

Chemoselective Preparation of 1,2,3-triazole and Isoxazoles Bisfunctional Derivatives and Its Application in Peptidomimetic Synthesis

Teng-fei Niu^a, Mei-fang Lv^a, Liang wang^b, Wen-bin Yi^a, and Chun Cai^{a*}

^aChemical Engineering College, Nanjing University of Science and Technology, Nanjing, 210094, P. R. China.

^bJiangsu Province Key Laboratory of Fine Petrochemical Engineering, Changzhou University, Changzhou 213164, P. R. China

Crystallographic data

Crystallographic data of complexes **6a** was collected at 296 K on a Bruker SMART CCD system equipped with graphite-monochromated Mo-K α radiation ($\lambda = 0.071073$ nm) using ω - ϕ scan technique. Diffraction data were integrated by the SAINT program, which was also used for intensity corrections for Lorentz and polarization effects. Semi-empirical absorption correction was applied using SADABS. The structures were solved by direct methods and all non-hydrogen atoms were refined anisotropically on F^2 by full-matrix least-squares using the SHELXL-97 crystallographic software package

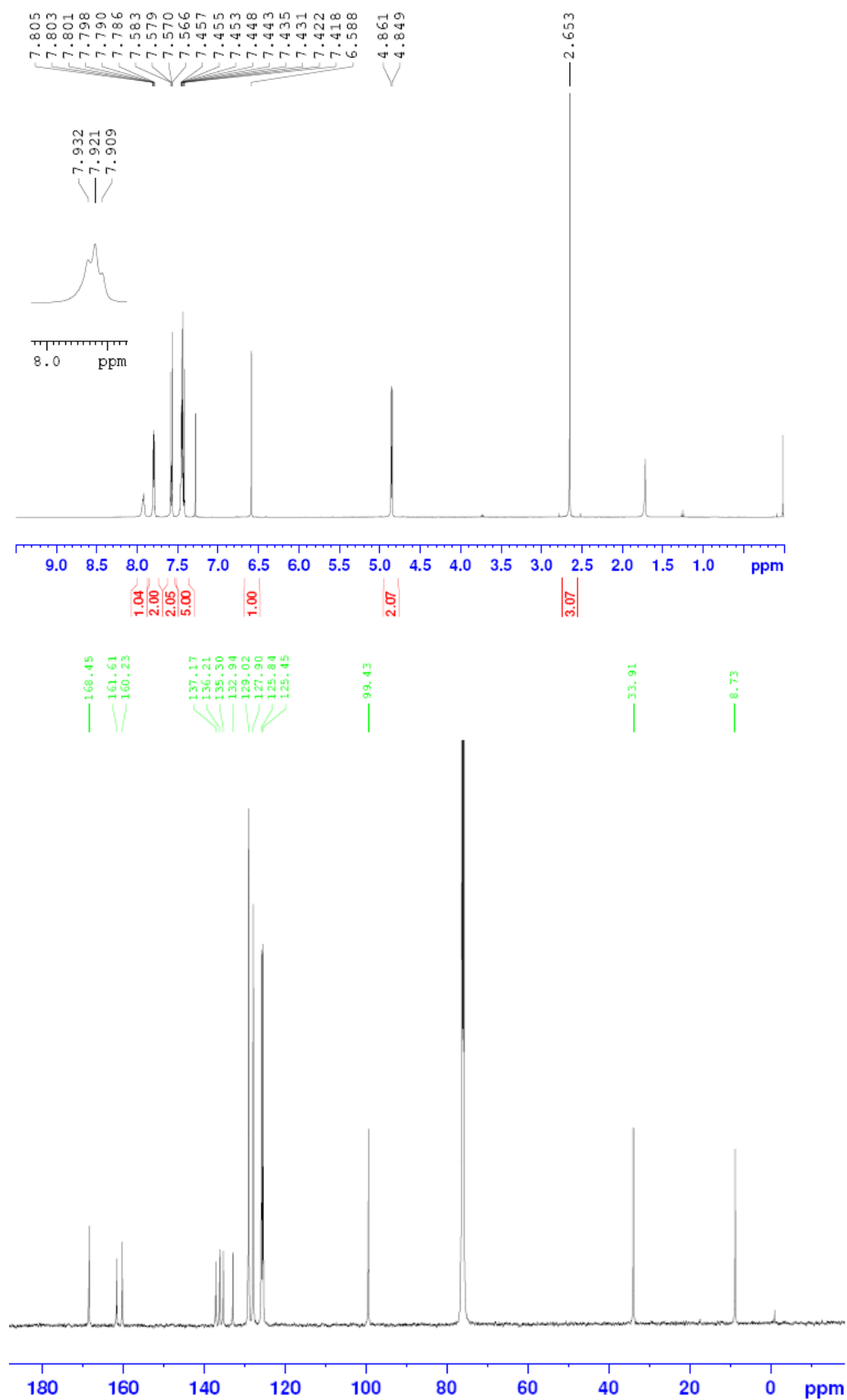
| complex | 1 |
|--|---|
| Formula | C ₂₀ H ₁₆ ClN ₅ O ₂ |
| Formula weight | 393.83 |
| Crystal system | Monoclinic |
| space group | <i>P2(1)/C</i> |
| a (Å) | 17.877(6) |
| b (Å) | 9.516(3) |
| c (Å) | 10.966(3) |
| α (°) | 90.00 |
| β (°) | 91.469(5) |
| γ (°) | 90.00 |
| Volume(Å ³) | 1864.8(10) |
| Z | 4 |
| T, (K) | 296(2) |
| μ (mm ⁻¹) | 0.232 |
| D _{calcd} (g/m ³) | 1.403 |

| | |
|------------------------|---------------------|
| F(000) | 816 |
| Reflections | 3218 |
| collected | |
| Unique | 2358 |
| reflections | |
| Goof | 1.025 |
| $R_1[I > 2\sigma(I)]$ | 0.0582 |
| $wR_2[I > 2\sigma(I)]$ | 0.1813 ^a |

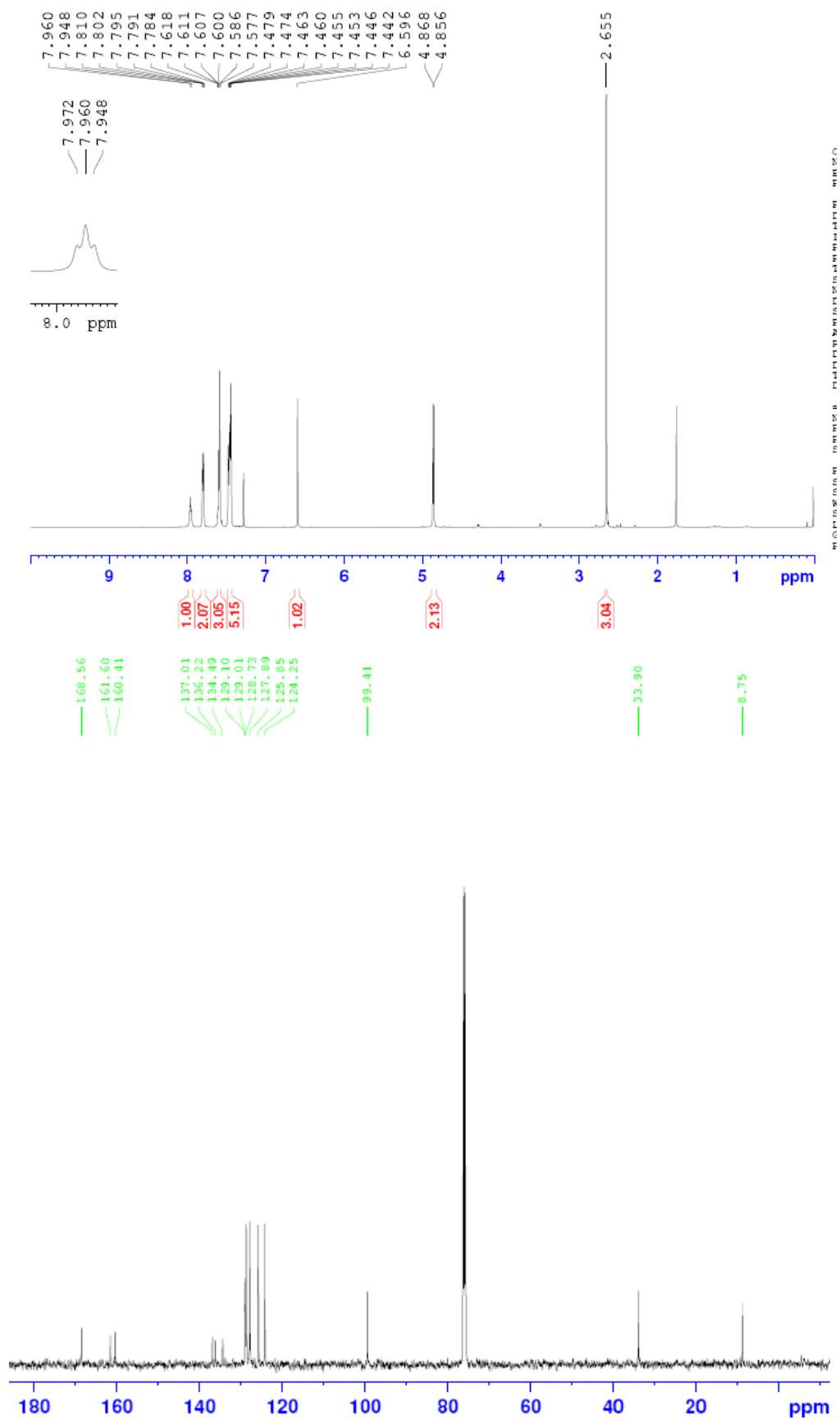
^a $w = 1/[\sigma^2(F_0)^2 + (0.1404P)^2 + 0.0000P]$, where $P = (F_0^2 + 2F_c^2)/3$

