

# **Synthesis of furan-3-carbonitriles by cyclization of cyano-substituted $\alpha,\beta$ -enones with potassium dinitromethanide**

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**SUPPLEMENTARY INFORMATION**

## Crystallographic data

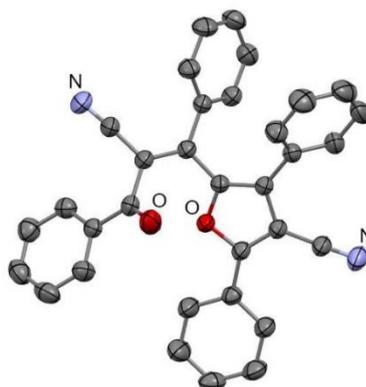


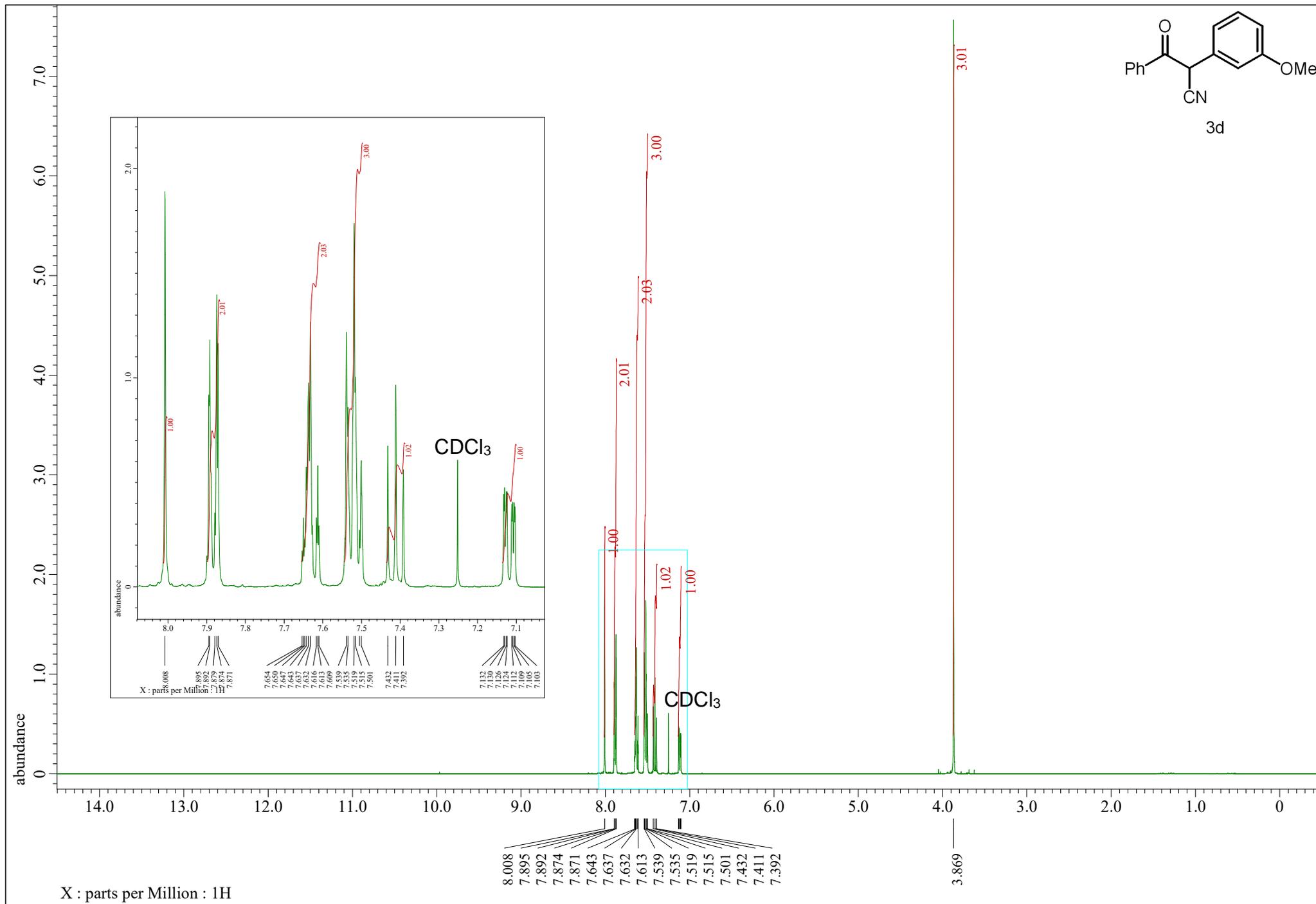
Table 1. Crystallographic data and structure refinement for **6a**.

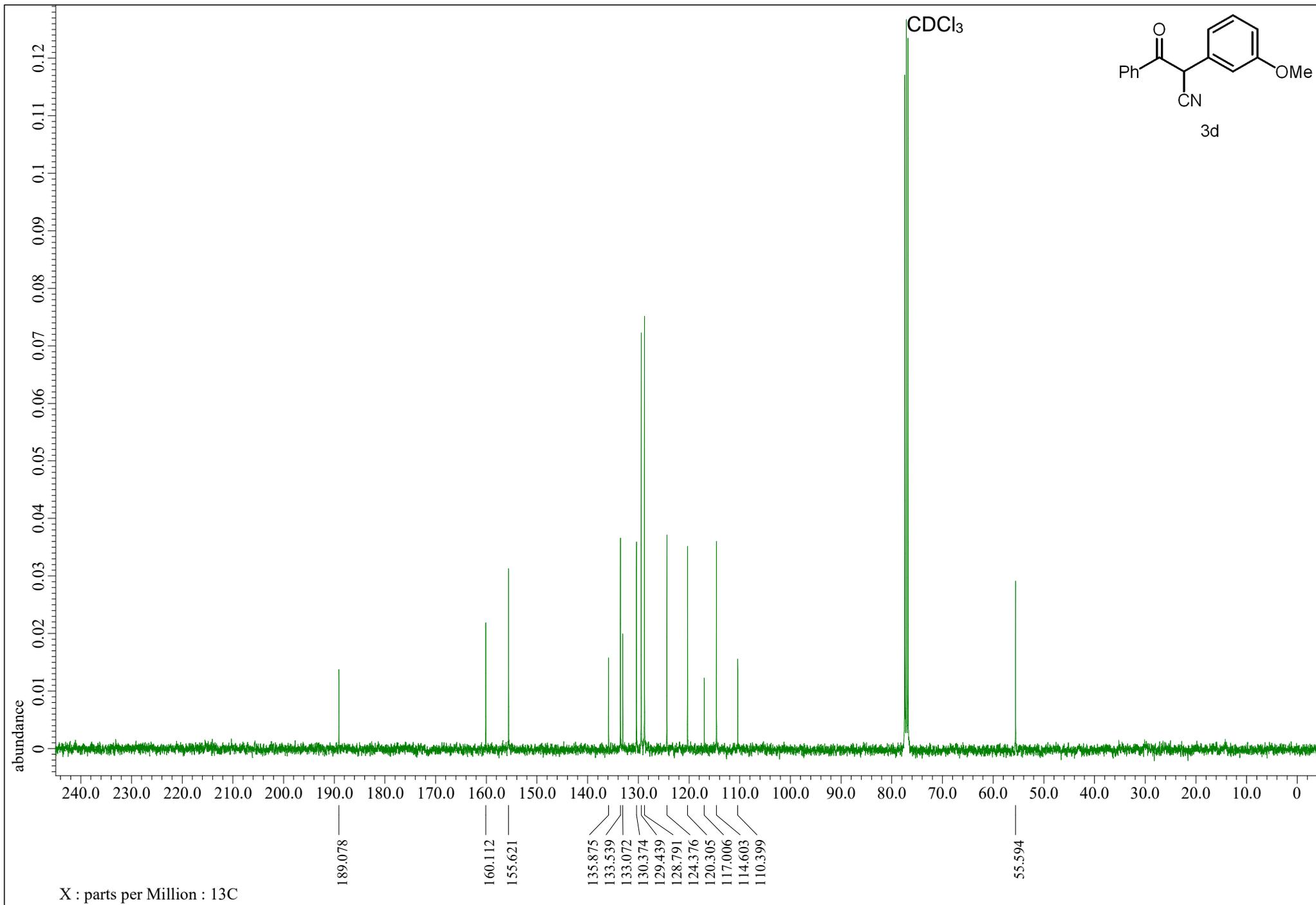
CCDC Number	2327101
Crystal data	
Chemical formula	$C_{33}H_{20}N_2O_2$
$M_r$	476.51
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	293
$a, b, c$ (Å)	10.2963 (3), 10.8281 (3), 13.1188 (4)
$\alpha, \beta, \gamma$ (°)	68.569 (3), 70.093 (3), 67.089 (3)
$V$ (Å <sup>3</sup> )	1220.09 (7)
$Z$	2
$F(000)$	496
$D_x$ (Mg m <sup>-3</sup> )	1.297
Radiation type	Cu $K\alpha$
No. of reflections for cell measurement	16448
$\theta$ range (°) for cell measurement	4.6–76.1
$\mu$ (mm <sup>-1</sup> )	0.65
Crystal shape	Plate
Colour	Yellow
Crystal size (mm)	0.36 × 0.32 × 0.19
Data collection	
Diffractometer	SuperNova, Dual, Cu at home/near, AtlasS2
Radiation source	micro-focus sealed X-ray tube, SuperNova (Cu) X-ray Source
Monochromator	Mirror
Detector resolution (pixels mm <sup>-1</sup> )	5.2529
Scan method	$\omega$ scans

Absorption correction	Gaussian <i>CrysAlis PRO</i> 1.171.42.49 (Rigaku Oxford Diffraction, 2022) Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
$T_{\min}$ , $T_{\max}$	0.348, 1.000
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	25669, 5103, 4787
$R_{\text{int}}$	0.018
$\theta$ values ( $^{\circ}$ )	$\theta_{\max} = 76.4$ , $\theta_{\min} = 3.7$
$(\sin \theta/\lambda)_{\max}$ ( $\text{\AA}^{-1}$ )	0.630
Range of $h$ , $k$ , $l$	$h = -11 \rightarrow 12$ , $k = -13 \rightarrow 13$ , $l = -15 \rightarrow 16$
Refinement	
Refinement on	$F^2$
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , $S$	0.036, 0.098, 1.04
No. of reflections	5103
No. of parameters	335
No. of restraints	0
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F^2) + (0.0462P)^2 + 0.217P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ ( $e \text{\AA}^{-3}$ )	0.21, -0.16

