

Supporting Information

Domino alkyne insertion/aldol reaction/aromatization of 2-alkynyl indole-3-carbaldehyde with 1,3-diketones: Entry to 2-indolyl phenols

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1. X-ray Crystallography of 3a.

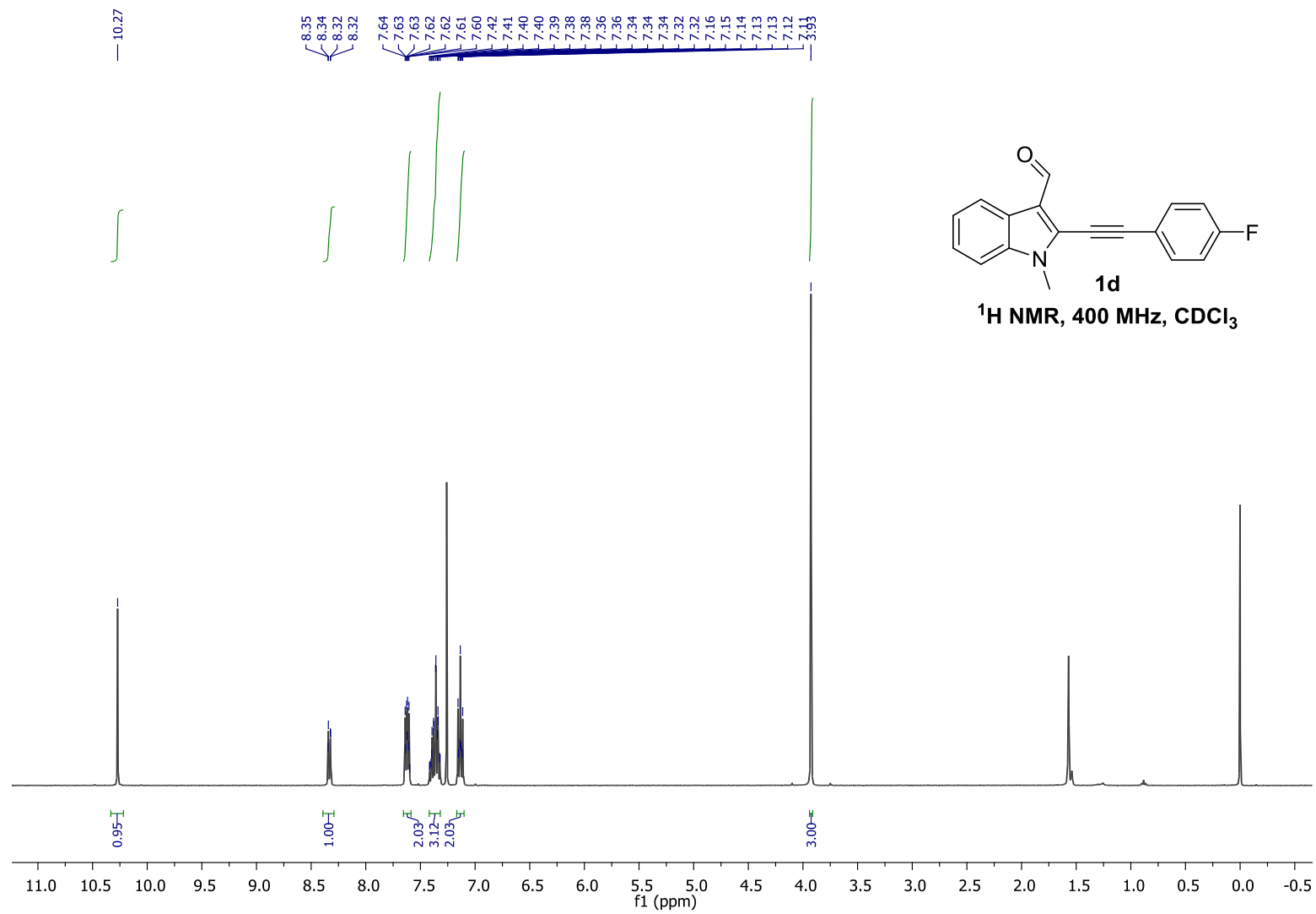
Data for the compound **3a** was collected at room temperature on a Bruker D8 QUEST instrument with an I μ S Mo microsource ($\lambda = 0.7107$ Å) and a PHOTON-100 detector. The raw data frames were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs [1]. The structure was solved using intrinsic phasing method [2] and further refined with the SHELXL [2] program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms. The O-bound H atom was located in difference Fourier maps and their positions and isotropic displacement parameters were located and refined. All C bound H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H or $1.2U_{\text{eq}}(\text{C})$ for other H atoms].

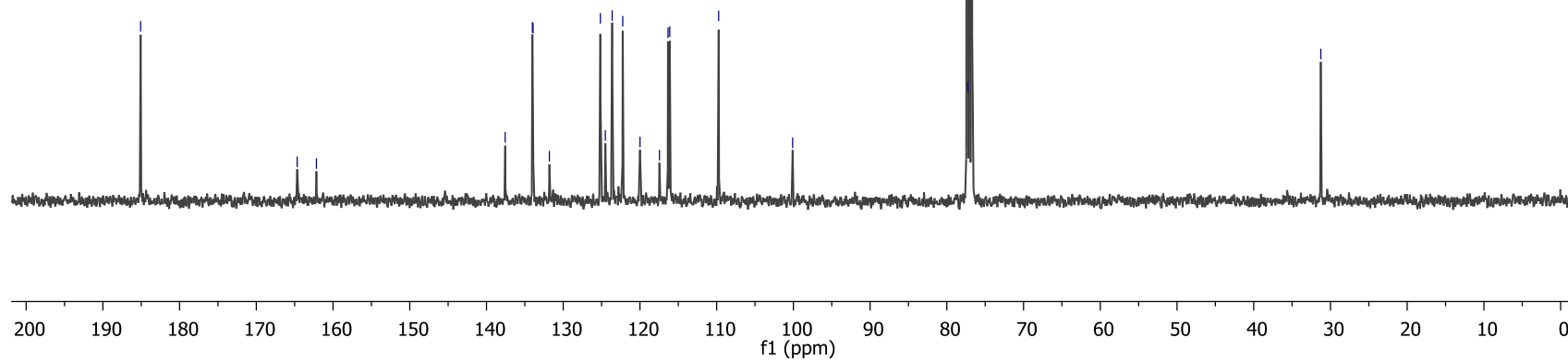
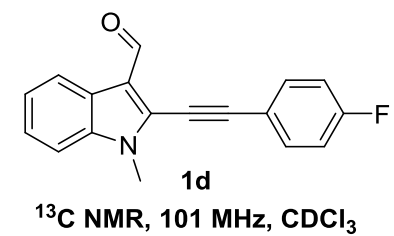
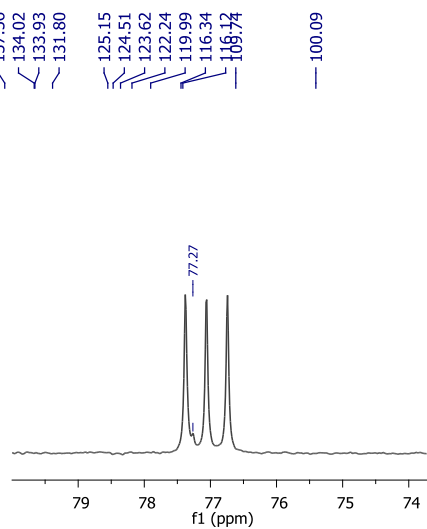
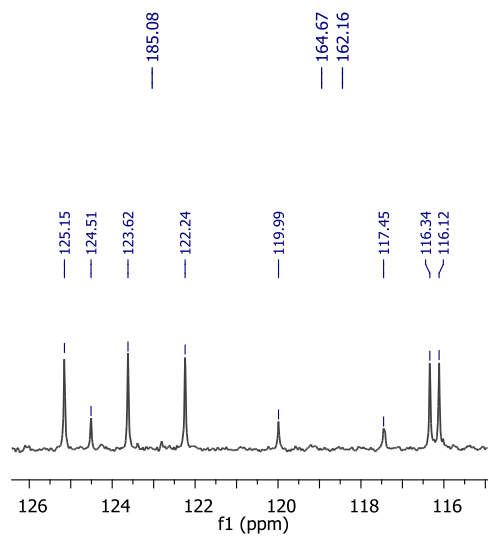
Crystal structure determination of 3a

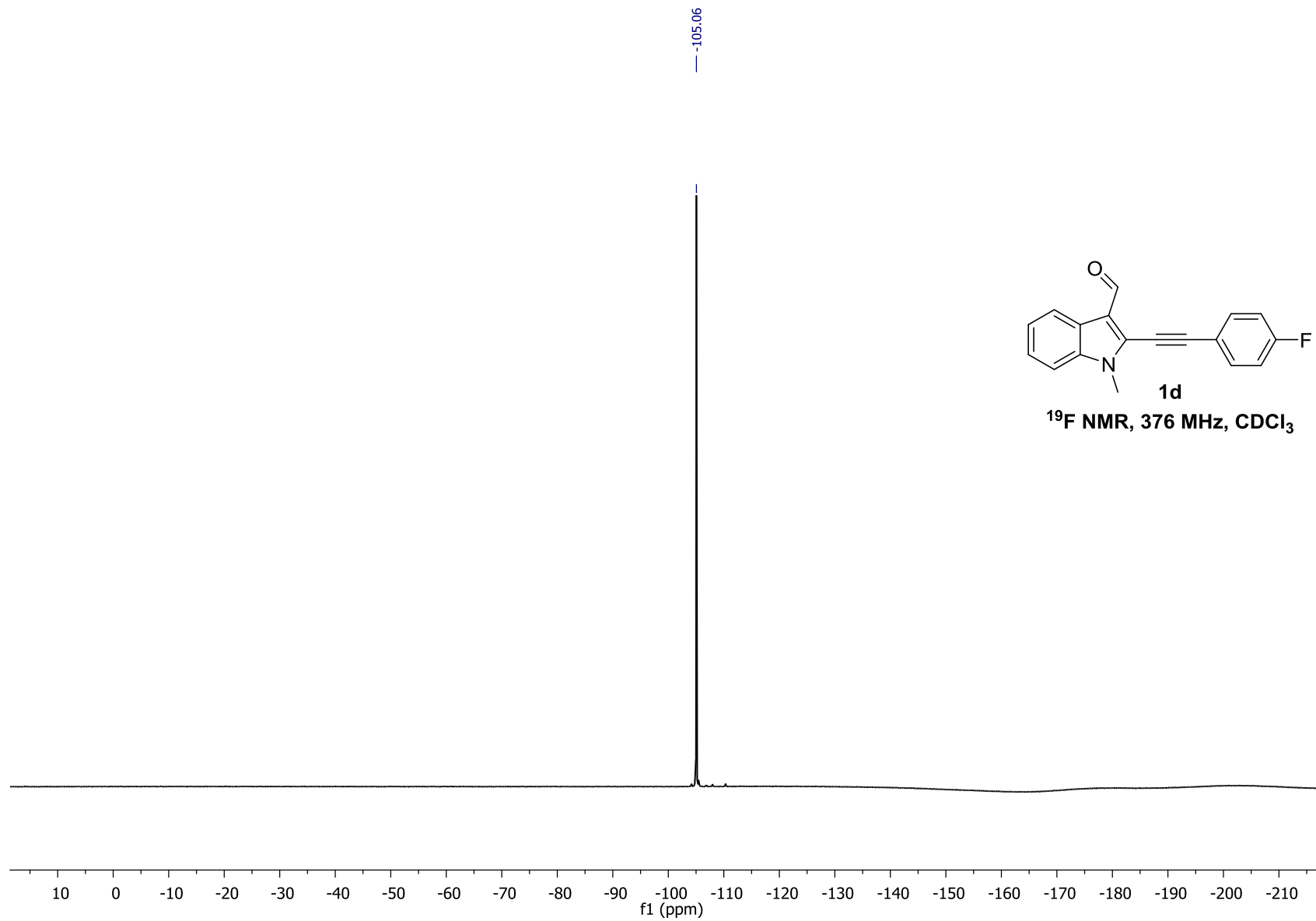
Crystal Data for $\text{C}_{23}\text{H}_{19}\text{NO}_2$ ($M = 341.413$ g/mol): monoclinic, space group $\text{P}2_1/\text{n}$ (no. 14), $a = 10.5837(11)$ Å, $b = 14.4099(13)$ Å, $c = 12.4674(13)$ Å, $\beta = 90.773(4)^\circ$, $V = 1901.2(3)$ Å³, $Z = 4$, $T = 294.15$ K, $\mu(\text{Mo K}\alpha) = 0.076$ mm⁻¹, $D_{\text{calc}} = 1.193$ g/cm³, 35526 reflections measured ($4.32^\circ \leq 2\theta \leq 60.86^\circ$), 5015 unique ($R_{\text{int}} = 0.0692$, $R_{\text{sigma}} = 0.0425$) which were used in all calculations. The final R_1 was 0.0667 ($I >= 2u(I)$) and wR_2 was 0.1689 (all data). CCDC 2217042 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk].

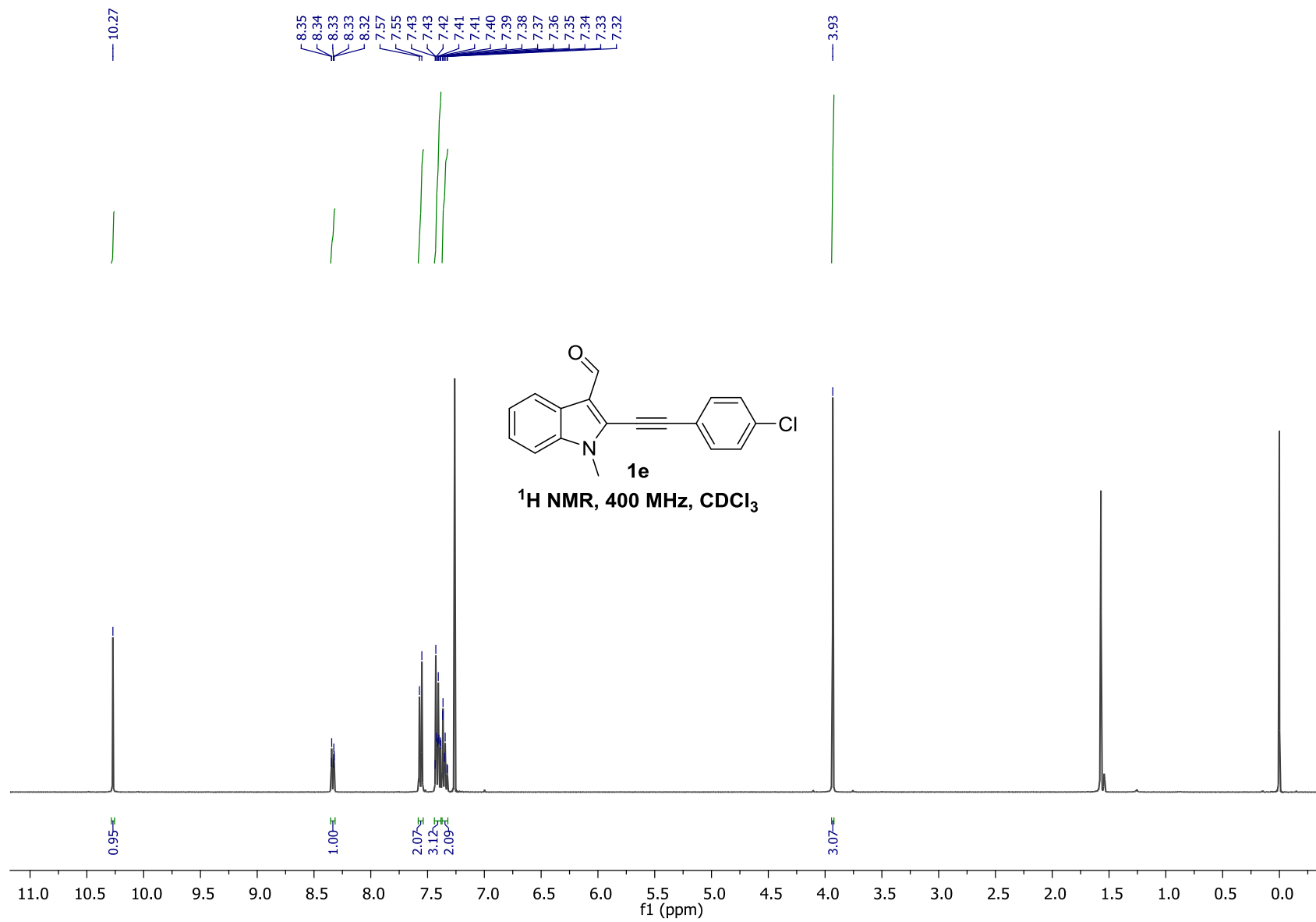
1. Bruker (2001). SAINT (Version 6.28a) & SMART (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.
2. Sheldrick G. M. (2015) Acta Crystallogr C71: 3-8.

