

Supporting Information

Bromodimethylsulfonium bromide (BDMS) as a Potential Candidate for Photocatalytic Selective Oxidation of Benzylic Alcohols Using Oxygen and Visible Light

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General Information

All chemicals and solvents used in this study were of analytical reagent grade, and they were used without further purification. The catalyst bromodimethylsulfonium bromide (BDMS) used in the present work was synthesized with the help of standard literature procedure.¹ The compound 2-chlorobenzyl 4-methylbenzenesulfonate was synthesized according to the literature procedure.² All the ¹H and ¹³C NMR spectra were recorded at 200 MHz and 50 MHz respectively.

Absorption Spectra of BDMS:

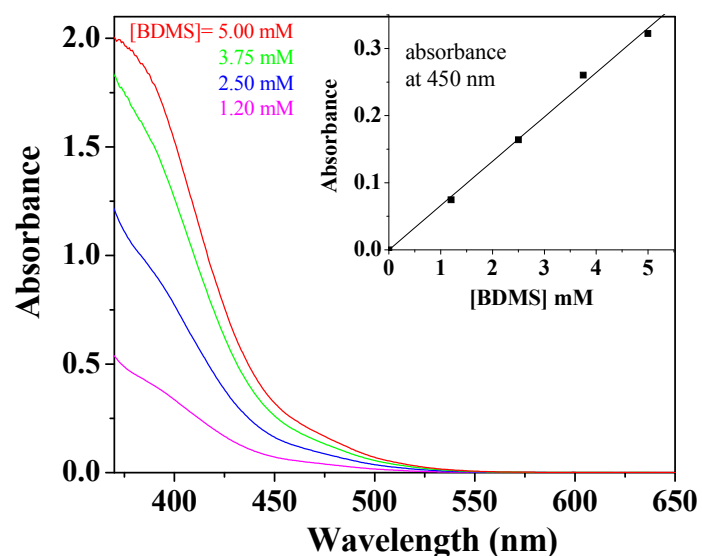


Figure 1. UV-visible spectra of BDMS in acetonitrile at different concentration (inset- the linear plot of absorbance vs concentration of BDMS at 450 nm).

Measurement of the intensity of 45 W Household CFL by using potassium ferrioxalate as an actinometer:

The intensity (I_0) of the lamp (Philips 45 W household white CFL) used in this photocatalytic study, was measured by following standard procedure utilizing potassium ferrioxalate as the actinometer.^{3,4} In a typical procedure, 10 ml (V_1) of 0.006 M solution of potassium ferrioxalate was taken in a 15 ml pyrex vial and placed 5 cm away from the visible light source. The ferrioxalate solution (V_1) was irradiated under efficient stirring. After 1 min, 1 ml (V_2) of the irradiated solution was transferred into a 10 ml (V_3) volumetric flask containing a mixture of 4 ml of 0.1 % 1.10-phenanthroline solution (store in the dark) and 0.5 ml of buffer solution (stock solution: 82 g NaOAc, 10 ml conc. H_2SO_4 , diluted to 1 L with distilled water) which was then diluted to the mark with distilled water. A reference was also prepared in the same way except that it has not been irradiated. Both solutions are kept in the dark for an hour until full colour development is achieved. Then, absorption spectra of these solutions were recorded by using UV-Vis spectrophotometer. Then the absorbance of the first (A_i) minus that of the second (A_d) sample is measured at 510 nm (1 cm path length, $\epsilon_{510} = 11100 \text{ dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$). After that the intensity (I_0) was calculated from the following **equation 1**.

$$I_0 = N_A \frac{(A_i - A_d) \times V_1 \times 10^{-3} \times V_3}{\Phi_\lambda \times \epsilon_{510} \times V_2 \times t} \quad \text{Einstein} \cdot \text{S}^{-1}$$

where, $\Phi_\lambda = 1.11$, at 436 nm and
 N_A is the Avogadro's number

(1)

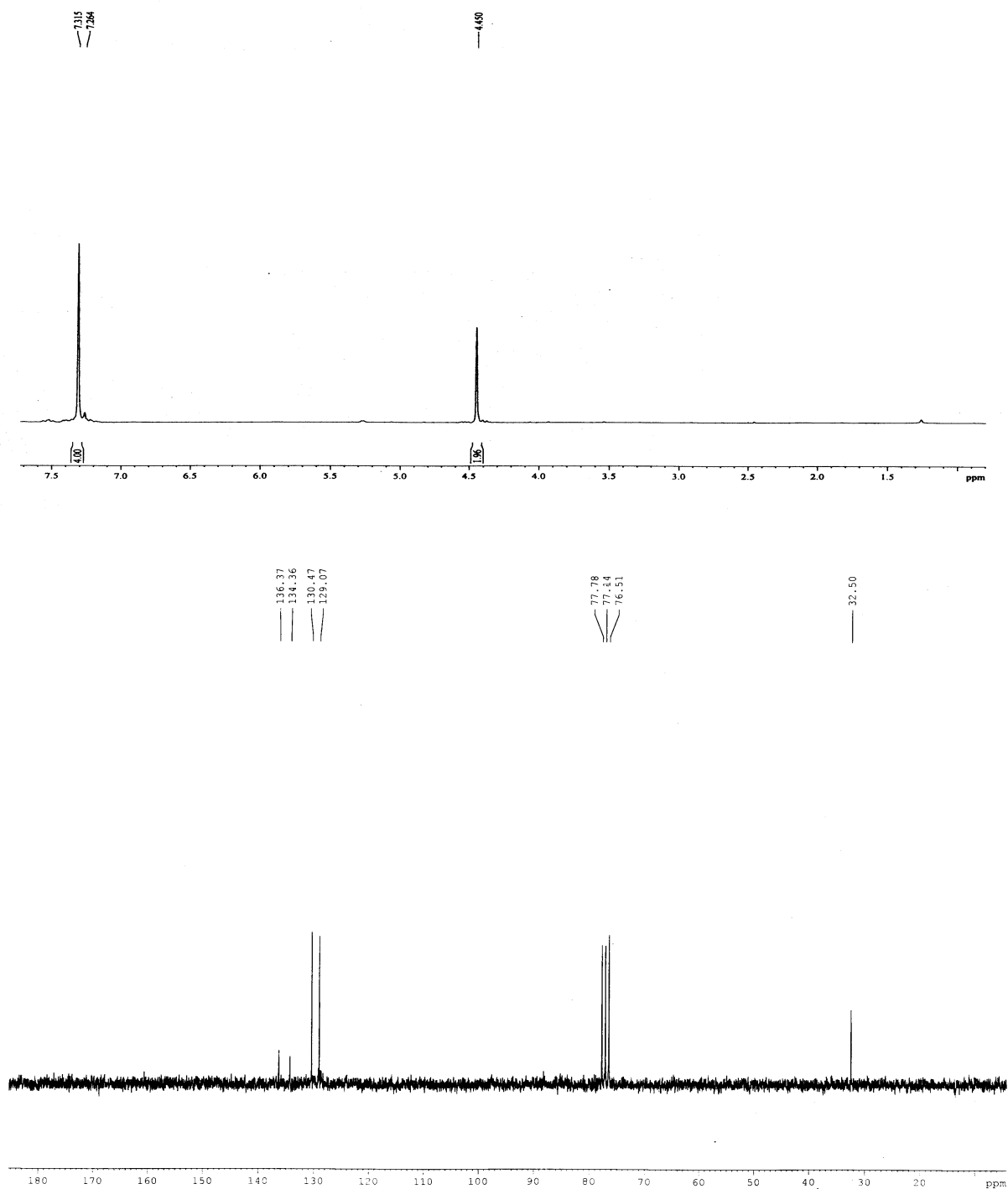
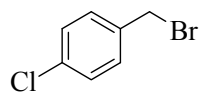
It was found that the intensity of the lamp 45 W CFL used was $2.98 \times 10^{16} \text{ Einstein S}^{-1}$.

