53.4(3) |
| C(24)-C(1)-C(10)-C(9) | 71.7(3) | C(8)-C(9)-C(14)-O(3) | -127.0(3) |
| C(8)-C(9)-C(10)-C(11) | -164.8(3) | C(25)-C(9)-C(14)-O(3) | -6.6(4) |
| C(25)-C(9)-C(10)-C(11) | 75.9(3) | C(10)-C(9)-C(14)-O(3) | 117.5(3) |

**Table 58** (Continued)

| | | | |
|---|---|---|---|
| C(8)-C(9)-C(14)-C(15) | -60.6(4) | C(16)-O(4)-C(17)-C(13) | -40.1(4) |
| C(25)-C(9)-C(14)-C(15) | 59.8(4) | C(14)-C(13)-C(17)-O(4) | 54.8(3) |
| C(10)-C(9)-C(14)-C(15) | -176.1(3) | C(26)-C(13)-C(17)-O(4) | -64.7(3) |
| C(8)-C(9)-C(14)-C(13) | 96.3(3) | C(12)-C(13)-C(17)-O(4) | 171.8(3) |
| C(25)-C(9)-C(14)-C(13) | -143.4(3) | C(14)-C(13)-C(17)-C(18) | 173.9(3) |
| C(10)-C(9)-C(14)-C(13) | -19.2(3) | C(26)-C(13)-C(17)-C(18) | 54.5(3) |
| C(14)-O(3)-C(15)-C(16) | 110.7(3) | C(12)-C(13)-C(17)-C(18) | -69.1(3) |
| C(13)-C(14)-C(15)-O(3) | 100.1(3) | O(4)-C(17)-C(18)-C(21) | -147.3(3) |
| C(9)-C(14)-C(15)-O(3) | -102.2(3) | C(13)-C(17)-C(18)-C(21) | 89.2(4) |
| O(3)-C(14)-C(15)-C(16) | -105.5(4) | O(4)-C(17)-C(18)-C(19) | 29.9(5) |
| C(13)-C(14)-C(15)-C(16) | -5.4(5) | C(13)-C(17)-C(18)-C(19) | -93.6(4) |
| C(9)-C(14)-C(15)-C(16) | 152.3(3) | C(21)-C(18)-C(19)-C(20) | 1.0(5) |
| C(17)-O(4)-C(16)-O(5) | 177.5(3) | C(17)-C(18)-C(19)-C(20) | -176.7(3) |
| C(17)-O(4)-C(16)-C(15) | -0.7(5) | C(18)-C(19)-C(20)-O(6) | -1.5(5) |
| O(3)-C(15)-C(16)-O(5) | 137.5(4) | C(21)-O(6)-C(20)-C(19) | 1.5(5) |
| C(14)-C(15)-C(16)-O(5) | -153.4(3) | C(19)-C(18)-C(21)-O(6) | -0.1(4) |
| O(3)-C(15)-C(16)-O(4) | -44.4(4) | C(17)-C(18)-C(21)-O(6) | 177.6(3) |
| C(14)-C(15)-C(16)-O(4) | 24.7(5) | C(20)-O(6)-C(21)-C(18) | -0.8(4) |
| C(16)-O(4)-C(17)-C(18) | -165.2(3) | | |

**Table 59** Crystal data and structure refinement for compound XC2

| | |
|---|---|
| Identification code | XC2 |
| Empirical formula | $C_{27}H_{34}O_8$ |
| Formula weight | 486.54 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Orthorhombic, P2(1)2(1)2(1) |
| Unit cell dimensions | a = 9.5760(5) Å alpha = 90° |
| | b = 11.3600(6) Å beta = 90° |
| | c = 22.4325(12) Å gamma = 90° |
| Volume | 2440.3(2) $Å^3$ |
| Z, Calculated density | 4, 1.324 $mg/m^3$ |
| Absorption coefficient | 0.097 $mm^{-1}$ |
| F(000) | 1040 |
| Theta range for data collection | 1.82 to 28.24° |
| Limiting indice | -12<=h<=12, -15<=k<=14, -29<=l<=29 |
| Reflections collected / unique | 21531 / 5882 [R(int) = 0.0265] |
| Completeness to theta = 28.24 | 98.9 % |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 5882 / 0 / 321 |
| Goodness-of-fit on $F^2$ | 1.076 |
| Final R indices [I>2sigma(I)] | R1 = 0.0514, wR2 = 0.1183 |
| R indices (all data) | R1 = 0.0572, wR2 = 0.1213 |
| Absolute structure parameter | -0.2(9) |
| Largest diff. peak and hole | 0.281 and -0.163 e. $Å^{-3}$ |

**Table 60** Bond lengths [Å] and angles [°] for compound XC2

| | | | |
|---|---|---|---|
| O(1)-C(22) | 1.325(3) | C(5)-C(6) | 1.542(3) |
| O(1)-C(23) | 1.444(3) | C(5)-H(5A) | 0.9800 |
| O(2)-C(22) | 1.198(3) | C(6)-C(7) | 1.532(3) |
| O(3)-C(1) | 1.209(2) | C(6)-H(6A) | 0.9800 |
| O(4)-C(8) | 1.442(2) | C(7)-C(8) | 1.537(2) |
| O(4)-C(5) | 1.447(2) | C(7)-H(7B) | 0.9700 |
| O(5)-C(15) | 1.341(2) | C(7)-H(7C) | 0.9700 |
| O(5)-C(16) | 1.460(2) | C(8)-C(9) | 1.544(2) |
| O(6)-C(15) | 1.203(2) | C(8)-C(13) | 1.556(2) |
| O(7)-C(13) | 1.429(2) | C(9)-C(10) | 1.534(3) |
| O(7)-H(7A) | 0.8200 | C(9)-H(9A) | 0.9800 |
| O(8)-C(19) | 1.346(3) | C(10)-C(11) | 1.527(3) |
| O(8)-C(20) | 1.359(3) | C(10)-H(10A) | 0.9700 |
| C(1)-C(6) | 1.506(3) | C(10)-H(10B) | 0.9700 |
| C(1)-C(2) | 1.517(3) | C(11)-C(12) | 1.535(3) |
| C(2)-C(24) | 1.536(3) | C(11)-H(11A) | 0.9700 |
| C(2)-C(3) | 1.579(3) | C(11)-H(11B) | 0.9700 |
| C(2)-C(9) | 1.582(3) | C(12)-C(27) | 1.538(3) |
| C(3)-C(21) | 1.537(3) | C(12)-C(16) | 1.544(3) |
| C(3)-C(4) | 1.574(3) | C(12)-C(13) | 1.559(2) |
| C(3)-H(3A) | 0.9800 | C(13)-C(14) | 1.523(3) |
| C(4)-C(5) | 1.527(3) | C(14)-C(15) | 1.495(3) |
| C(4)-C(26) | 1.530(3) | C(14)-H(14A) | 0.9700 |
| C(4)-C(25) | 1.545(3) | C(14)-H(14B) | 0.9700 |

**Table 60** (Continued)

| | | | |
|---|---|---|---|
| C(16)-C(17) | 1.507(3) | C(27)-H(27B) | 0.9600 |
| C(16)-H(16A) | 0.9800 | C(27)-H(27C) | 0.9600 |
| C(17)-C(20) | 1.334(3) | C(22)-O(1)-C(23) | 116.90(19) |
| C(17)-C(18) | 1.421(3) | C(8)-O(4)-C(5) | 108.23(12) |
| C(18)-C(19) | 1.340(3) | C(15)-O(5)-C(16) | 121.28(15) |
| C(18)-H(18A) | 0.9300 | C(13)-O(7)-H(7A) | 109.5 |
| C(19)-H(19A) | 0.9300 | C(19)-O(8)-C(20) | 105.79(18) |
| C(20)-H(20A) | 0.9300 | O(3)-C(1)-C(6) | 123.3(2) |
| C(21)-C(22) | 1.502(3) | O(3)-C(1)-C(2) | 124.5(2) |
| C(21)-H(21A) | 0.9700 | C(6)-C(1)-C(2) | 112.24(16) |
| C(21)-H(21B) | 0.9700 | C(1)-C(2)-C(24) | 110.29(17) |
| C(23)-H(23A) | 0.9600 | C(1)-C(2)-C(3) | 104.68(15) |
| C(23)-H(23B) | 0.9600 | C(24)-C(2)-C(3) | 112.67(17) |
| C(23)-H(23C) | 0.9600 | C(1)-C(2)-C(9) | 109.38(16) |
| C(24)-H(24A) | 0.9600 | C(24)-C(2)-C(9) | 107.71(16) |
| C(24)-H(24B) | 0.9600 | C(3)-C(2)-C(9) | 112.08(14) |
| C(24)-H(24C) | 0.9600 | C(21)-C(3)-C(4) | 110.18(15) |
| C(25)-H(25A) | 0.9600 | C(21)-C(3)-C(2) | 114.34(16) |
| C(25)-H(25B) | 0.9600 | C(4)-C(3)-C(2) | 114.03(15) |
| C(25)-H(25C) | 0.9600 | C(21)-C(3)-H(3A) | 105.8 |
| C(26)-H(26A) | 0.9600 | C(4)-C(3)-H(3A) | 105.8 |
| C(26)-H(26B) | 0.9600 | C(2)-C(3)-H(3A) | 105.8 |
| C(26)-H(26C) | 0.9600 | C(5)-C(4)-C(26) | 109.63(15) |
| C(27)-H(27A) | 0.9600 | C(5)-C(4)-C(25) | 106.54(16) |

**Table 60** (Continued)

| | | | |
|---|---|---|---|
| C(26)-C(4)-C(25) | 108.76(16) | C(7)-C(8)-C(9) | 109.24(15) |
| C(5)-C(4)-C(3) | 109.25(14) | O(4)-C(8)-C(13) | 107.78(13) |
| C(26)-C(4)-C(3) | 108.38(16) | C(7)-C(8)-C(13) | 113.70(14) |
| C(25)-C(4)-C(3) | 114.21(16) | C(9)-C(8)-C(13) | 113.22(14) |
| O(4)-C(5)-C(4) | 110.29(14) | C(10)-C(9)-C(8) | 112.20(15) |
| O(4)-C(5)-C(6) | 106.03(14) | C(10)-C(9)-C(2) | 113.06(16) |
| C(4)-C(5)-C(6) | 113.23(15) | C(8)-C(9)-C(2) | 113.03(14) |
| O(4)-C(5)-H(5A) | 109.1 | C(10)-C(9)-H(9A) | 105.9 |
| C(4)-C(5)-H(5A) | 109.1 | C(8)-C(9)-H(9A) | 105.9 |
| C(6)-C(5)-H(5A) | 109.1 | C(2)-C(9)-H(9A) | 105.9 |
| C(1)-C(6)-C(7) | 105.66(16) | C(11)-C(10)-C(9) | 112.31(16) |
| C(1)-C(6)-C(5) | 110.32(16) | C(11)-C(10)-H(10A) | 109.1 |
| C(7)-C(6)-C(5) | 102.38(14) | C(9)-C(10)-H(10A) | 109.1 |
| C(1)-C(6)-H(6A) | 112.6 | C(11)-C(10)-H(10B) | 109.1 |
| C(7)-C(6)-H(6A) | 112.6 | C(9)-C(10)-H(10B) | 109.1 |
| C(5)-C(6)-H(6A) | 112.6 | H(10A)-C(10)-H(10B) | 107.9 |
| C(6)-C(7)-C(8) | 99.62(14) | C(10)-C(11)-C(12 | 113.56(15) |
| C(6)-C(7)-H(7B) | 111.8 | C(10)-C(11)-H(11A) | 108.9 |
| C(8)-C(7)-H(7B) | 111.8 | C(12)-C(11)-H(11A) | 108.9 |
| C(6)-C(7)-H(7C) | 111.8 | C(10)-C(11)-H(11B) | 108.9 |
| C(8)-C(7)-H(7C) | 111.8 | C(12)-C(11)-H(11B) | 108.9 |
| H(7B)-C(7)-H(7C) | 109.6 | H(11A)-C(11)-H(11B) | 107.7 |
| O(4)-C(8)-C(7) | 102.08(13) | C(11)-C(12)-C(27) | 108.98(15) |
| O(4)-C(8)-C(9) | 110.20(13) | C(11)-C(12)-C(16) | 109.99(14) |

**Table 60** (Continued)

| | | | |
|---|---|---|---|
| C(27)-C(12)-C(16) | 110.38(16) | C(12)-C(16)-H(16A) | 107.5 |
| C(11)-C(12)-C(13) | 108.47(15) | C(20)-C(17)-C(18) | 105.16(18) |
| C(27)-C(12)-C(13) | 110.64(15) | C(20)-C(17)-C(16) | 126.12(19) |
| C(16)-C(12)-C(13) | 108.36(14) | C(18)-C(17)-C(16) | 128.62(18) |
| O(7)-C(13)-C(14) | 111.23(15) | C(19)-C(18)-C(17) | 106.8(2) |
| O(7)-C(13)-C(8) | 107.15(15) | C(19)-C(18)-H(18A) | 126.6 |
| C(14)-C(13)-C(8) | 110.94(15) | C(17)-C(18)-H(18A) | 126.6 |
| O(7)-C(13)-C(12) | 105.63(14) | C(18)-C(19)-O(8) | 110.7(2) |
| C(14)-C(13)-C(12) | 108.32(15) | C(18)-C(19)-H(19A) | 124.7 |
| C(8)-C(13)-C(12) | 113.47(14) | O(8)-C(19)-H(19A) | 124.7 |
| C(15)-C(14)-C(13) | 116.06(16) | C(17)-C(20)-O(8) | 111.6(2) |
| C(15)-C(14)-H(14A) | 108.3 | C(17)-C(20)-H(20A) | 124.2 |
| C(13)-C(14)-H(14A) | 108.3 | O(8)-C(20)-H(20A) | 124.2 |
| C(15)-C(14)-H(14B) | 108.3 | C(22)-C(21)-C(3) | 117.51(17) |
| C(13)-C(14)-H(14B) | 108.3 | C(22)-C(21)-H(21A) | 107.9 |
| H(14A)-C(14)-H(14B) | 107.4 | C(3)-C(21)-H(21A) | 107.9 |
| O(6)-C(15)-O(5) | 117.4(2) | C(22)-C(21)-H(21B) | 107.9 |
| O(6)-C(15)-C(14) | 123.2(2) | C(3)-C(21)-H(21B) | 107.9 |
| O(5)-C(15)-C(14) | 119.17(17) | H(21A)-C(21)-H(21B) | 107.2 |
| O(5)-C(16)-C(17) | 104.57(15) | O(2)-C(22)-O(1) | 122.6(2) |
| O(5)-C(16)-C(12) | 113.44(14) | O(2)-C(22)-C(21) | 125.2(2) |
| C(17)-C(16)-C(12) | 115.82(15) | O(1)-C(22)-C(21) | 112.01(17) |
| O(5)-C(16)-H(16A) | 107.5 | O(1)-C(23)-H(23A) | 109.5 |
| C(17)-C(16)-H(16A) | 107.5 | O(1)-C(23)-H(23B) | 109.5 |

**Table 60** (Continued)

| | | | |
|---|---|---|---|
| H(23A)-C(23)-H(23B) | 109.5 | H(25A)-C(25)-H(25C) | 109.5 |
| O(1)-C(23)-H(23C) | 109.5 | H(25B)-C(25)-H(25C) | 109.5 |
| H(23A)-C(23)-H(23C) | 109.5 | C(4)-C(26)-H(26A) | 109.5 |
| H(23B)-C(23)-H(23C) | 109.5 | C(4)-C(26)-H(26B) | 109.5 |
| C(2)-C(24)-H(24A) | 109.5 | H(26A)-C(26)-H(26B) | 109.5 |
| C(2)-C(24)-H(24B) | 109.5 | C(4)-C(26)-H(26C) | 109.5 |
| H(24A)-C(24)-H(24B) | 109.5 | H(26A)-C(26)-H(26C) | 109.5 |
| C(2)-C(24)-H(24C) | 109.5 | H(26B)-C(26)-H(26C) | 109.5 |
| H(24A)-C(24)-H(24C) | 109.5 | C(12)-C(27)-H(27A) | 109.5 |
| H(24B)-C(24)-H(24C) | 109.5 | C(12)-C(27)-H(27B) | 109.5 |
| C(4)-C(25)-H(25A) | 109.5 | H(27A)-C(27)-H(27B) | 109.5 |
| C(4)-C(25)-H(25B) | 109.5 | C(12)-C(27)-H(27C) | 109.5 |
| H(25A)-C(25)-H(25B) | 109.5 | H(27A)-C(27)-H(27C) | 109.5 |
| C(4)-C(25)-H(25C) | 109.5 | H(27B)-C(27)-H(27C) | 109.5 |

Symmetry transformations used to generate equivalent atoms:

**Table 61** Torsion angles [°] for compound XC2.

| | | | |
|---|---|---|---|
| O(3)-C(1)-C(2)-C(24) | -14.5(3) | C(25)-C(4)-C(5)-C(6) | 64.25(19) |
| C(6)-C(1)-C(2)-C(24) | 166.81(17) | C(3)-C(4)-C(5)-C(6) | -59.59(19) |
| O(3)-C(1)-C(2)-C(3) | 107.0(2) | O(3)-C(1)-C(6)-C(7) | 111.5(2) |
| C(6)-C(1)-C(2)-C(3) | -71.74(19) | C(2)-C(1)-C(6)-C(7) | -69.80(19) |
| O(3)-C(1)-C(2)-C(9) | -132.8(2) | O(3)-C(1)-C(6)-C(5) | -138.6(2) |
| C(6)-C(1)-C(2)-C(9) | 48.5(2) | C(2)-C(1)-C(6)-C(5) | 40.2(2) |
| C(1)-C(2)-C(3)-C(21) | -93.00(19) | O(4)-C(5)-C(6)-C(1) | -94.03(17) |
| C(24)-C(2)-C(3)-C(21) | 26.9(2) | C(4)-C(5)-C(6)-C(1) | 27.0(2) |
| C(9)-C(2)-C(3)-C(21) | 148.55(17) | O(4)-C(5)-C(6)-C(7) | 18.05(18) |
| C(1)-C(2)-C(3)-C(4) | 35.0(2) | C(4)-C(5)-C(6)-C(7) | 139.11(16) |
| C(24)-C(2)-C(3)-C(4) | 154.90(17) | C(1)-C(6)-C(7)-C(8) | 77.12(18) |
| C(9)-C(2)-C(3)-C(4) | -83.42(19) | C(5)-C(6)-C(7)-C(8) | -38.39(18) |
| C(21)-C(3)-C(4)-C(5) | 155.52(16) | C(5)-O(4)-C(8)-C(7) | -36.47(17) |
| C(2)-C(3)-C(4)-C(5) | 25.4(2) | C(5)-O(4)-C(8)-C(9) | 79.50(16) |
| C(21)-C(3)-C(4)-C(26) | -85.08(19) | C(5)-O(4)-C(8)-C(13) | -156.50(13) |
| C(2)-C(3)-C(4)-C(26) | 144.79(16) | C(6)-C(7)-C(8)-O(4) | 46.10(17) |
| C(21)-C(3)-C(4)-C(25) | 36.3(2) | C(6)-C(7)-C(8)-C(9) | -70.56(17) |
| C(2)-C(3)-C(4)-C(25) | -93.80(19) | C(6)-C(7)-C(8)-C(13) | 161.90(15) |
| C(8)-O(4)-C(5)-C(4) | -111.38(15) | O(4)-C(8)-C(9)-C(10) | 73.03(18) |
| C(8)-O(4)-C(5)-C(6) | 11.56(17) | C(7)-C(8)-C(9)-C(10) | -175.58(15) |
| C(26)-C(4)-C(5)-O(4) | -59.60(19) | C(13)-C(8)-C(9)-C(10) | -47.8(2) |
| C(25)-C(4)-C(5)-O(4) | -177.13(15) | O(4)-C(8)-C(9)-C(2) | -56.25(18) |
| C(3)-C(4)-C(5)-O(4) | 59.03(19) | C(7)-C(8)-C(9)-C(2) | 55.14(19) |
| C(26)-C(4)-C(5)-C(6) | -178.22(15) | C(13)-C(8)-C(9)-C(2) | -177.04(15) |

**Table 61** (Continued)

| | | | |
|---|---|---|---|
| C(1)-C(2)-C(9)-C(10) | -170.00(15) | C(11)-C(12)-C(13)-C(14) | -176.49(15) |
| C(24)-C(2)-C(9)-C(10) | 70.1(2) | C(27)-C(12)-C(13)-C(14) | 64.03(19) |
| C(3)-C(2)-C(9)-C(10) | -54.4(2) | C(16)-C(12)-C(13)-C(14) | -57.11(18) |
| C(1)-C(2)-C(9)-C(8) | -41.16(19) | C(11)-C(12)-C(13)-C(8) | -52.84(18) |
| C(24)-C(2)-C(9)-C(8) | -161.04(17) | C(27)-C(12)-C(13)-C(8) | -172.32(16) |
| C(3)-C(2)-C(9)-C(8) | 74.48(19) | C(16)-C(12)-C(13)-C(8) | 66.54(19) |
| C(8)-C(9)-C(10)-C(11) | 50.6(2) | O(7)-C(13)-C(14)-C(15) | 162.77(16) |
| C(2)-C(9)-C(10)-C(11) | 179.91(15) | C(8)-C(13)-C(14)-C(15) | -78.1(2) |
| C(9)-C(10)-C(11)-C(12) | -56.8(2) | C(12)-C(13)-C(14)-C(15) | 47.1(2) |
| C(10)-C(11)-C(12)-C(27) | 176.95(17) | C(16)-O(5)-C(15)-O(6) | -161.03(18) |
| C(10)-C(11)-C(12)-C(16) | -61.9(2) | C(16)-O(5)-C(15)-C(14) | 25.0(3) |
| C(10)-C(11)-C(12)-C(13) | 56.4(2) | C(13)-C(14)-C(15)-O(6) | 155.6(2) |
| O(4)-C(8)-C(13)-O(7) | 171.79(13) | C(13)-C(14)-C(15)-O(5) | -30.8(3) |
| C(7)-C(8)-C(13)-O(7) | 59.40(19) | C(15)-O(5)-C(16)-C(17) | -164.33(17) |
| C(9)-C(8)-C(13)-O(7) | -66.06(17) | C(15)-O(5)-C(16)-C(12) | -37.2(2) |
| O(4)-C(8)-C(13)-C(14) | 50.20(18) | C(11)-C(12)-C(16)-O(5) | 171.17(14) |
| C(7)-C(8)-C(13)-C(14) | -62.2(2) | C(27)-C(12)-C(16)-O(5) | -68.55(19) |
| C(9)-C(8)-C(13)-C(14) | 172.35(14) | C(13)-C(12)-C(16)-O(5) | 52.74(19) |
| O(4)-C(8)-C(13)-C(12) | -72.02(17) | C(11)-C(12)-C(16)-C(17) | -67.9(2) |
| C(7)-C(8)-C(13)-C(12) | 175.59(15) | C(27)-C(12)-C(16)-C(17) | 52.4(2) |
| C(9)-C(8)-C(13)-C(12) | 50.14(19) | C(13)-C(12)-C(16)-C(17) | 173.70(16) |
| C(11)-C(12)-C(13)-O(7) | 64.25(18) | O(5)-C(16)-C(17)-C(20) | -141.8(2) |
| C(27)-C(12)-C(13)-O(7) | -55.2(2) | C(12)-C(16)-C(17)-C(20) | 92.5(3) |
| C(16)-C(12)-C(13)-O(7) | -176.37(14) | O(5)-C(16)-C(17)-C(18) | 34.1(3) |

**Table 61** (Continued)

| | | | |
|---|---|---|---|
| C(12)-C(16)-C(17)-C(18) | -91.5(3) | C(19)-O(8)-C(20)-C(17) | -0.9(3) |
| C(20)-C(17)-C(18)-C(19) | 0.0(3) | C(4)-C(3)-C(21)-C(22) | 149.44(18) |
| C(16)-C(17)-C(18)-C(19) | -176.6(2) | C(2)-C(3)-C(21)-C(22) | -80.6(2) |
| C(17)-C(18)-C(19)-O(8) | -0.5(3) | C(23)-O(1)-C(22)-O(2) | 0.3(4) |
| C(20)-O(8)-C(19)-C(18) | 0.9(3) | C(23)-O(1)-C(22)-C(21) | -174.5(2) |
| C(18)-C(17)-C(20)-O(8) | 0.5(3) | C(3)-C(21)-C(22)-O(2) | 150.4(3) |
| C(16)-C(17)-C(20)-O(8) | 177.29(19) | C(3)-C(21)-C(22)-O(1) | -34.9(3) |

Symmetry transformations used to generate equivalent atoms:

**Table 62** Crystal data and structure refinement for compound XC4

| | |
|---|---|
| Identification code | XC4 |
| Empirical formula | $C_{30}H_{52}O_4$ |
| Formula weight | 476.72 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | P2(1)2(1)2(1), Orthorhombic |
| Unit cell dimensions | a = 10.5917(15) Å alpha = 90° |
| | b = 14.4818(19) Å beta = 90° |
| | c = 18.205(3) Å gamma = 90° |
| Volume | 2792.5(7) $Å^3$ |
| Z, Calculated density | 4, 1.134 $mg/m^3$ |
| Absorption coefficient | 0.073 $mm^{-1}$ |
| F(000) | 1056 |
| Theta range for data collection | 1.80 to 25.00° |
| Limiting indices | -12<=h<=12, -17<=k<=16, -21<=l<=21 |
| Reflections collected / unique | 14727 / 4892 [R(int) = 0.0771] |
| Completeness to theta = 25.00 | 99.5 % |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 4892 / 0 / 315 |
| Goodness-of-fit on $F^2$ | 1.027 |
| Final R indices [I>2sigma(I)] | R1 = 0.0826, wR2 = 0.1629 |
| R indices (all data) | R1 = 0.1351, wR2 = 0.1877 |
| Absolute structure parameter | 1(3) |
| Largest diff. peak and hole | 0.240 and -0.222 e. $Å^{-3}$ |

**Table 63** Bond lengths [Å] and angles [°] for compound XC4

| | | | |
|---|---|---|---|
| O(1)-C(3) | 1.437(5) | C(6)-H(6A) | 0.9700 |
| O(1)-H(1A) | 0.8200 | C(6)-H(6B) | 0.9700 |
| O(2)-C(20) | 1.431(5) | C(7)-C(8) | 1.324(6) |
| O(2)-H(2A) | 0.8200 | C(7)-H(7A) | 0.9300 |
| O(3)-C(21) | 1.433(6) | C(8)-C(14) | 1.512(6) |
| O(3)-H(3A) | 0.8200 | C(8)-C(9) | 1.534(6) |
| O(4)-C(22) | 1.434(6) | C(9)-C(11) | 1.536(6) |
| O(4)-H(4A) | 0.8200 | C(9)-C(10) | 1.560(6) |
| C(1)-C(2) | 1.521(6) | C(9)-H(9A) | 0.9800 |
| C(1)-C(10) | 1.527(6) | C(10)-C(27) | 1.541(6) |
| C(1)-H(1B) | 0.9700 | C(11)-C(12) | 1.541(6) |
| C(1)-H(1C) | 0.9700 | C(11)-H(11A) | 0.9700 |
| C(2)-C(3) | 1.481(6) | C(11)-H(11B) | 0.9700 |
| C(2)-H(2B) | 0.9700 | C(12)-C(13) | 1.523(6) |
| C(2)-H(2C) | 0.9700 | C(12)-H(12A) | 0.9700 |
| C(3)-C(4) | 1.536(6) | C(12)-H(12B) | 0.9700 |
| C(3)-H(3B) | 0.9800 | C(13)-C(14) | 1.547(6) |
| C(4)-C(25) | 1.532(6) | C(13)-C(29) | 1.552(6) |
| C(4)-C(26) | 1.537(6) | C(13)-C(17) | 1.555(6) |
| C(4)-C(5) | 1.561(6) | C(14)-C(15) | 1.544(7) |
| C(5)-C(6) | 1.538(6) | C(14)-C(28) | 1.551(7) |
| C(5)-C(10) | 1.544(6) | C(15)-C(16) | 1.553(6) |
| C(5)-H(5A) | 0.9800 | C(15)-H(15A) | 0.9700 |
| C(6)-C(7) | 1.505(6) | C(15)-H(15B) | 0.9700 |

**Table 63** (Continued)

| | | | |
|---|---|---|---|
| C(16)-C(17) | 1.524(7) | C(25)-H(25B) | 0.9600 |
| C(16)-H(16A) | 0.9700 | C(25)-H(25C) | 0.9600 |
| C(16)-H(16B) | 0.9700 | C(26)-H(26A) | 0.9600 |
| C(17)-C(18) | 1.544(6) | C(26)-H(26B) | 0.9600 |
| C(17)-H(17A) | 0.9800 | C(26)-H(26C) | 0.9600 |
| C(18)-C(30) | 1.518(7) | C(27)-H(27A) | 0.9600 |
| C(18)-C(19) | 1.554(6) | C(27)-H(27B) | 0.9600 |
| C(18)-H(18A) | 0.9800 | C(27)-H(27C) | 0.9600 |
| C(19)-C(20) | 1.514(6) | C(28)-H(28A) | 0.9600 |
| C(19)-H(19A) | 0.9700 | C(28)-H(28B) | 0.9600 |
| C(19)-H(19B) | 0.9700 | C(28)-H(28C) | 0.9600 |
| C(20)-C(21) | 1.517(7) | C(29)-H(29A) | 0.9600 |
| C(20)-H(20A) | 0.9800 | C(29)-H(29B) | 0.9600 |
| C(21)-C(22) | 1.519(7) | C(29)-H(29C) | 0.9600 |
| C(21)-H(21A) | 0.9800 | C(30)-H(30A) | 0.9600 |
| C(22)-C(23) | 1.493(8) | C(30)-H(30B) | 0.9600 |
| C(22)-C(24) | 1.516(7) | C(30)-H(30C) | 0.9600 |
| C(23)-H(23A) | 0.9600 | C(3)-O(1)-H(1A) | 109.5 |
| C(23)-H(23B) | 0.9600 | C(20)-O(2)-H(2A) | 109.5 |
| C(23)-H(23C) | 0.9600 | C(21)-O(3)-H(3A) | 109.5 |
| C(24)-H(24A) | 0.9600 | C(22)-O(4)-H(4A) | 109.5 |
| C(24)-H(24B) | 0.9600 | C(2)-C(1)-C(10) | 113.5(4) |
| C(24)-H(24C) | 0.9600 | C(2)-C(1)-H(1B) | 108.9 |
| C(25)-H(25A) | 0.9600 | C(10)-C(1)-H(1B) | 108.9 |

**Table 63** (Continued)

| | | | |
|---|---|---|---|
| C(2)-C(1)-H(1C) | 108.9 | C(6)-C(5)-H(5A) | 104.2 |
| C(10)-C(1)-H(1C) | 108.9 | C(10)-C(5)-H(5A) | 104.2 |
| H(1B)-C(1)-H(1C) | 107.7 | C(4)-C(5)-H(5A) | 104.2 |
| C(3)-C(2)-C(1) | 110.0(4) | C(7)-C(6)-C(5) | 112.1(4) |
| C(3)-C(2)-H(2B) | 109.7 | C(7)-C(6)-H(6A) | 109.2 |
| C(1)-C(2)-H(2B) | 109.7 | C(5)-C(6)-H(6A) | 109.2 |
| C(3)-C(2)-H(2C) | 109.7 | C(7)-C(6)-H(6B) | 109.2 |
| C(1)-C(2)-H(2C) | 109.7 | C(5)-C(6)-H(6B) | 109.2 |
| H(2B)-C(2)-H(2C) | 108.2 | H(6A)-C(6)-H(6B) | 107.9 |
| O(1)-C(3)-C(2) | 111.2(4) | C(8)-C(7)-C(6) | 125.4(4) |
| O(1)-C(3)-C(4) | 111.5(3) | C(8)-C(7)-H(7A) | 117.3 |
| C(2)-C(3)-C(4) | 114.1(4) | C(6)-C(7)-H(7A) | 117.3 |
| O(1)-C(3)-H(3B) | 106.5 | C(7)-C(8)-C(14) | 123.4(4) |
| C(2)-C(3)-H(3B) | 106.5 | C(7)-C(8)-C(9) | 119.6(4) |
| C(4)-C(3)-H(3B) | 106.5 | C(14)-C(8)-C(9) | 117.0(4) |
| C(25)-C(4)-C(3) | 110.6(4) | C(8)-C(9)-C(11) | 110.7(4) |
| C(25)-C(4)-C(26) | 106.9(4) | C(8)-C(9)-C(10) | 112.3(4) |
| C(3)-C(4)-C(26) | 107.8(4) | C(11)-C(9)-C(10) | 114.8(4) |
| C(25)-C(4)-C(5) | 115.4(4) | C(8)-C(9)-H(9A) | 106.1 |
| C(3)-C(4)-C(5) | 106.2(3) | C(11)-C(9)-H(9A) | 106.1 |
| C(26)-C(4)-C(5) | 109.6(4) | C(10)-C(9)-H(9A) | 106.1 |
| C(6)-C(5)-C(10) | 111.0(4) | C(1)-C(10)-C(27) | 110.5(4) |
| C(6)-C(5)-C(4) | 112.2(3) | C(1)-C(10)-C(5) | 109.1(3) |
| C(10)-C(5)-C(4) | 119.2(4) | C(27)-C(10)-C(5) | 113.4(4) |

**Table 63** (Continued)

| | | | |
|---|---|---|---|
| C(1)-C(10)-C(9) | 108.9(3) | C(8)-C(14)-C(28) | 107.6(4) |
| C(27)-C(10)-C(9) | 110.0(4) | C(15)-C(14)-C(28) | 108.2(4) |
| C(5)-C(10)-C(9) | 104.8(3) | C(13)-C(14)-C(28) | 112.3(4) |
| C(9)-C(11)-C(12) | 114.7(4) | C(14)-C(15)-C(16) | 102.9(4) |
| C(9)-C(11)-H(11A) | 108.6 | C(14)-C(15)-H(15A) | 111.2 |
| C(12)-C(11)-H(11A) | 108.6 | C(16)-C(15)-H(15A) | 111.2 |
| C(9)-C(11)-H(11B) | 108.6 | C(14)-C(15)-H(15B) | 111.2 |
| C(12)-C(11)-H(11B) | 108.6 | C(16)-C(15)-H(15B) | 111.2 |
| H(11A)-C(11)-H(11B) | 107.6 | H(15A)-C(15)-H(15B) | 109.1 |
| C(13)-C(12)-C(11) | 114.9(4) | C(17)-C(16)-C(15) | 108.1(4) |
| C(13)-C(12)-H(12A) | 108.5 | C(17)-C(16)-H(16A) | 110.1 |
| C(11)-C(12)-H(12A) | 108.5 | C(15)-C(16)-H(16A) | 110.1 |
| C(13)-C(12)-H(12B) | 108.5 | C(17)-C(16)-H(16B) | 110.1 |
| C(11)-C(12)-H(12B) | 108.5 | C(15)-C(16)-H(16B) | 110.1 |
| H(12A)-C(12)-H(12B) | 107.5 | H(16A)-C(16)-H(16B) | 108.4 |
| C(12)-C(13)-C(14) | 109.3(4) | C(16)-C(17)-C(18) | 113.9(4) |
| C(12)-C(13)-C(29) | 109.7(4) | C(16)-C(17)-C(13) | 103.7(4) |
| C(14)-C(13)-C(29) | 110.5(4) | C(18)-C(17)-C(13) | 119.0(4) |
| C(12)-C(13)-C(17) | 118.1(4) | C(16)-C(17)-H(17A) | 106.5 |
| C(14)-C(13)-C(17) | 101.4(3) | C(18)-C(17)-H(17A) | 106.5 |
| C(29)-C(13)-C(17) | 107.6(3) | C(13)-C(17)-H(17A) | 106.5 |
| C(8)-C(14)-C(15) | 116.1(4) | C(30)-C(18)-C(17) | 113.8(4) |
| C(8)-C(14)-C(13) | 110.6(4) | C(30)-C(18)-C(19) | 110.4(4) |
| C(15)-C(14)-C(13) | 102.1(3) | C(17)-C(18)-C(19) | 108.6(4) |

**Table 63** (Continued)

| | | | |
|---|---|---|---|
| C(30)-C(18)-H(18A) | 108.0 | O(4)-C(22)-C(21) | 106.5(4) |
| C(17)-C(18)-H(18A) | 108.0 | C(23)-C(22)-C(21) | 112.6(4) |
| C(19)-C(18)-H(18A) | 108.0 | C(24)-C(22)-C(21) | 110.7(5) |
| C(20)-C(19)-C(18) | 115.1(4) | C(22)-C(23)-H(23A) | 109.5 |
| C(20)-C(19)-H(19A) | 108.5 | C(22)-C(23)-H(23B) | 109.5 |
| C(18)-C(19)-H(19A) | 108.5 | H(23A)-C(23)-H(23B) | 109.5 |
| C(20)-C(19)-H(19B) | 108.5 | C(22)-C(23)-H(23C) | 109.5 |
| C(18)-C(19)-H(19B) | 108.5 | H(23A)-C(23)-H(23C) | 109.5 |
| H(19A)-C(19)-H(19B) | 107.5 | H(23B)-C(23)-H(23C) | 109.5 |
| O(2)-C(20)-C(19) | 108.0(4) | C(22)-C(24)-H(24A) | 109.5 |
| O(2)-C(20)-C(21) | 110.6(4) | C(22)-C(24)-H(24B) | 109.5 |
| C(19)-C(20)-C(21) | 112.3(4) | H(24A)-C(24)-H(24B) | 109.5 |
| O(2)-C(20)-H(20A) | 108.6 | C(22)-C(24)-H(24C) | 109.5 |
| C(19)-C(20)-H(20A) | 108.6 | H(24A)-C(24)-H(24C) | 109.5 |
| C(21)-C(20)-H(20A) | 108.6 | H(24B)-C(24)-H(24C) | 109.5 |
| O(3)-C(21)-C(20) | 109.0(4) | C(4)-C(25)-H(25A) | 109.5 |
| O(3)-C(21)-C(22) | 109.8(4) | C(4)-C(25)-H(25B) | 109.5 |
| C(20)-C(21)-C(22) | 116.2(4) | H(25A)-C(25)-H(25B) | 109.5 |
| O(3)-C(21)-H(21A) | 107.1 | C(4)-C(25)-H(25C) | 109.5 |
| C(20)-C(21)-H(21A) | 107.1 | H(25A)-C(25)-H(25C) | 109.5 |
| C(22)-C(21)-H(21A) | 107.1 | H(25B)-C(25)-H(25C) | 109.5 |
| O(4)-C(22)-C(23) | 109.2(5) | C(4)-C(26)-H(26A) | 109.5 |
| O(4)-C(22)-C(24) | 106.5(4) | C(4)-C(26)-H(26B) | 109.5 |
| C(23)-C(22)-C(24) | 110.9(6) | H(26A)-C(26)-H(26B) | 109.5 |

**Table 63** (Continued)

| | | | |
|---|---|---|---|
| C(4)-C(26)-H(26C) | 109.5 | H(28B)-C(28)-H(28C) | 109.5 |
| H(26A)-C(26)-H(26C) | 109.5 | C(13)-C(29)-H(29A) | 109.5 |
| H(26B)-C(26)-H(26C) | 109.5 | C(13)-C(29)-H(29B) | 109.5 |
| C(10)-C(27)-H(27A) | 109.5 | H(29A)-C(29)-H(29B) | 109.5 |
| C(10)-C(27)-H(27B) | 109.5 | C(13)-C(29)-H(29C) | 109.5 |
| H(27A)-C(27)-H(27B) | 109.5 | H(29A)-C(29)-H(29C) | 109.5 |
| C(10)-C(27)-H(27C) | 109.5 | H(29B)-C(29)-H(29C) | 109.5 |
| H(27A)-C(27)-H(27C) | 109.5 | C(18)-C(30)-H(30A) | 109.5 |
| H(27B)-C(27)-H(27C) | 109.5 | C(18)-C(30)-H(30B) | 109.5 |
| C(14)-C(28)-H(28A) | 109.5 | H(30A)-C(30)-H(30B) | 109.5 |
| C(14)-C(28)-H(28B) | 109.5 | C(18)-C(30)-H(30C) | 109.5 |
| H(28A)-C(28)-H(28B) | 109.5 | H(30A)-C(30)-H(30C) | 109.5 |
| C(14)-C(28)-H(28C) | 109.5 | H(30B)-C(30)-H(30C) | 109.5 |
| H(28A)-C(28)-H(28C) | 109.5 | | |

Symmetry transformations used to generate equivalent atoms:

**Table 64** Torsion angles [°] for compound XC4

| | | | |
|---|---|---|---|
| C(10)-C(1)-C(2)-C(3) | 58.3(5) | C(2)-C(1)-C(10)-C(27) | 76.7(5) |
| C(1)-C(2)-C(3)-O(1) | 170.6(4) | C(2)-C(1)-C(10)-C(5) | -48.6(5) |
| C(1)-C(2)-C(3)-C(4) | -62.2(5) | C(2)-C(1)-C(10)-C(9) | -162.5(4) |
| O(1)-C(3)-C(4)-C(25) | 55.4(5) | C(6)-C(5)-C(10)-C(1) | 178.3(4) |
| C(2)-C(3)-C(4)-C(25) | -71.6(5) | C(4)-C(5)-C(10)-C(1) | 45.6(5) |
| O(1)-C(3)-C(4)-C(26) | -61.2(4) | C(6)-C(5)-C(10)-C(27) | 54.7(5) |
| C(2)-C(3)-C(4)-C(26) | 171.8(4) | C(4)-C(5)-C(10)-C(27) | -78.1(5) |
| O(1)-C(3)-C(4)-C(5) | -178.6(3) | C(6)-C(5)-C(10)-C(9) | -65.3(4) |
| C(2)-C(3)-C(4)-C(5) | 54.3(5) | C(4)-C(5)-C(10)-C(9) | 162.0(4) |
| C(25)-C(4)-C(5)-C(6) | -56.4(5) | C(8)-C(9)-C(10)-C(1) | 172.5(4) |
| C(3)-C(4)-C(5)-C(6) | -179.4(4) | C(11)-C(9)-C(10)-C(1) | -59.8(5) |
| C(26)-C(4)-C(5)-C(6) | 64.4(5) | C(8)-C(9)-C(10)-C(27) | -66.3(5) |
| C(25)-C(4)-C(5)-C(10) | 75.8(5) | C(11)-C(9)-C(10)-C(27) | 61.3(5) |
| C(3)-C(4)-C(5)-C(10) | -47.1(5) | C(8)-C(9)-C(10)-C(5) | 55.9(4) |
| C(26)-C(4)-C(5)-C(10) | -163.4(4) | C(11)-C(9)-C(10)-C(5) | -176.4(4) |
| C(10)-C(5)-C(6)-C(7) | 43.1(5) | C(8)-C(9)-C(11)-C(12) | -51.2(6) |
| C(4)-C(5)-C(6)-C(7) | 179.2(4) | C(10)-C(9)-C(11)-C(12) | -179.6(4) |
| C(5)-C(6)-C(7)-C(8) | -10.0(7) | C(9)-C(11)-C(12)-C(13) | 21.5(7) |
| C(6)-C(7)-C(8)-C(14) | -176.5(5) | C(11)-C(12)-C(13)-C(14) | 35.1(6) |
| C(6)-C(7)-C(8)-C(9) | 1.7(8) | C(11)-C(12)-C(13)-C(29) | -86.1(5) |
| C(7)-C(8)-C(9)-C(11) | -155.9(4) | C(11)-C(12)-C(13)-C(17) | 150.2(4) |
| C(14)-C(8)-C(9)-C(11) | 22.4(5) | C(7)-C(8)-C(14)-C(15) | -32.6(7) |
| C(7)-C(8)-C(9)-C(10) | -26.1(6) | C(9)-C(8)-C(14)-C(15) | 149.2(4) |
| C(14)-C(8)-C(9)-C(10) | 152.2(4) | C(7)-C(8)-C(14)-C(13) | -148.3(5) |

**Table 64** (Continued)

| | | | |
|---|---|---|---|
| C(9)-C(8)-C(14)-C(13) | 33.6(5) | C(12)-C(13)-C(17)-C(18) | 75.4(5) |
| C(7)-C(8)-C(14)-C(28) | 88.8(6) | C(14)-C(13)-C(17)-C(18) | -165.3(4) |
| C(9)-C(8)-C(14)-C(28) | -89.4(5) | C(29)-C(13)-C(17)-C(18) | -49.4(6) |
| C(12)-C(13)-C(14)-C(8) | -63.5(5) | C(16)-C(17)-C(18)-C(30) | -176.0(4) |
| C(29)-C(13)-C(14)-C(8) | 57.3(5) | C(13)-C(17)-C(18)-C(30) | -53.2(6) |
| C(17)-C(13)-C(14)-C(8) | 171.1(4) | C(16)-C(17)-C(18)-C(19) | 60.7(5) |
| C(12)-C(13)-C(14)-C(15) | 172.4(4) | C(13)-C(17)-C(18)-C(19) | -176.6(4) |
| C(29)-C(13)-C(14)-C(15) | -66.9(5) | C(30)-C(18)-C(19)-C(20) | 71.2(6) |
| C(17)-C(13)-C(14)-C(15) | 47.0(4) | C(17)-C(18)-C(19)-C(20) | -163.4(4) |
| C(12)-C(13)-C(14)-C(28) | 56.7(5) | C(18)-C(19)-C(20)-O(2) | -155.8(4) |
| C(29)-C(13)-C(14)-C(28) | 177.4(4) | C(18)-C(19)-C(20)-C(21) | 81.9(5) |
| C(17)-C(13)-C(14)-C(28) | -68.8(5) | O(2)-C(20)-C(21)-O(3) | -58.9(5) |
| C(8)-C(14)-C(15)-C(16) | -158.0(4) | C(19)-C(20)-C(21)-O(3) | 61.8(5) |
| C(13)-C(14)-C(15)-C(16) | -37.6(5) | O(2)-C(20)-C(21)-C(22) | 65.8(6) |
| C(28)-C(14)-C(15)-C(16) | 81.0(5) | C(19)-C(20)-C(21)-C(22) | -173.5(4) |
| C(14)-C(15)-C(16)-C(17) | 14.3(6) | O(3)-C(21)-C(22)-O(4) | 66.2(5) |
| C(15)-C(16)-C(17)-C(18) | 145.3(4) | C(20)-C(21)-C(22)-O(4) | -58.1(6) |
| C(15)-C(16)-C(17)-C(13) | 14.5(5) | O(3)-C(21)-C(22)-C(23) | -174.1(6) |
| C(12)-C(13)-C(17)-C(16) | -156.9(4) | C(20)-C(21)-C(22)-C(23) | 61.6(7) |
| C(14)-C(13)-C(17)-C(16) | -37.6(4) | O(3)-C(21)-C(22)-C(24) | -49.2(6) |
| C(29)-C(13)-C(17)-C(16) | 78.3(5) | C(20)-C(21)-C(22)-C(24) | -173.5(5) |