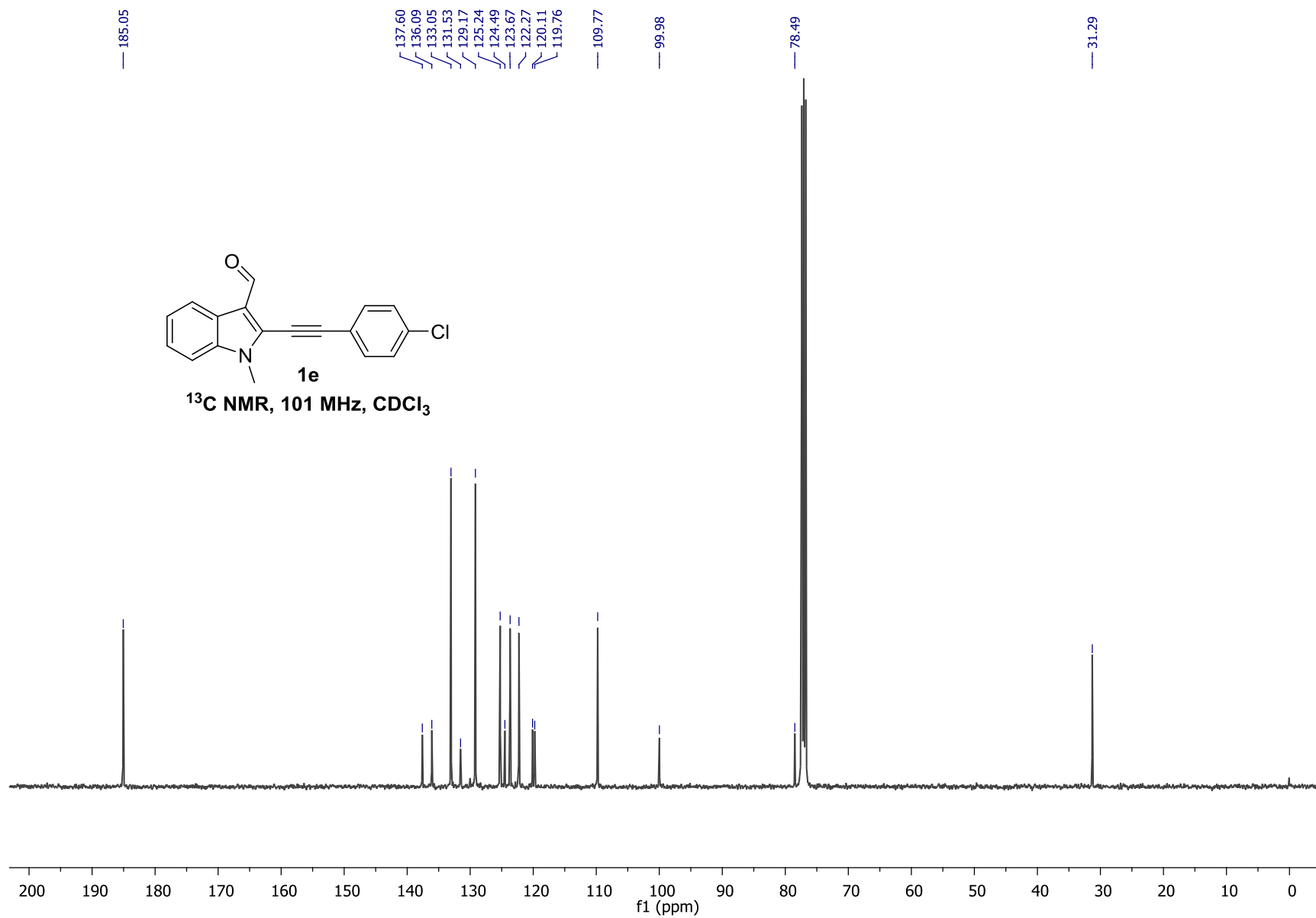
2. ^1H and ^{13}C NMR spectra new starting Materials

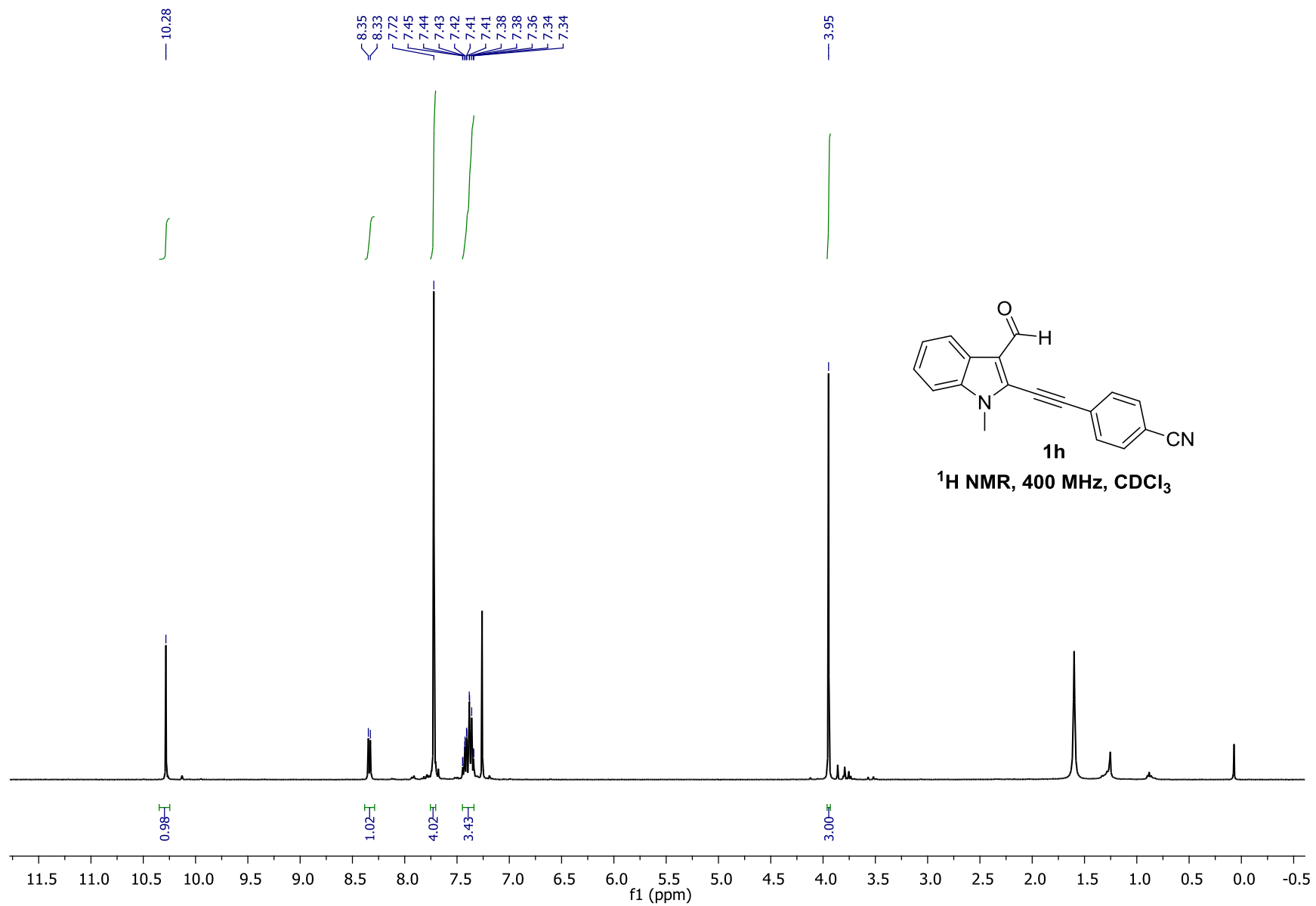


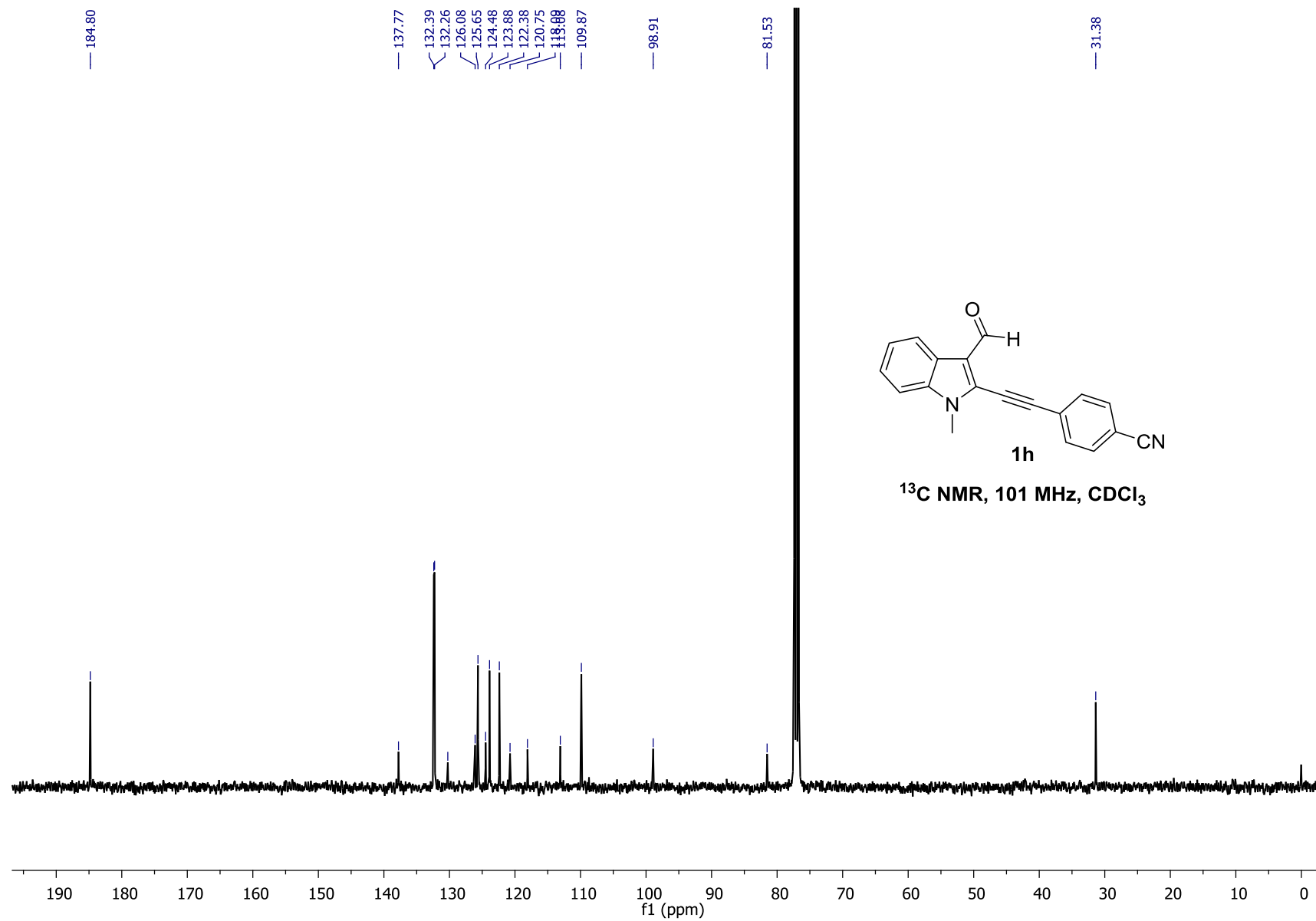


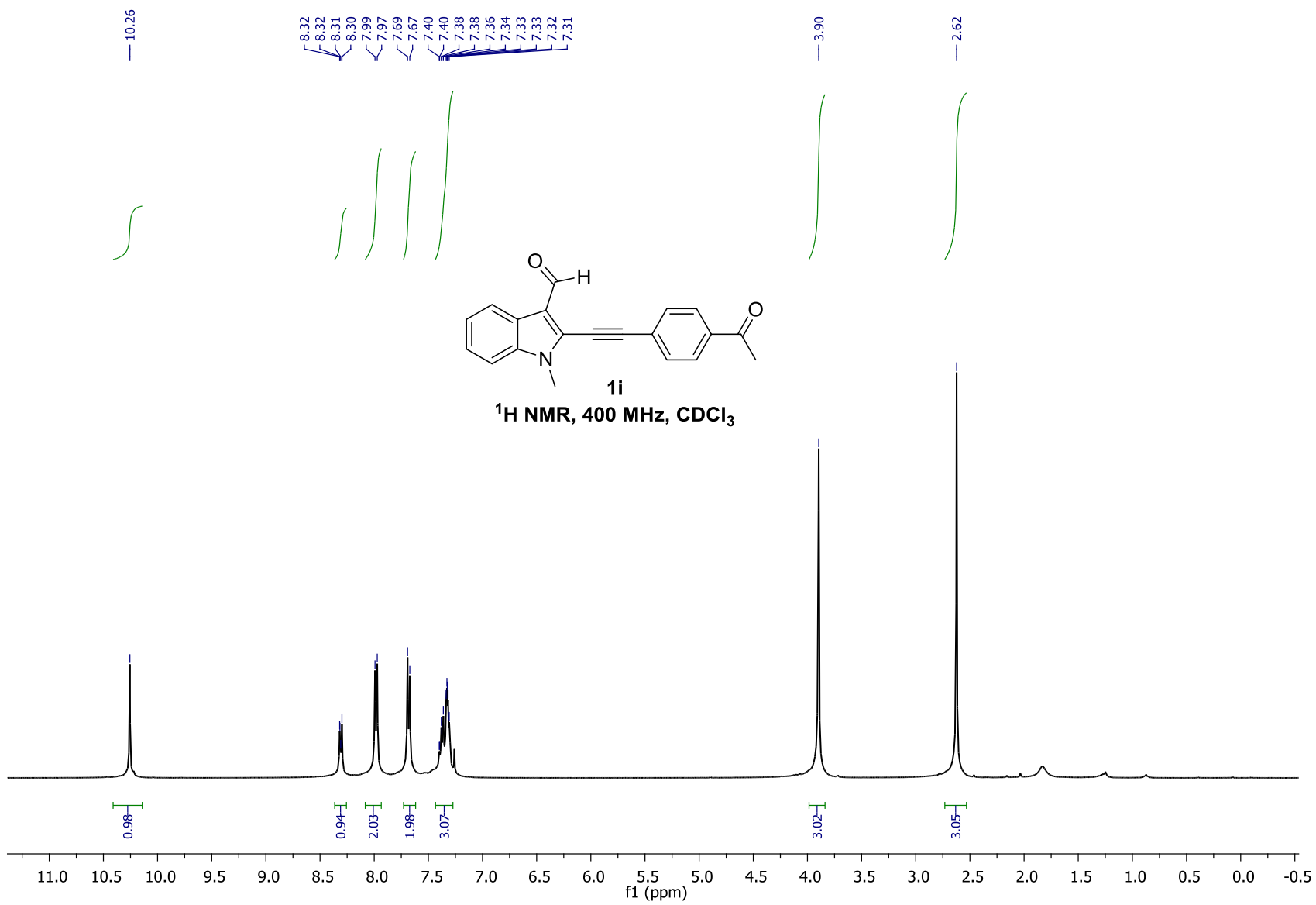


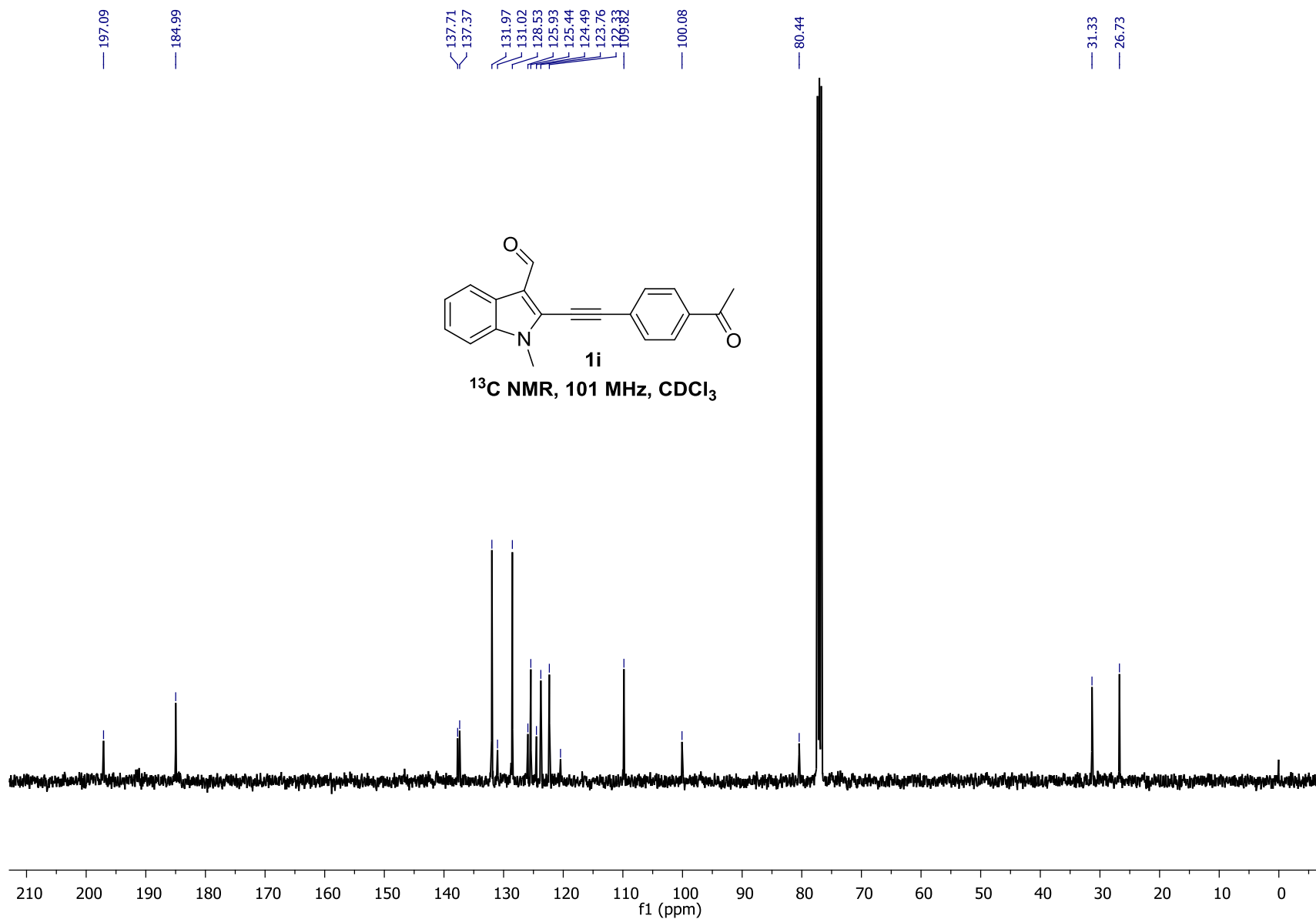


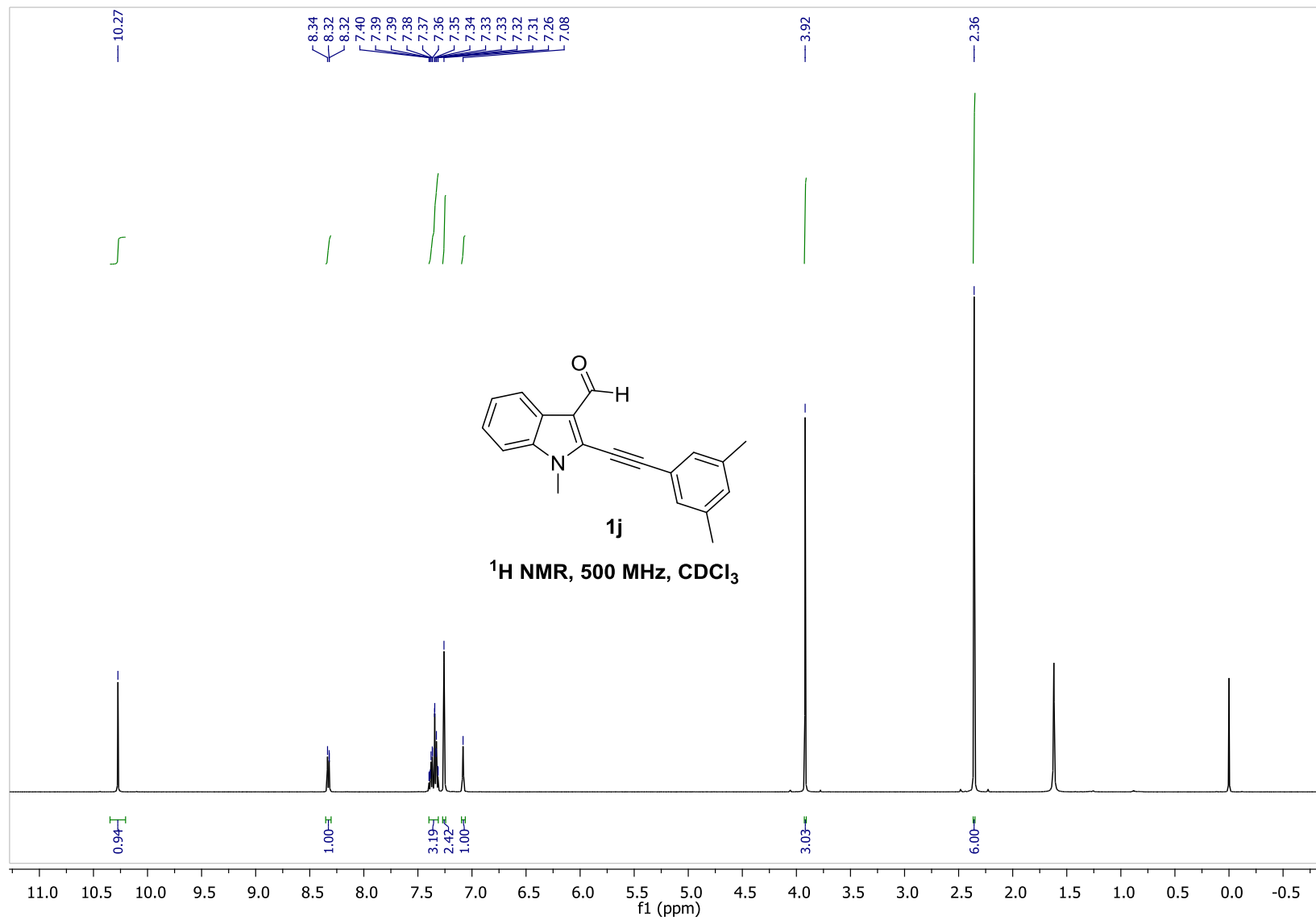


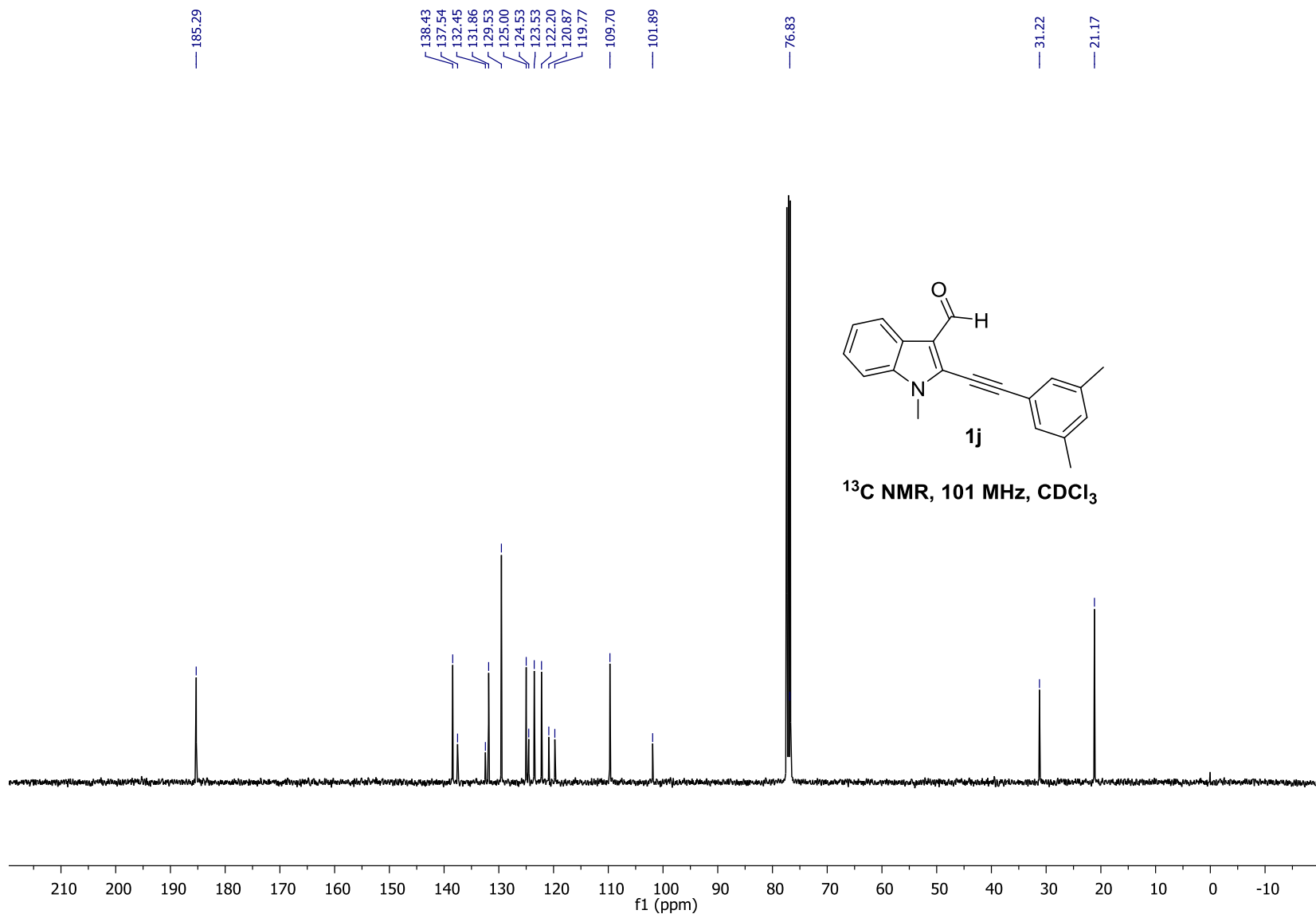




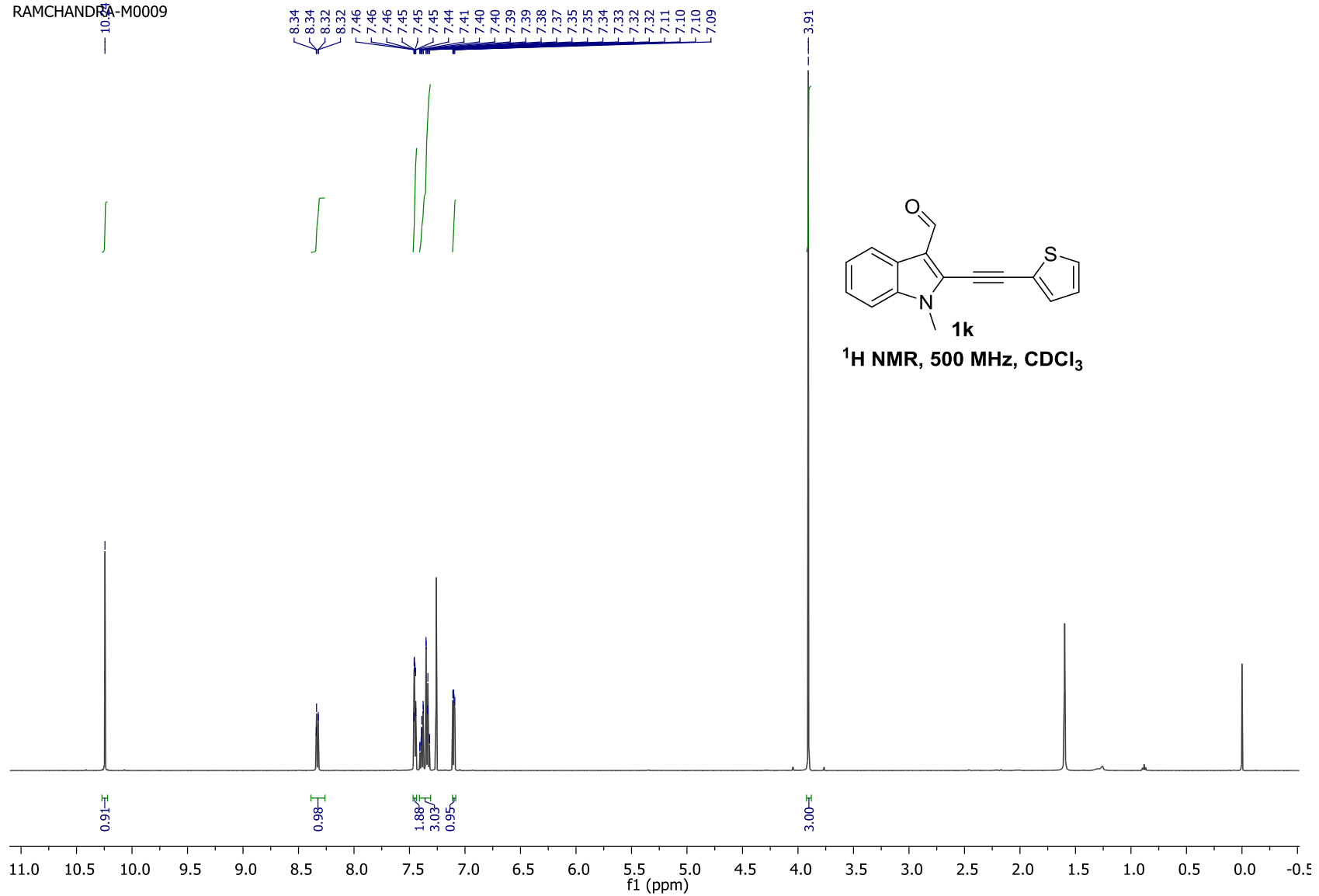


