

Supplementary Material (ESI)

In(OTf)₃ catalyzed tandem aza-Piancatelli rearrangement/Michael reaction sequence for the synthesis of 3,4-dihydro-2*H*-benzo[*b*][1,4]thiazine and oxazine derivatives

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P. Purushotham Reddy,^c A. C. Kunwar^c

Table of Contents

1. Copies of ¹H and ¹³C NMR spectra of products S2-S26

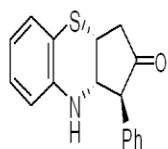
Details about the X-crystallography:

X-ray data for compounds AN45 were collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated MoK α radiation ($\lambda=0.71073\text{\AA}$) with ω -scan method.¹ Preliminary lattice parameters and orientation matrices were obtained from four sets of frames. Integration and scaling of intensity data were accomplished using SAINT program.¹ The structures were solved by Direct Methods using SHELXS97² and refinement was carried out by full-matrix least-squares technique using SHELXL97.² Anisotropic displacement parameters were included for all non-hydrogen atoms. N-bound H atom was located in a difference Fourier density map and refined isotropically. All other H atoms were located in difference density maps, but were positioned geometrically and included as riding atoms, with C-H = 0.93 (aromatic), 0.96 (methyl) or 0.97 \AA (methylene) and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the methyl groups and $1.2U_{\text{eq}}(\text{C})$ otherwise. The methyl groups were allowed to rotate but not to tip.

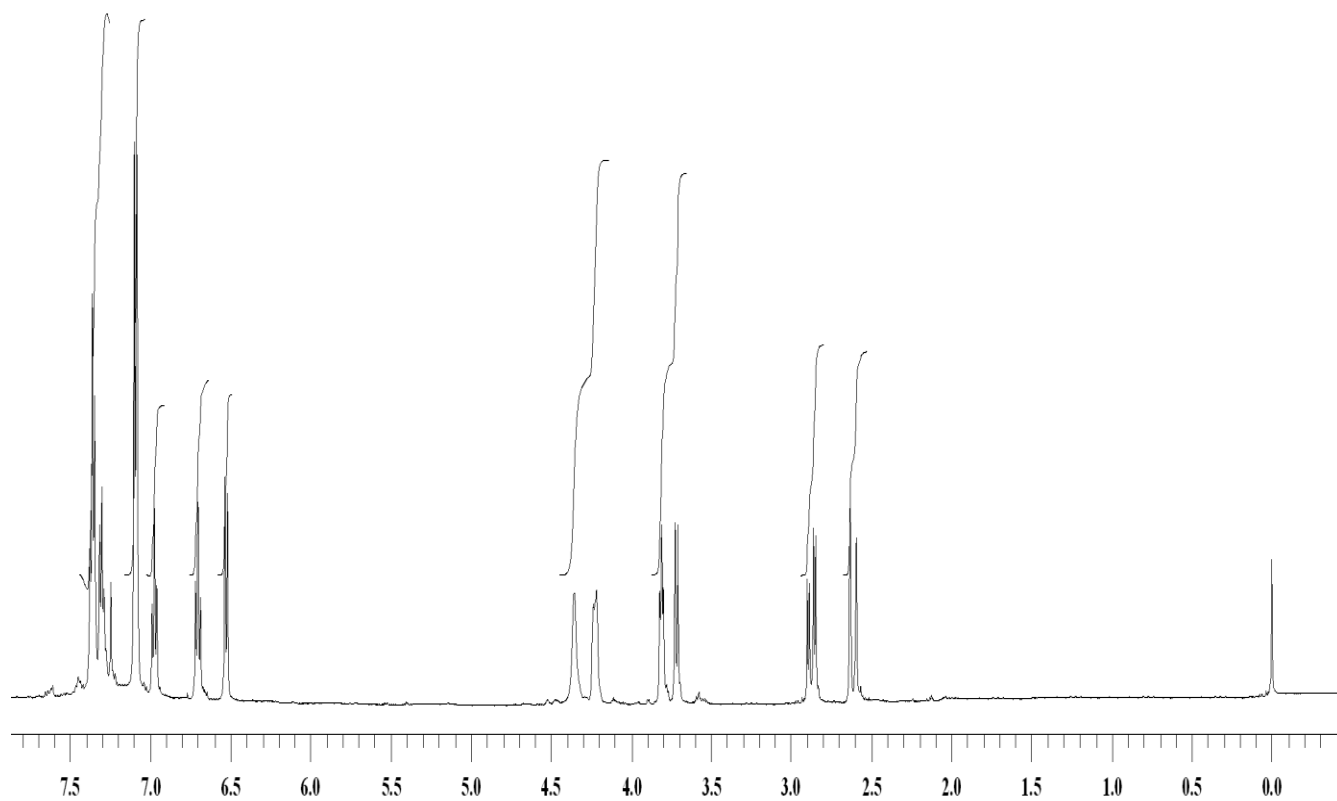
1. SMART & SAINT. Software Reference manuals. Versions 6.28a & 5.625, Bruker Analytical X-ray Systems Inc., Madison, Wisconsin, U.S.A., 2001.
2. Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

Figure caption: The molecular structure of (**3g**), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

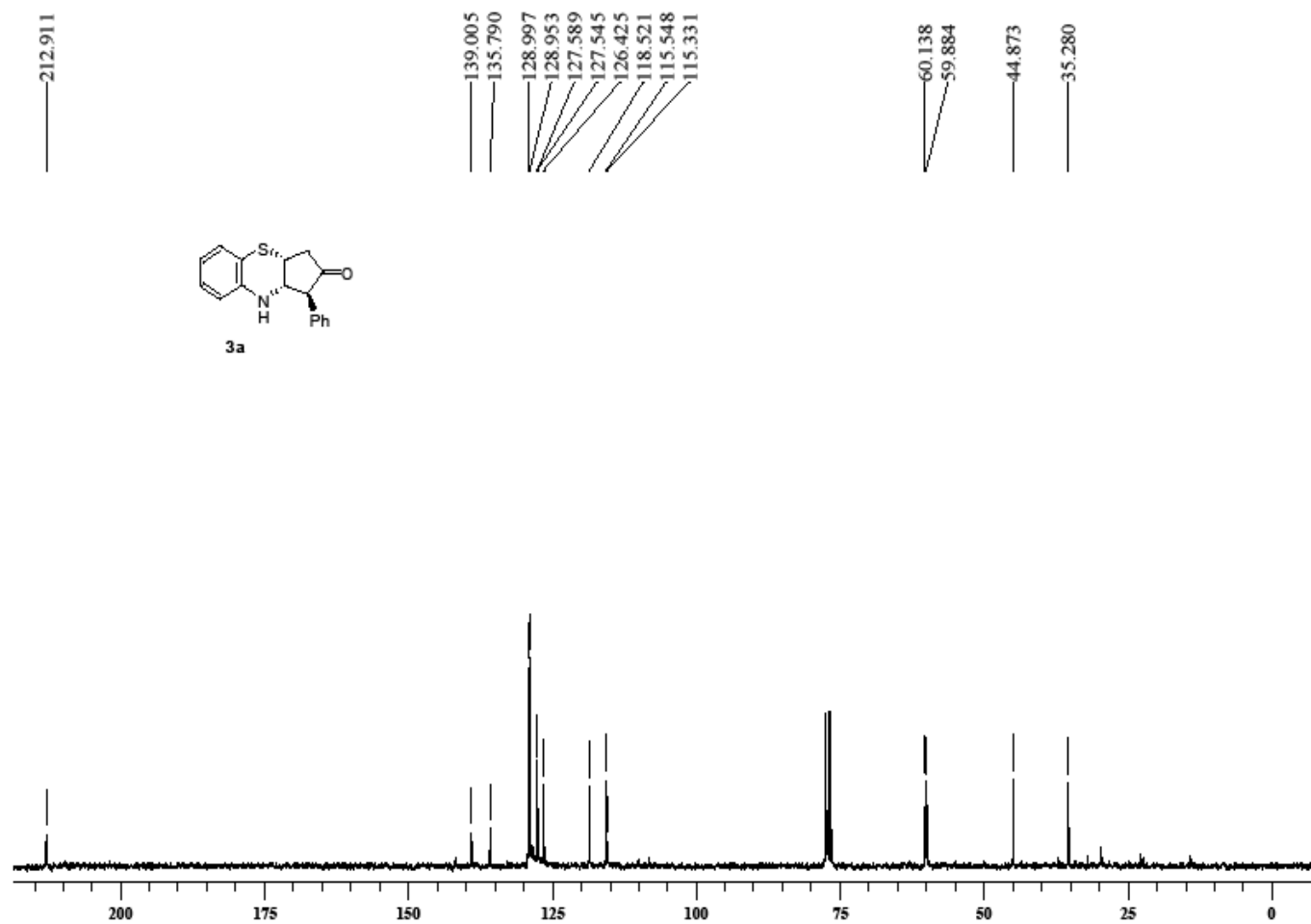
¹H NMR Spectrum of Compound 3a.