References:

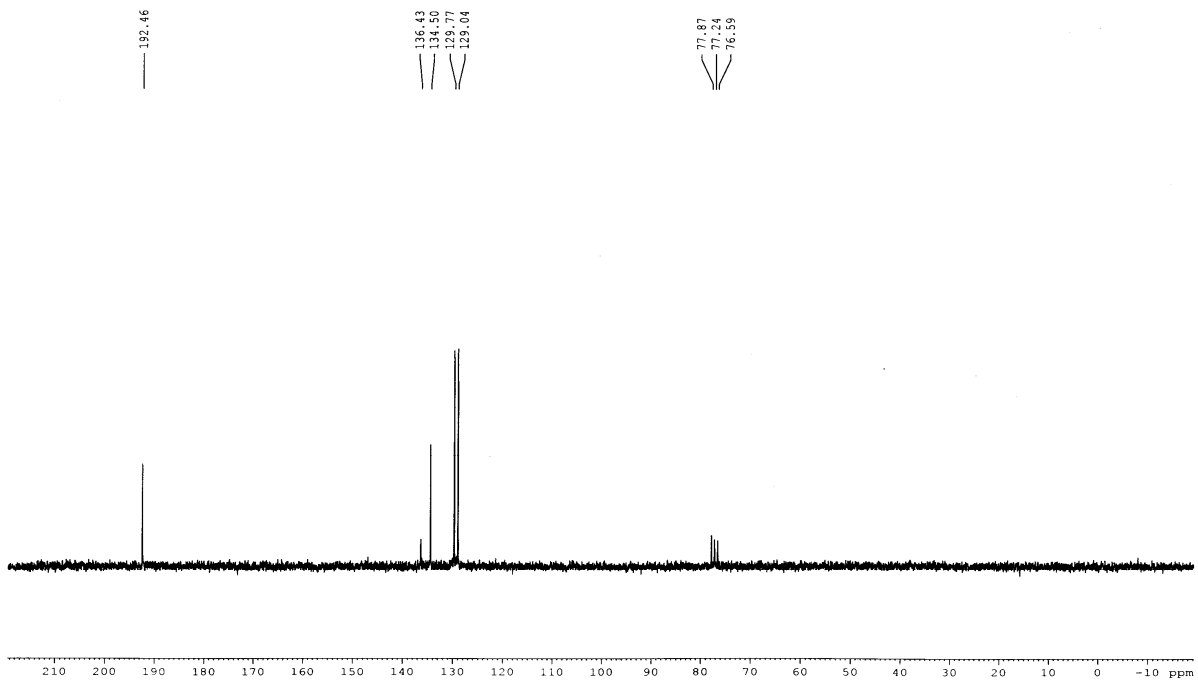
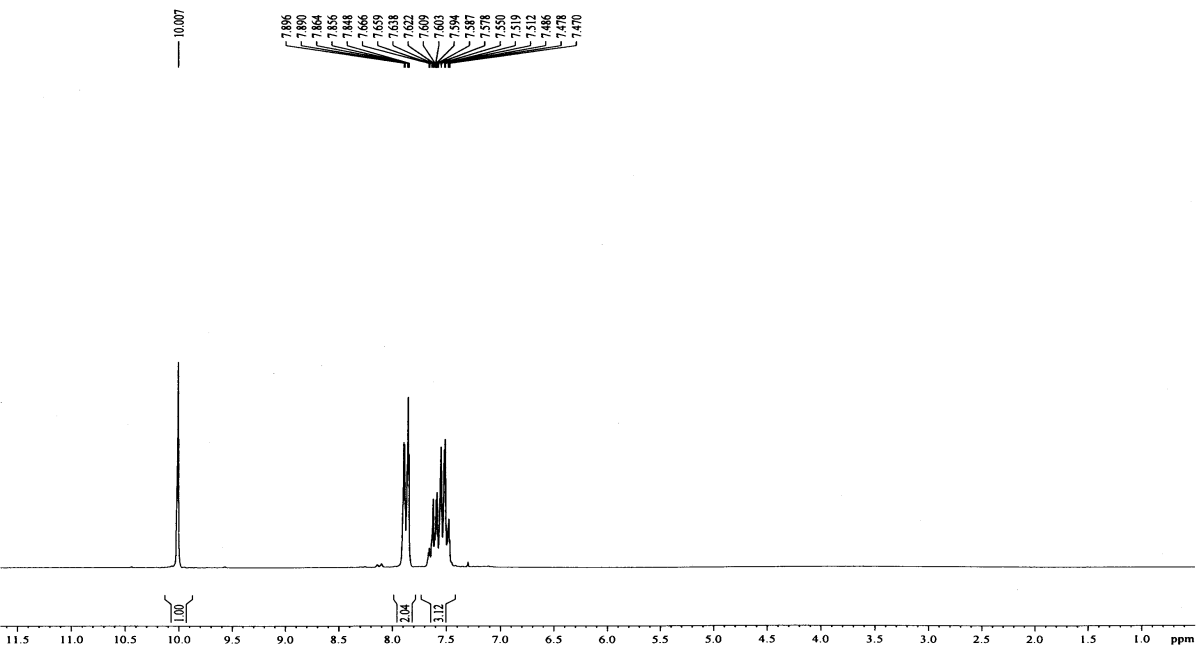
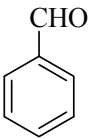
1. A. T. Khan, Md A. Ali, P. Goswami, L. H. Choudhury, *J. Org. Chem.* 2006, **71**, 8961-8963.
2. F. Kazemi, A. R. Massah, M. Javaherian, *Tetrahedron* 2007, **63**, 5083-5087.
3. C. G. Hatchard, C. A. Parker, *Proc. R. Soc. Lond., Ser.* **1956**, A235, 518-536.
4. R. Ananthakrishnan, S. Gazi, *Catal. Sci. Technol.* 2012, DOI: 10.1039/c2cy20050c.

¹H and ¹³C NMR spectra of compounds:

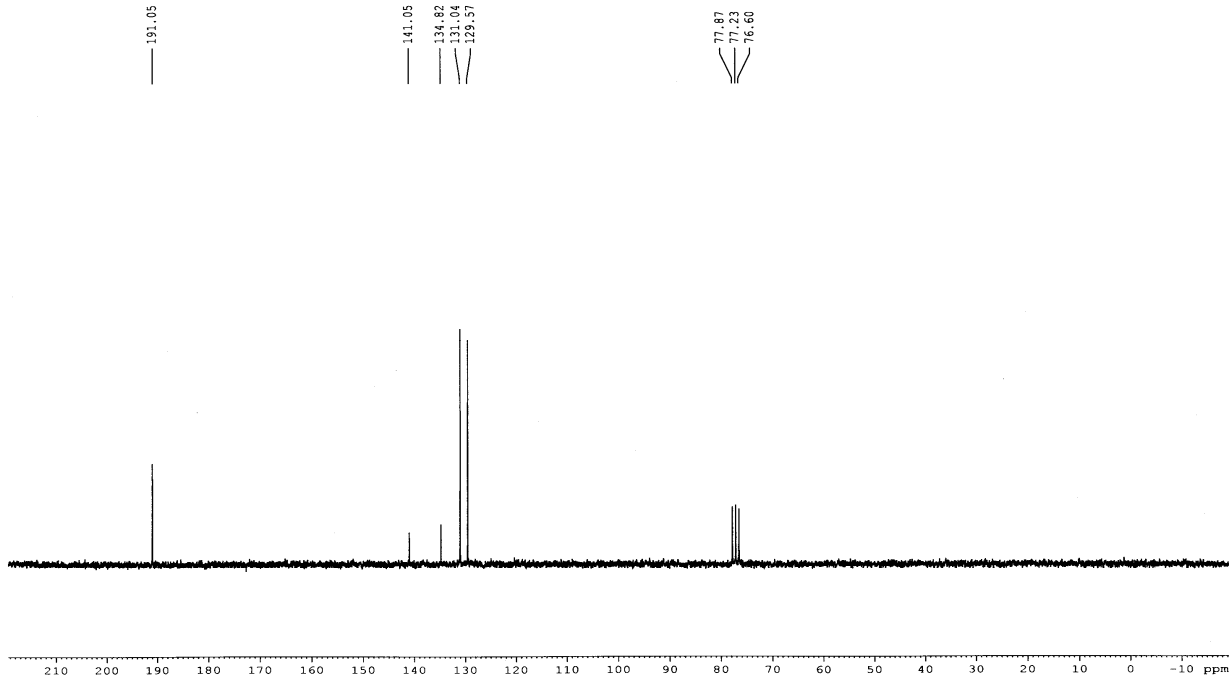
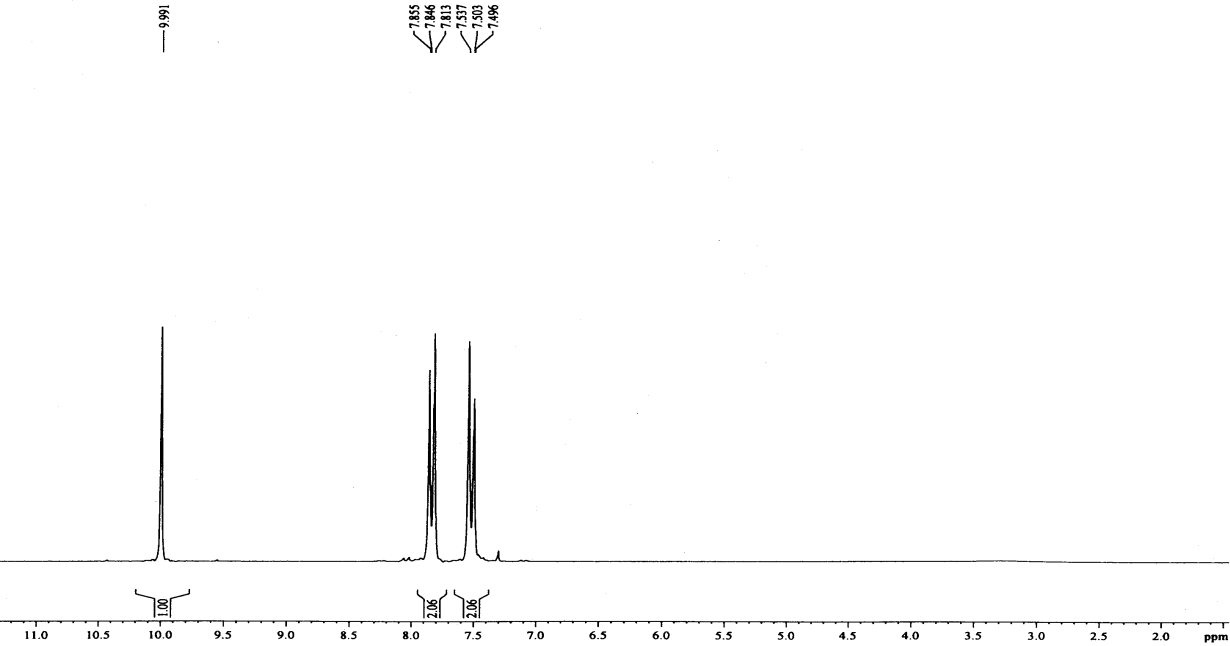
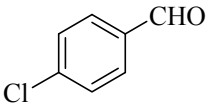
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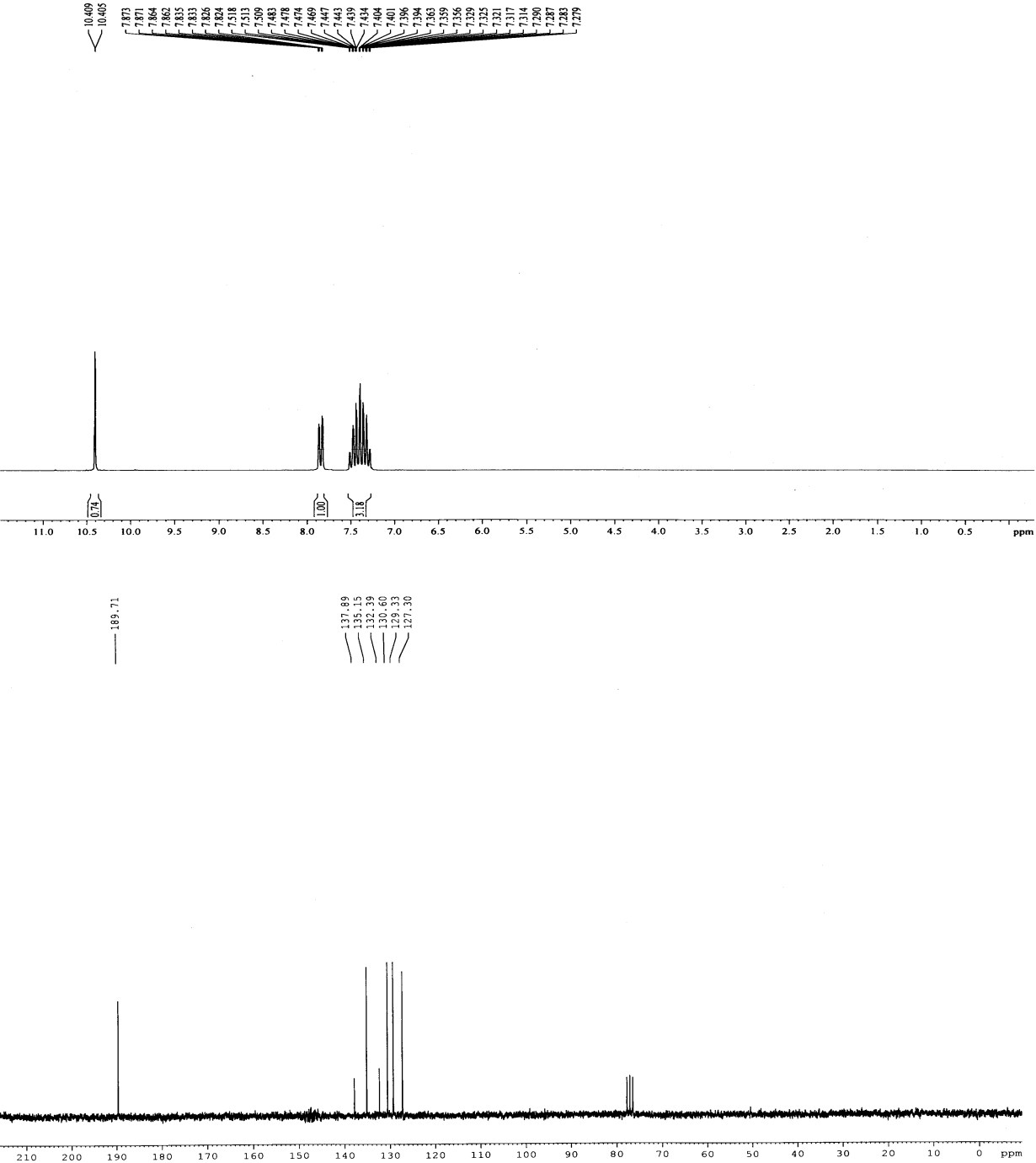
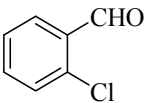
Benzaldehyde