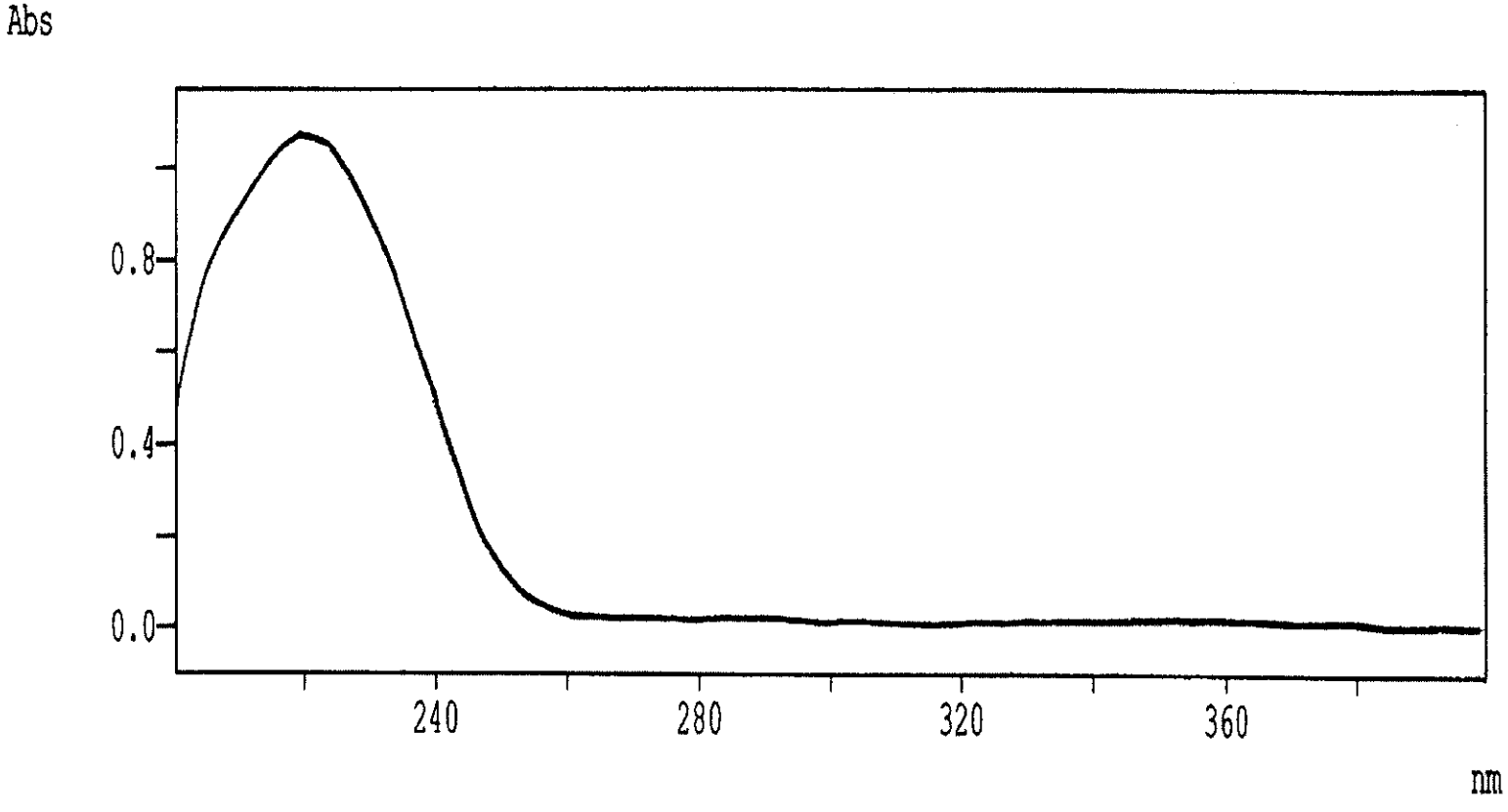


**Figure 5** UV (MeOH) spectrum of compound **XC1**

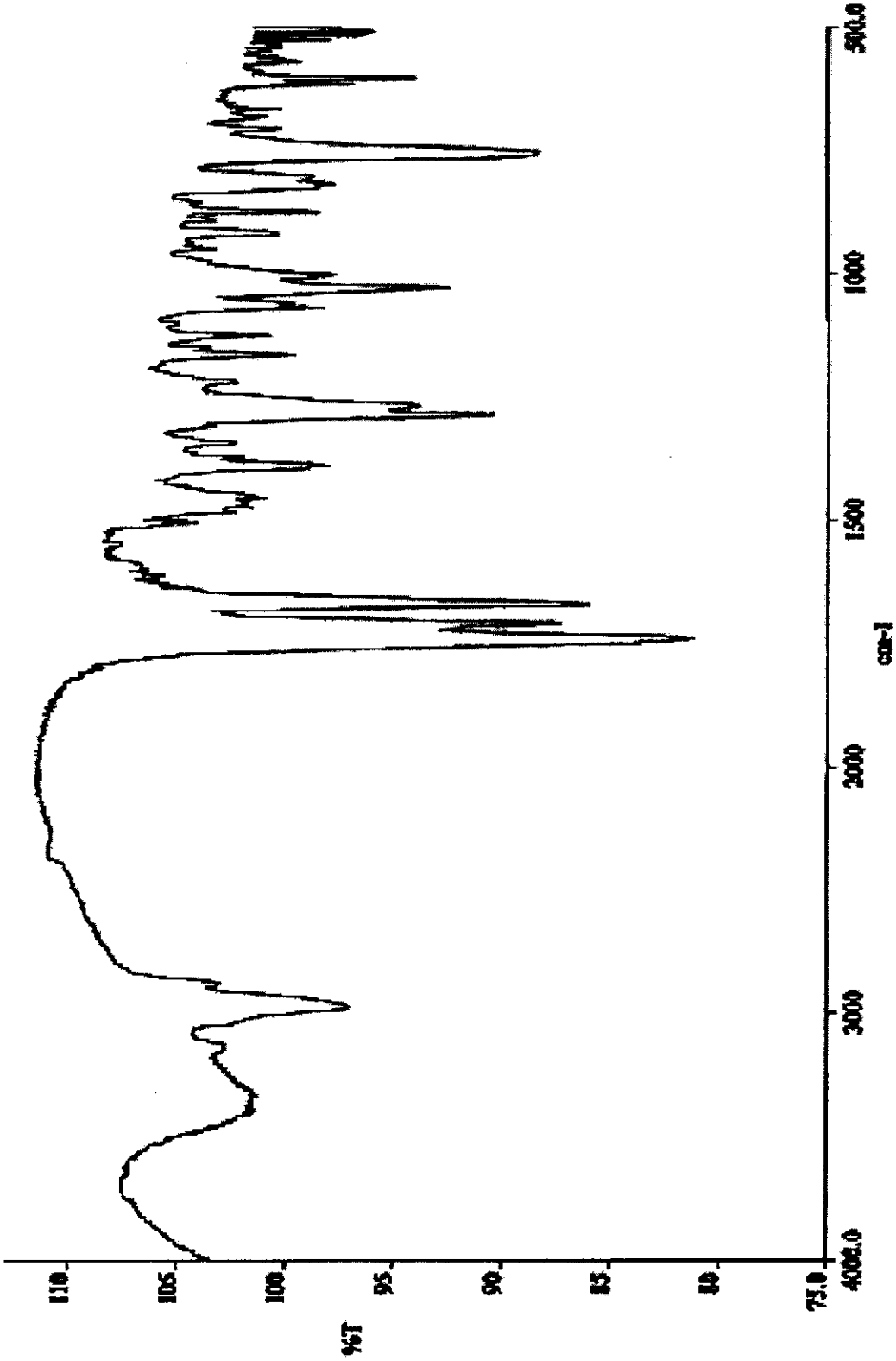


Figure 6 IR (Neat) spectrum of compound **XC1**

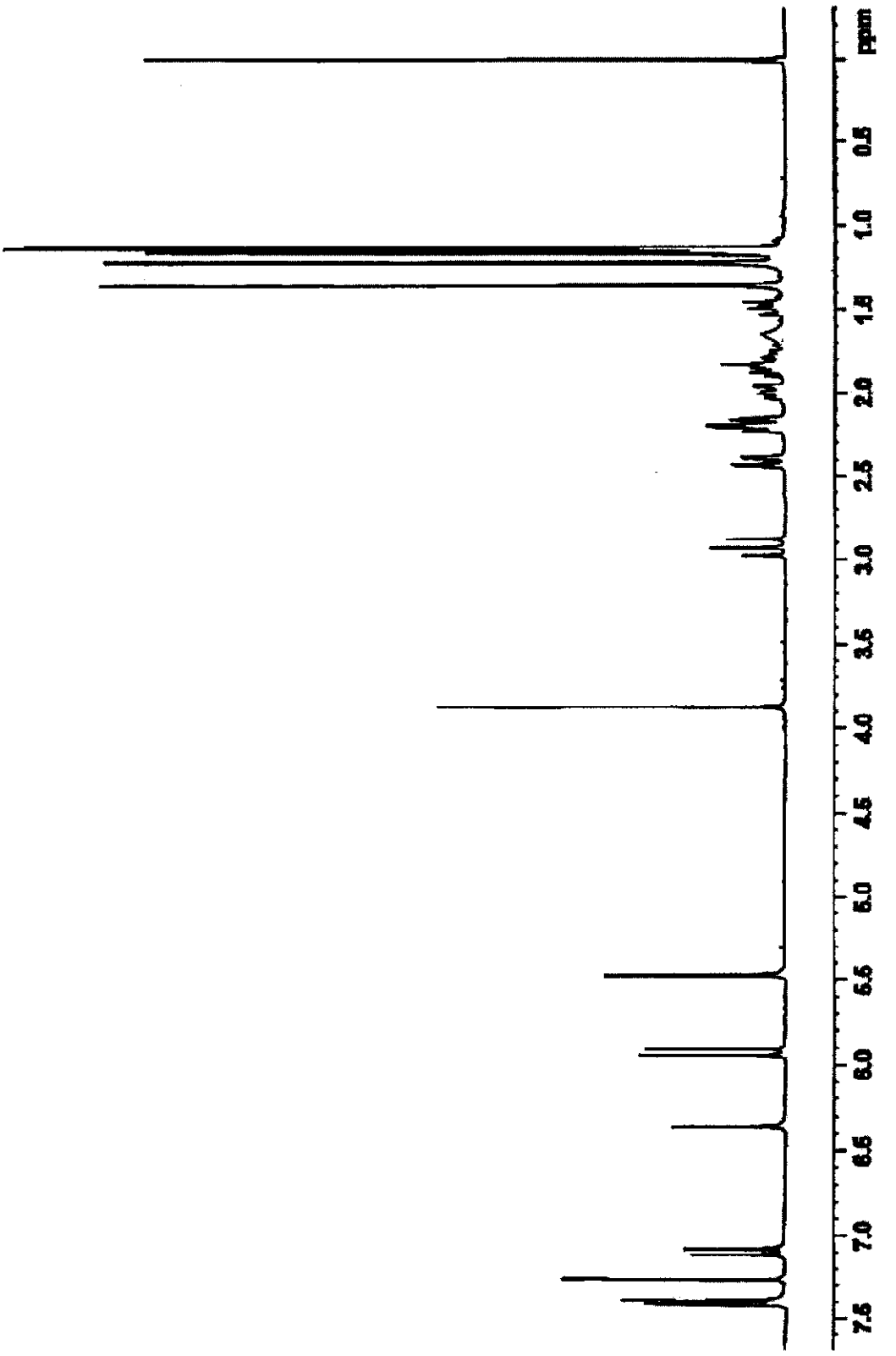


**Figure 7** $^{1}$H NMR (300 MHz, $CDCl_3$) spectrum of compound **XC1**

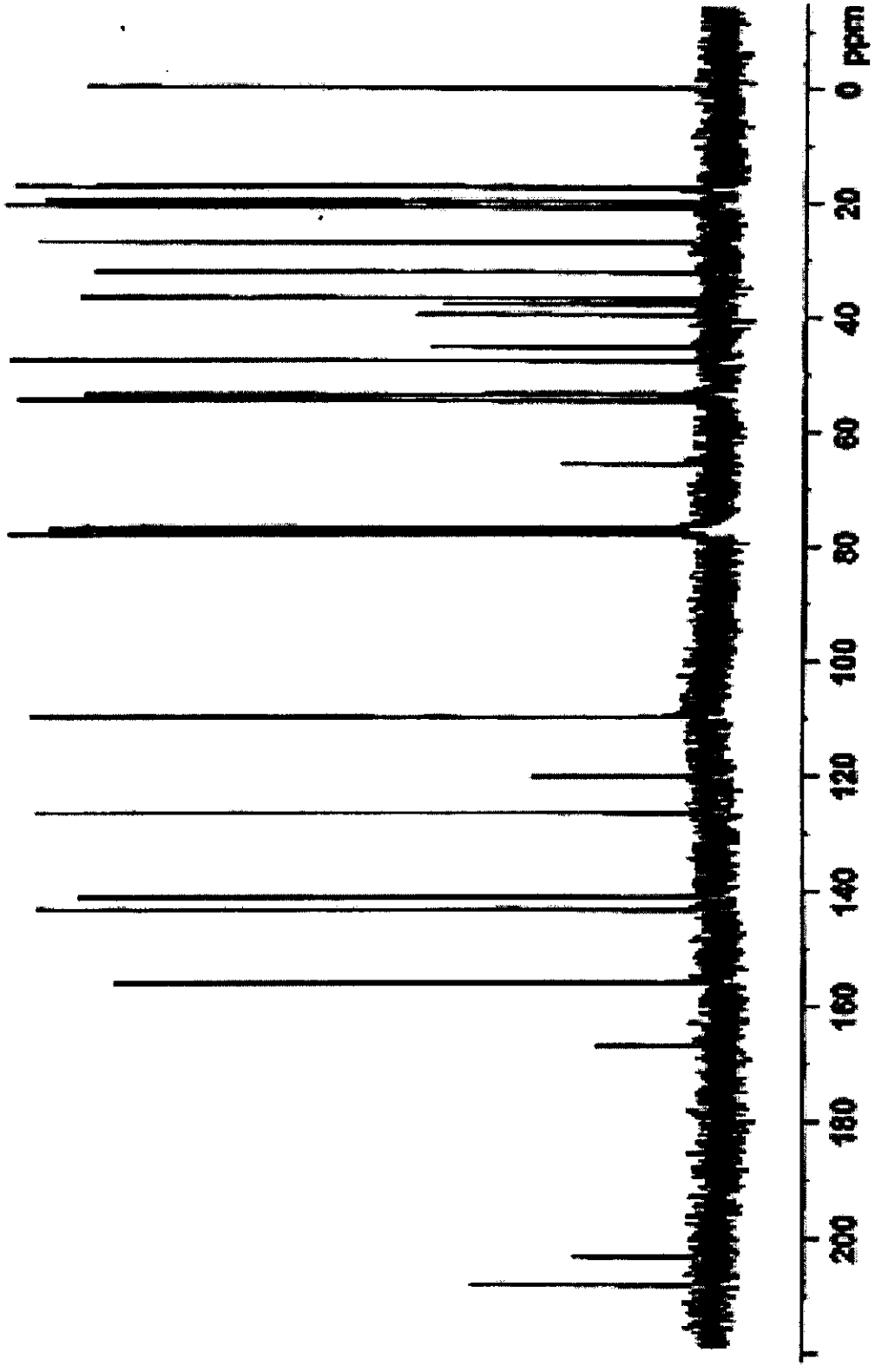


**Figure 8** $^{13}C$ NMR (75 MHz, $CDCl_3$) spectrum of compound **XC1**

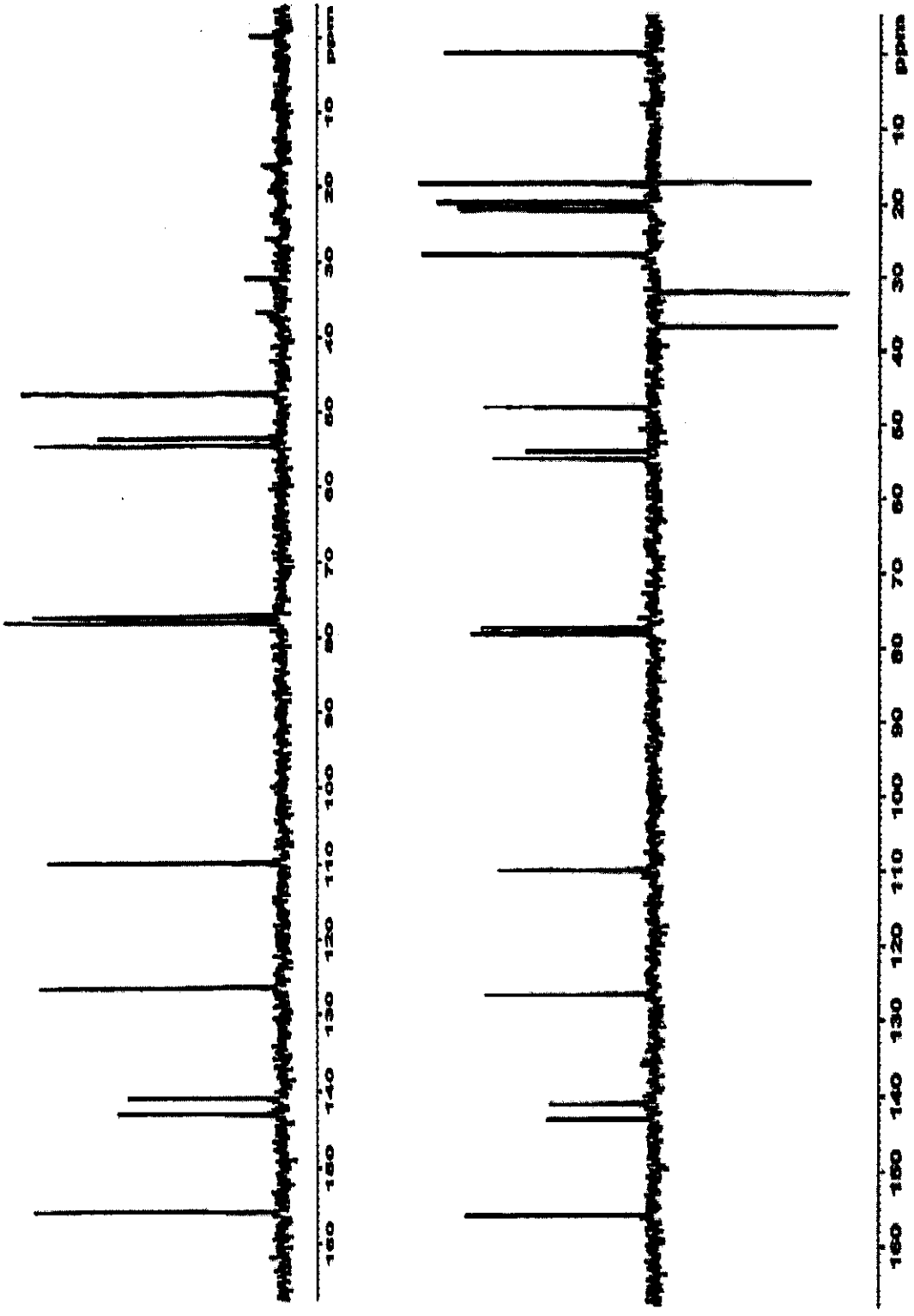


**Figure 9** DEPT ($CDCl_3$) spectrum of compound **XC1**

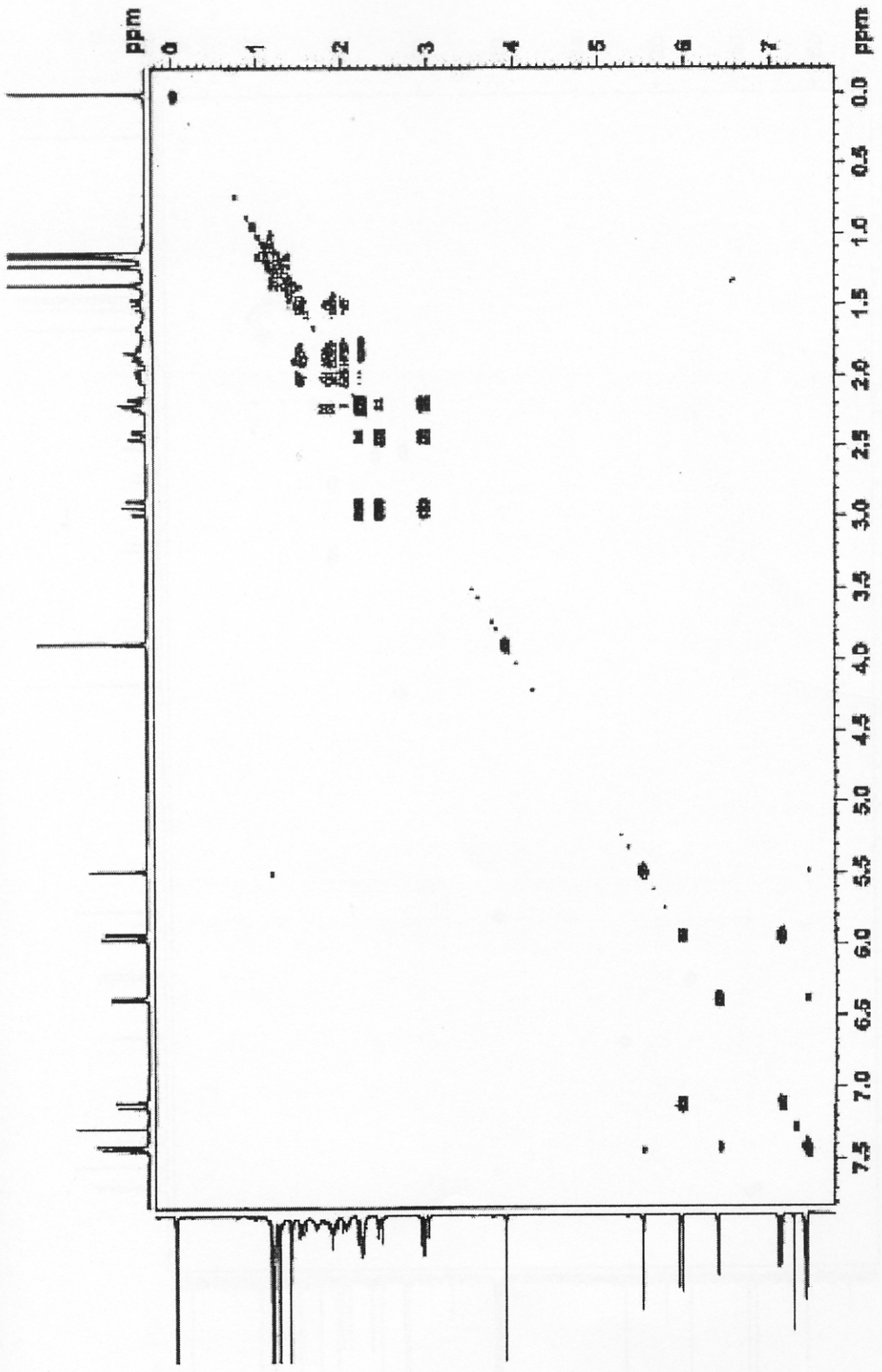


**Figure 10** 2D COSY spectrum of compound **XC1**

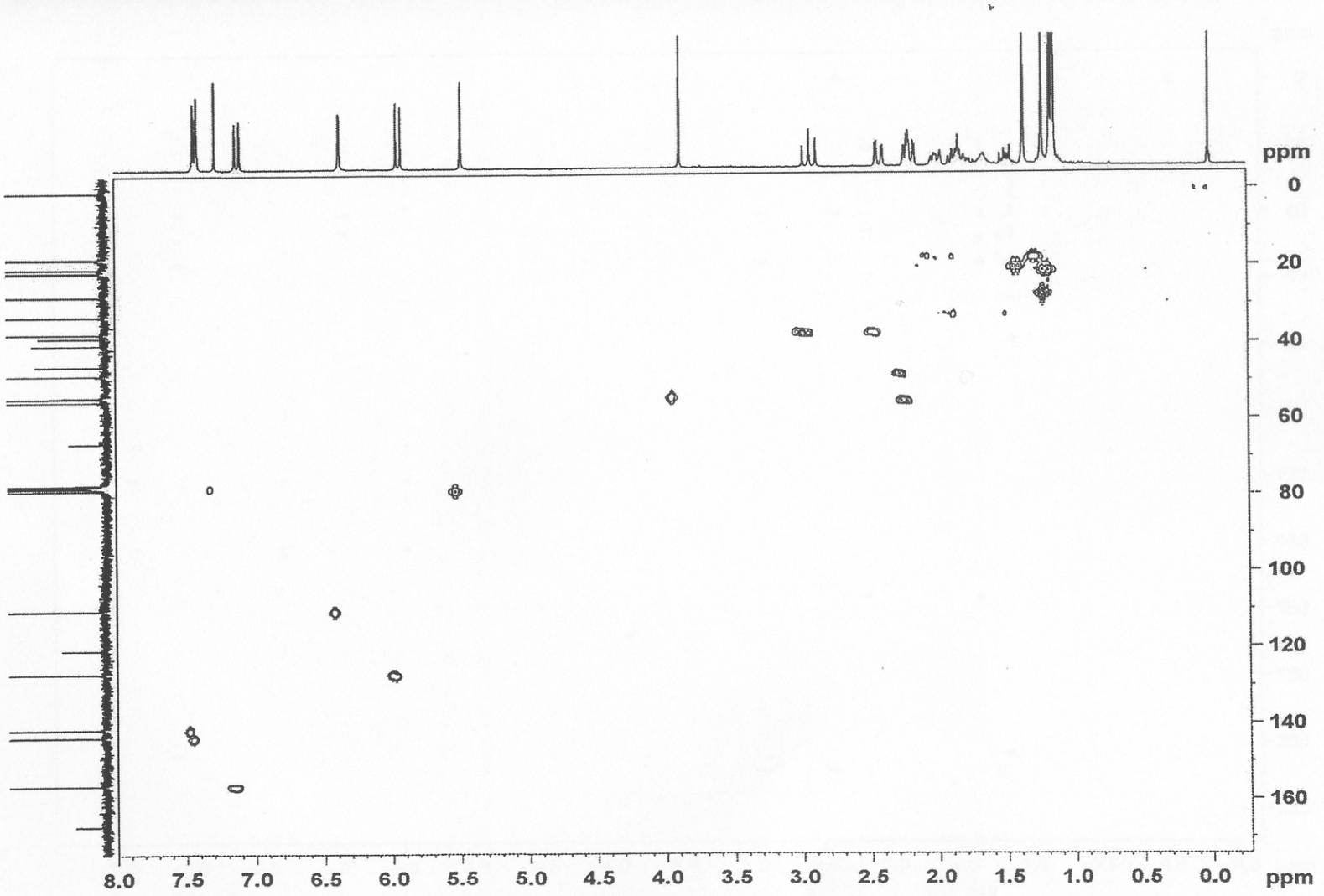


**Figure 11** 2D HMQC spectrum of compound **XC1**

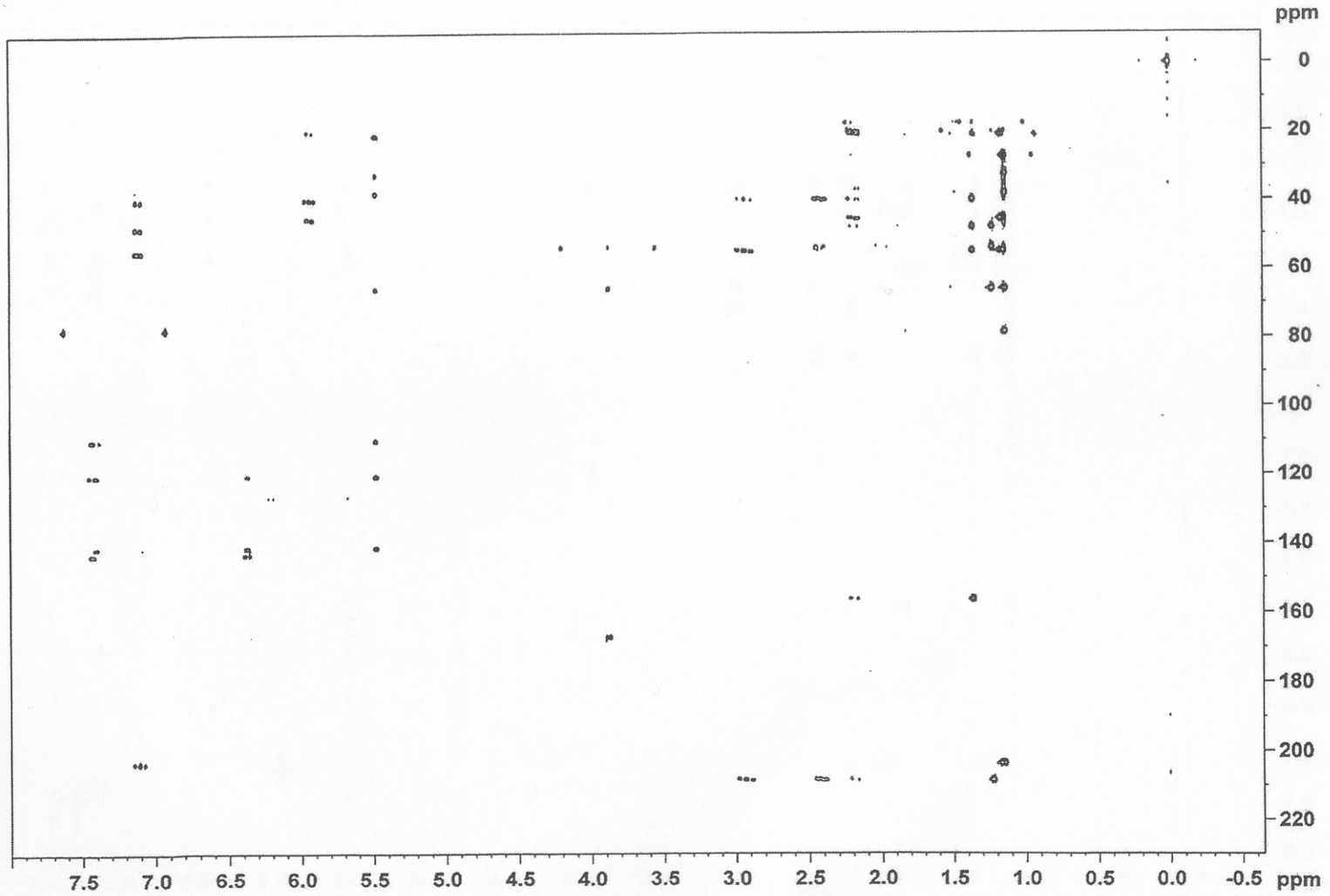


**Figure 12** 2D HMBC spectrum of compound **XC1**

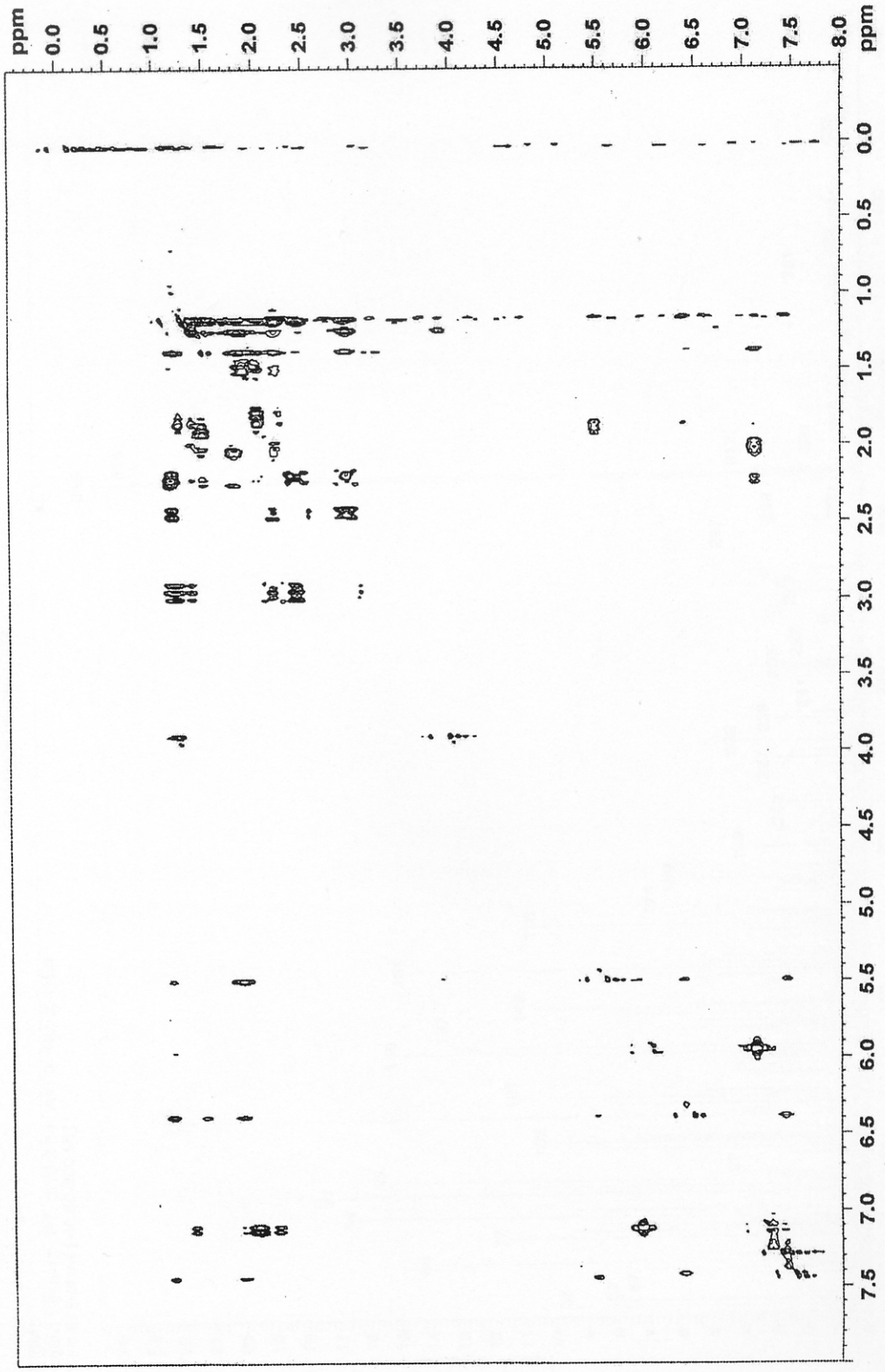


**Figure 13** NOESY spectrum of compound **XC1**

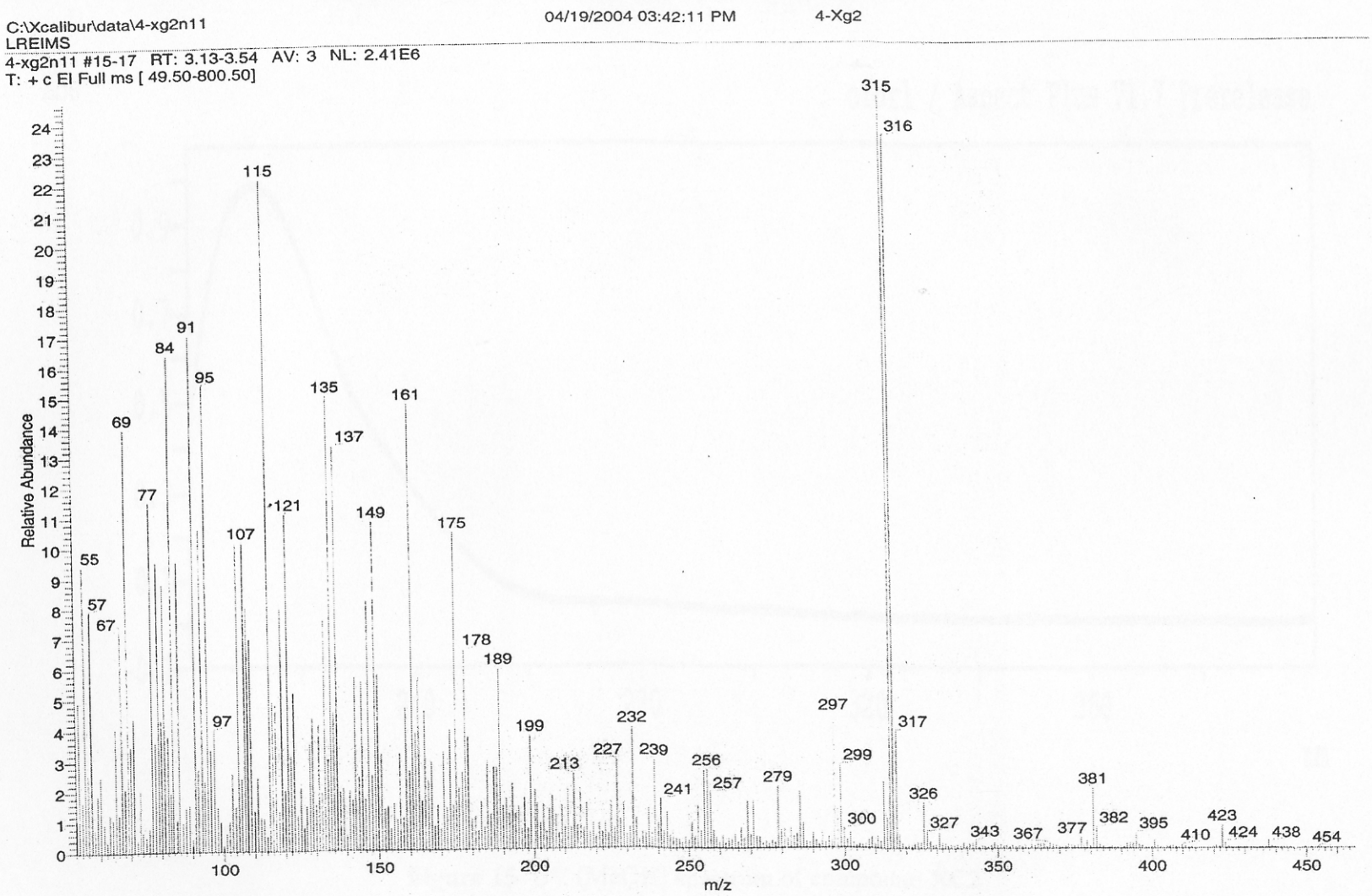


**Figure 14** Mass spectrum of compound **XC1**

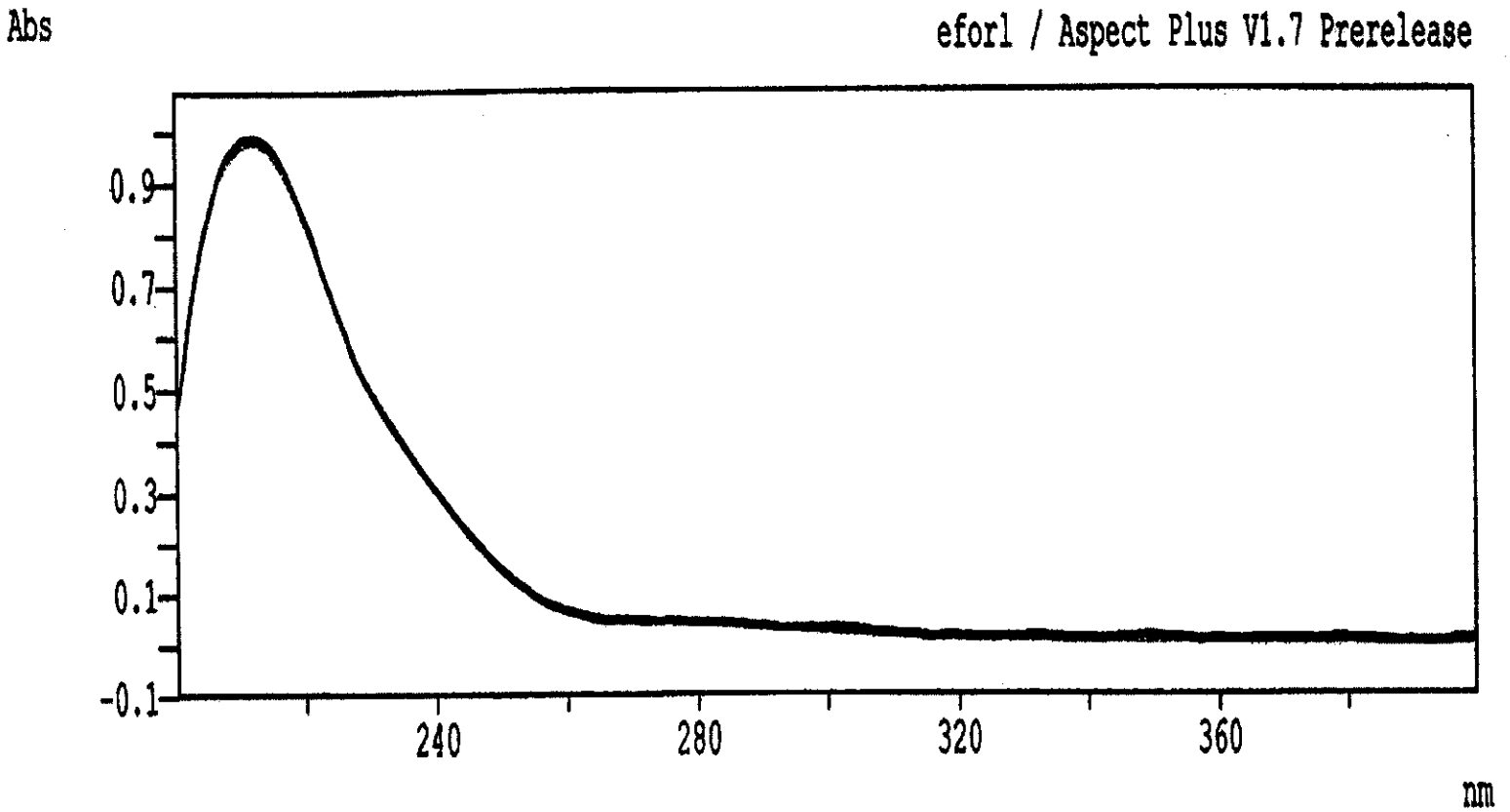


**Figure 15** UV (MeOH) spectrum of compound **XC2**

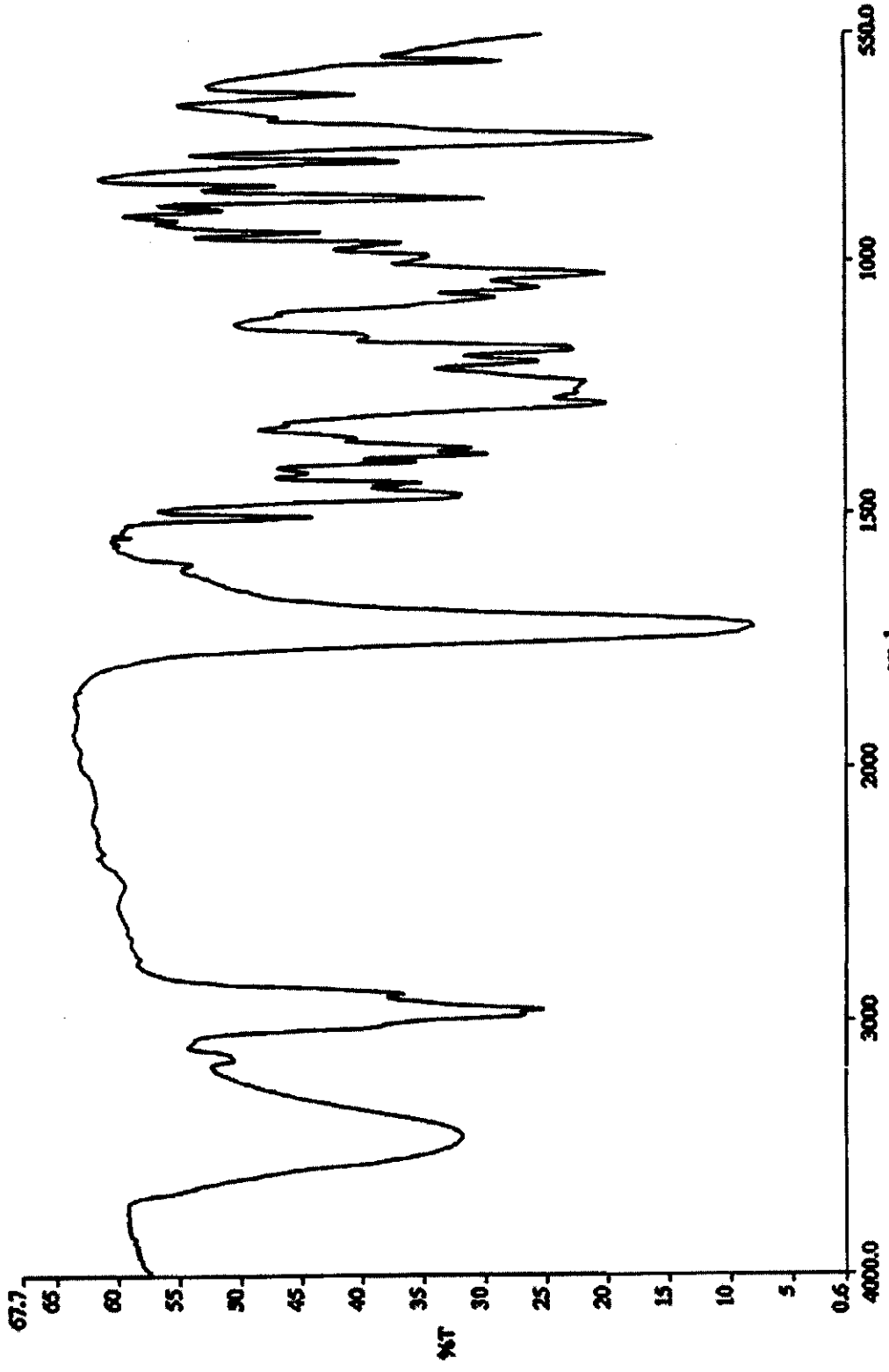


**Figure 16** IR (Neat) spectrum of compound **XC2**

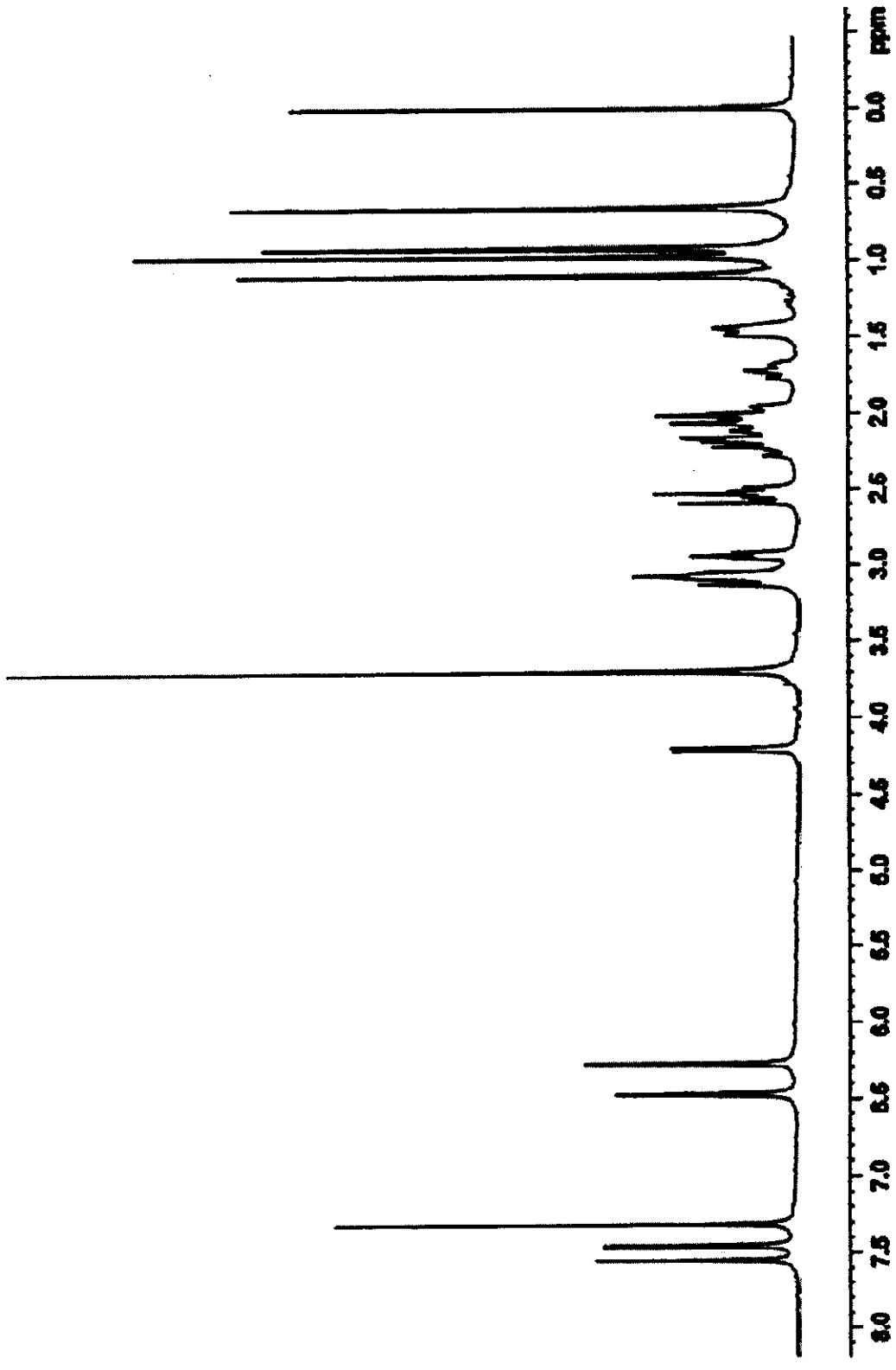