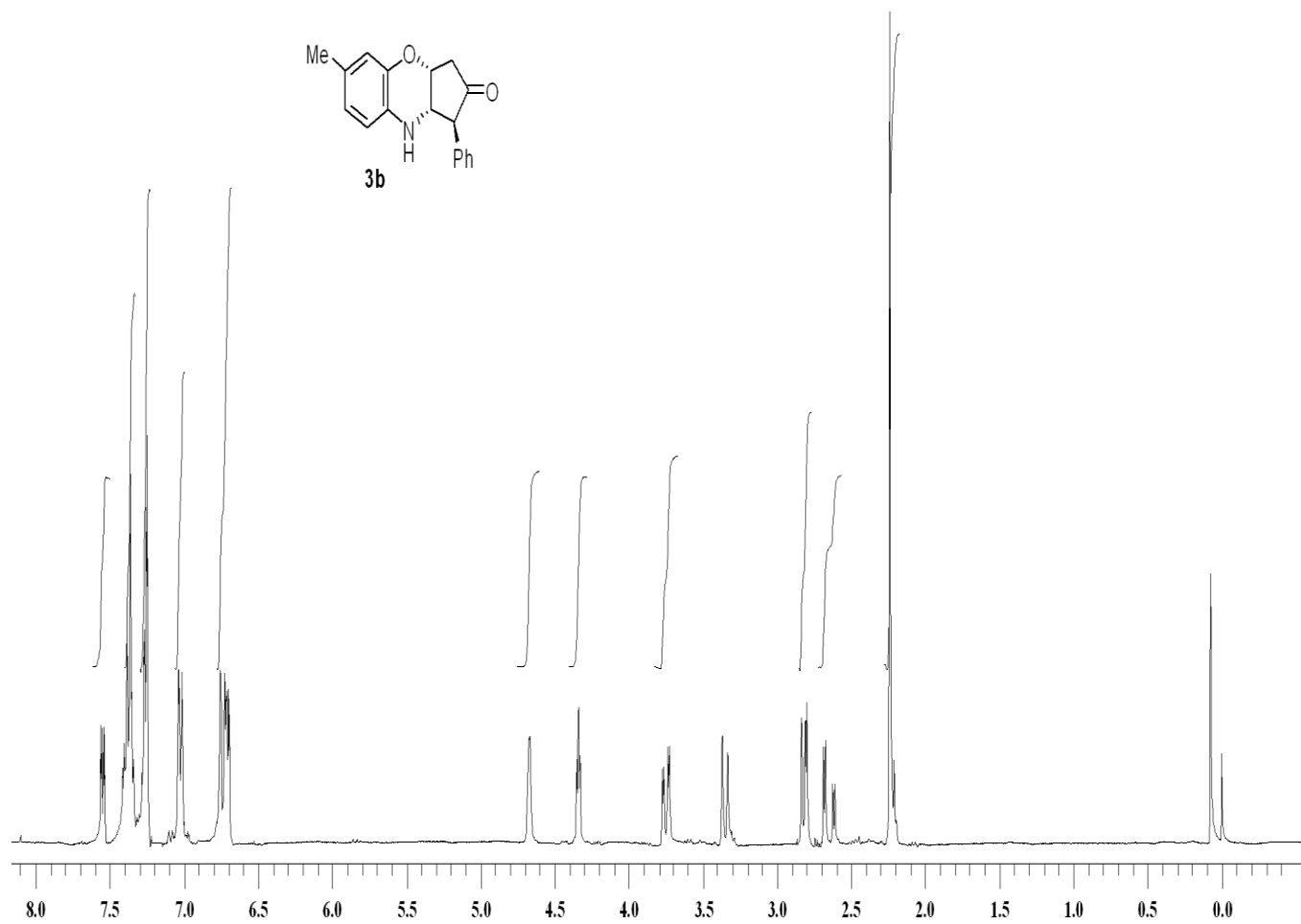
3a



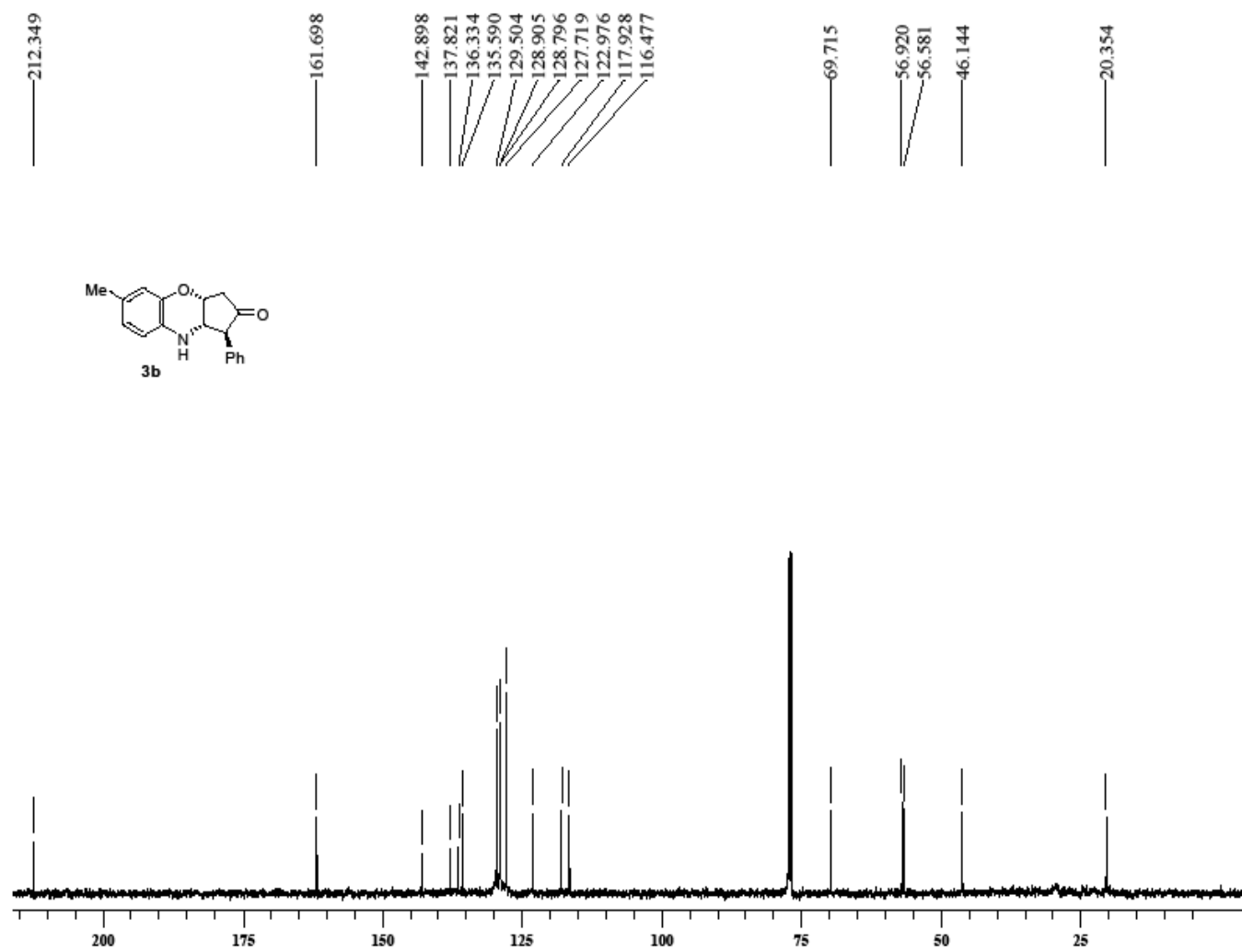
^{13}C spectrum of compound 3a:



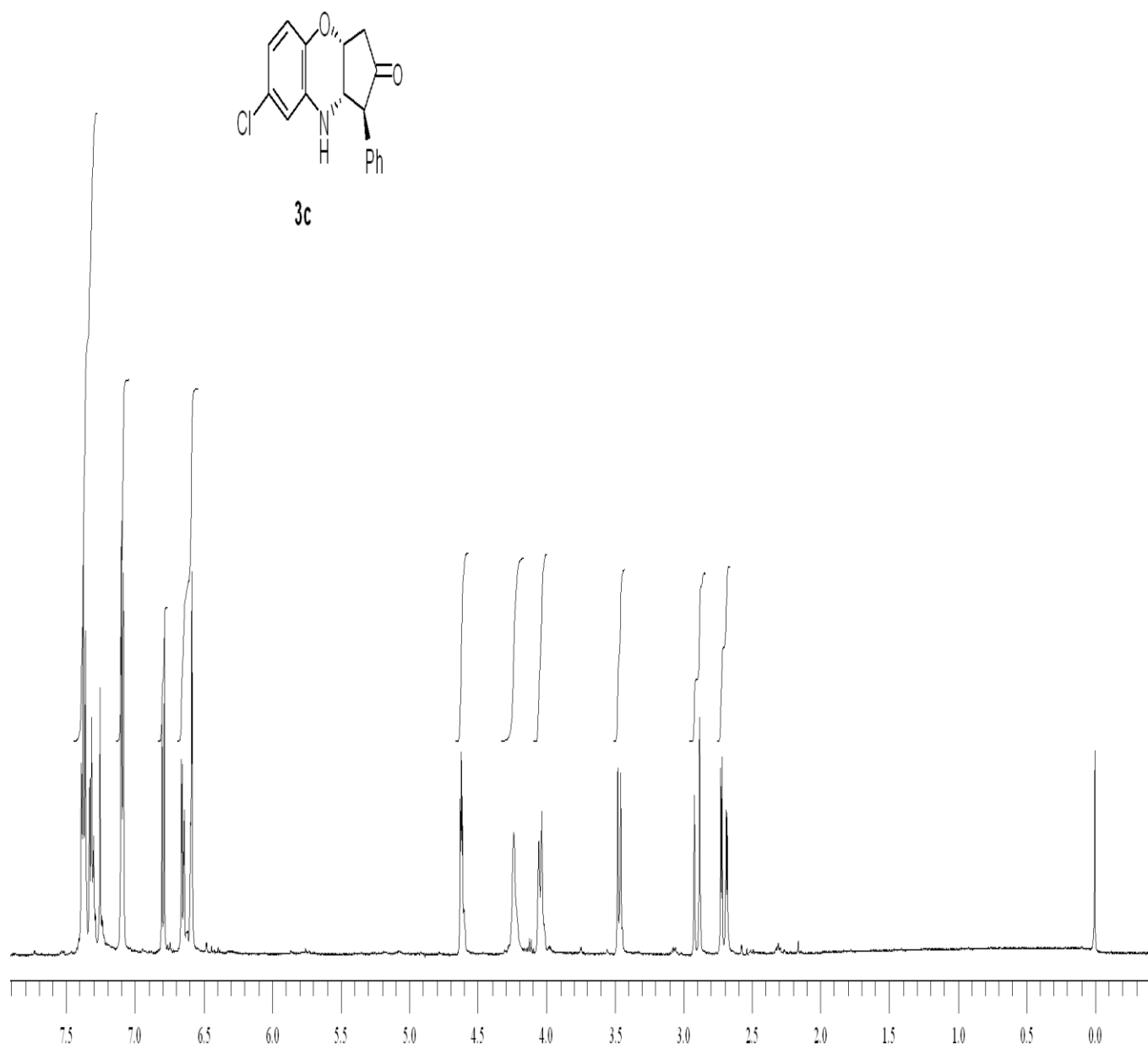
¹H NMR Spectrum of Compound 3b.



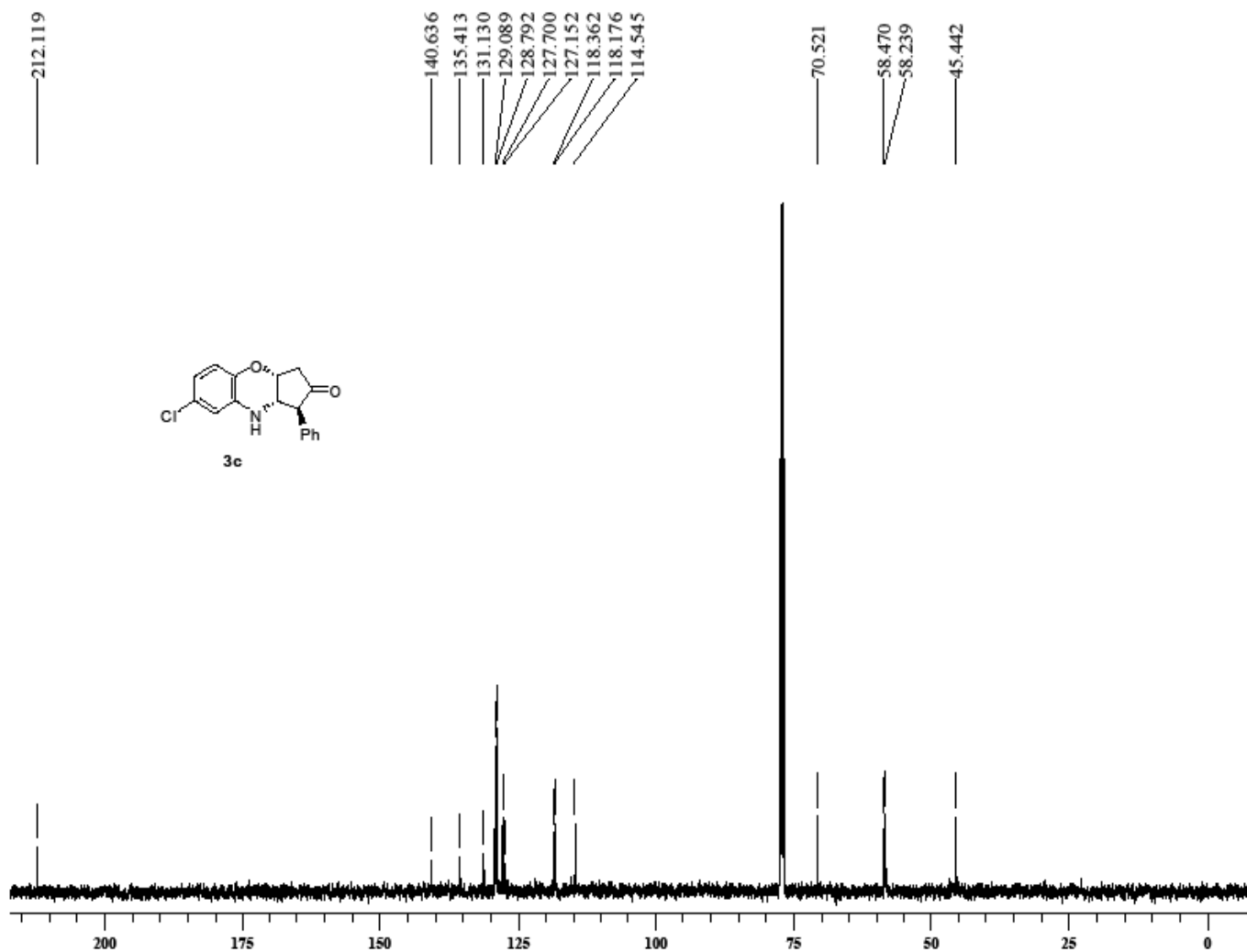
^{13}C spectrum of compound 3b:



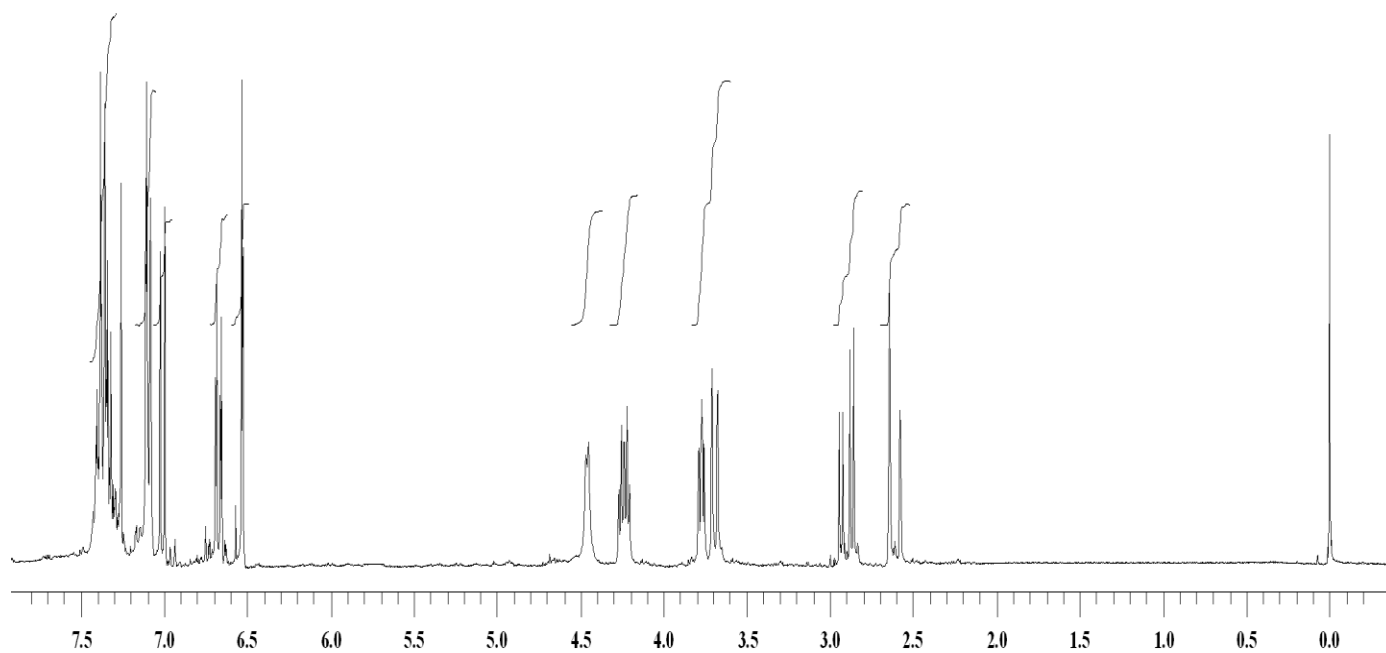
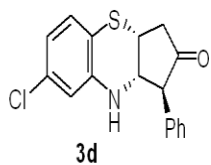
¹HNMR Spectrum of Compound 3c.



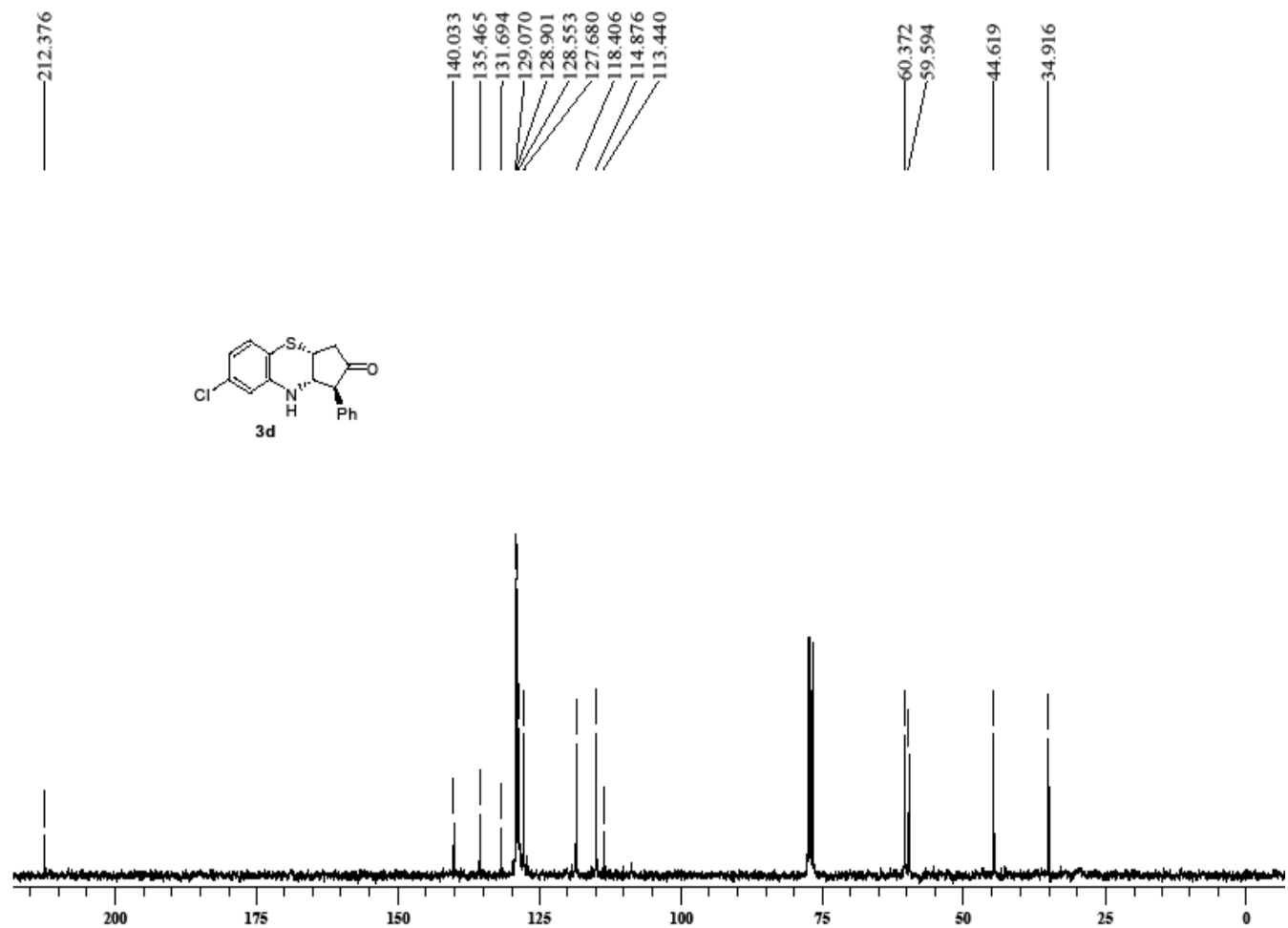
^{13}C spectrum of compound 3c:



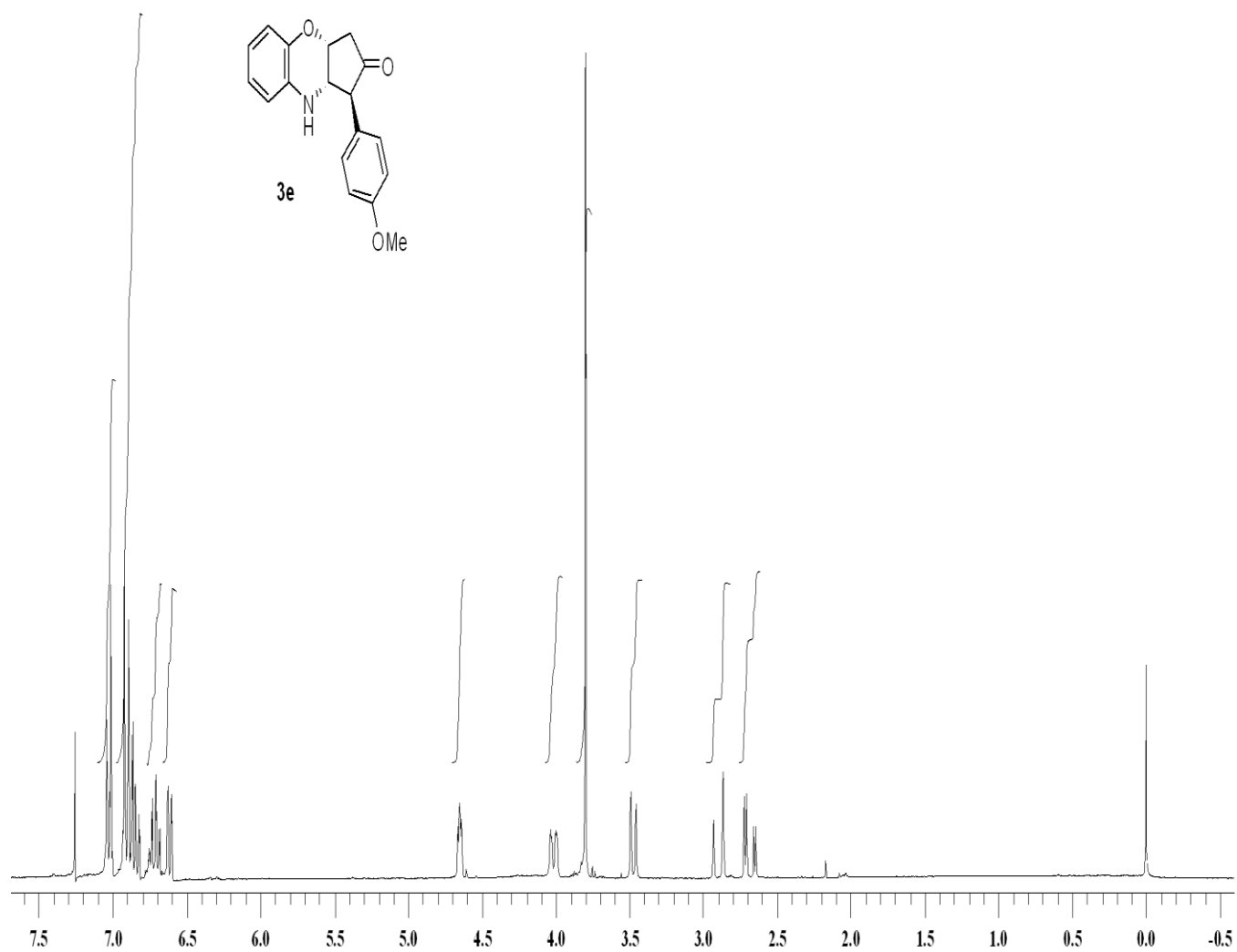
¹H NMR Spectrum of Compound 3d:



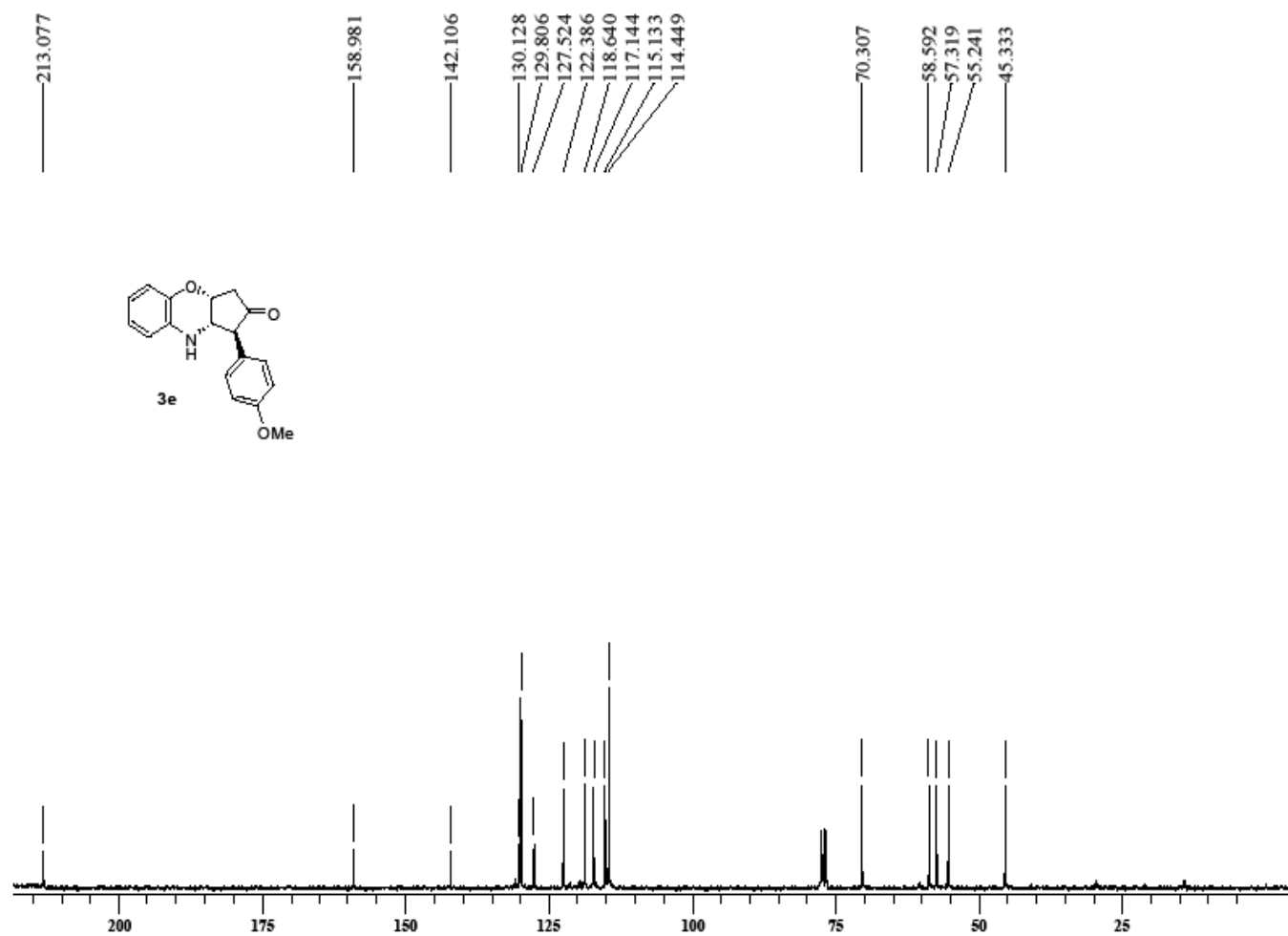
¹³C spectrum of compound 3d:



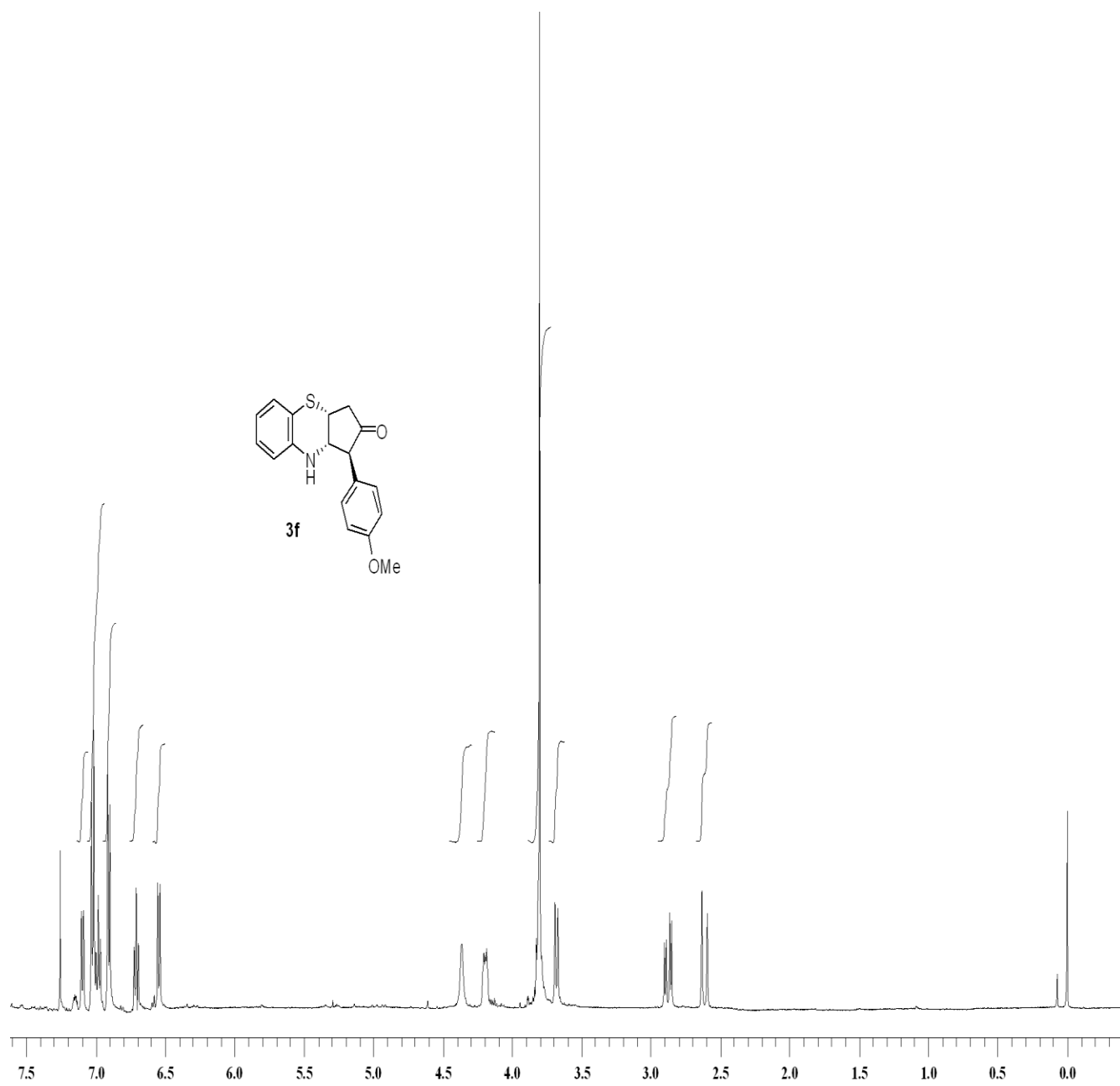
¹H NMR Spectrum of Compound 3e:



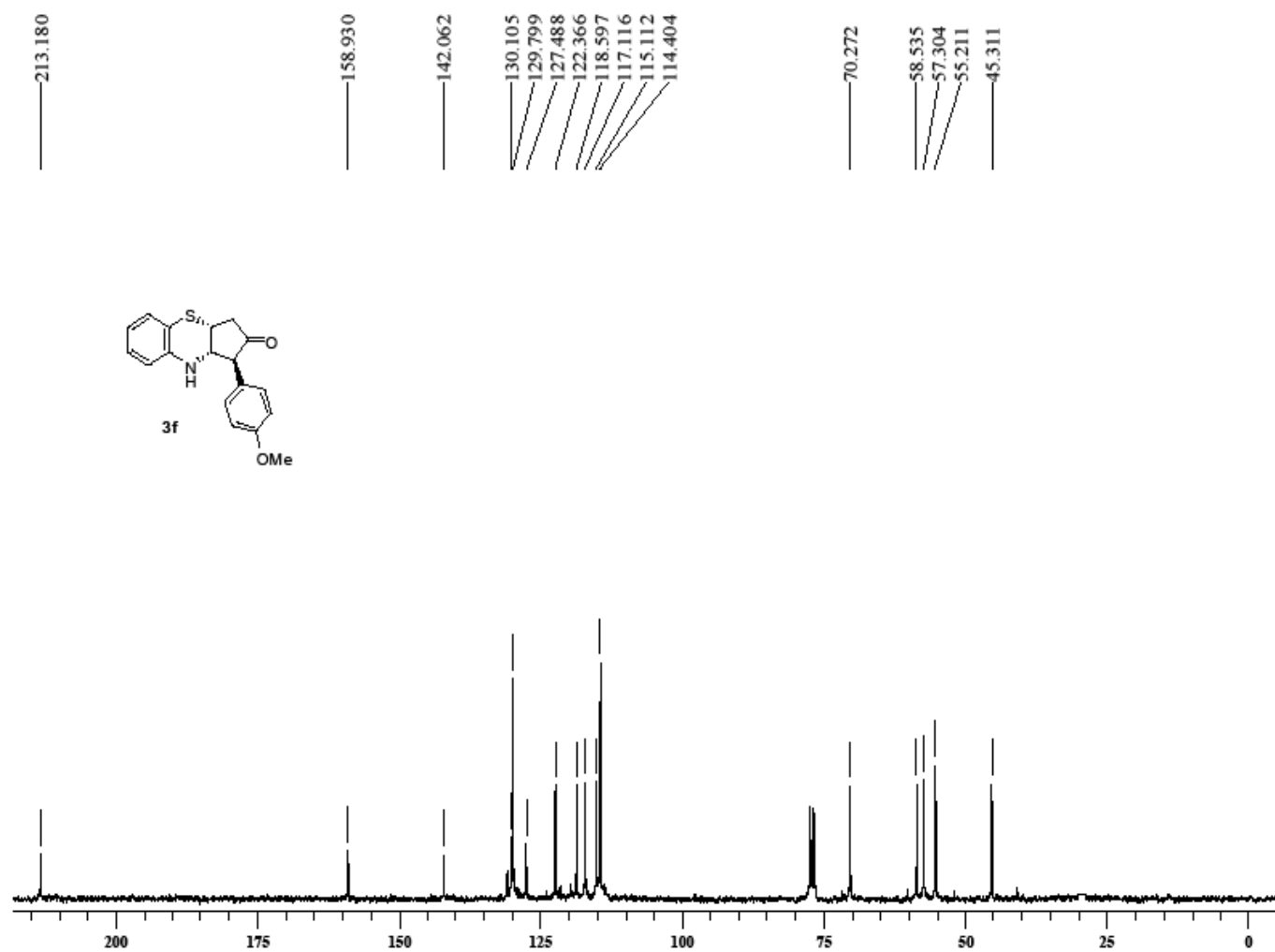
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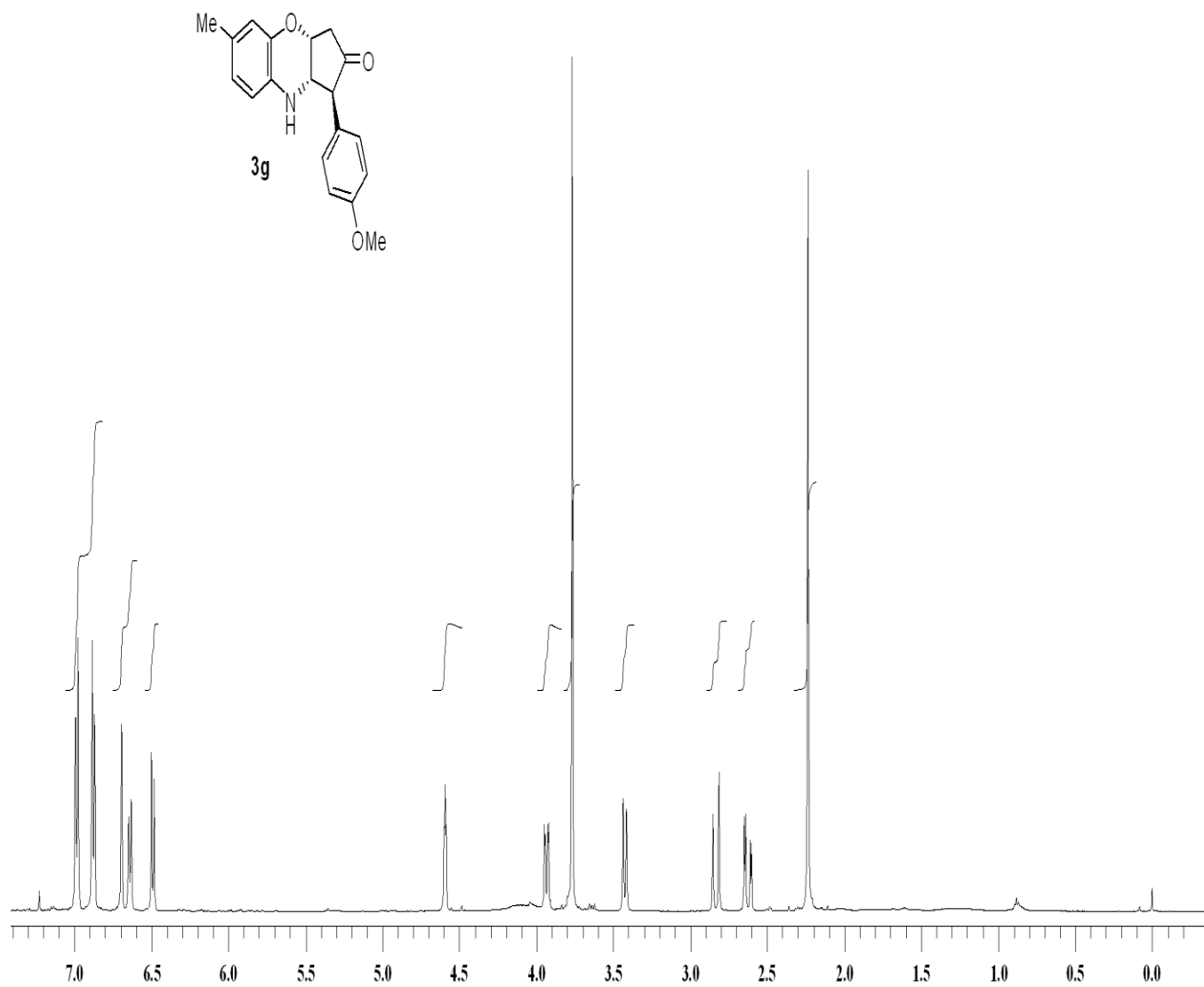
¹HNMR Spectrum of Compound 3f:



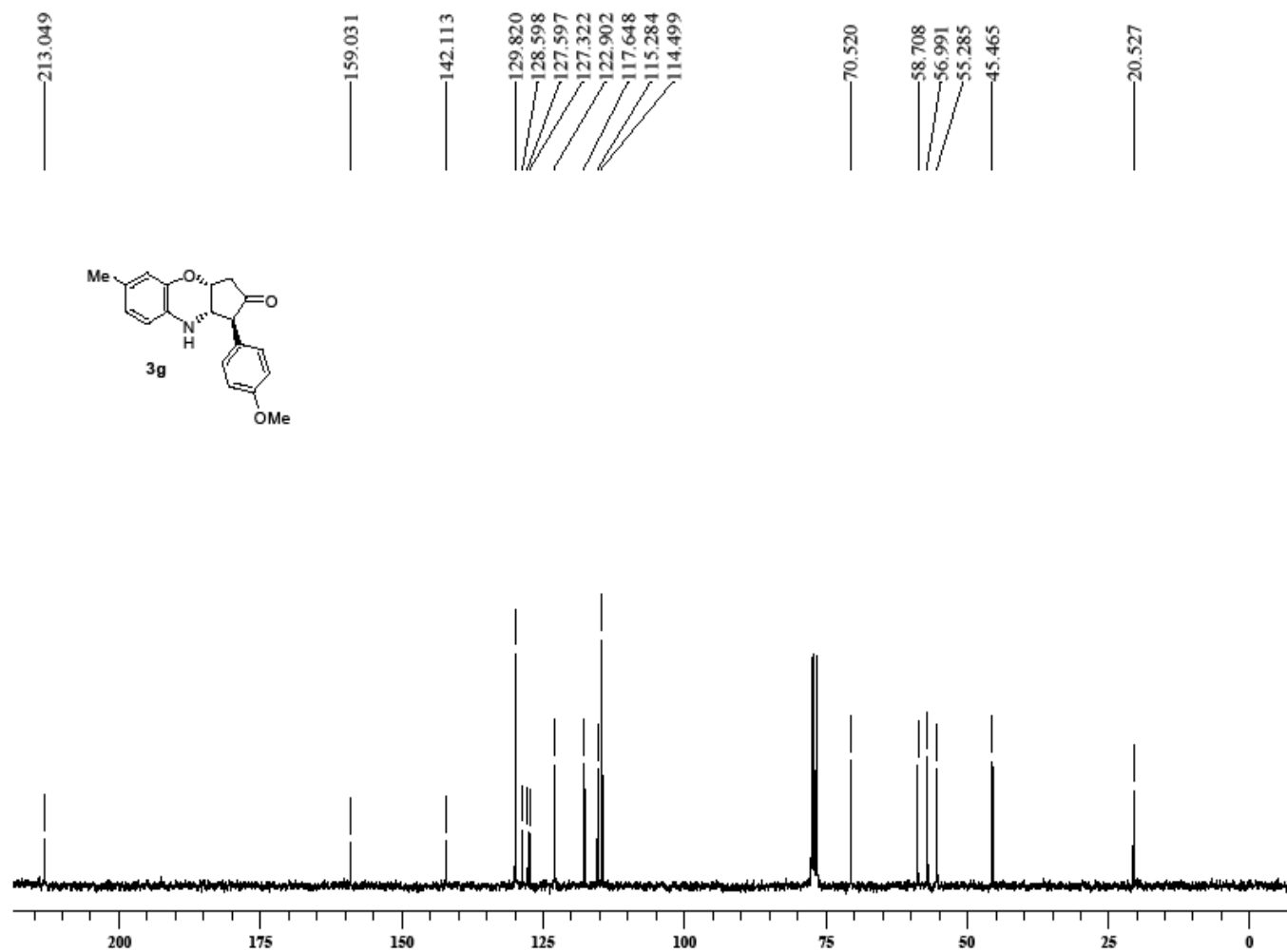
^{13}C spectrum of compound 3f:



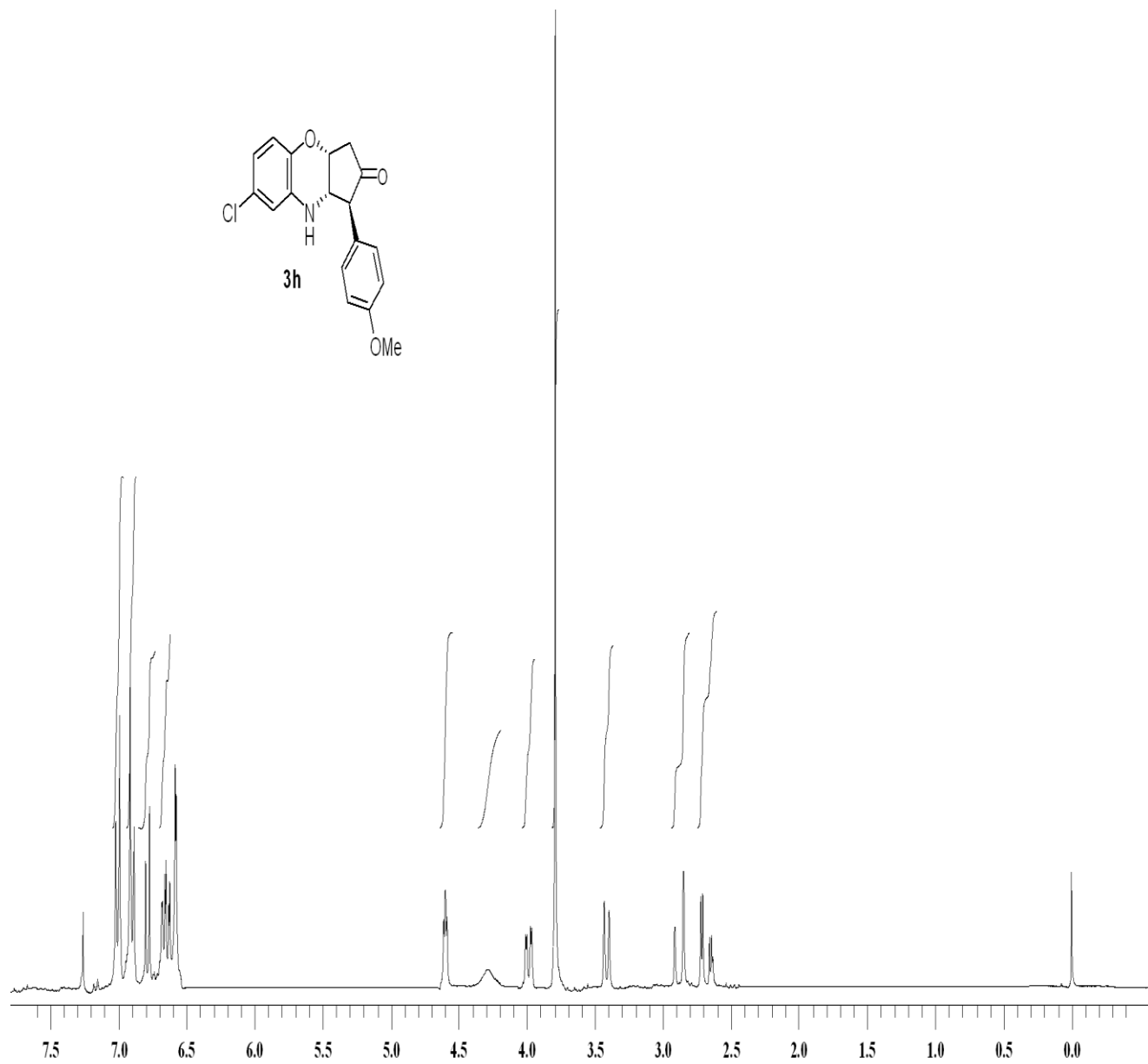
¹HNMR Spectrum of Compound 3g:



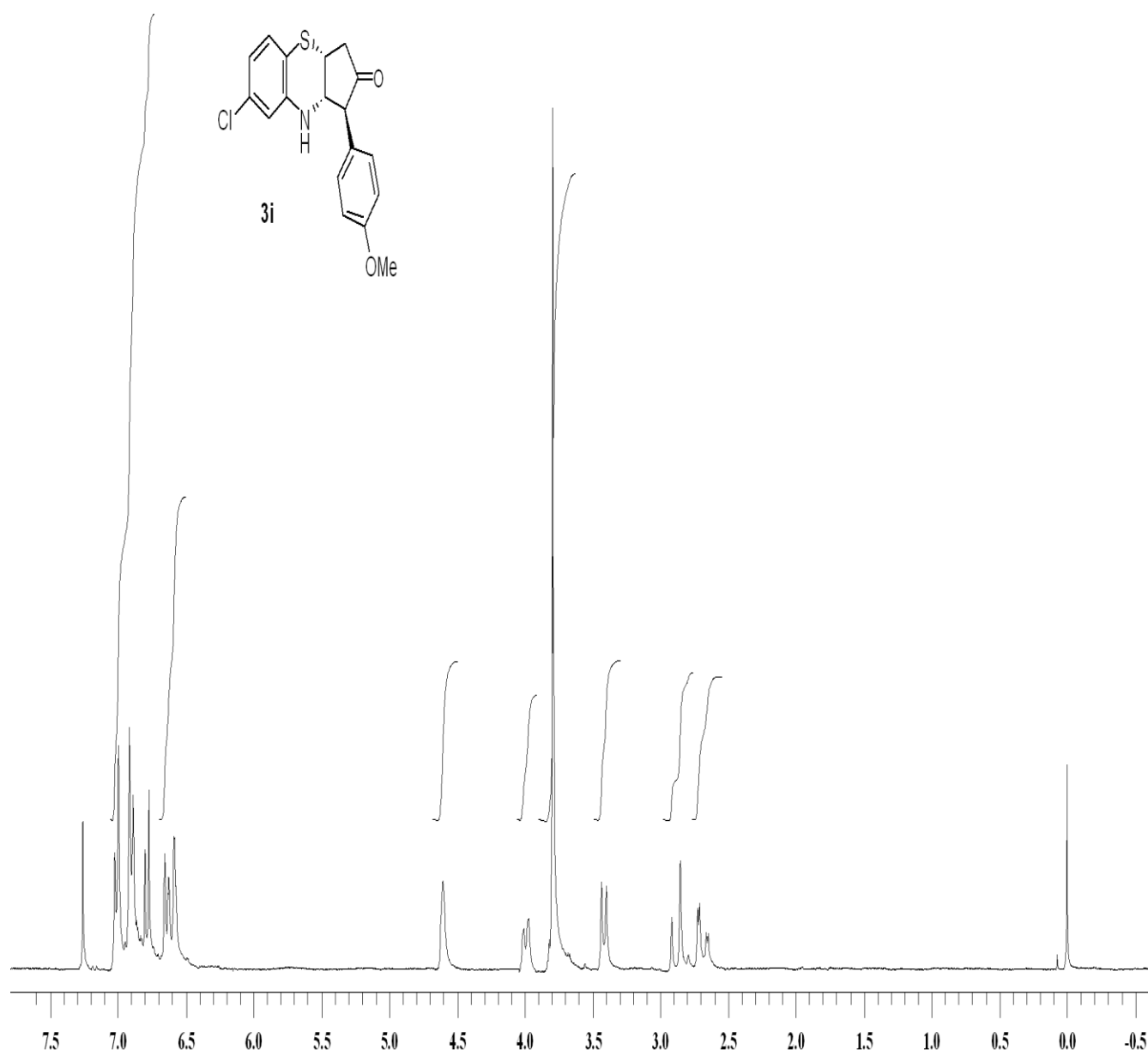
^{13}C spectrum of compound 3g:



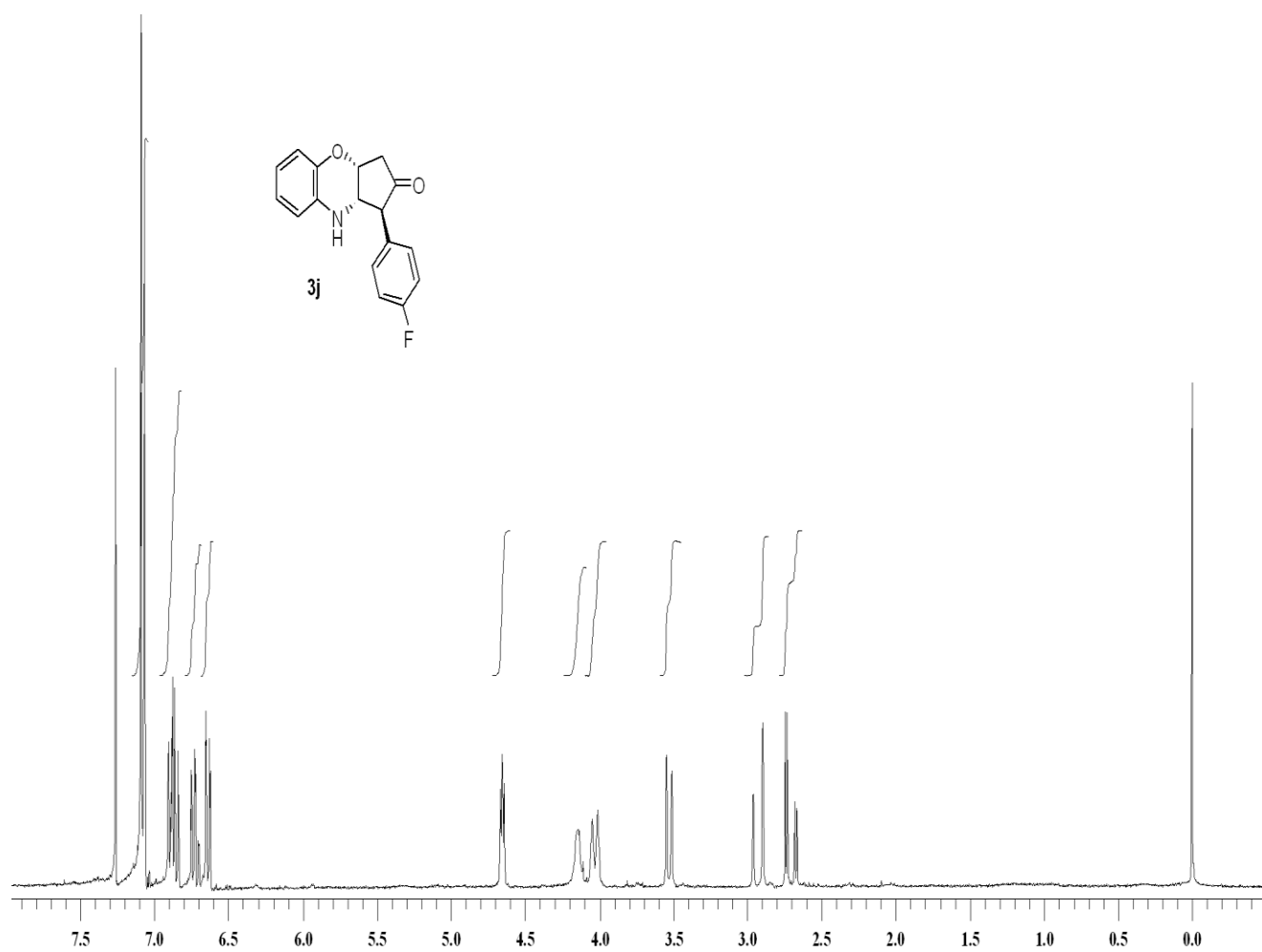
¹HNMR Spectrum of Compound 3h:



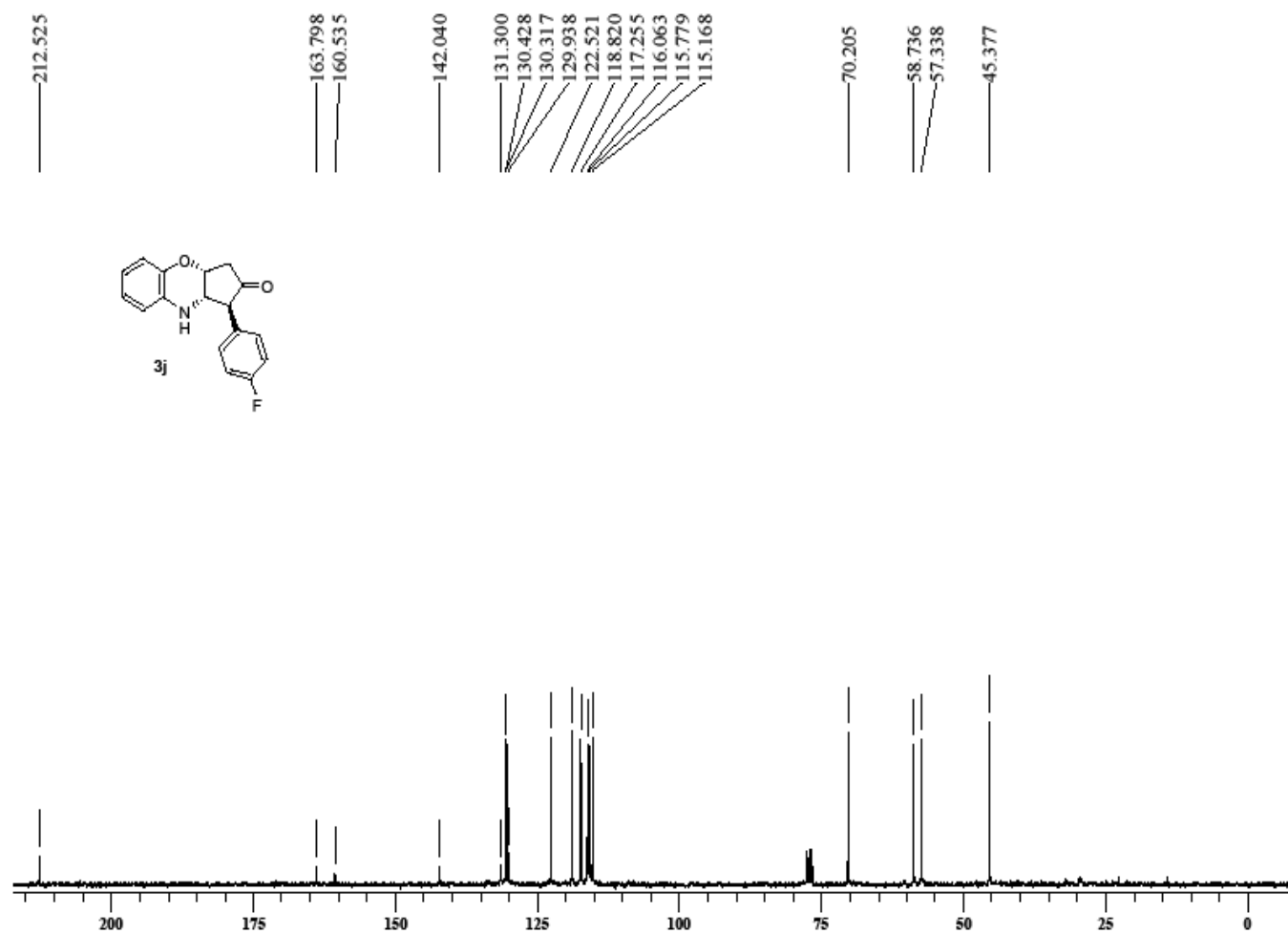
¹HNMR Spectrum of Compound 3i:



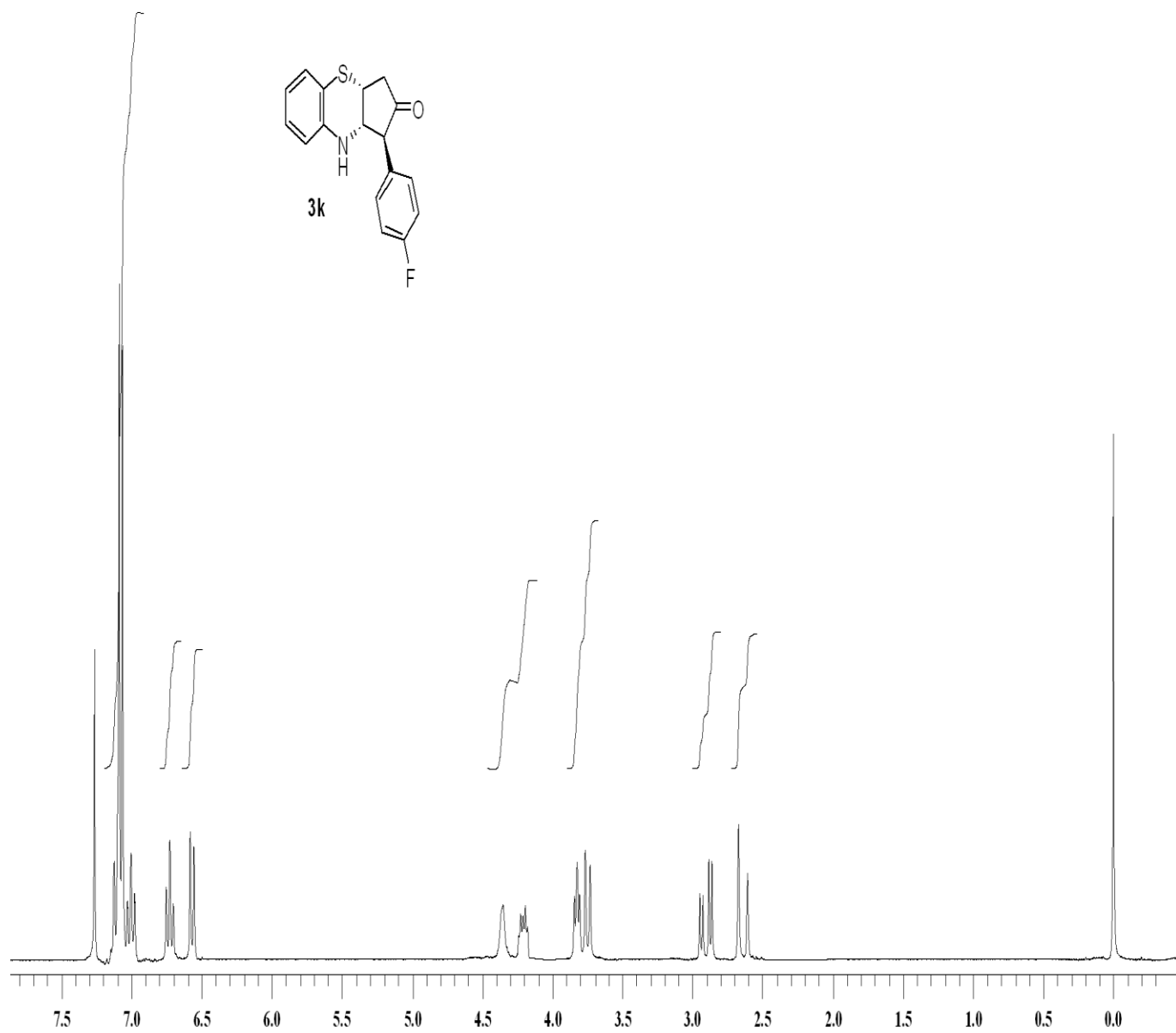
¹HNMR Spectrum of Compound 3j:



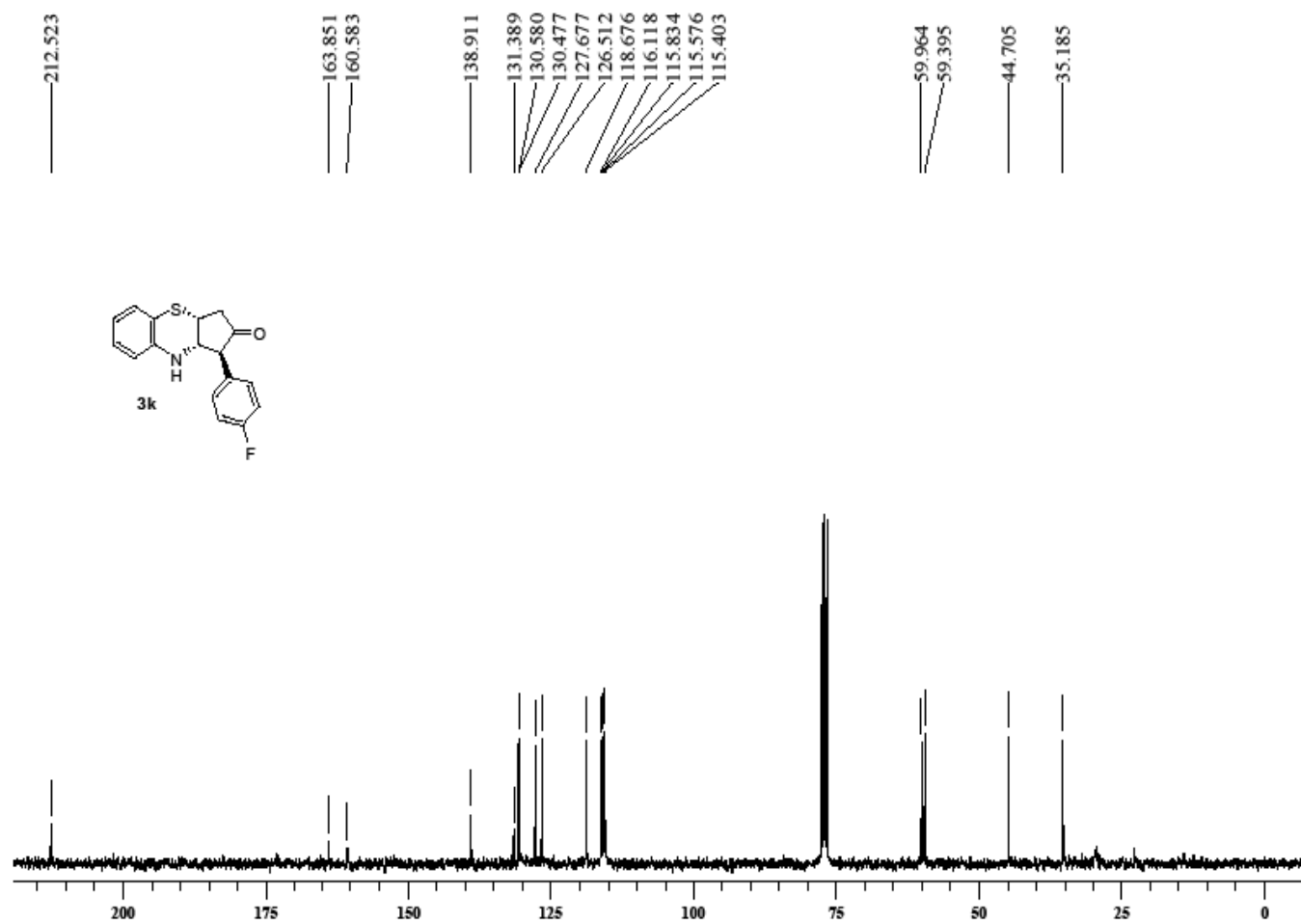
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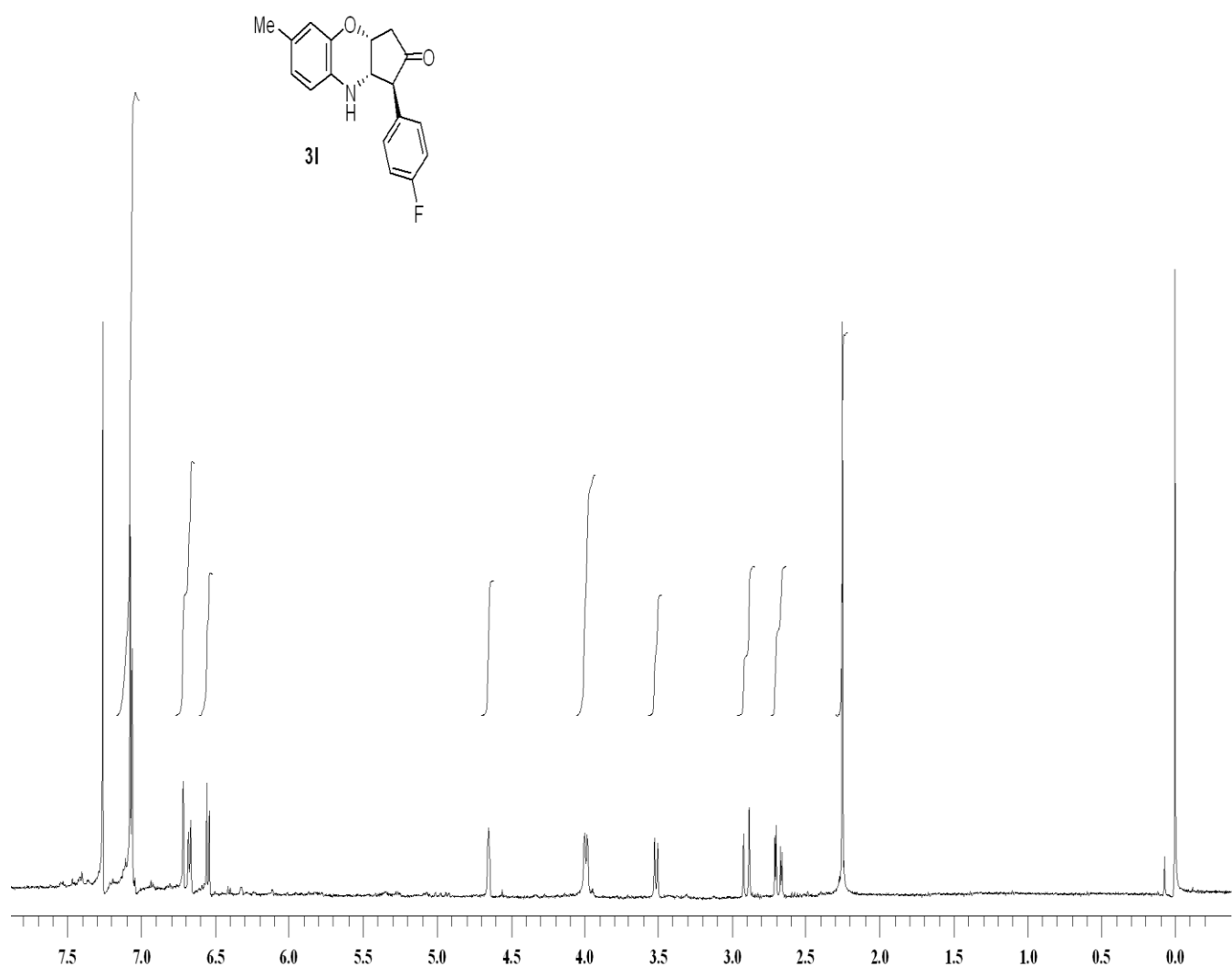
¹HNMR Spectrum of Compound 3k:



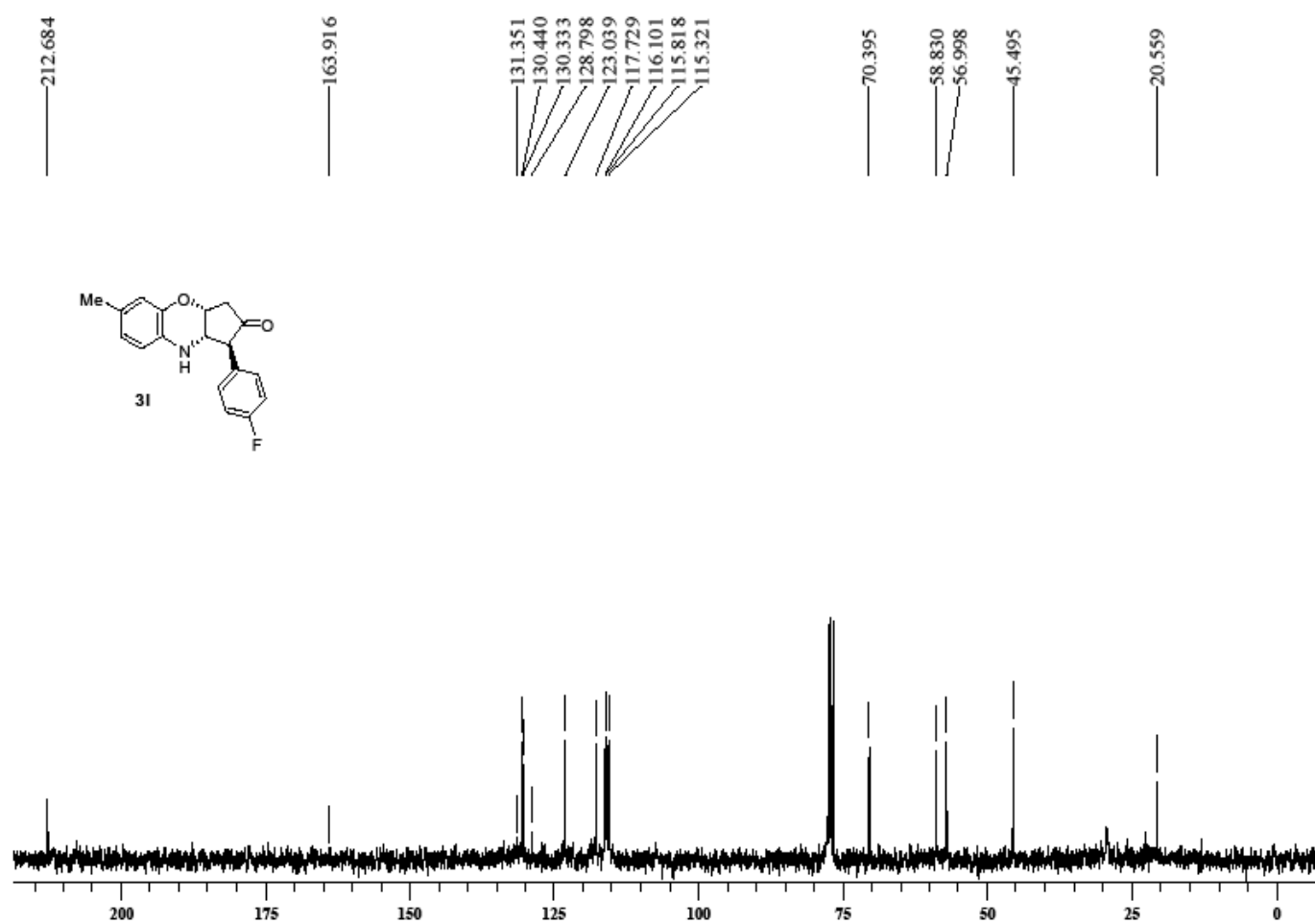
^{13}C spectrum of compound 3k:



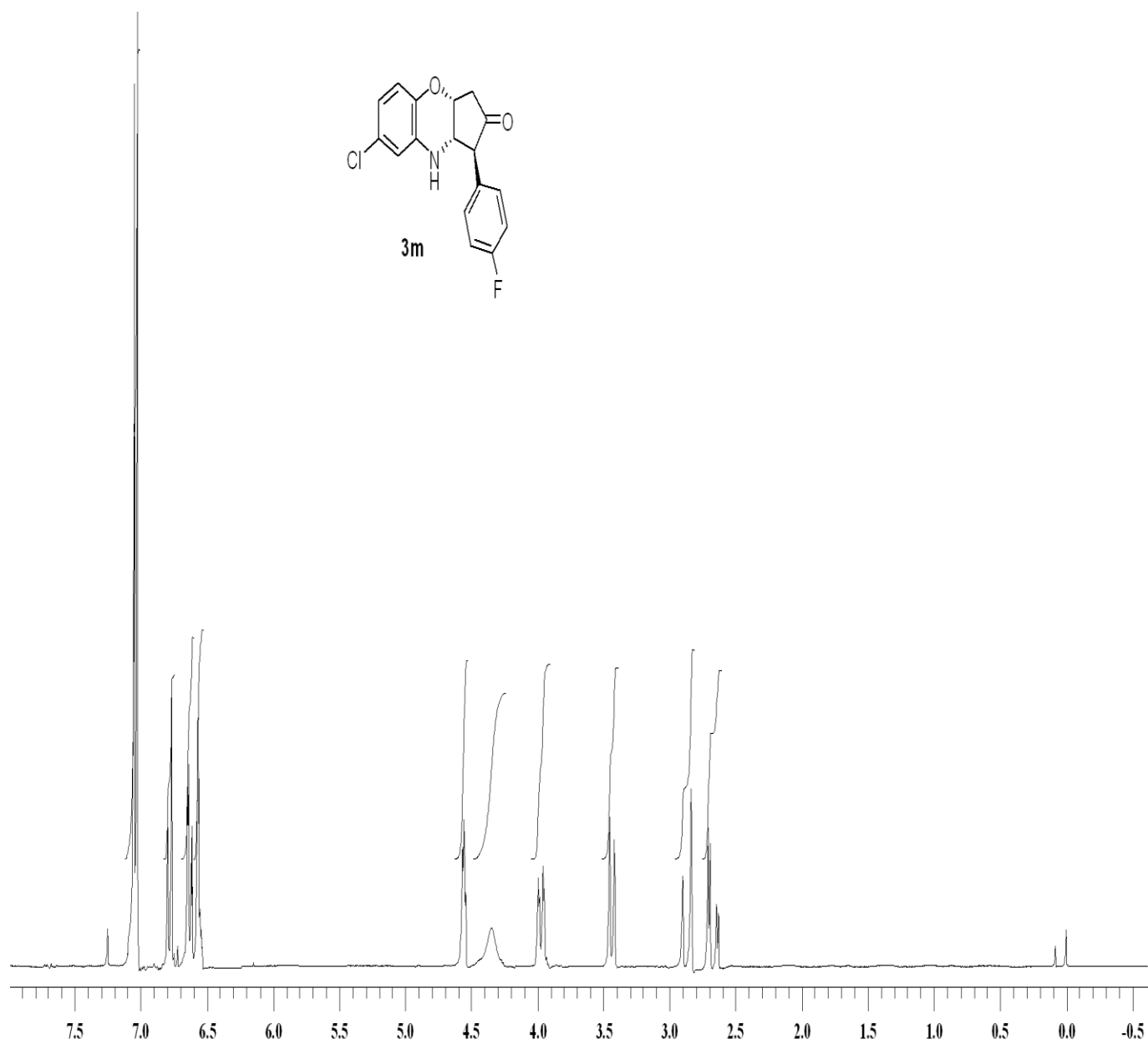
¹HNMR Spectrum of Compound 3l:



^{13}C spectrum of compound 3l:



¹H NMR Spectrum of Compound 3m:



^{13}C spectrum of compound 3m:

