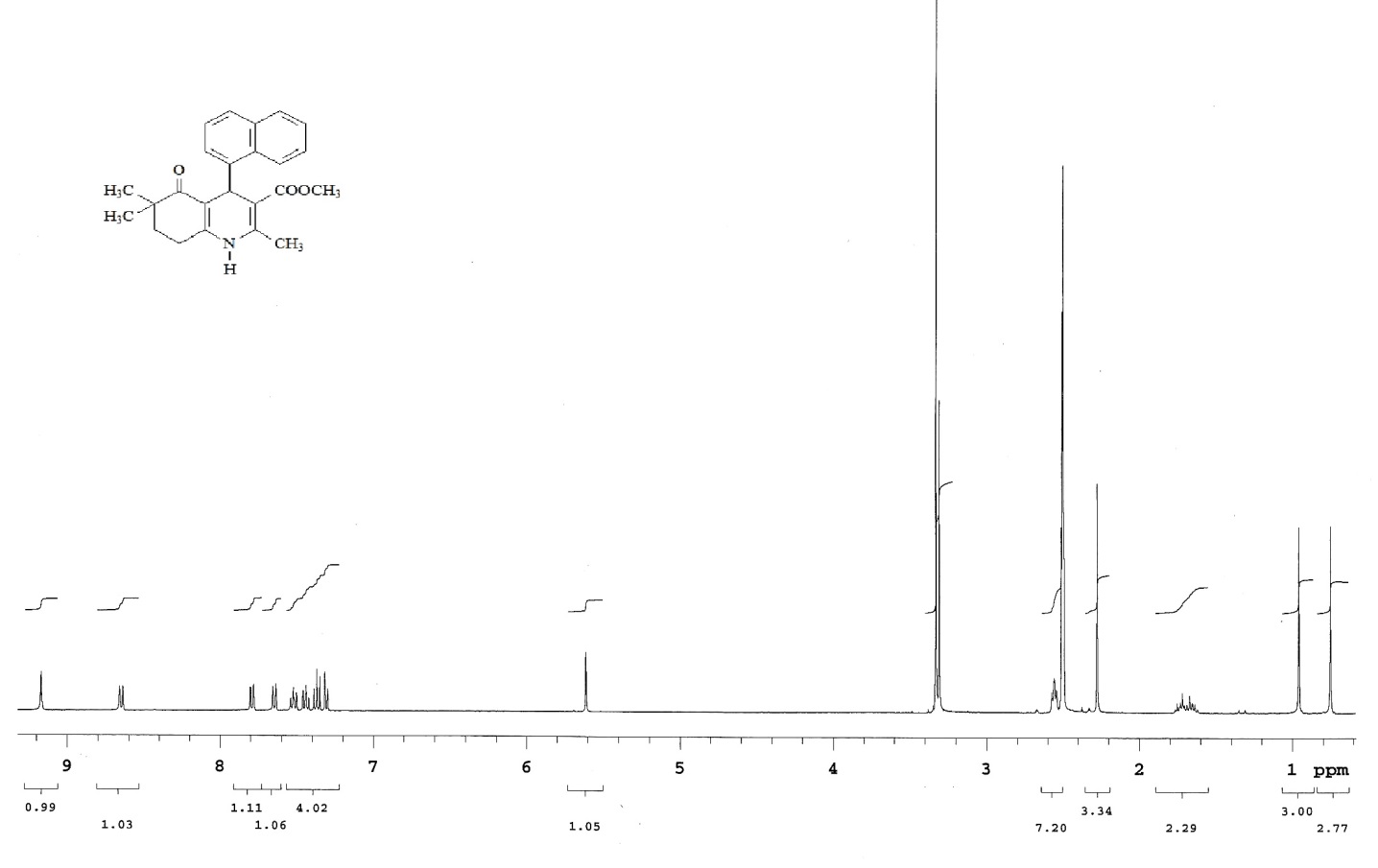
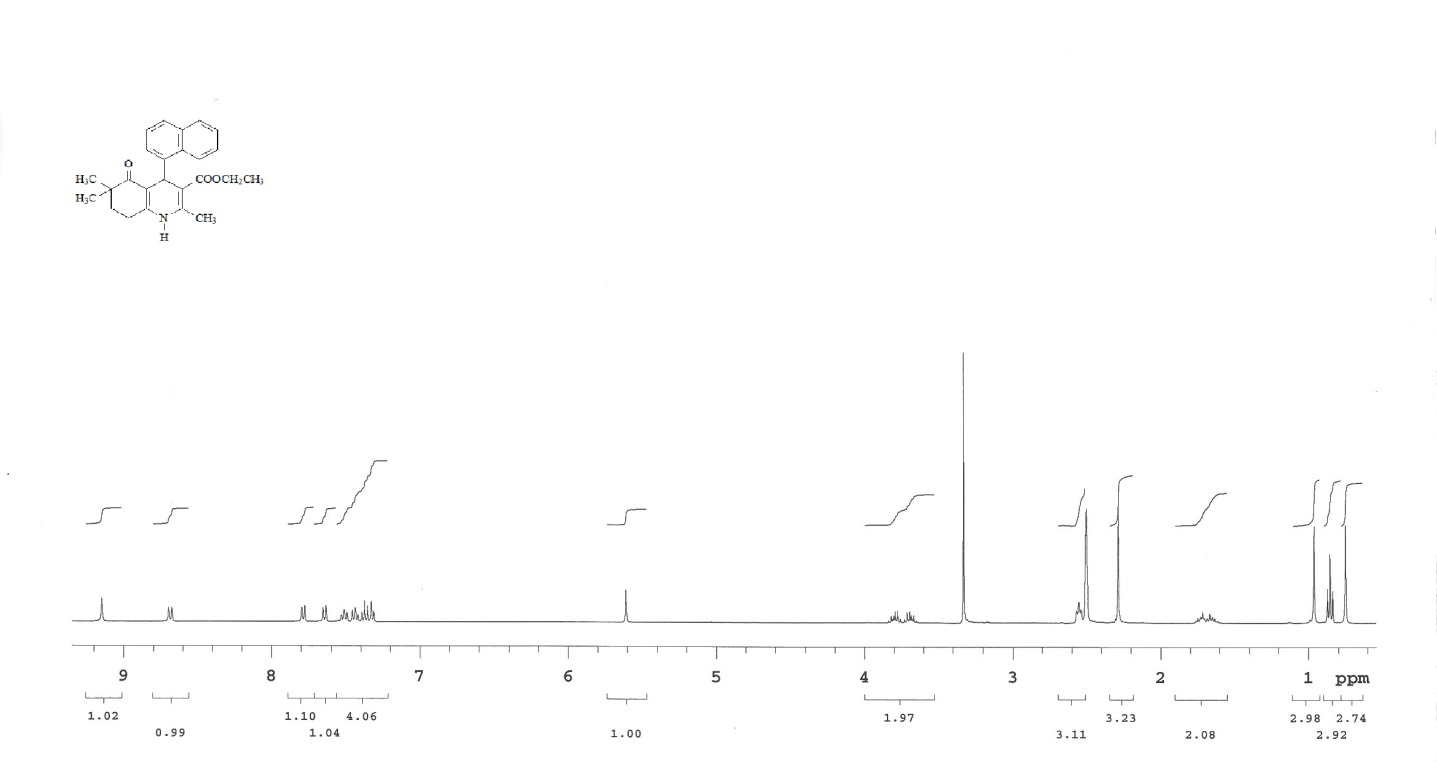
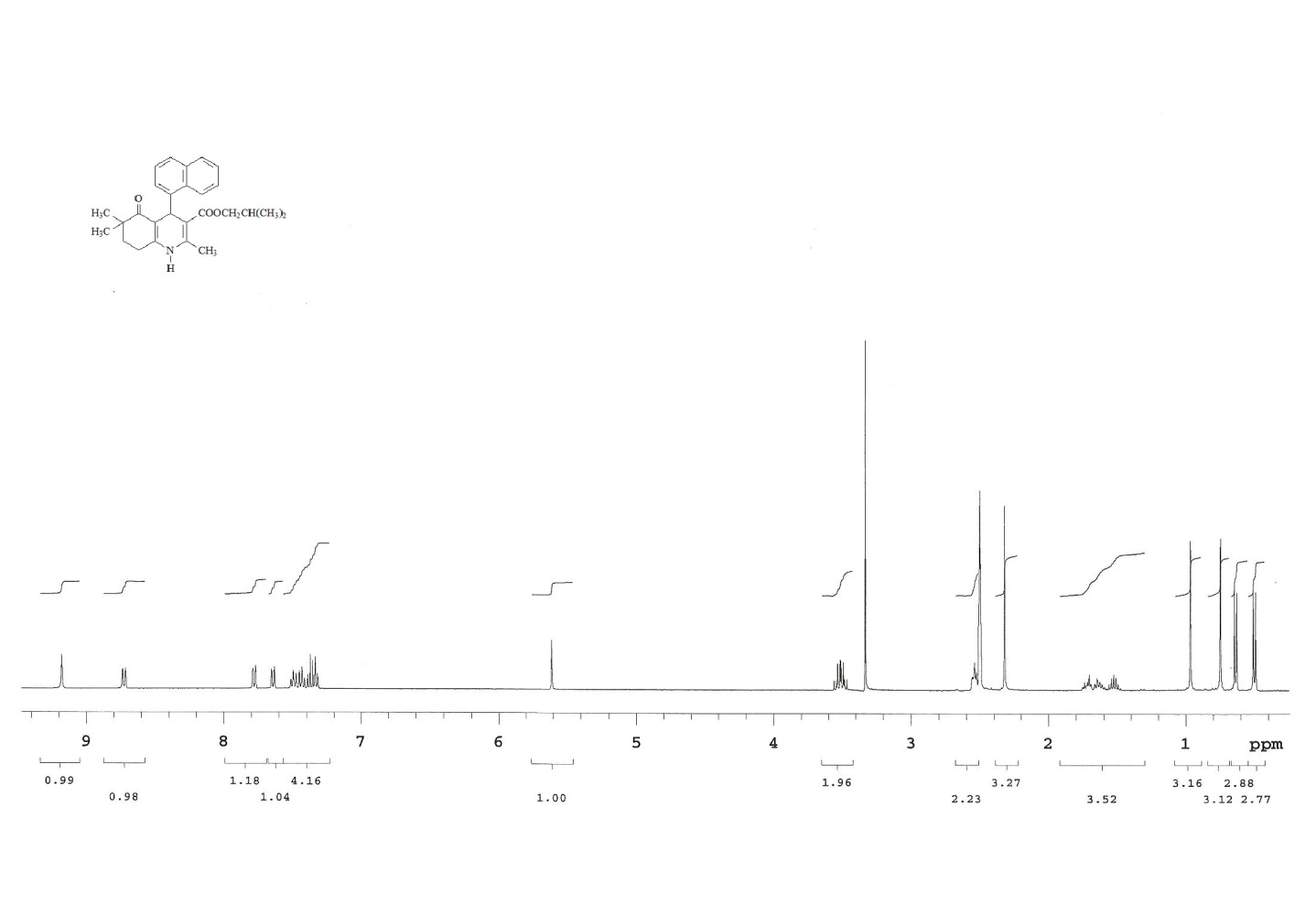
**Synthesis, Structural Characterization and Myorelaxant Activity of 4-Naphthyl-Hexahydroquinoline Derivatives Containing Different Ester Groups**