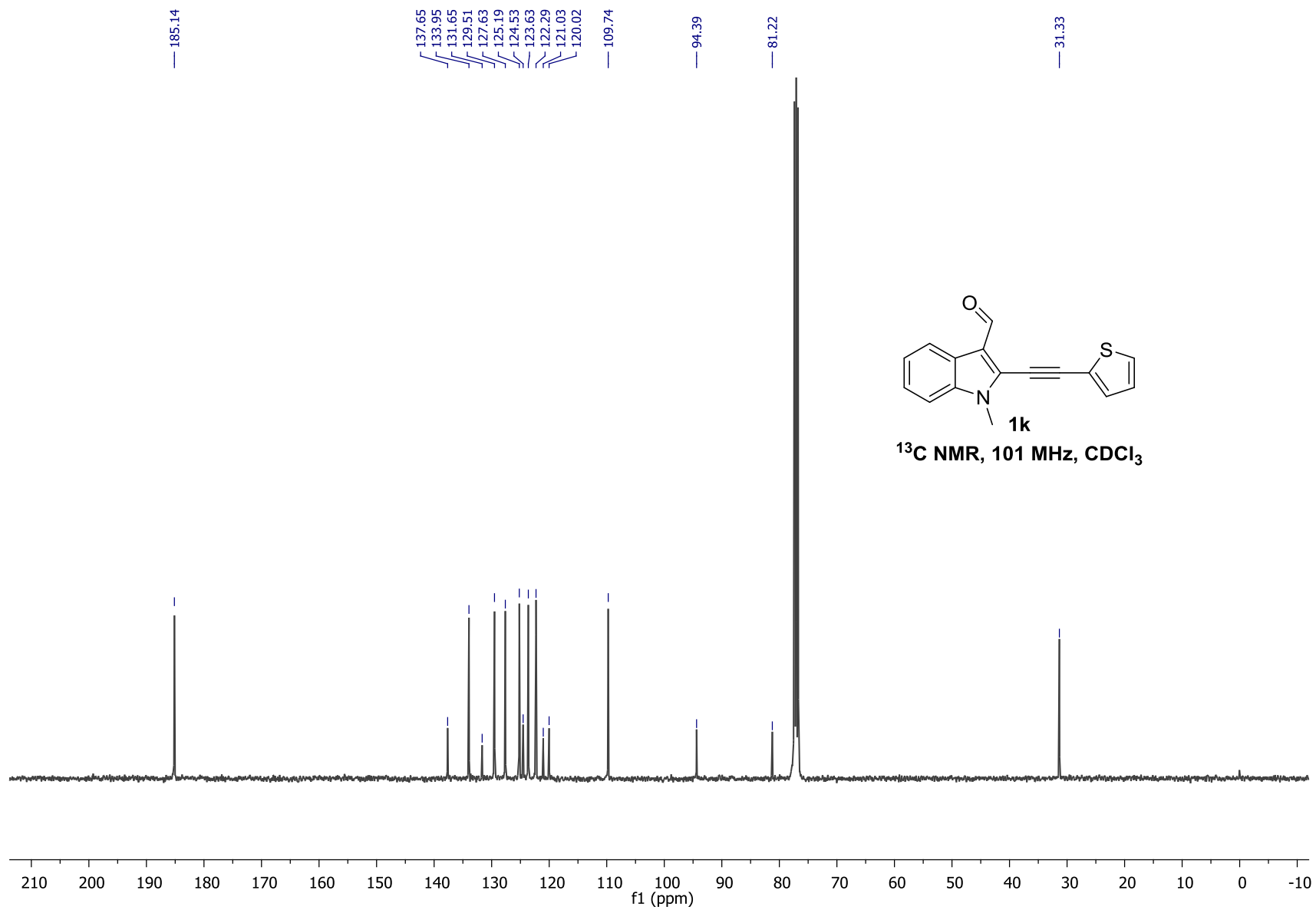


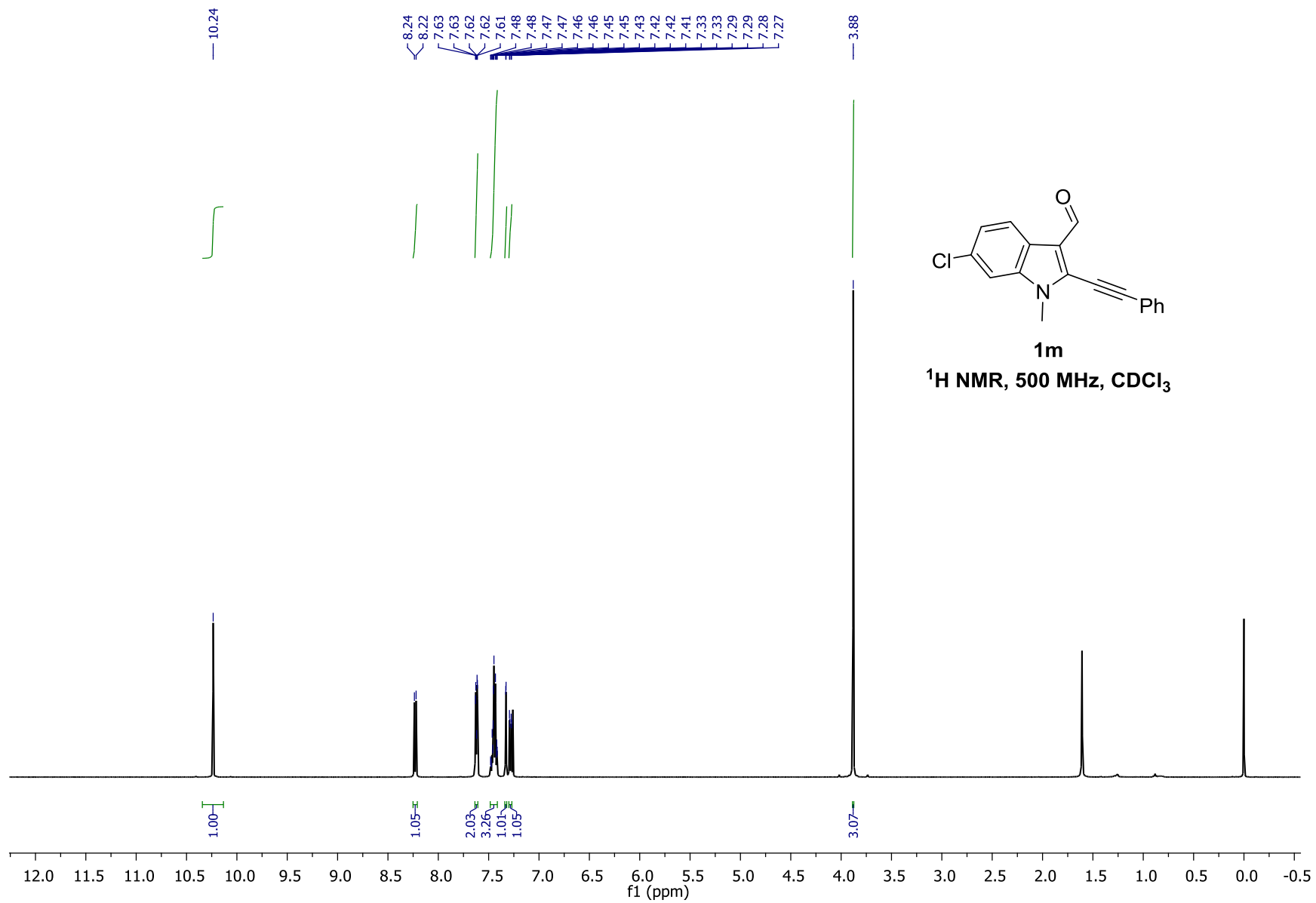


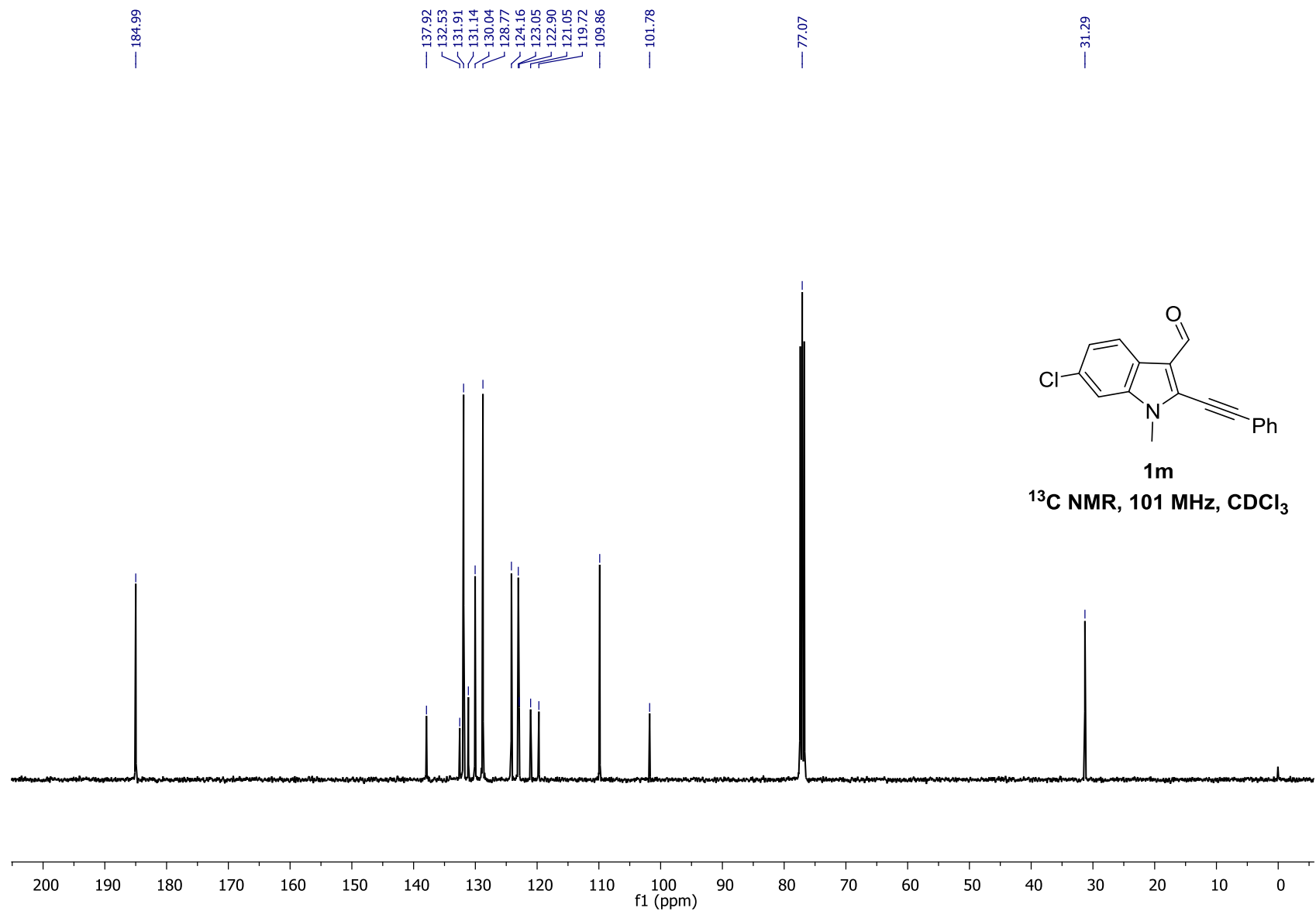


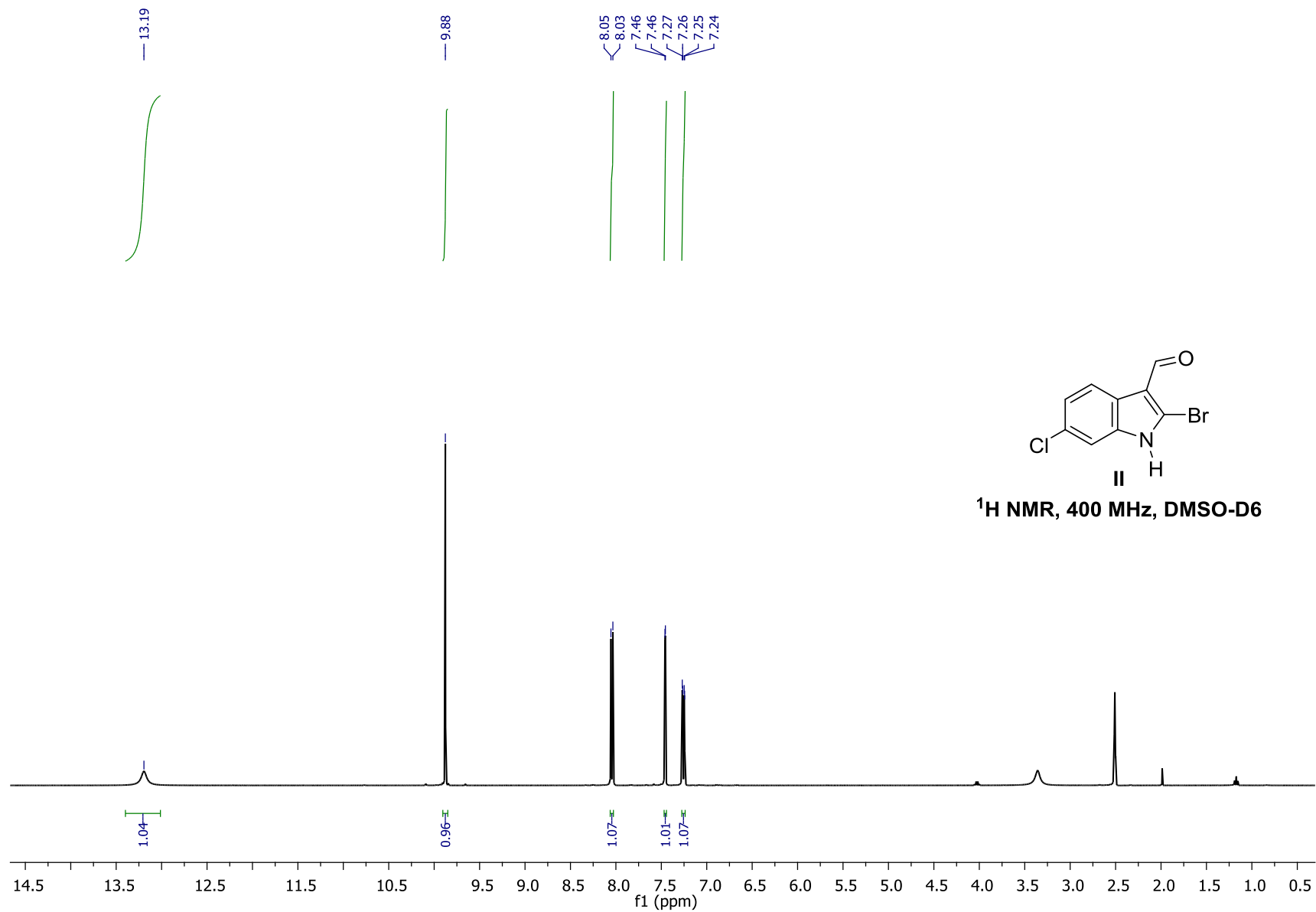
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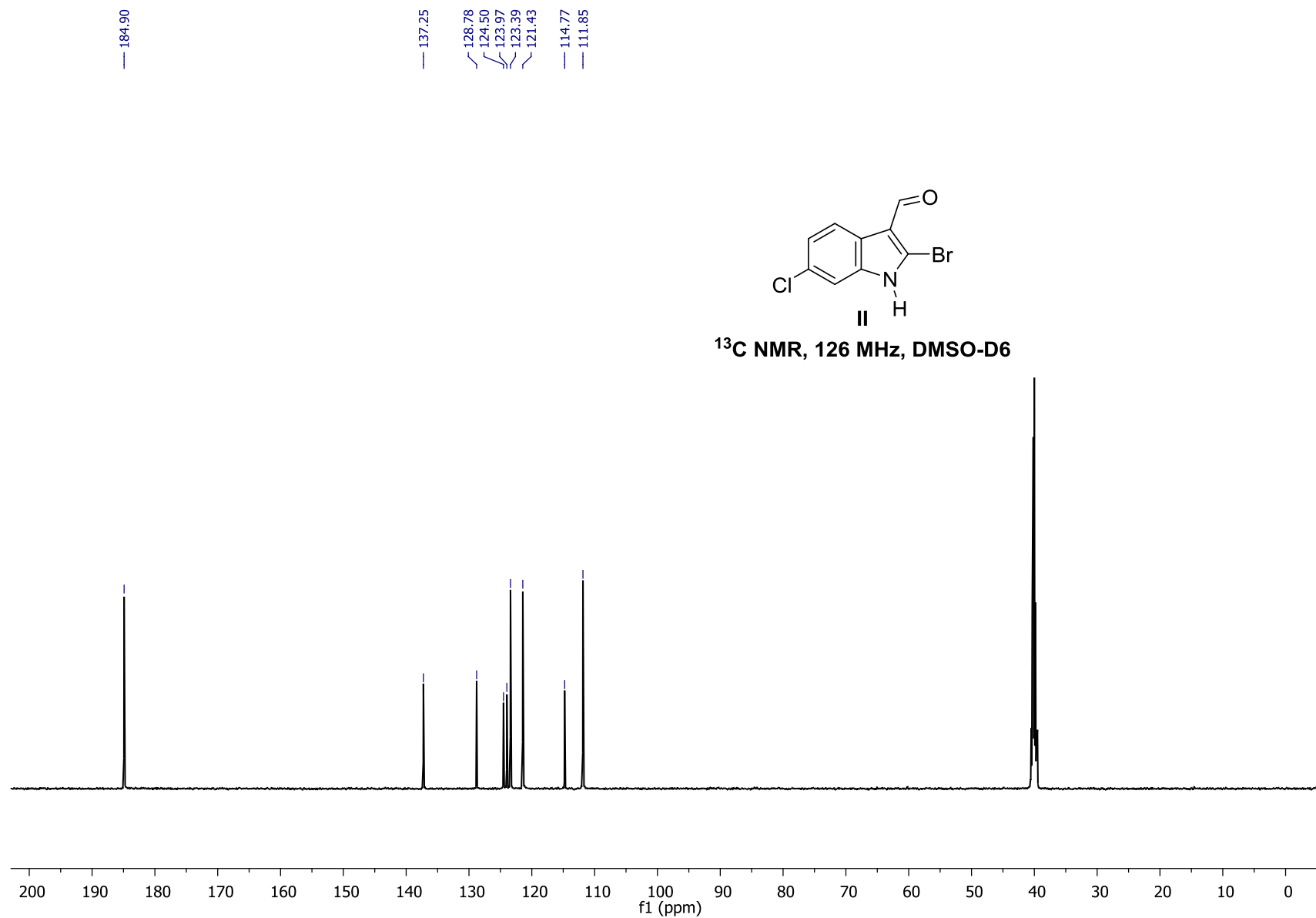


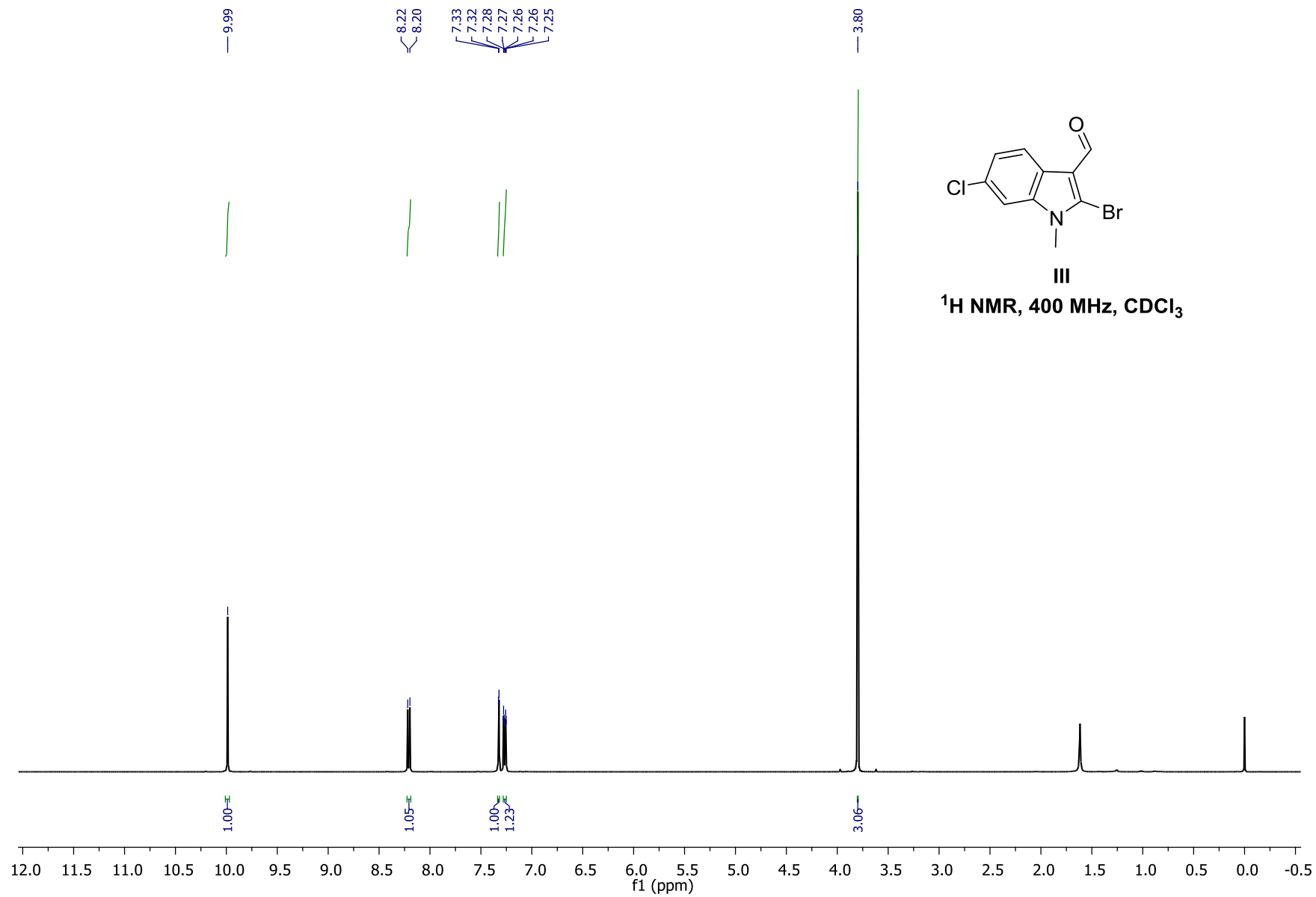




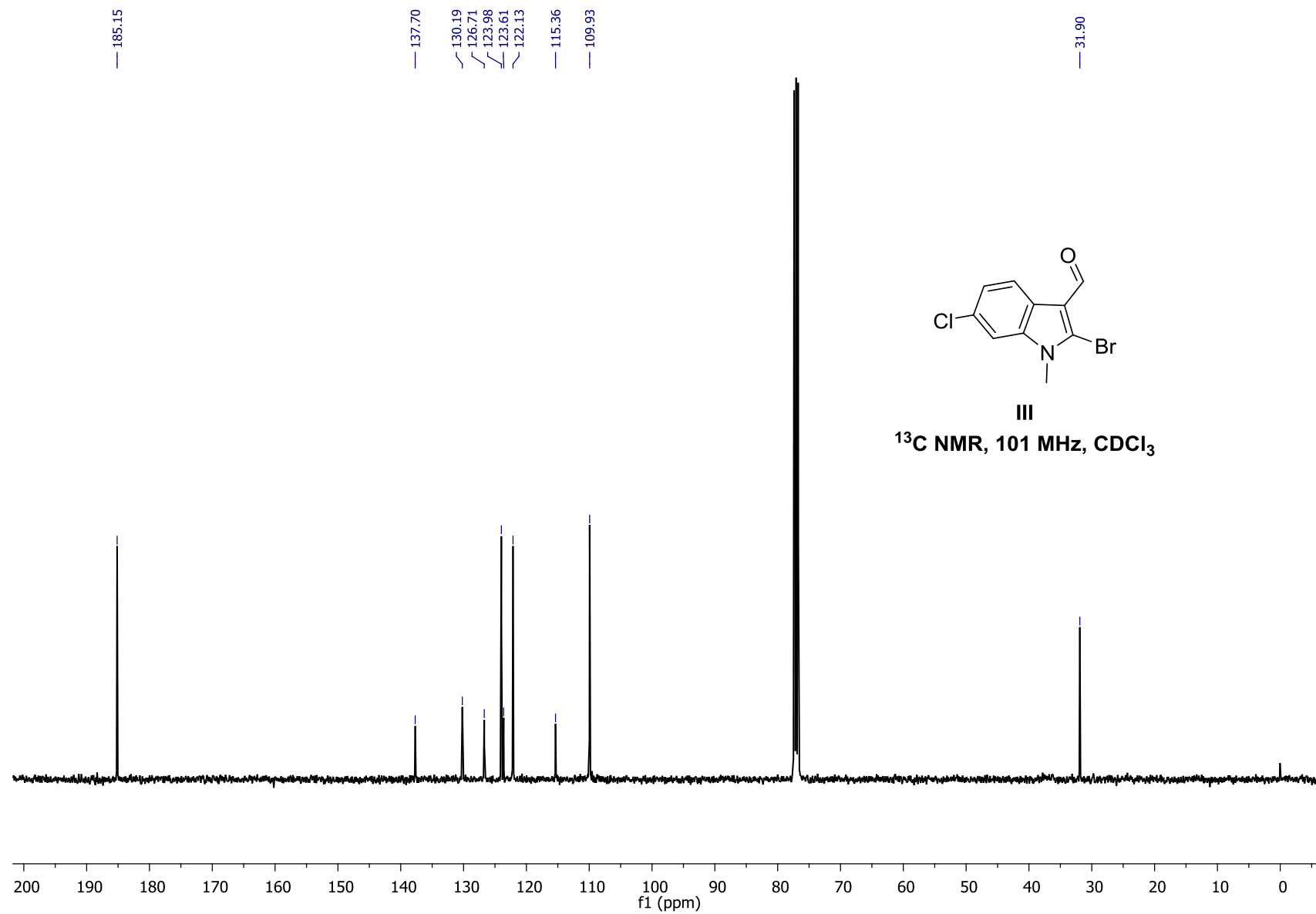




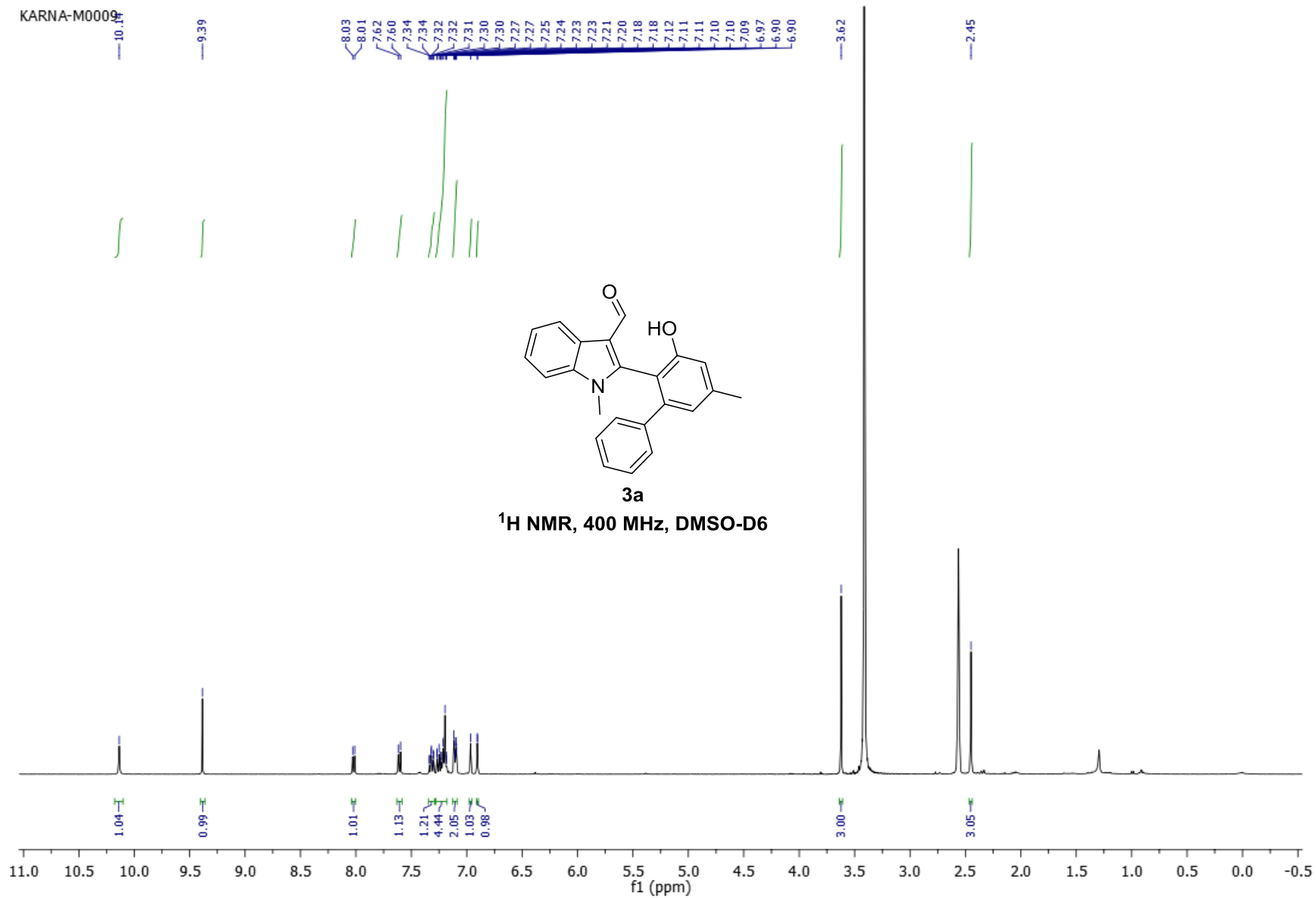




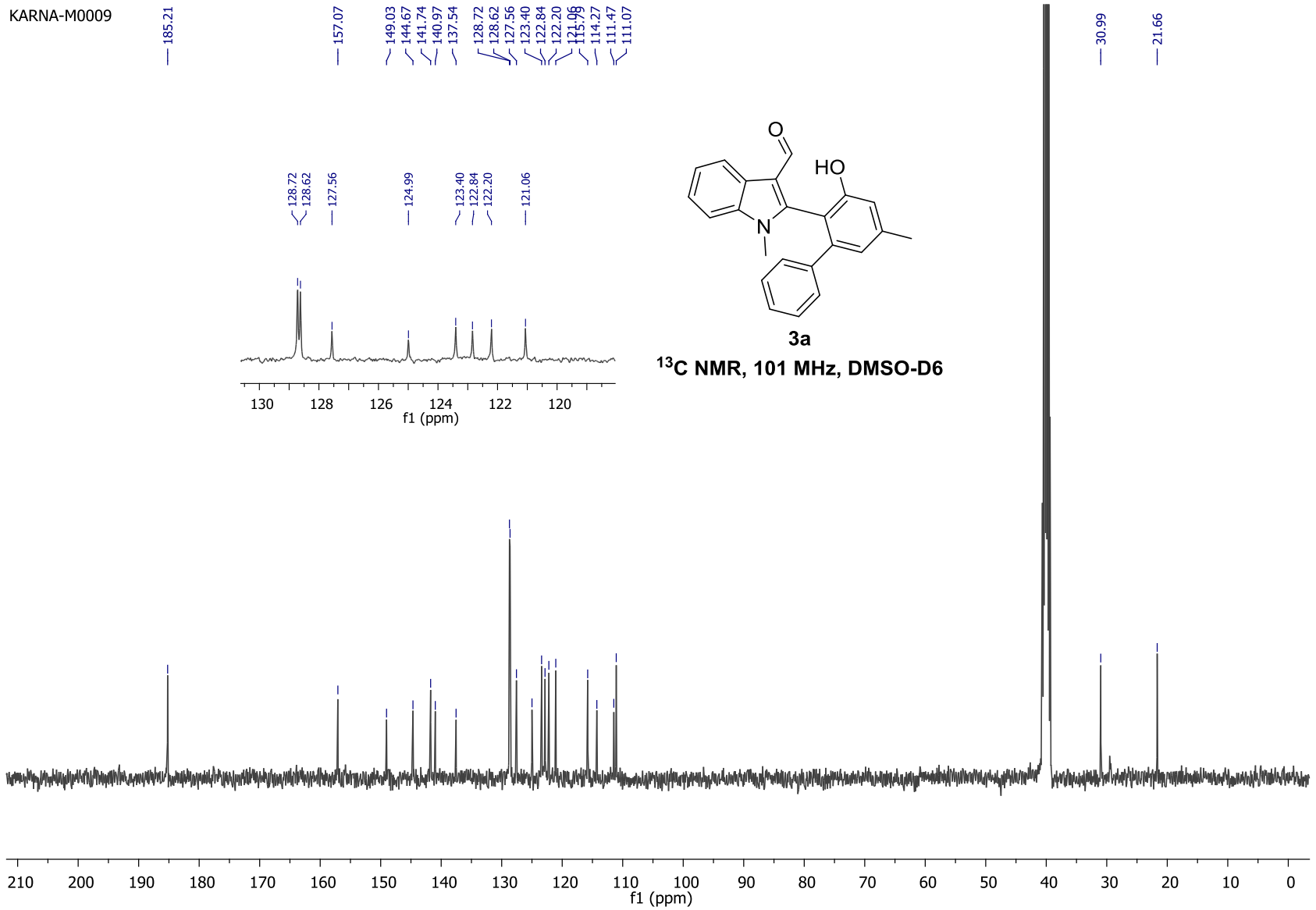
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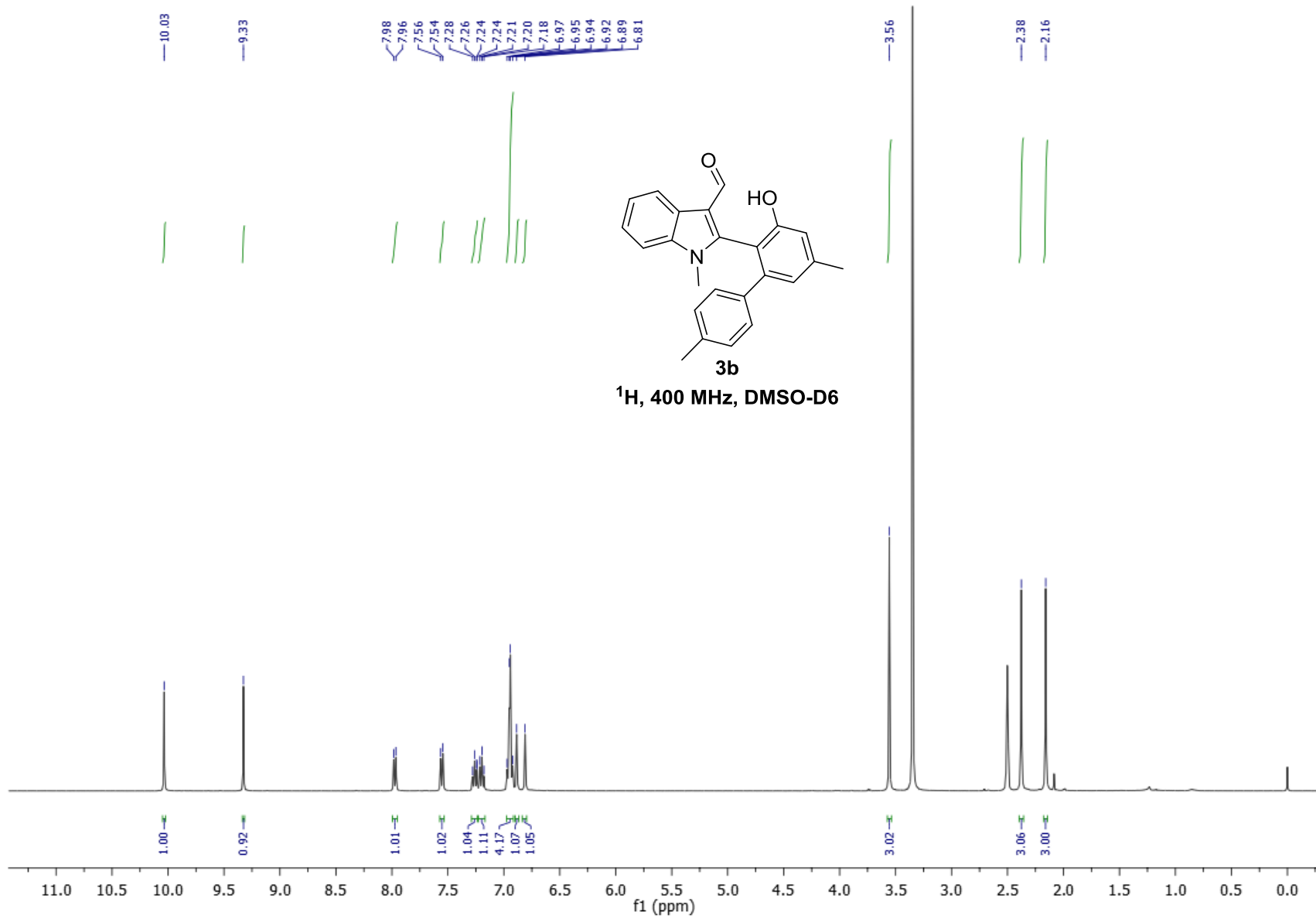


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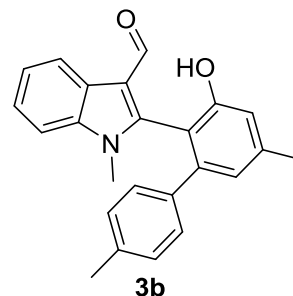
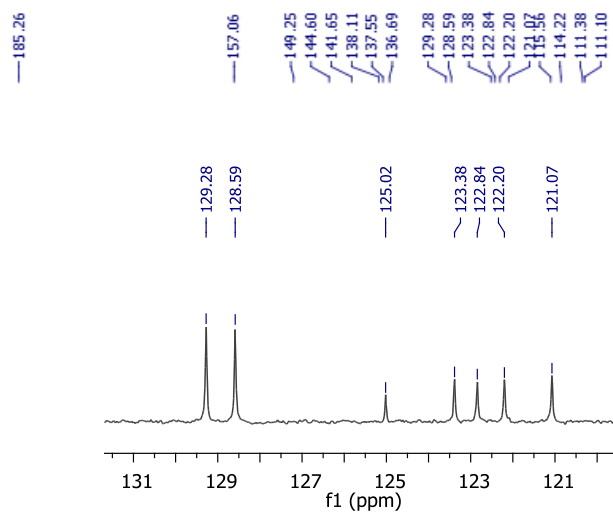


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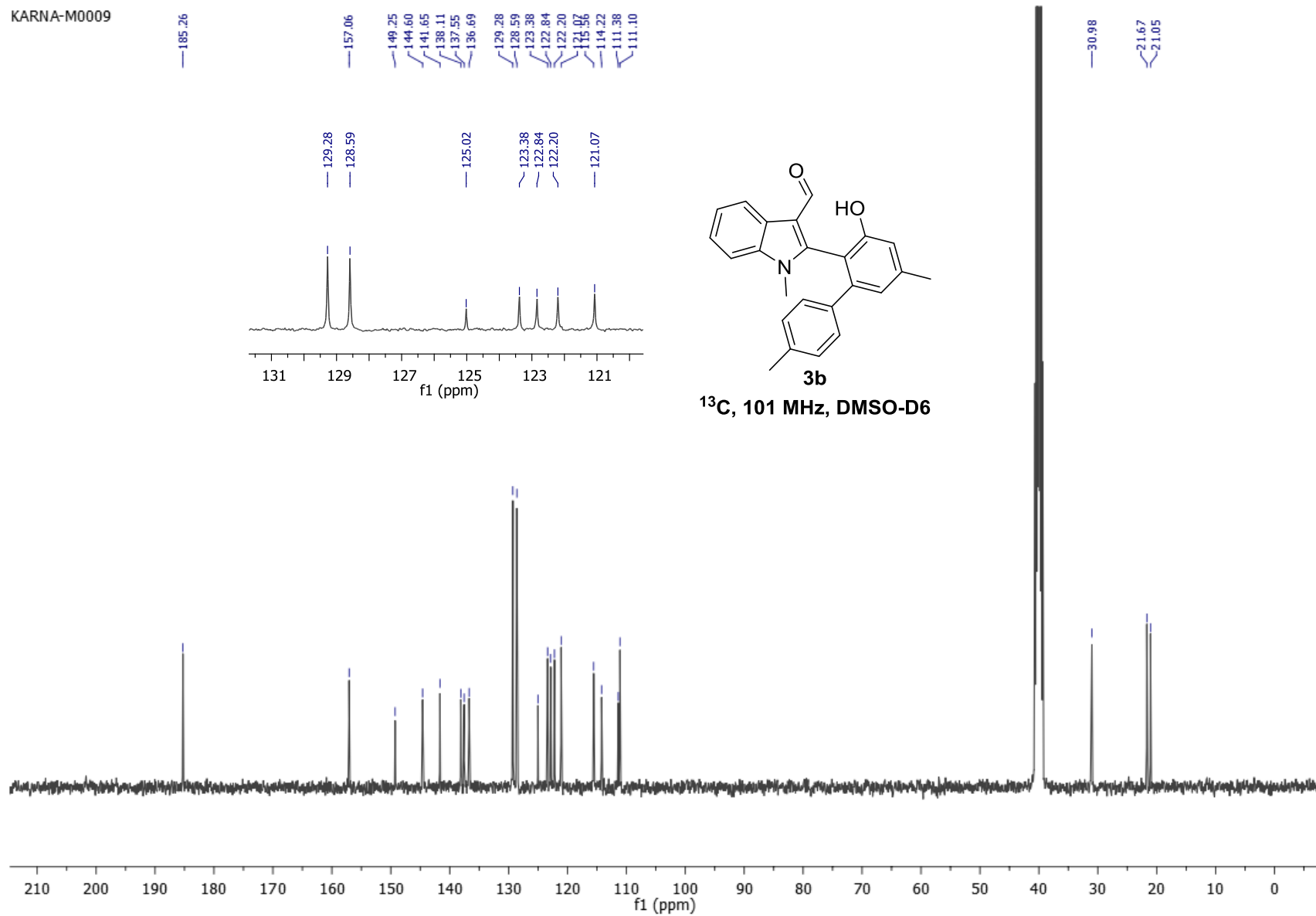




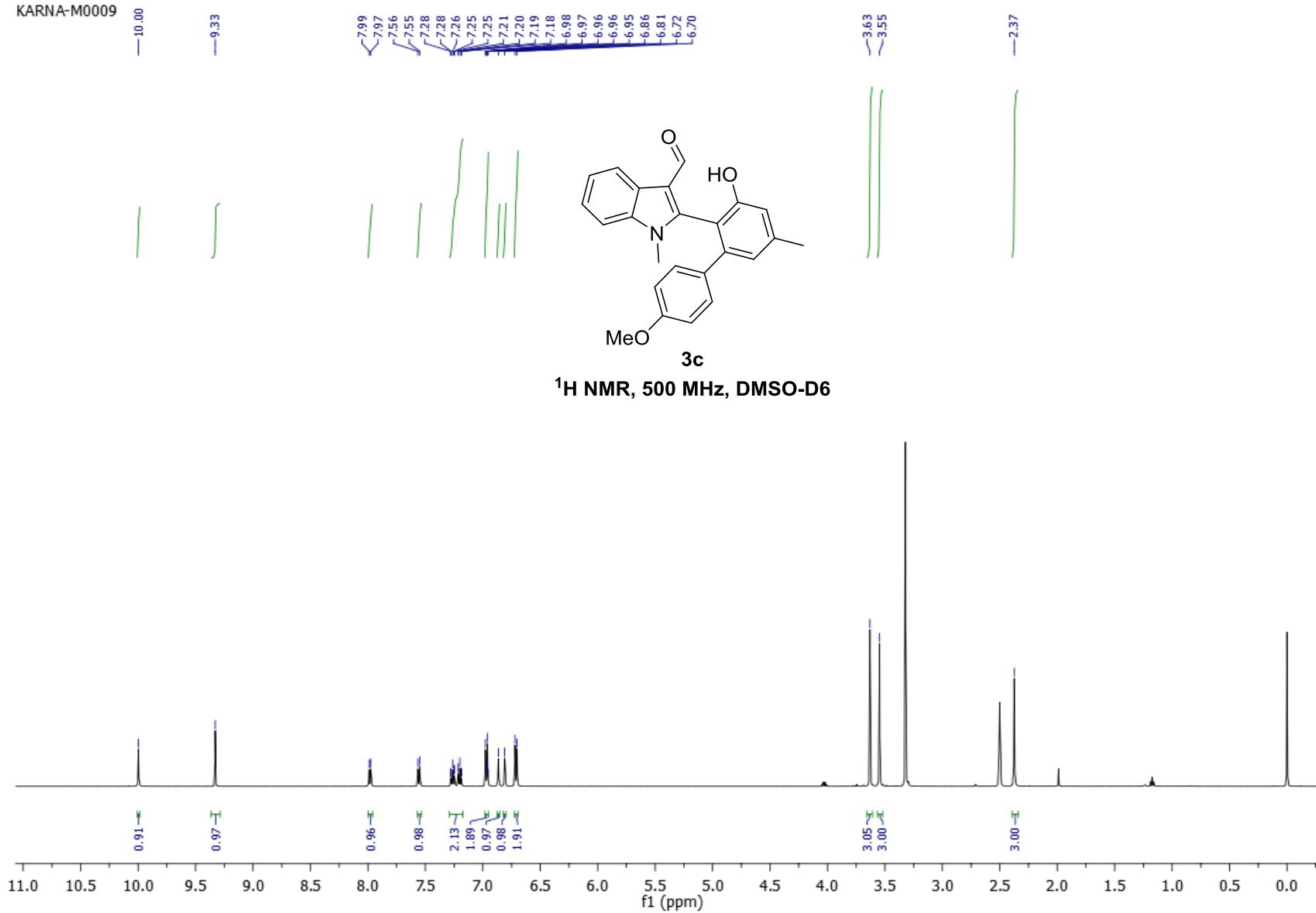
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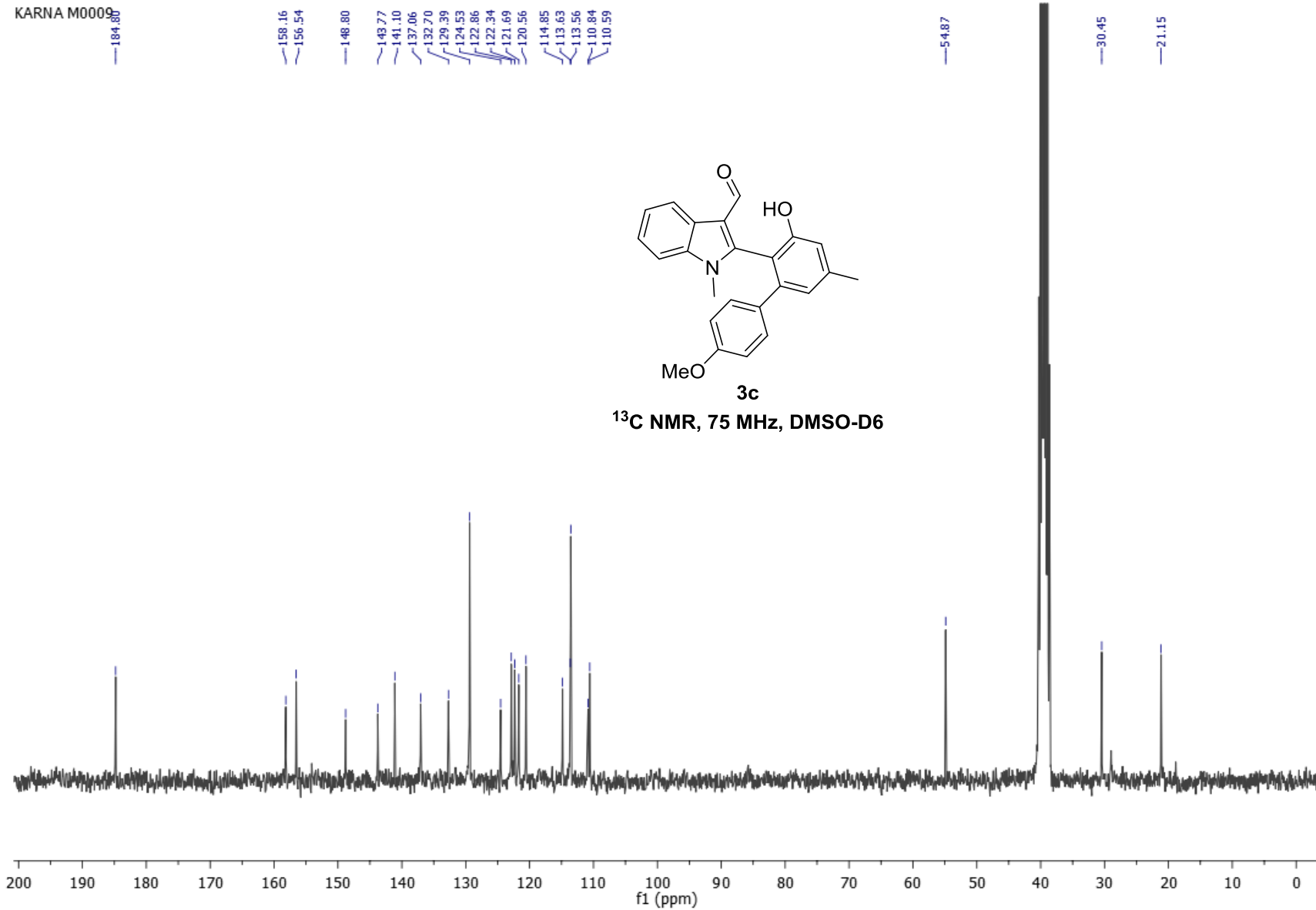
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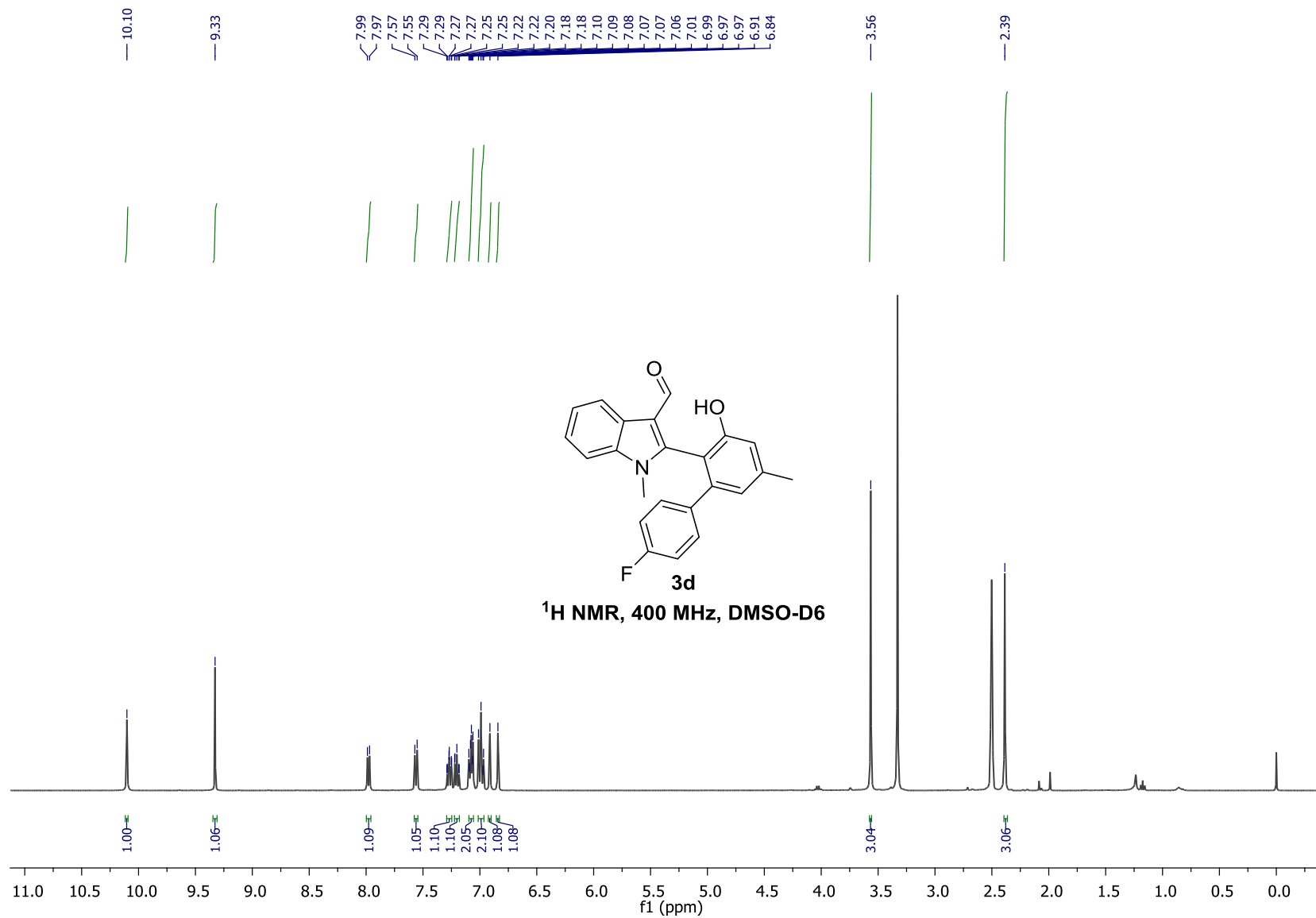