**Figure 17** $^{1}$H NMR (300 MHz, $CDCl_3$) spectrum of compound **XC2**

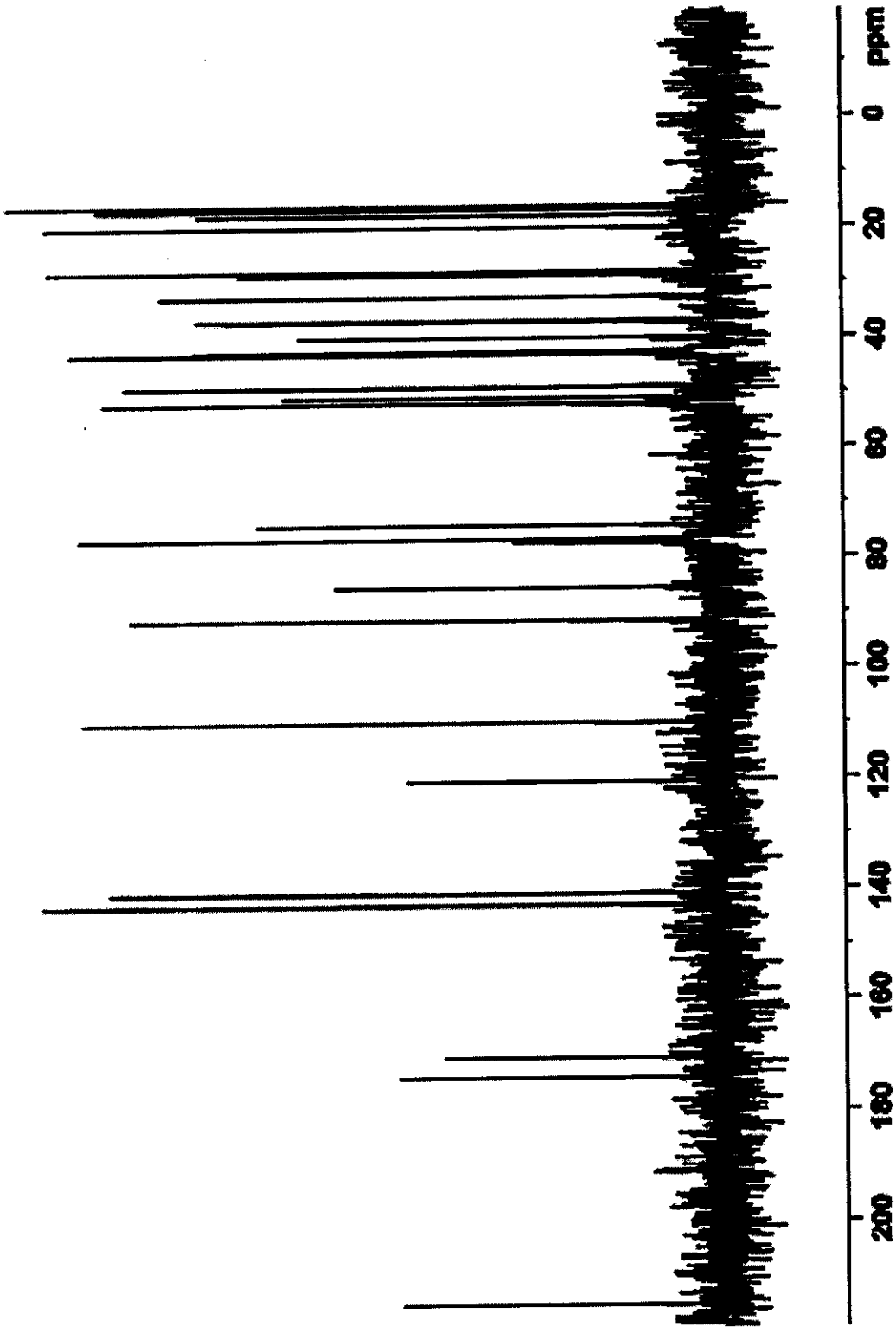


**Figure 18** $^{13}C$ NMR (75 MHz, $CDCl_3$) spectrum of compound **XC2**

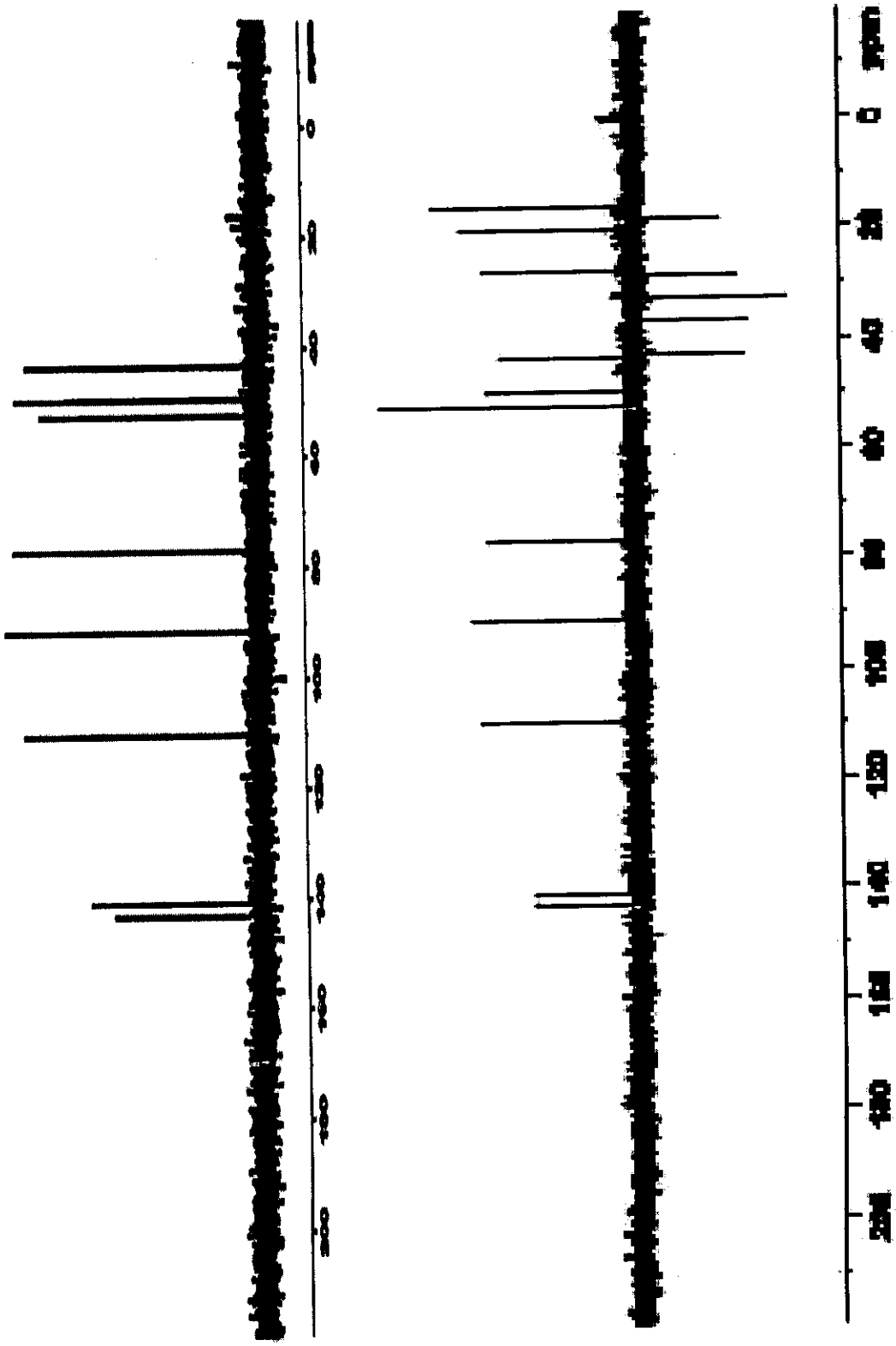

**Figure 19** DEPT ($CDCl_3$) spectrum of compound **XC2**

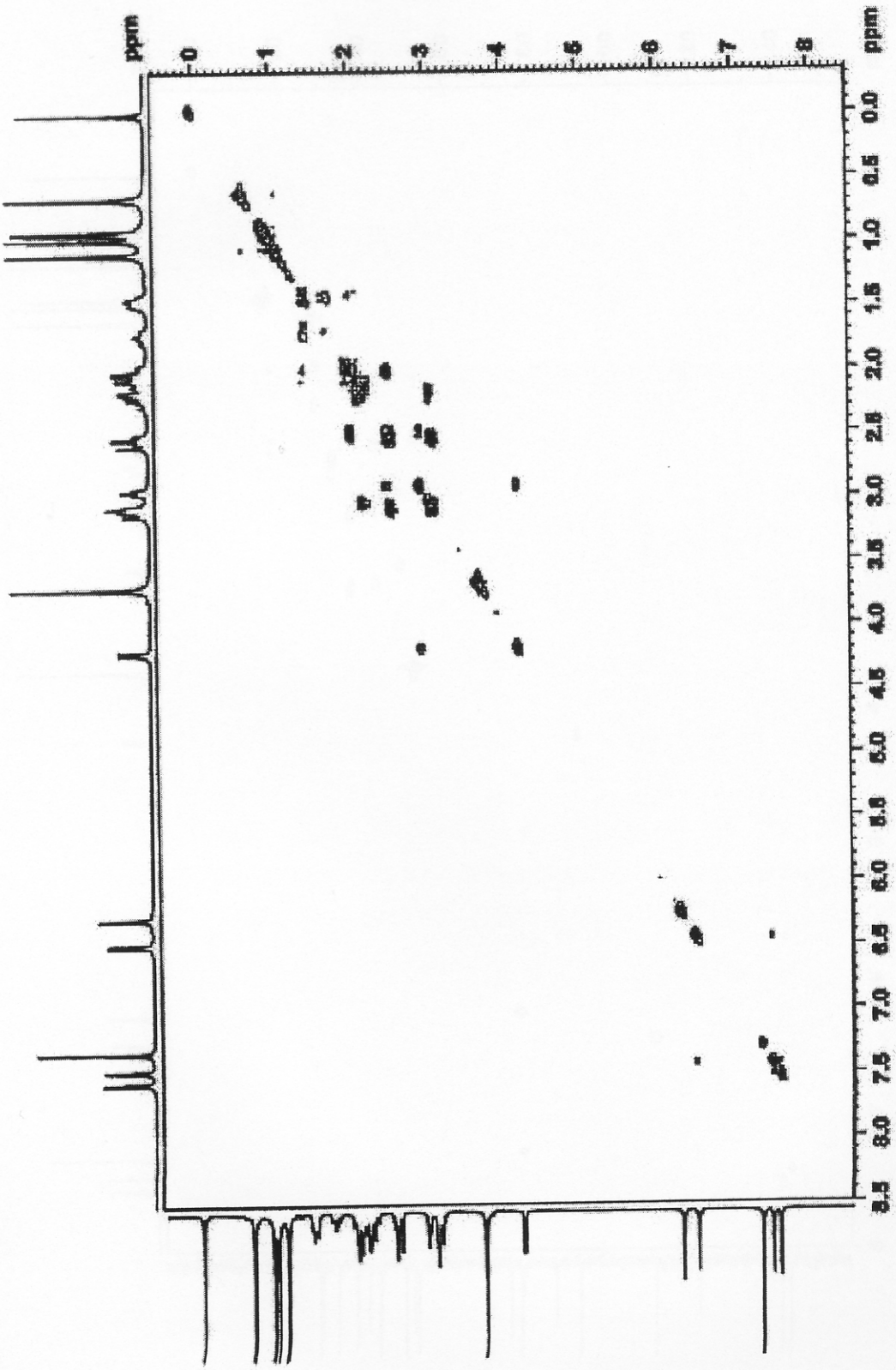


Figure 20 2D COSY spectrum of compound XC2

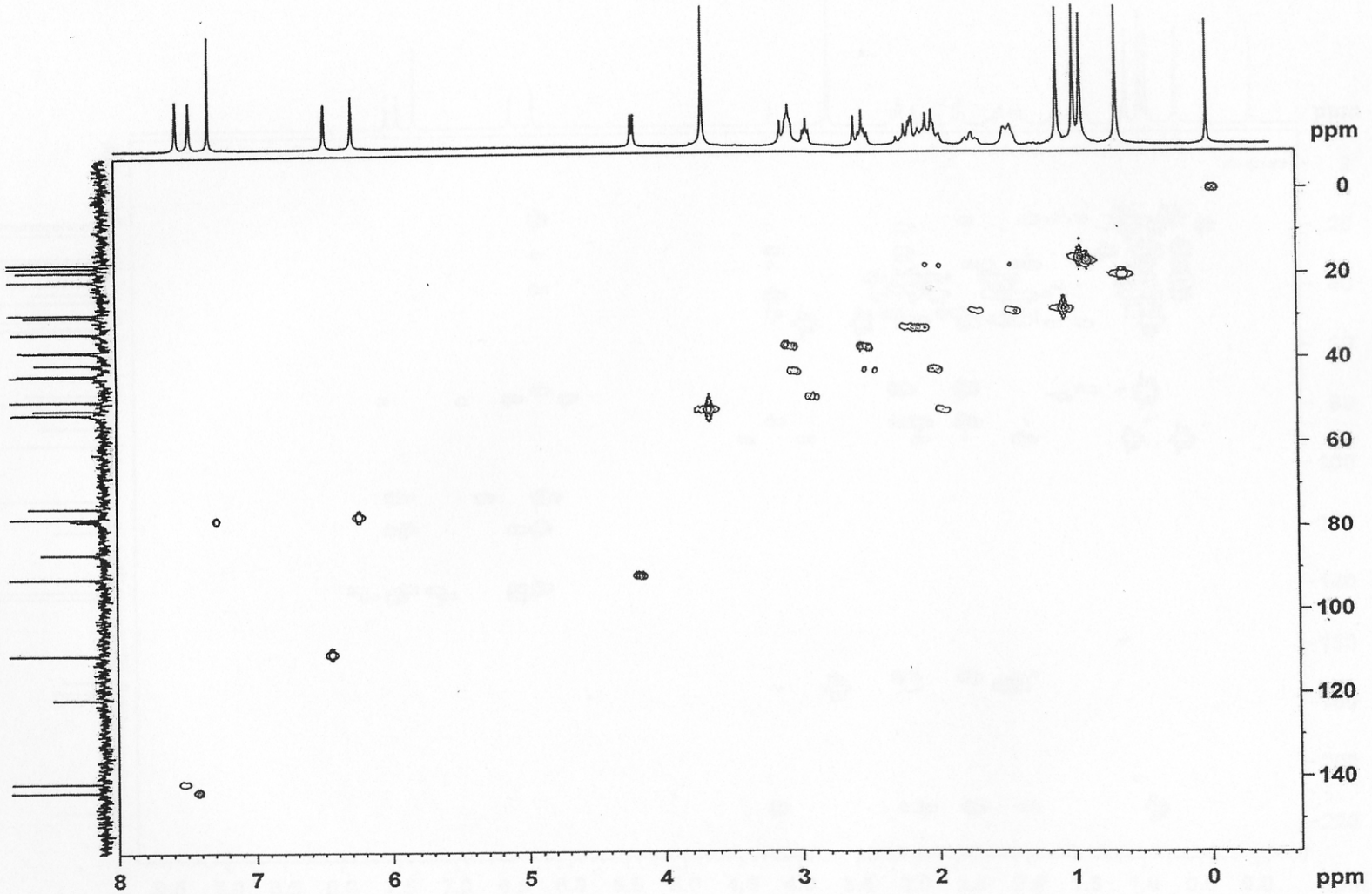


**Figure 21** 2D HMQC spectrum of compound **XC2**

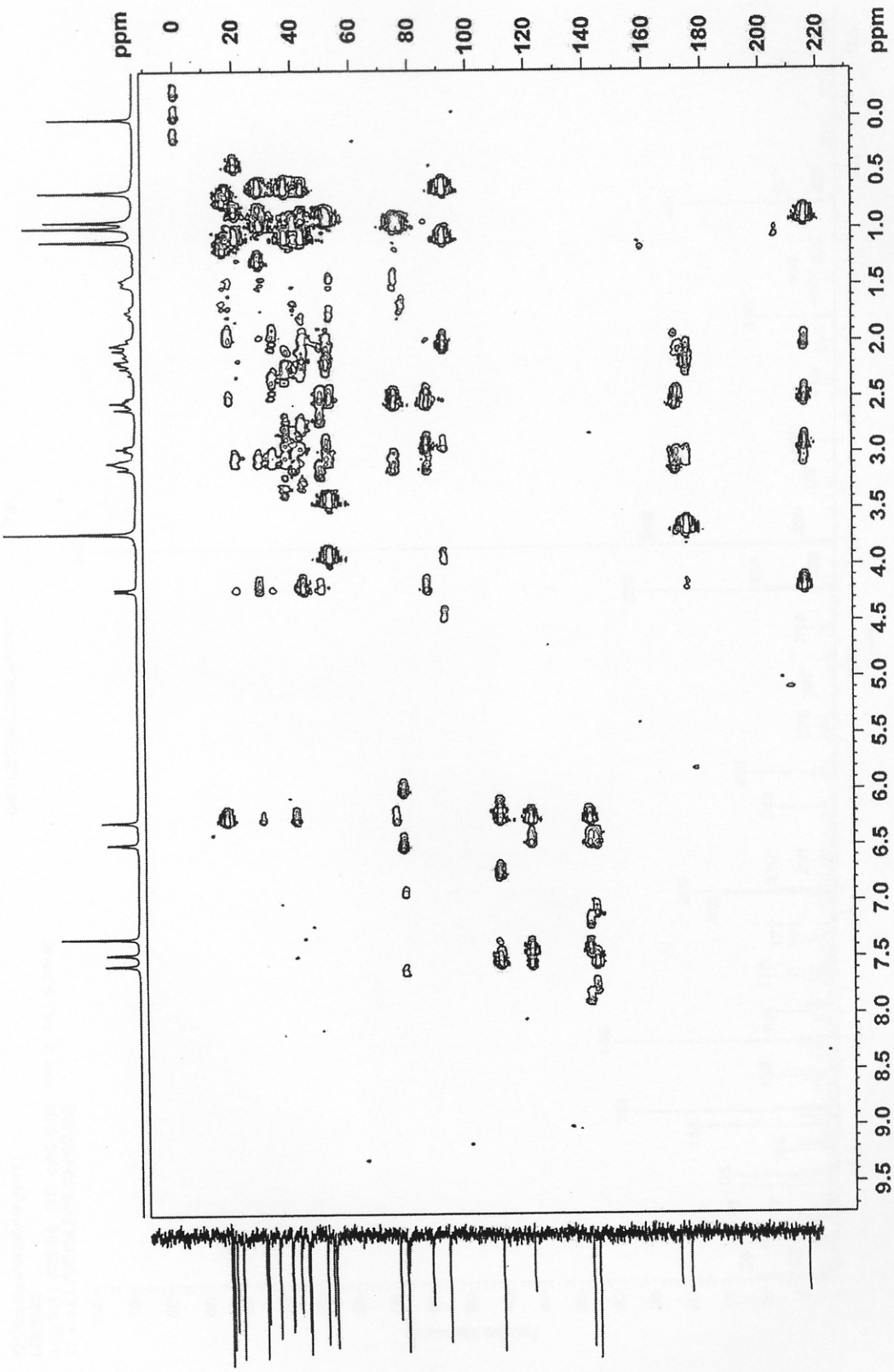


**Figure 22** 2D HMBC spectrum of compound **XC2**

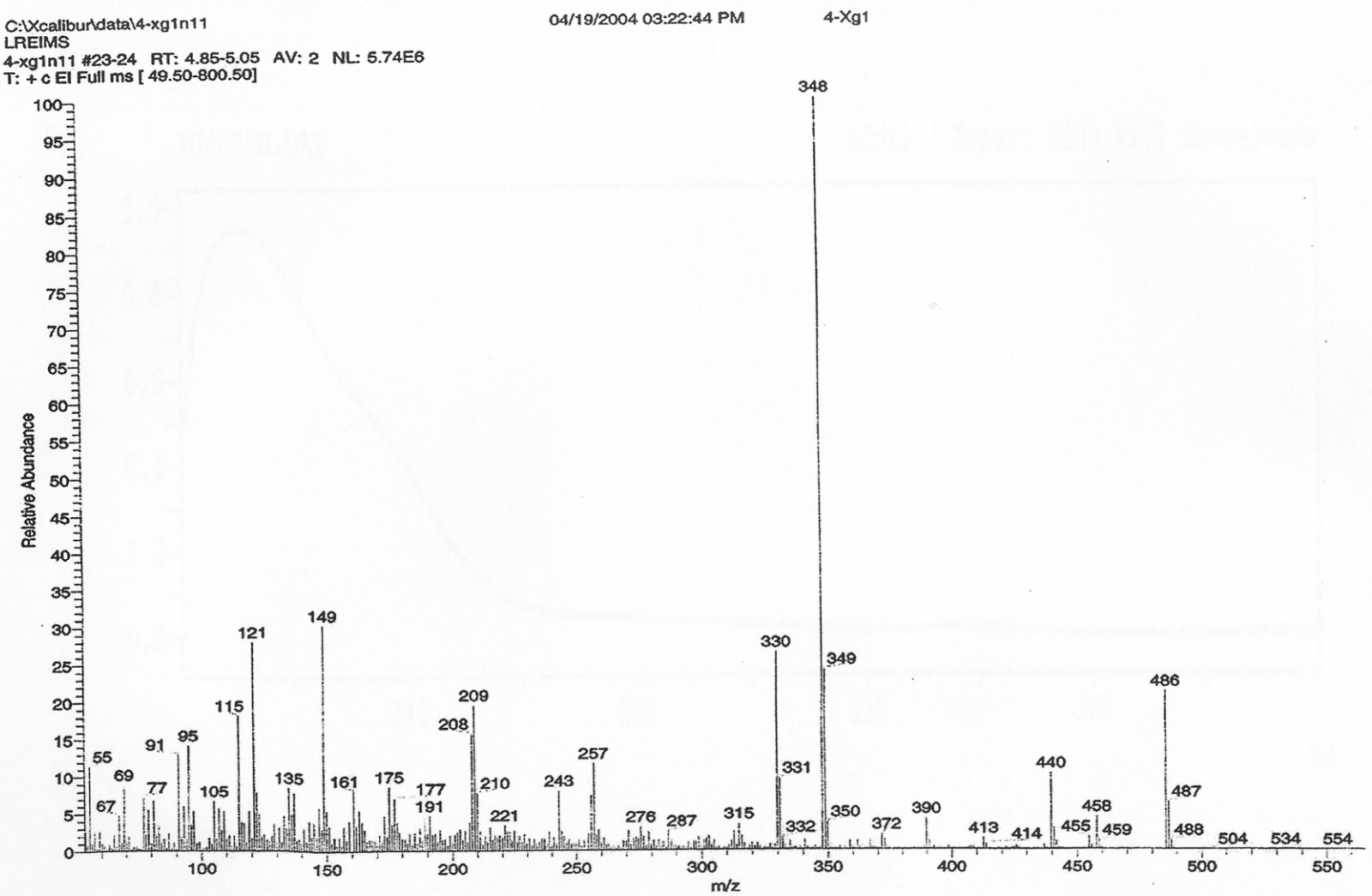


**Figure 23** Mass spectrum of compound **XC2**

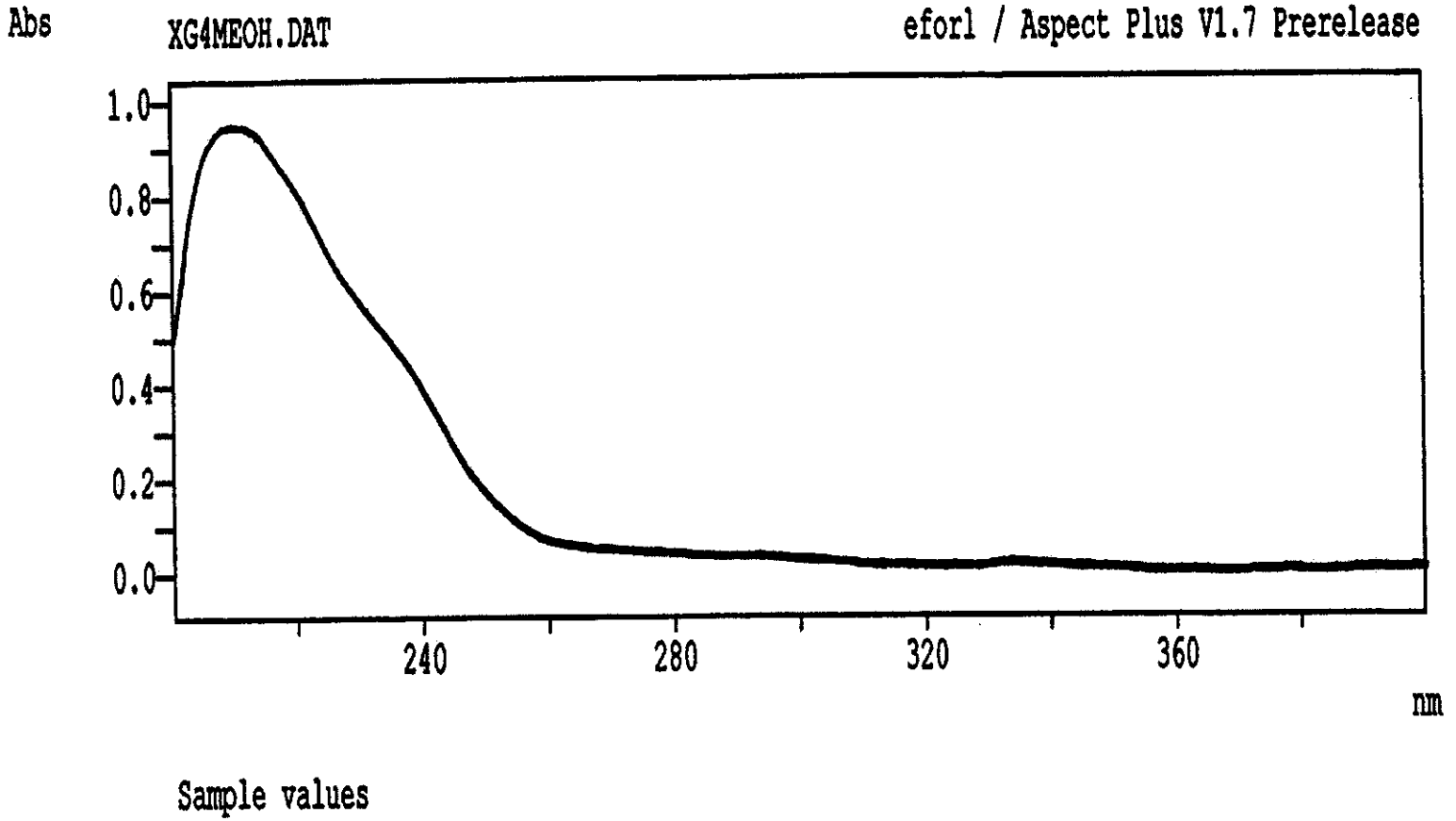


**Figure 24** UV (MeOH) spectrum of compound **XC3**

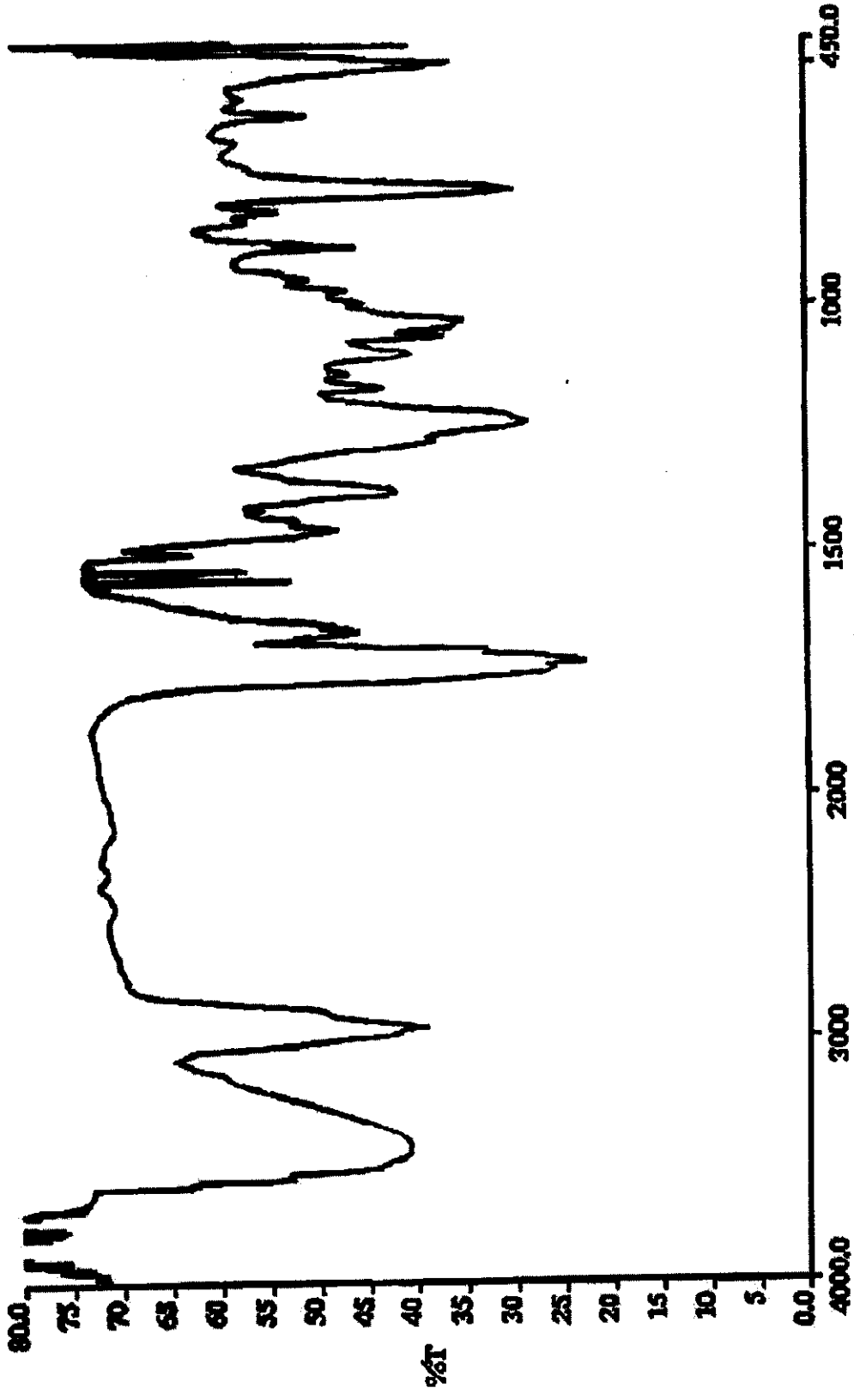


**Figure 25** IR (Neat) spectrum of compound **XC3**

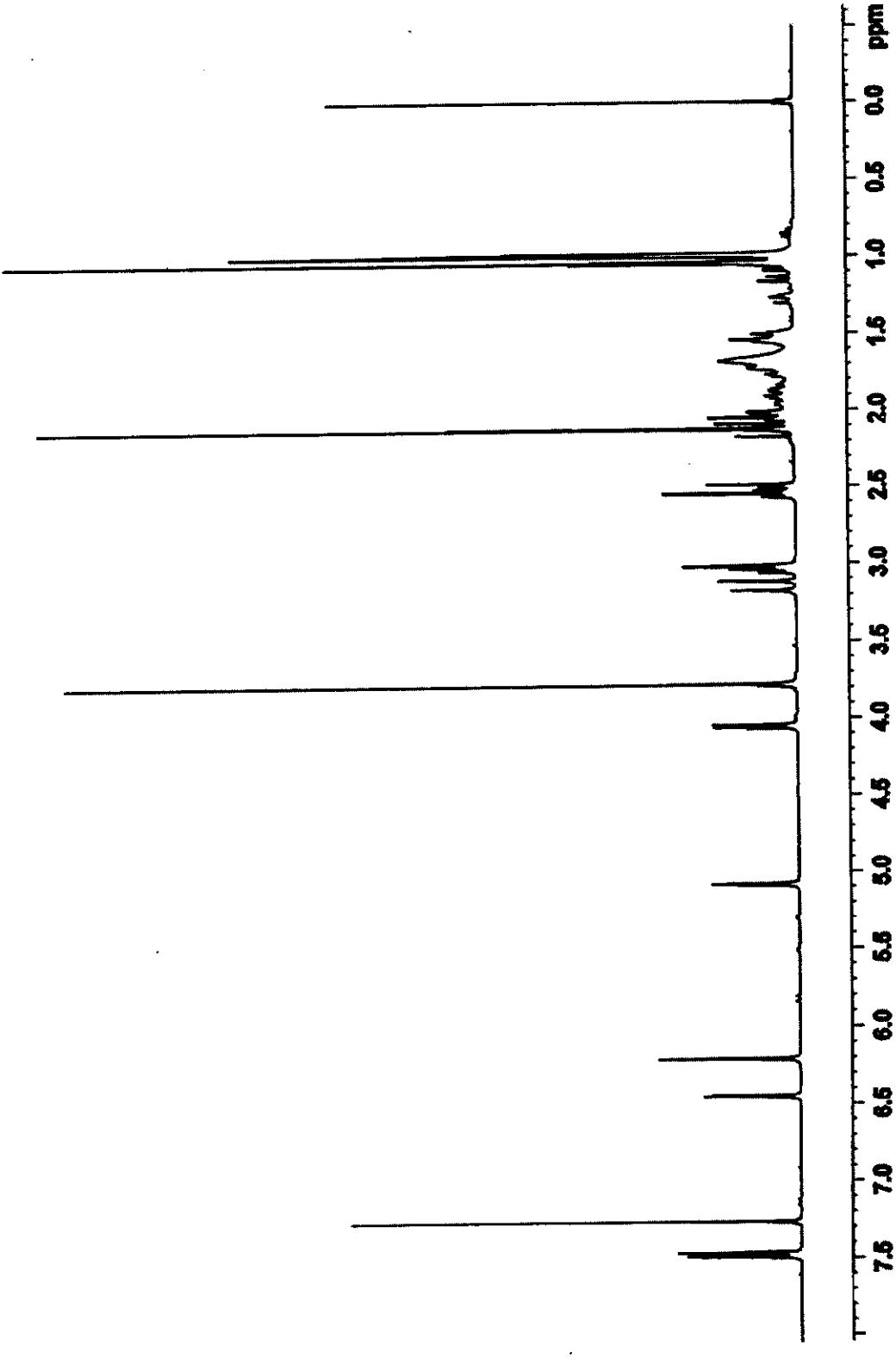


**Figure 26** $^{1}$H NMR (300 MHz, $CDCl_3$) spectrum of compound **XC3**

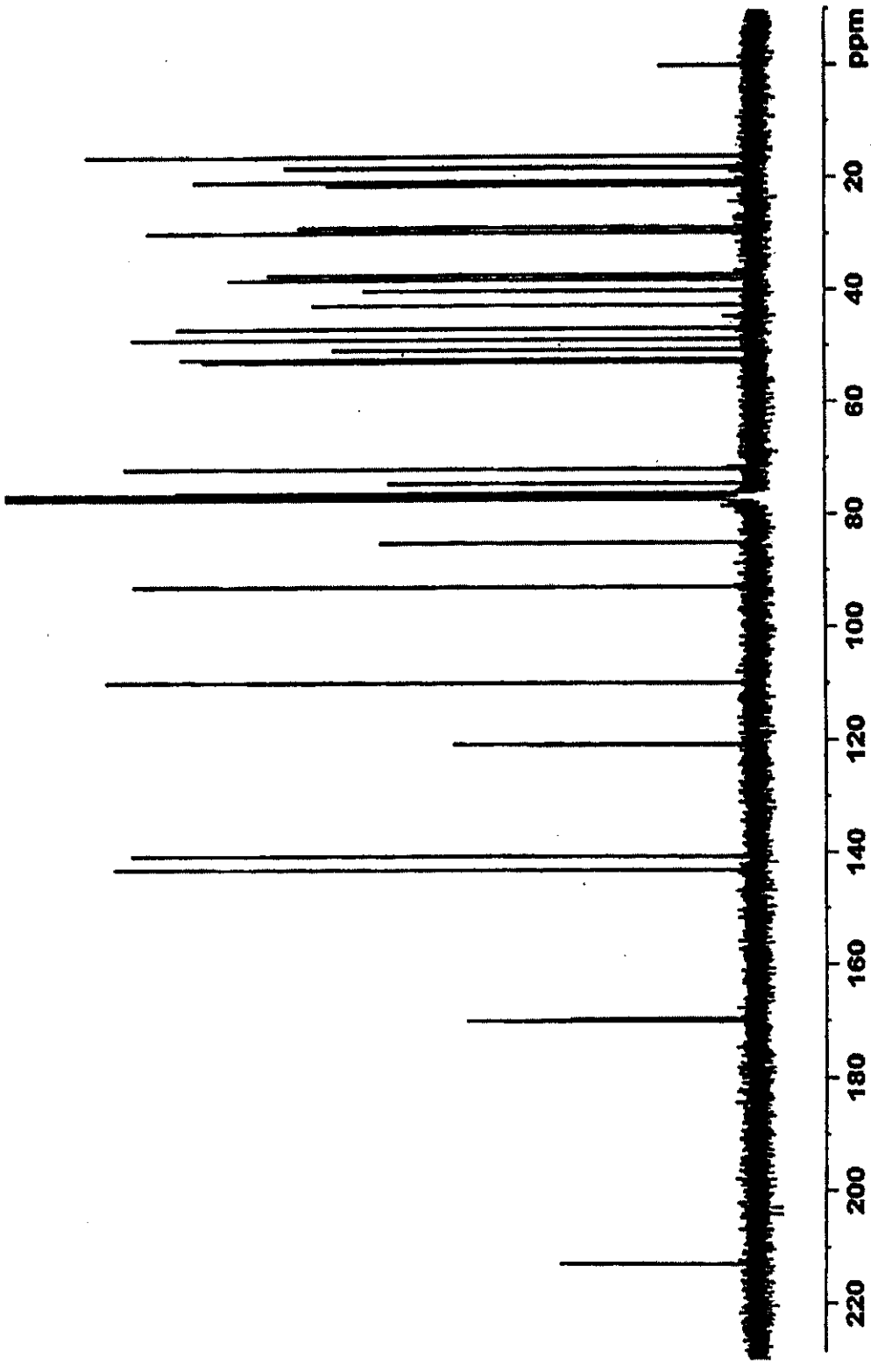


**Figure 27** $^{13}C$ NMR (75 MHz, $CDCl_3$) spectrum of compound **XC3**

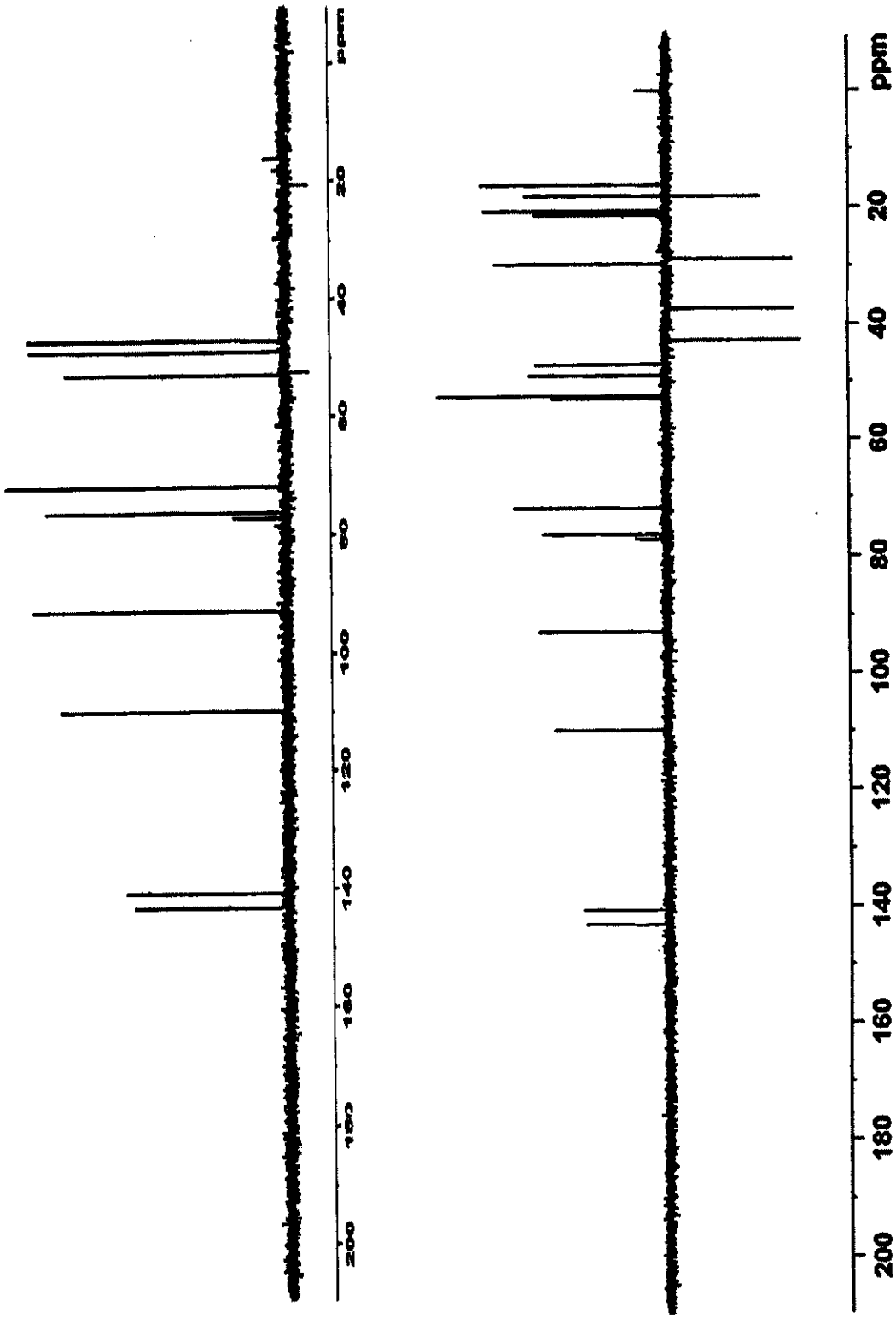


**Figure 28** DEPT ($CDCl_3$) spectrum of compound **XC3**

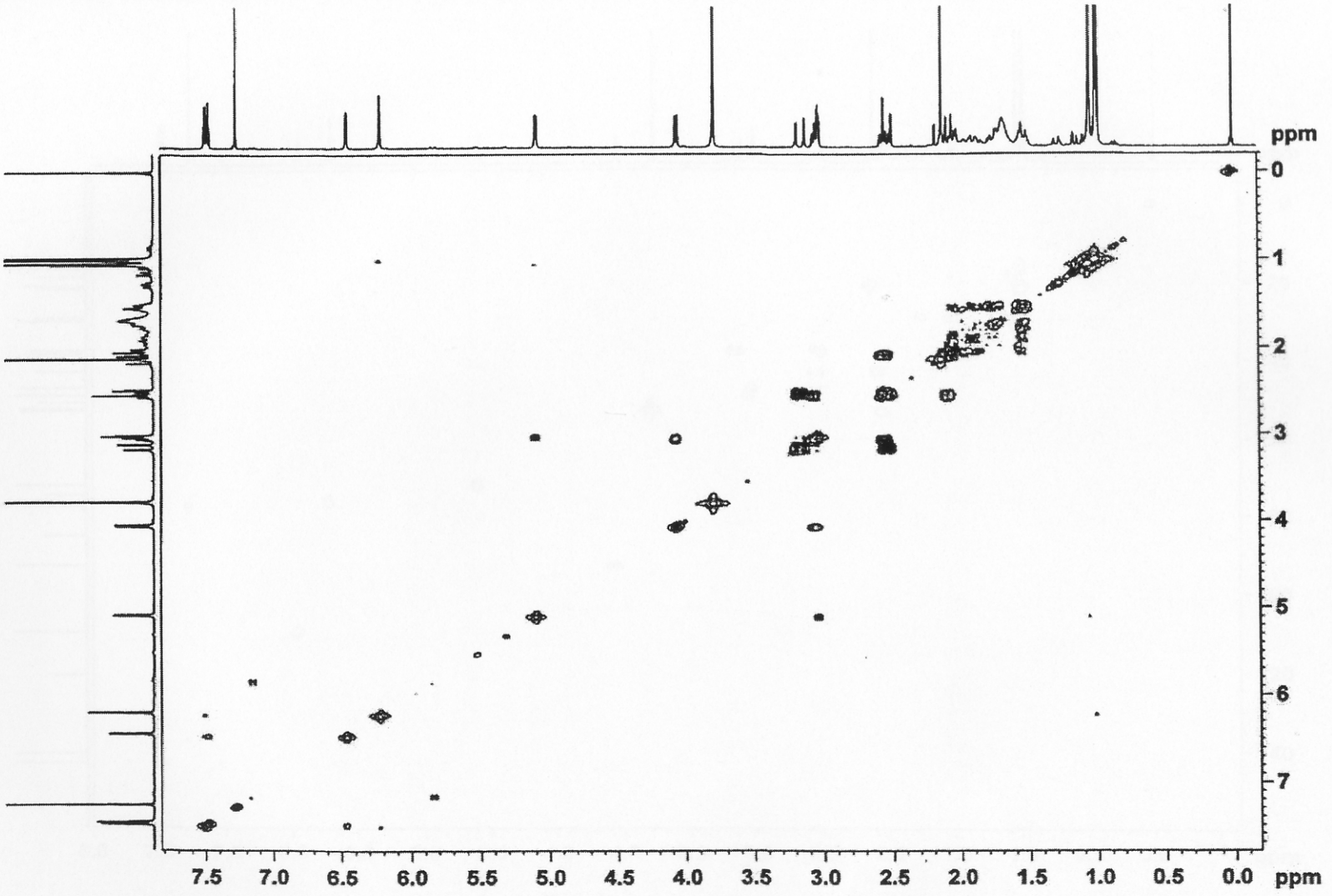