Copies of ¹H and ¹³C spectra of 6, 13, 14,15

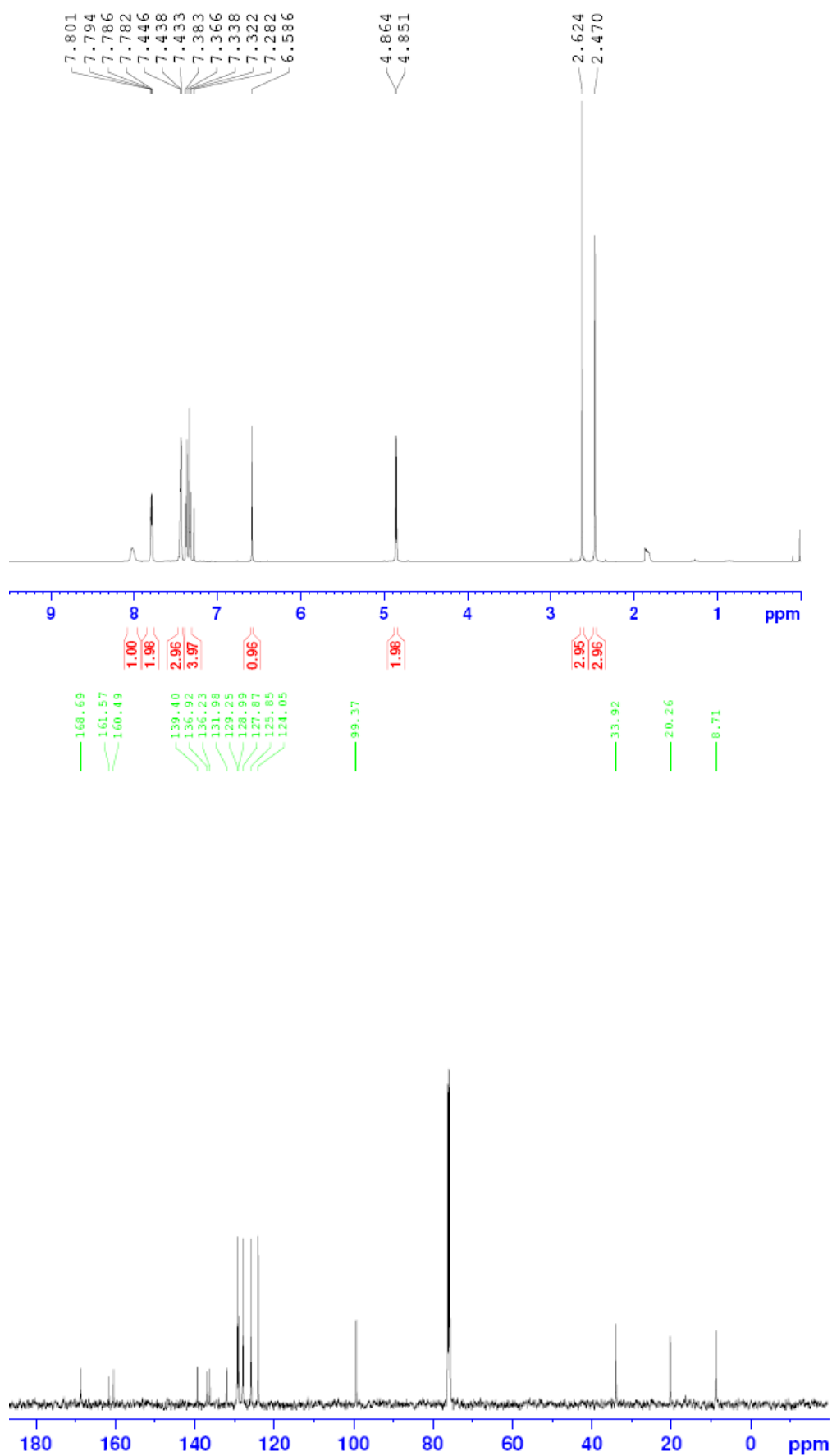
6a



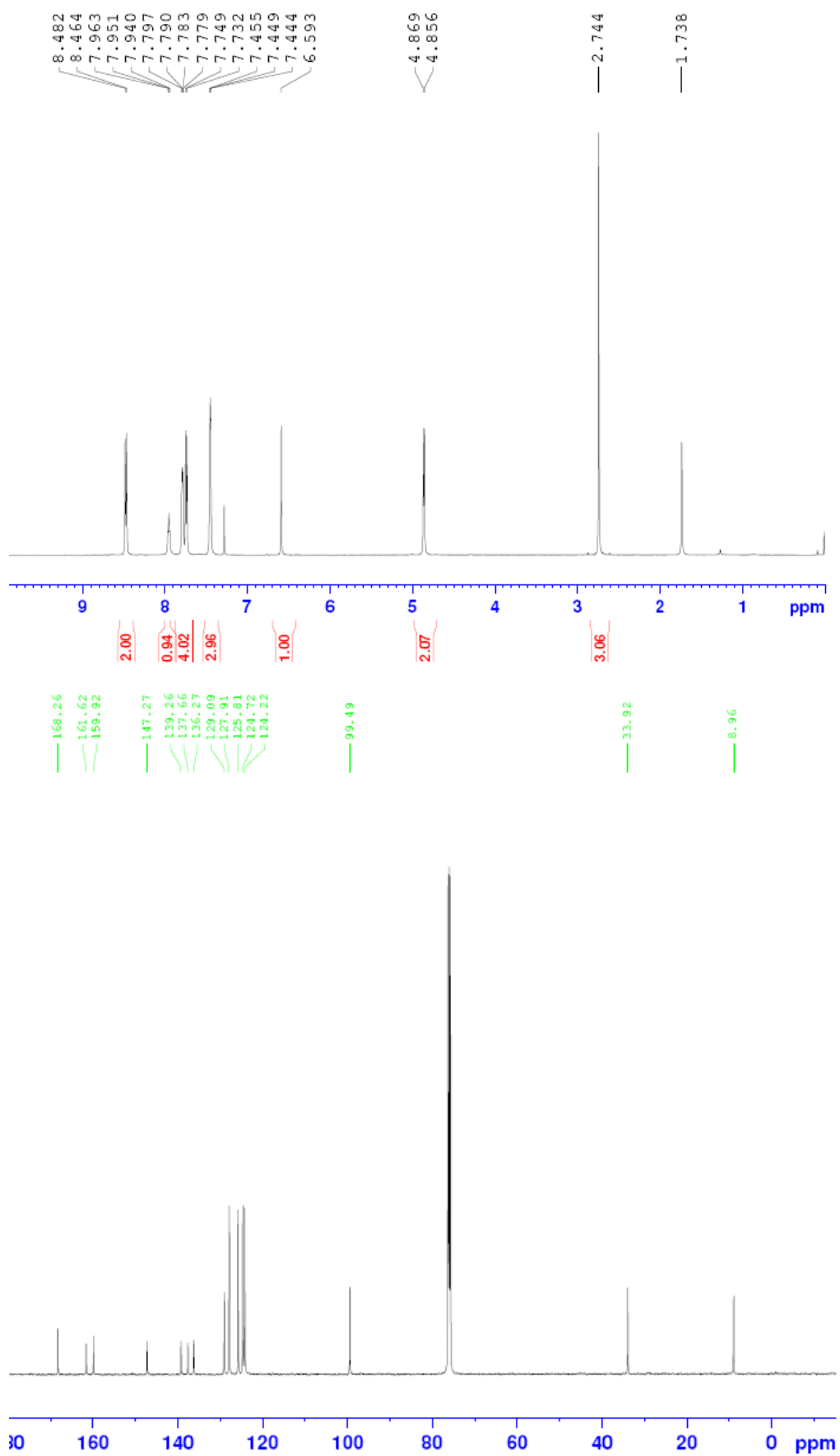