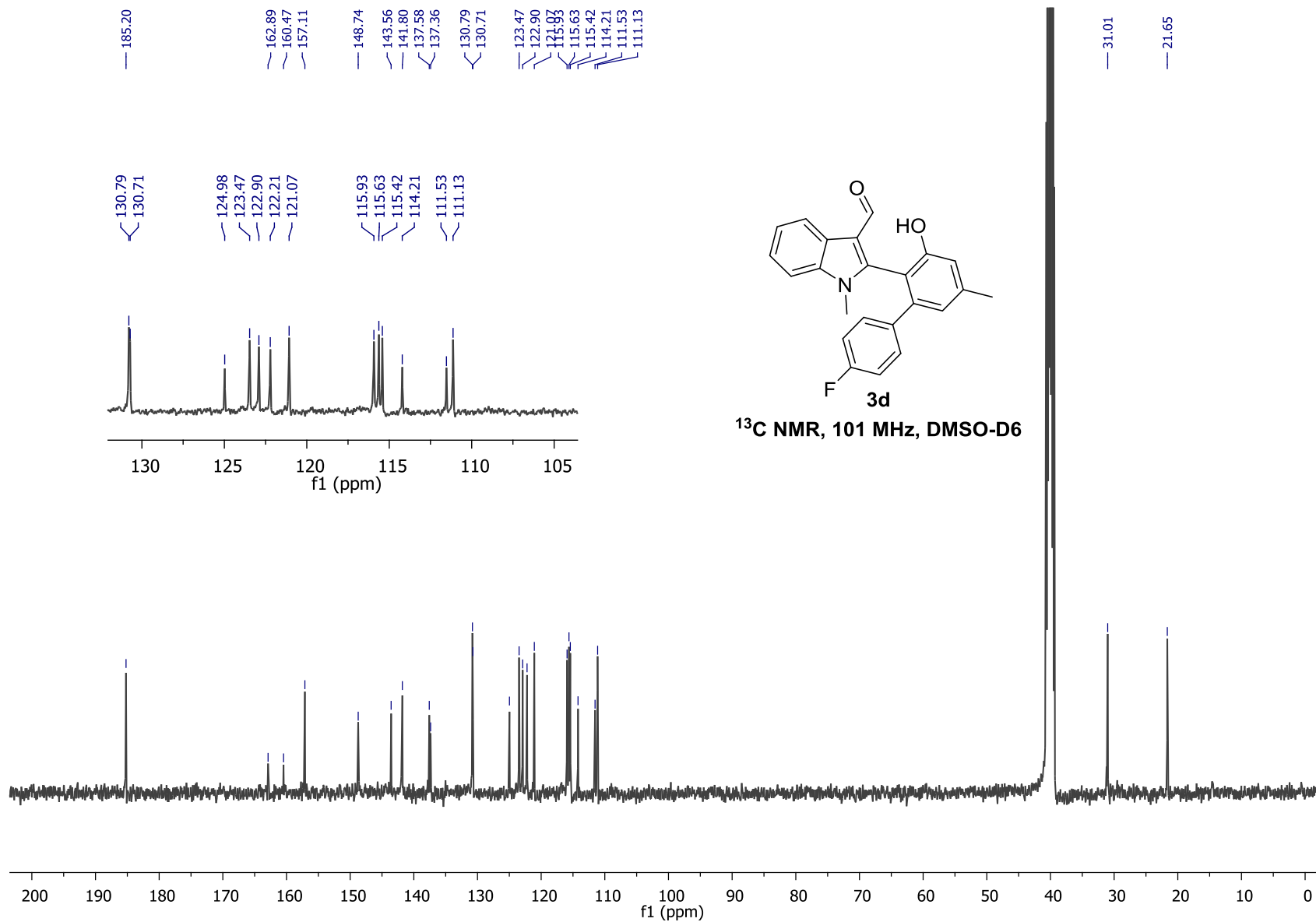
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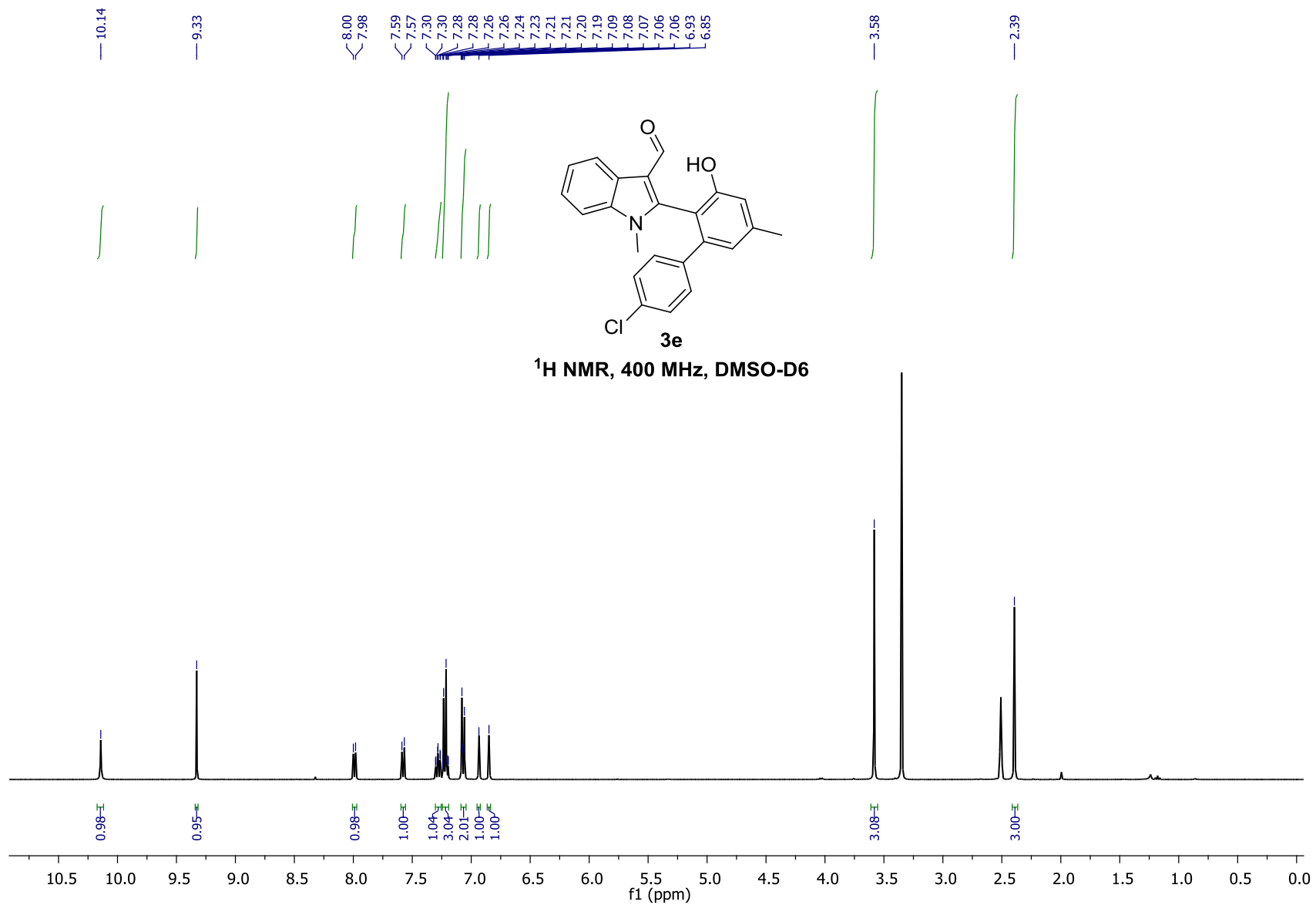


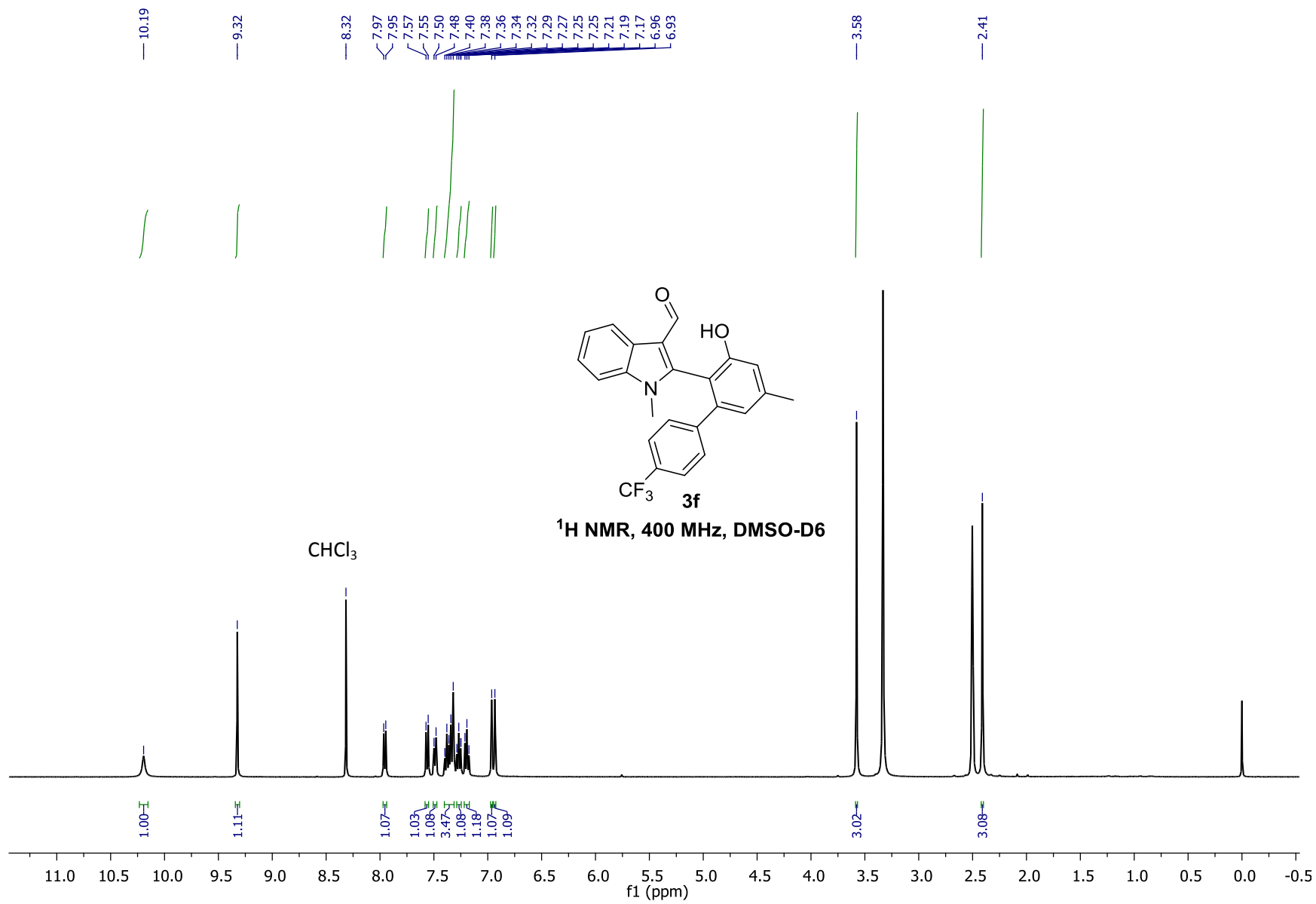
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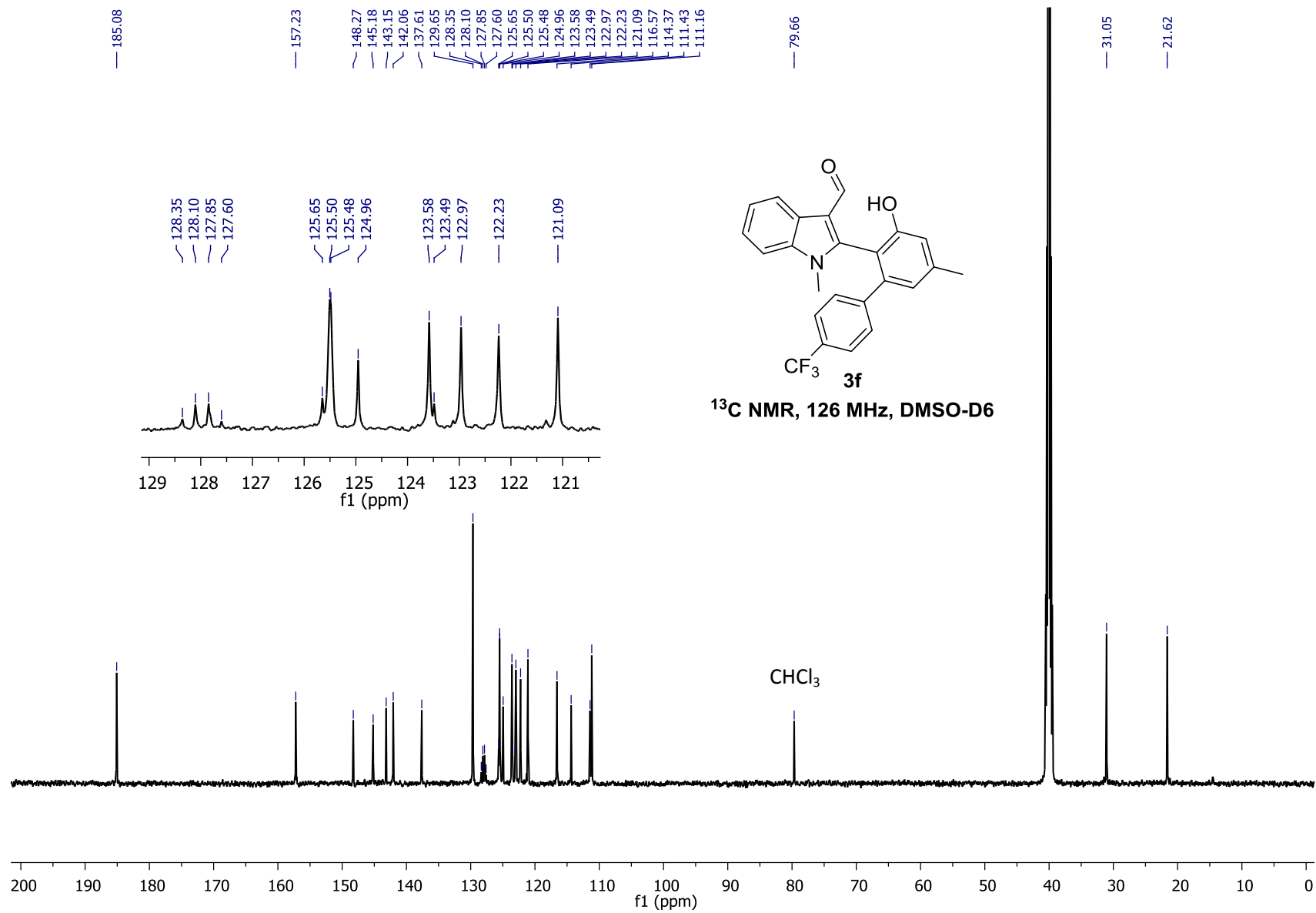