**Figure 29** 2D COSY spectrum of compound **XC3**

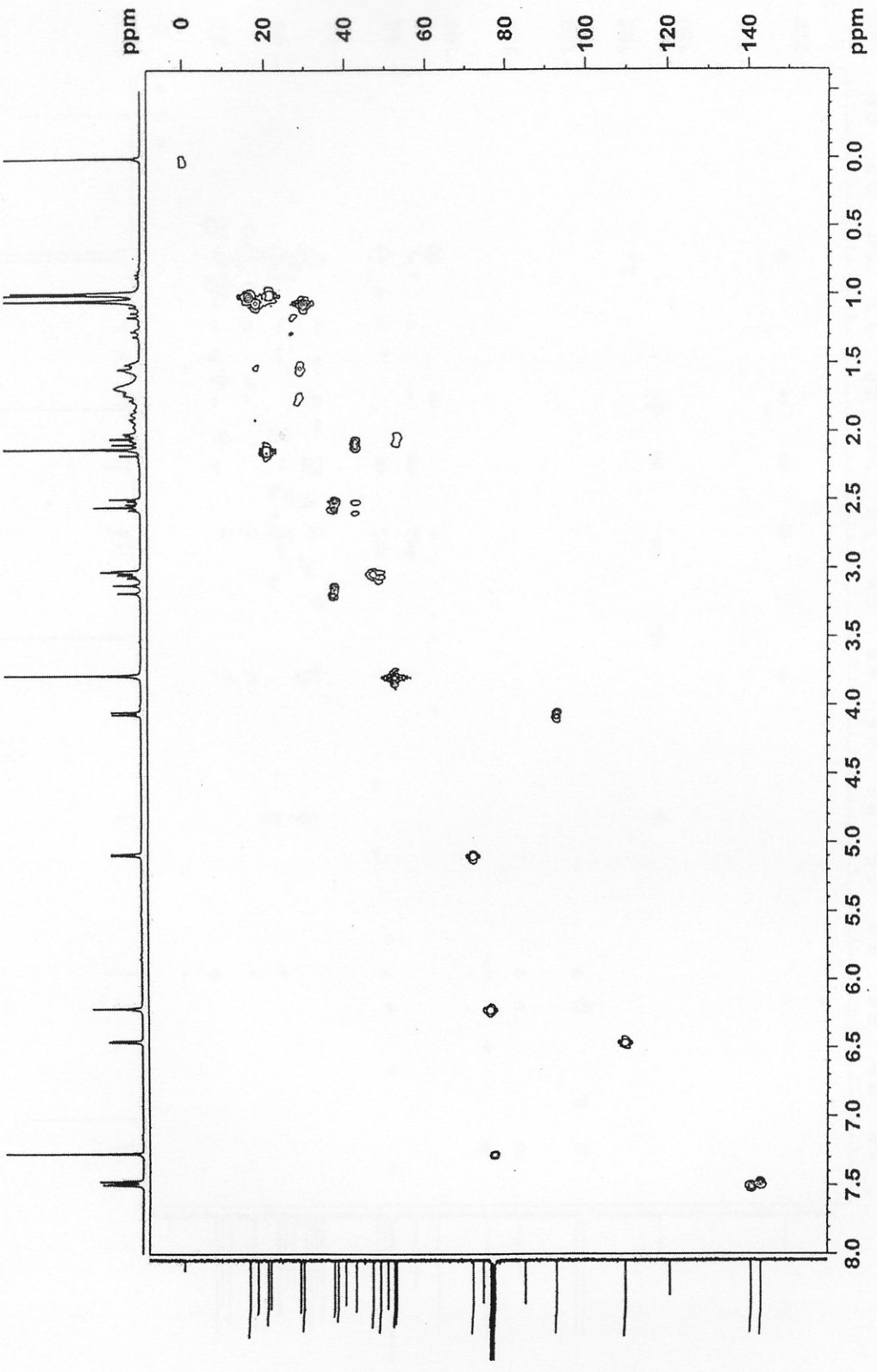


**Figure 30** 2D HMQC spectrum of compound **XC3**

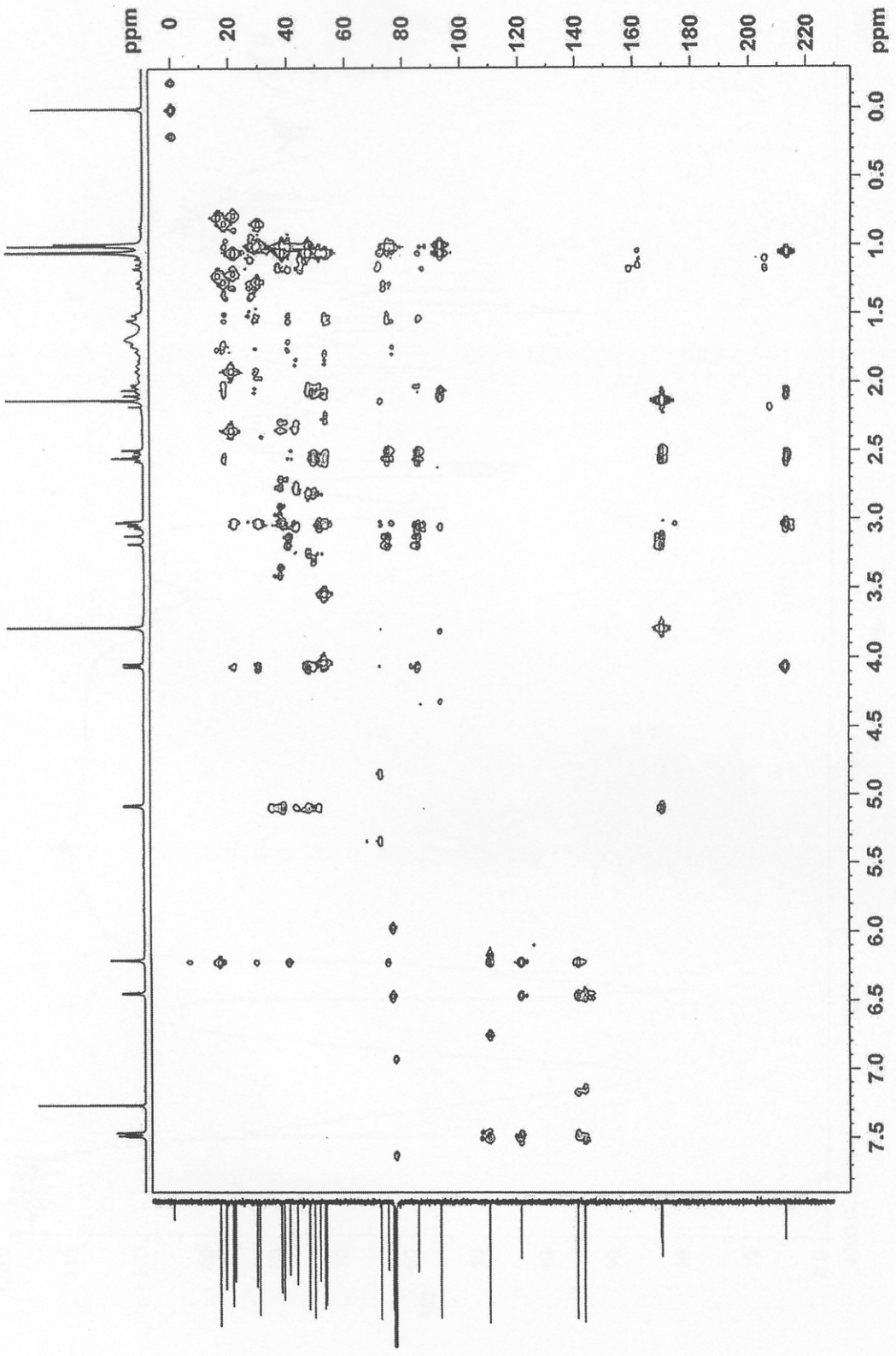


**Figure 31** 2D HMBC spectrum of compound **XC3**

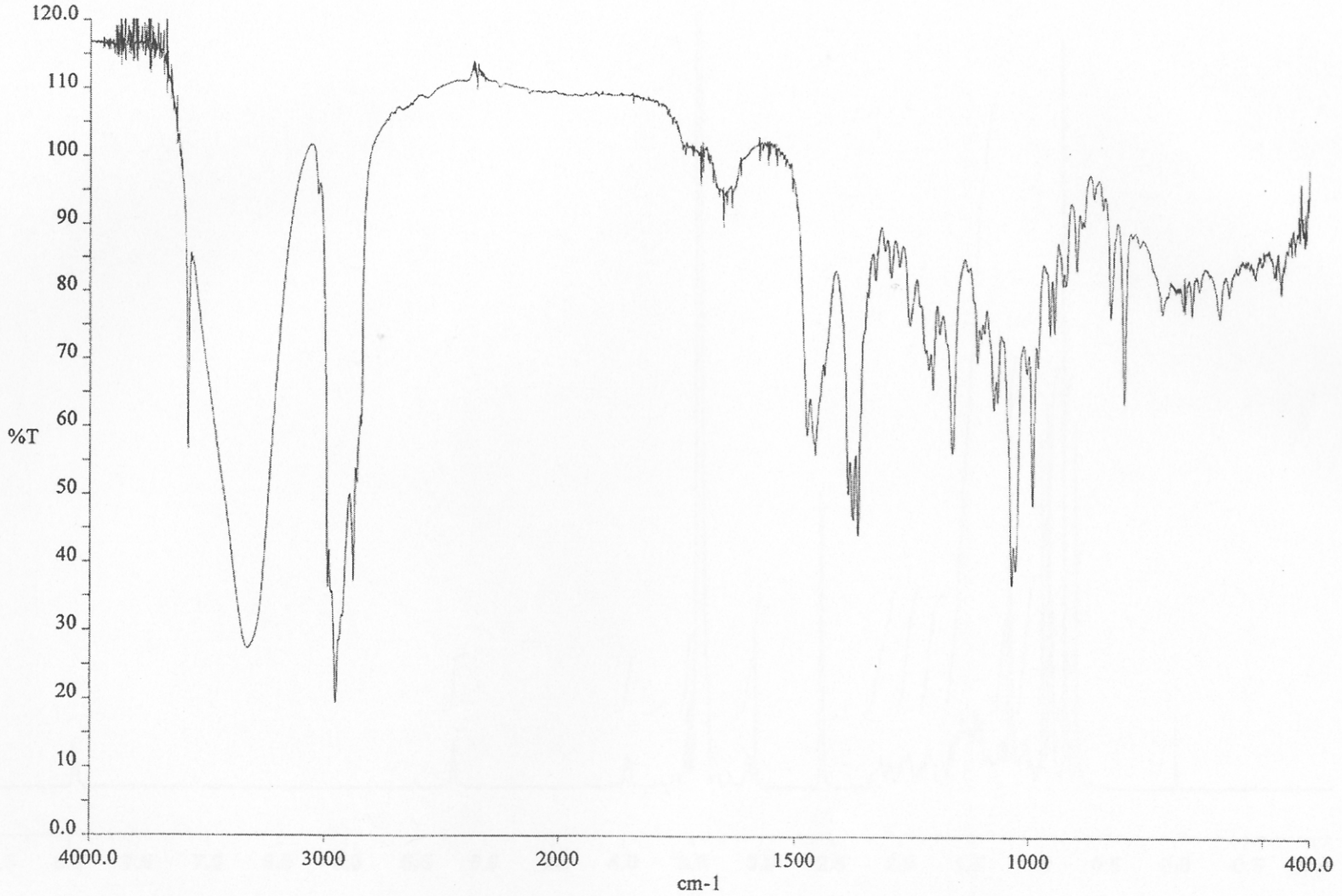


**Figure 32** IR (KBr) spectrum of compound **XC4**

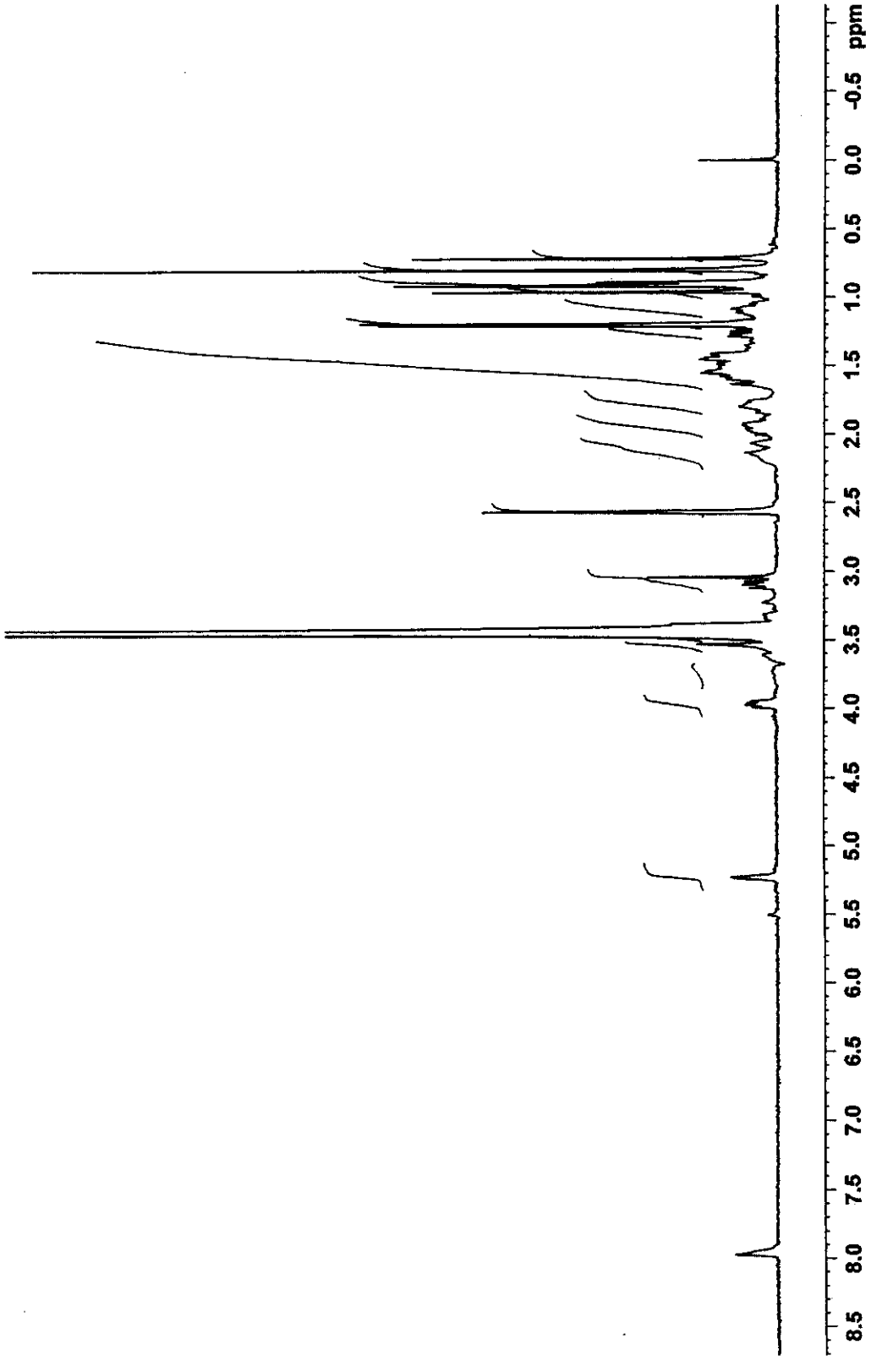


**Figure 33** $^{1}$H NMR (300 MHz, DMSO- $d_6$ and $CDCl_3$) spectrum of compound **XC4**

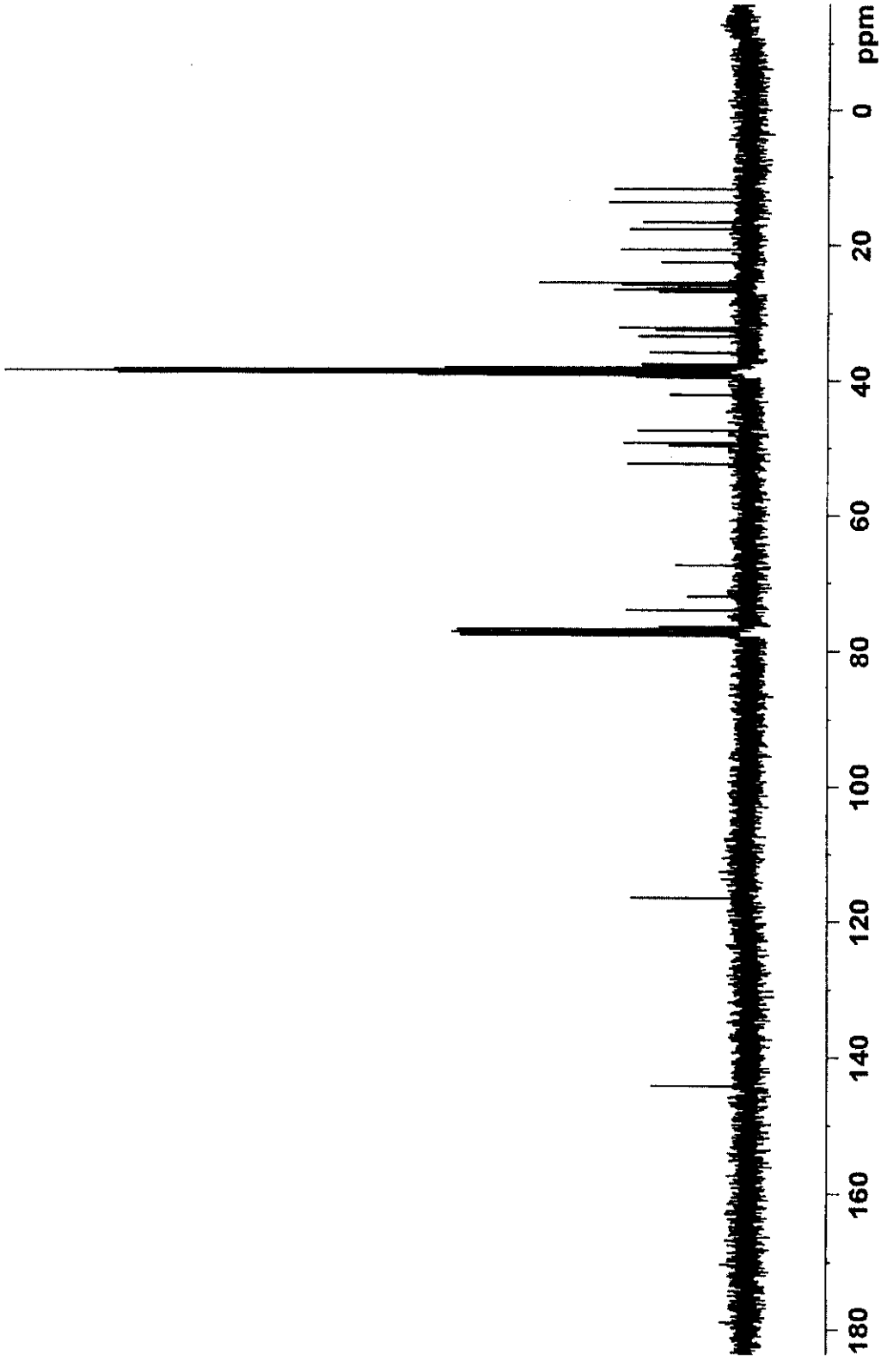


**Figure 34** $^{13}C$ NMR (75 MHz, DMSO- $d_6$ and $CDCl_3$) spectrum of compound **XC4**

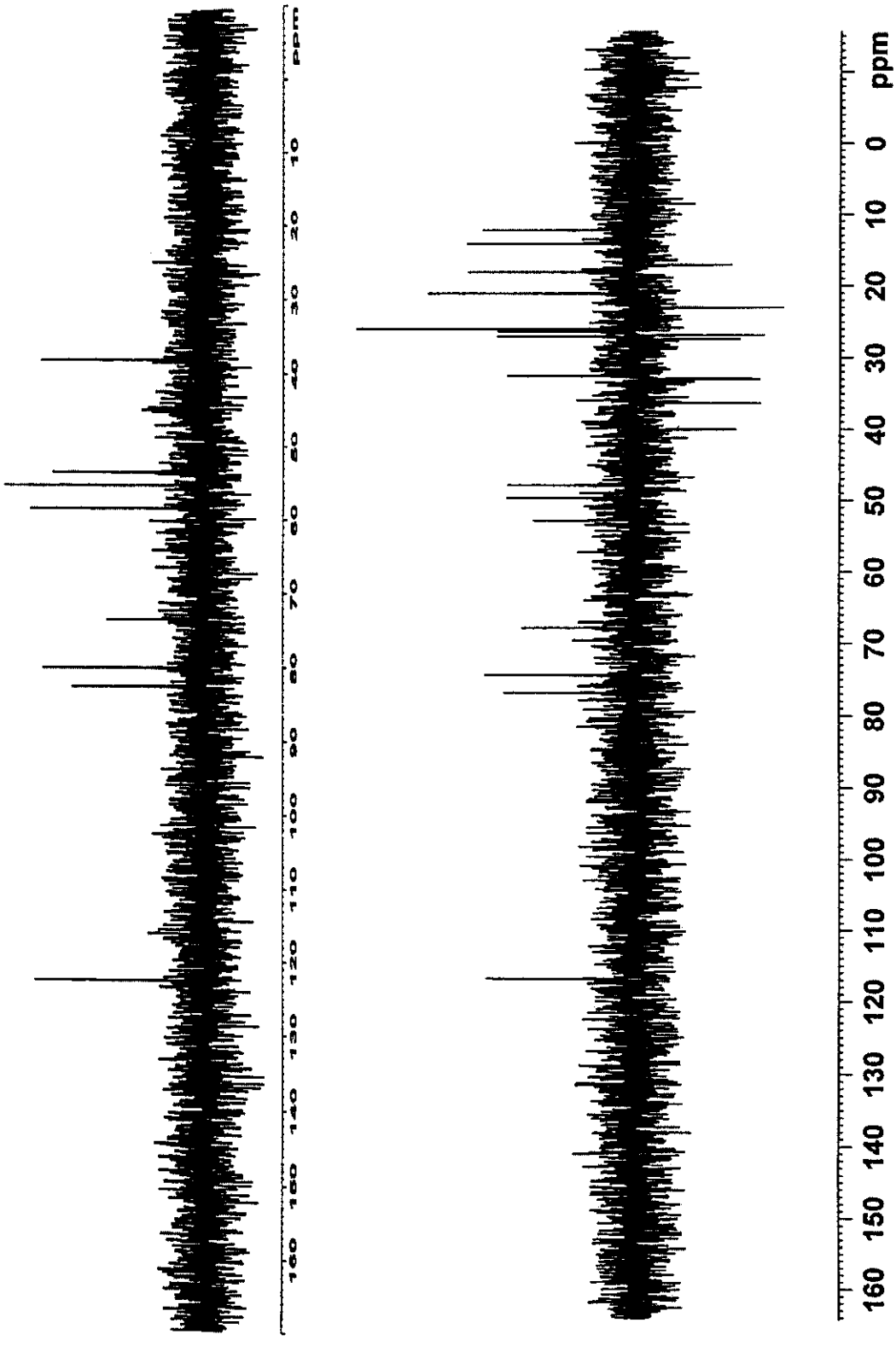


**Figure 35** DEPT (DMSO- $d_6$ and $CDCl_3$) spectrum of compound **XC4**

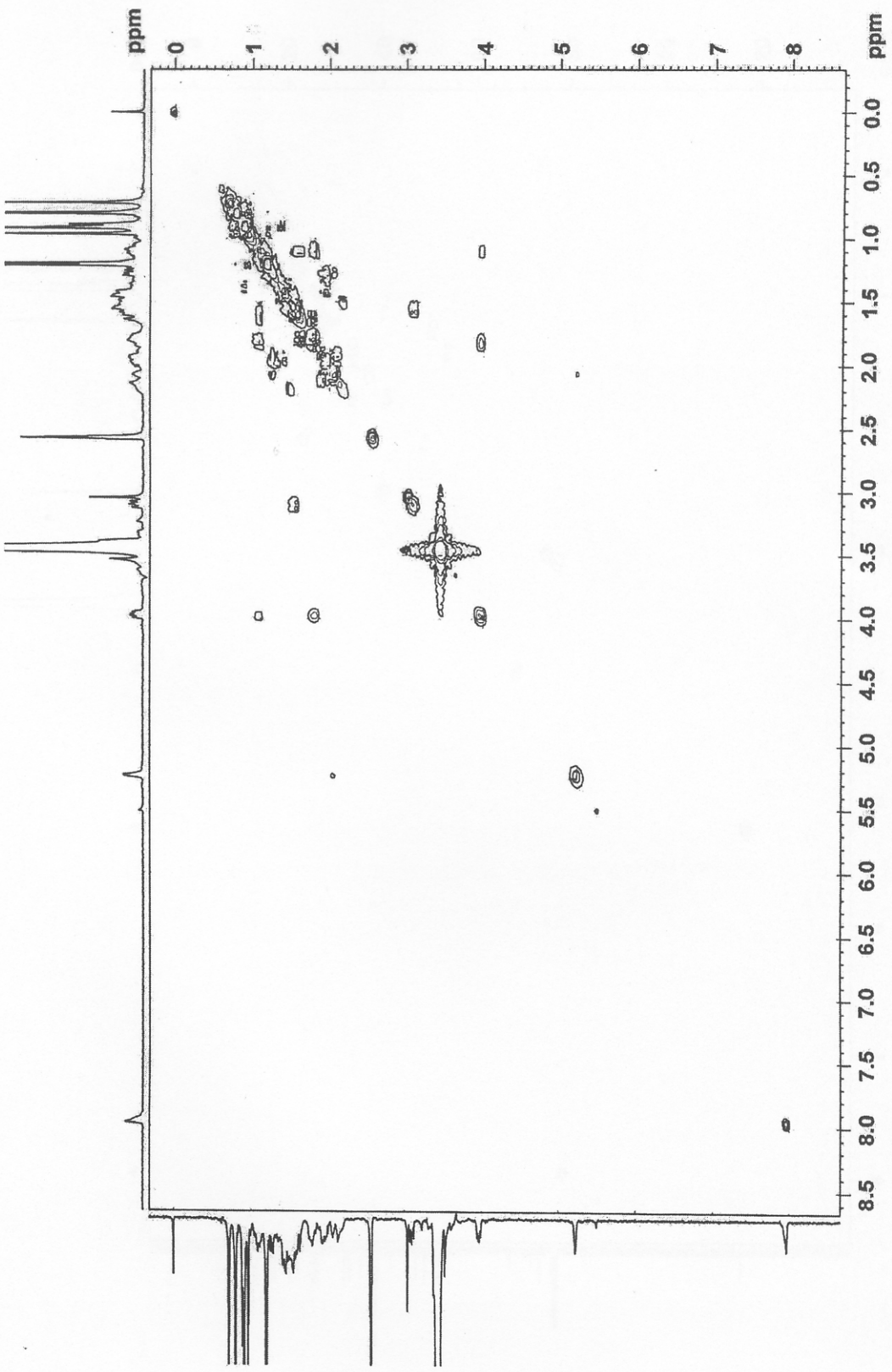


**Figure 36** 2D COSY spectrum of compound **XC4**

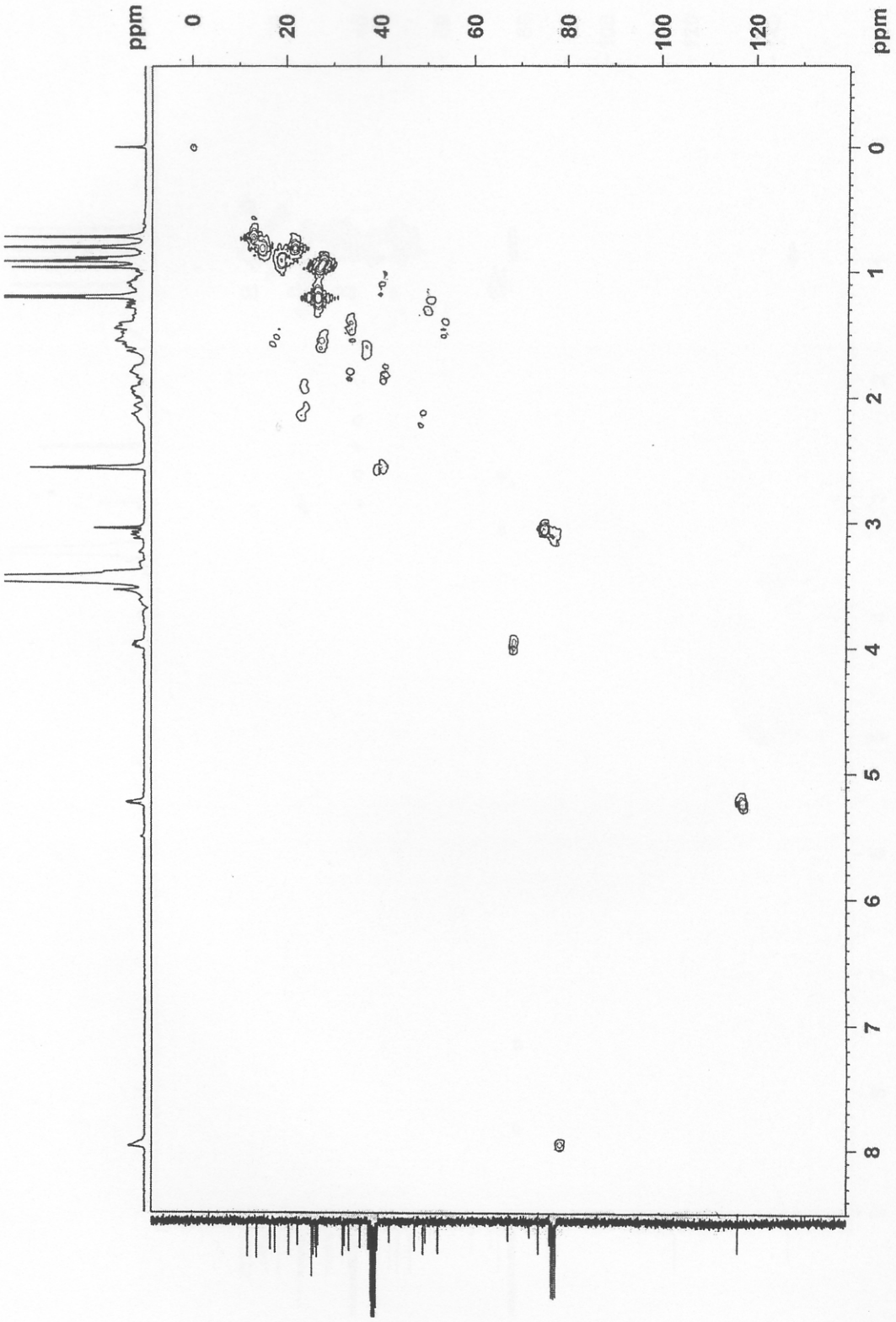


**Figure 37** 2D HMQC spectrum of compound **XC4**

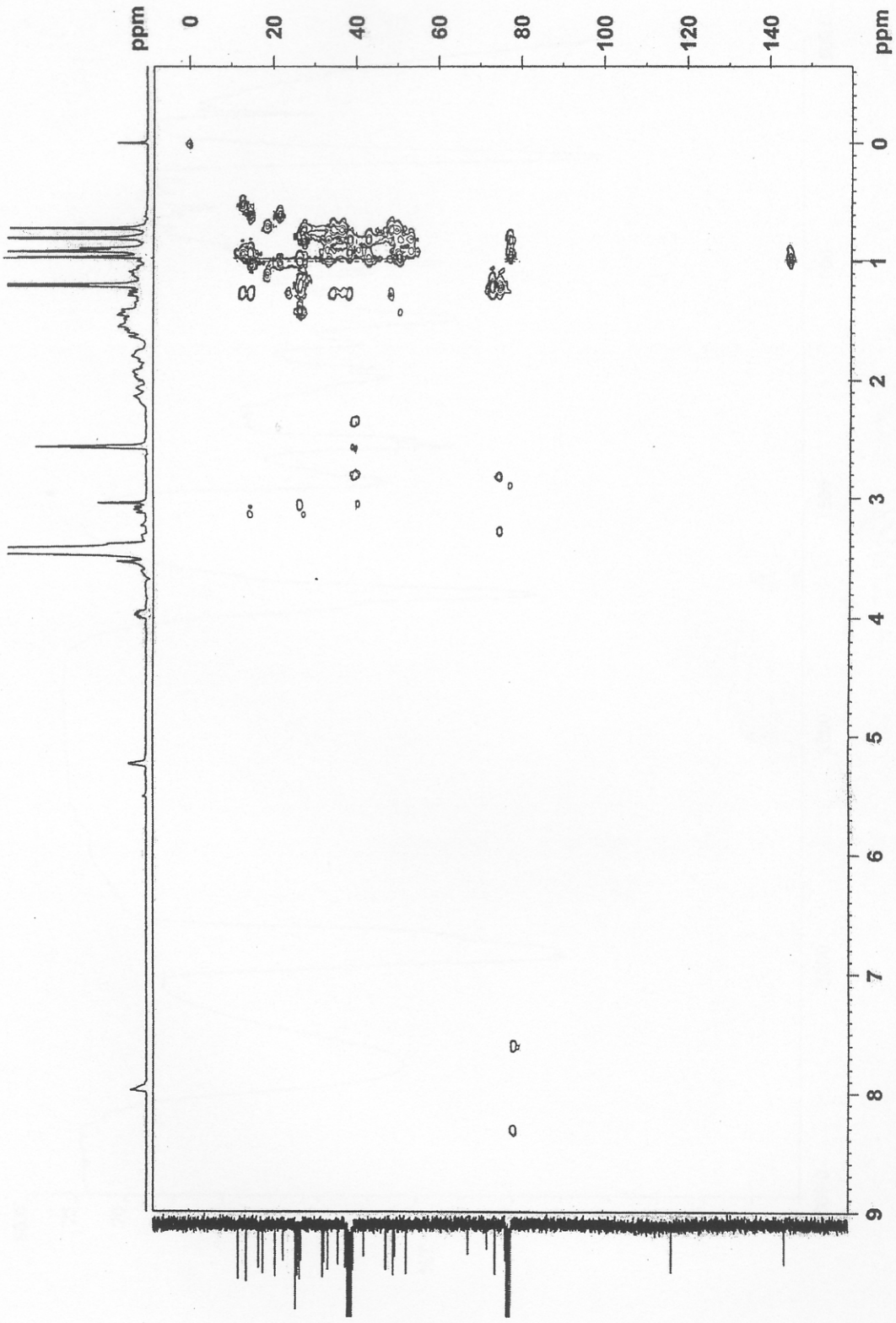


**Figure 38** 2D HMBC spectrum of compound **XC4**

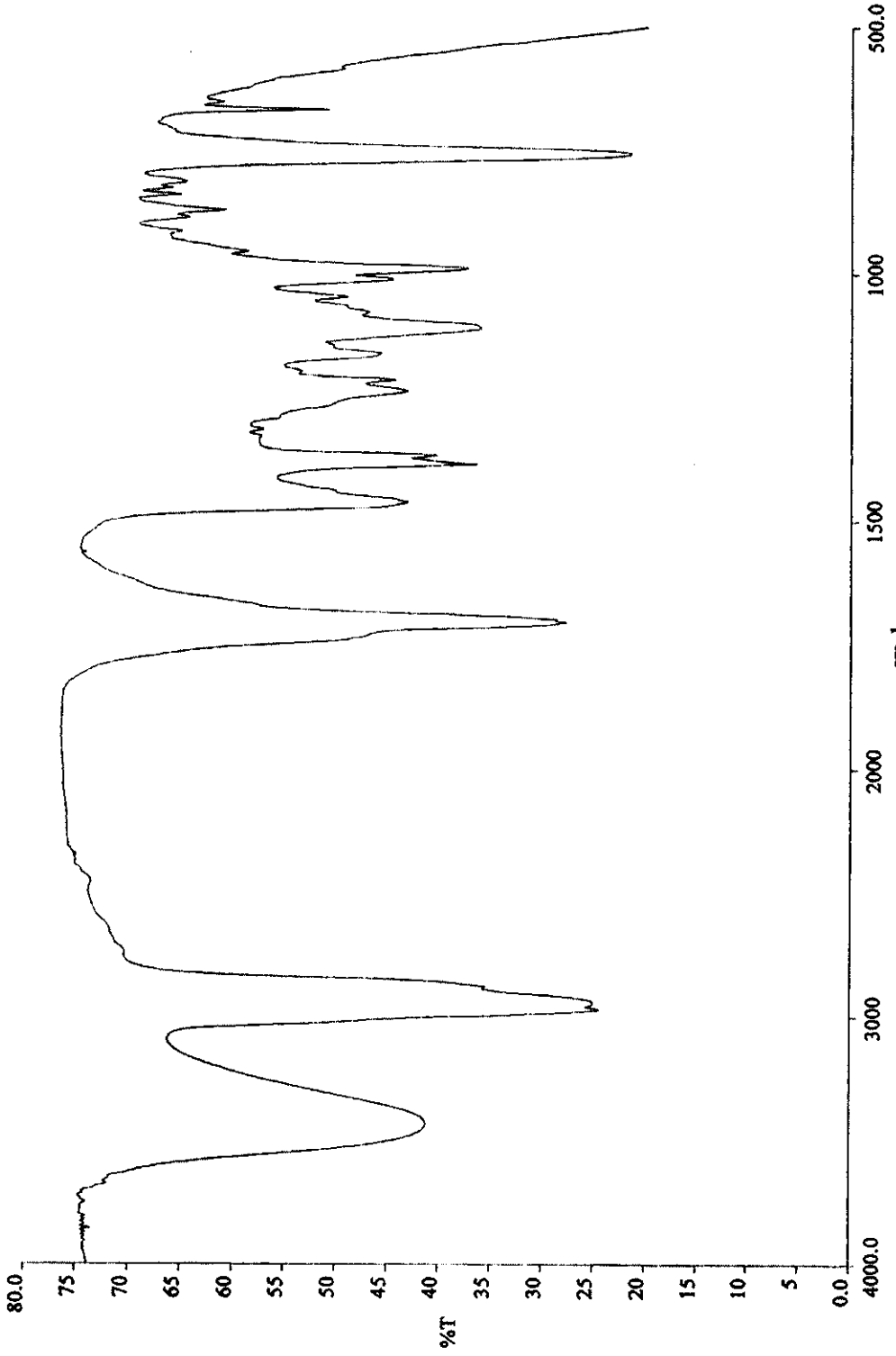


**Figure 39** IR (Neat) spectrum of compound **XC5**

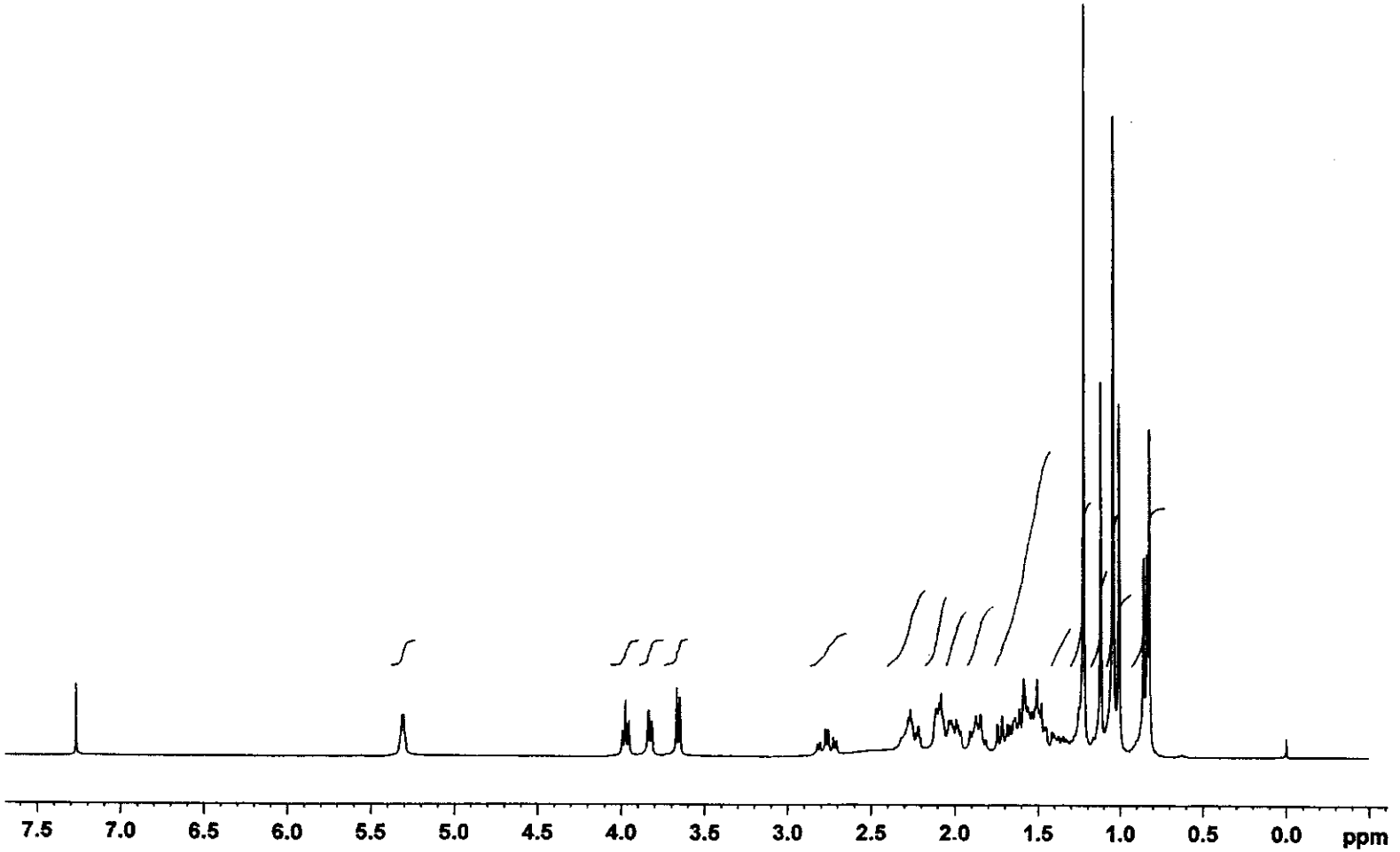


**Figure 40** $^{1}$H NMR (300 MHz, $CDCl_3$) spectrum of compound **XC5**

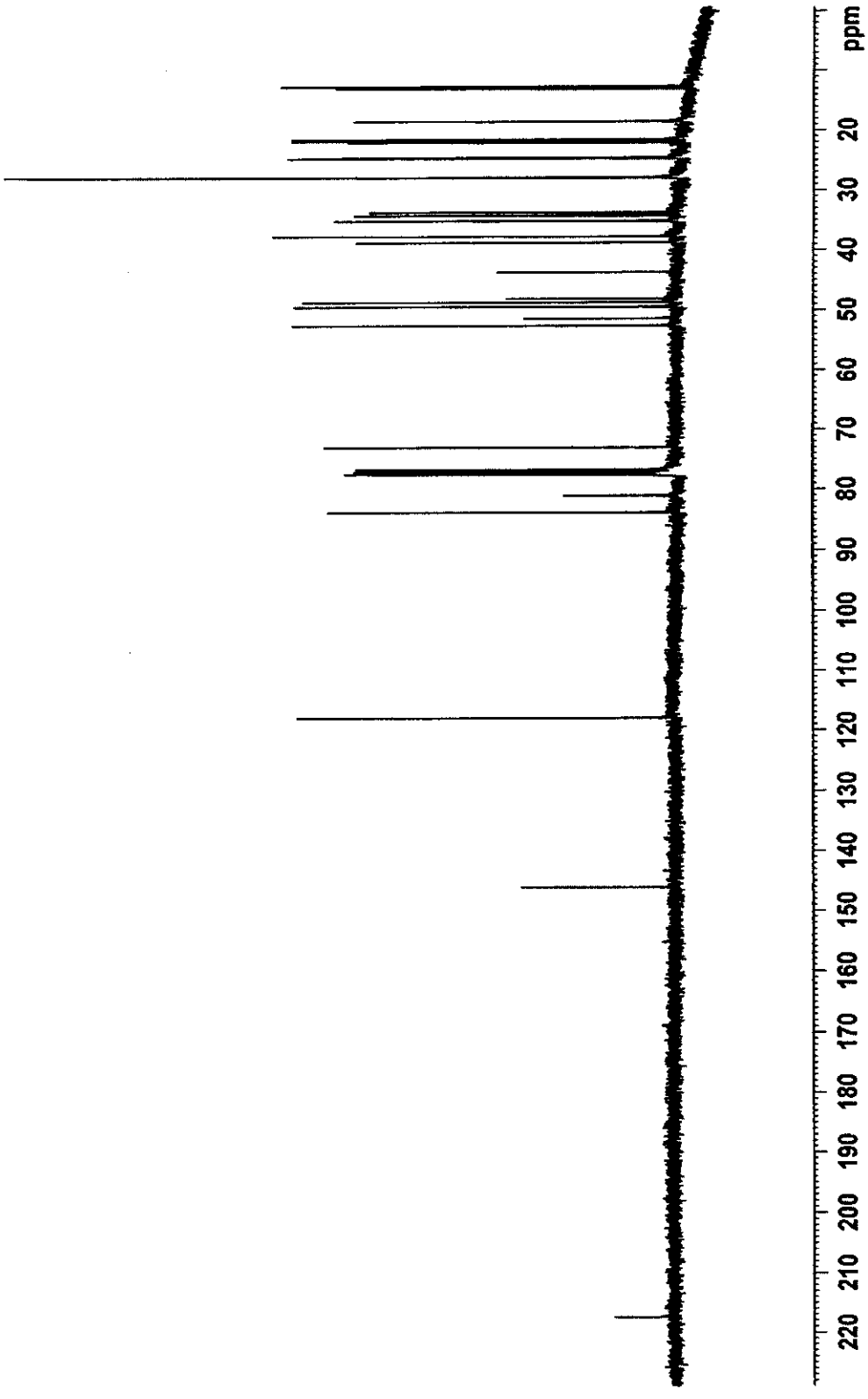


**Figure 41** $^{13}C$ NMR (75 MHz, $CDCl_3$) spectrum of compound **XC5**

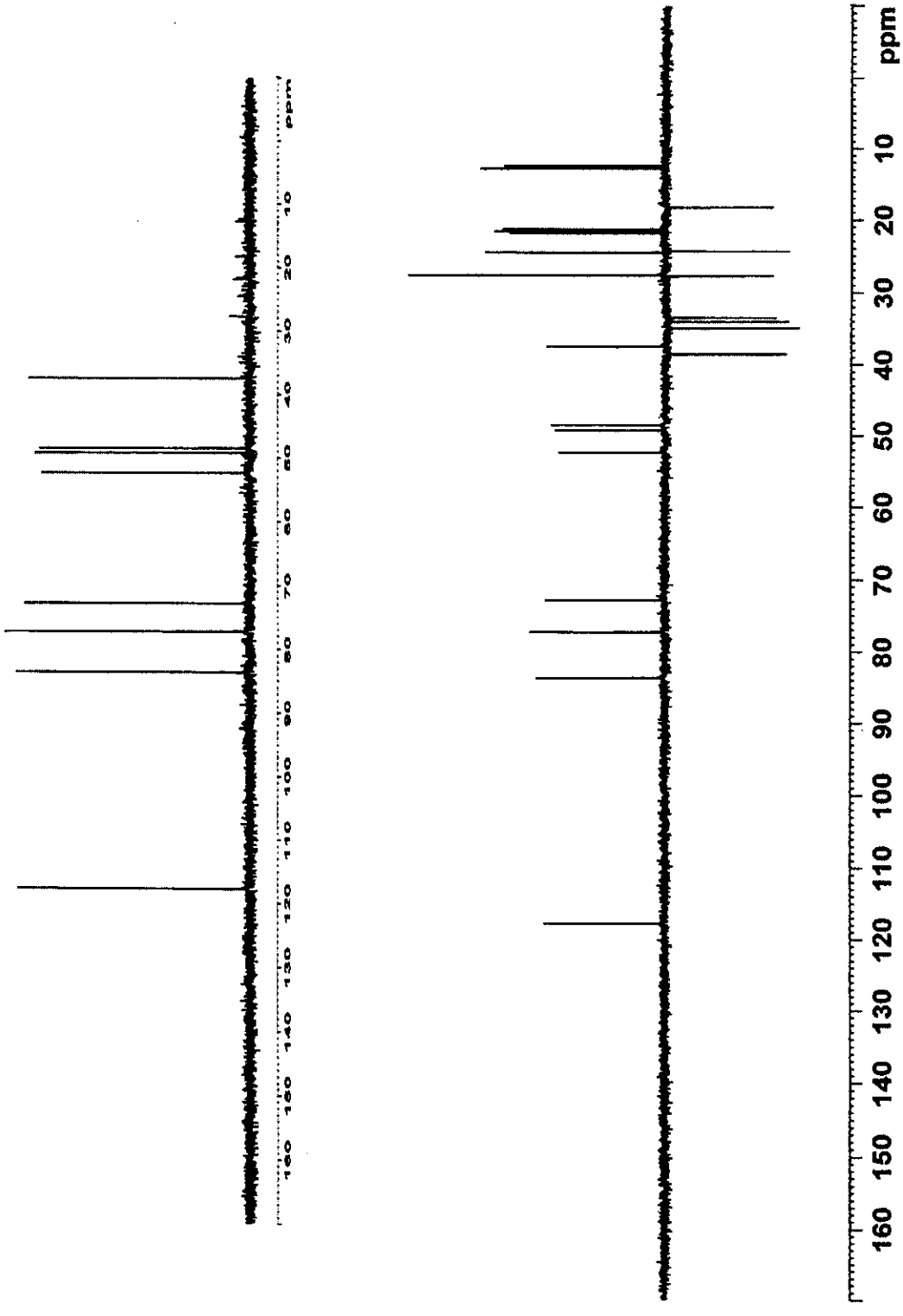


**Figure 42** DEPT ($CDCl_3$) spectrum of compound **XC5**

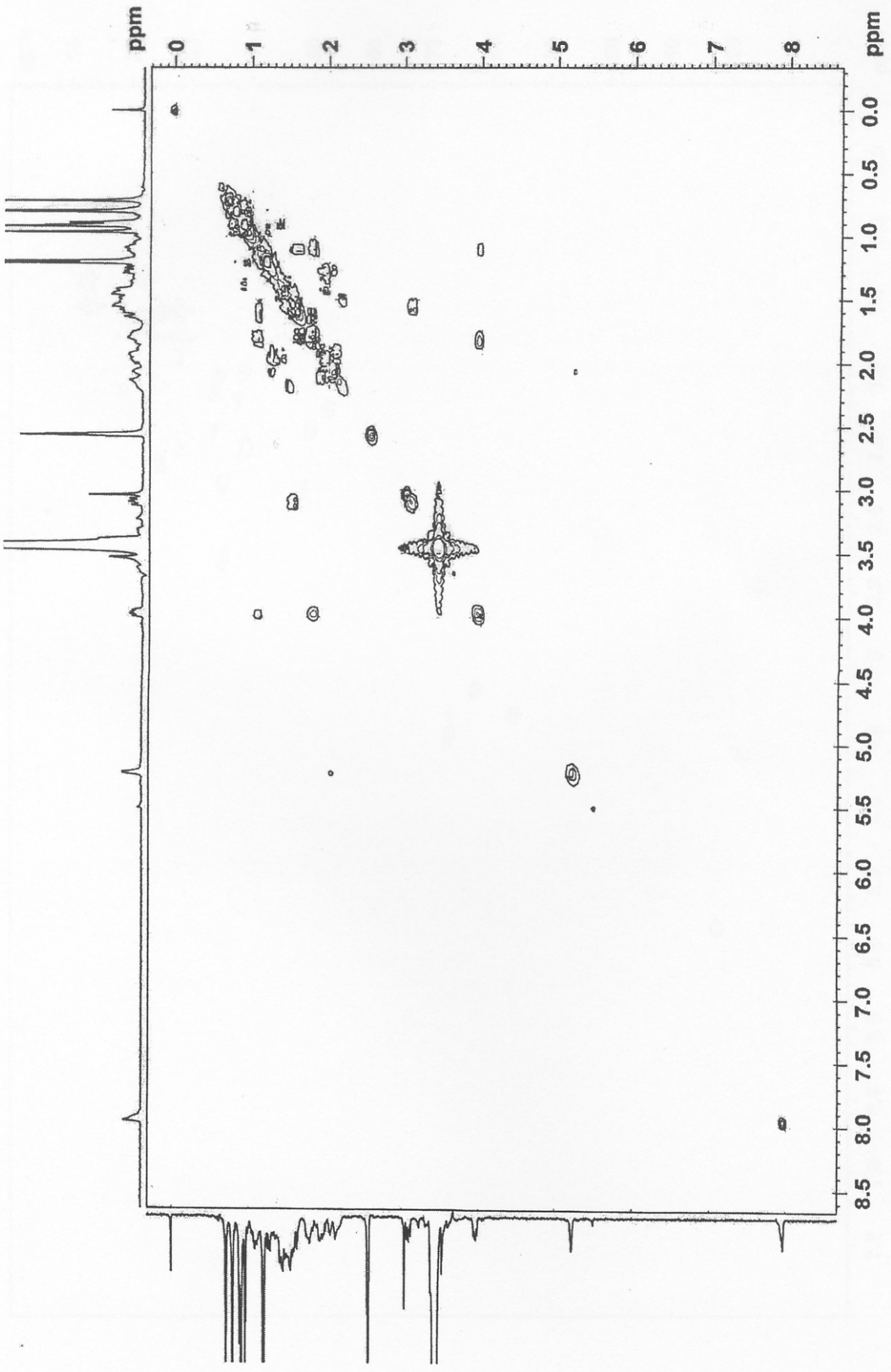


**Figure 43** 2D COSY spectrum of compound **XC5**

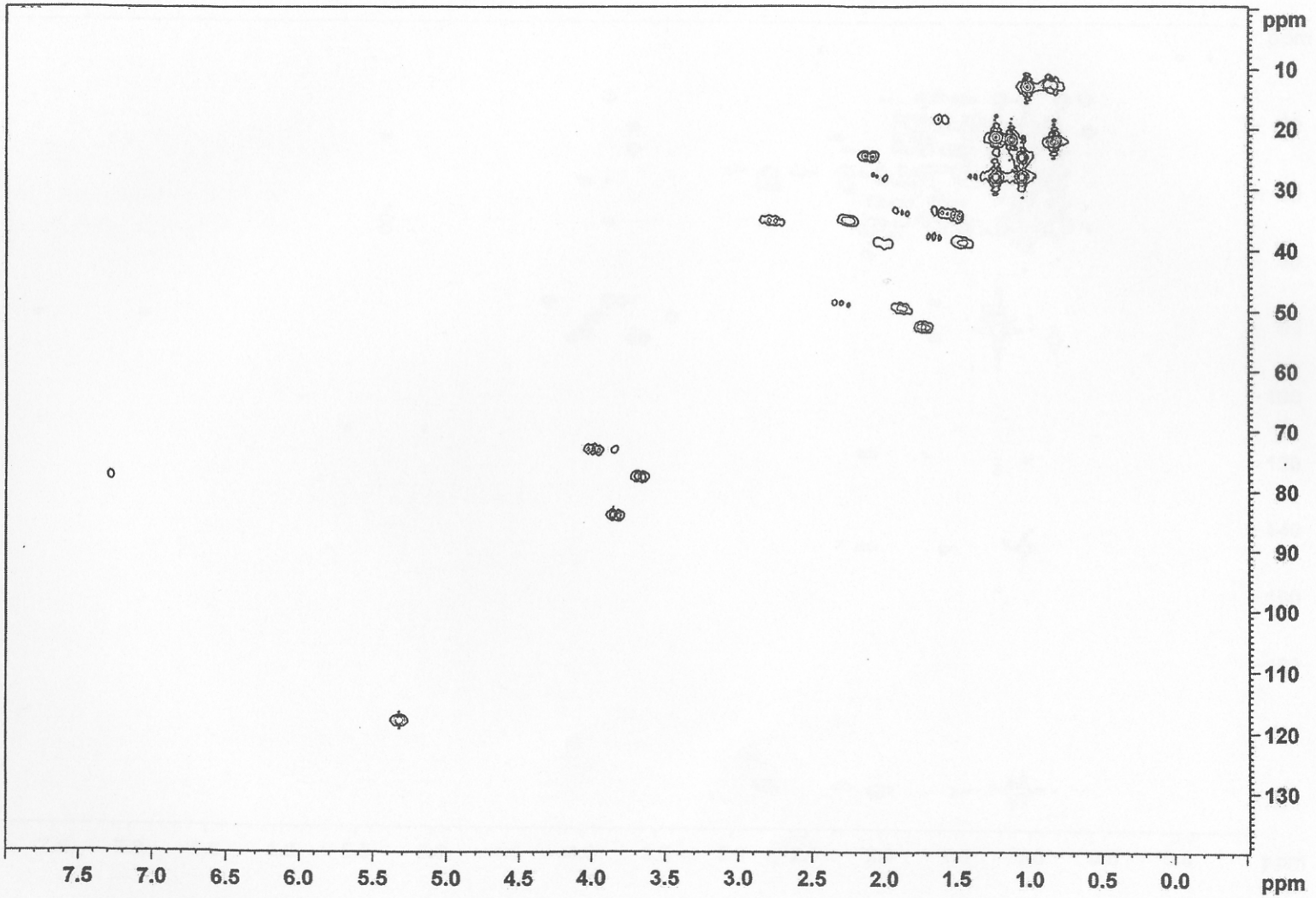


**Figure 44** 2D HMQC spectrum of compound **XC5**

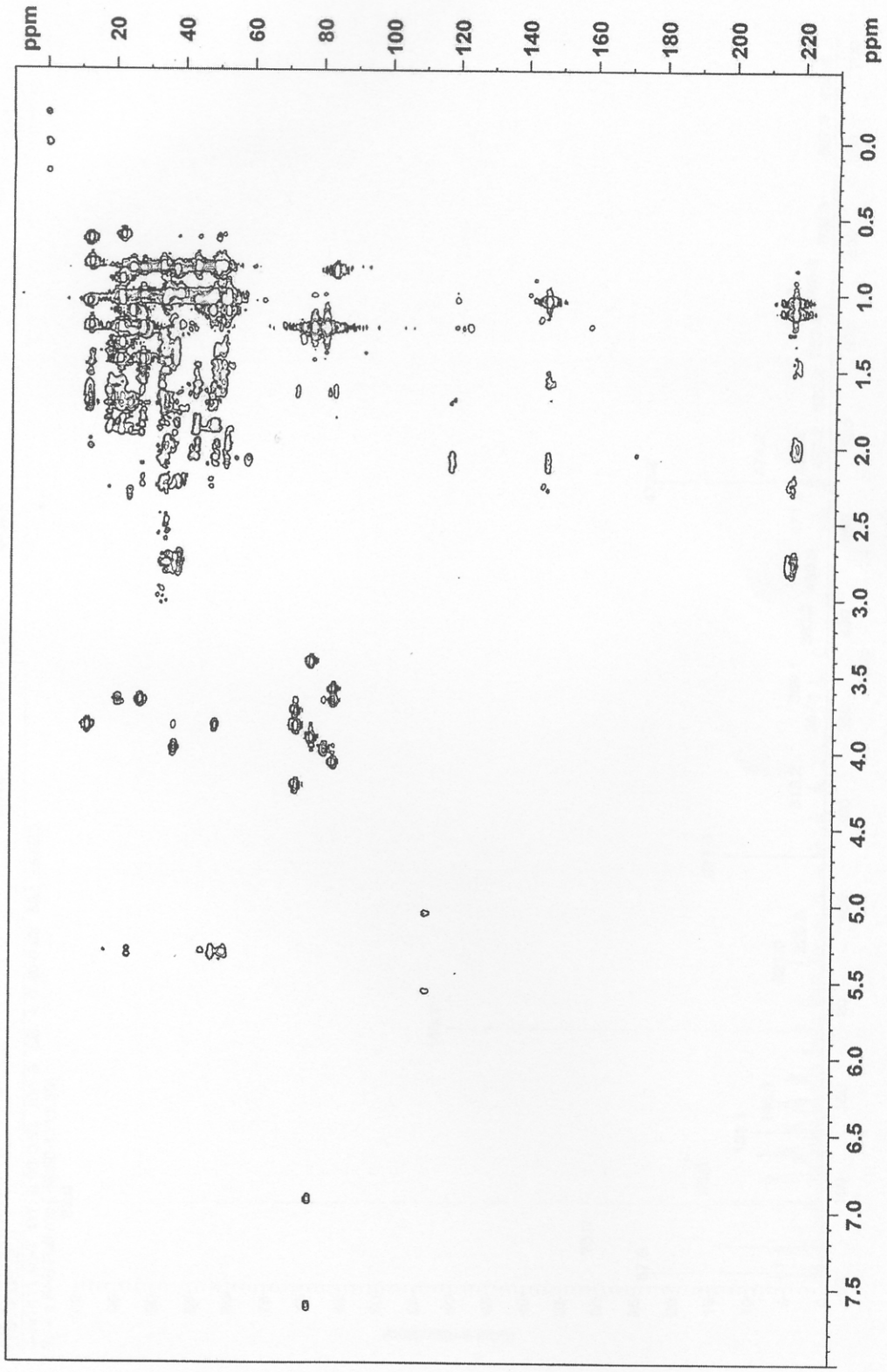


**Figure 45** 2D HMBC spectrum of compound **XC5**

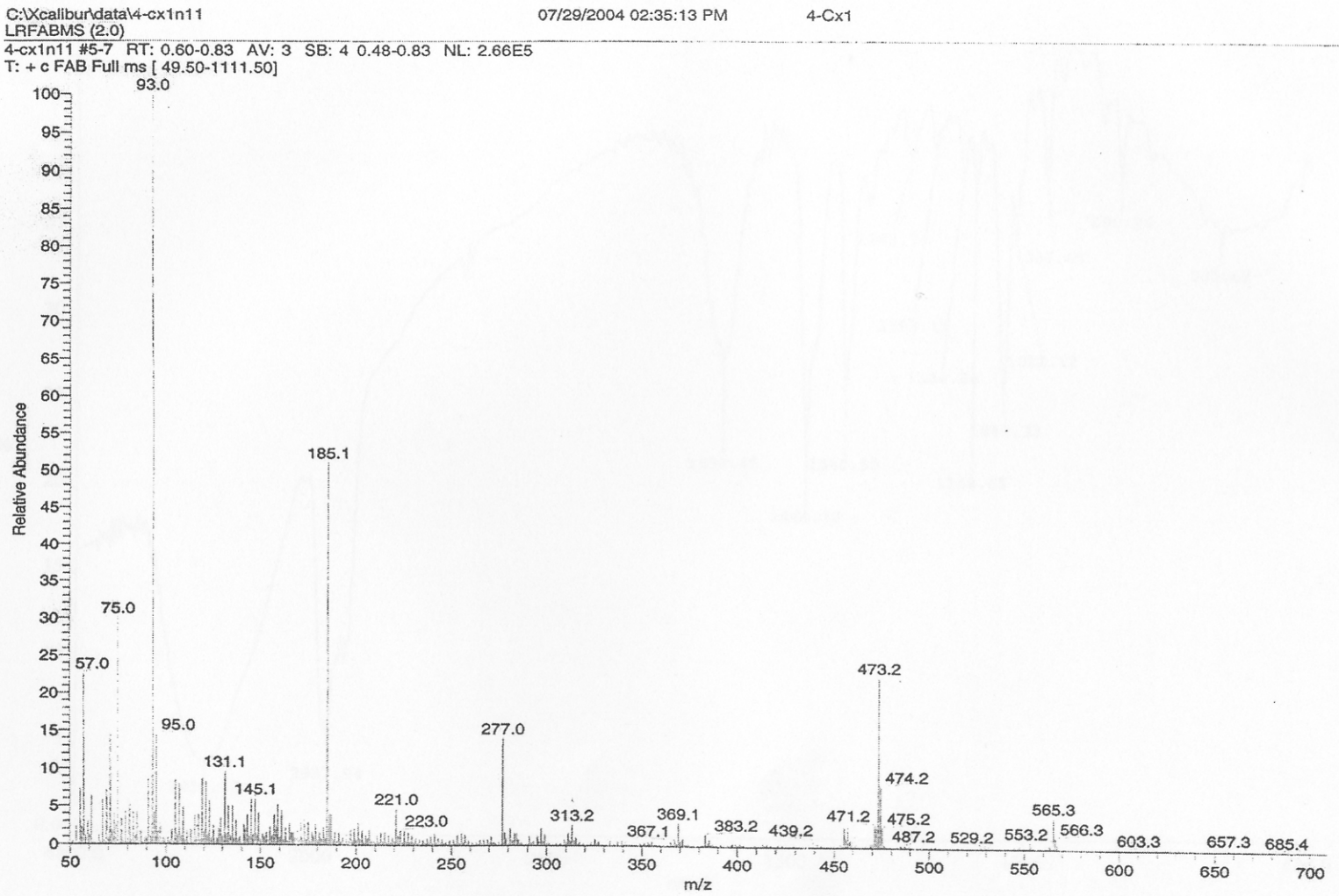


**Figure 46** Mass spectrum of compound **XC5**

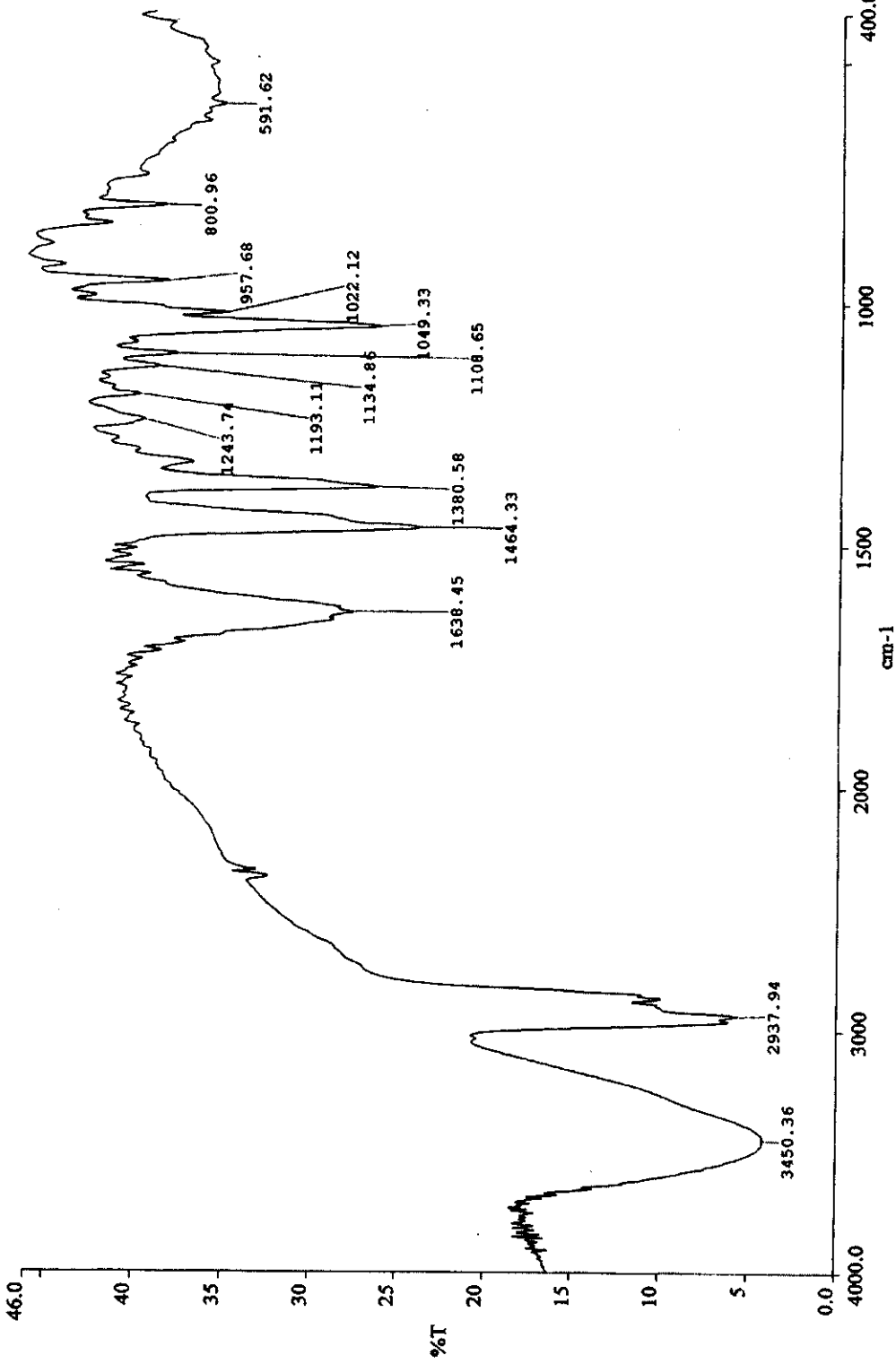


**Figure 47** IR (Neat) spectrum of compound **XC6**

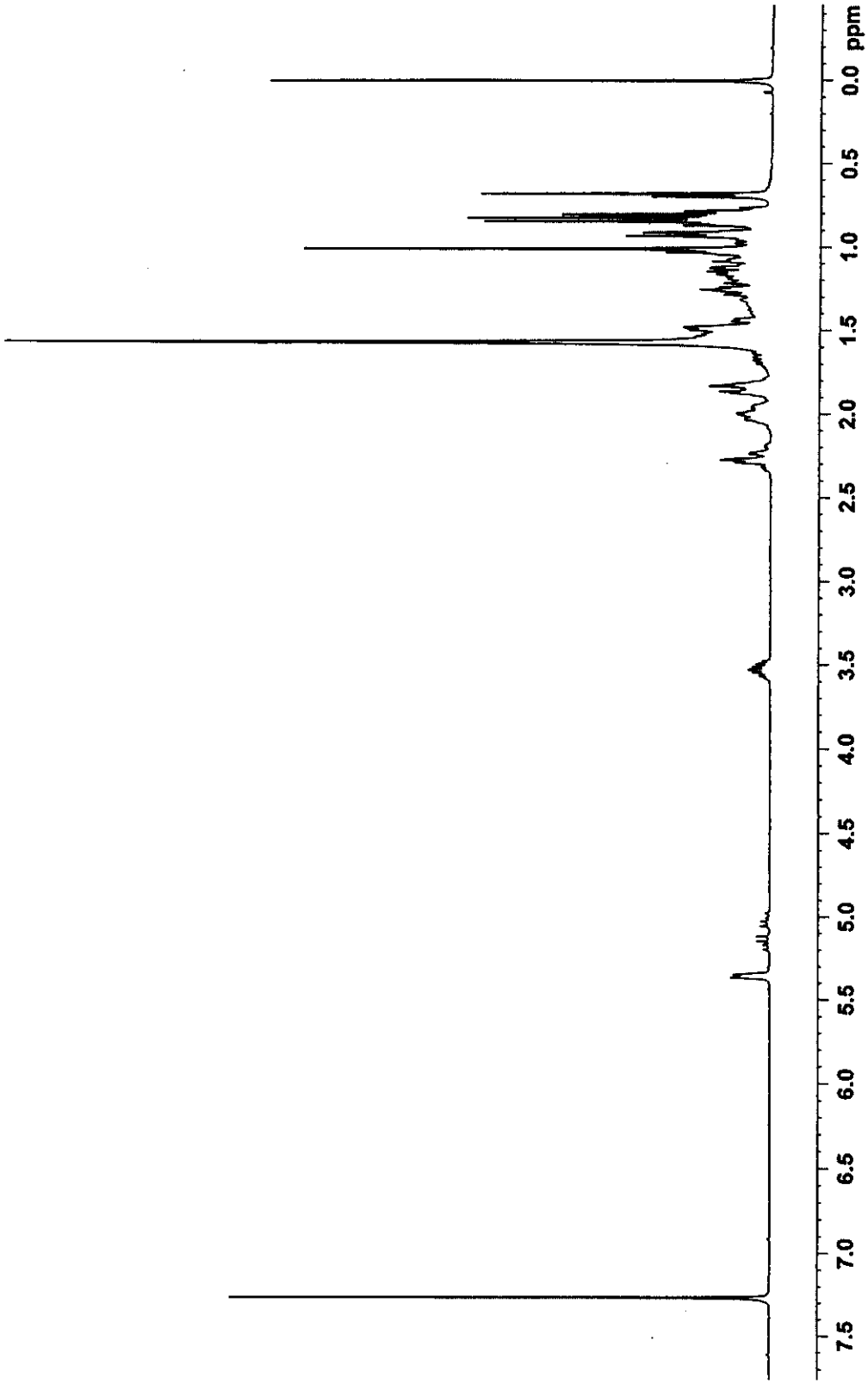


**Figure 48** $^{1}$H NMR (300 MHz, $CDCl_3$) spectrum of compound **XC6**

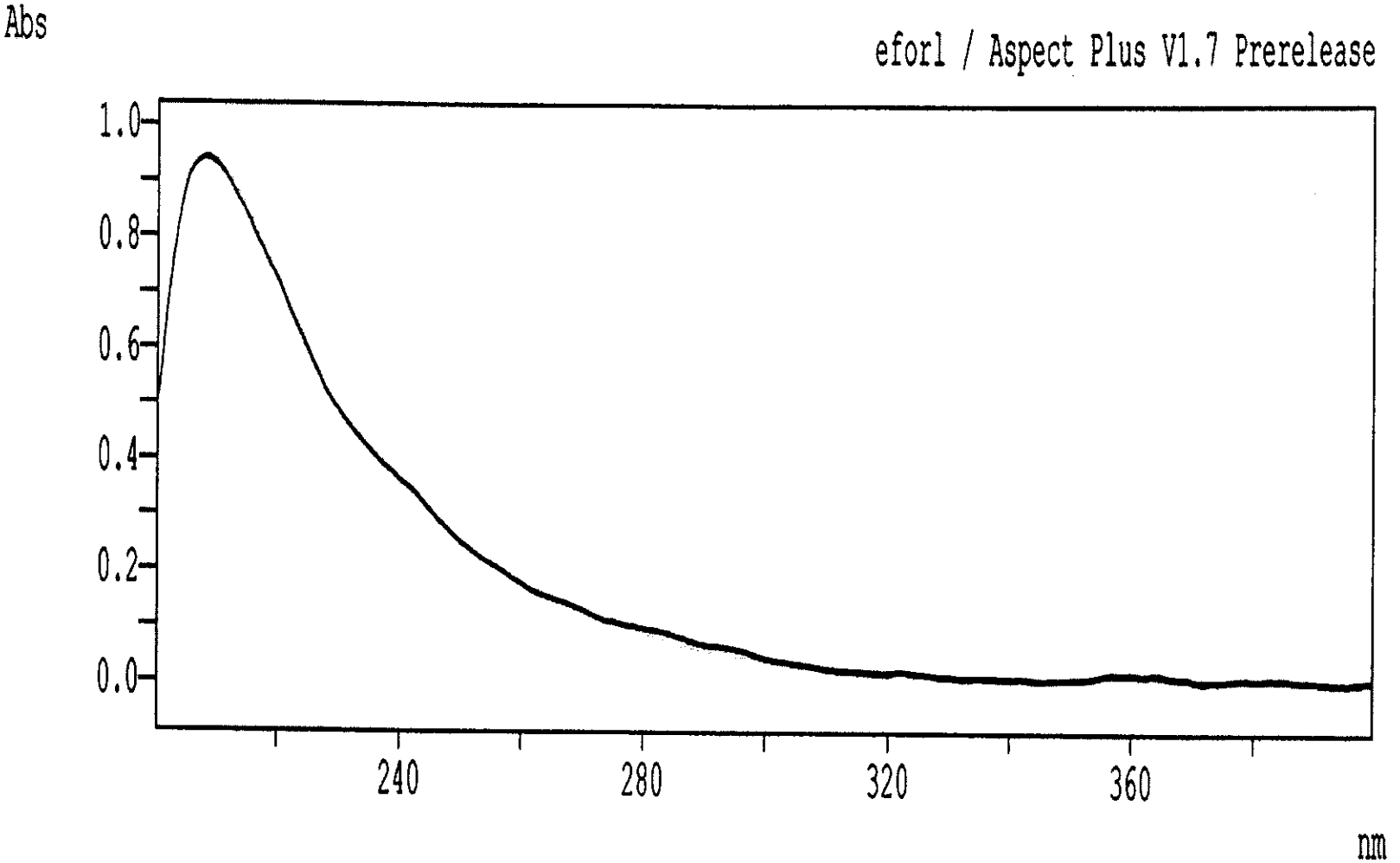


**Figure 49** UV (MeOH) spectrum of compound **XH1**

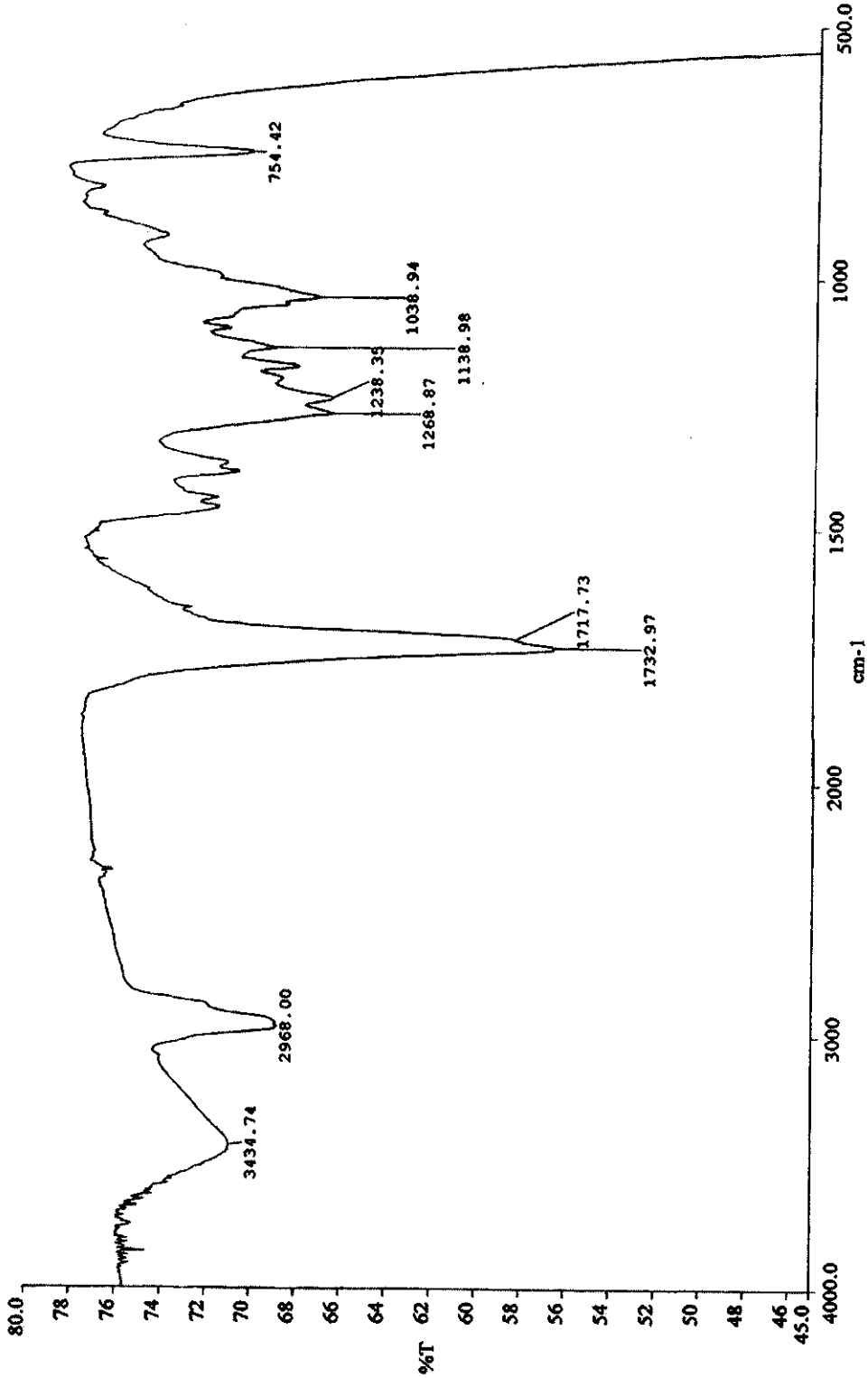


**Figure 50** IR (Neat) spectrum of compound **XH1**

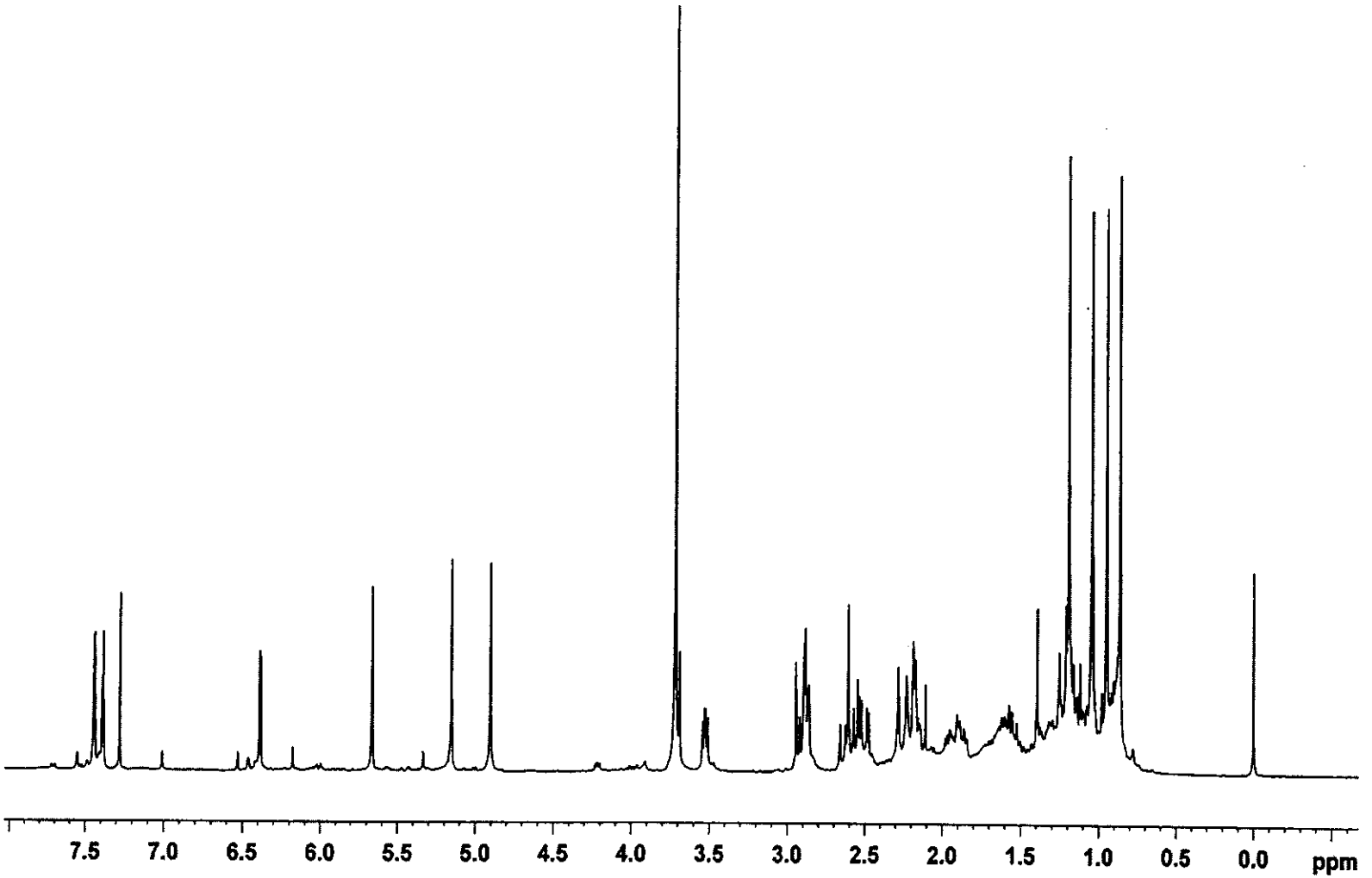


**Figure 51** $^{1}$H NMR (300 MHz, $CDCl_3$) spectrum of compound **XH1**

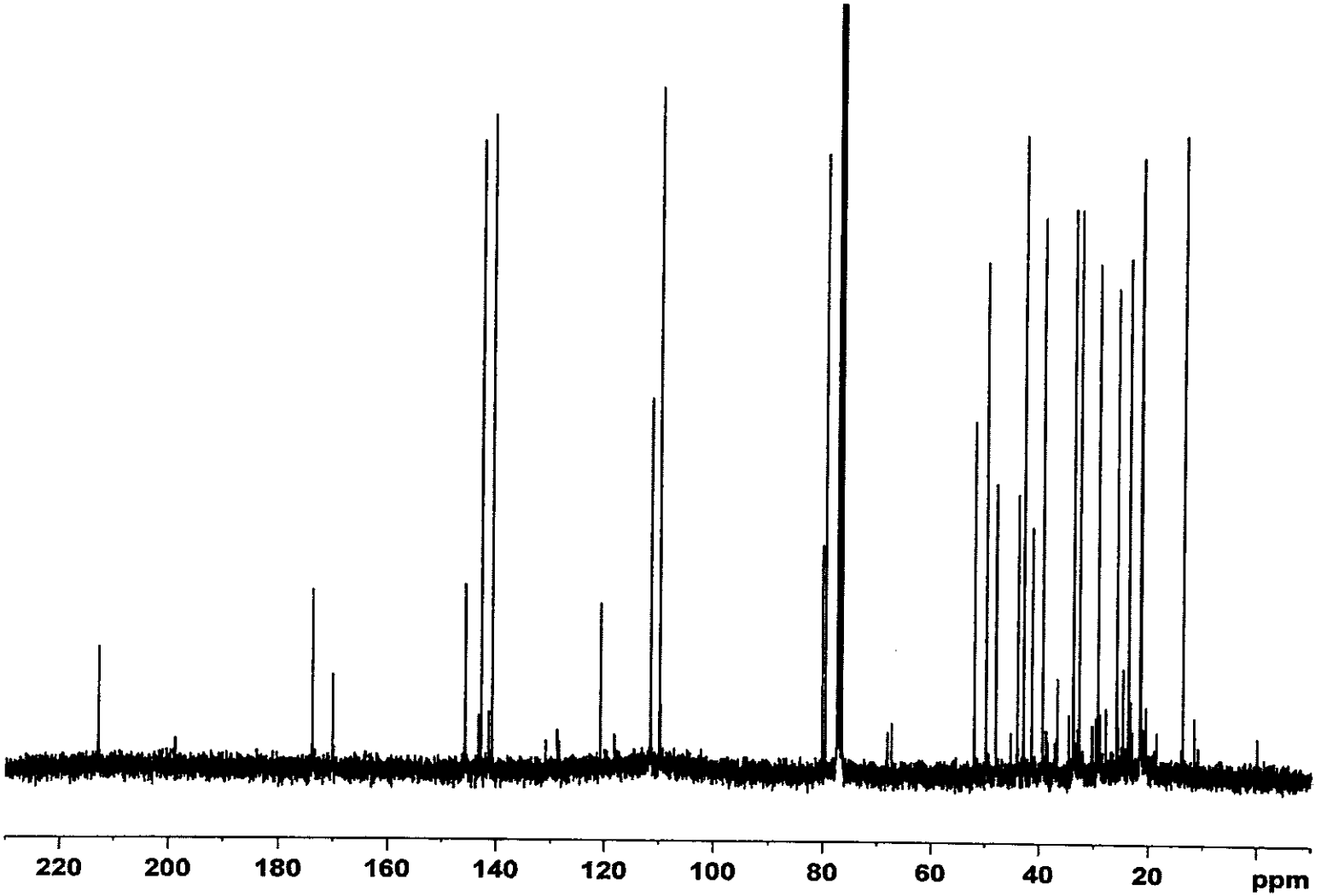


**Figure 52** $^{13}C$ NMR (75 MHz, $CDCl_3$) spectrum of compound **XH1**

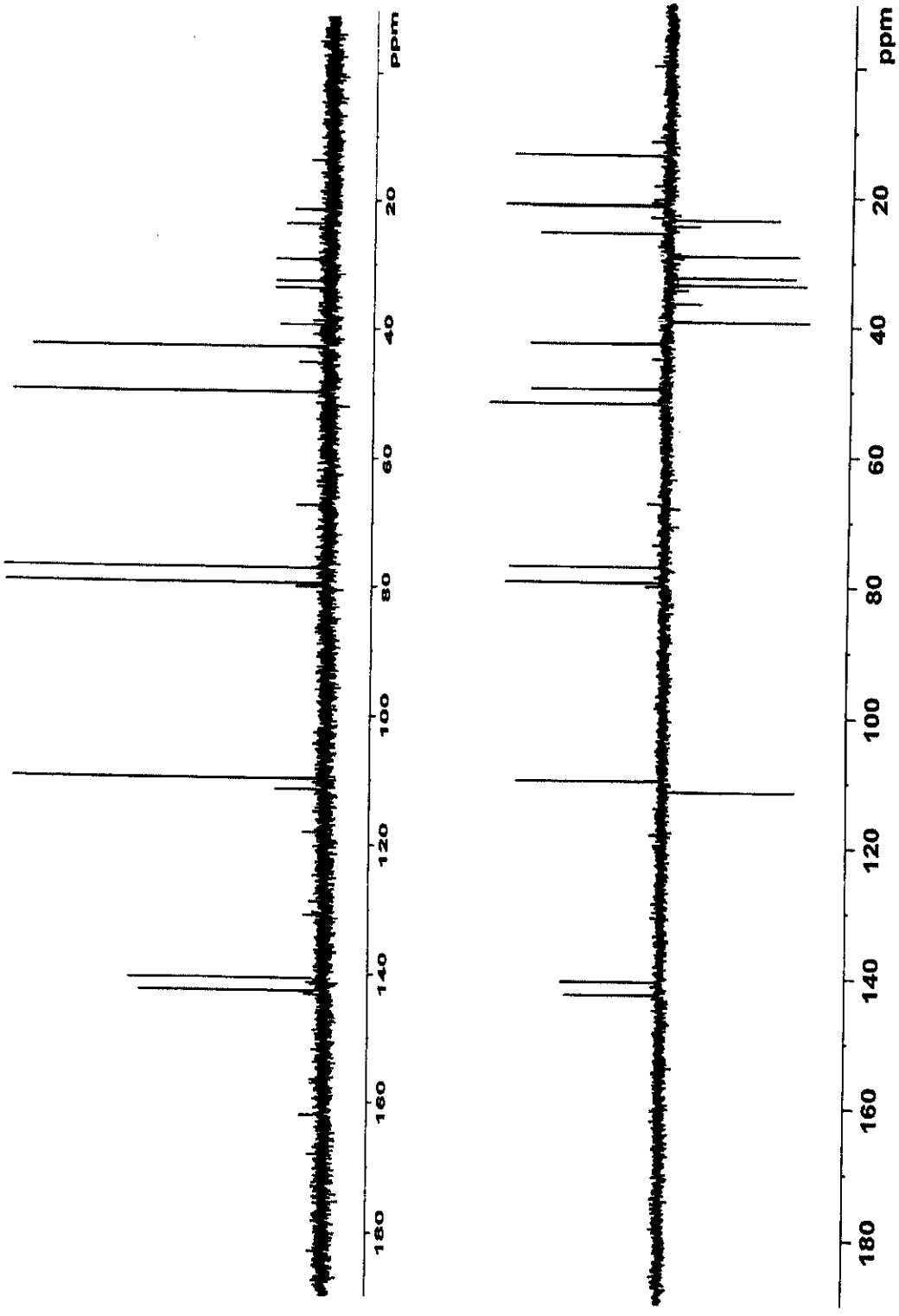


**Figure 53** DEPT ($CDCl_3$) spectrum of compound **XH1**

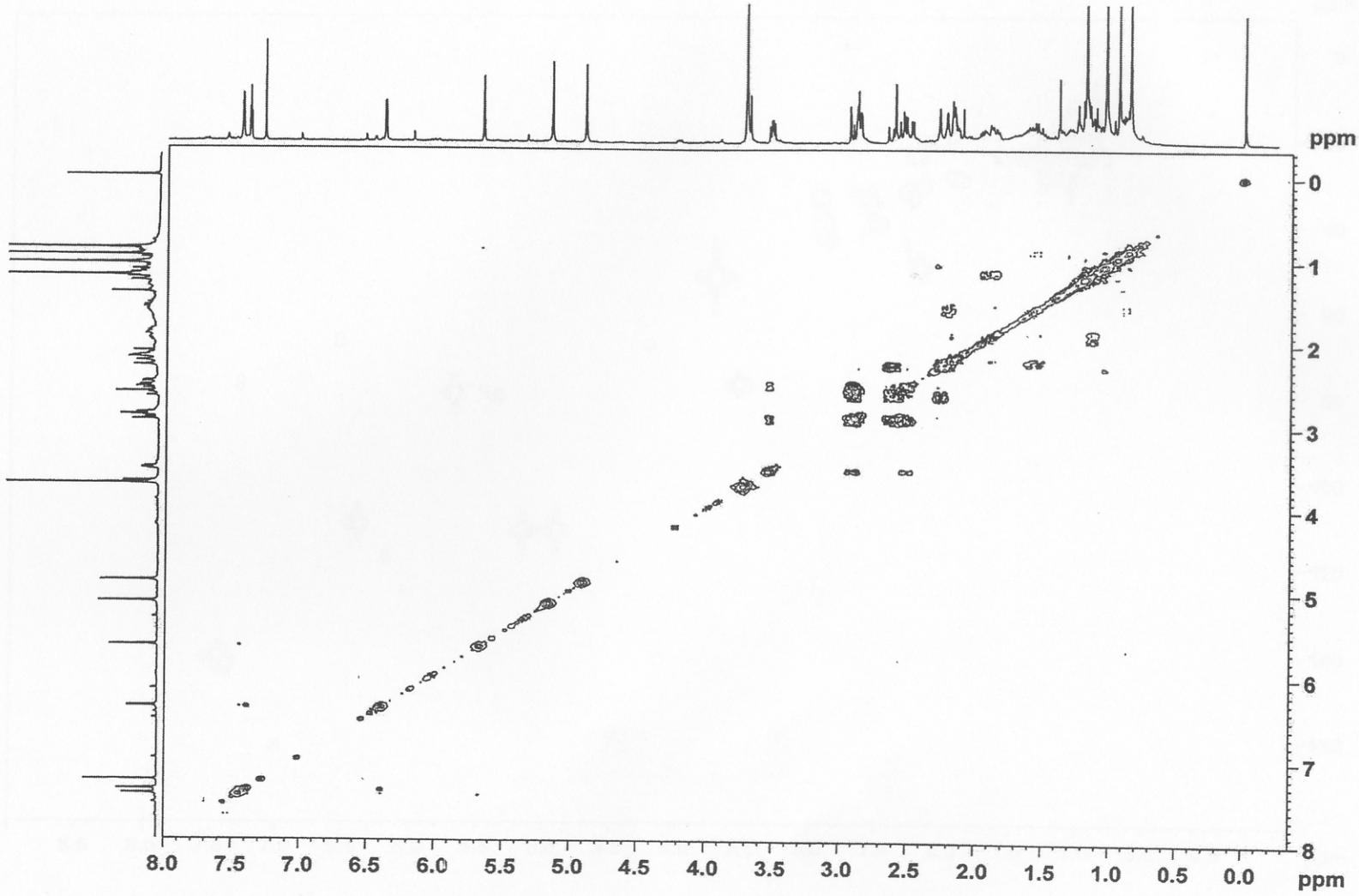


**Figure 54** 2D COSY spectrum of compound **XH1**

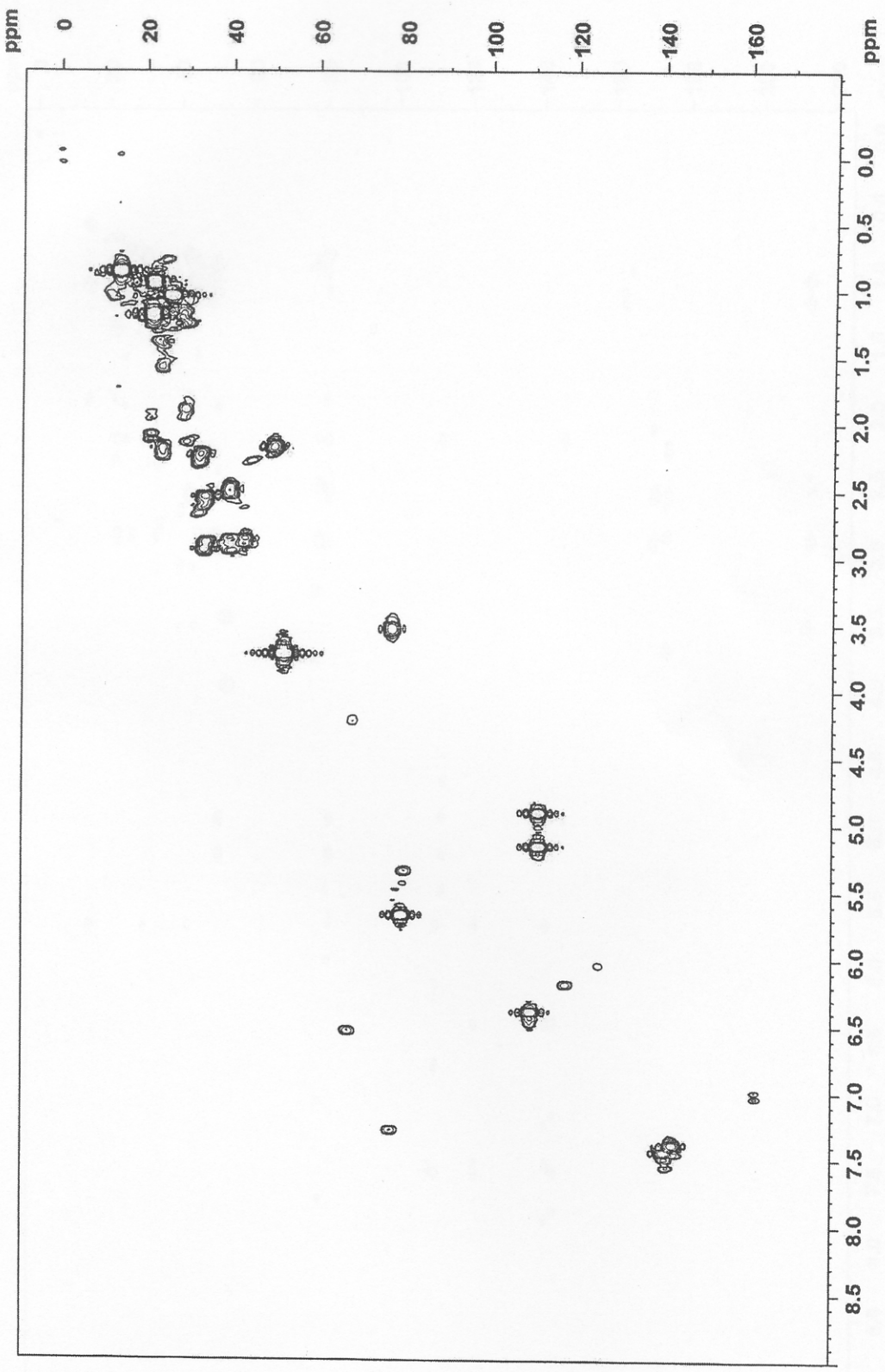


**Figure 55** 2D HMQC spectrum of compound **XH1**

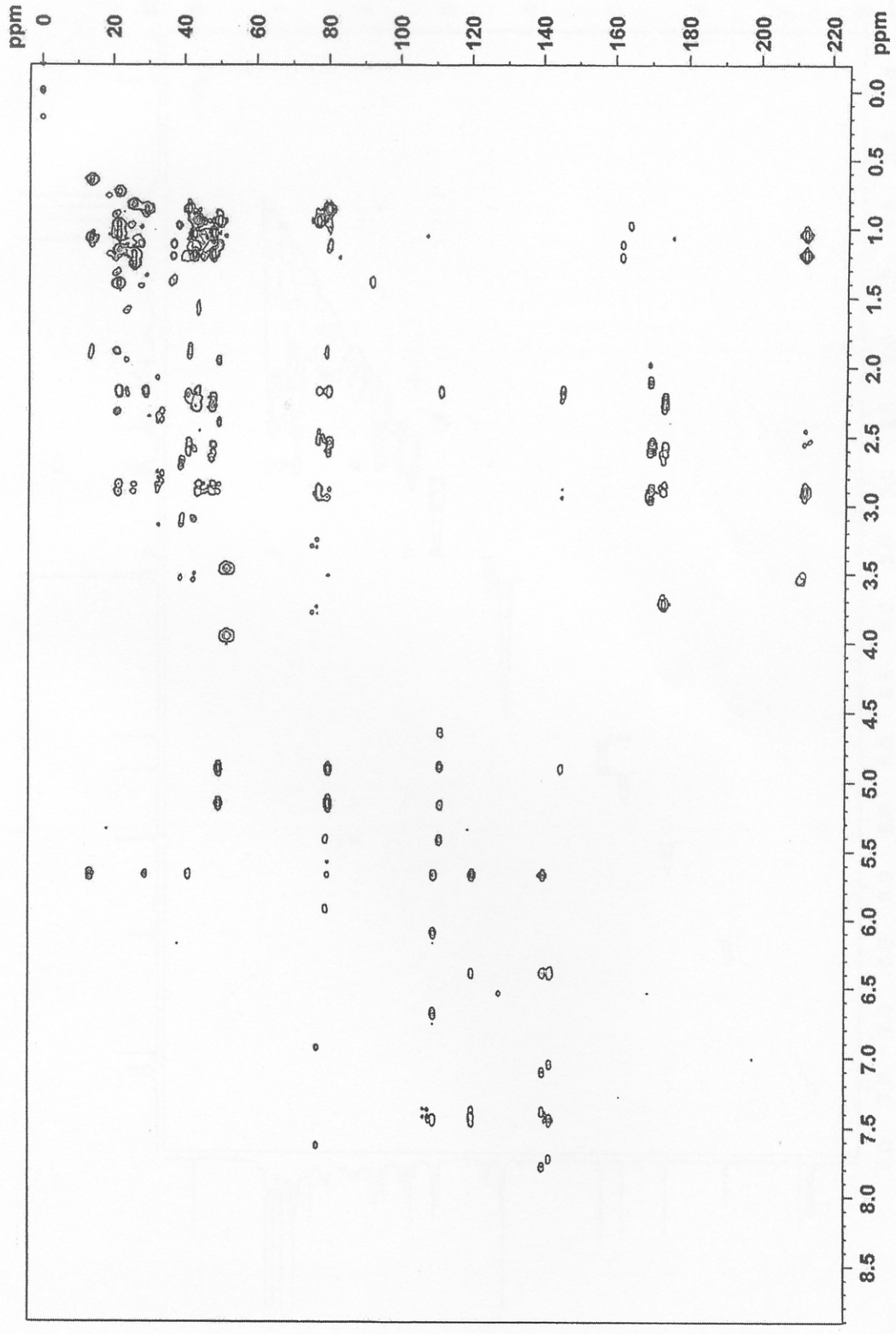


**Figure 56** 2D HMBC spectrum of compound **XH1**

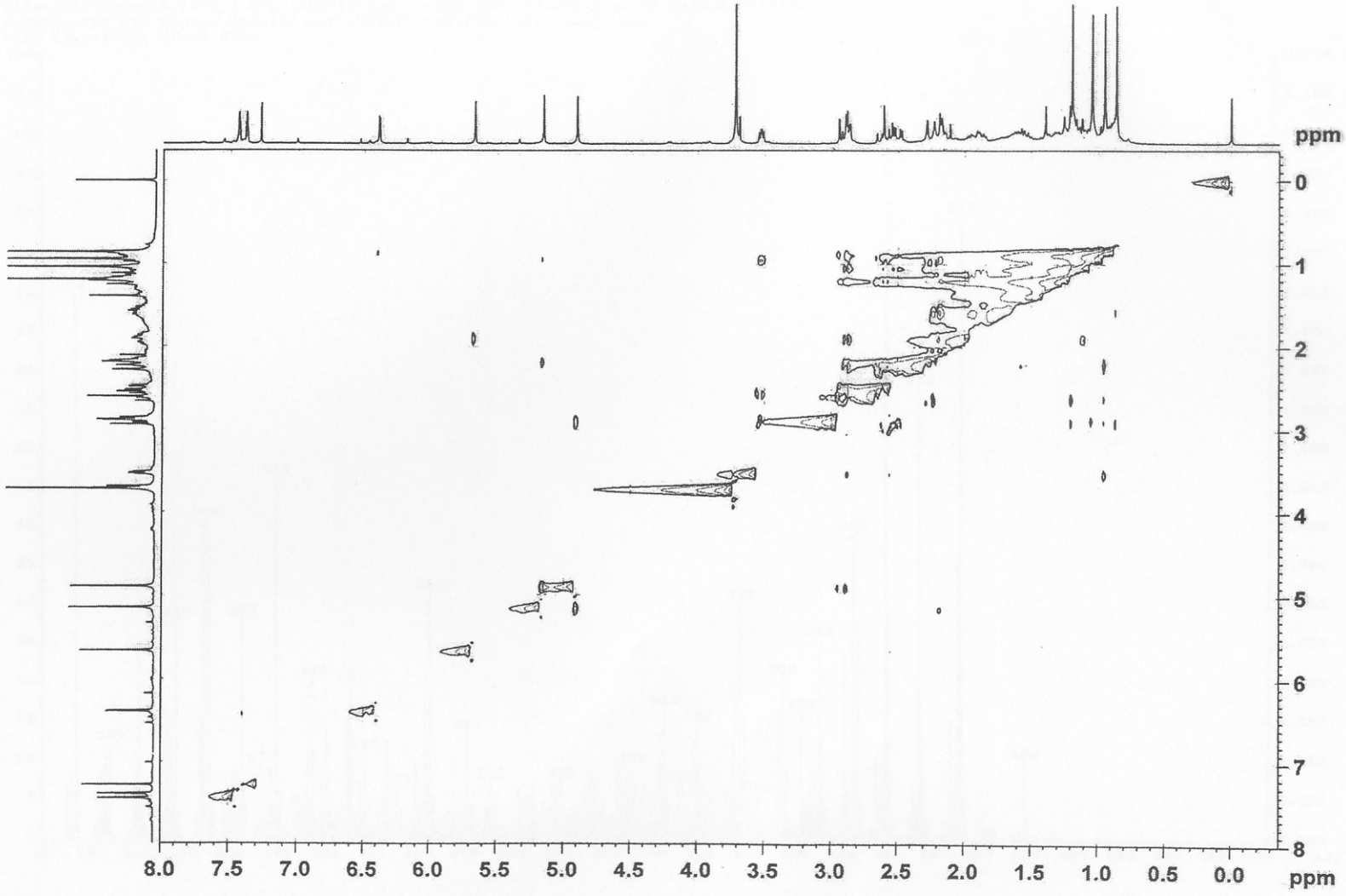


**Figure 57** NOESY spectrum of compound **XH1**

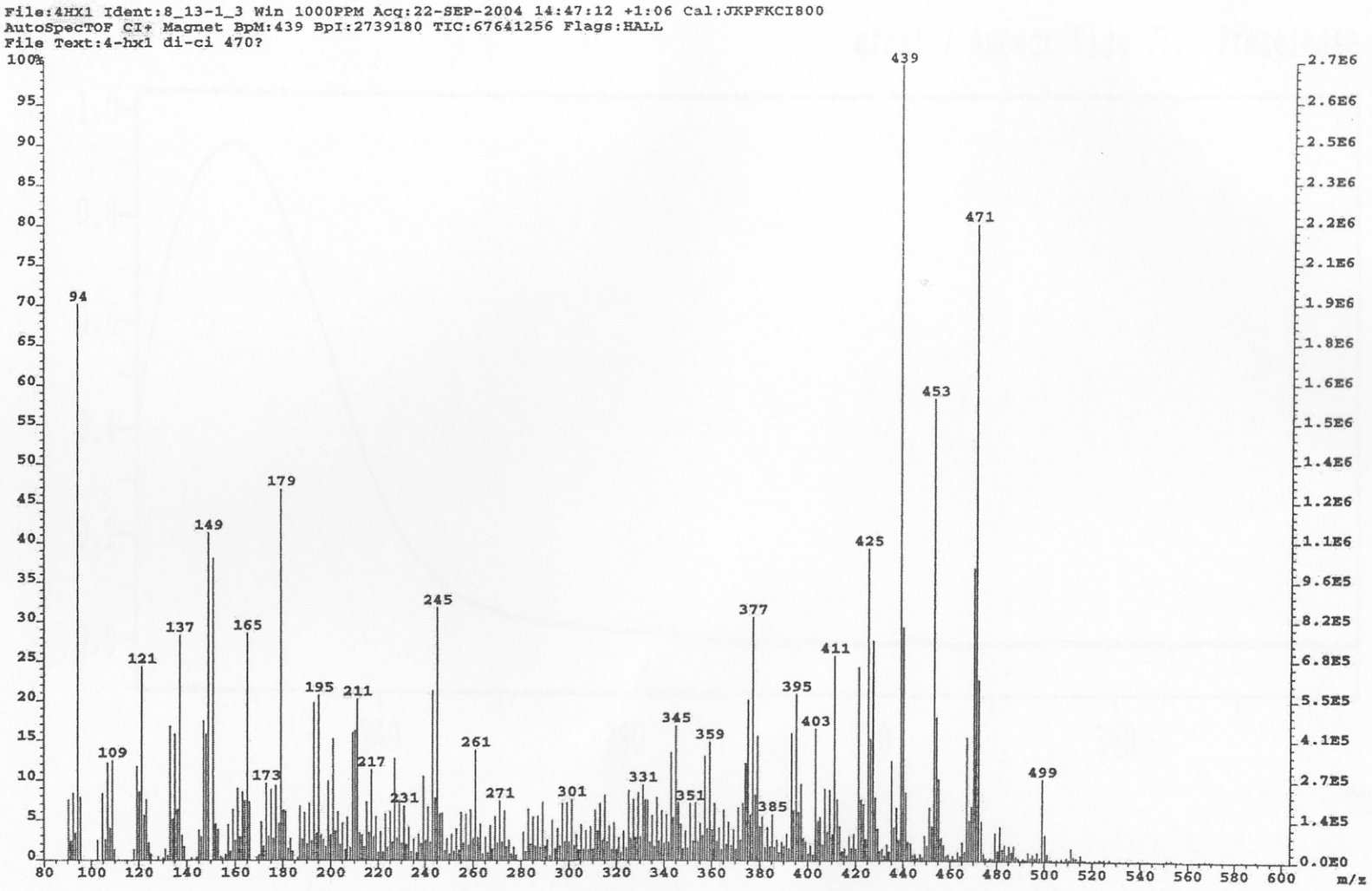


**Figure 58** Mass spectrum of compound **XH1**

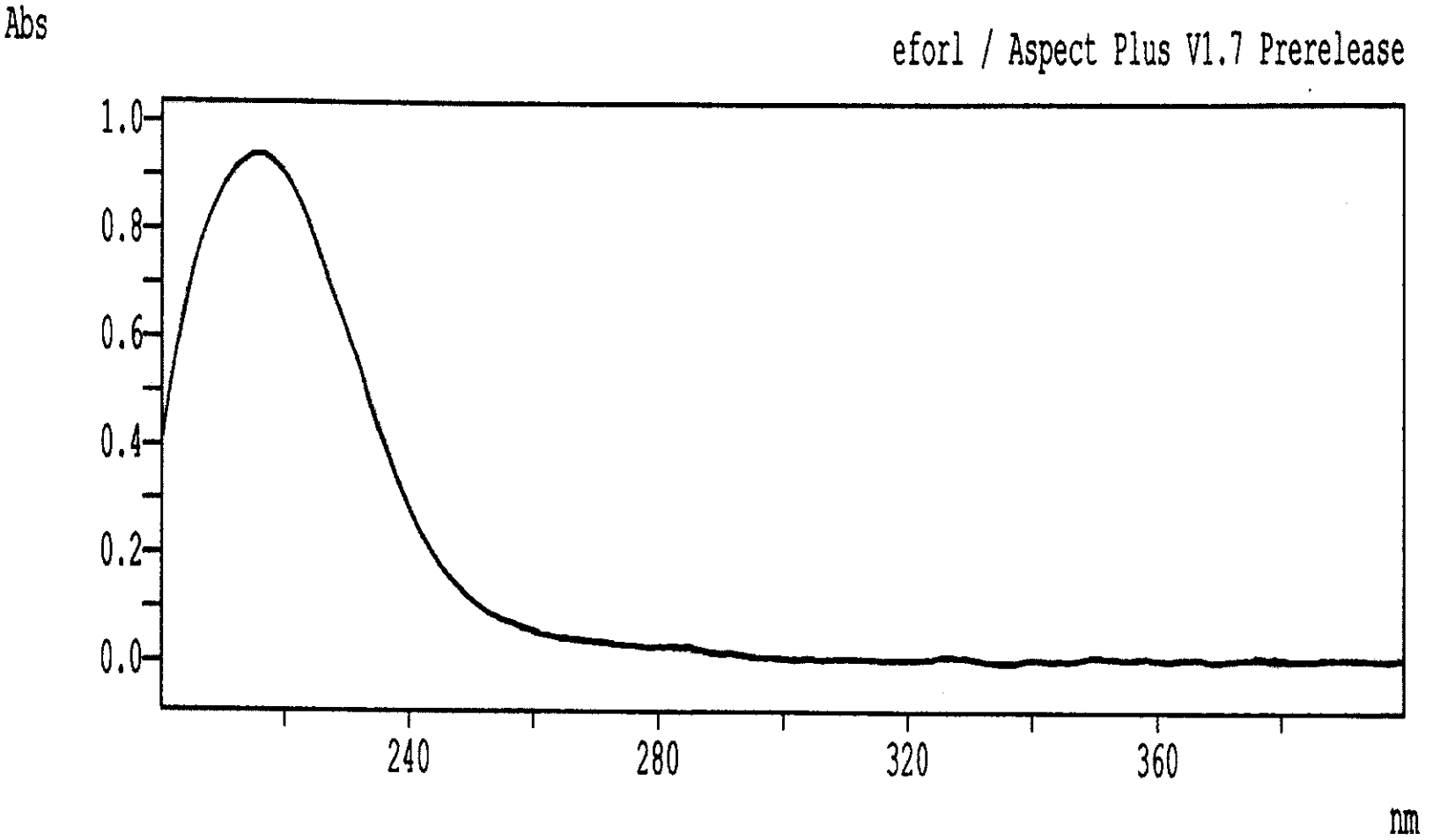


**Figure 59** UV (MeOH) spectrum of compound **XH2**

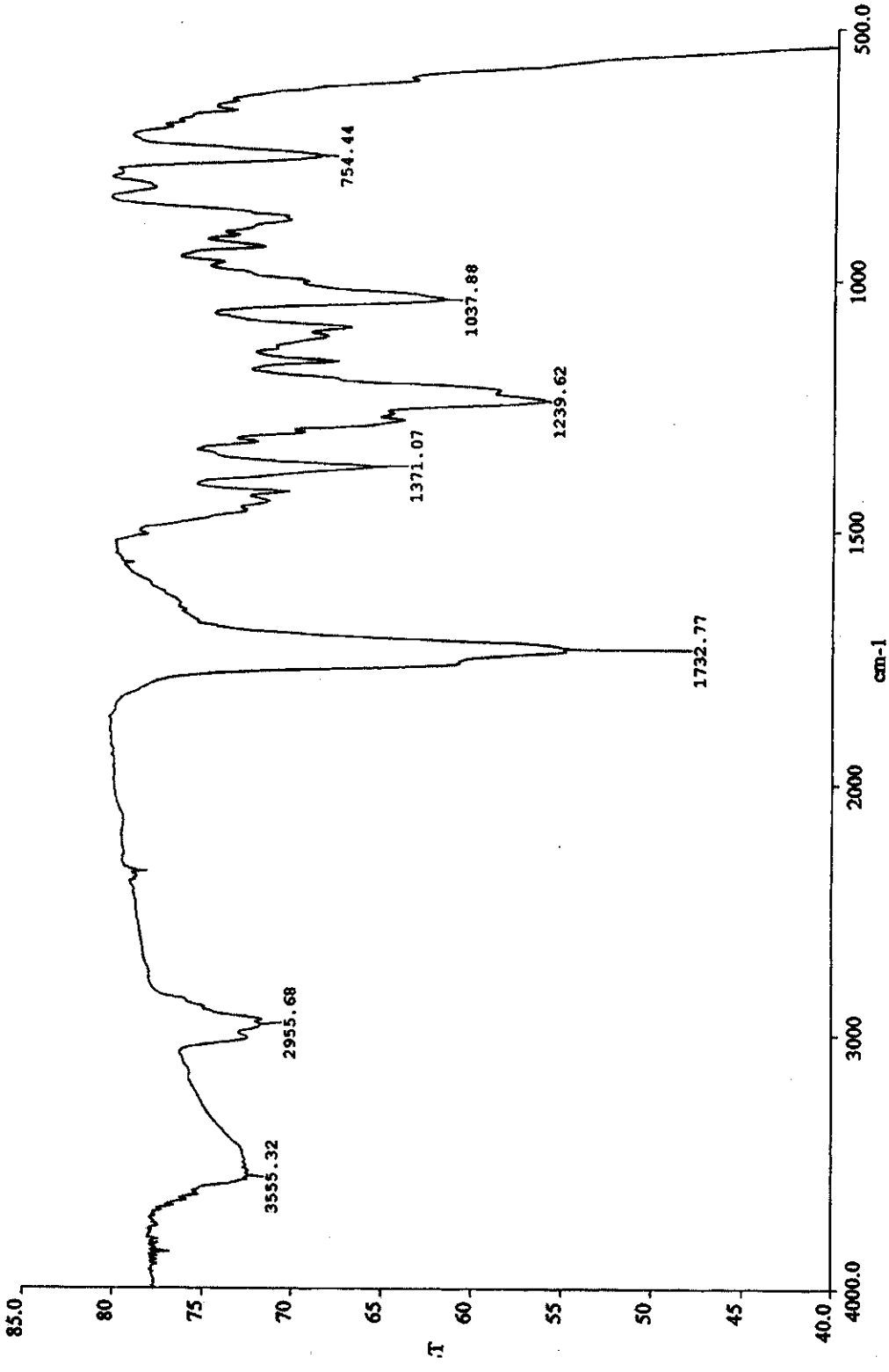


**Figure 60** IR (Neat) spectrum of compound **XH2**

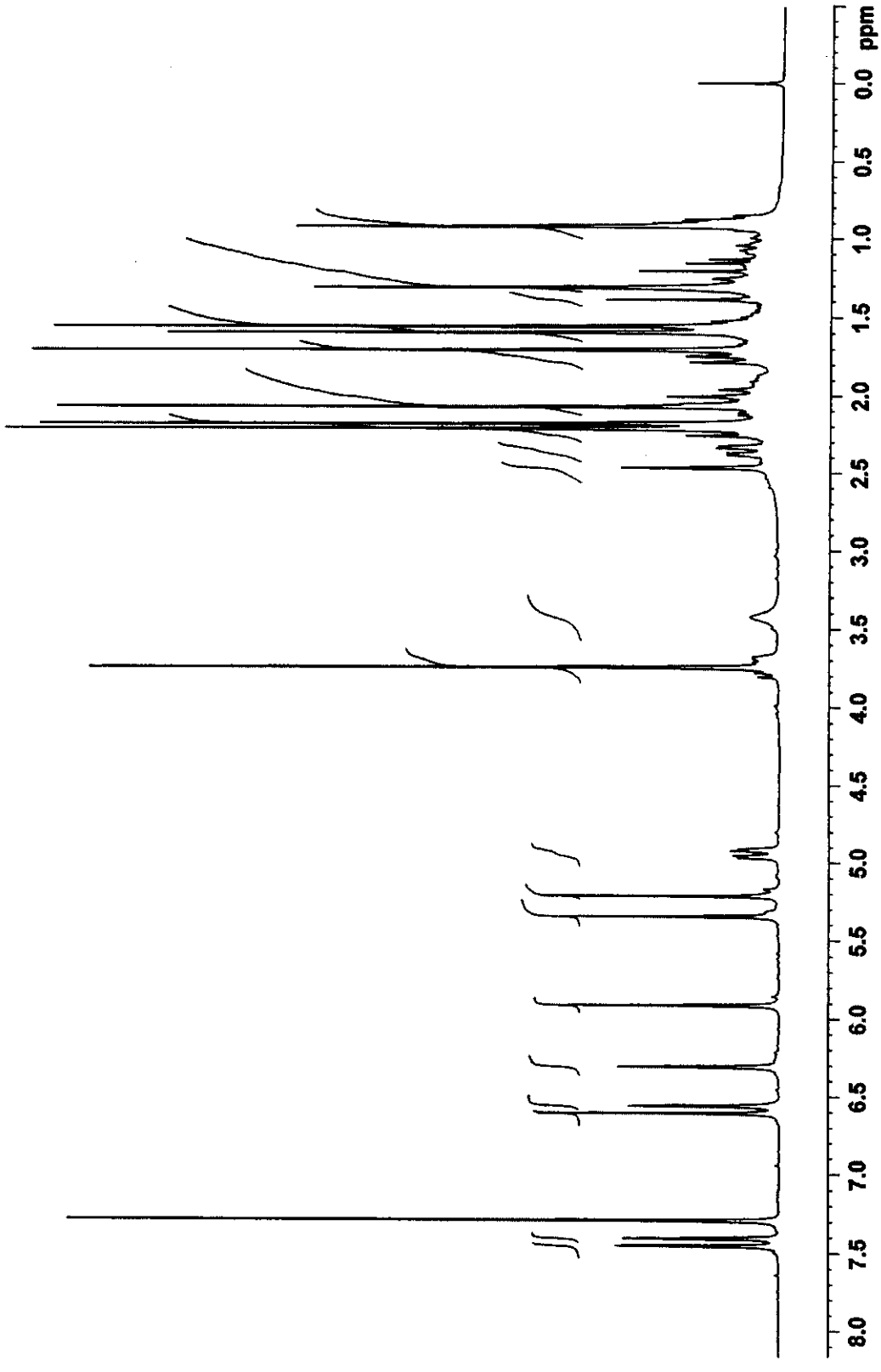


**Figure 61** $^{1}$H NMR (300 MHz, $CDCl_3$) spectrum of compound **XH2**

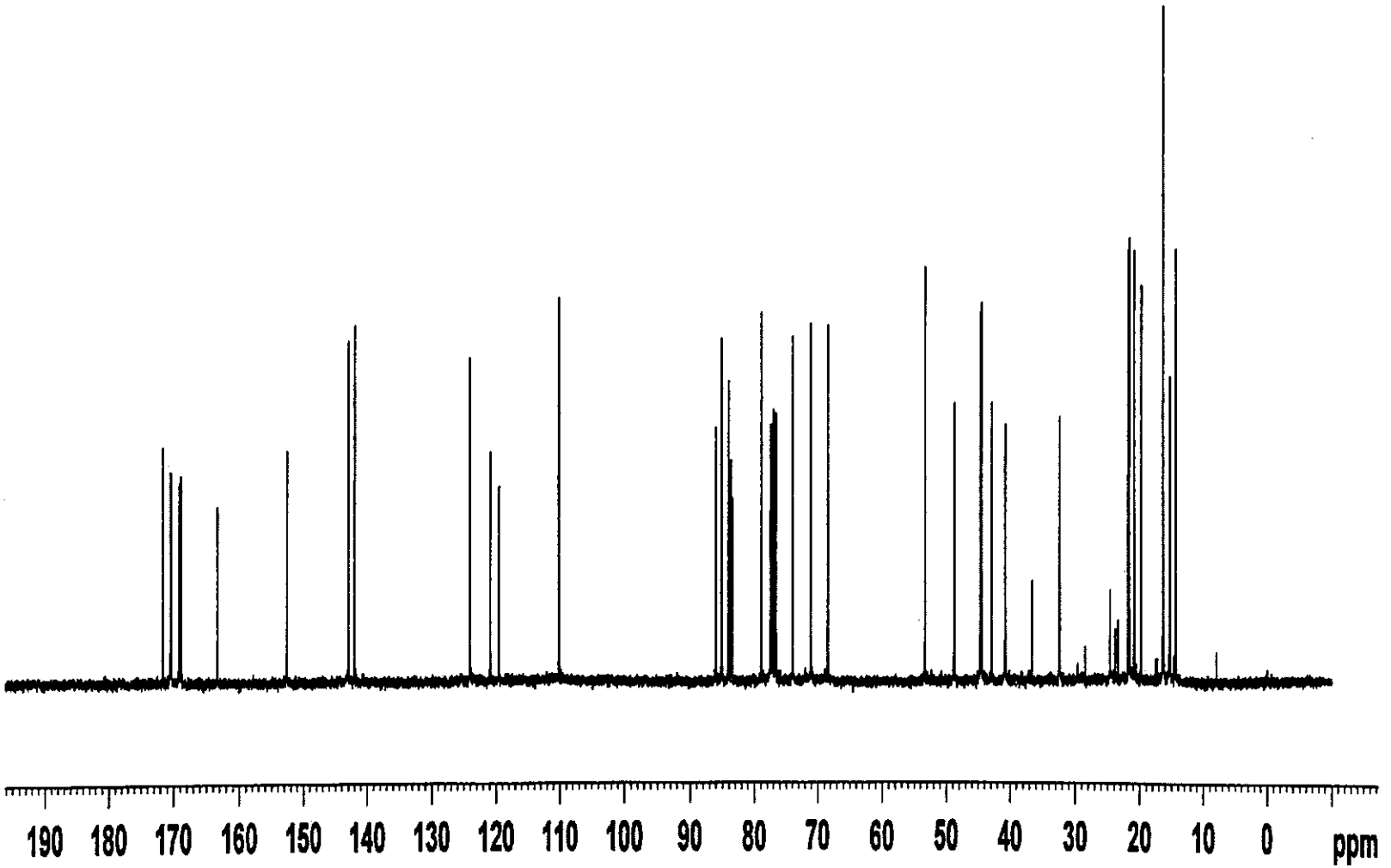


**Figure 62** $^{13}C$ NMR (75 MHz, $CDCl_3$) spectrum of compound **XH2**

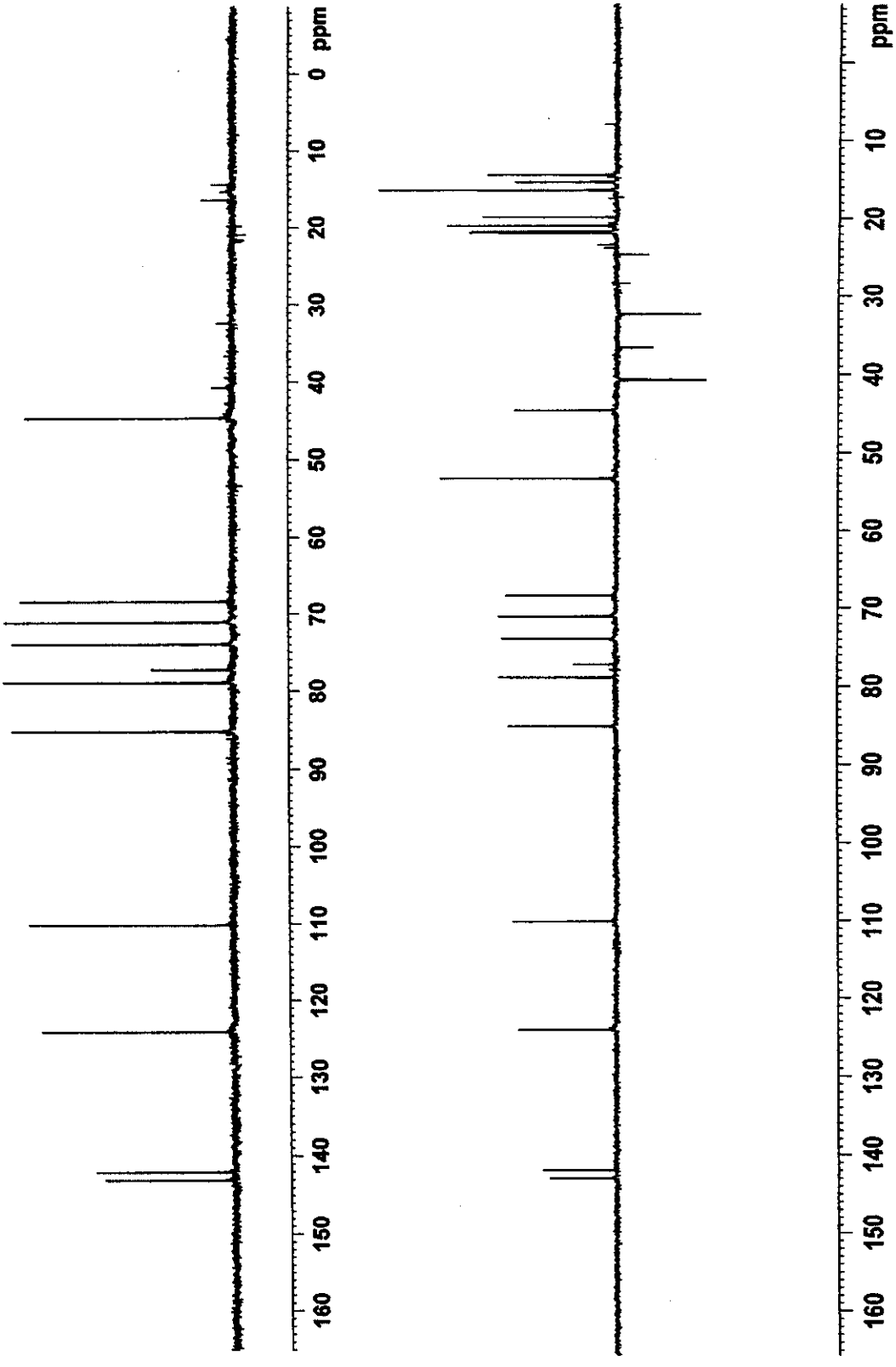


**Figure 63** DEPT ($CDCl_3$) spectrum of compound **XH2**

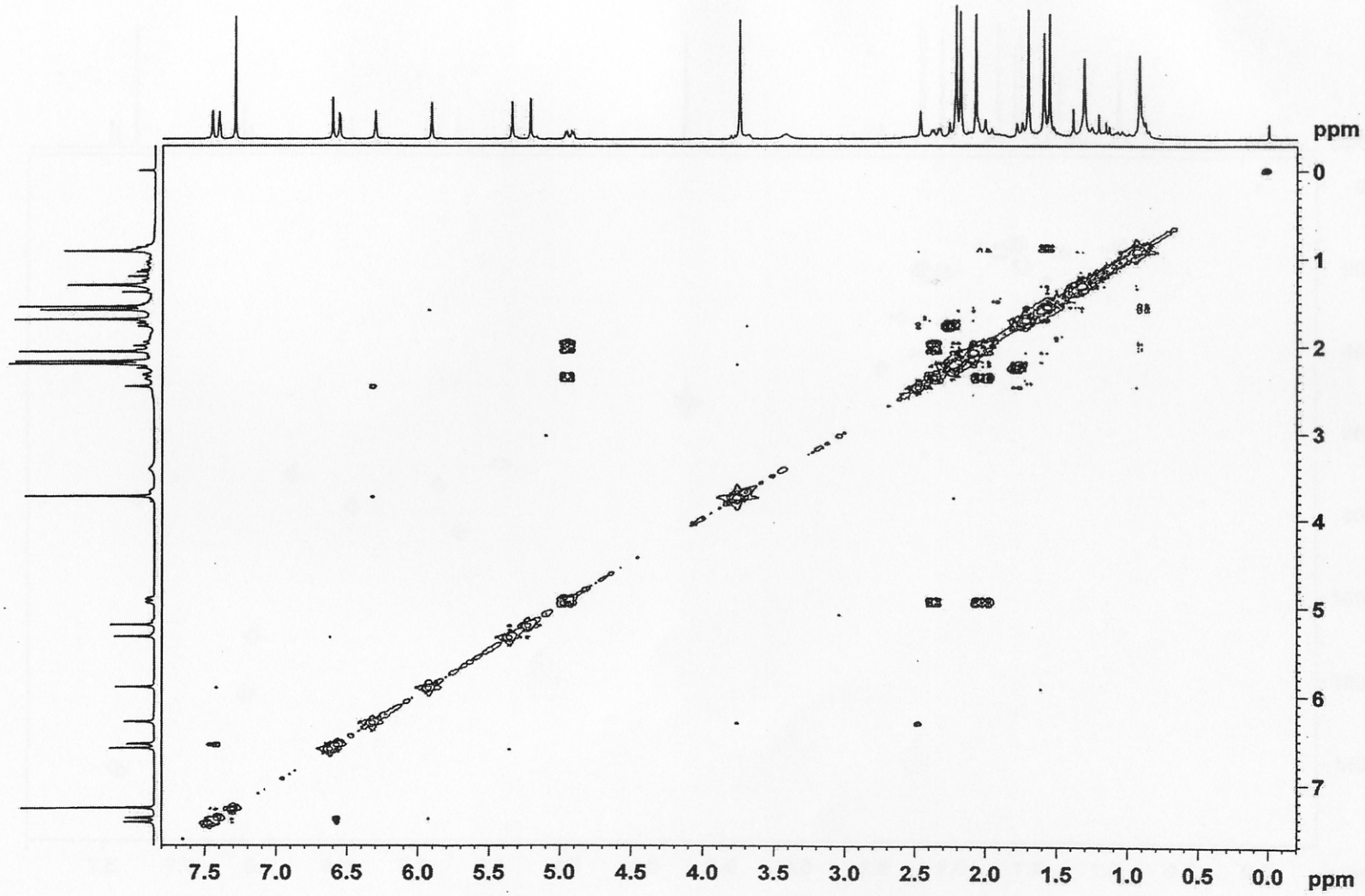


**Figure 64** 2D COSY spectrum of compound **XH2**

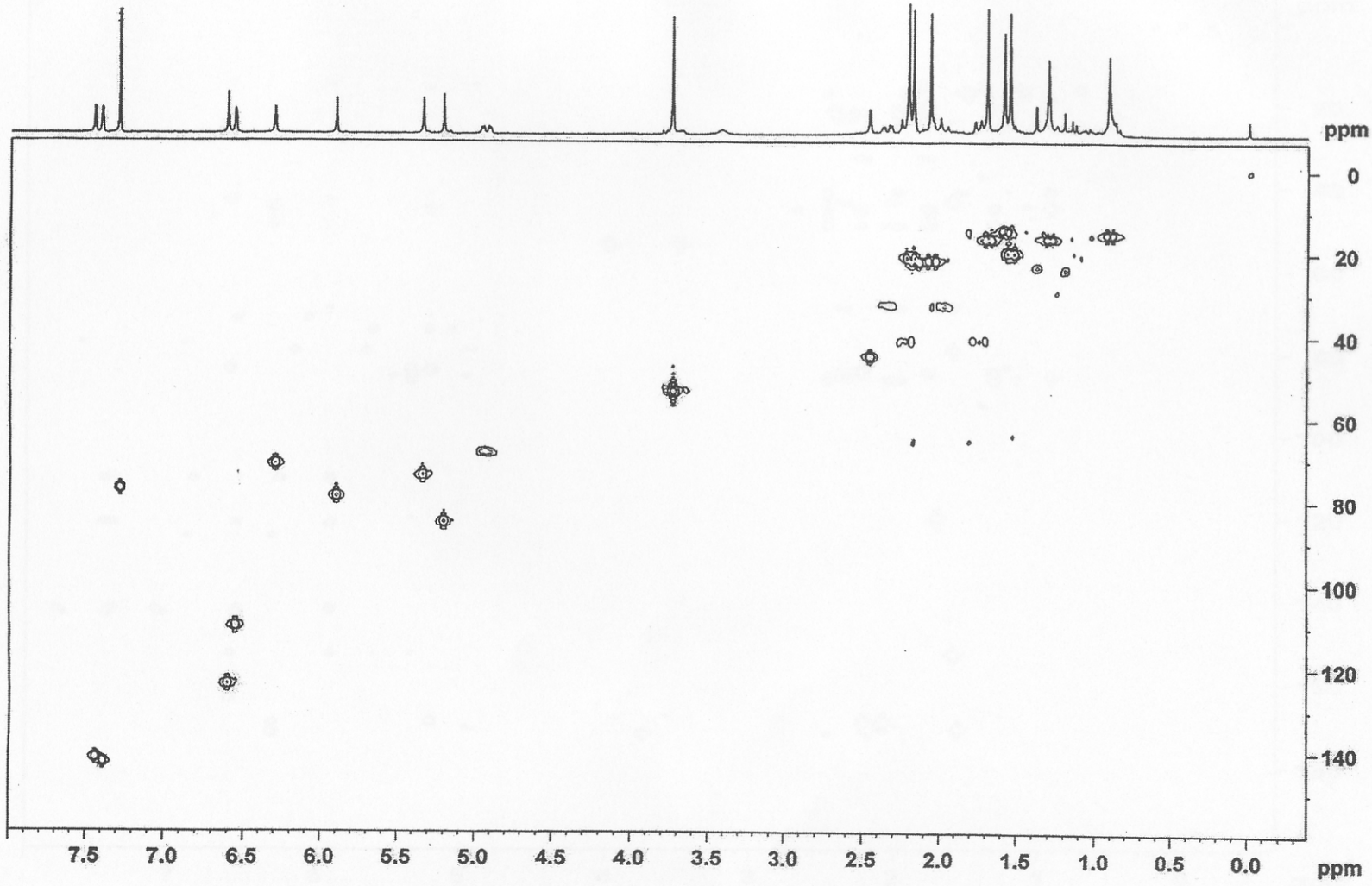


**Figure 65** 2D HMQC spectrum of compound **XH2**

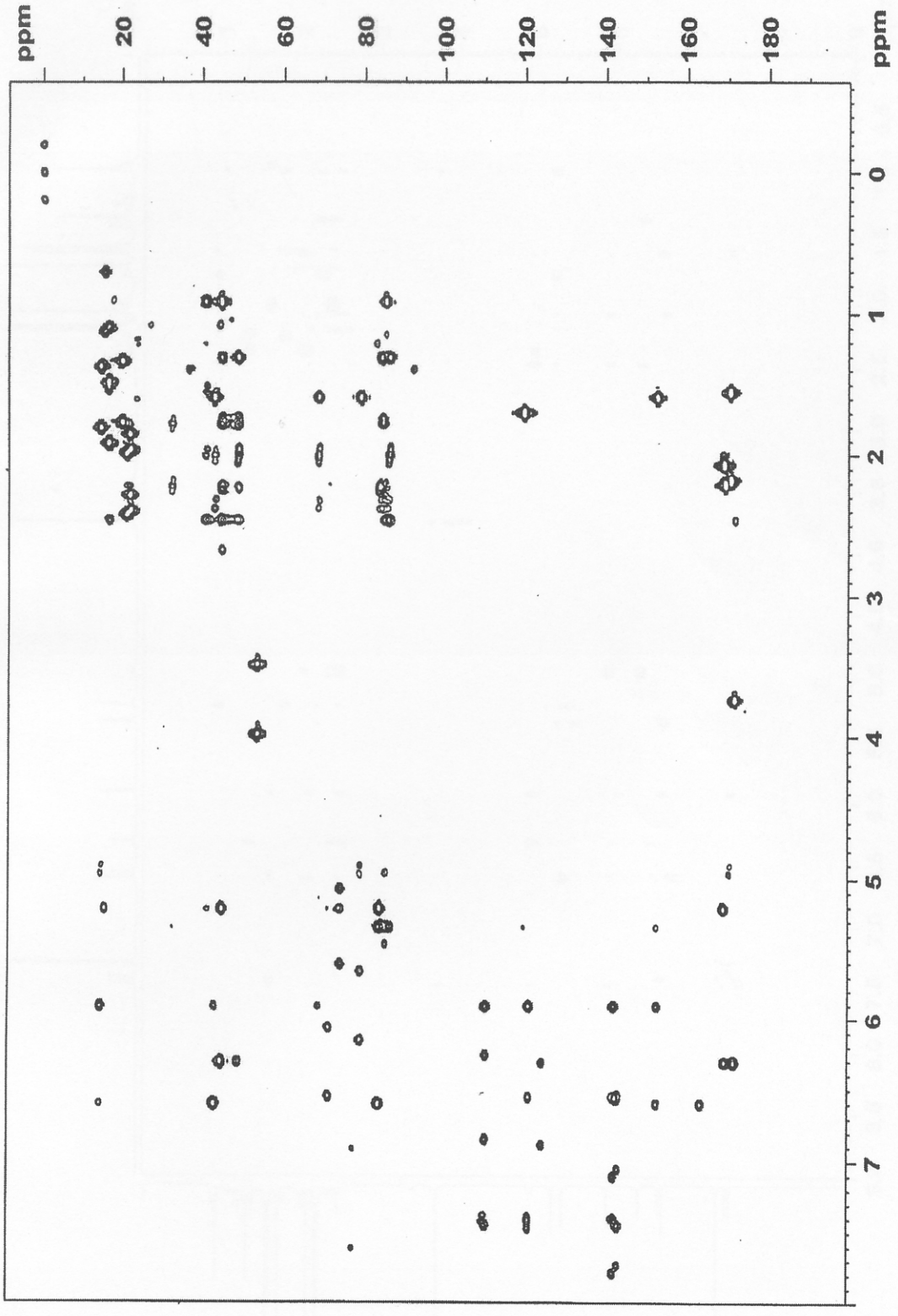