6b



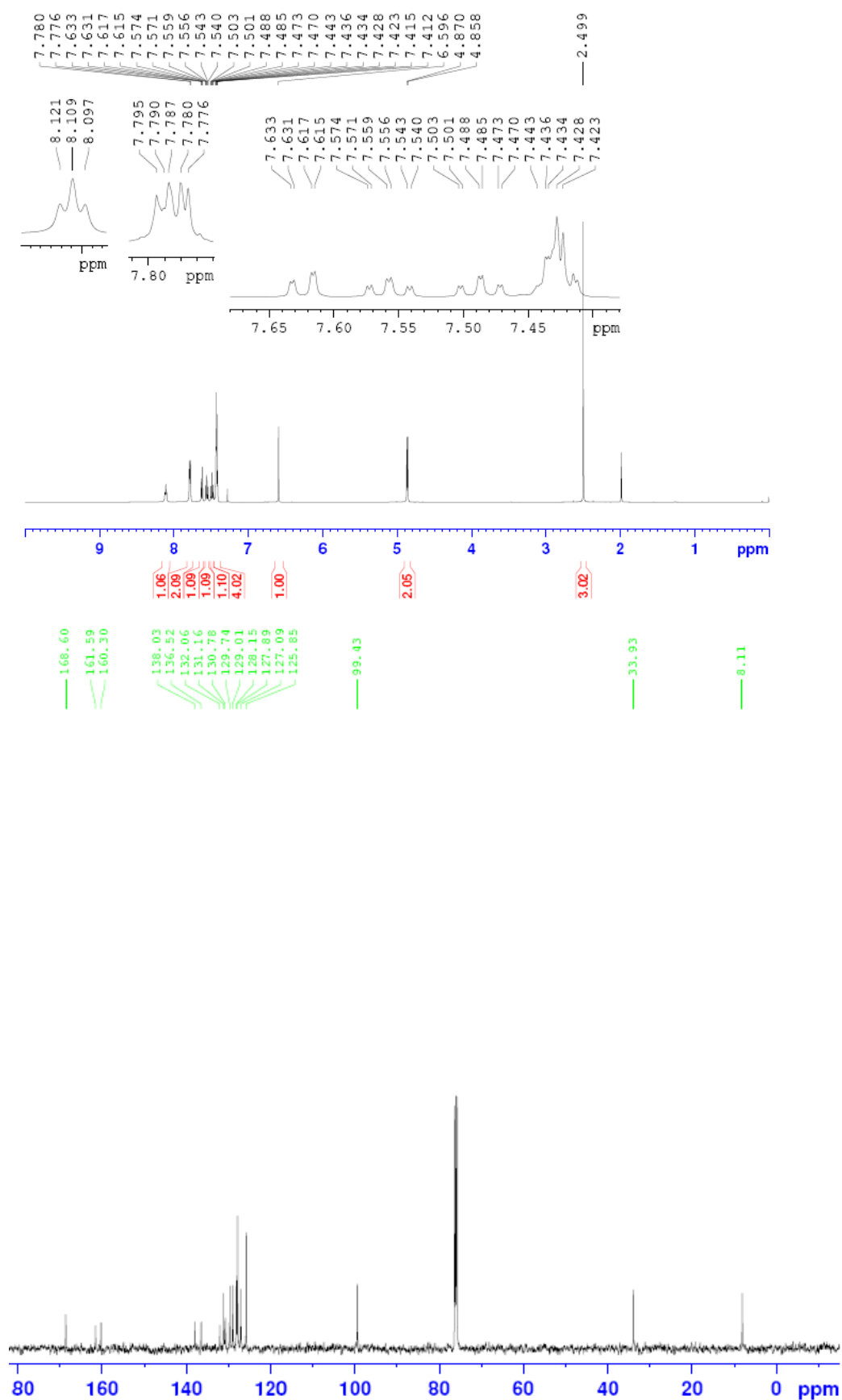
6c



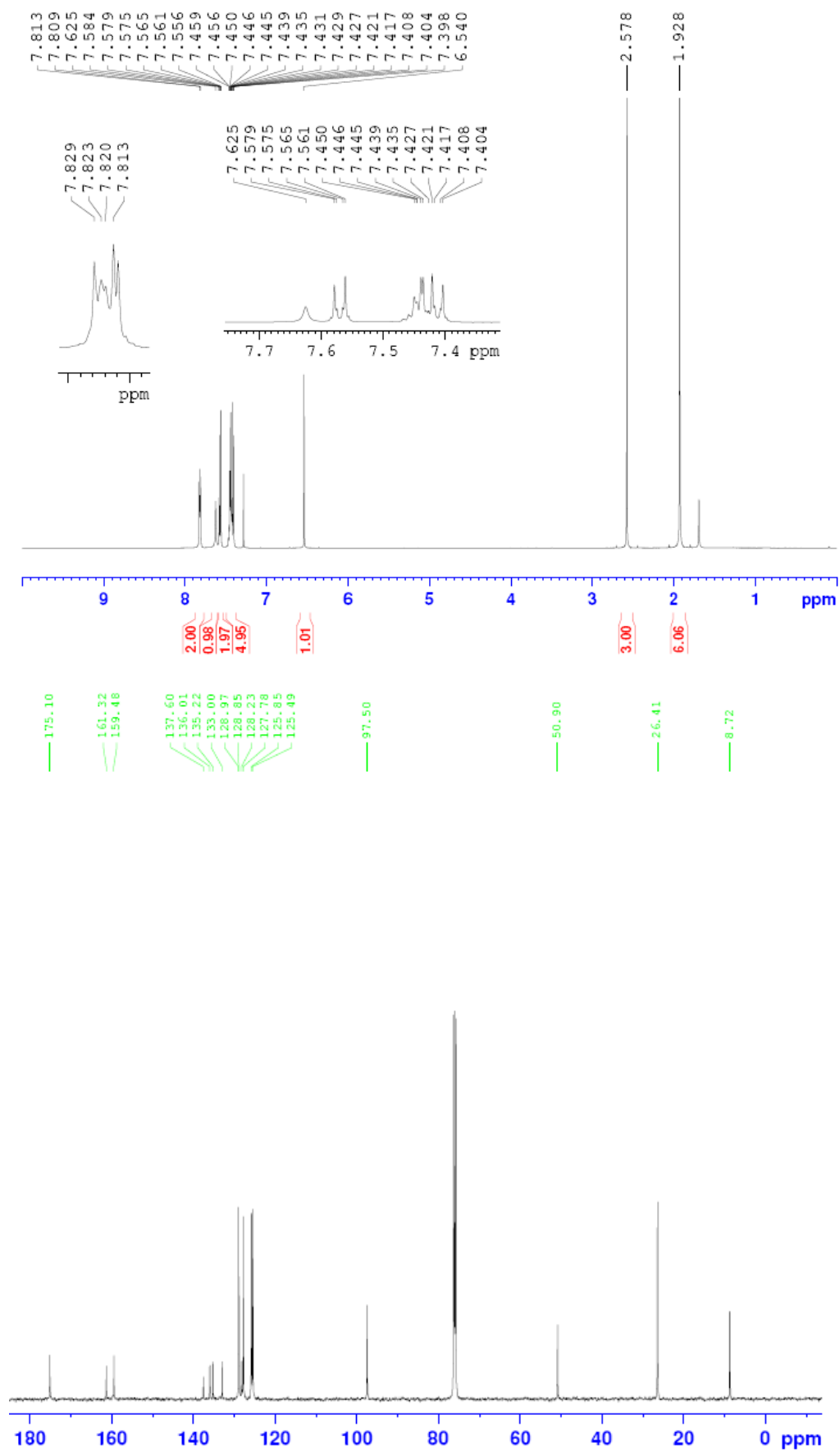
6d



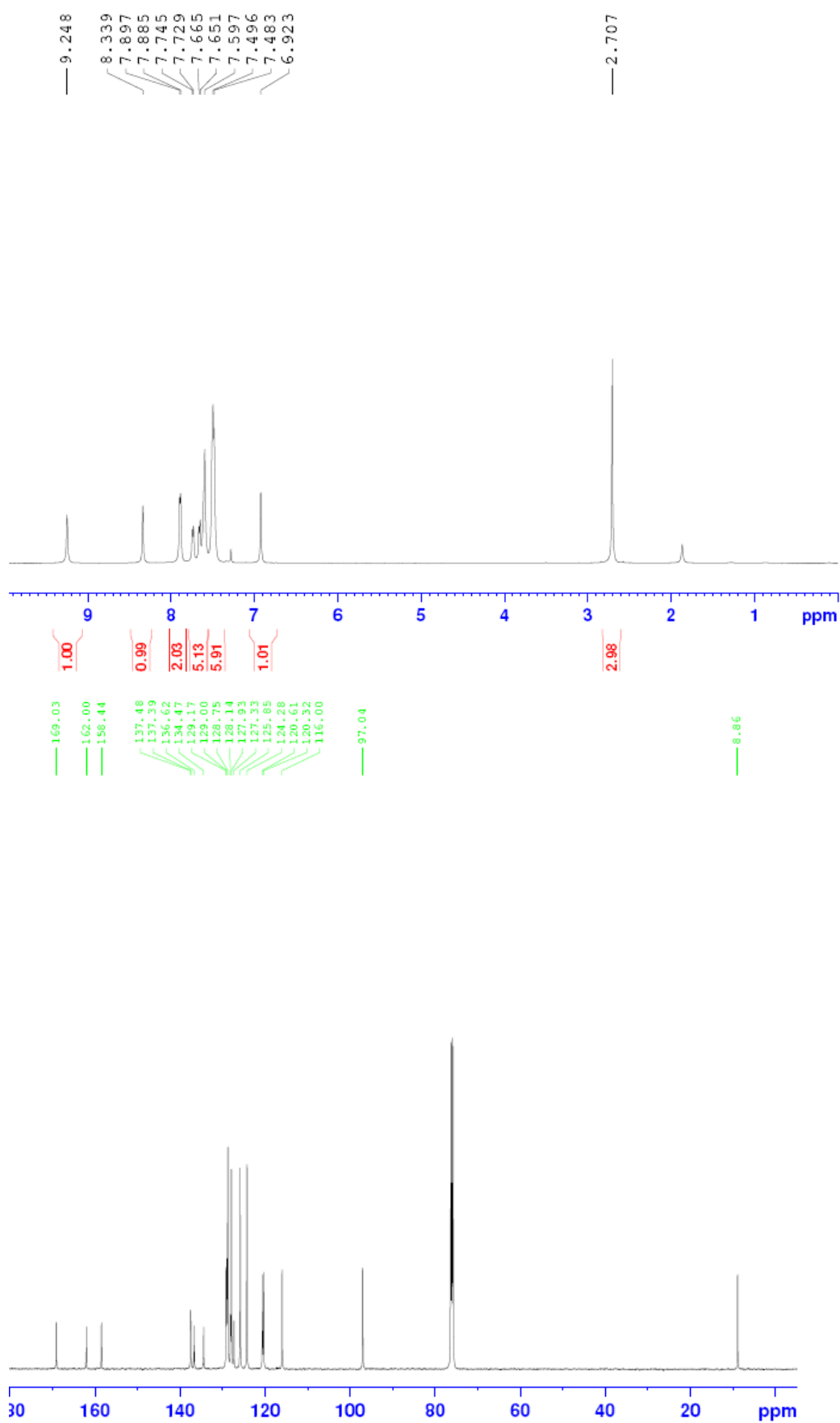
6e



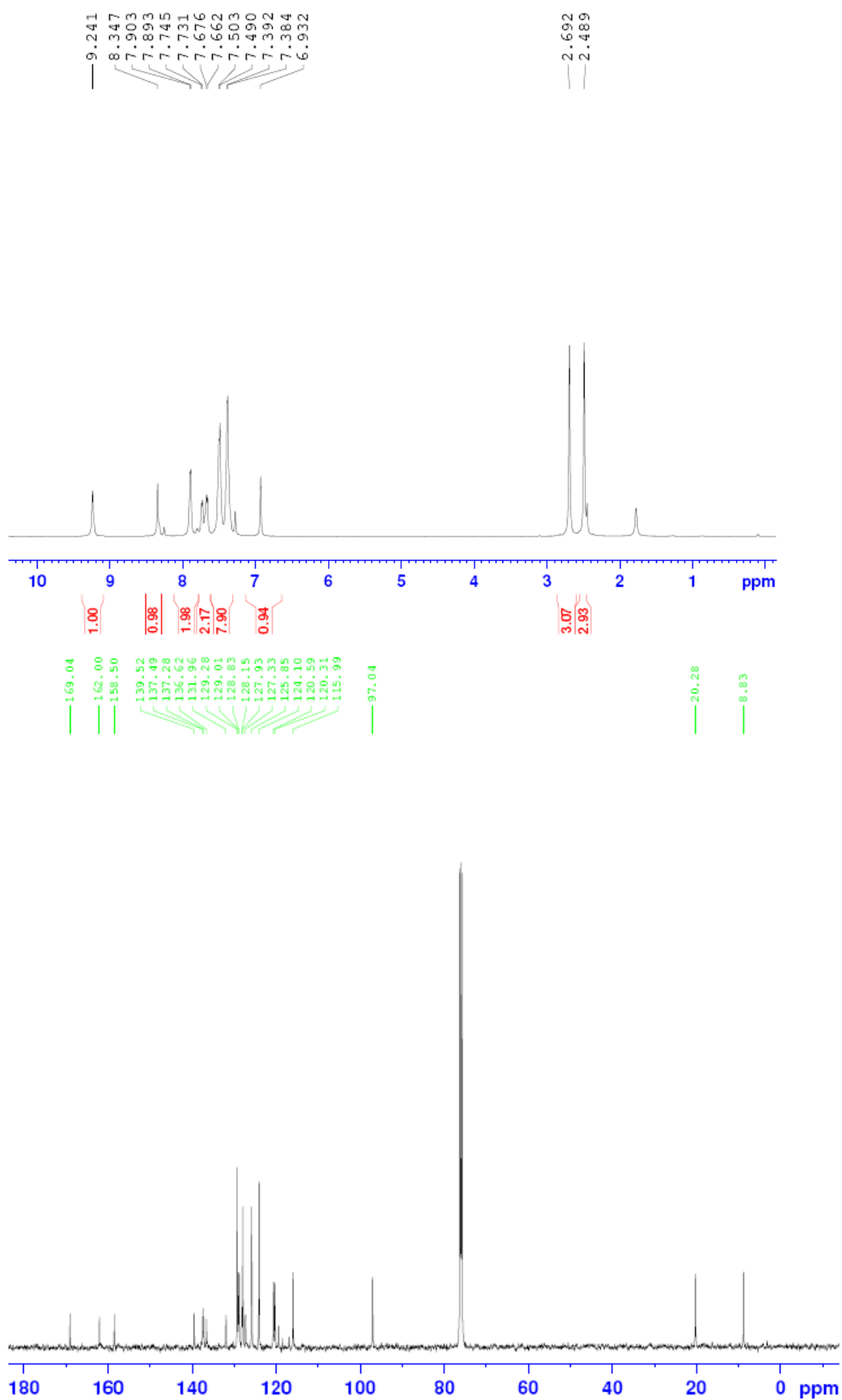
6f



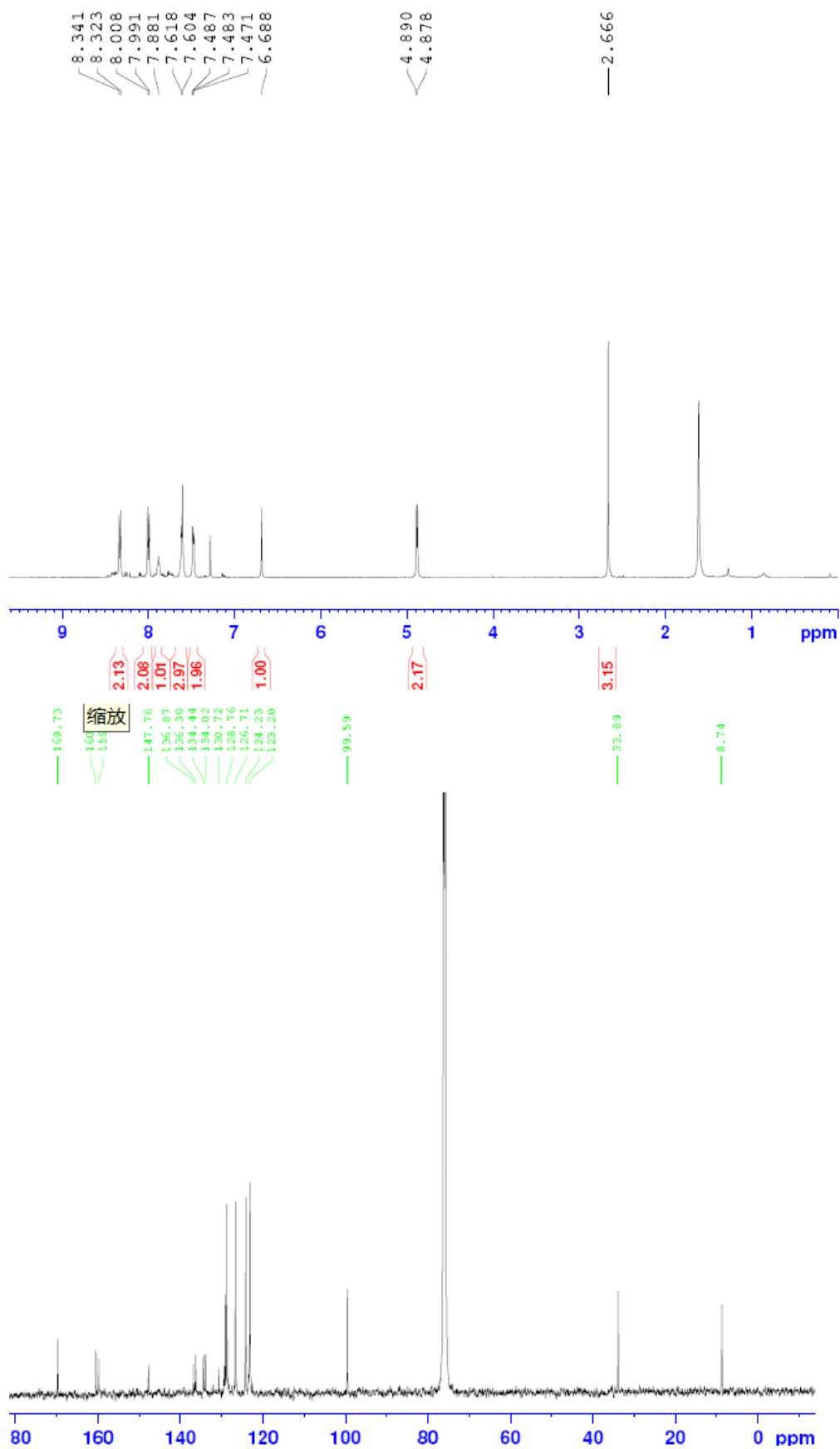
6g



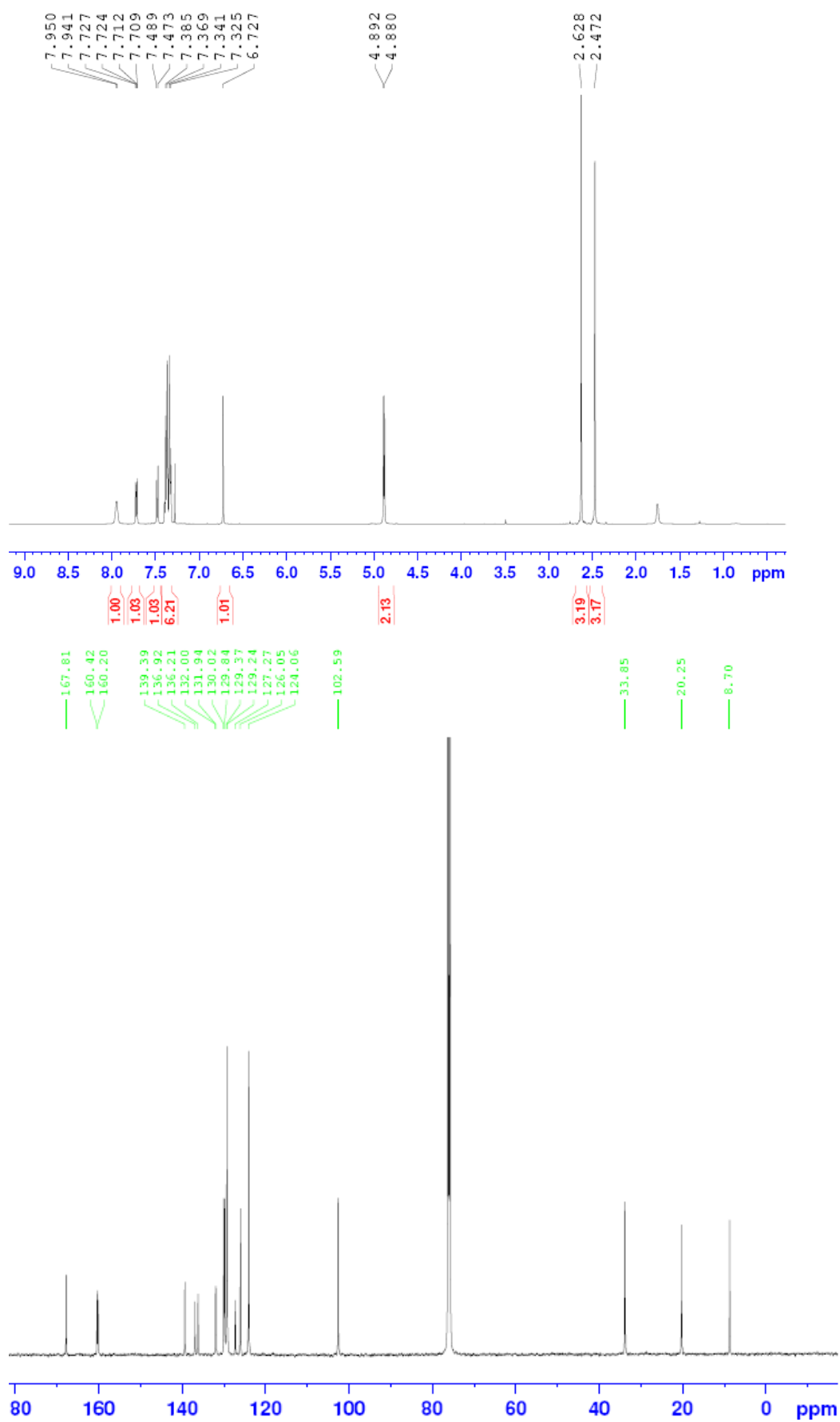
6h



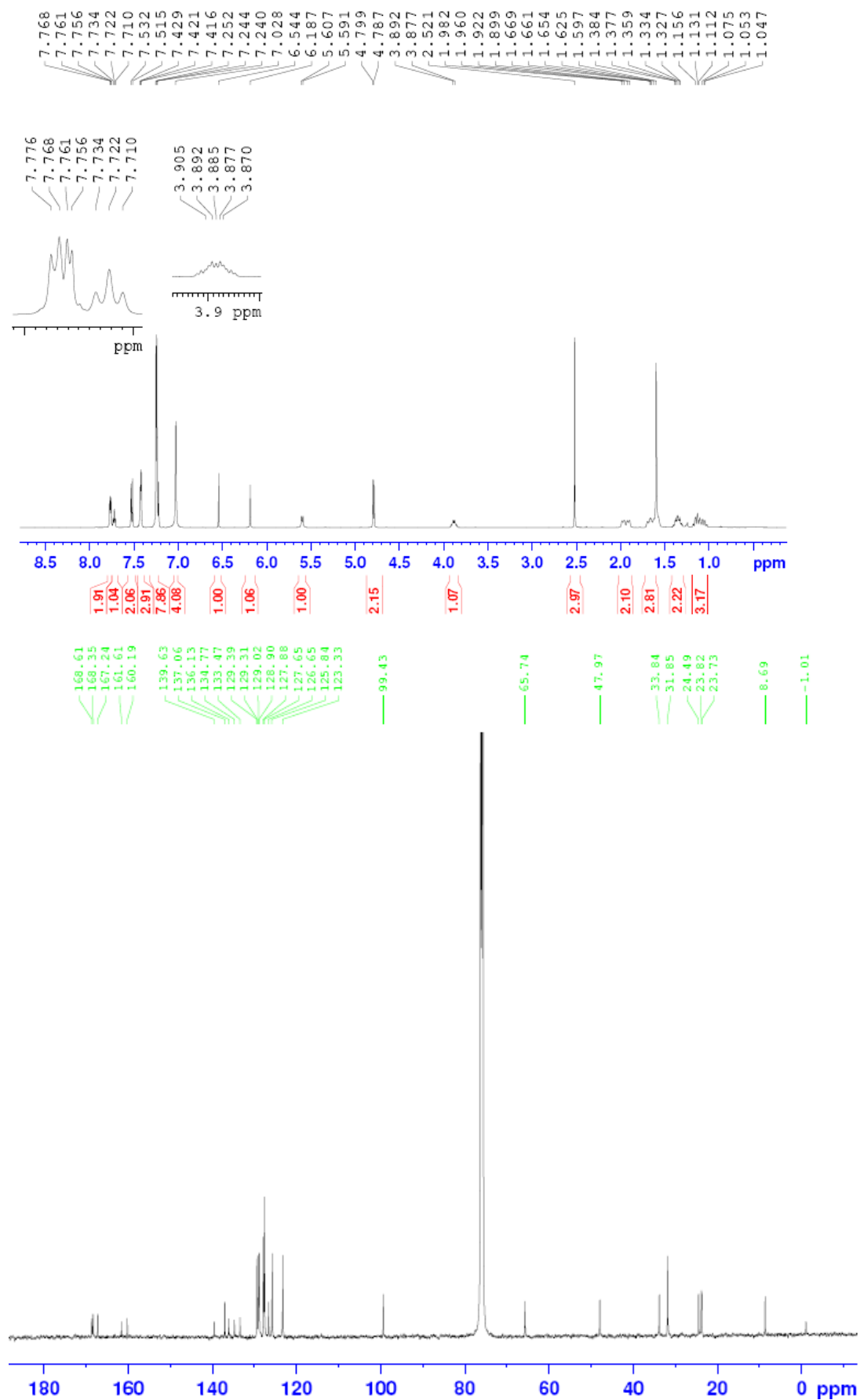
6i



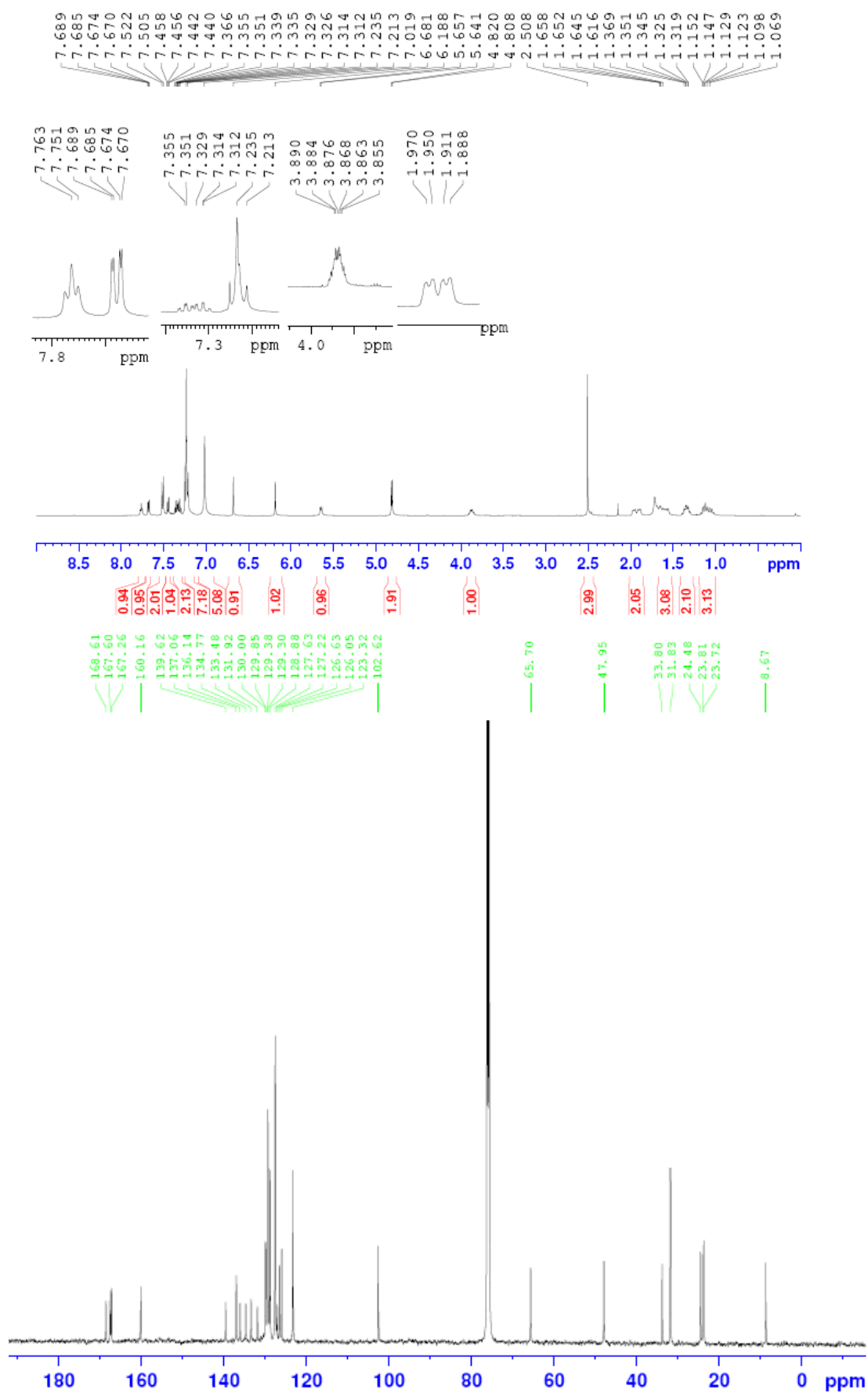
6j



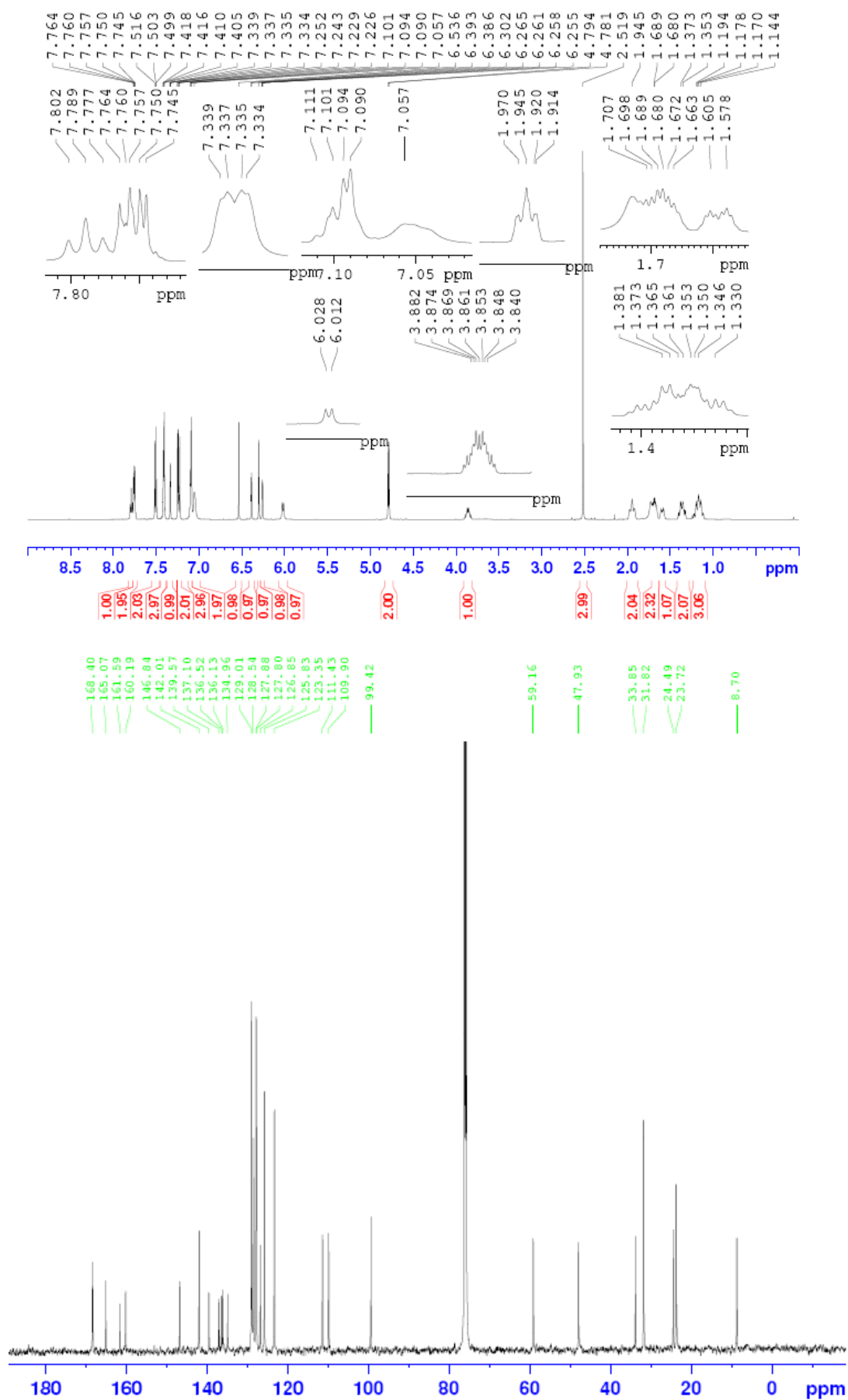
13a



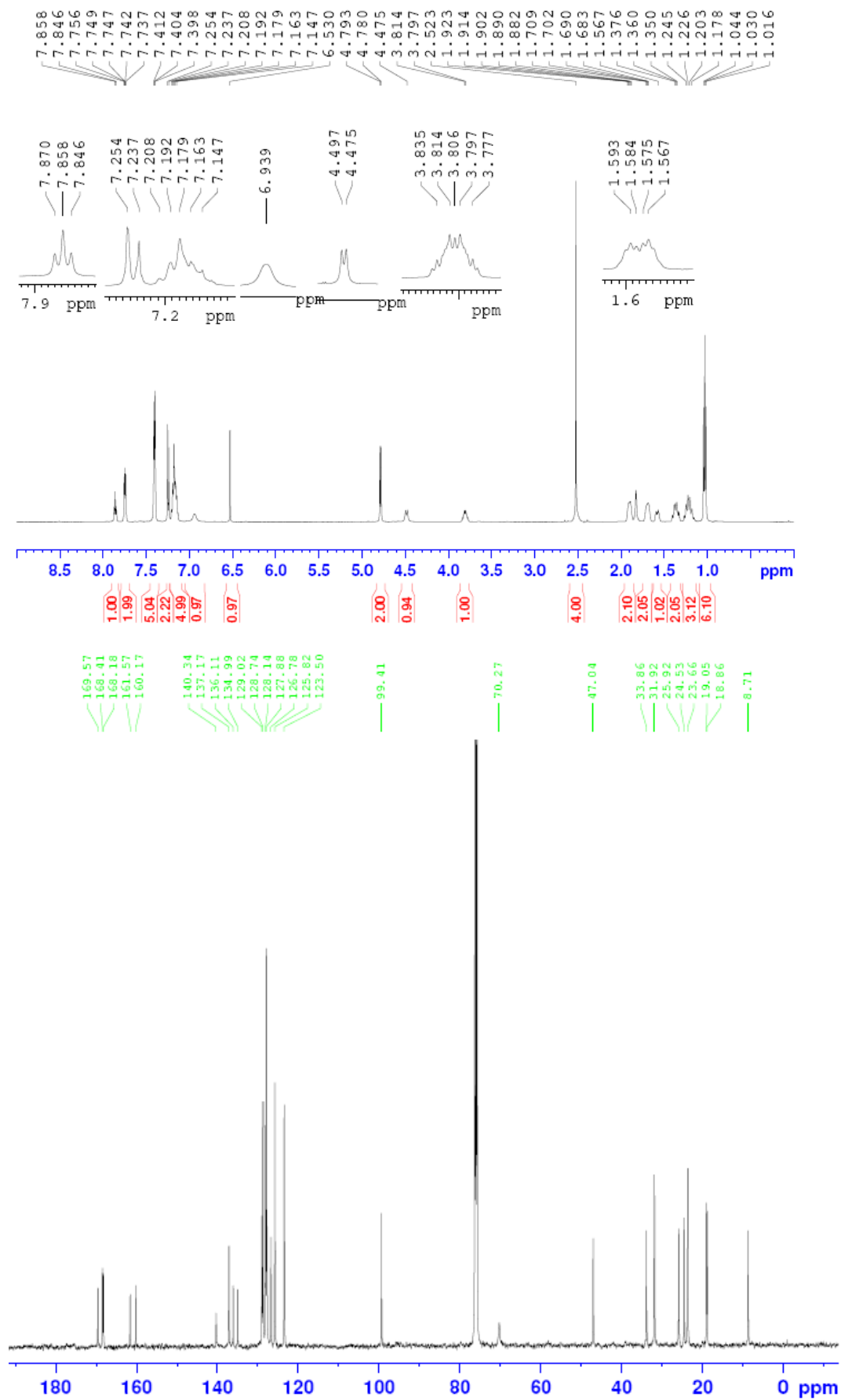
13b



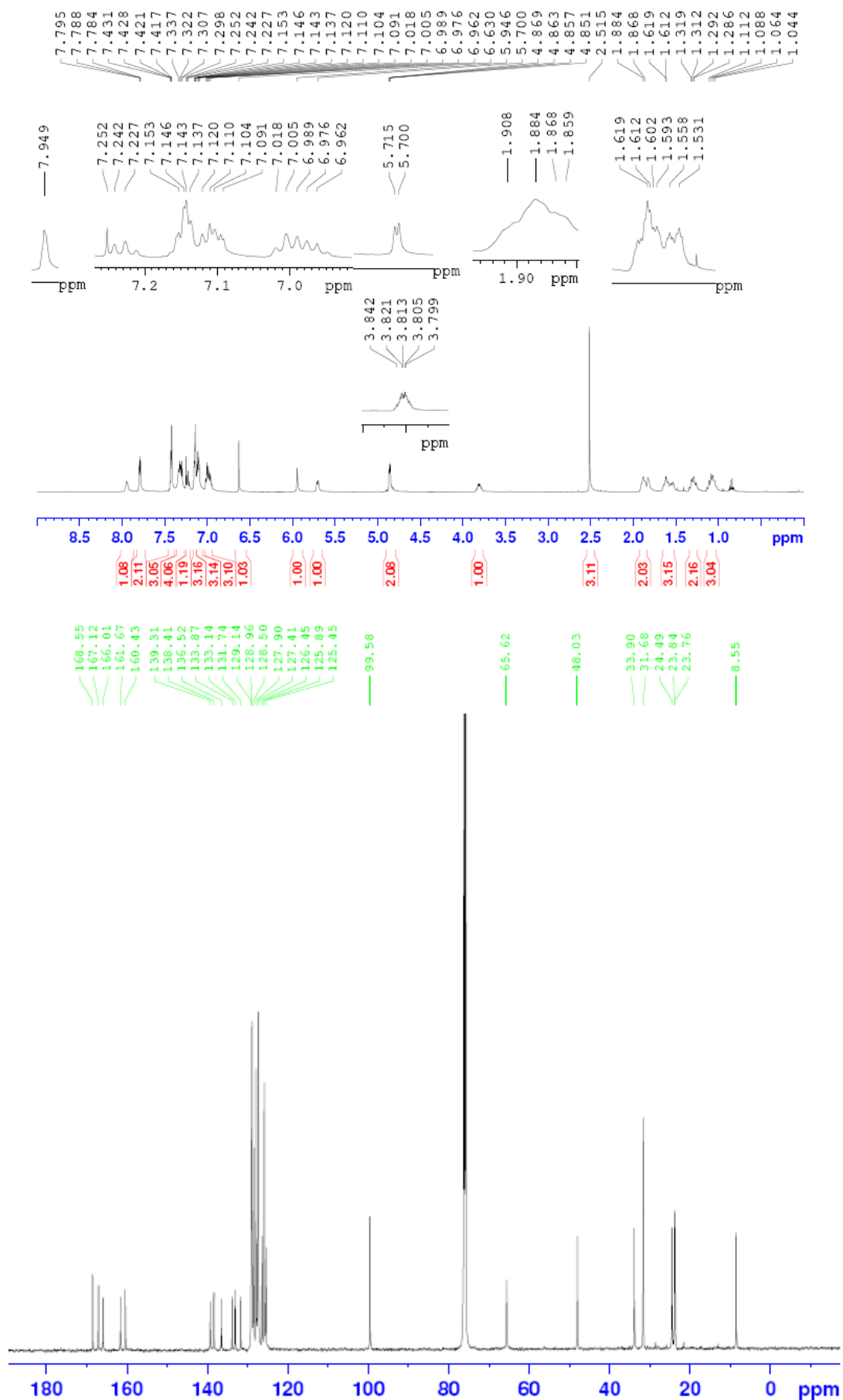
13c



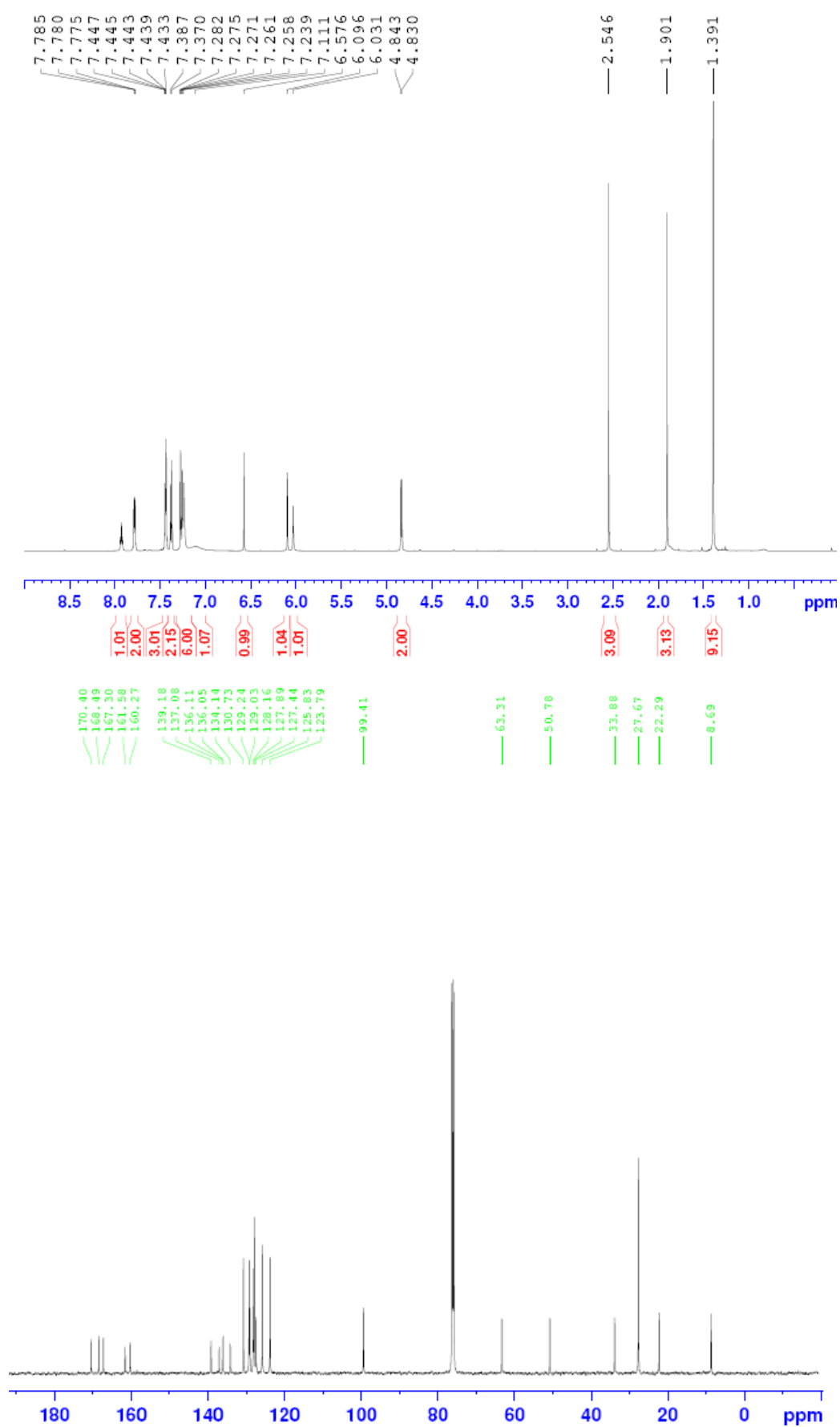
13d



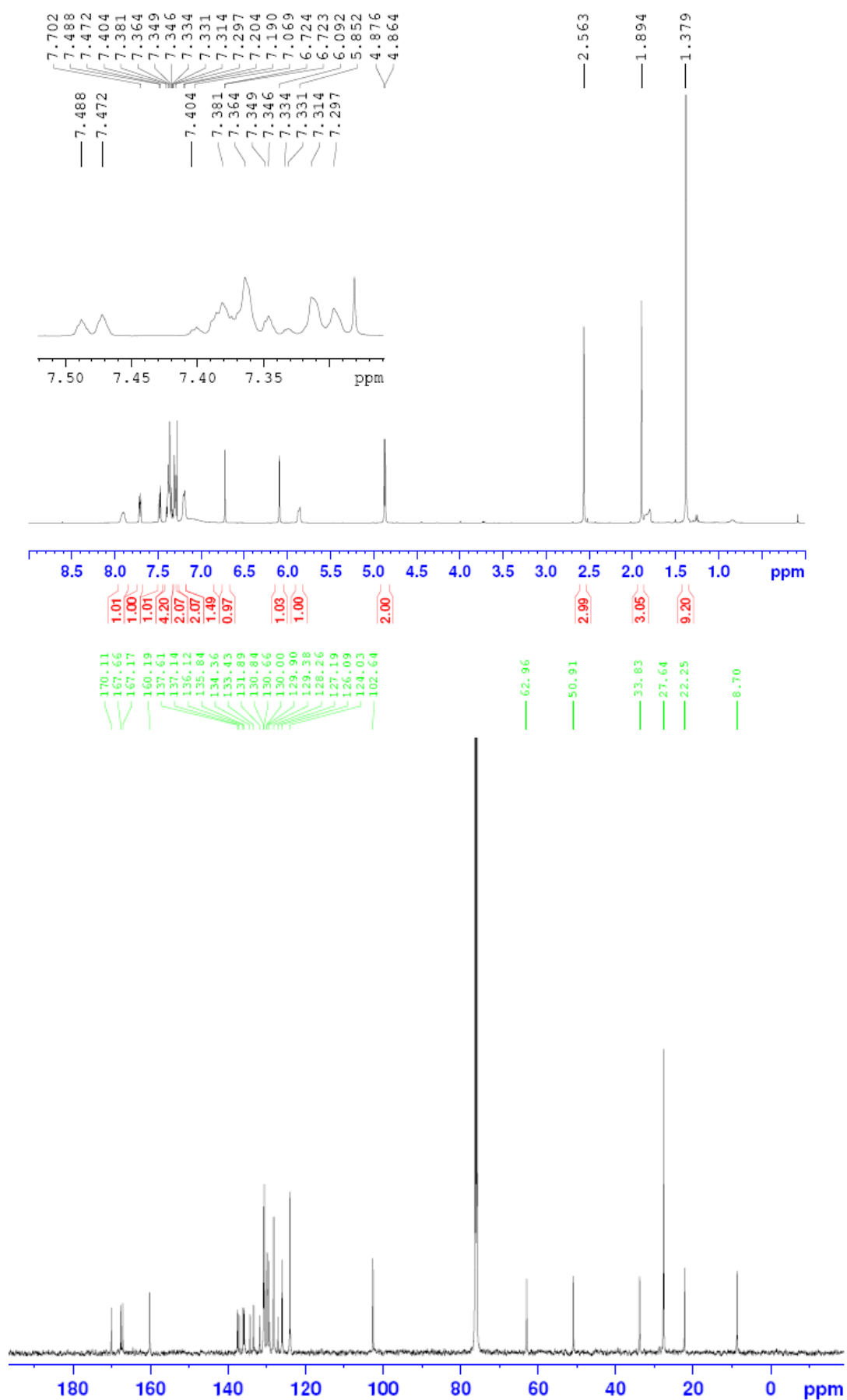
14a



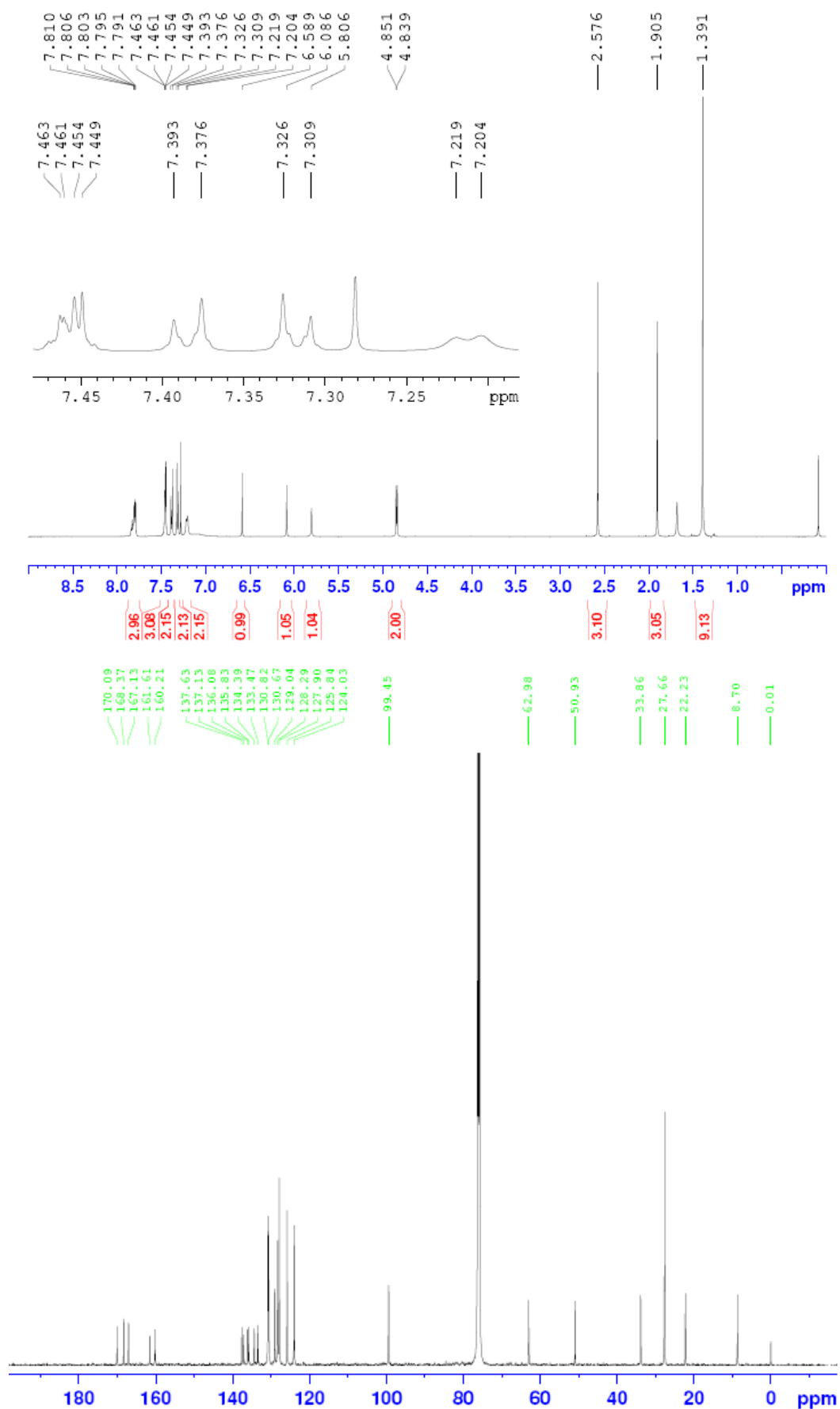
15a



15b



13c



15d