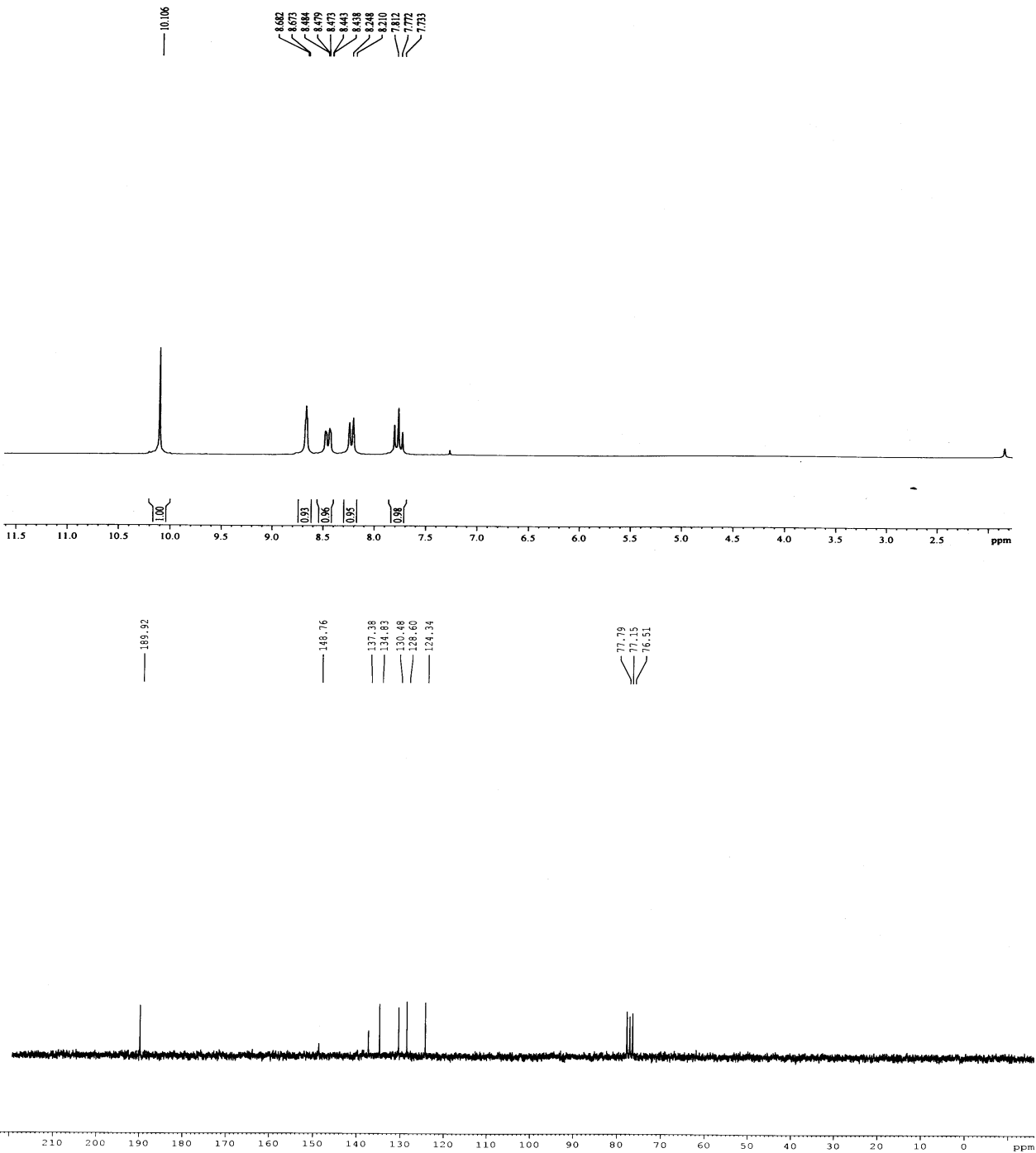
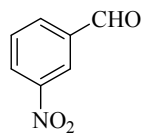
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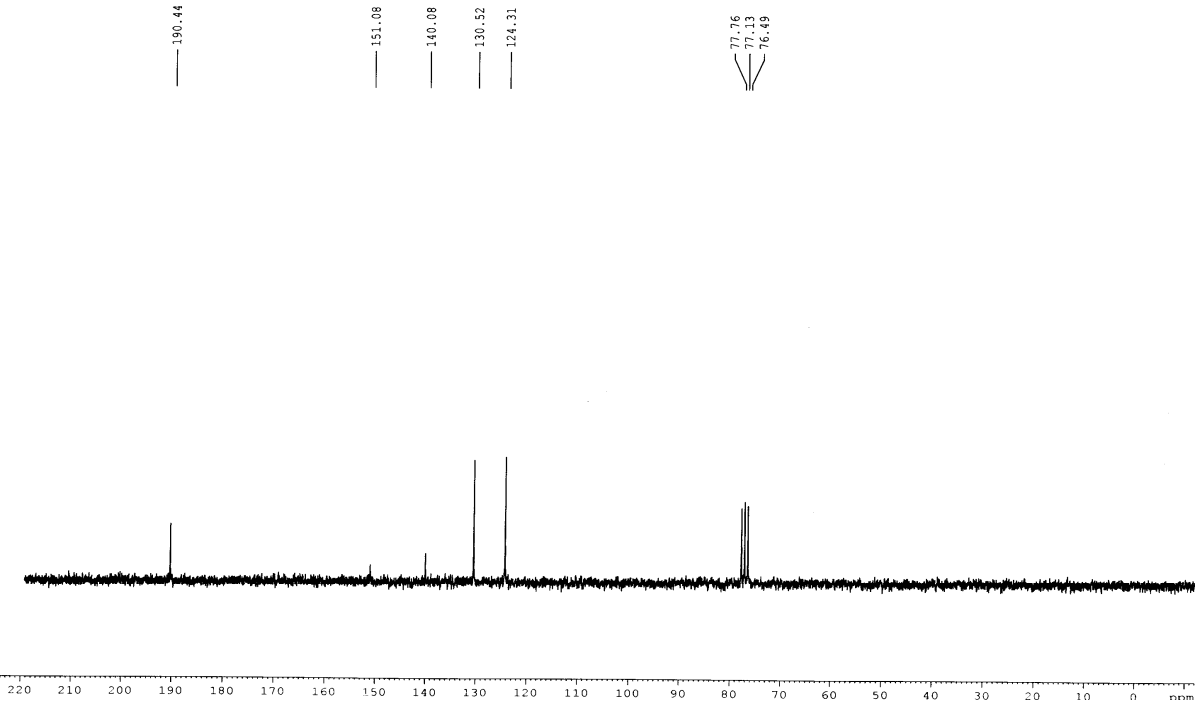
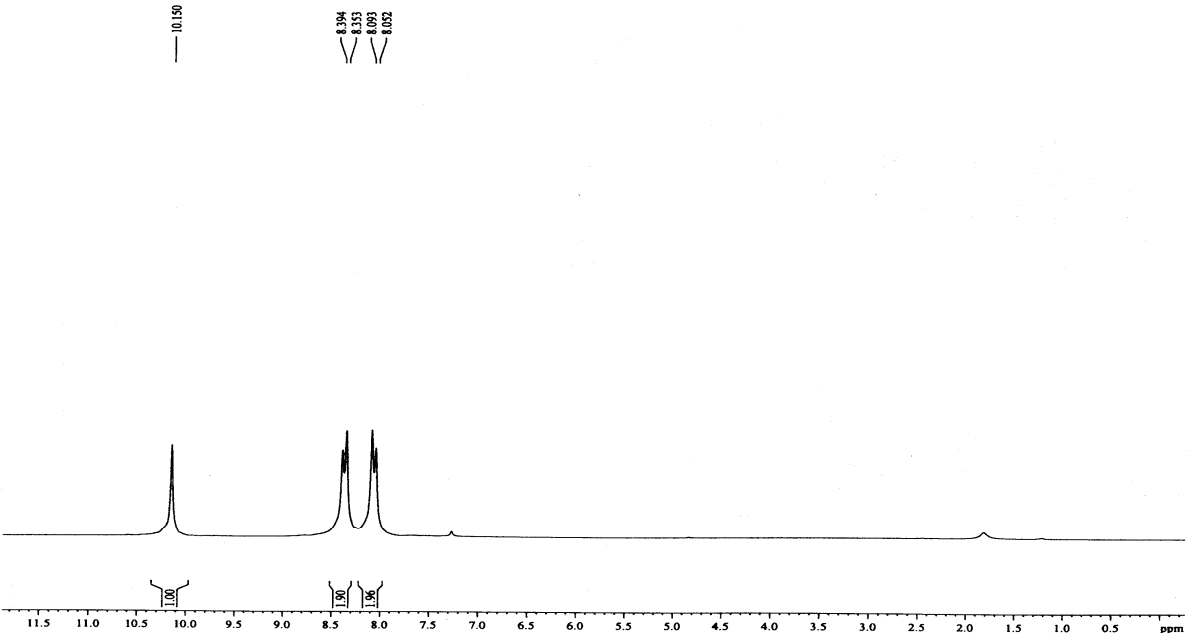
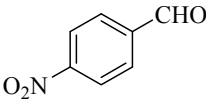
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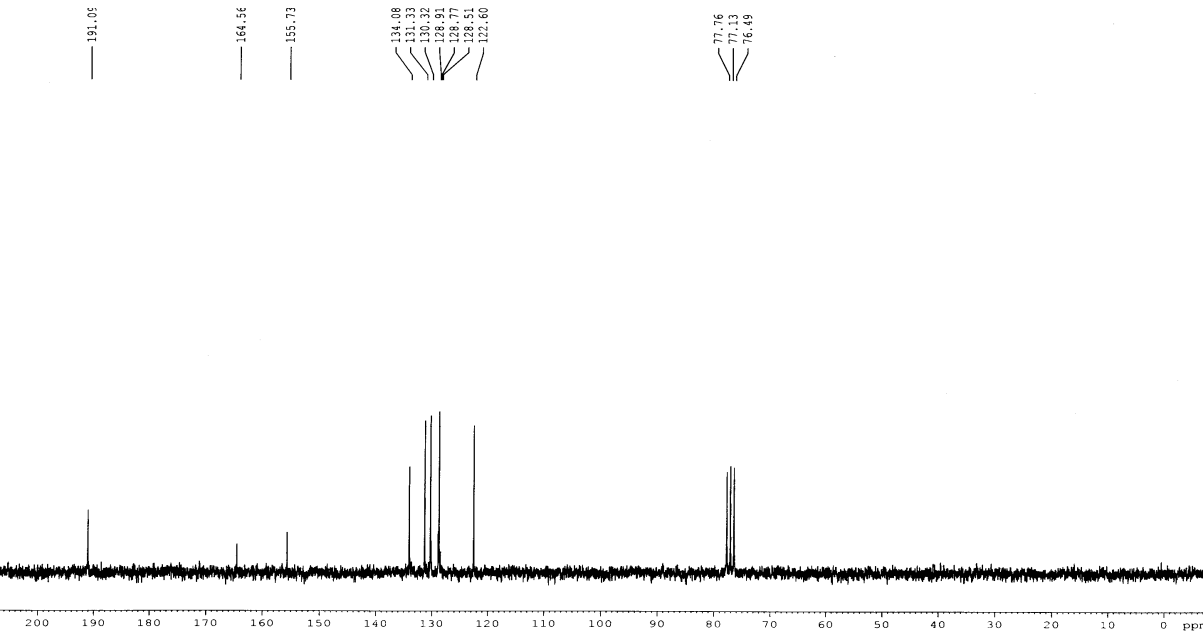
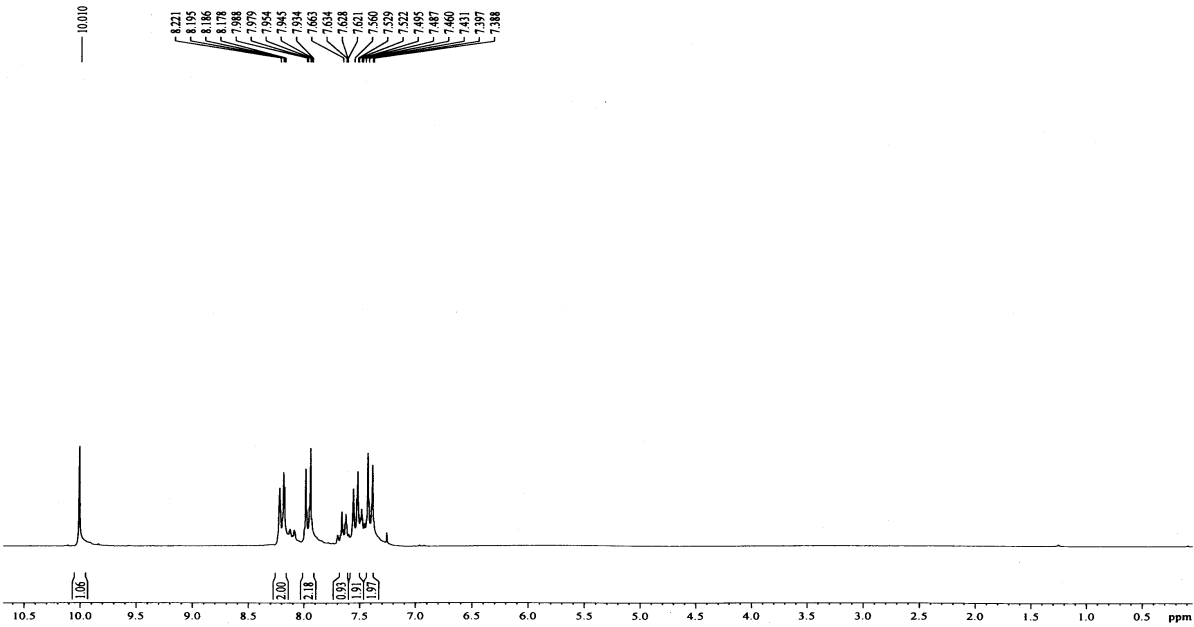
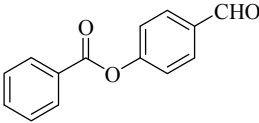
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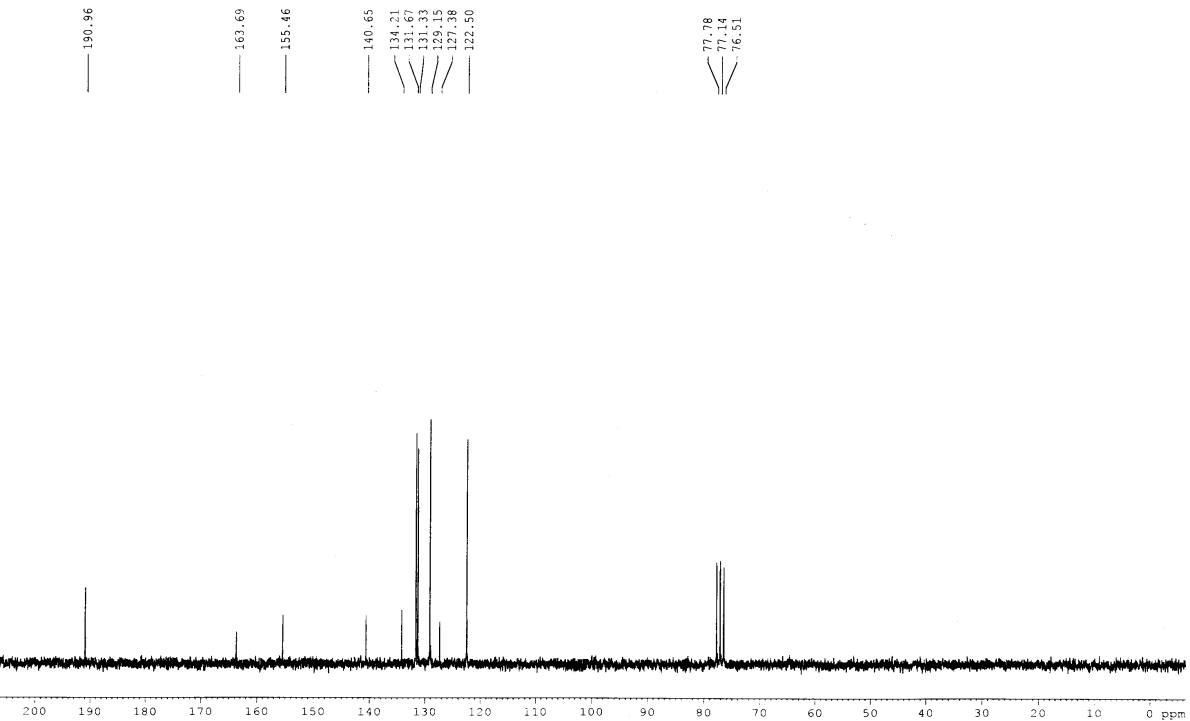
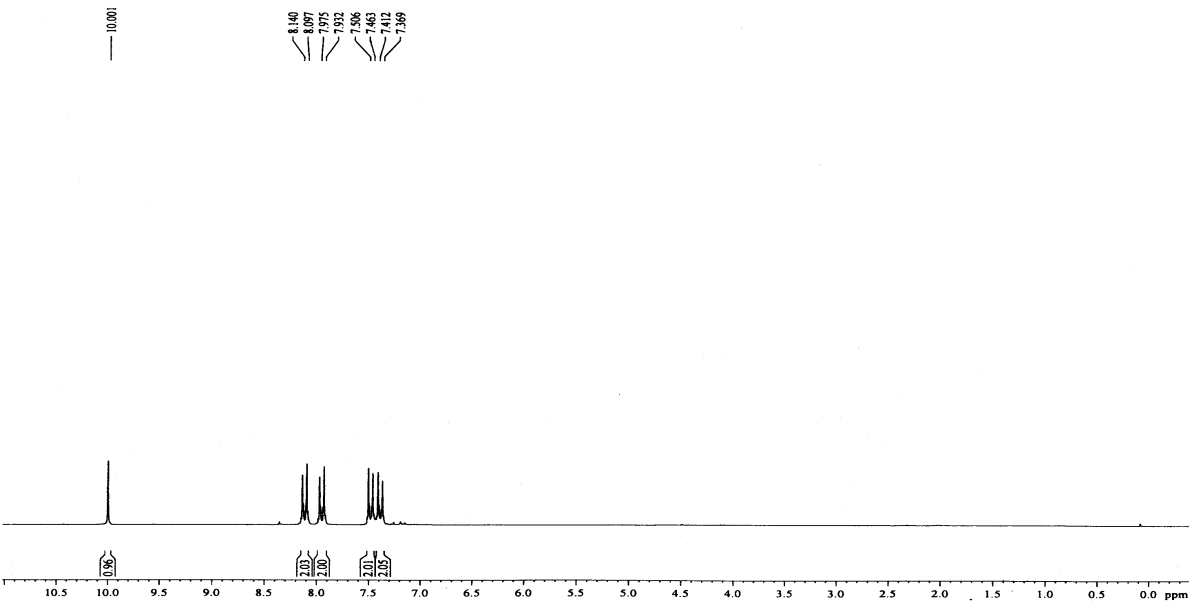
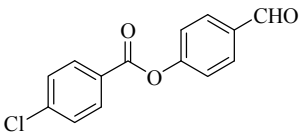
4-nitrobenzaldehyde