****

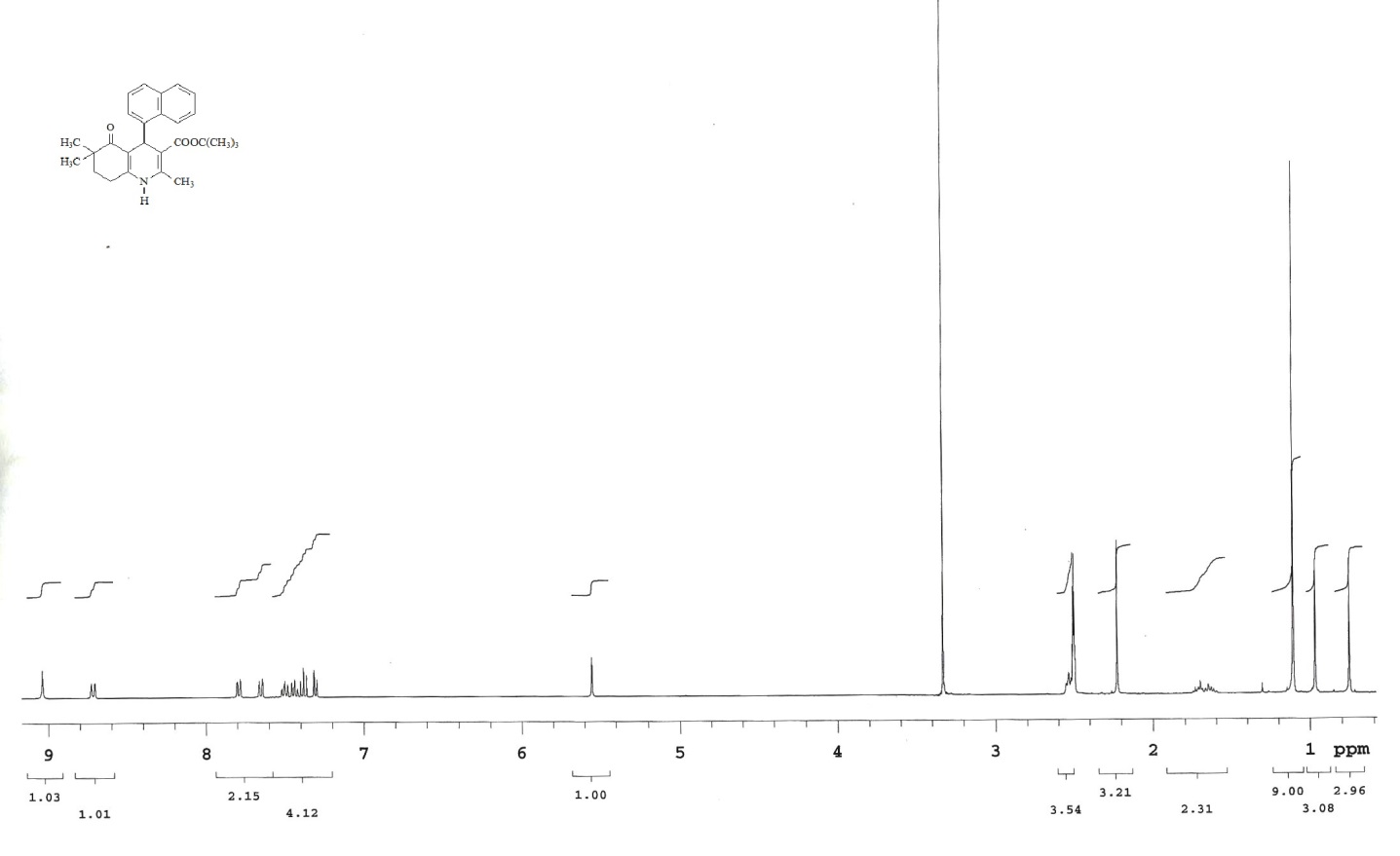
1H-NMR spectrum of compound **1**

****

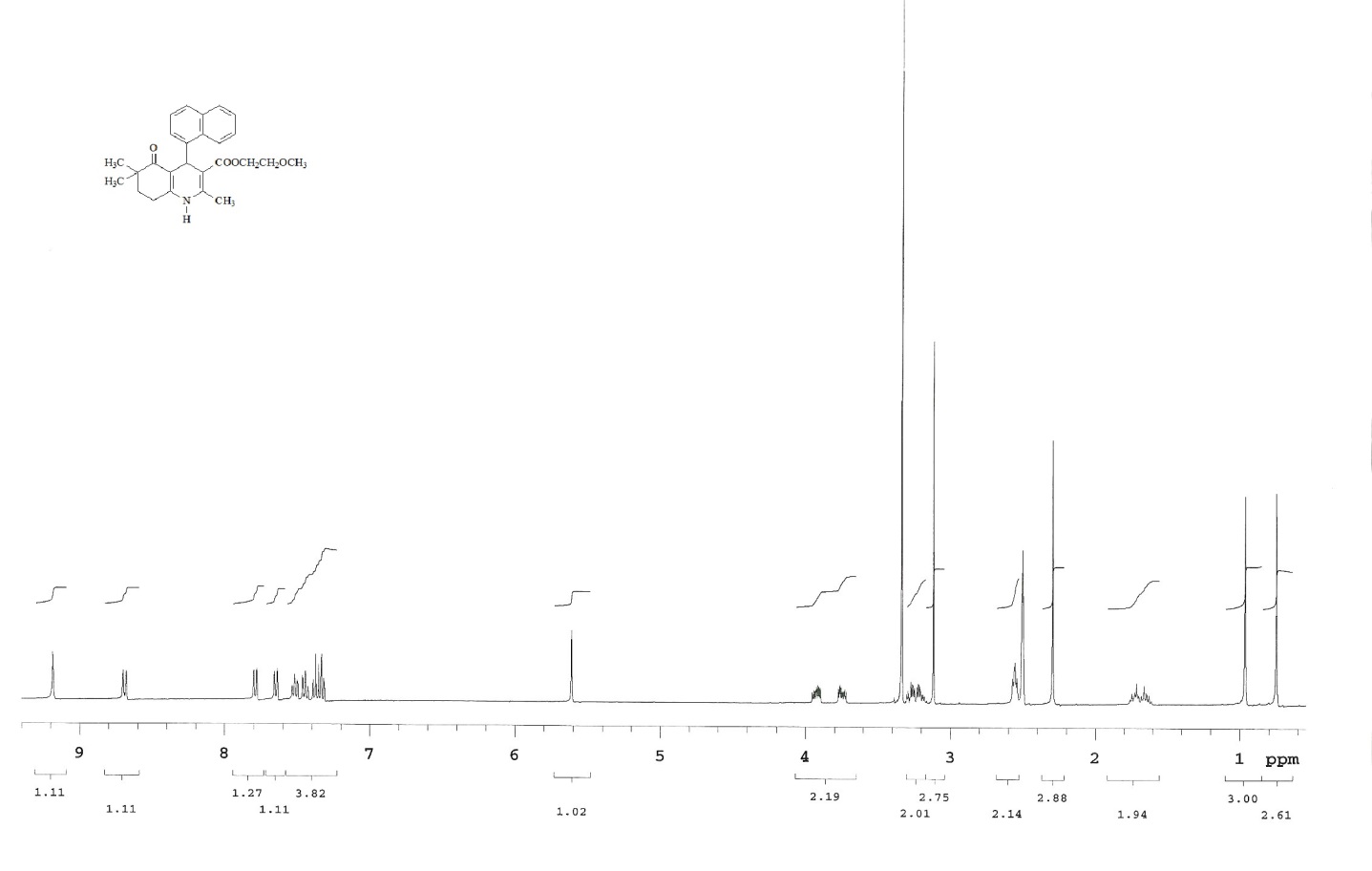
1H-NMR spectrum of compound **2**



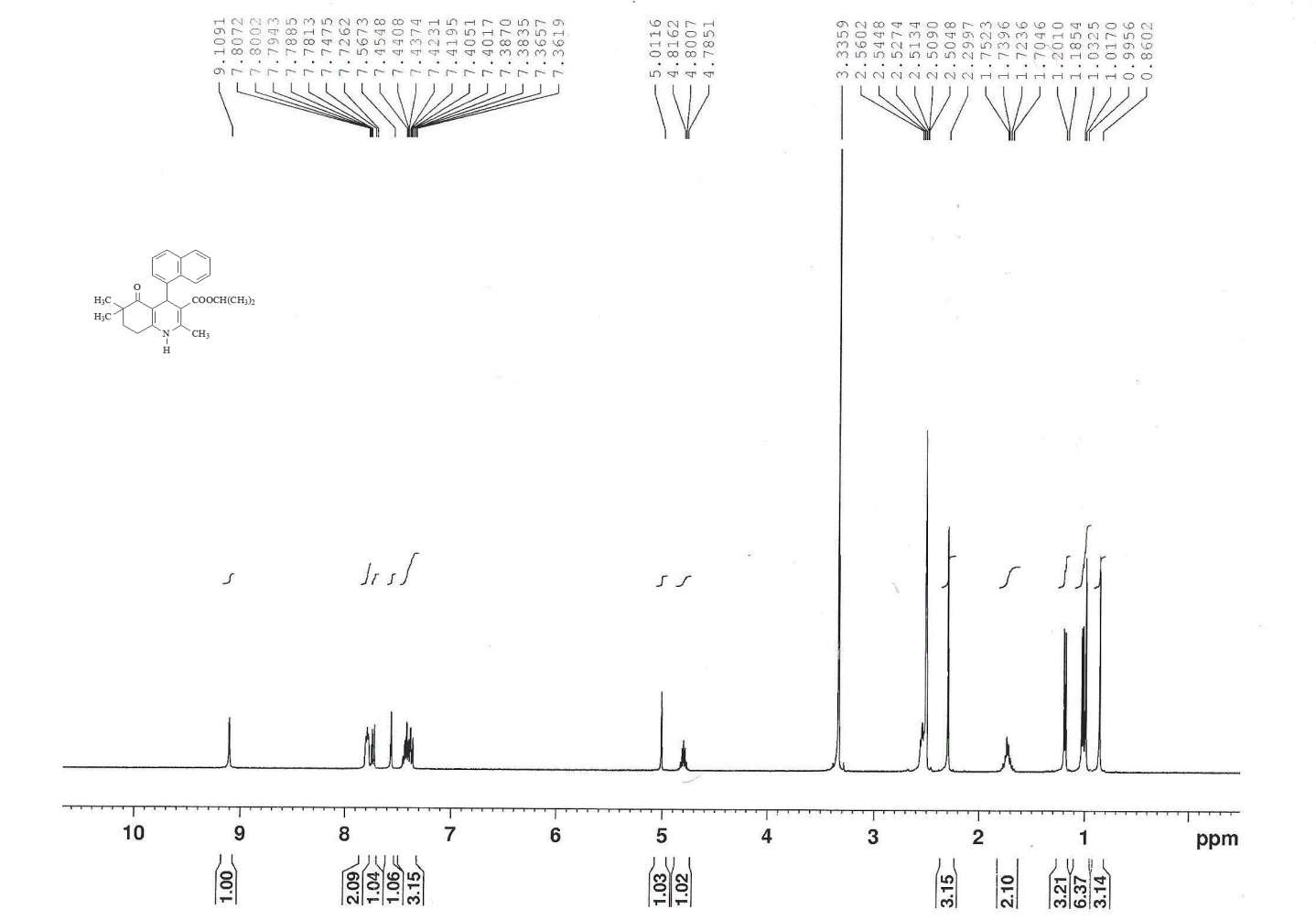
1H-NMR spectrum of compound **4**



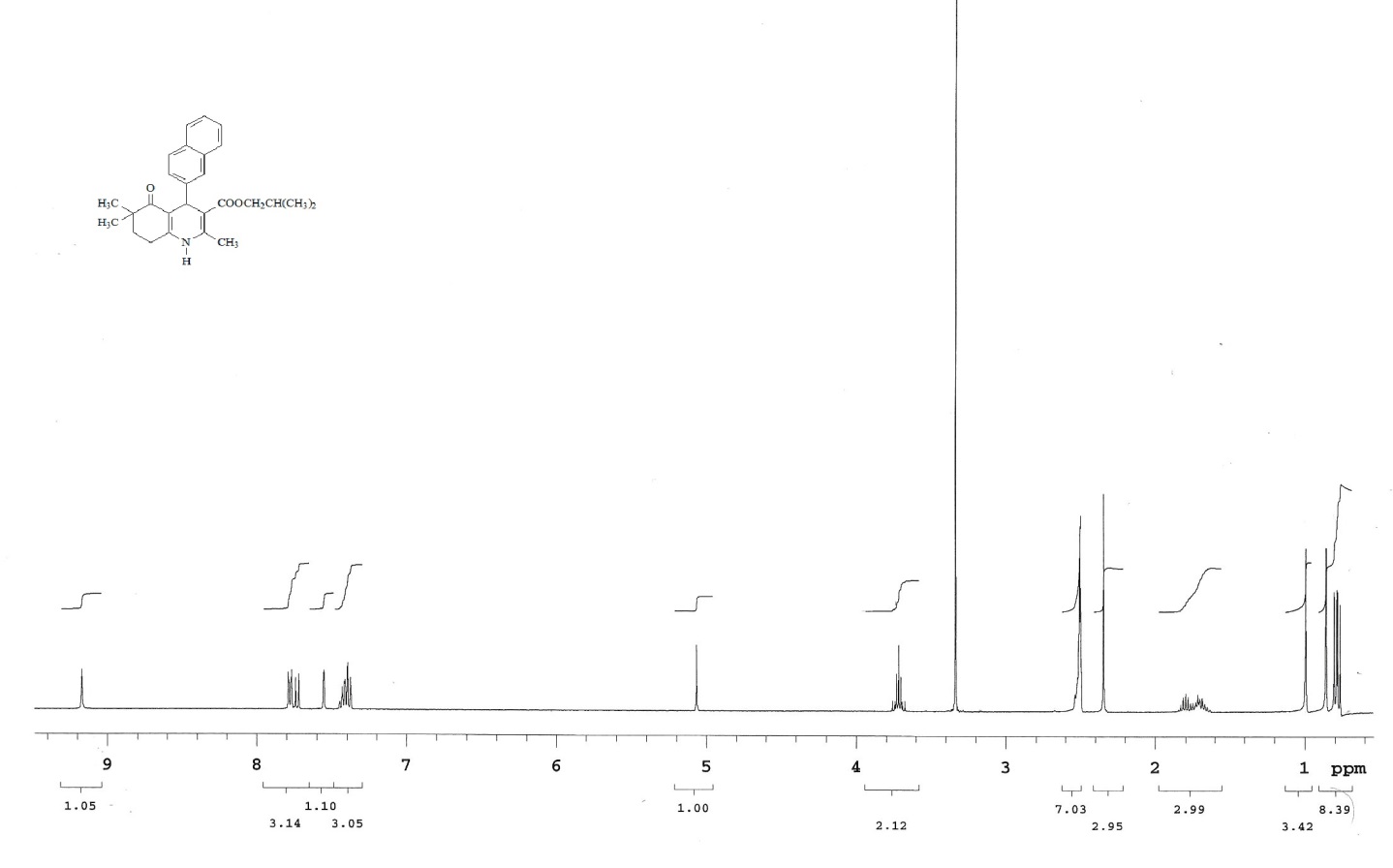
1H-NMR spectrum of compound **5**

****

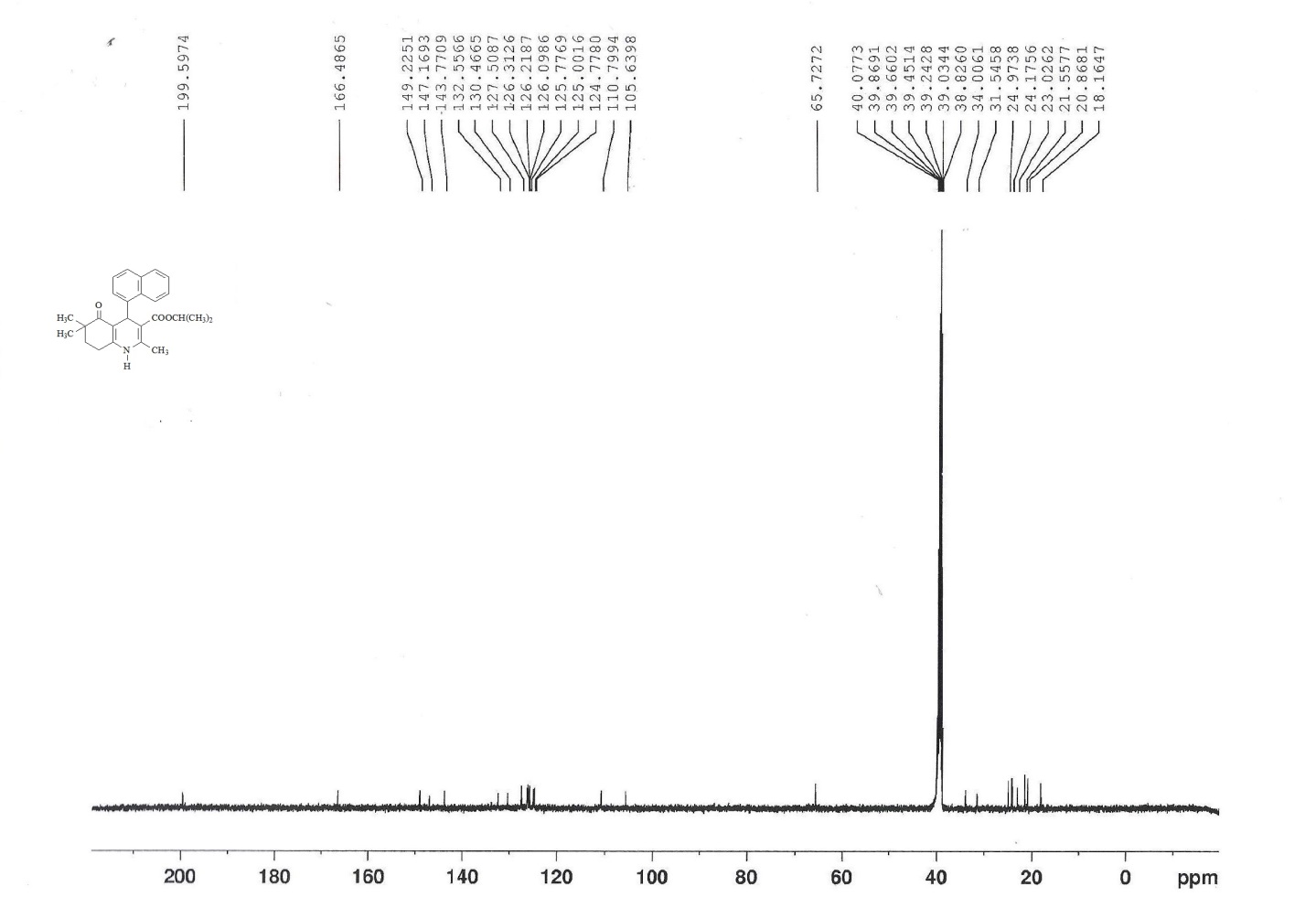
1H-NMR spectrum of compound **6**

****

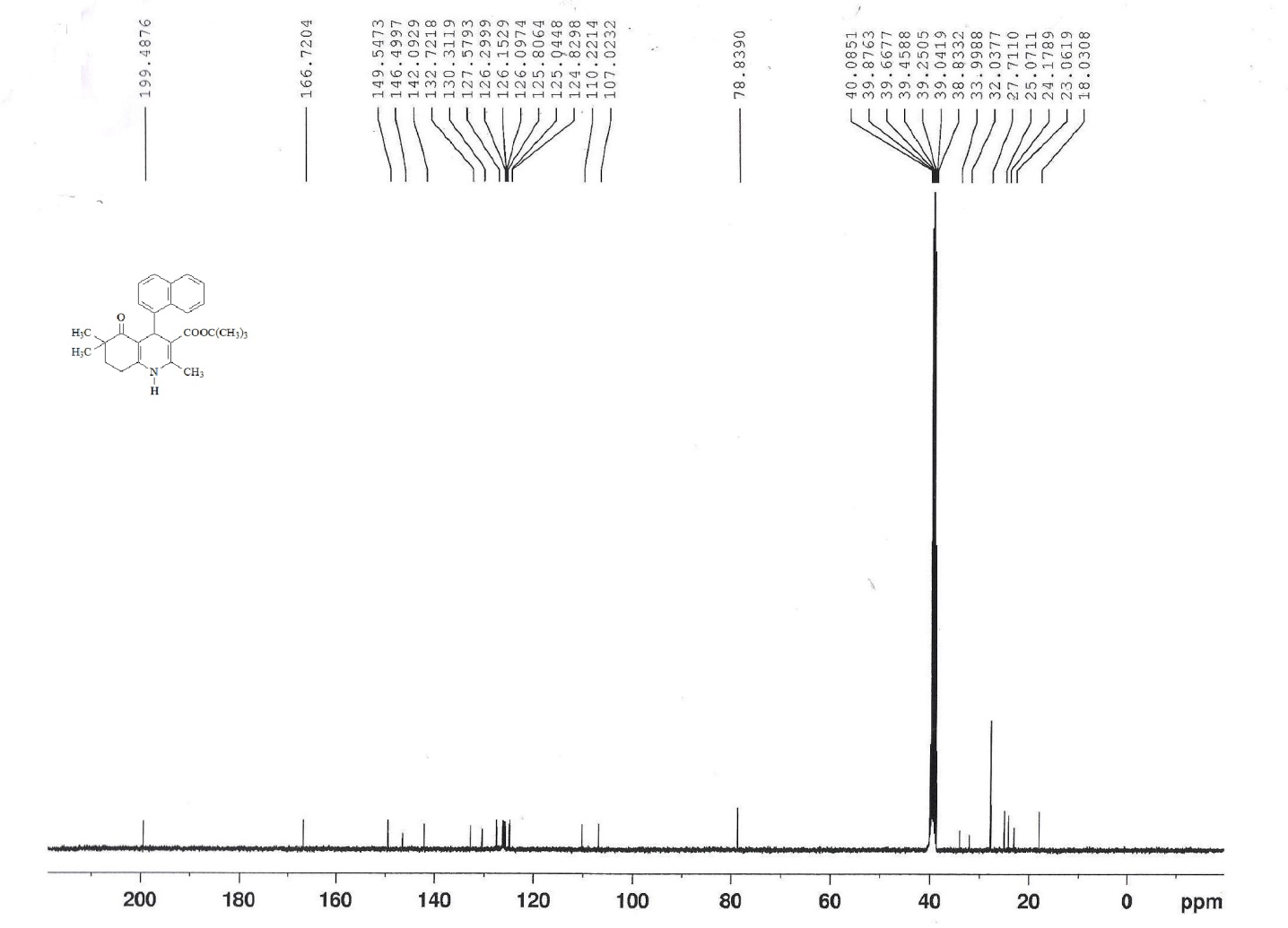
1H-NMR spectrum of compound **11**

****

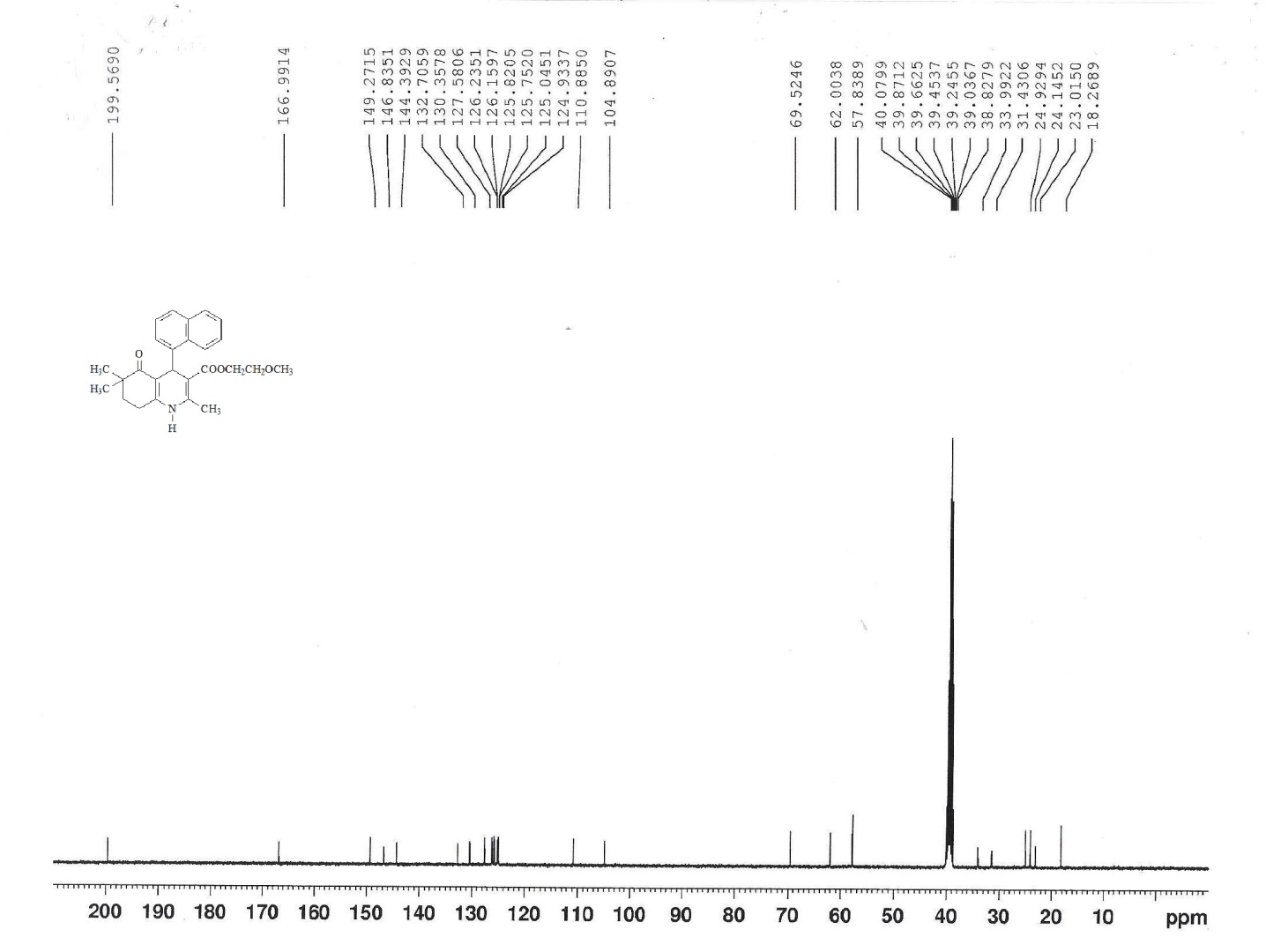
1H-NMR spectrum of compound **12**



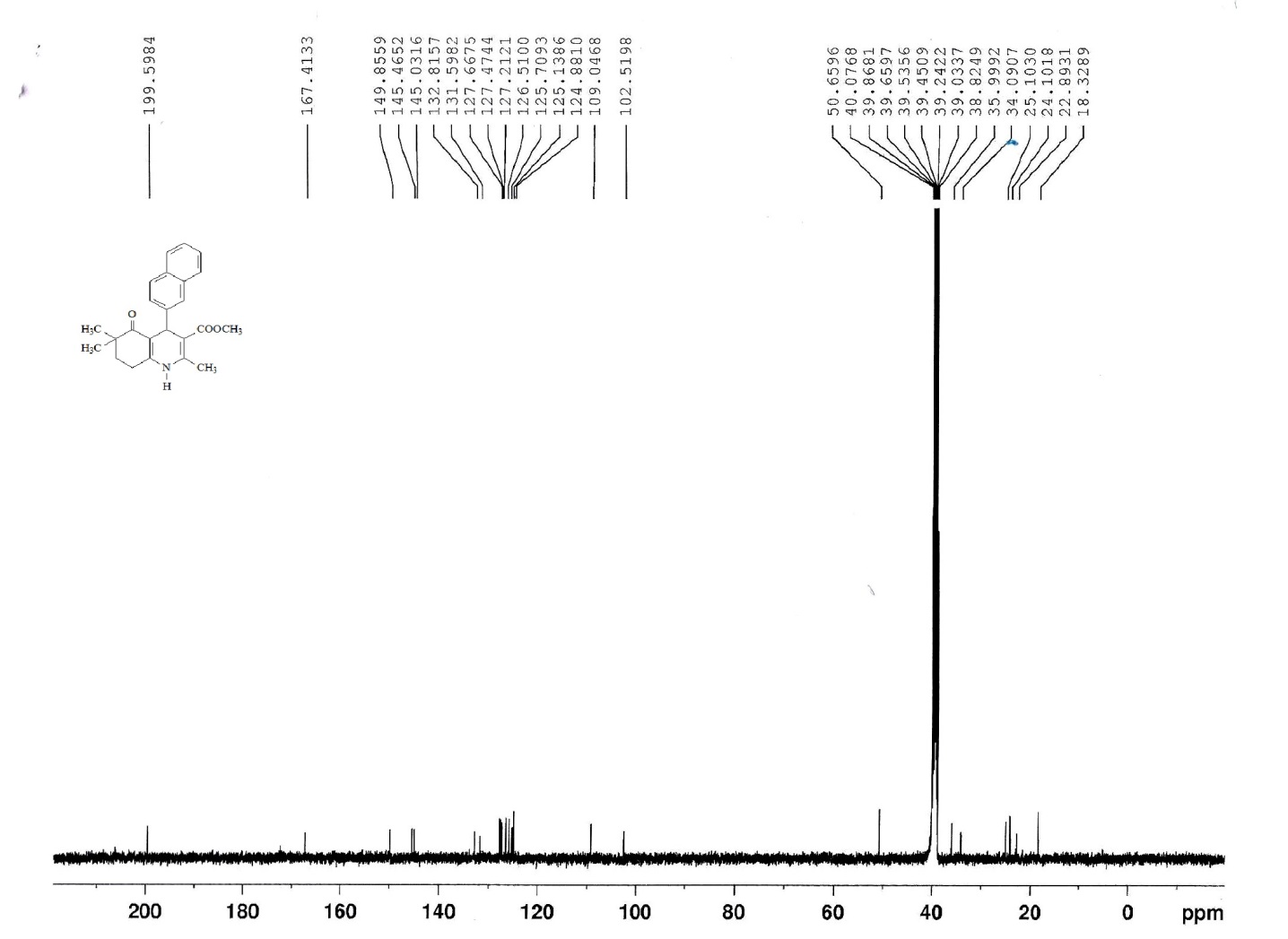
13C-NMR spectrum of compound **3**

****

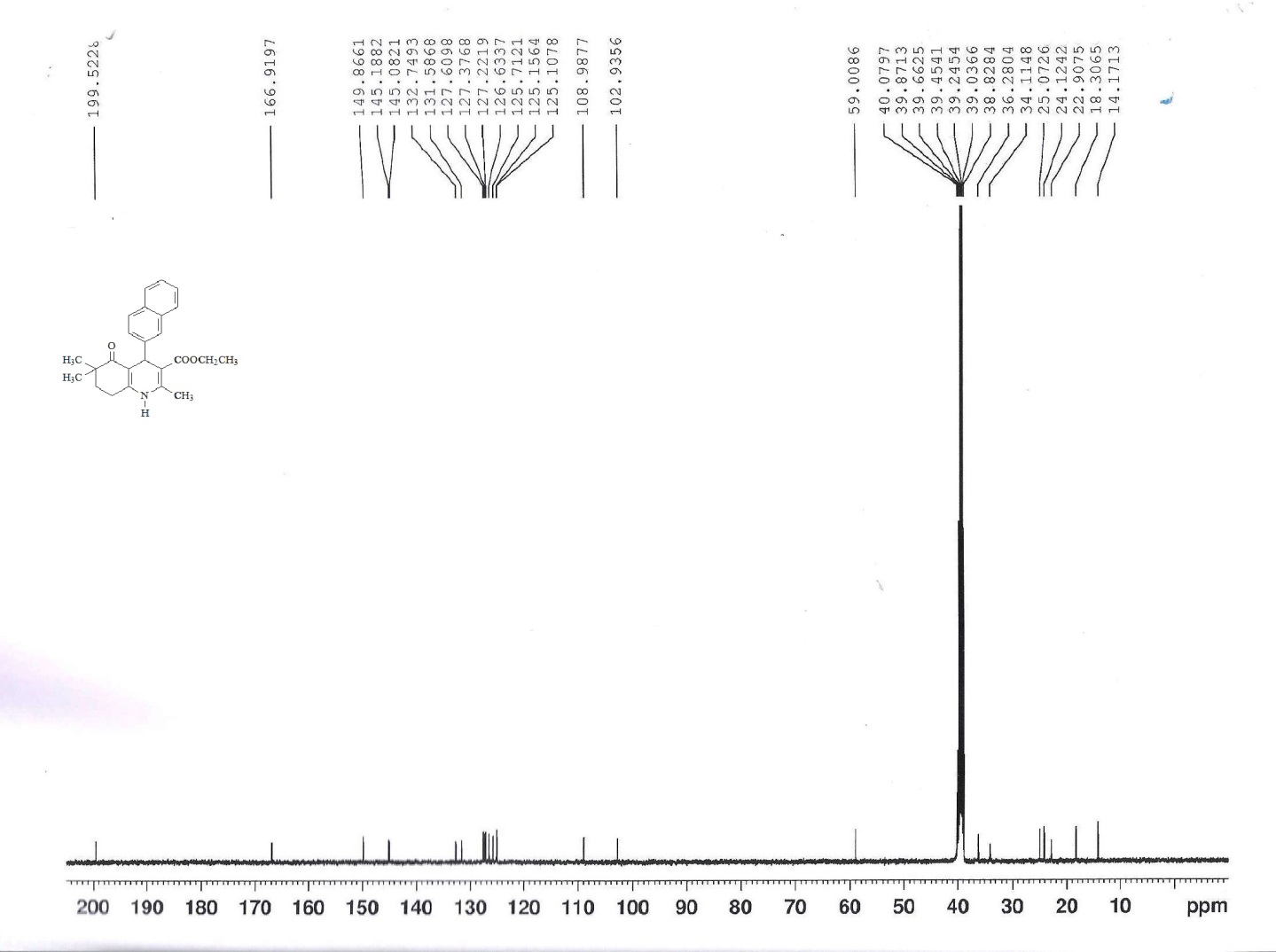
13C-NMR spectrum of compound **5**

****

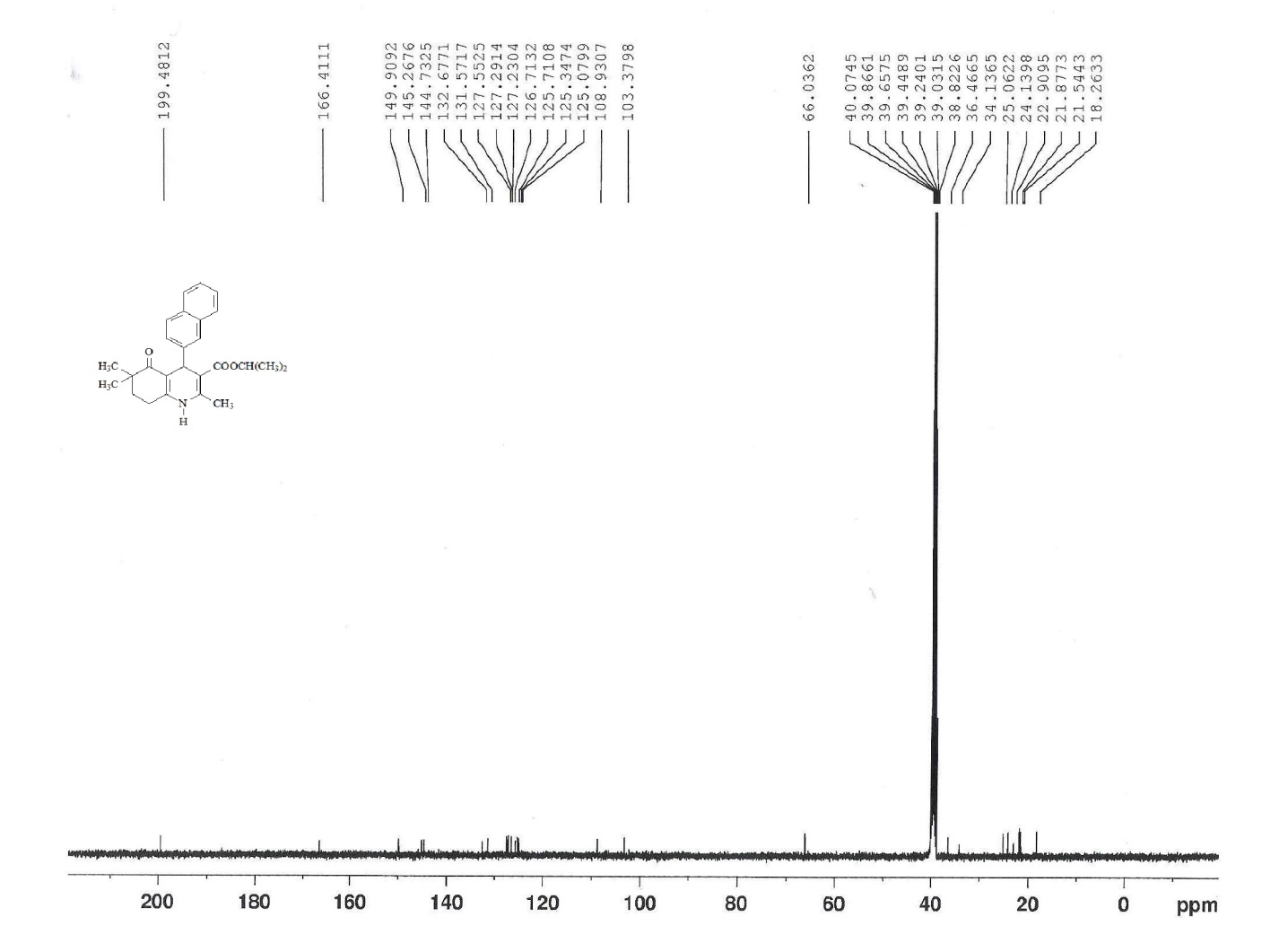
13C-NMR spectrum of compound **6**

****

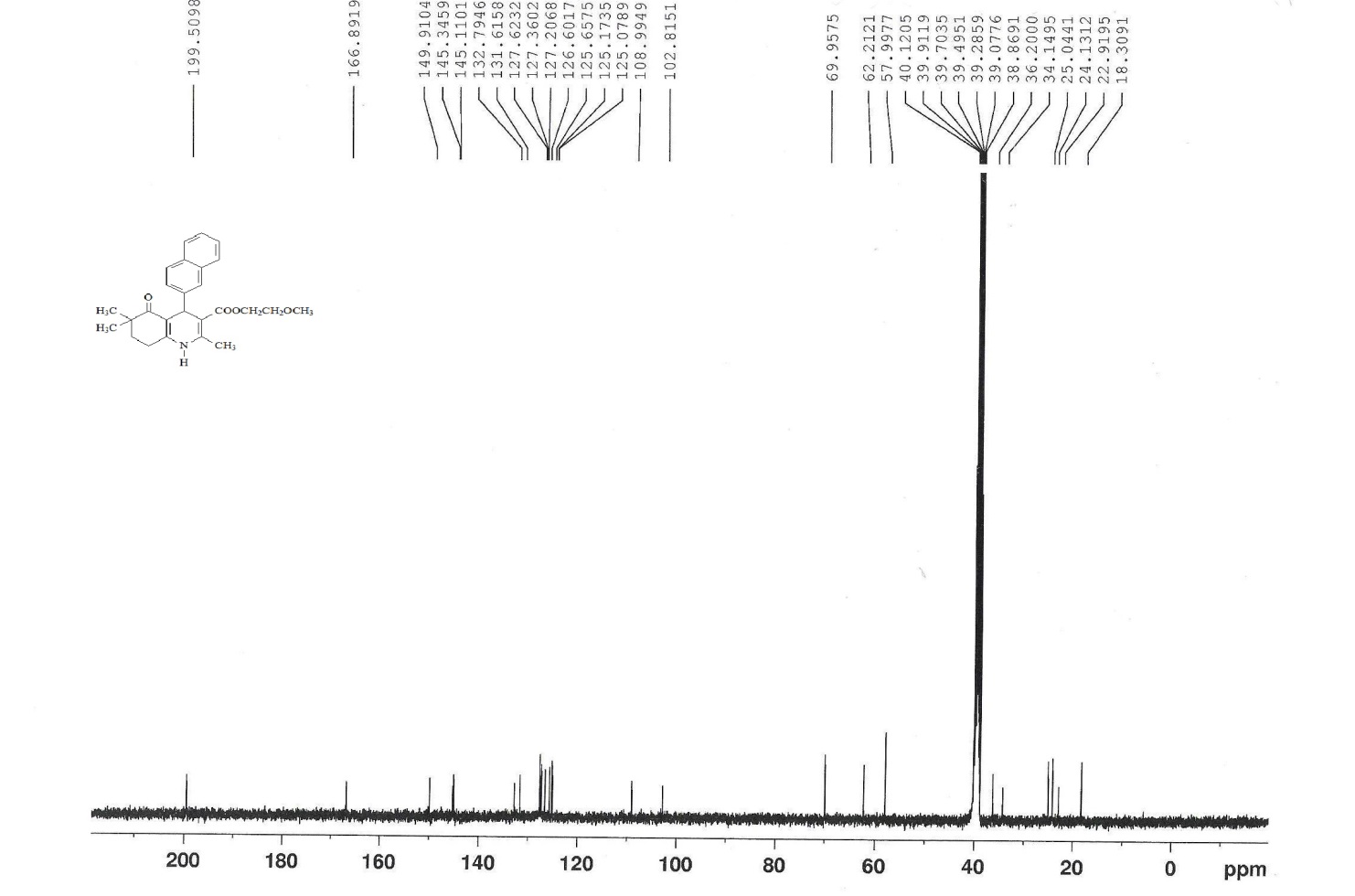
13C-NMR spectrum of compound **9**

****

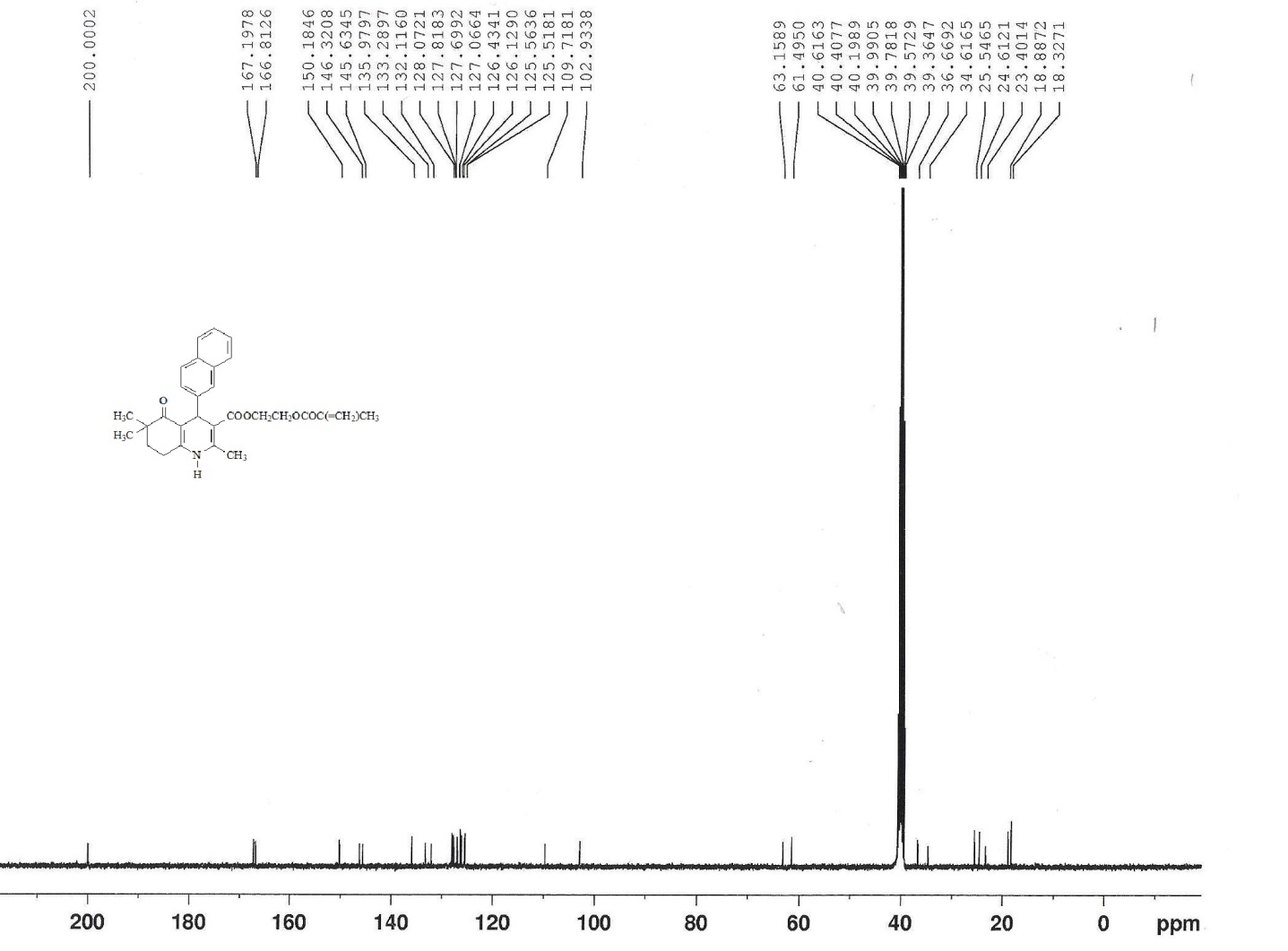
13C-NMR spectrum of compound **10**

****

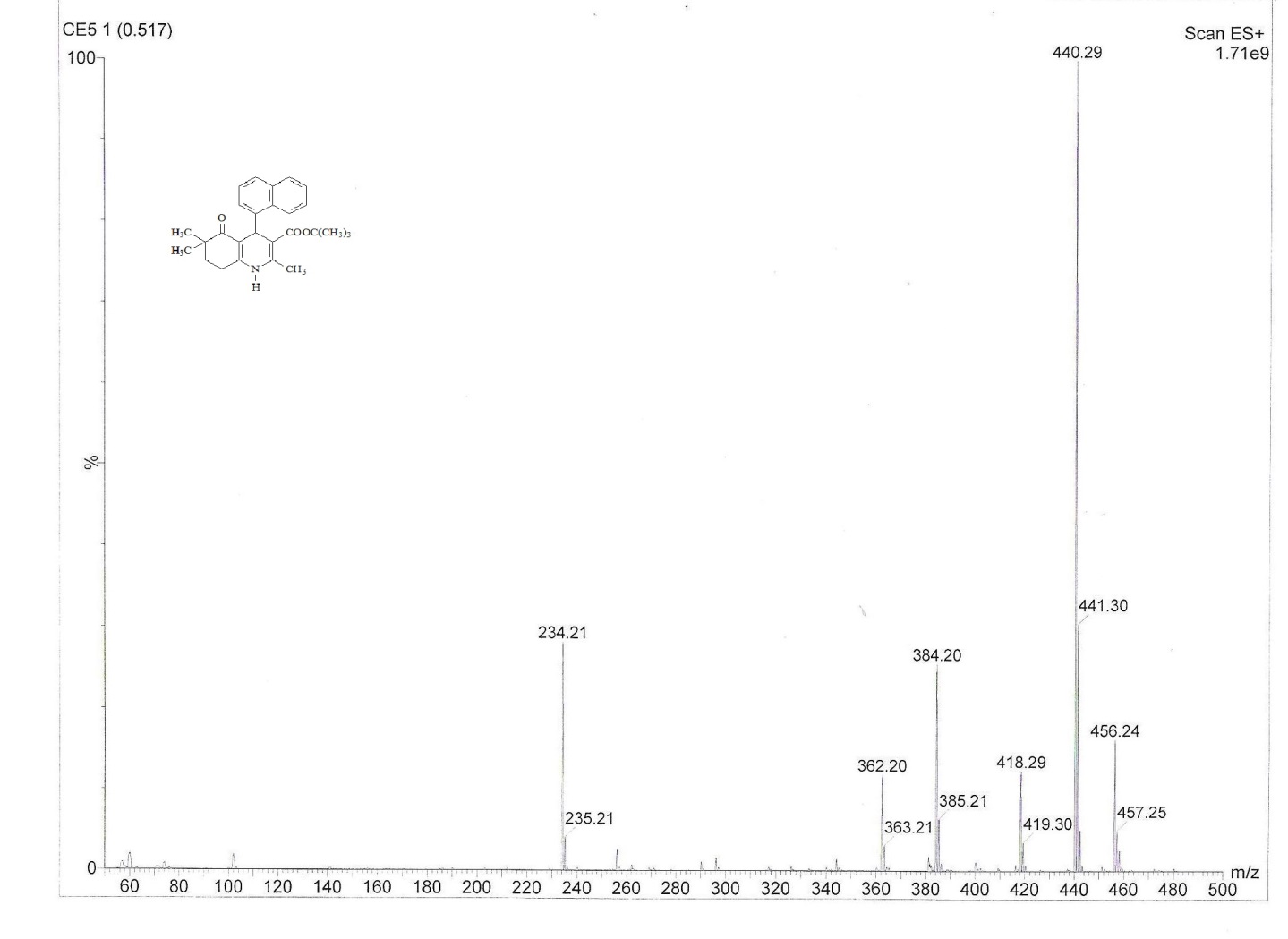
13C-NMR spectrum of compound **11**



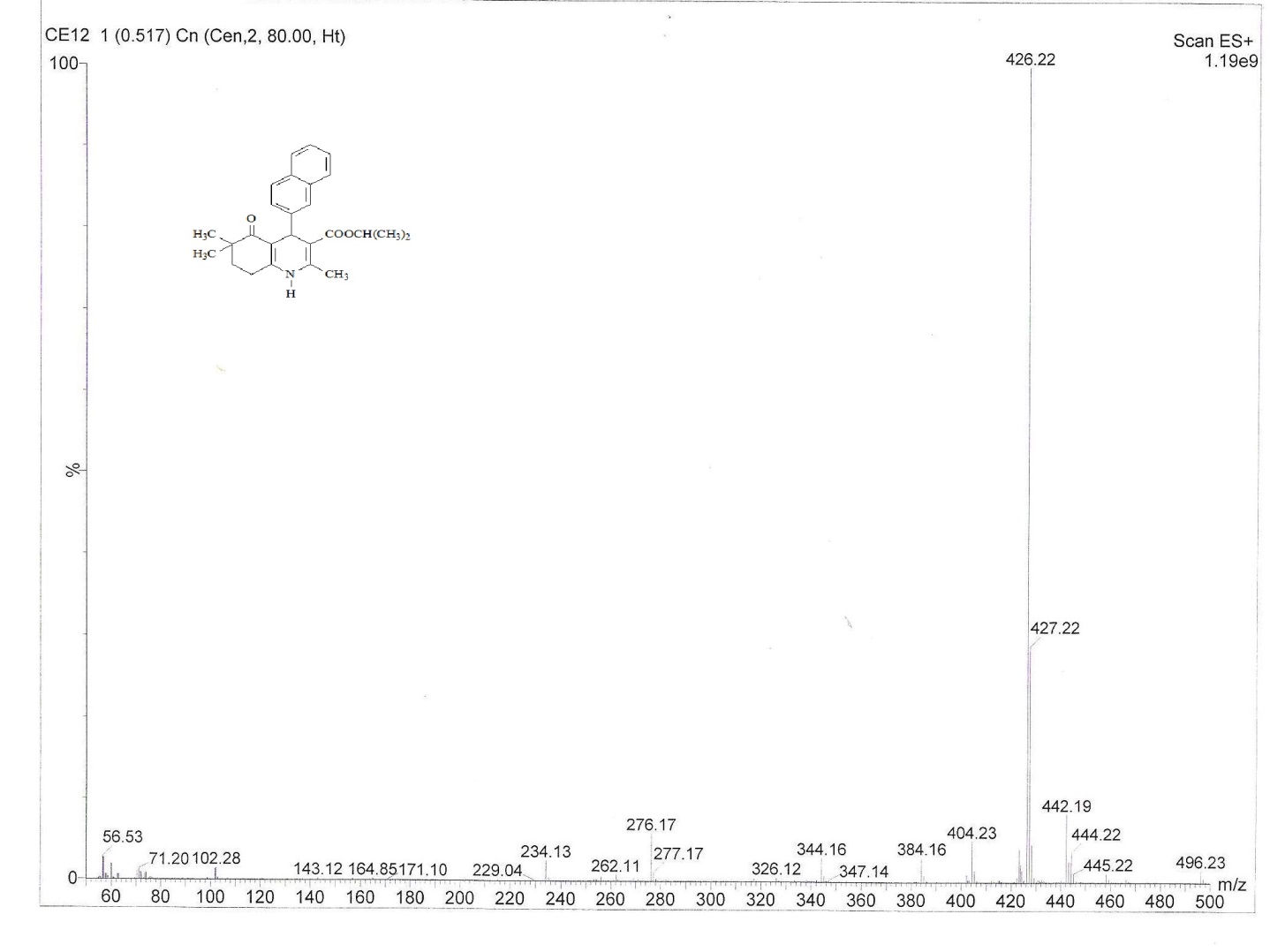
13C-NMR spectrum of compound **14**

****

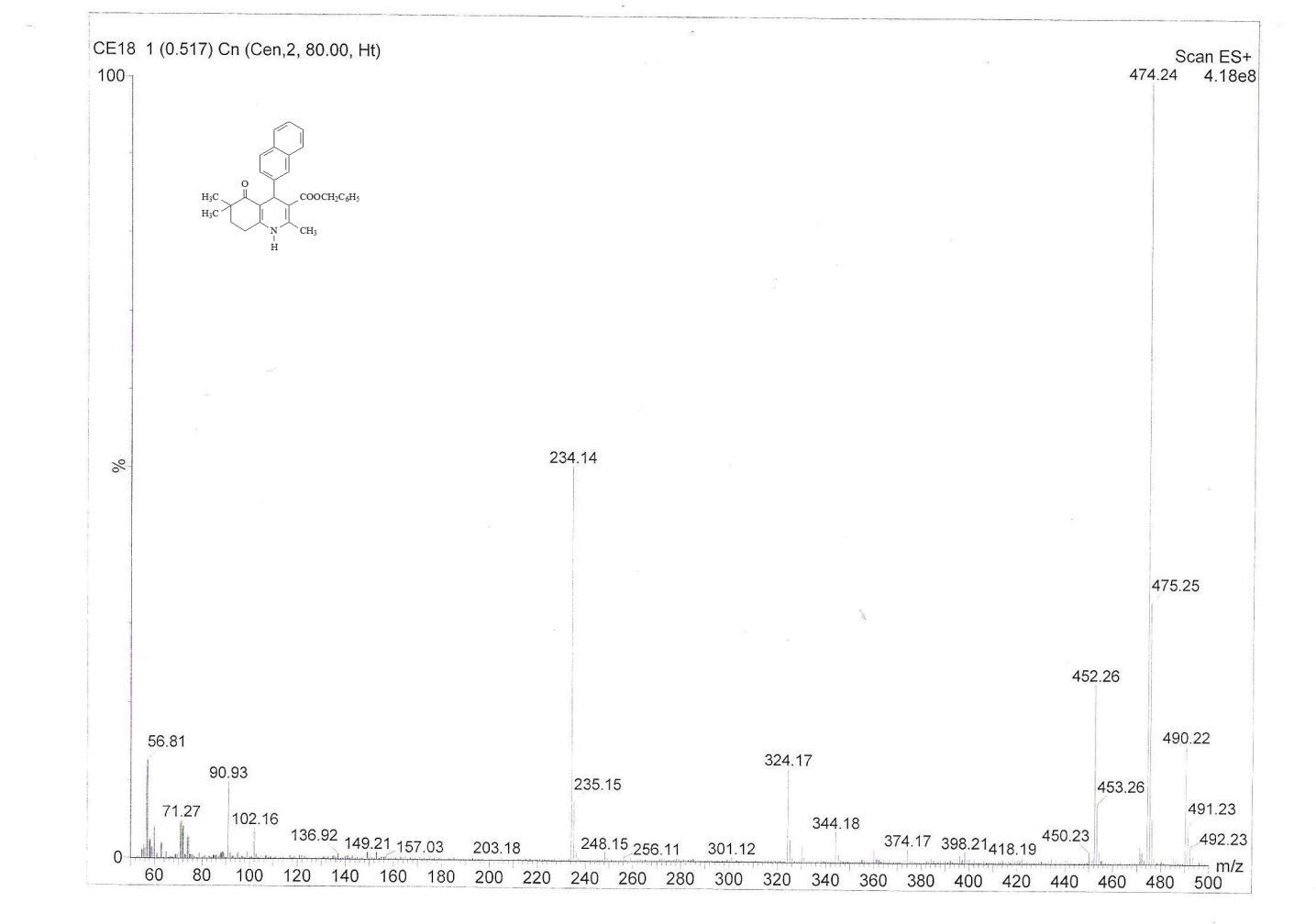
13C-NMR spectrum of compound **15**



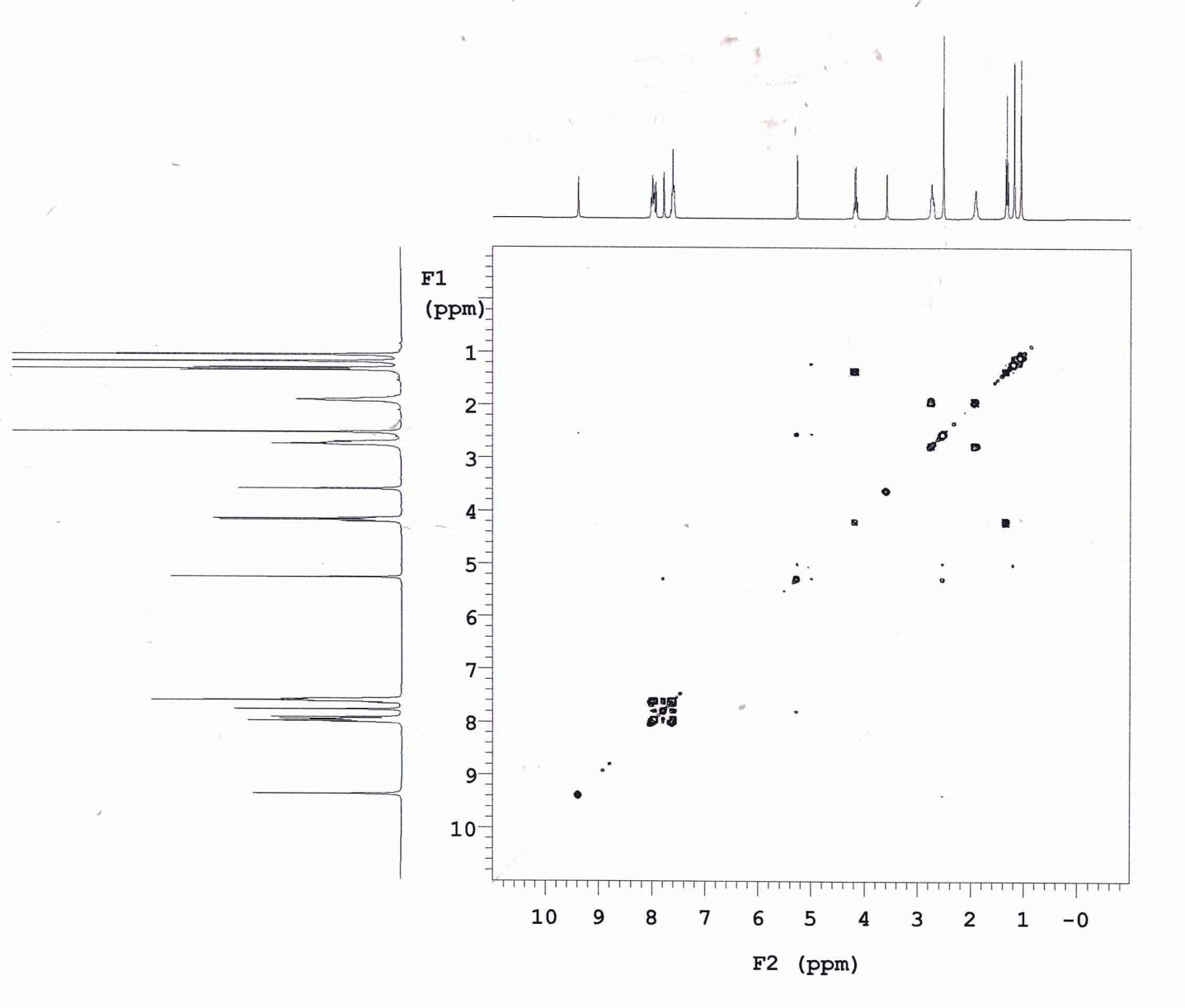
Mass spectrum of compound **5**



Mass spectrum of compound **11**

****

Mass spectrum of compound **16**



COSY spectrum of compound **2**

Crystal data and details of the structure determination of compound **10**

|  |  |
| --- | --- |
| -------------------------------------------------------------------------------------------------------------- | |
| Formula | [C25H27NO3](../../../AppData/Local/Temp/hu-ce1a%20_chemical_formula_moiety) |
| Molecular weight | [389.48](../../../AppData/Local/Temp/hu-ce1a%20_chemical_formula_weight) |
| Crystal system | Orthorhombic |
| Space group | [*Pbca*](../../../AppData/Local/Temp/hu-ce1a%20_symmetry_space_group_name_H-M) |
| a (Å), b (Å), c(Å) | [10.5179 (2)](../../../AppData/Local/Temp/hu-ce1a%20_cell_length_a), [12.1144 (3)](../../../AppData/Local/Temp/hu-ce1a%20_cell_length_b), [33.6297 (8)](../../../AppData/Local/Temp/hu-ce1a%20_cell_length_c) |
| α (°), β (°), γ (°) | 90, 90, 90 |
| Volume (Å3) | [4285.03 (18)](../../../AppData/Local/Temp/hu-ce1a%20_cell_volume) |
| Z | 8 |
| D (calculated) (gcm-3) | 1.207 |
| F000 | 1664 |
| Linear absorption coefficient (mm-1) | [0.63](../../../AppData/Local/Temp/hu-ce1a%20_exptl_absorpt_coefficient_mu) |
| Absorption correction type | multi-scan |
| Crystal size (mm) | 0.50 x 0.35 x 0.30 |
| Diffractions radiation type | CuKα |
| λ (Å) | 1.54184 |
| Monochromator | Graphite |
| Diffractions measurement device type | Xcalibur, Ruby, Gemini |
| Diffractions measurement device | ω scans |
| Total reflection number | 15413 |
| Independent reflection number | 4374 |
| Collected reflection for I > 2σ(I) | 3821 |
| Rint | [0.029](../../../AppData/Local/Temp/hu-ce1a%20_diffrn_reflns_av_R_equivalents) |
| h, k, l ranges | -12→12, -13→14, -38→41 |
| θmin , θmax range (°) | -4.96, 75.64 |
| Solution | Direct methods, SHELXS-97, SHELXL-97, SHELXTL |
| Least squares refine weighting details | *w* = 1/[*σ*2(*F*o2) + (0.0764*P*)2 + 1.7455*P*]  where *P* = (*F*o2 + 2*F*c2)/3 |
| Number of variable | 270 |
| R | 0.0479 |
| wR | 0.1326 |
| S(F2) | 1.043 |
| Δρmax , Δρmin (e/Å3) | 0.39, —0.23 |
| -------------------------------------------------------------------------------------------------------------- | |

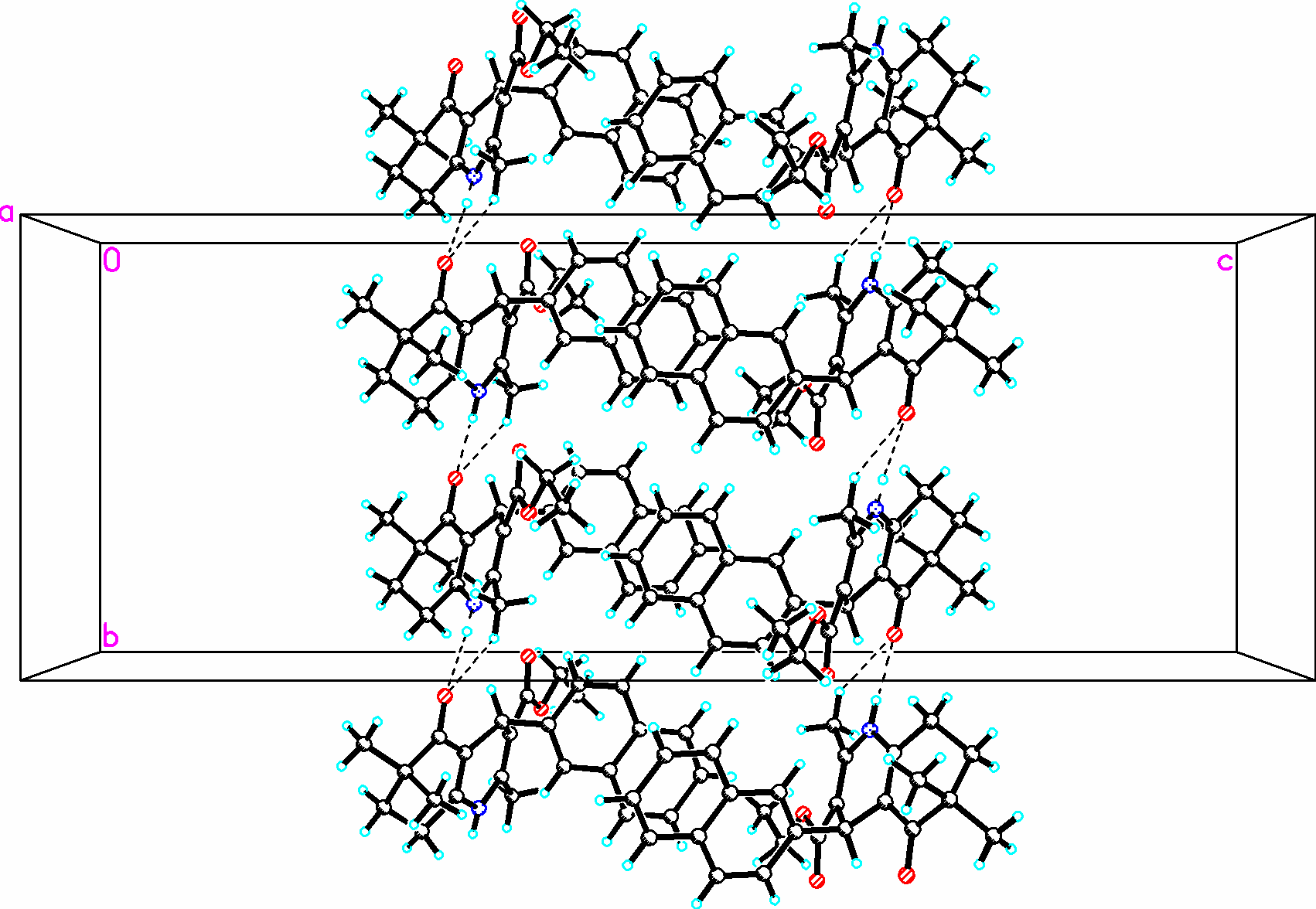
Selected bond lengths (Å), bond (°) and torsion angles (°).

|  |  |  |  |
| --- | --- | --- | --- |
| ---------------------------------------------------------------------------------------------------------------- | | | |
| O1—C5 | 1.2319 (19) | O3—C21 | 1.450 (2) |
| O2—C20 | 1.216 (2) | N1—C1 | 1.3642 (19) |
| O3—C20 | 1.3441 (18) | N1—C9 | 1.3905 (19) |
| C20—O3—C21 | 116.23 (13) | C11—C10—C7 | 121.60 (13) |
| C1—N1—C9 | 122.72 (13) | C19—C10—C7 | 119.49 (13) |
| N1—C1—C2 | 116.62 (13) | C10—C11—C12 | 121.39 (14) |
| O1—C5—C6 | 121.45 (13) | C15—C16—C17 | 120.98 (18) |
| O1—C5—C4 | 119.16 (13) | O2—C20—O3 | 122.15 (14) |
| C8—C9—N1 | 119.09 (13) | O2—C20—C8 | 123.13 (13) |
| C8—C9—C23 | 128.34 (14) | O3—C20—C8 | 114.71 (13) |
| N1—C9—C23 | 112.55 (13) | O3—C21—C22 | 107.31 (16) |
| C11—C10—C19 | 118.83 (14) |  |  |
| N1—C1—C2—C3 | 155.38 (13) | C1—N1—C9—C8 | −12.6 (2) |
| C1—C2—C3—C4 | 48.82 (17) | C1—N1—C9—C23 | 165.63 (14) |
| C3—C4—C5—O1 | −151.82 (14) | C21—O3—C20—O2 | −4.3 (2) |
| C25—C4—C5—O1 | 87.90 (17) | C21—O3—C20—C8 | 175.61 (16) |
| N1—C1—C6—C5 | −177.12 (13) | C9—C8—C20—O2 | −169.51 (15) |
| N1—C1—C6—C7 | 6.2 (2) | C7—C8—C20—O2 | 11.6 (2) |
| O1—C5—C6—C1 | 176.76 (14) | C9—C8—C20—O3 | 10.6 (2) |
| O1—C5—C6—C7 | −6.5 (2) | C7—C8—C20—O3 | −168.32 (13) |
| C20—C8—C9—N1 | 170.78 (13) | C20—O3—C21—C22 | −173.42 (18) |
| C7—C8—C9—N1 | −10.4 (2) |  |  |
| ---------------------------------------------------------------------------------------------------------------- | | | |

[Hydrogen-bond geometry (Å, °)](file:///C:\Users\Toshıba\AppData\Local\Temp\hu-ce1a%20_geom_hbond_atom_site_label_D)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ----------------------------------------------------------------------------------------------------------------- | | | | |
| D—H···A | D—H | H···A | D···A | D—H···A |
| ----------------------------------------------------------------------------------------------------------------- | | | | |
| C7—H7A···O2 | 0.98 | 2.45 | 2.8122(17) | 101.6 |
| N1—H1N···O1i | 0.83(2) | 1.99(2) | 2.8150(17) | 171.6(19) |
| C23—H23B···O1i | 0.96 | 2.52 | 3.346(2) | 143.7 |
| ----------------------------------------------------------------------------------------------------------------- | | | | |

Symmetry code: (i) −x+3/2, y+1/2, z.



The packing and hydrogen bonding of compound **10** in the unit cell, viewed along the a axis. Hydrogen bonds are shown as dashed lines.