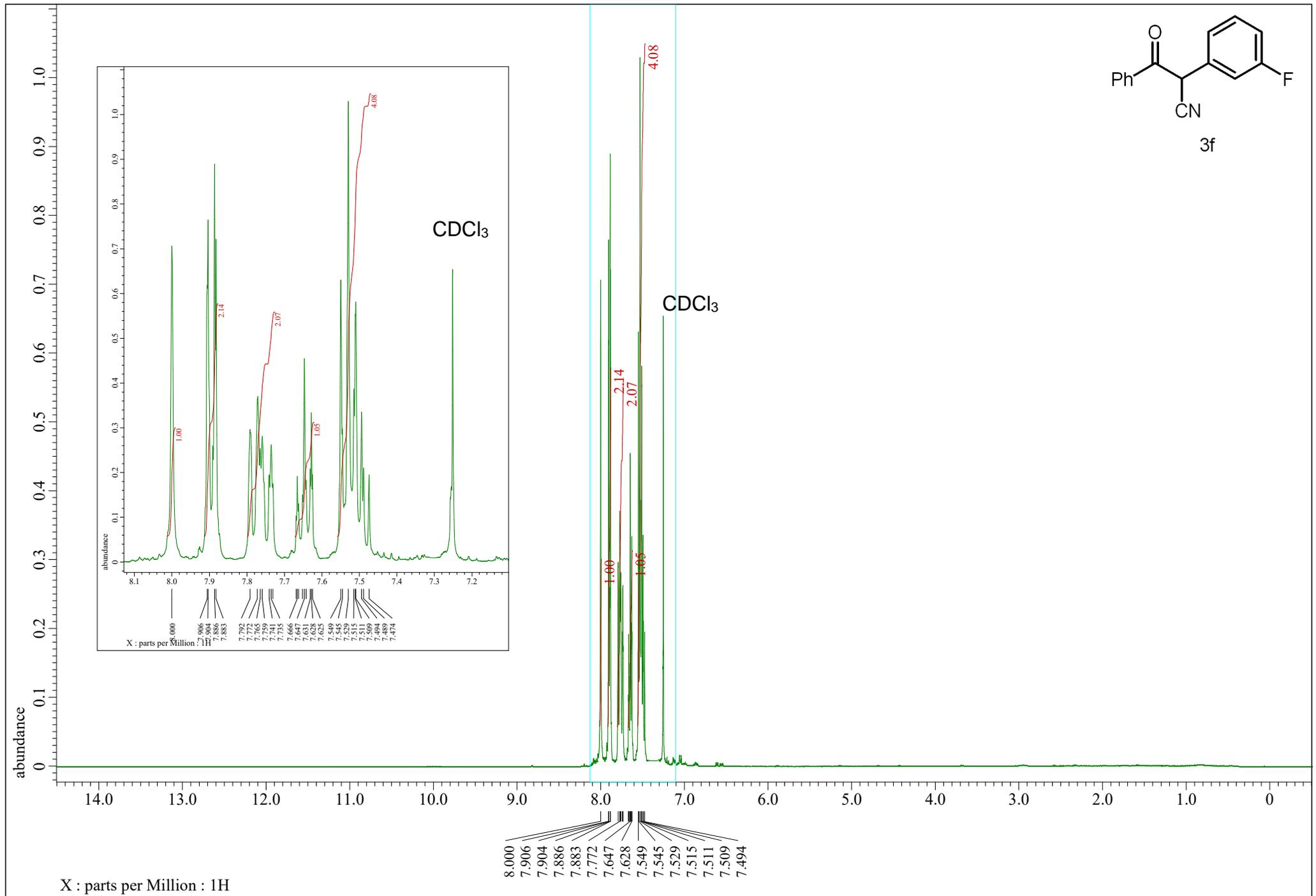
Computer programs: *CrysAlis PRO* 1.171.42.49 (Rigaku OD, 2022), *SHELXT* 2018/2 (Sheldrick, 2018), *SHELXL* 2019/2 (Sheldrick, 2015), *Olex2* 1.5 (Dolomanov *et al.*, 2009).

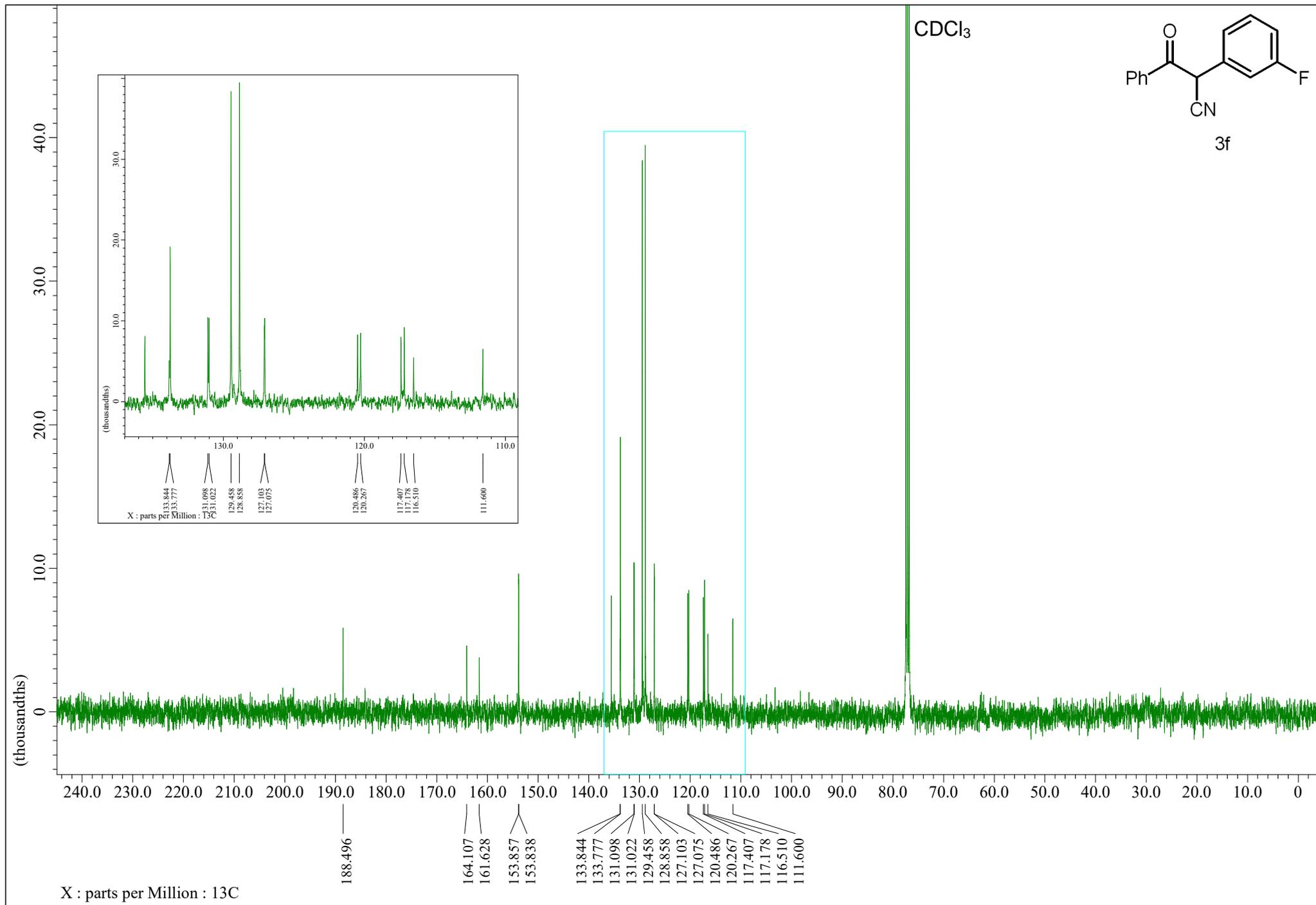
<sup>1</sup>H NMR



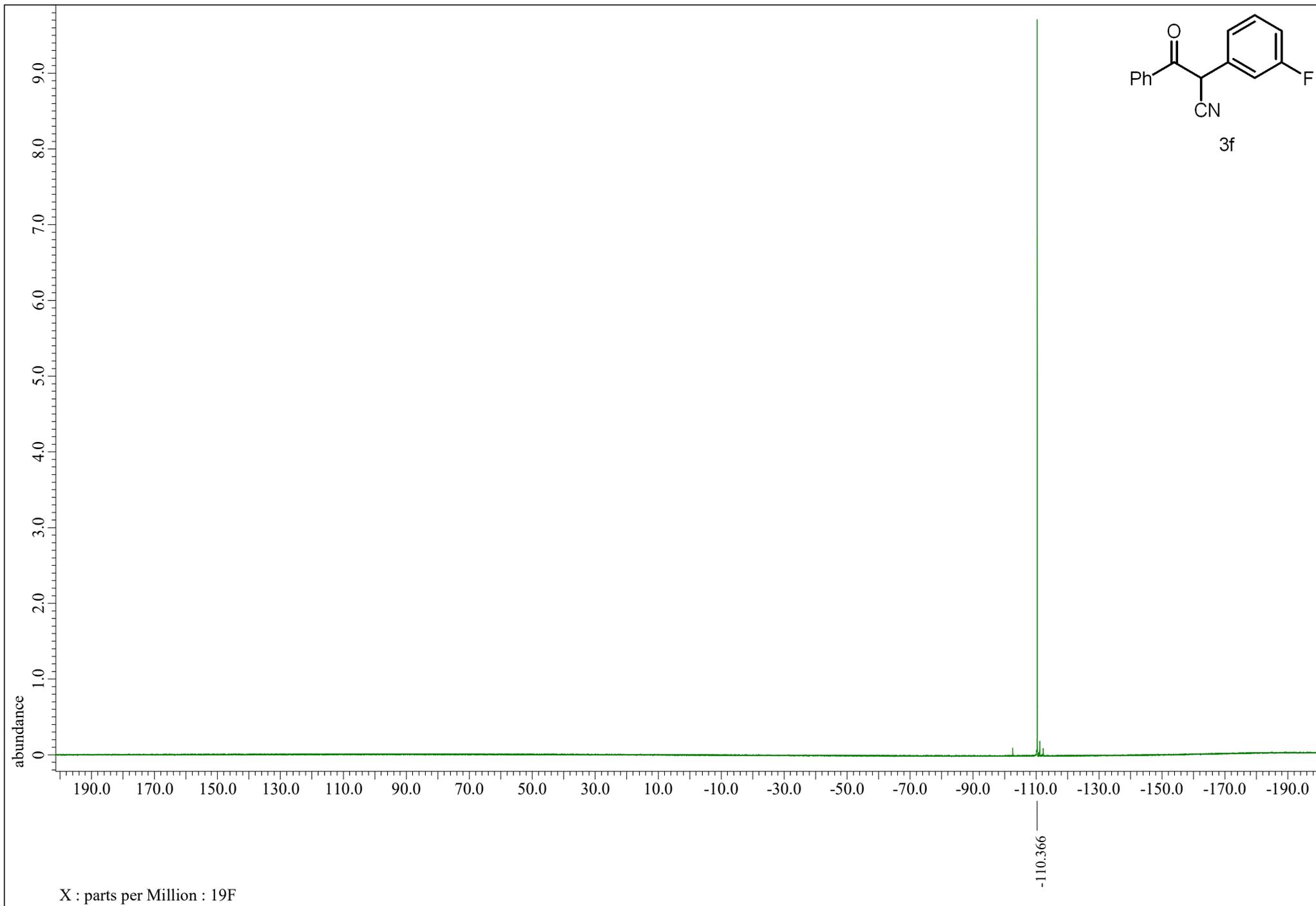


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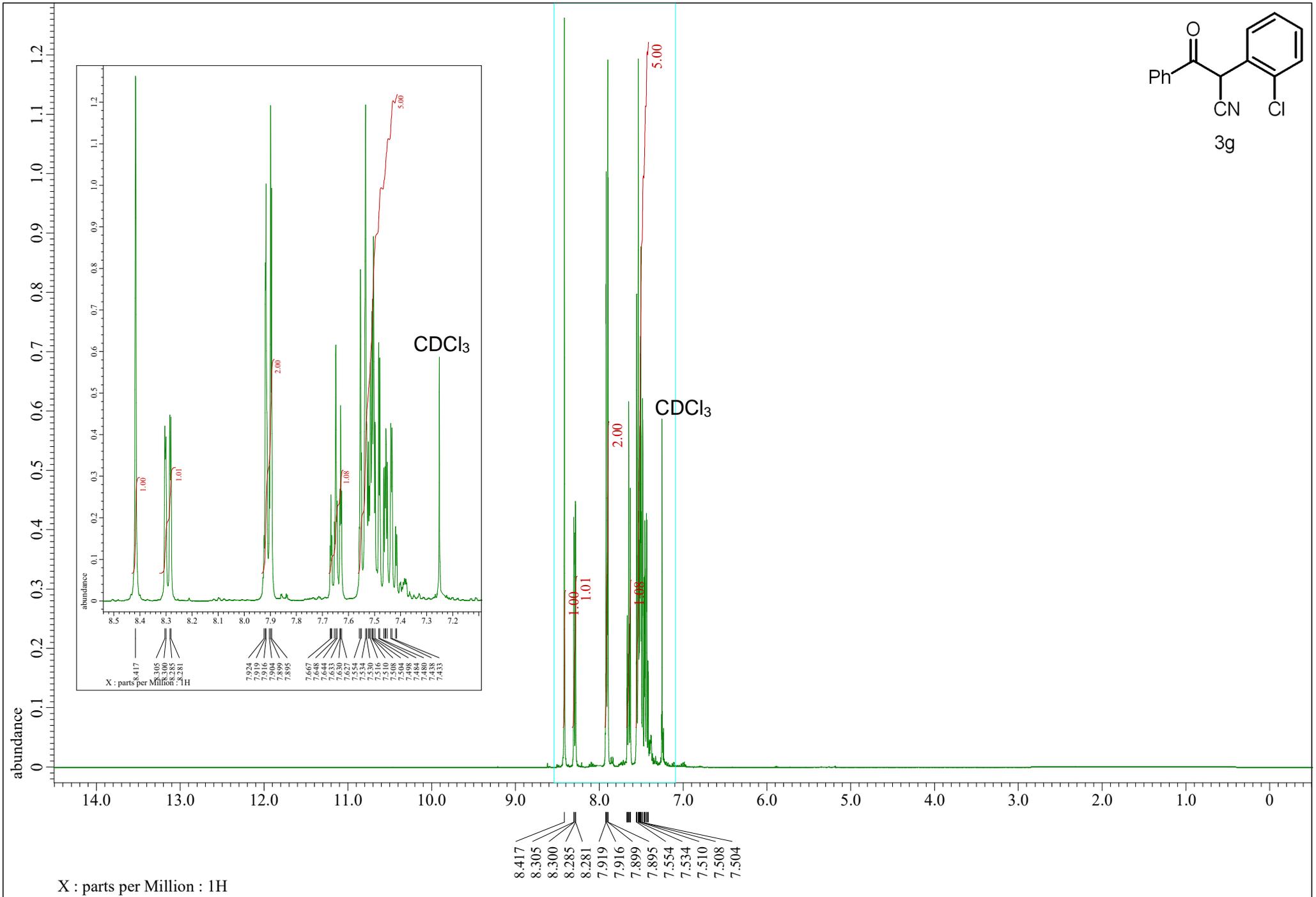




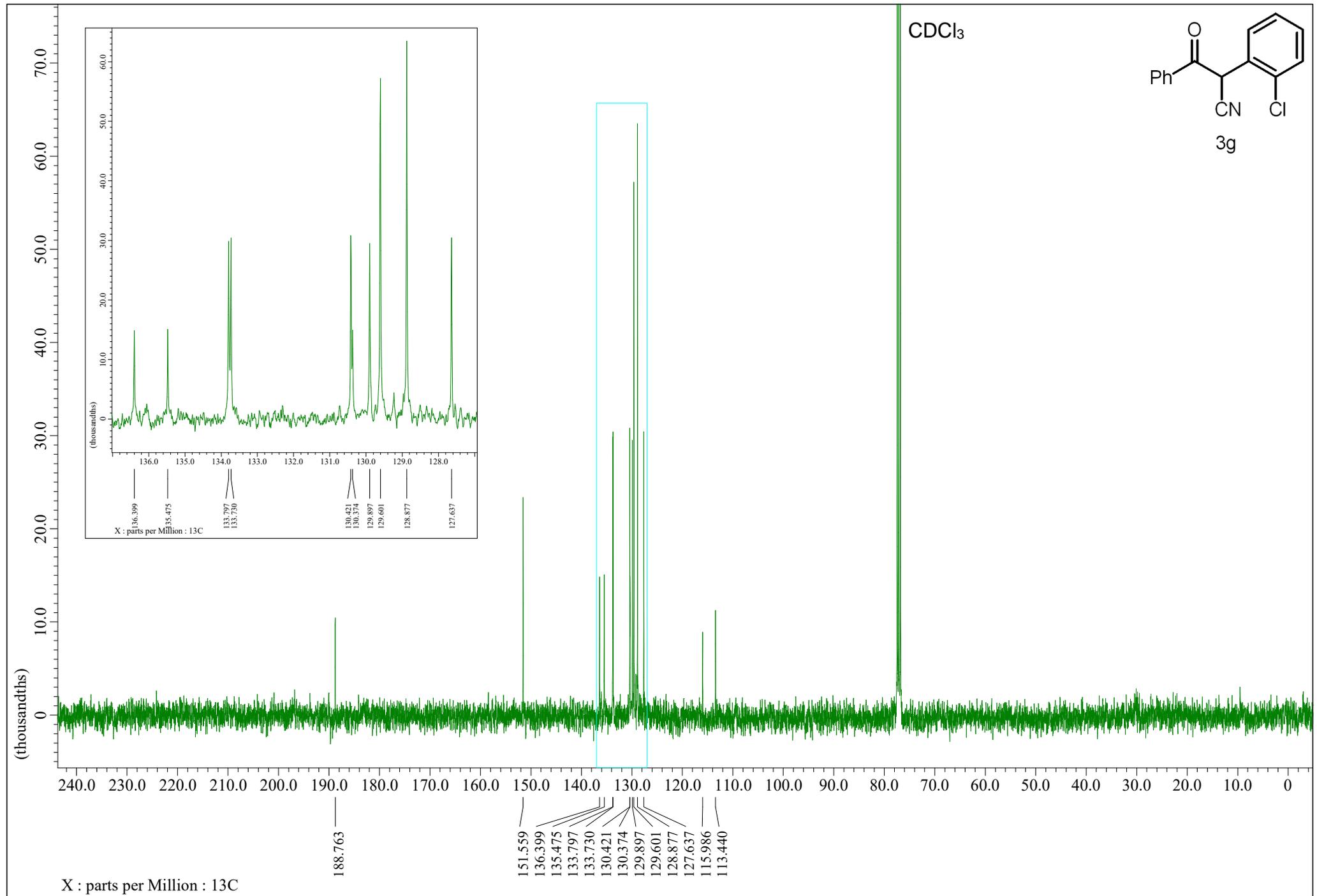
<sup>19</sup>F NMR



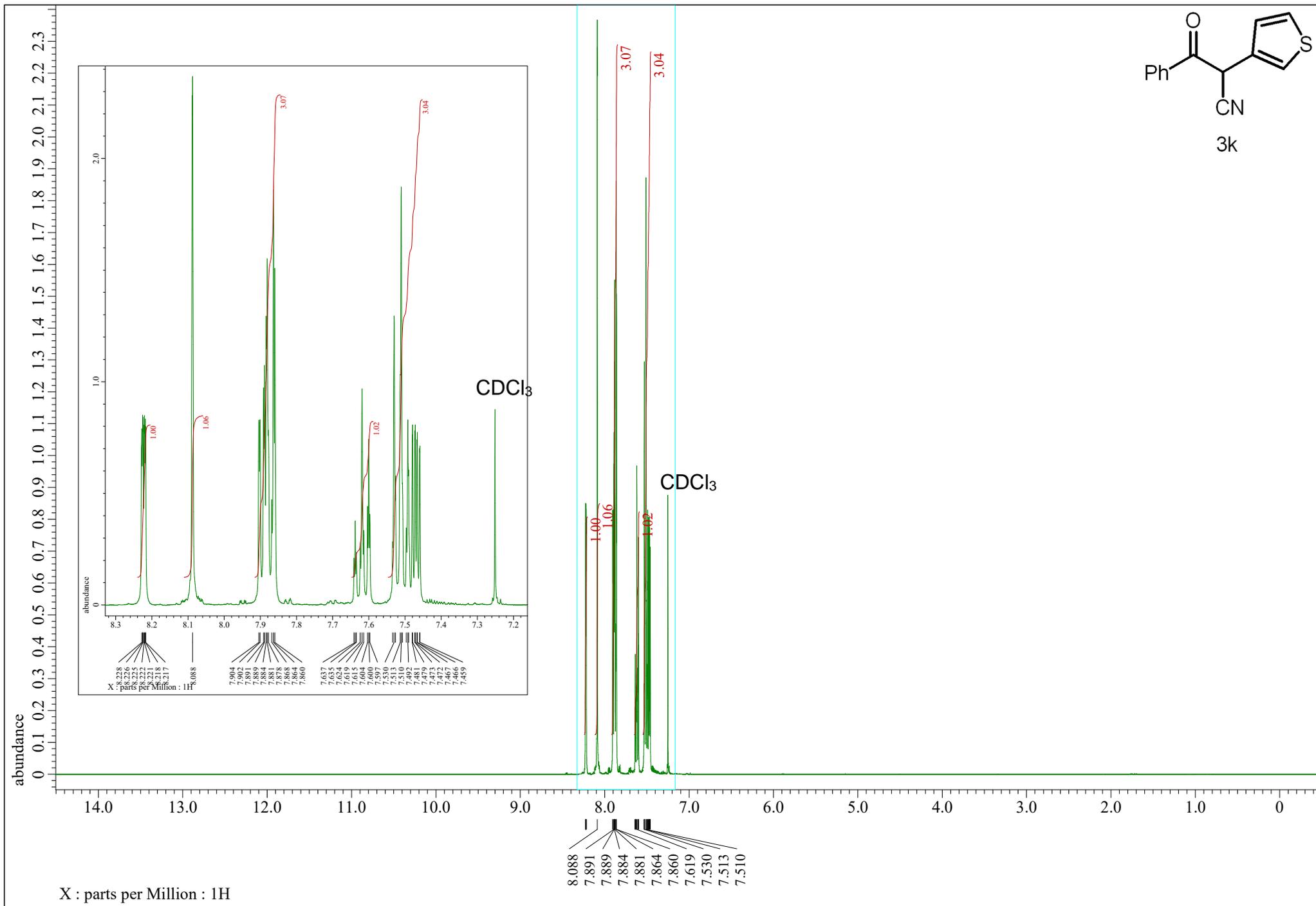
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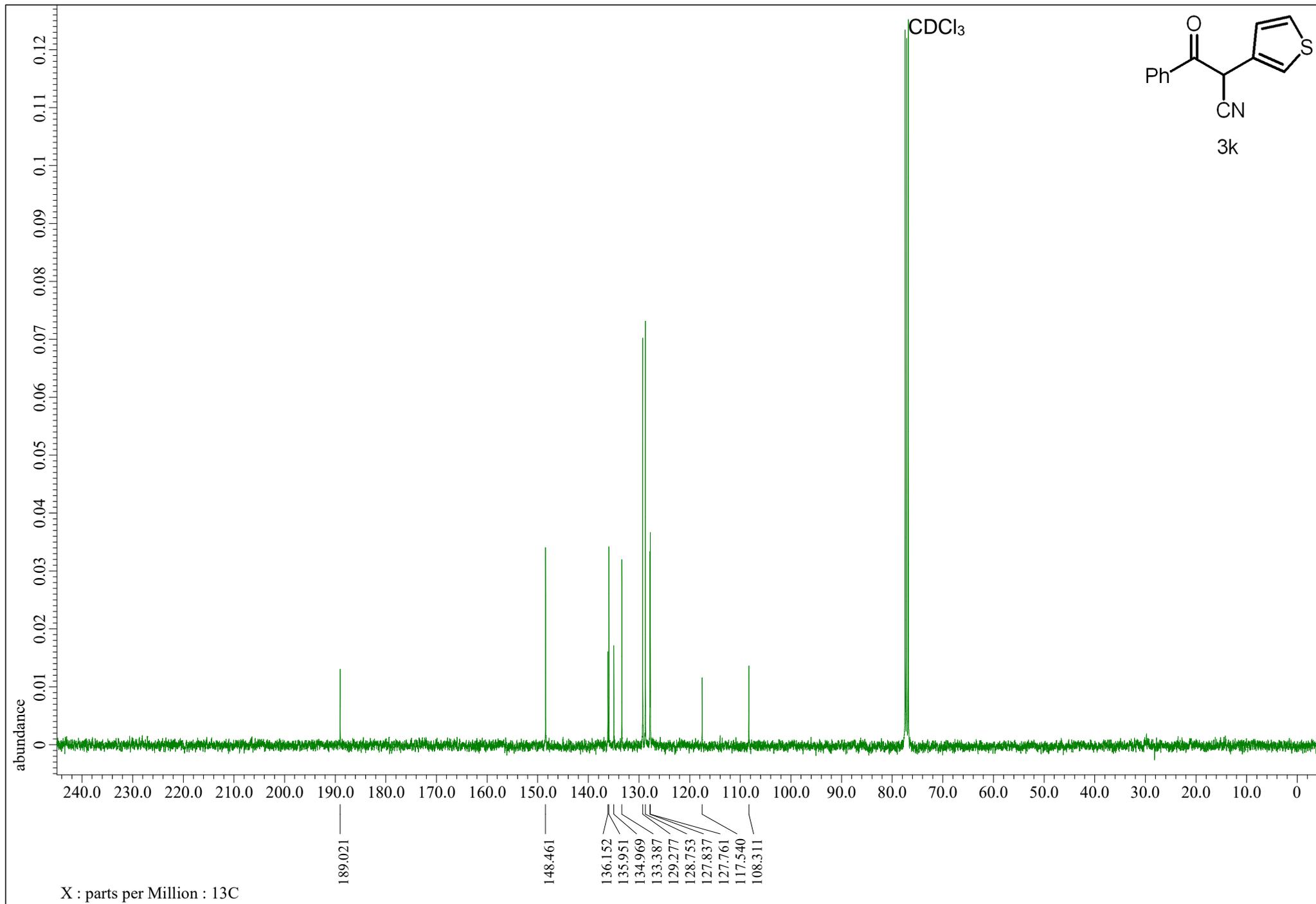


<sup>13</sup>C NMR

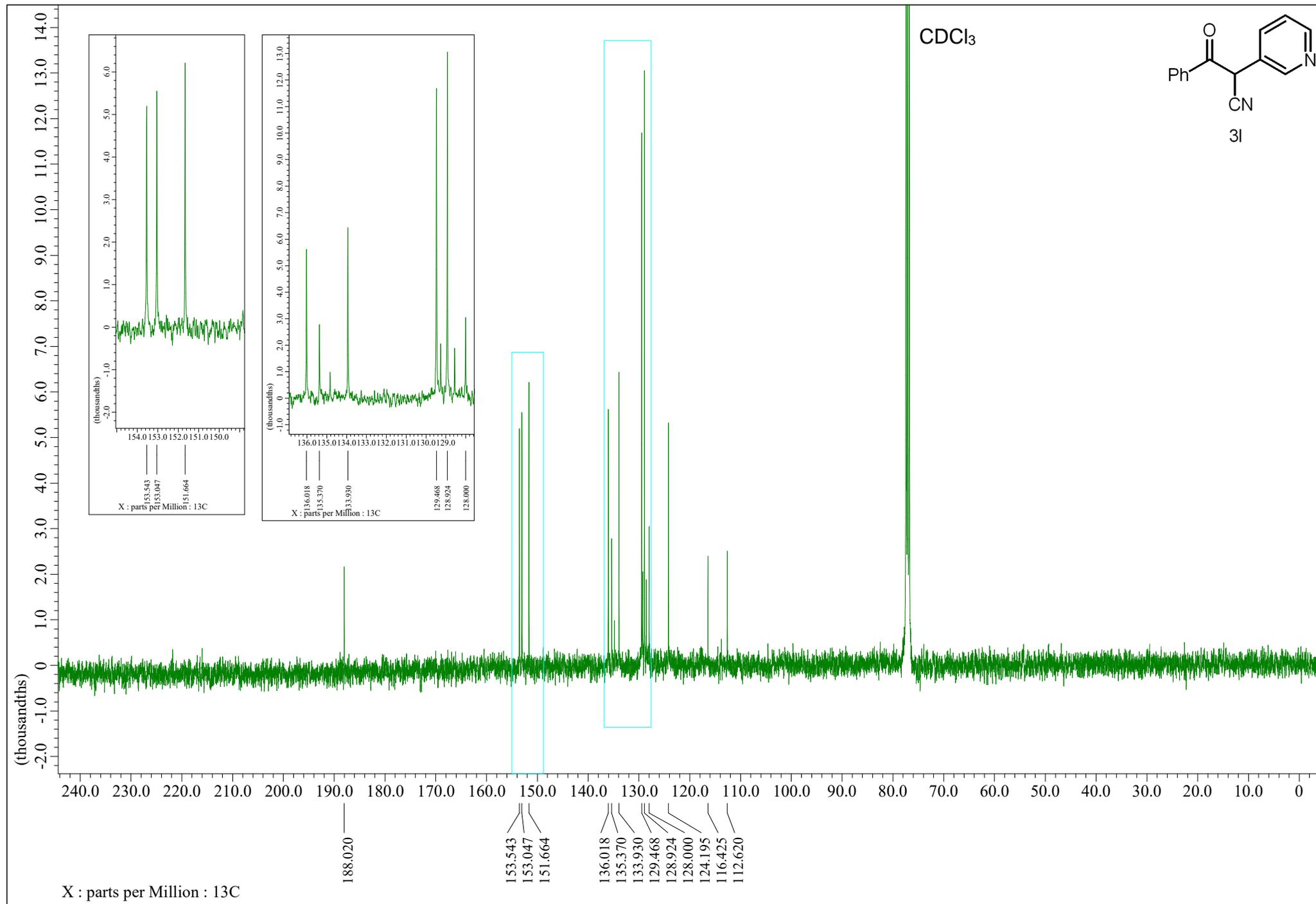


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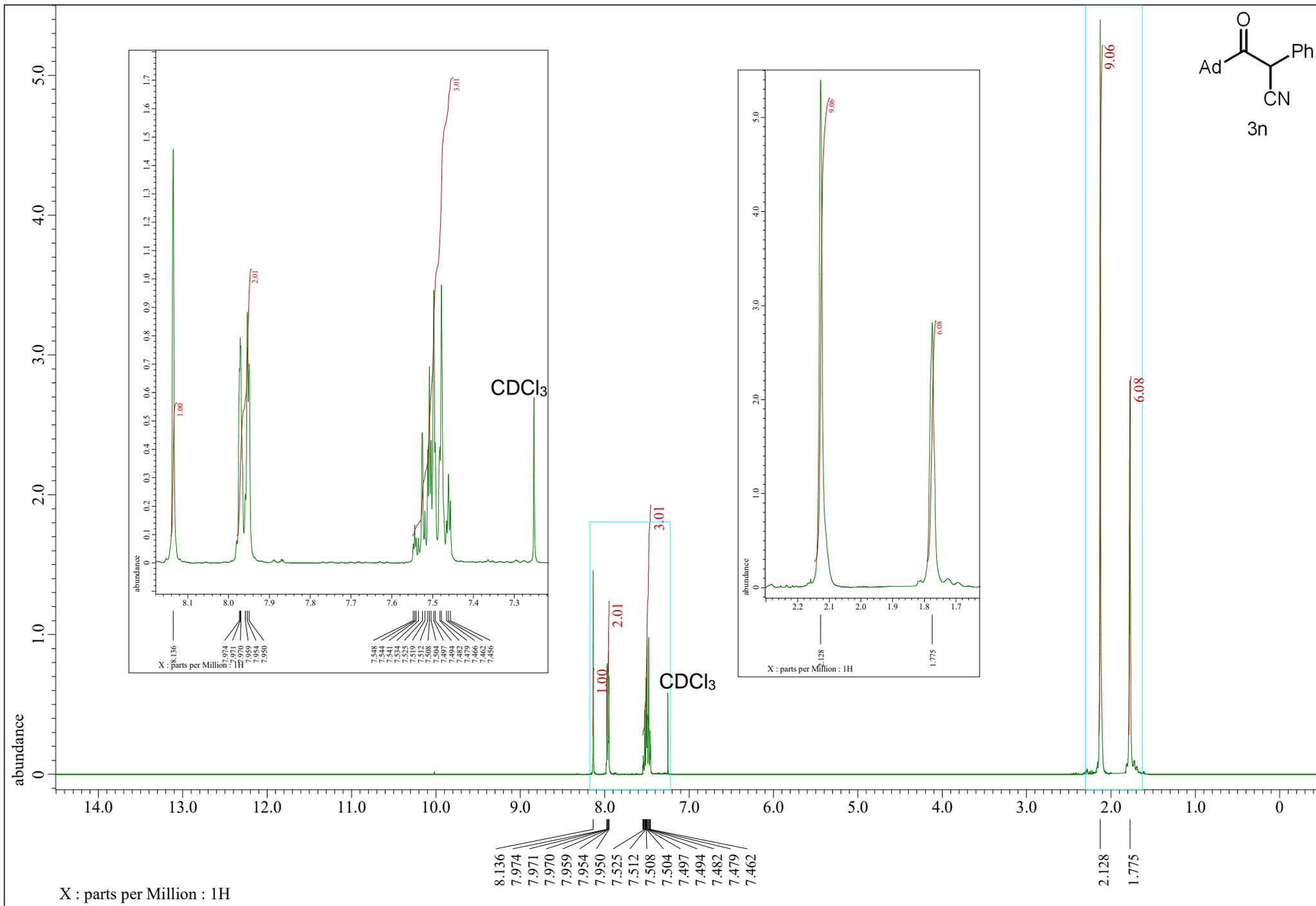


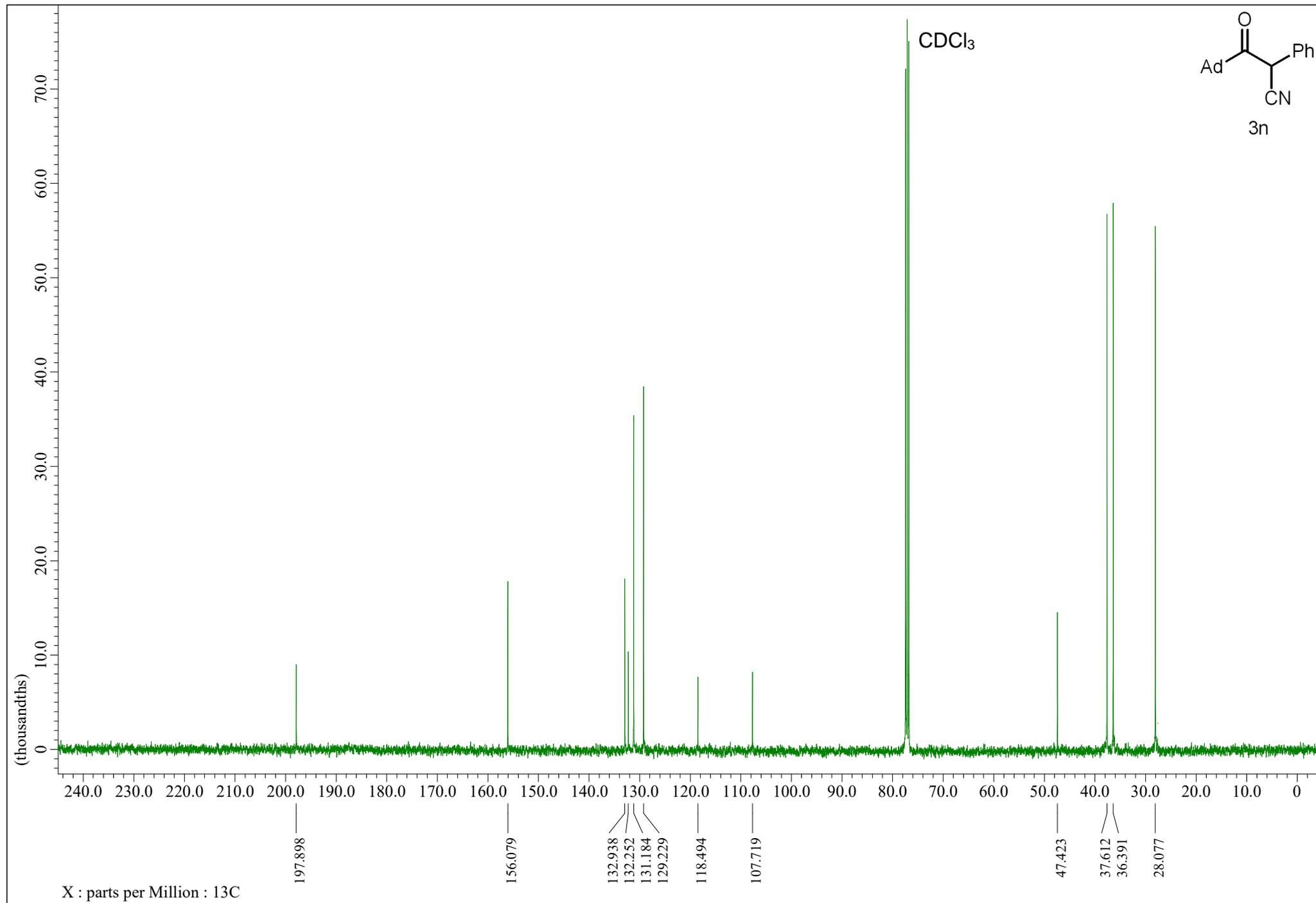




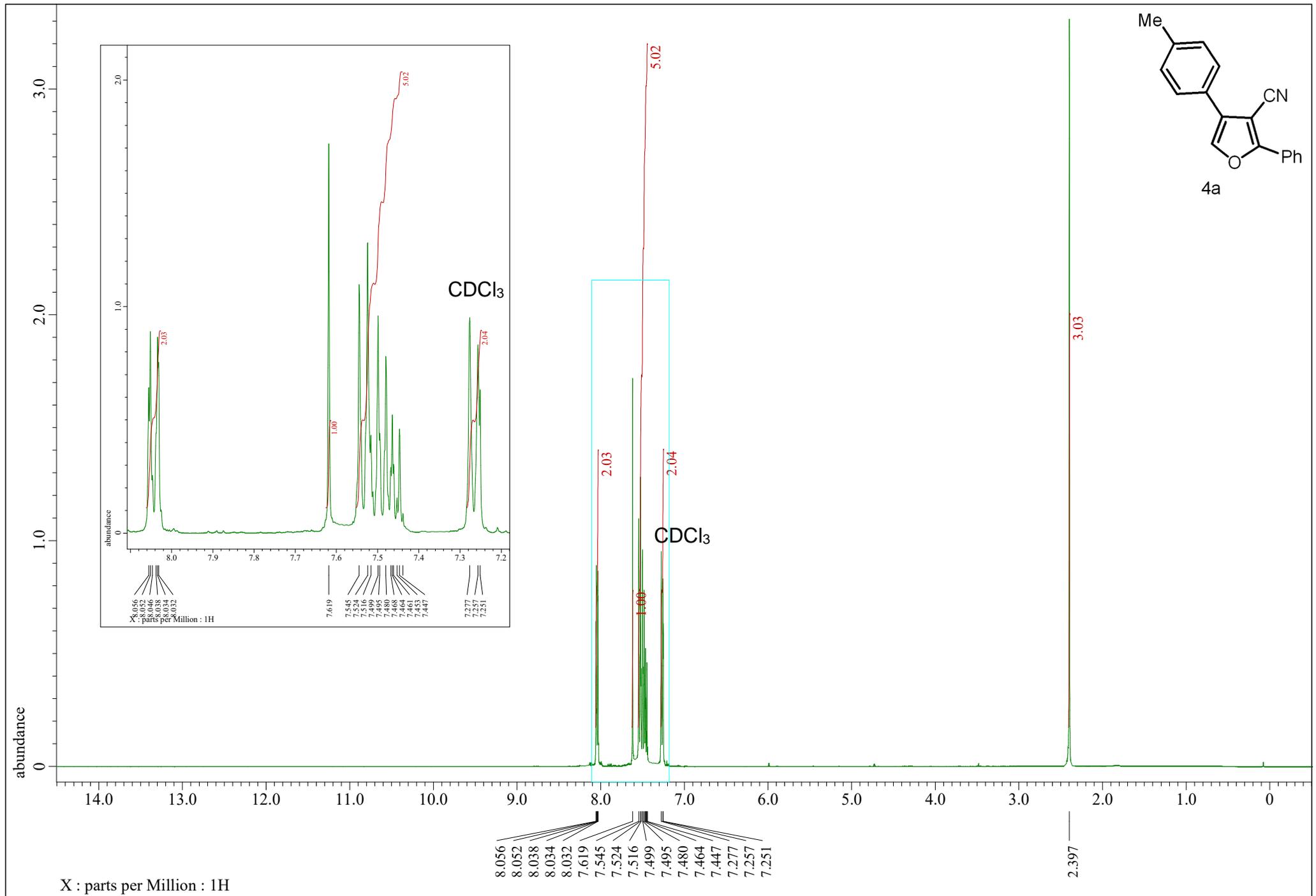


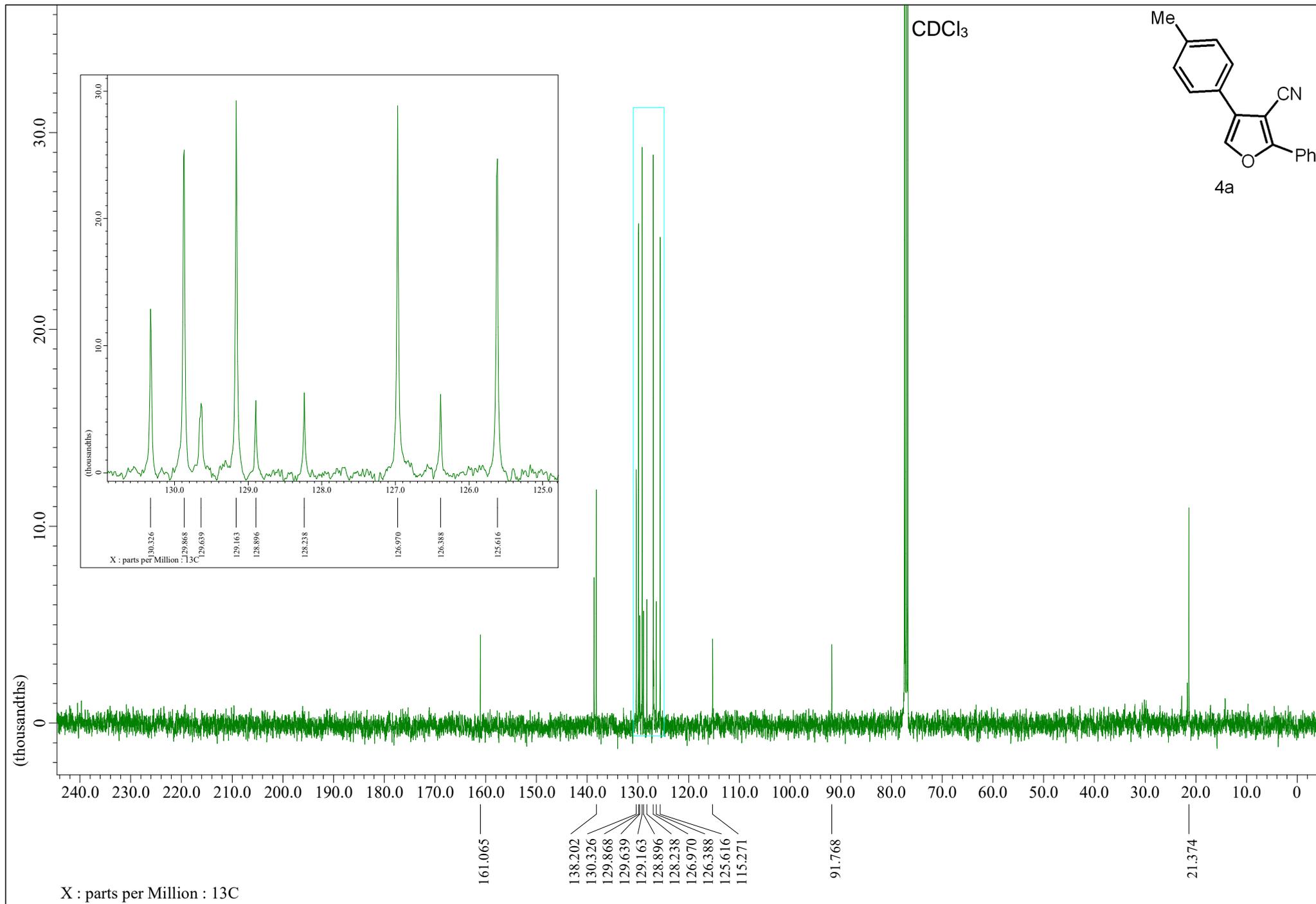
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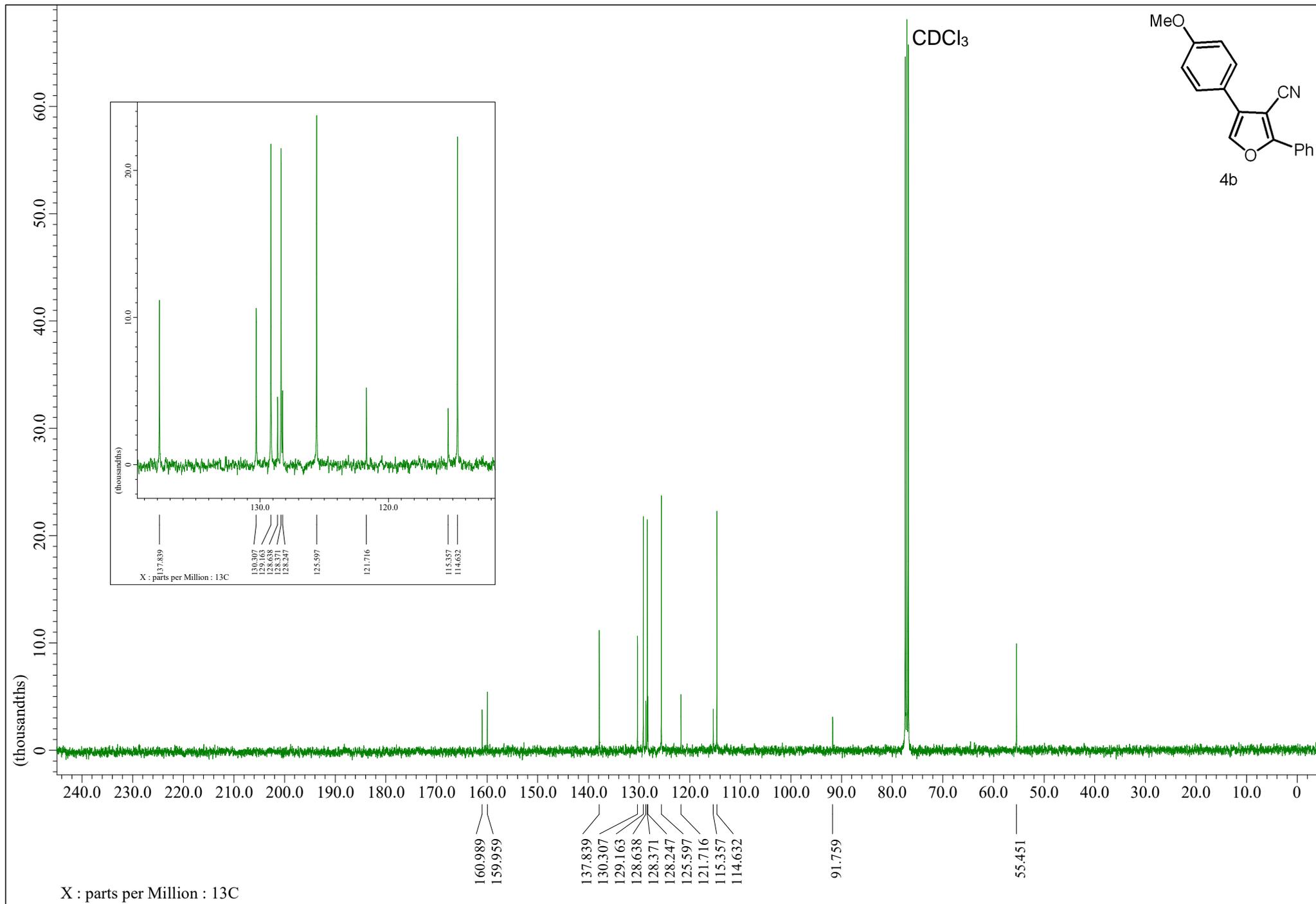


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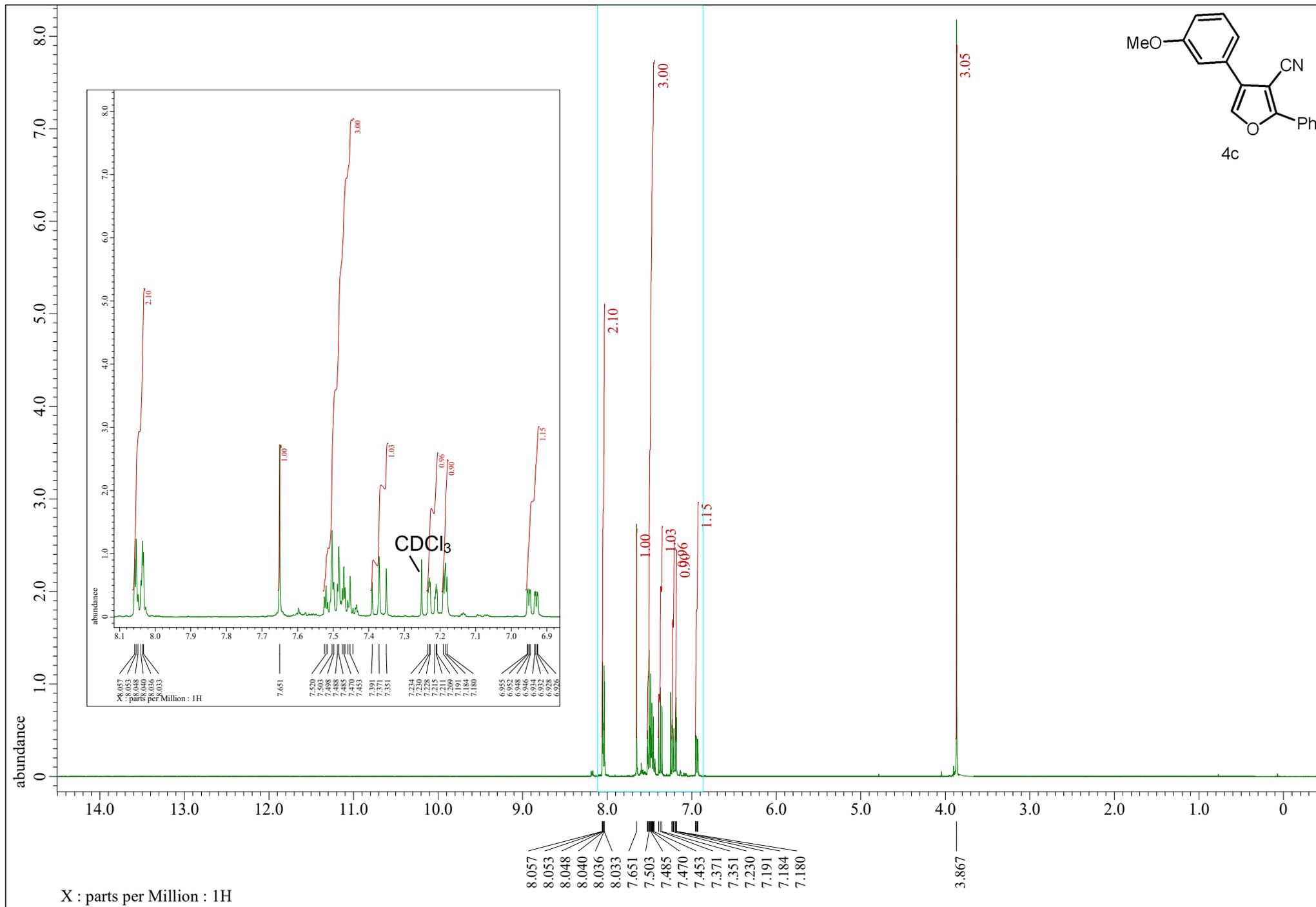


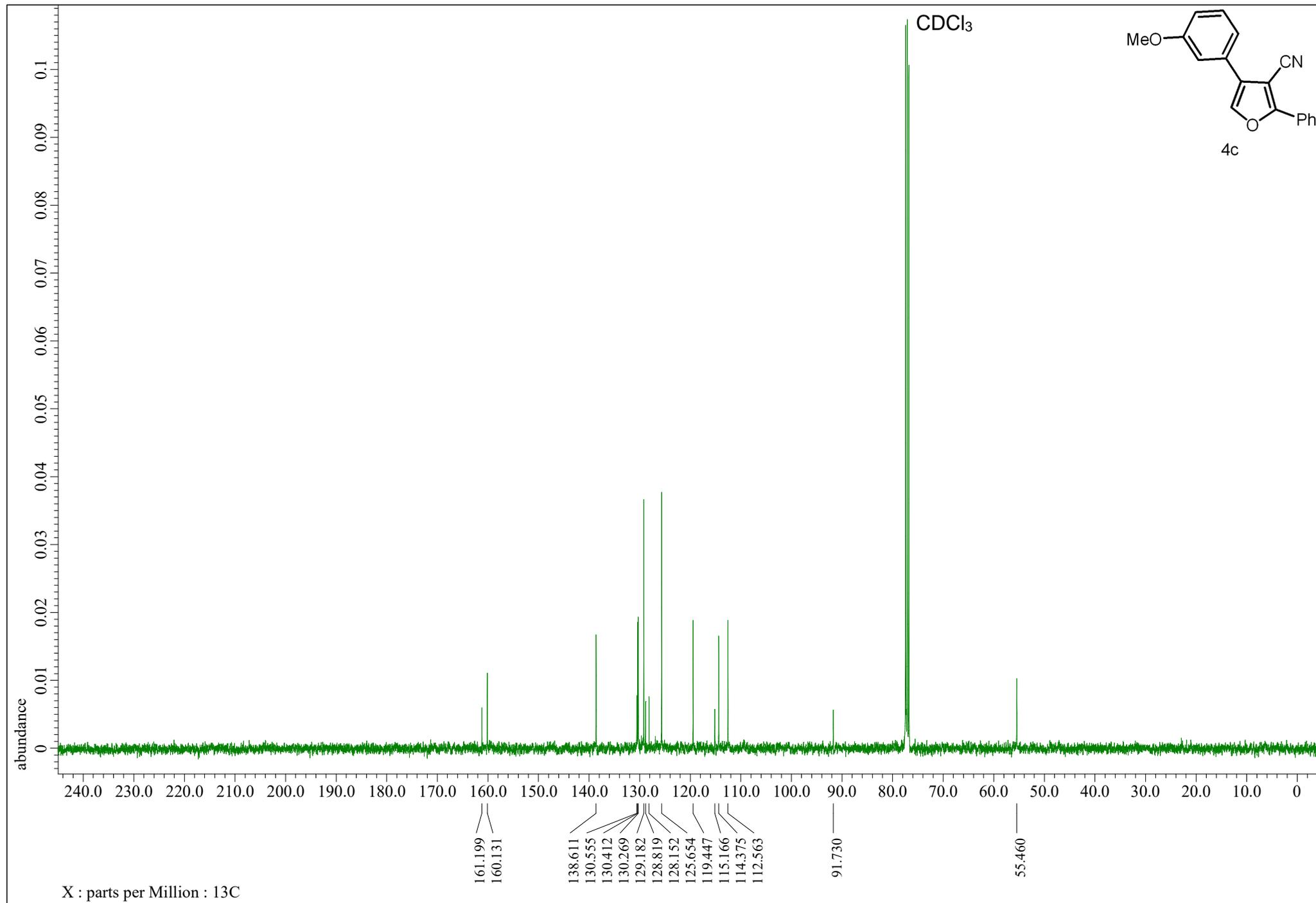




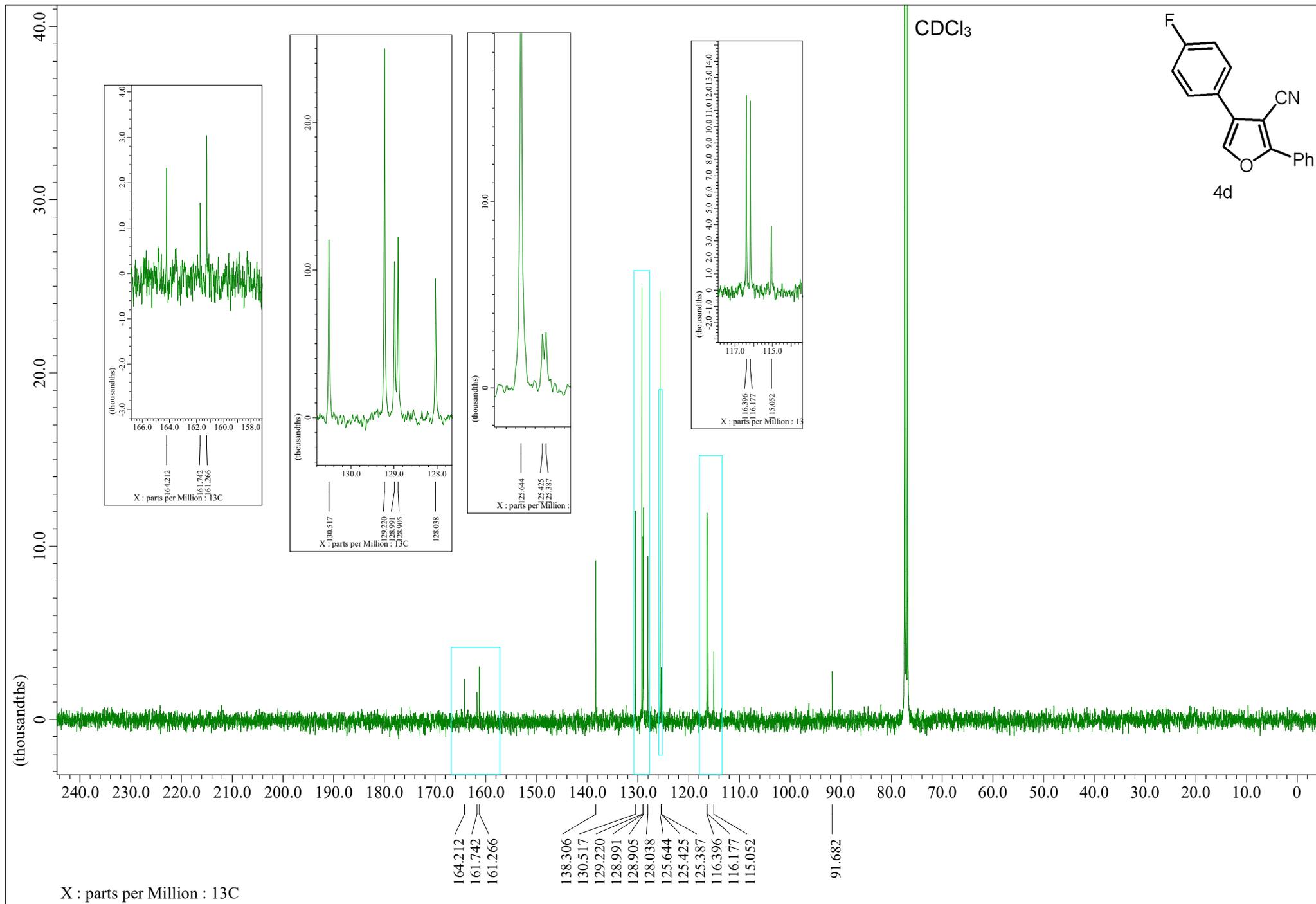


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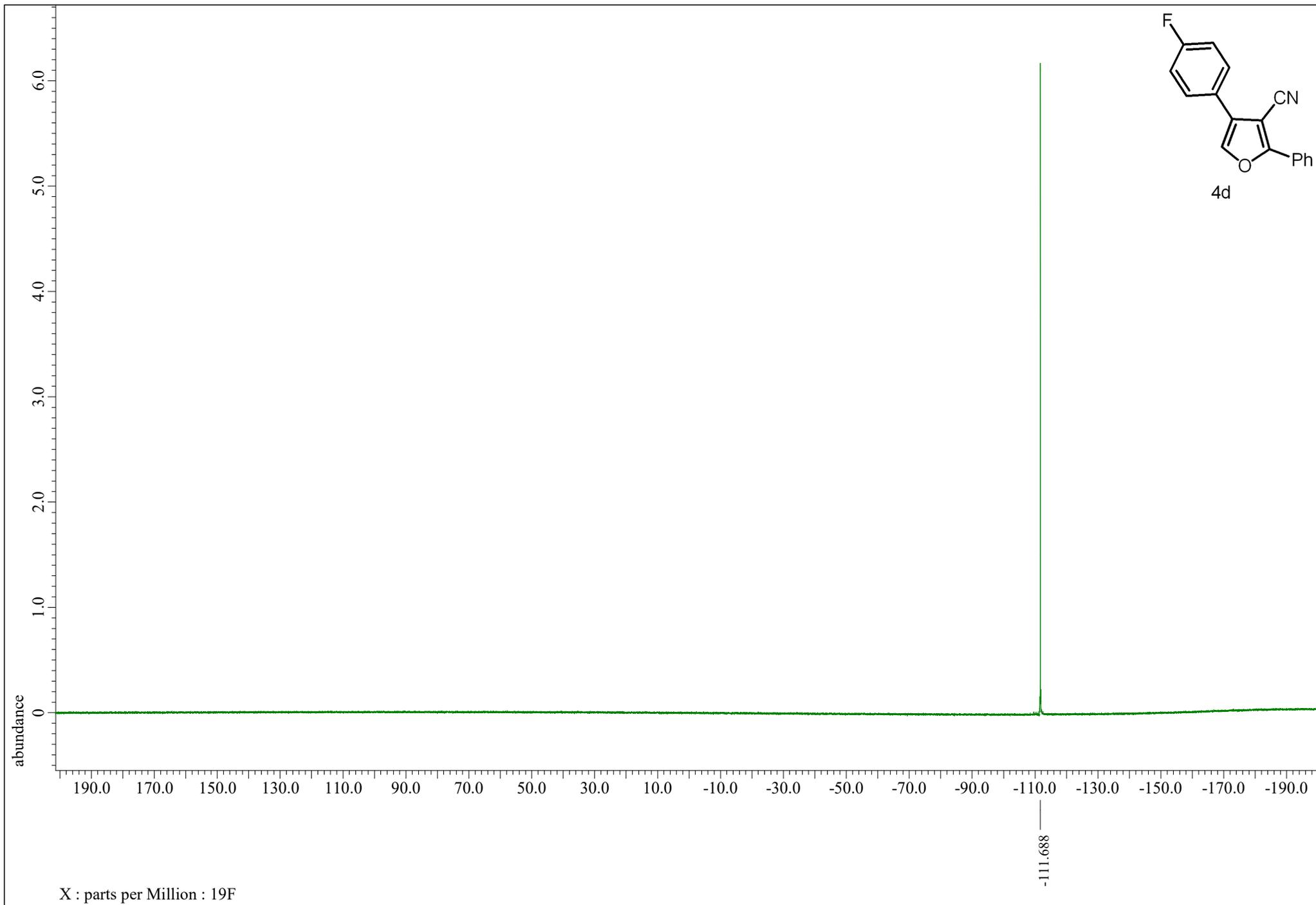