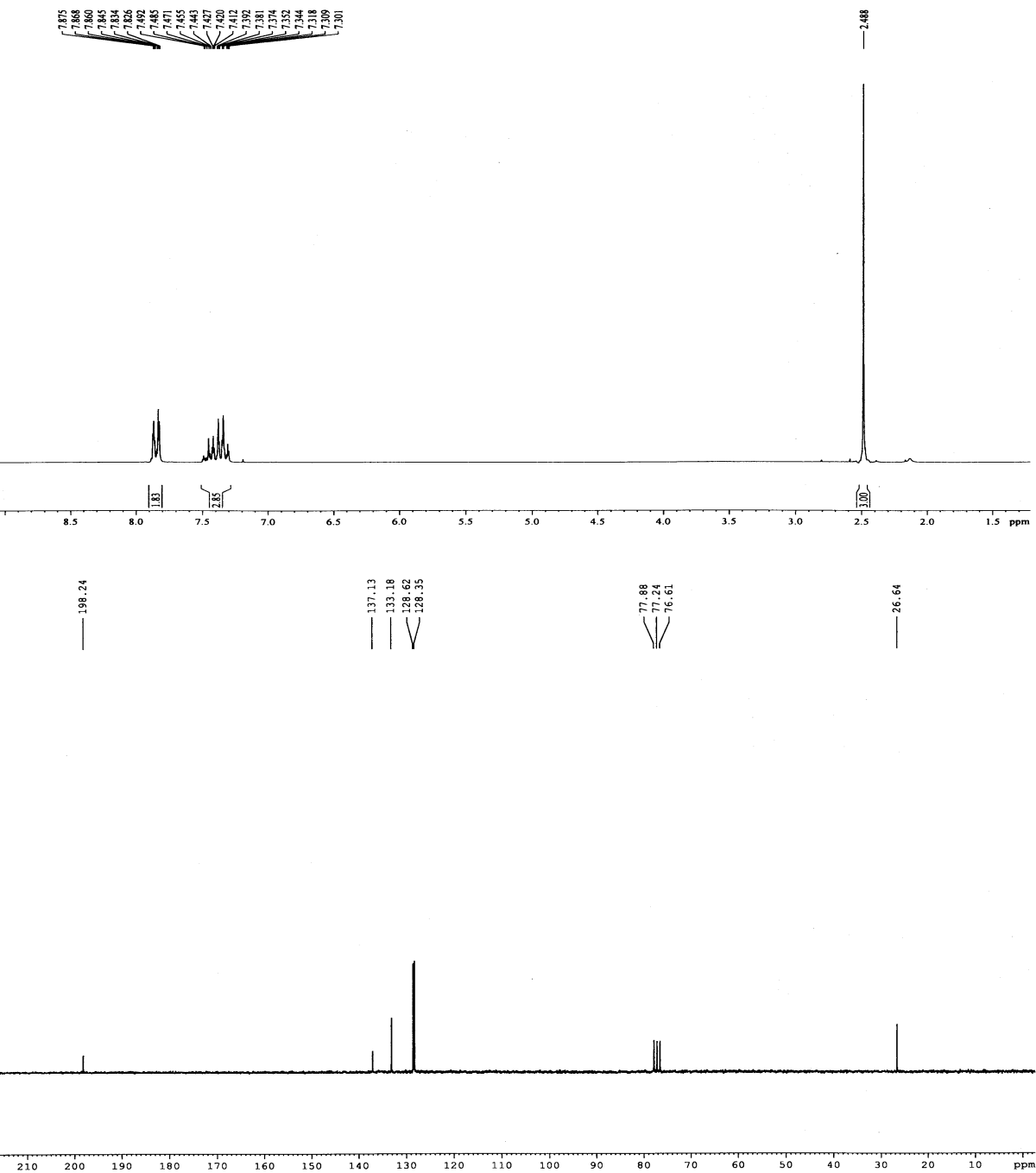
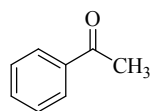
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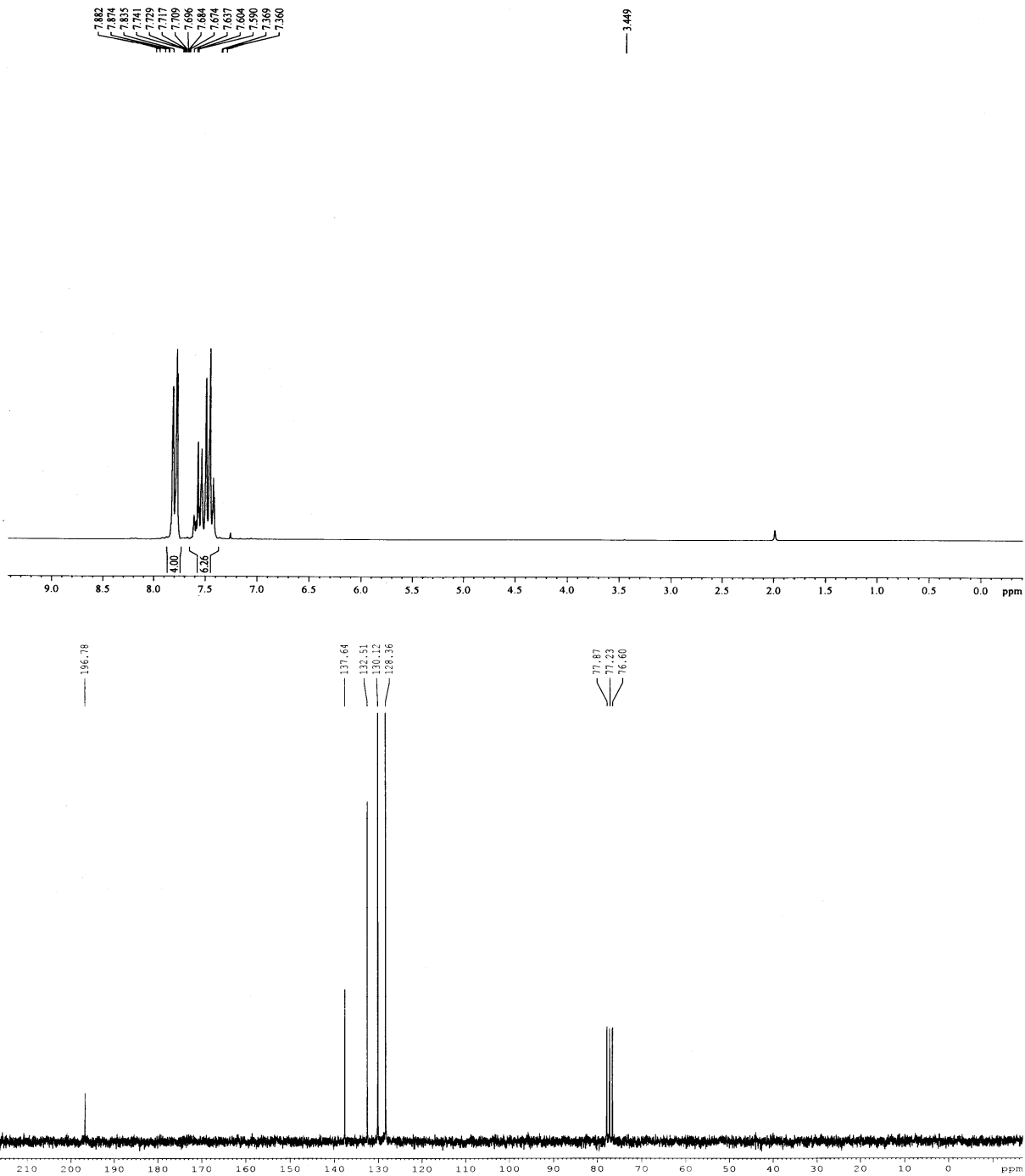
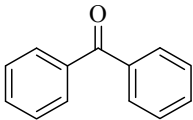
4-formylphenyl 4-chlorobenzoate