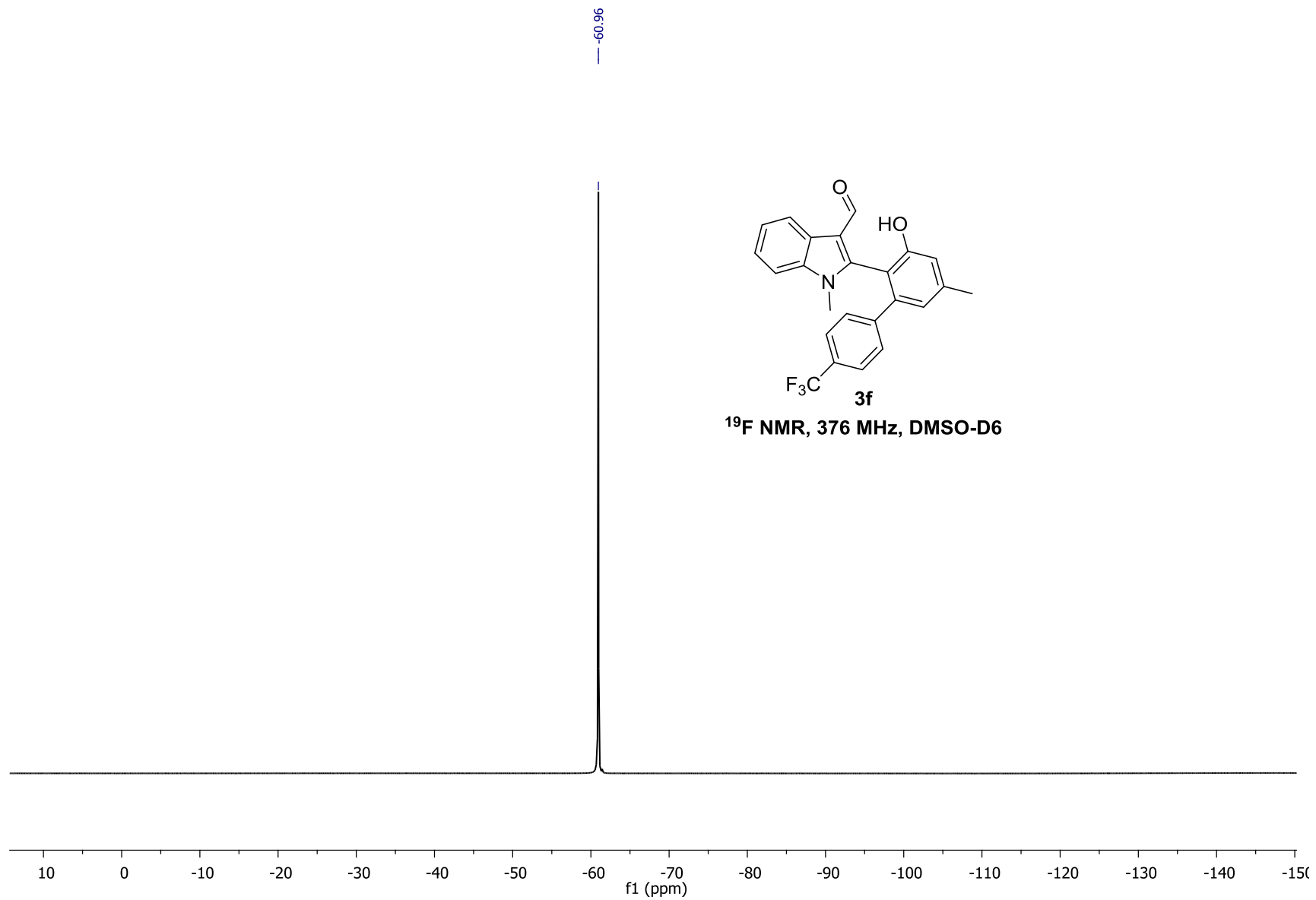


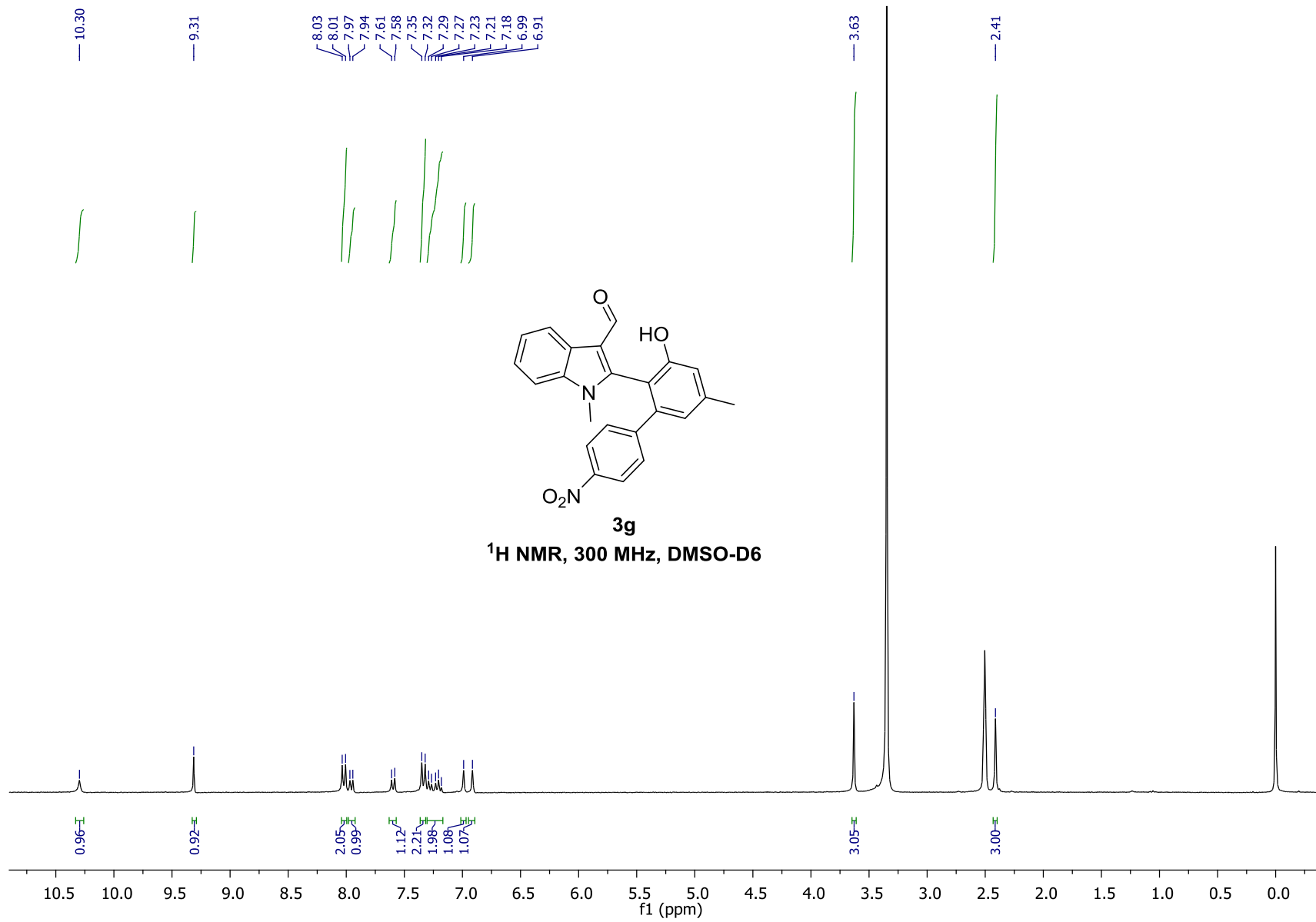




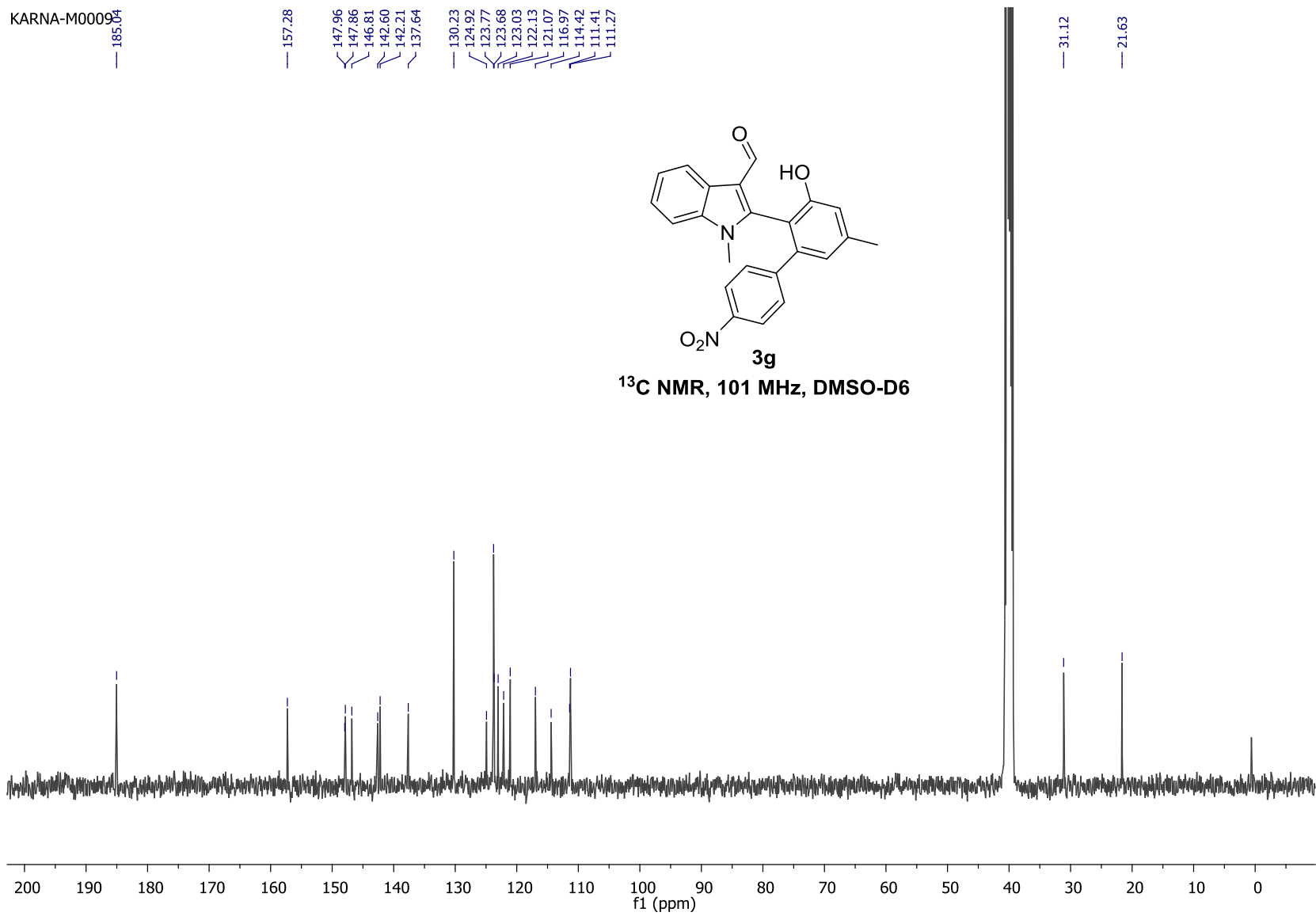




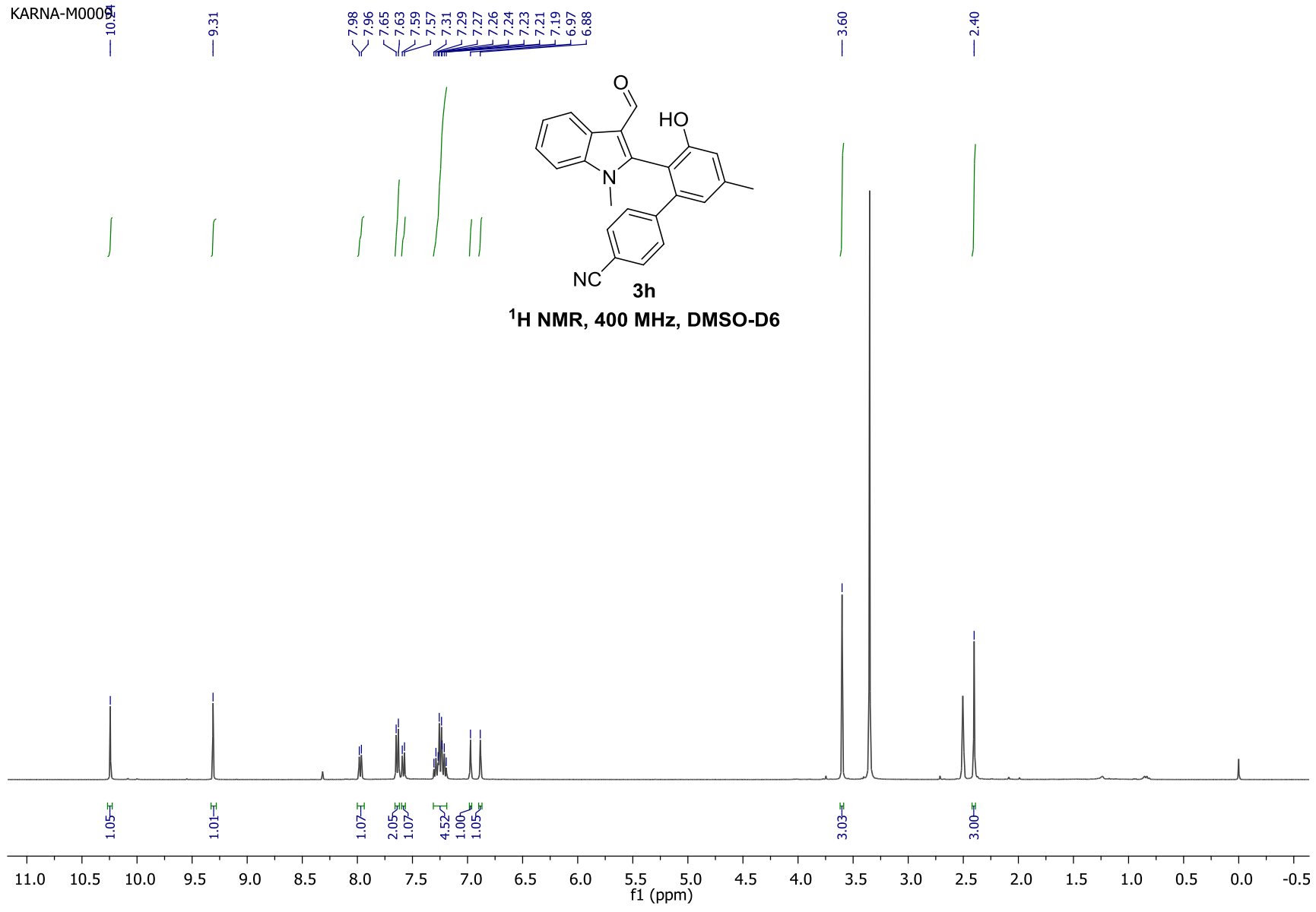


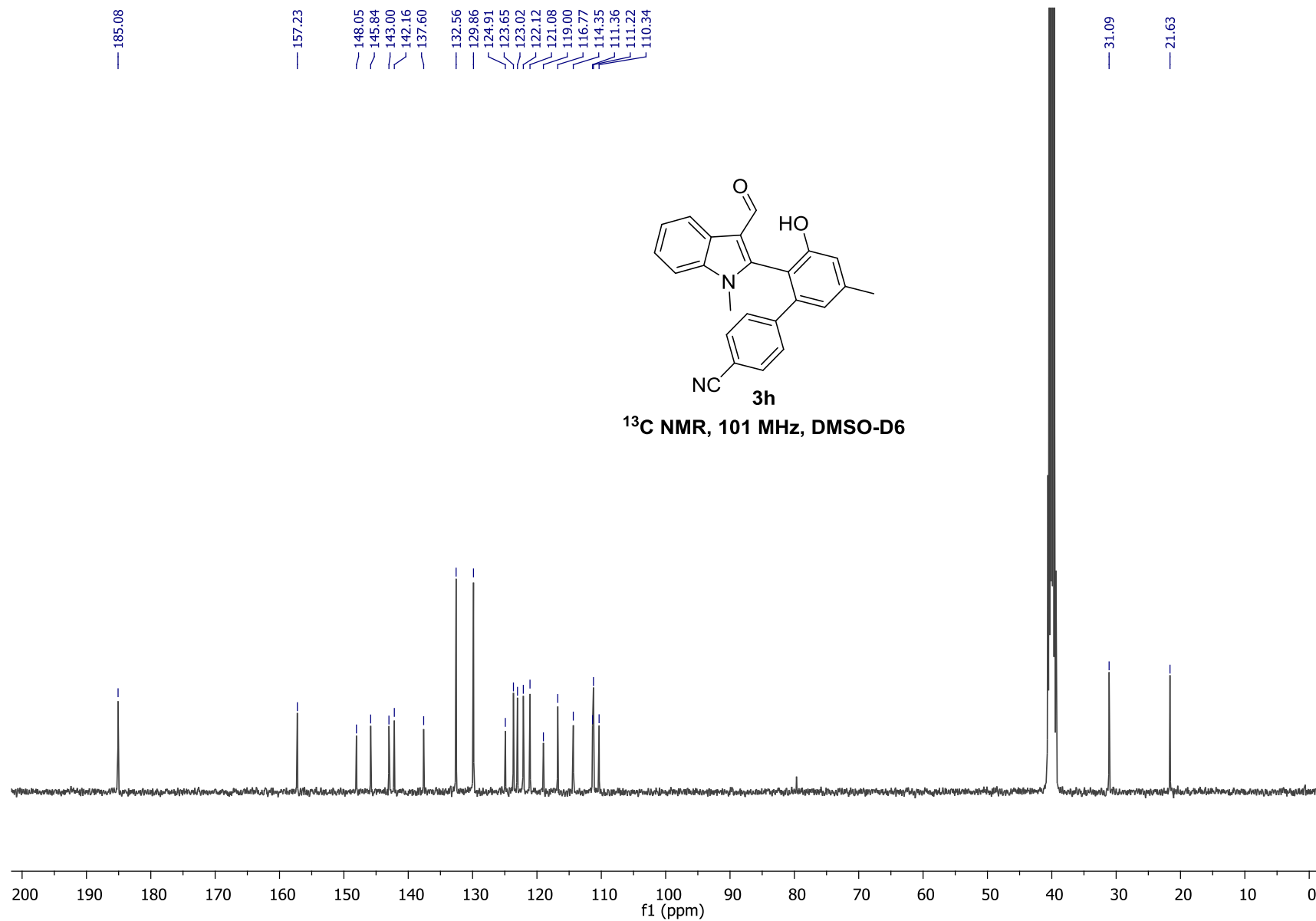


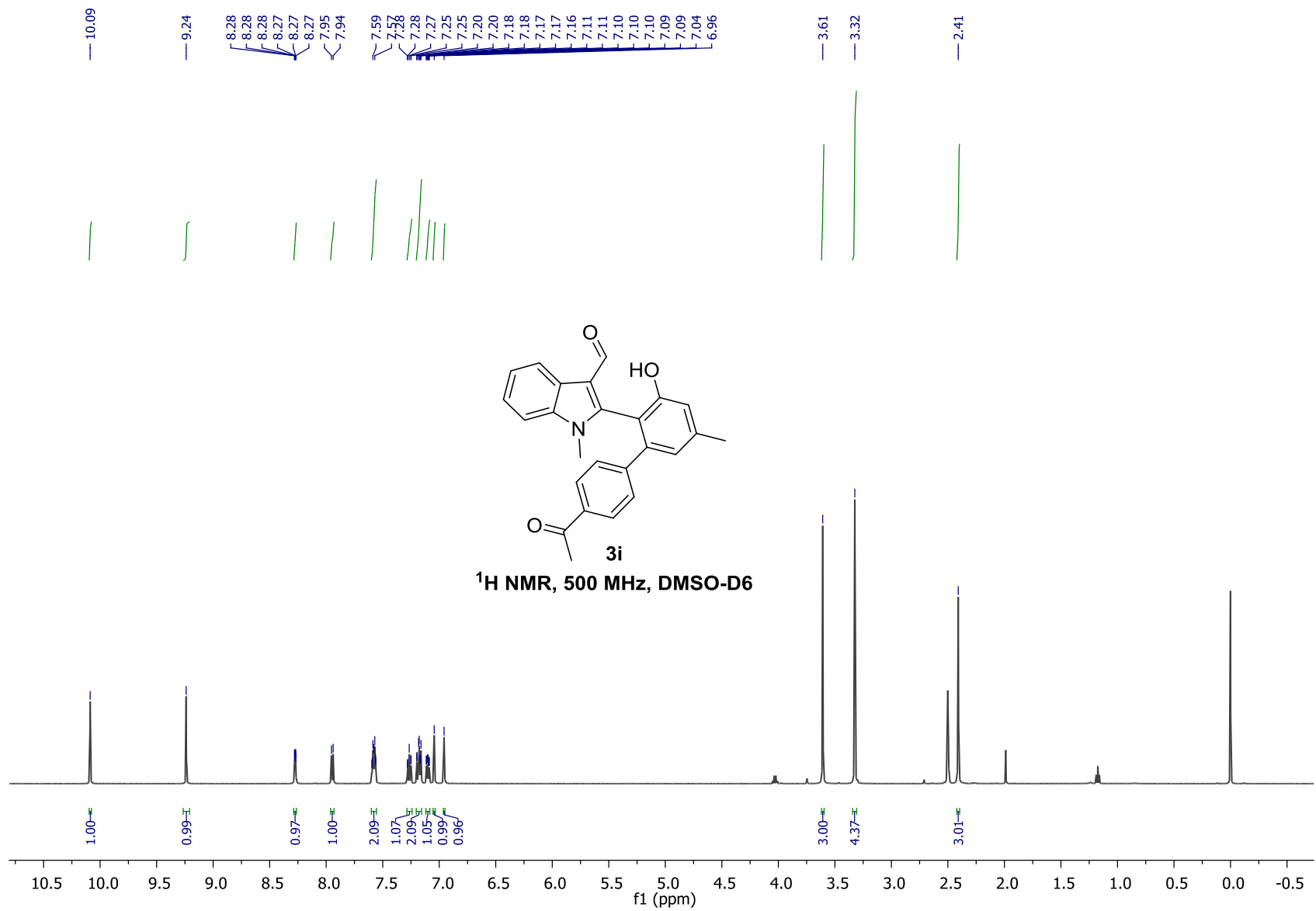
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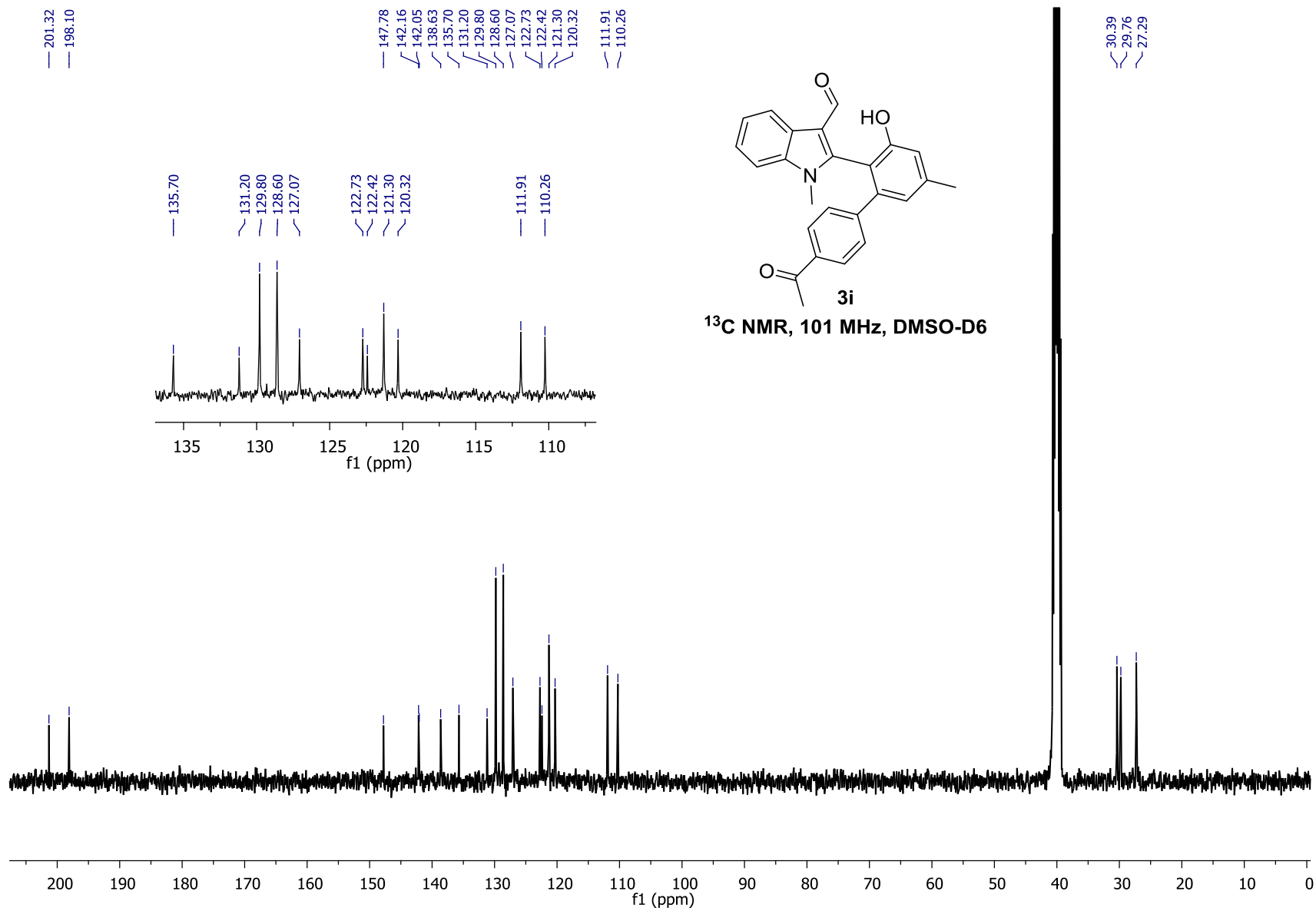