**Figure 66** 2D HMBC spectrum of compound **XH2**

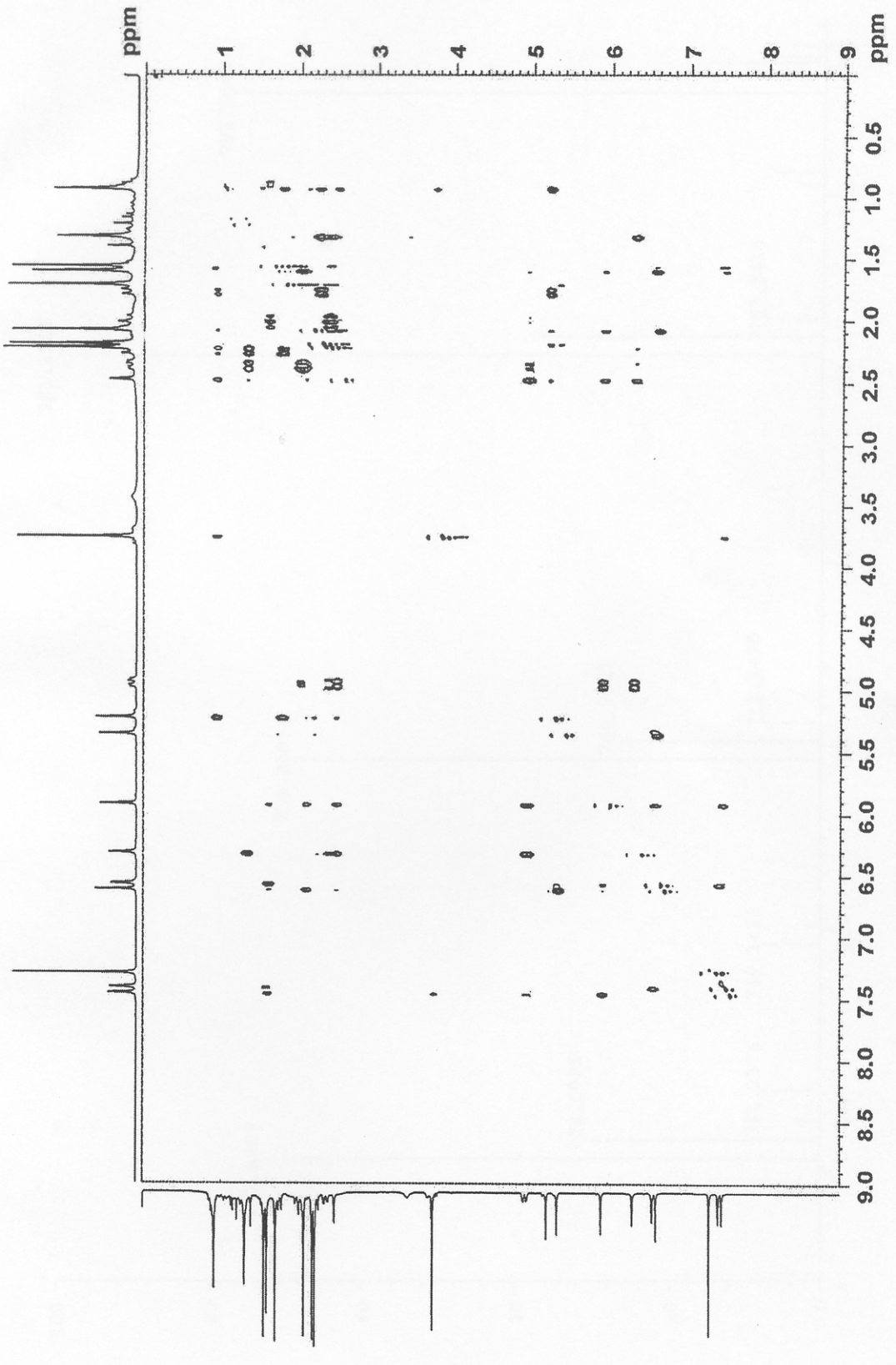


Figure 67 NOESY spectrum of compound **XH2**

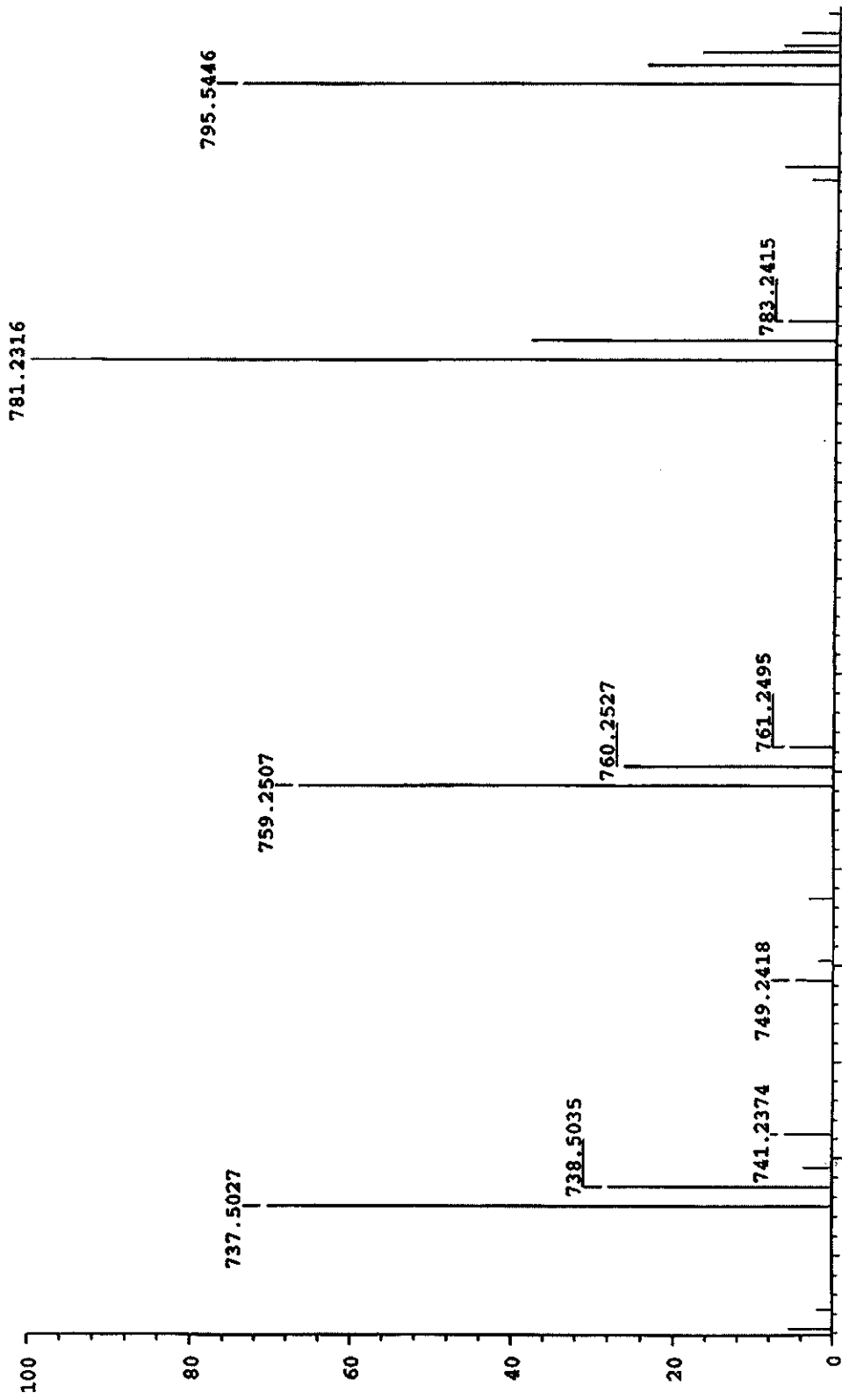


**Figure 68** Mass spectrum of compound **XH2**

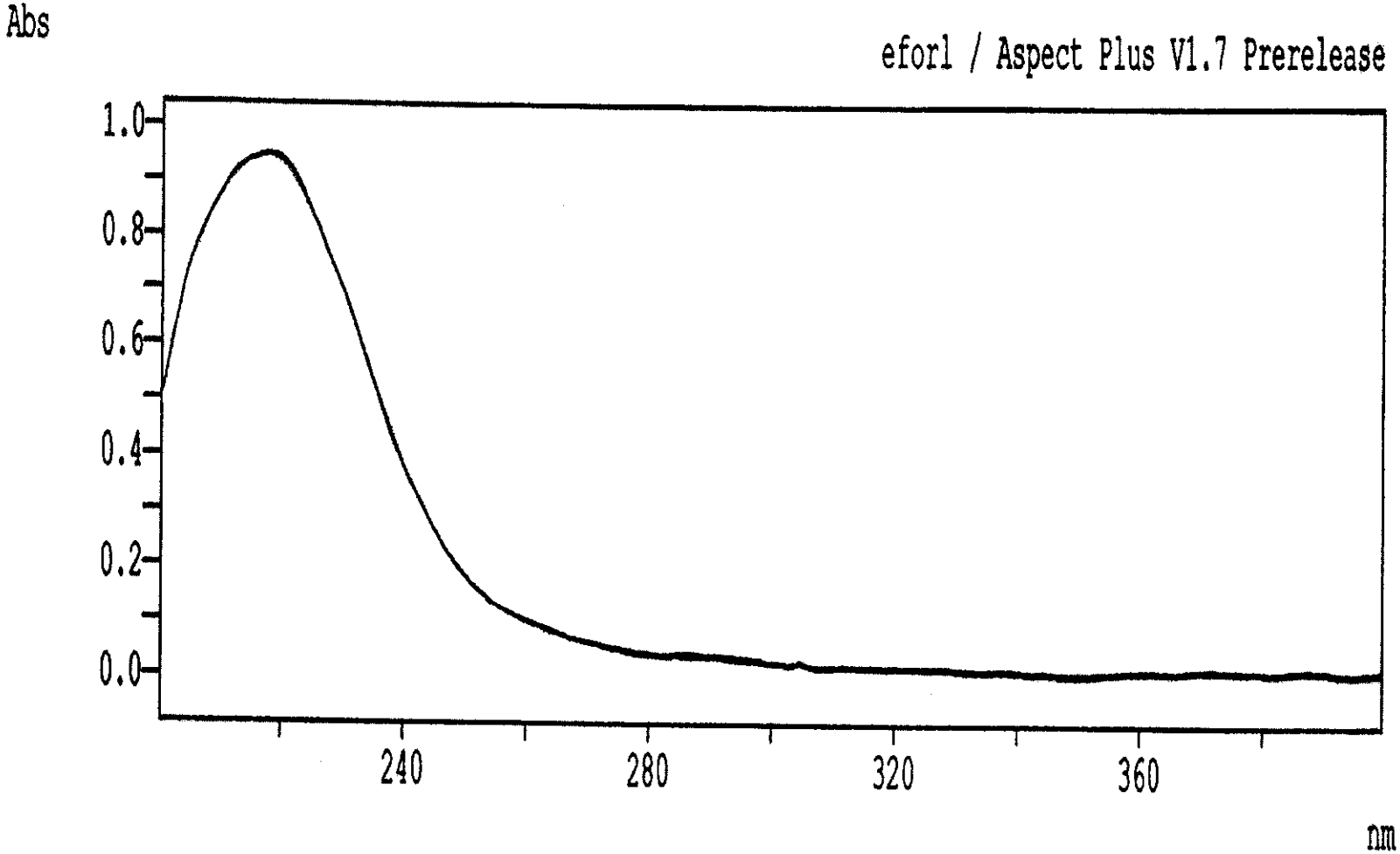


**Figure 69** UV (MeOH) spectrum of compound **XH3**

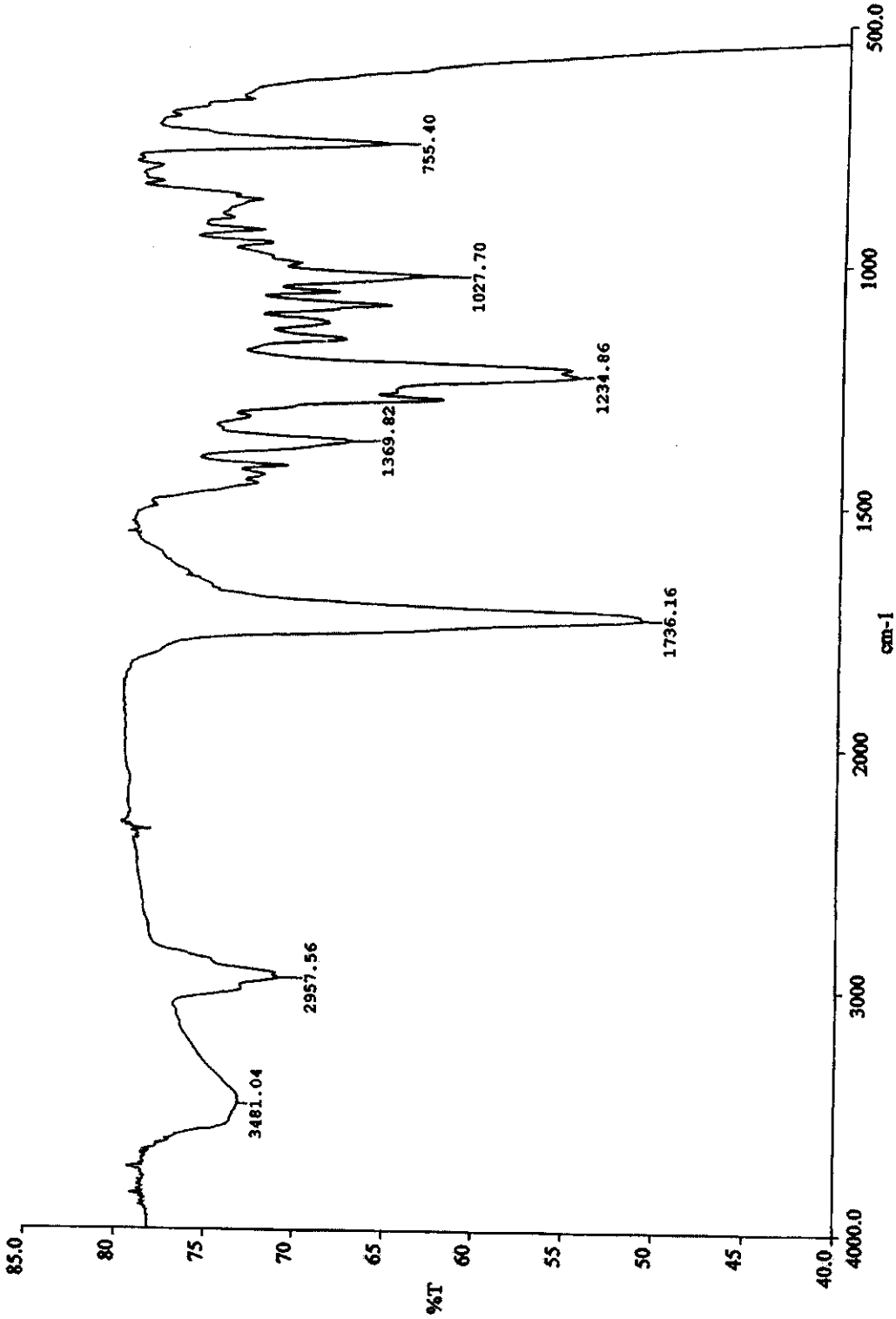


**Figure 70** IR (Neat) spectrum of compound **XH3**

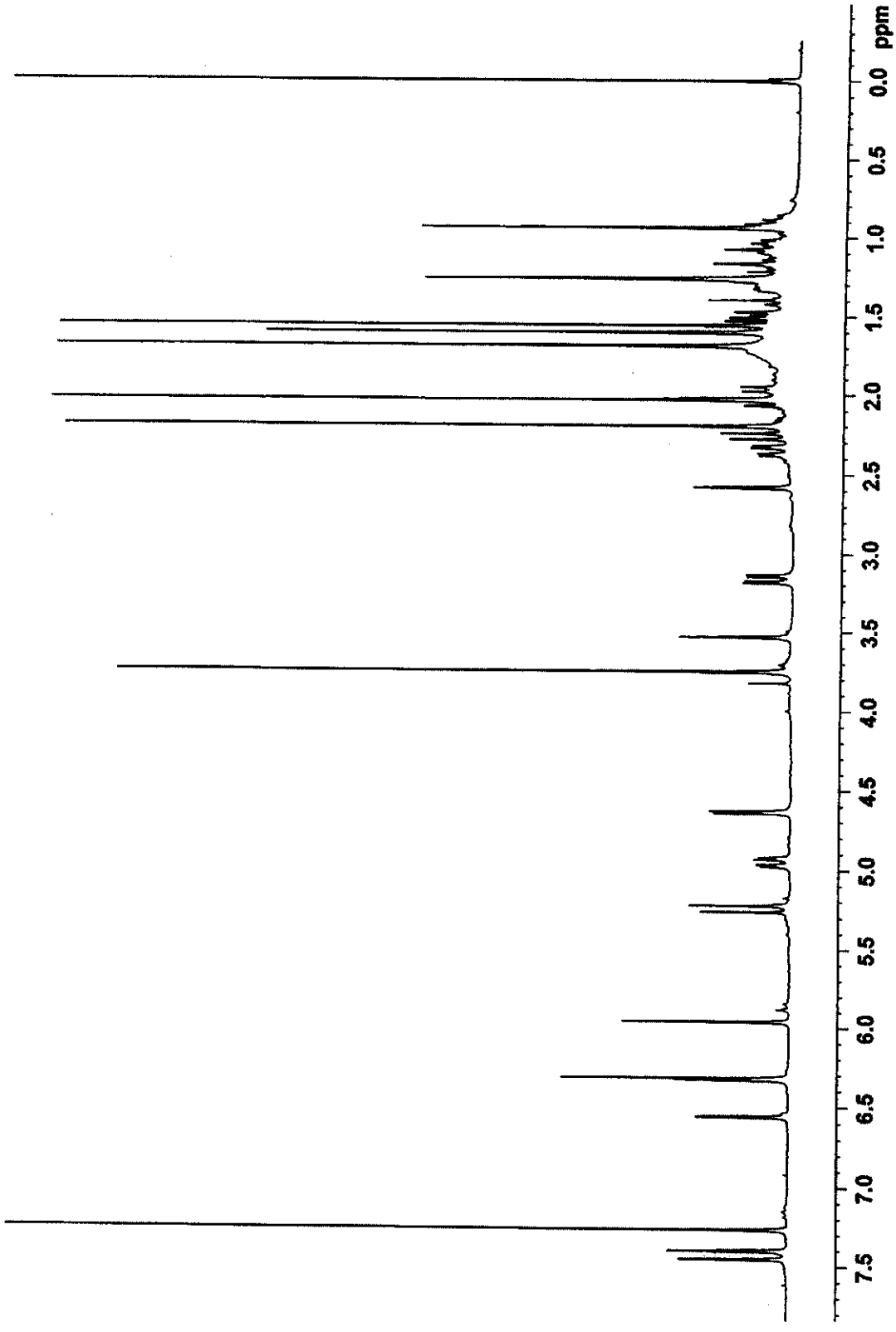


**Figure 71** $^{1}$H NMR (300 MHz, $CDCl_3$) spectrum of compound **XH3**

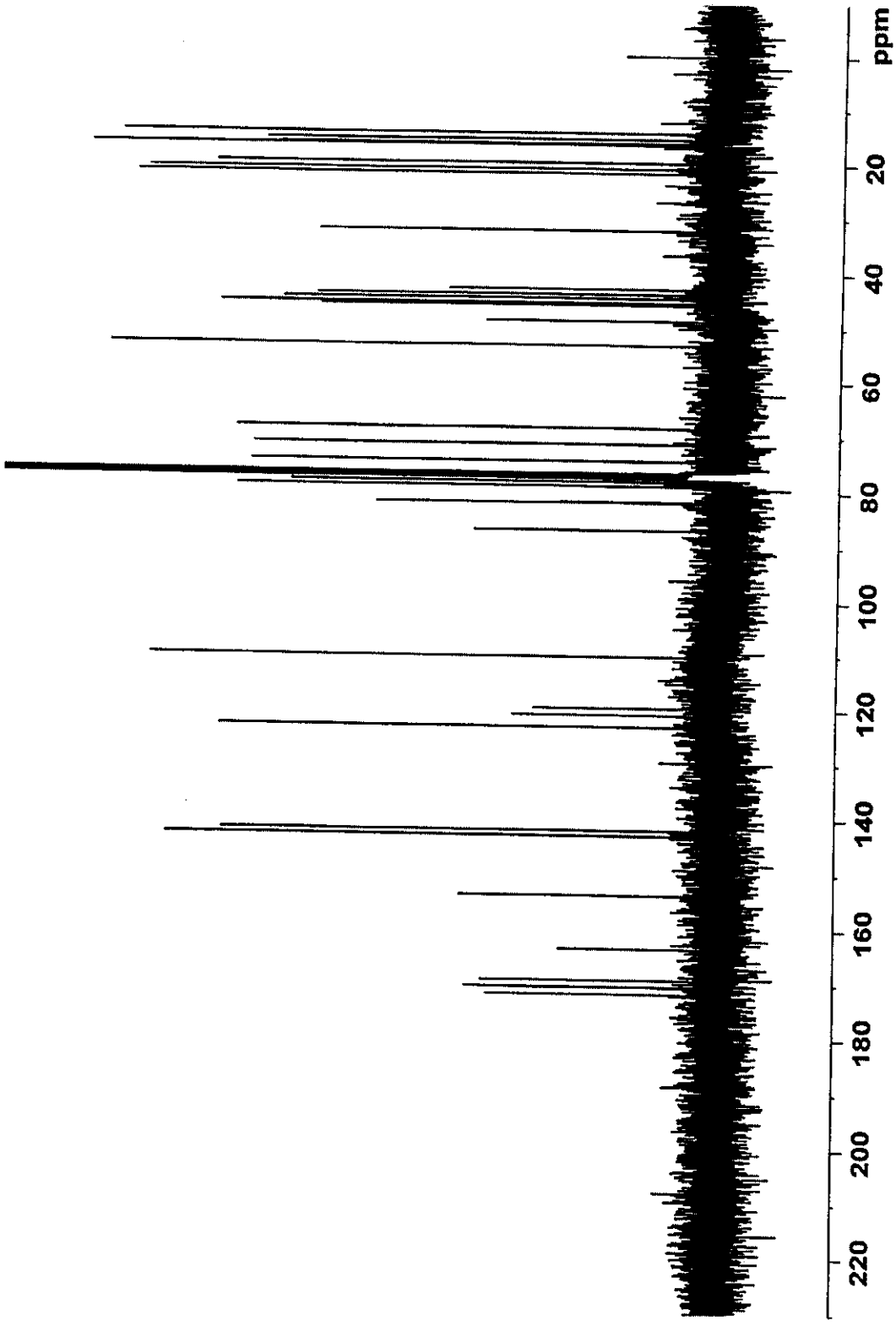


**Figure 72** $^{13}C$ NMR (75 MHz, $CDCl_3$) spectrum of compound **XH3**

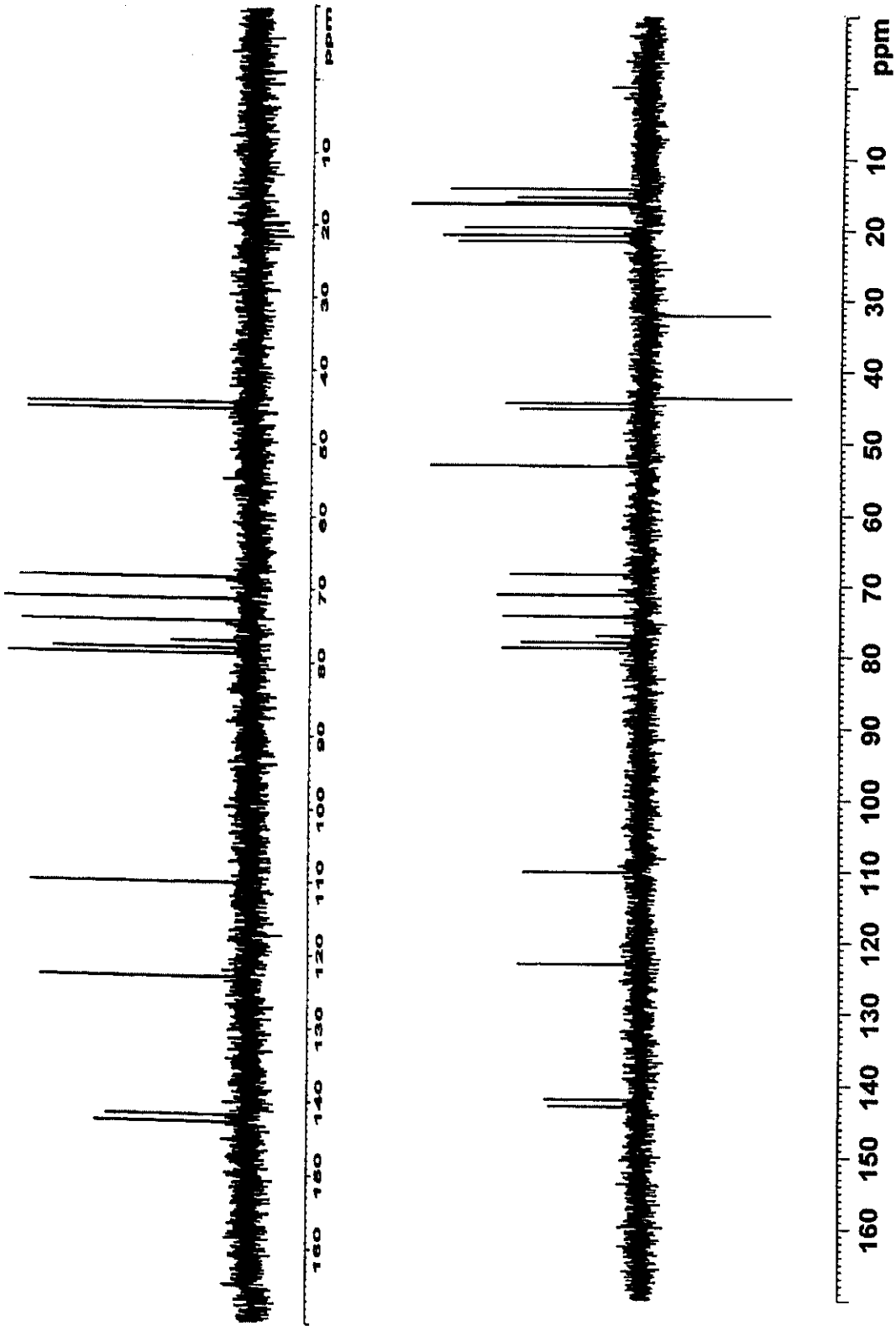


Figure 73 DEPT ($CDCl_3$) spectrum of compound **XH3**

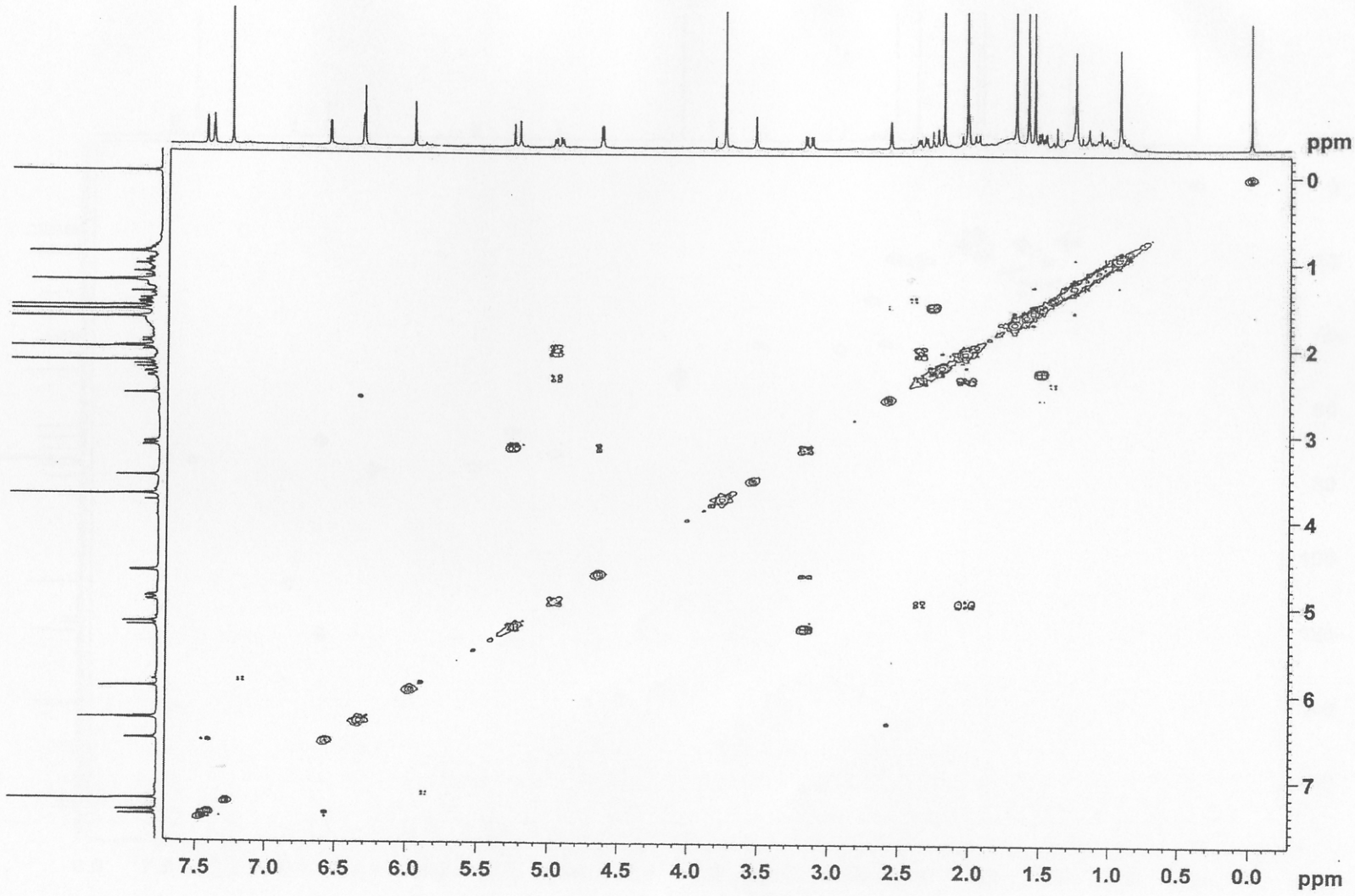


**Figure 74** 2D COSY spectrum of compound **XH3**

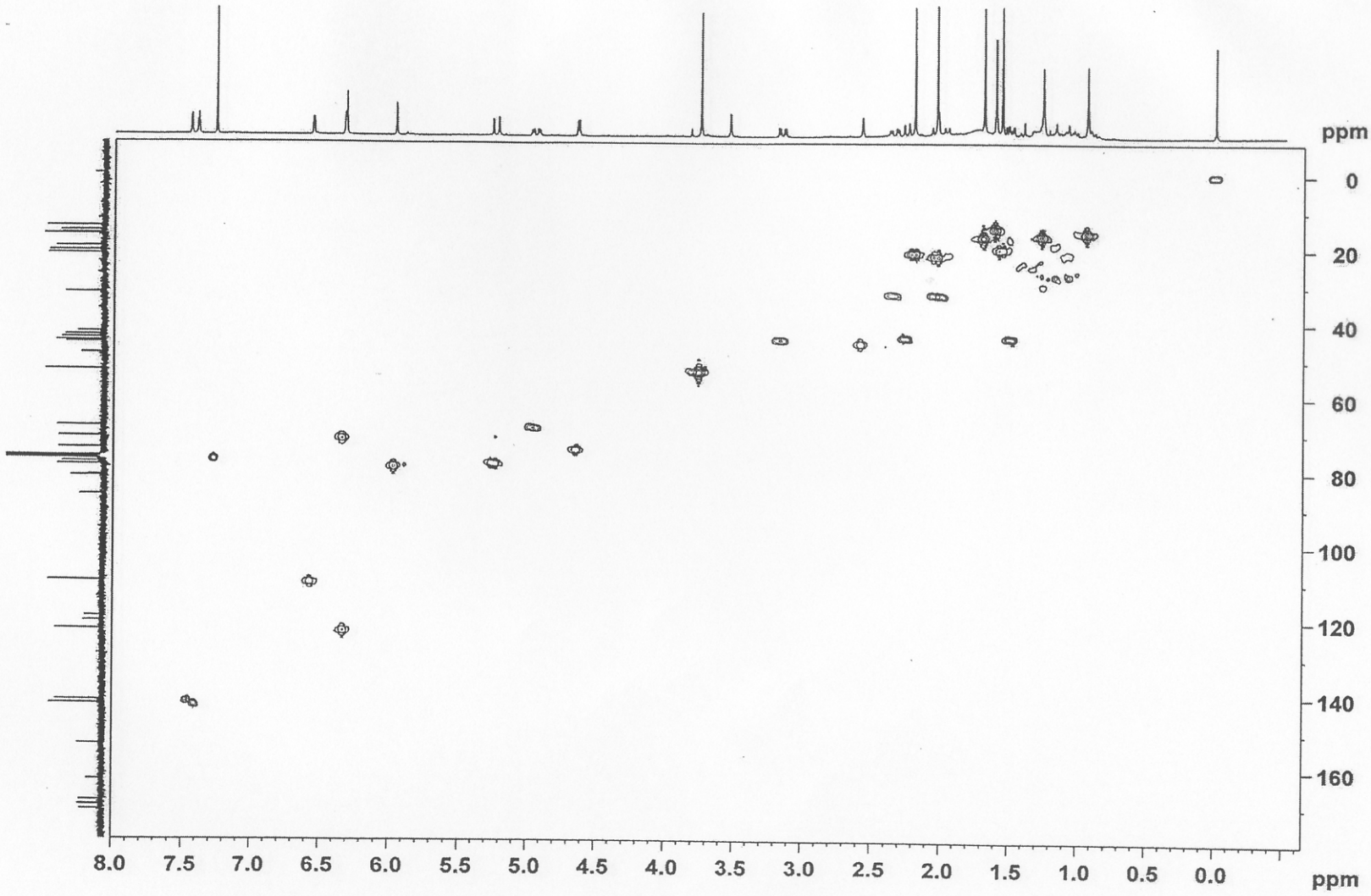


**Figure 75** 2D HMQC spectrum of compound **XH3**

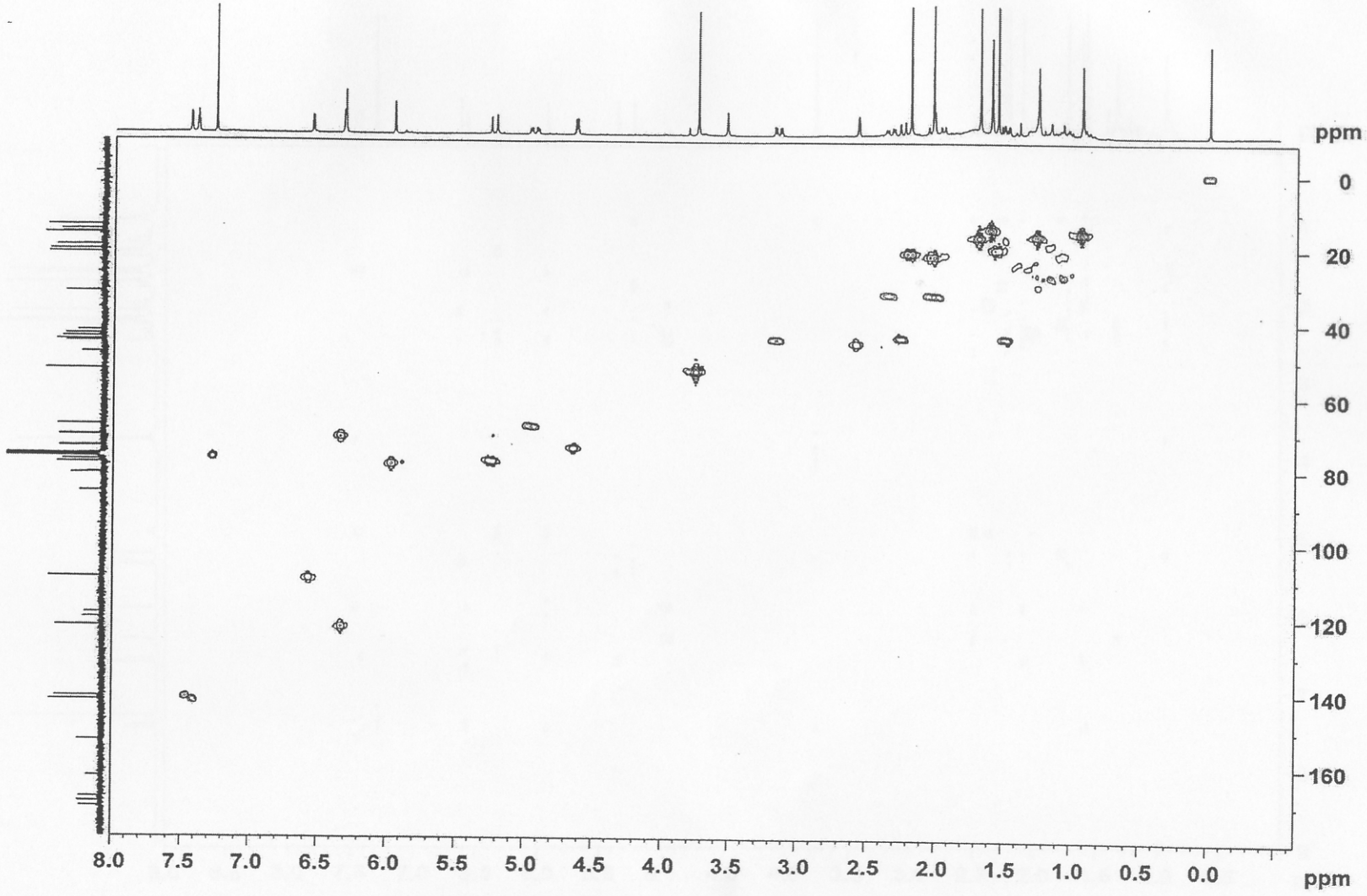


**Figure 76** 2D HMBC spectrum of compound **XH3**

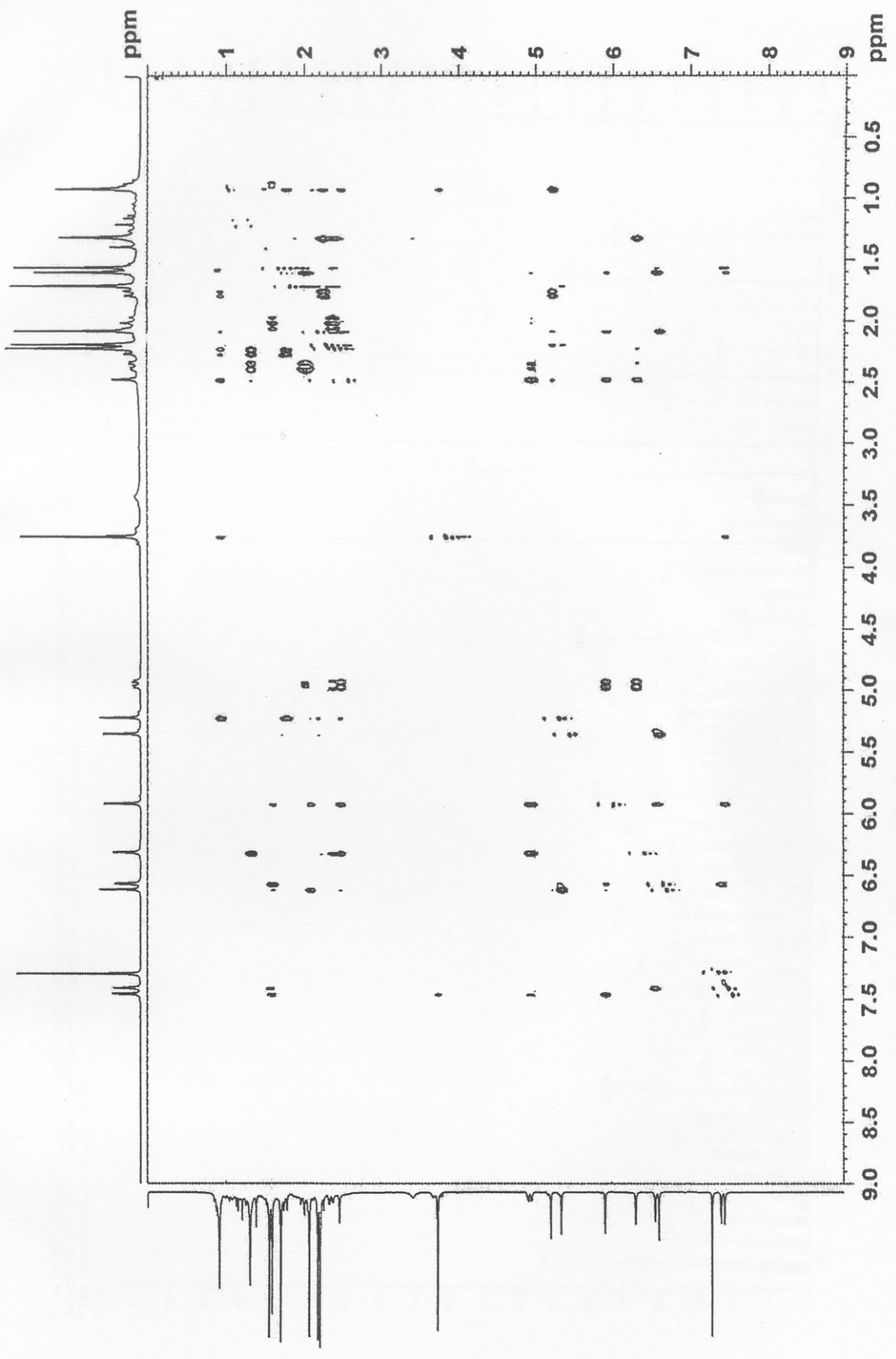


**Figure 77** NOESY spectrum of compound **XH3**

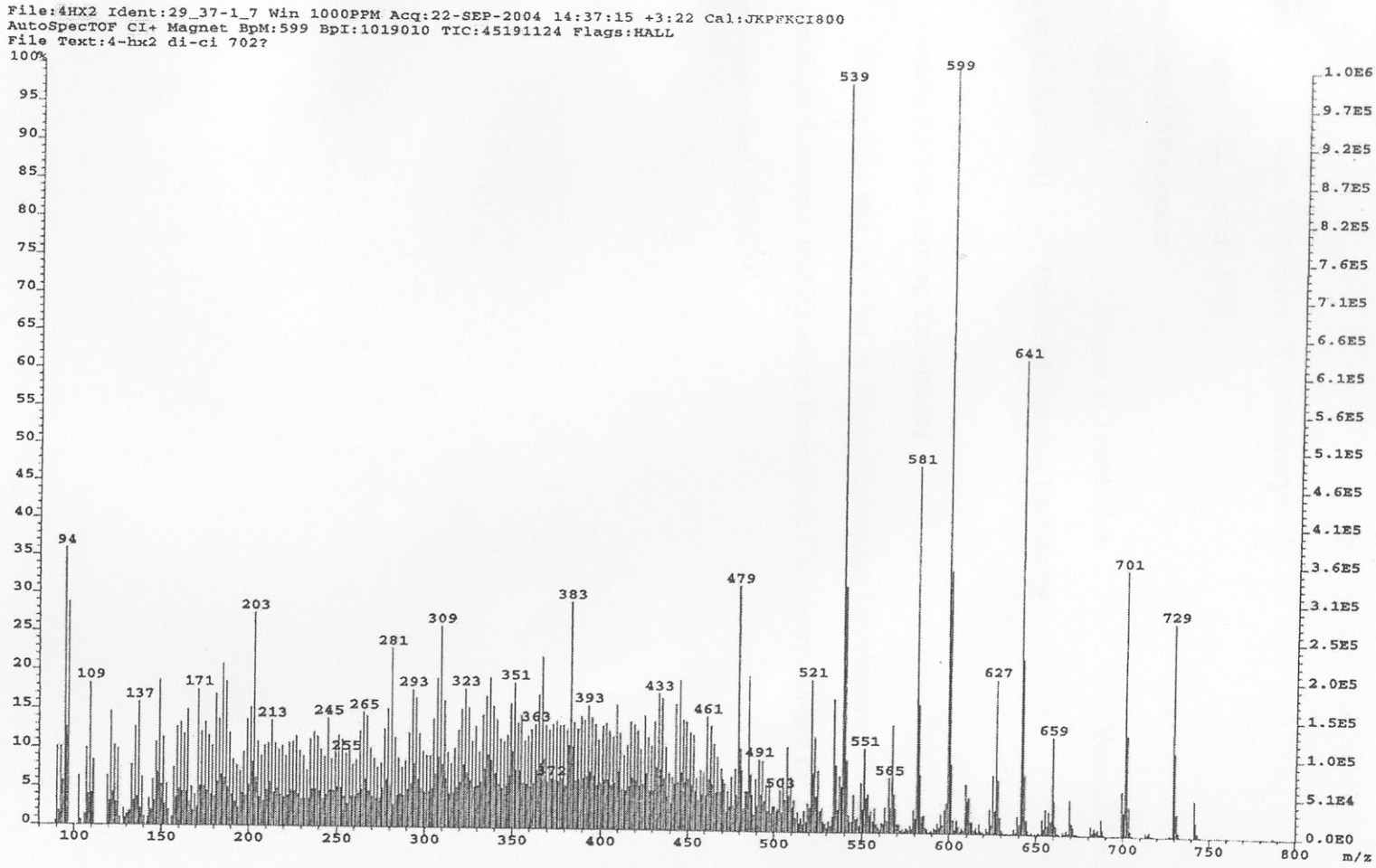


**Figure 78** Mass spectrum of compound **XH3**