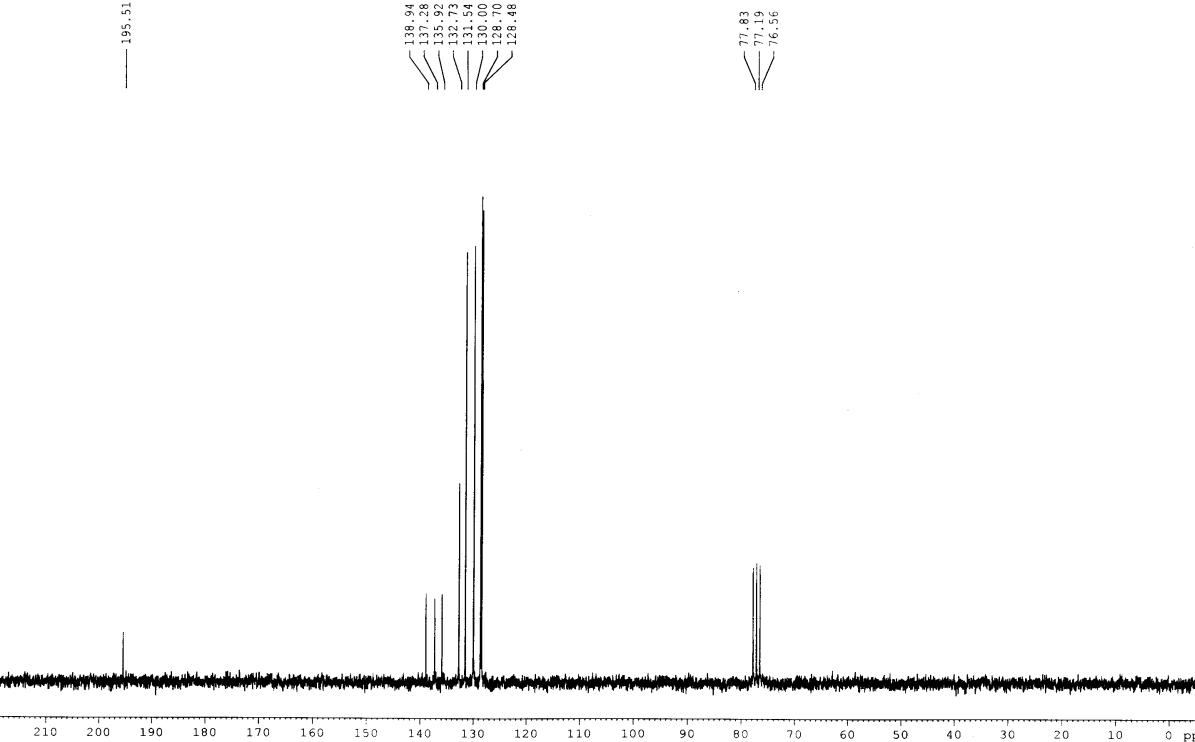
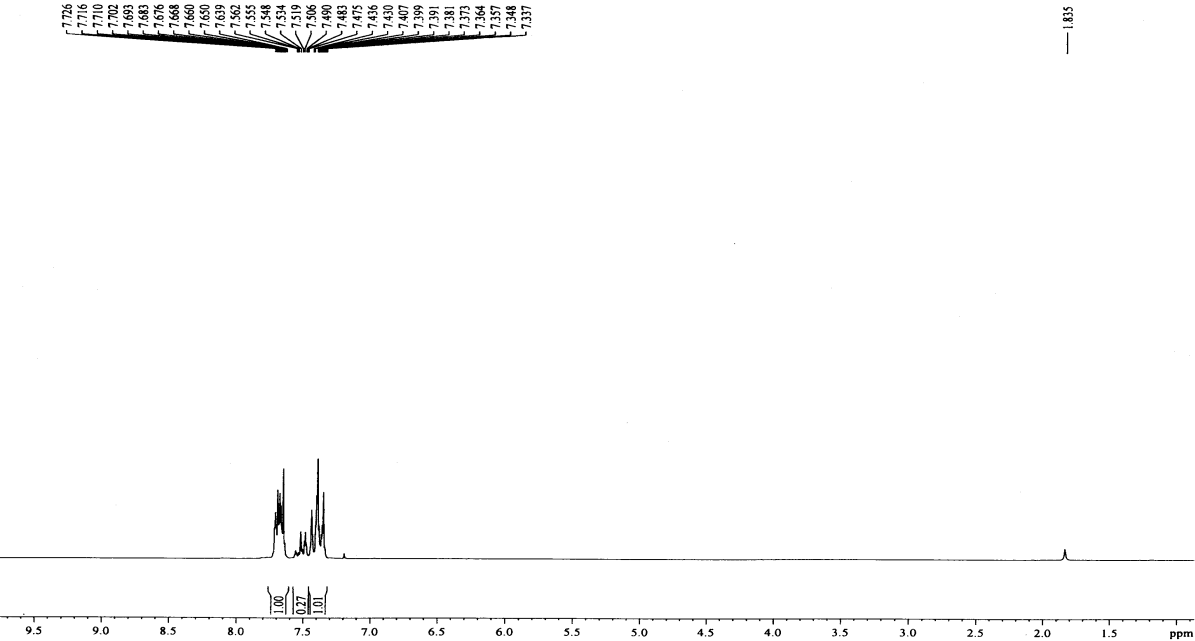
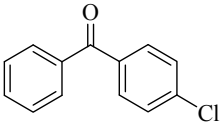
Acetophenone



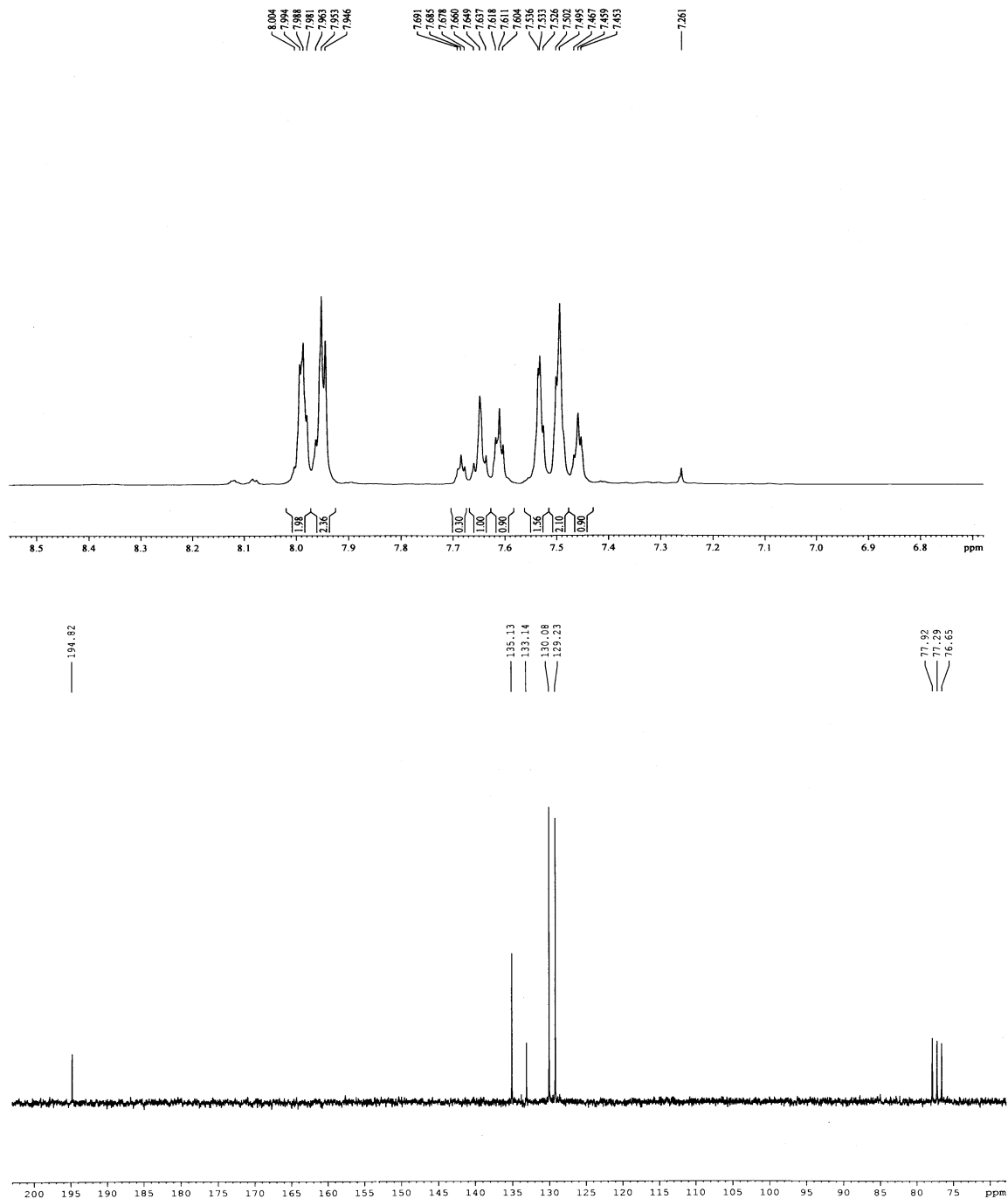
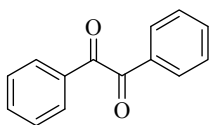
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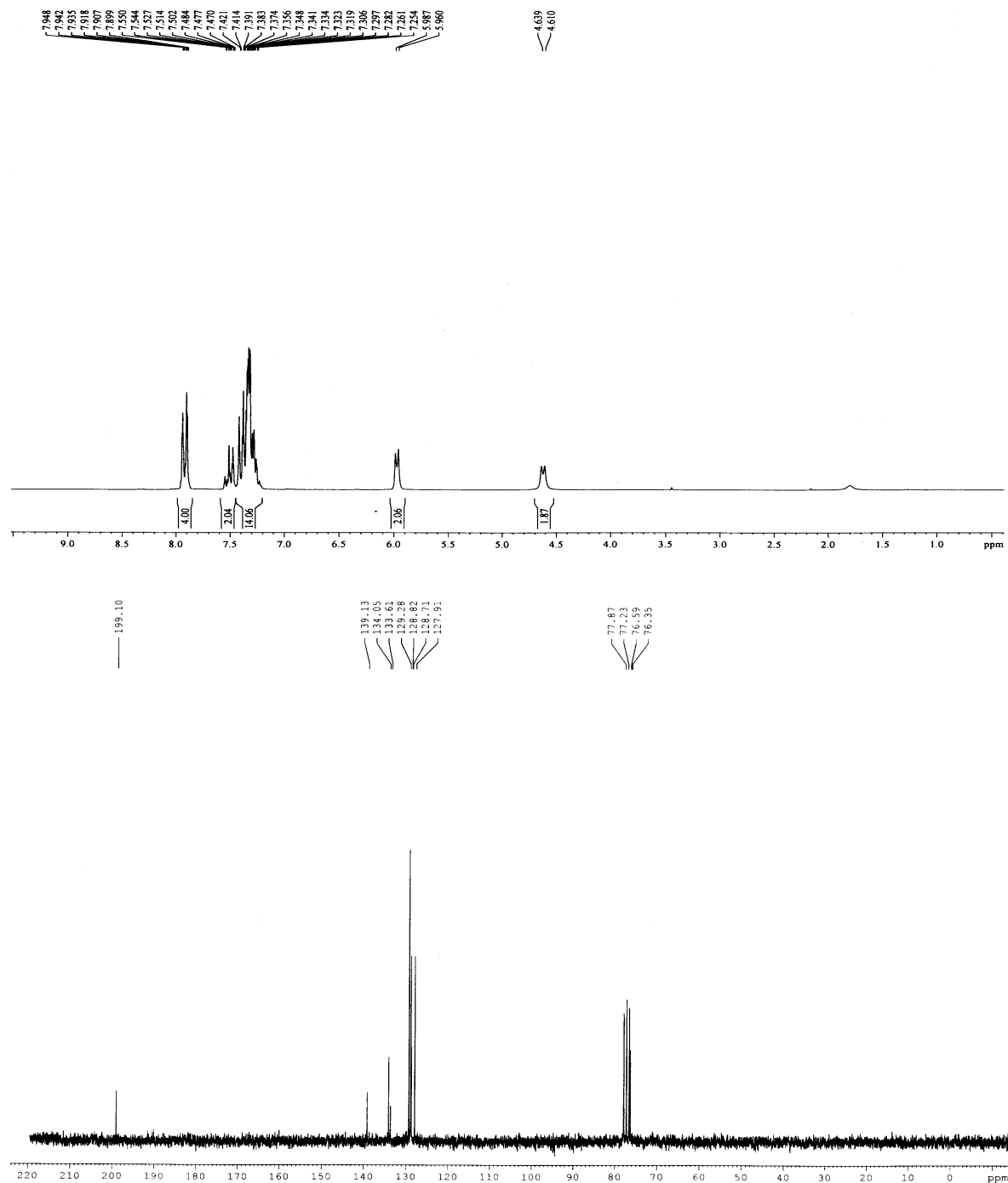
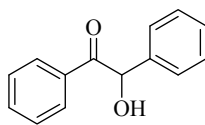
(4-chlorophenyl)(phenyl)methanone



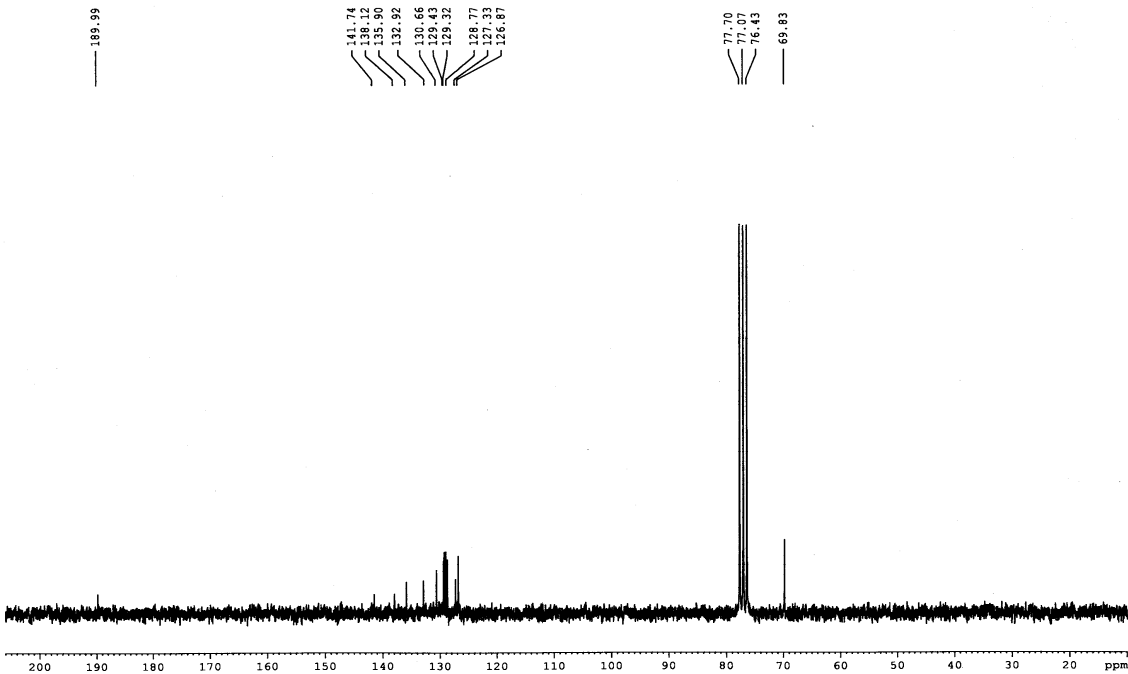
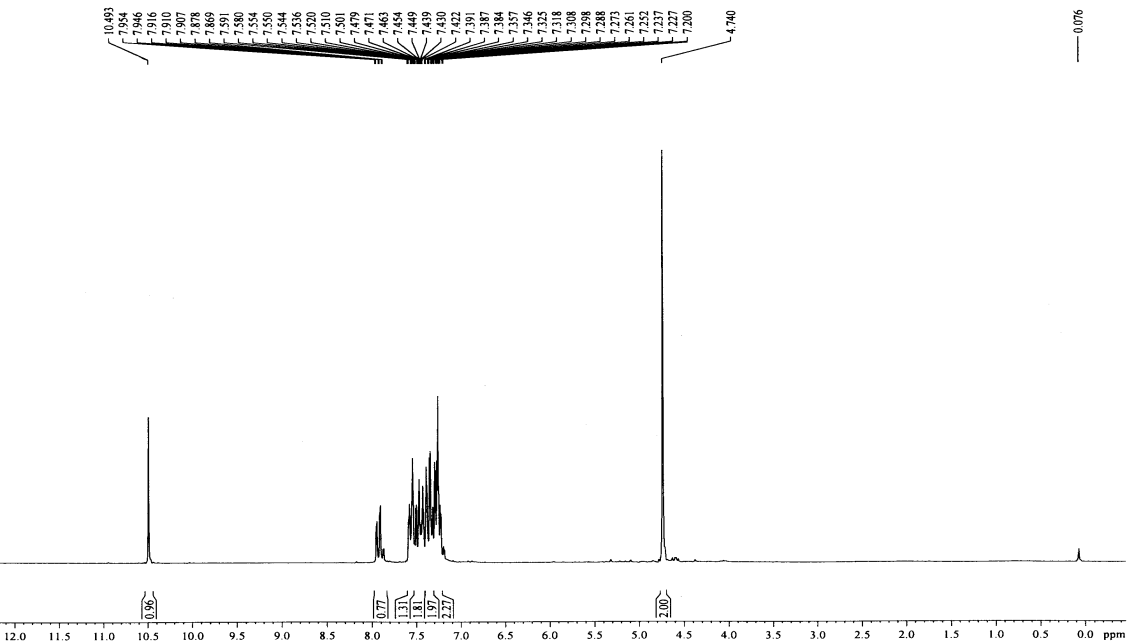
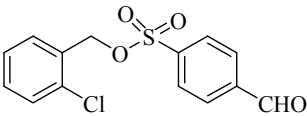
Benzyl



2-hydroxy-1,2-diphenylethanone



2-chlorobenzyl 4-formylbenzenesulfonate



2-chlorobenzyl 4-methylbenzenesulfonate