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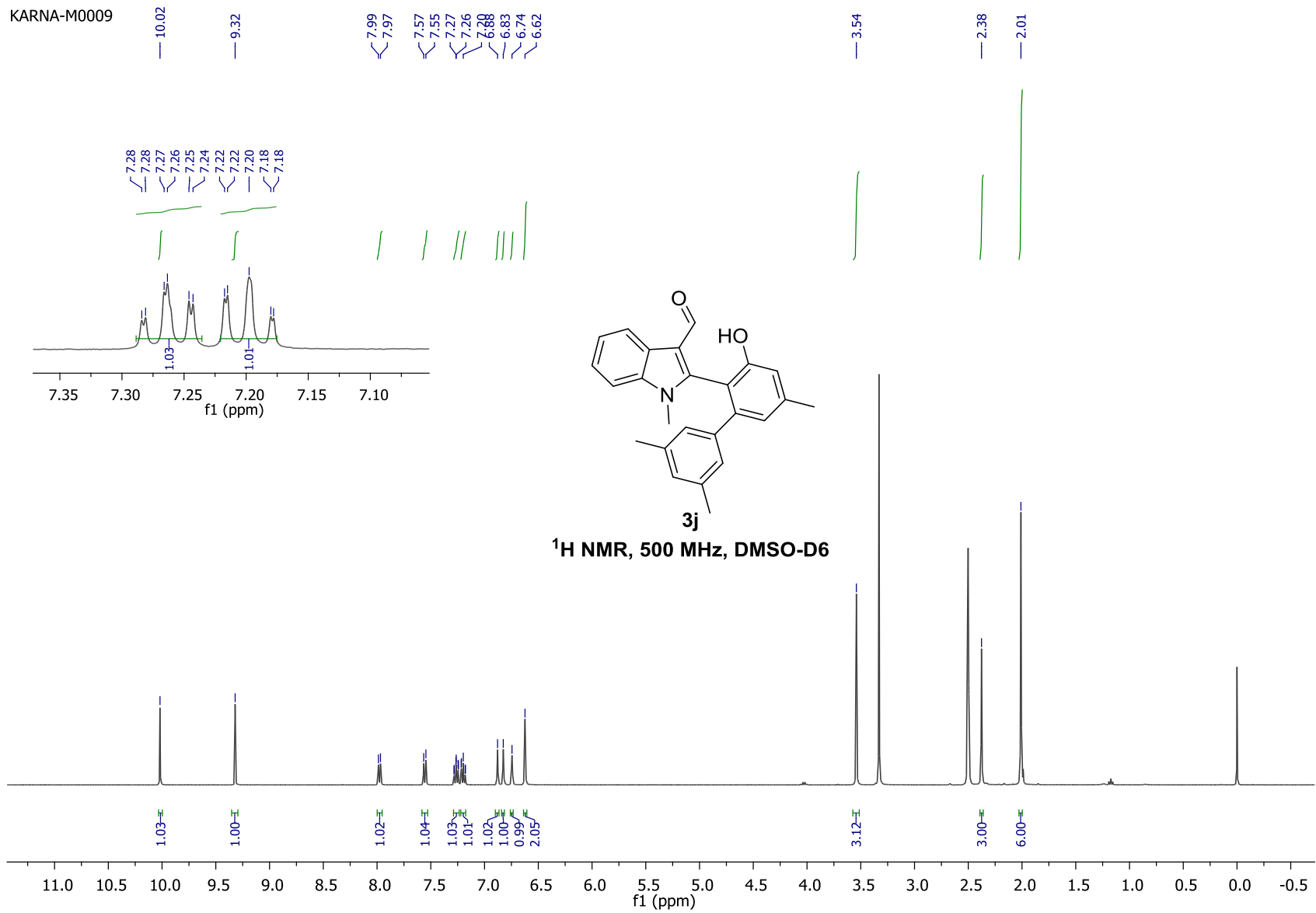


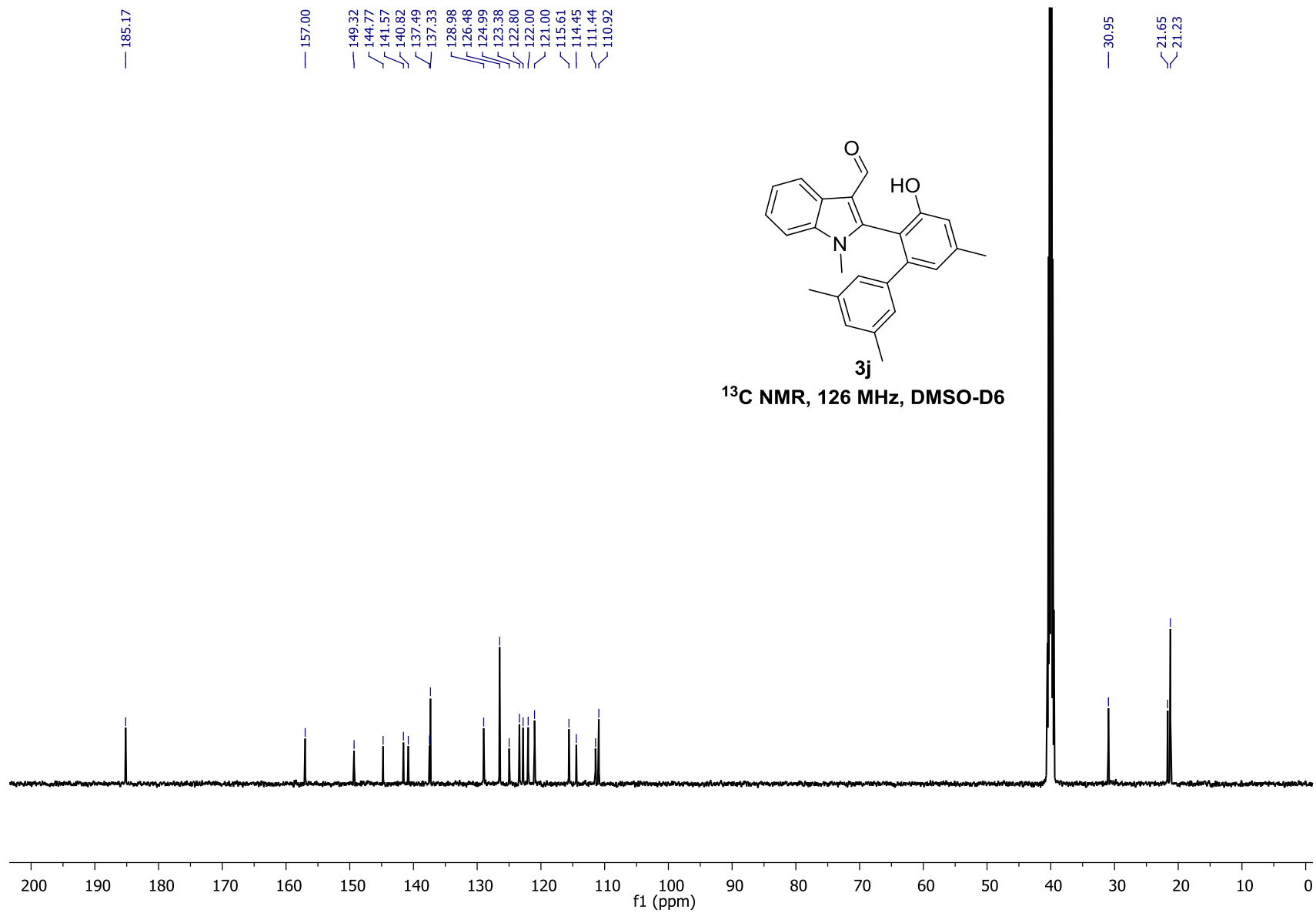


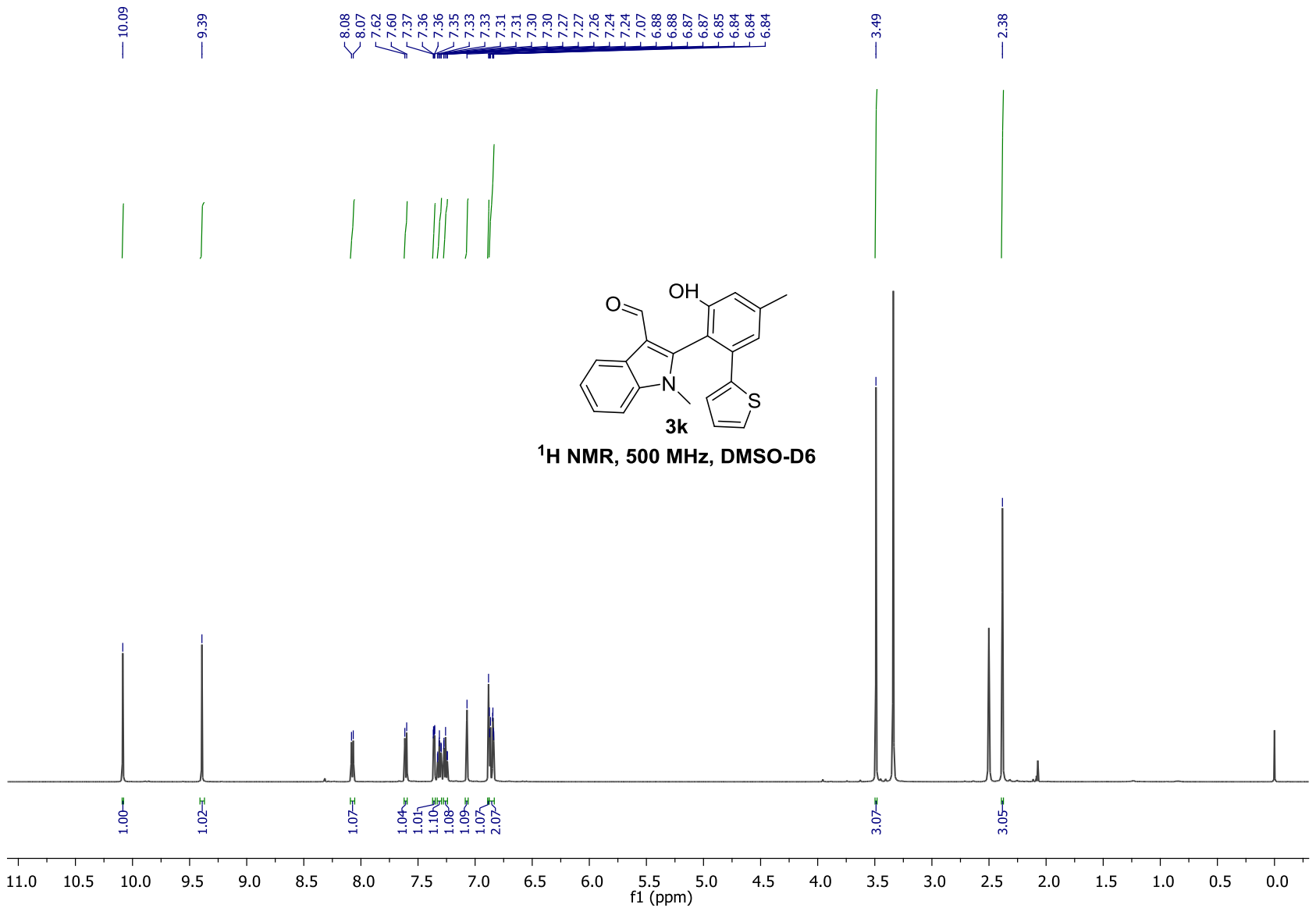




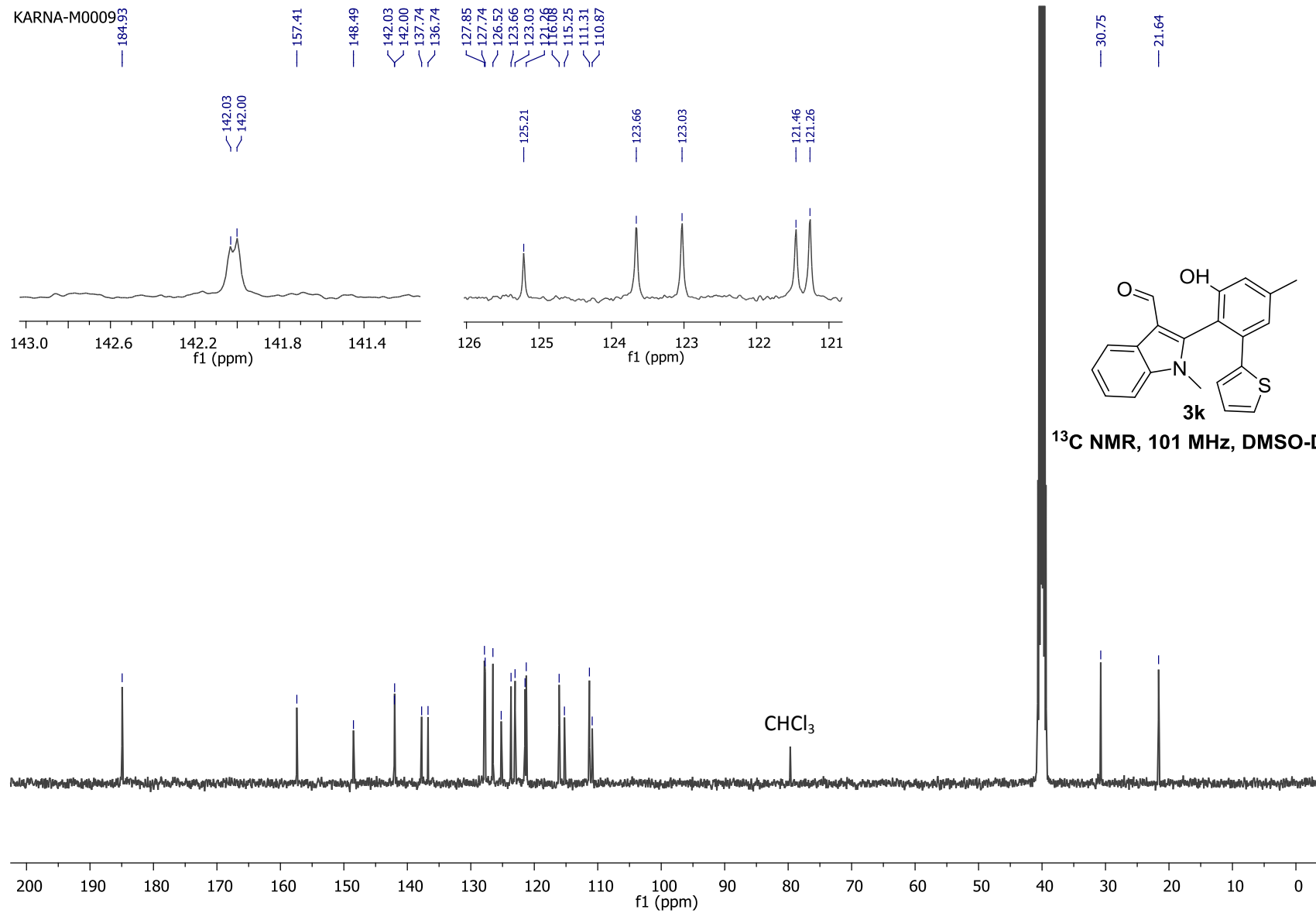
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