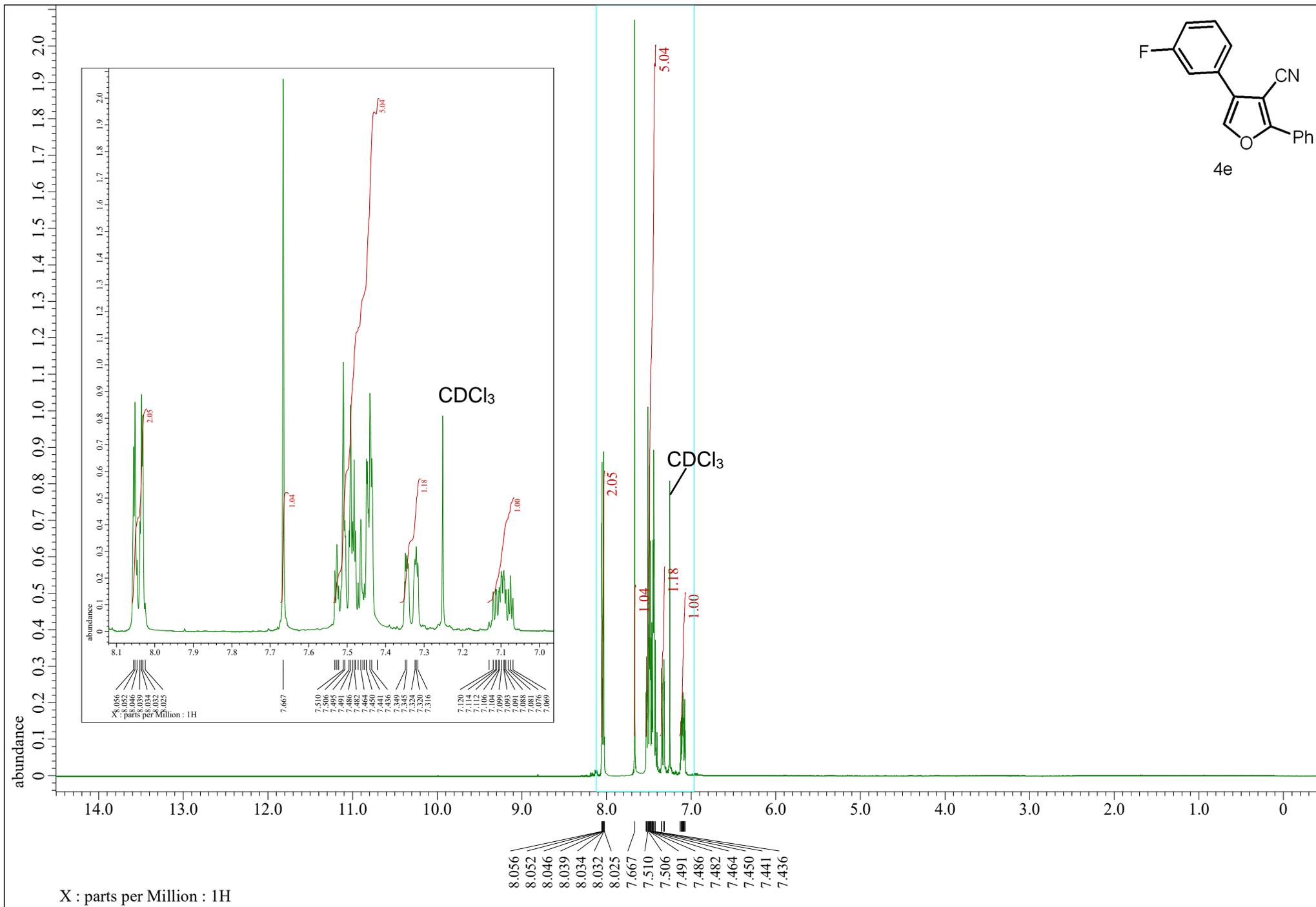




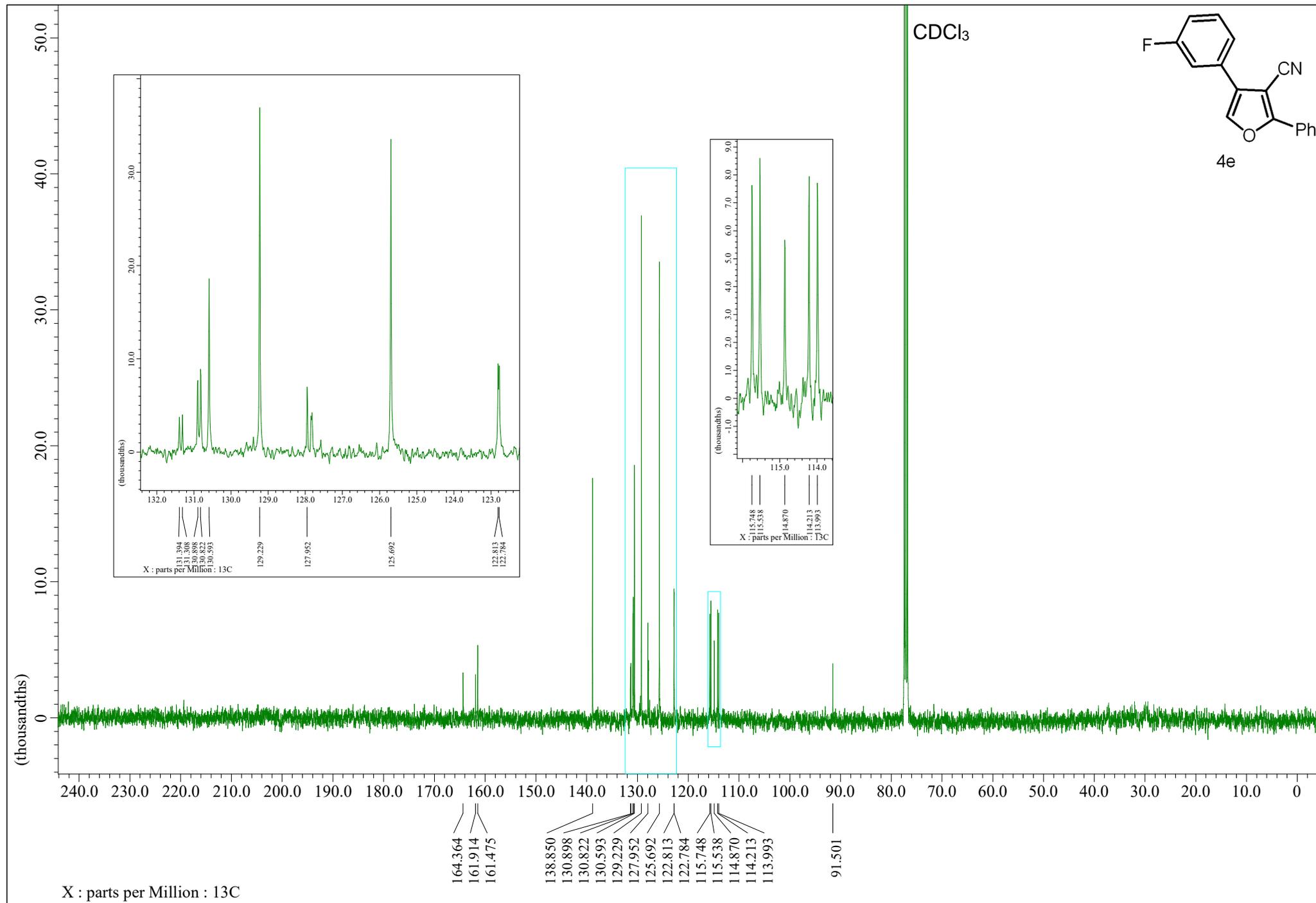
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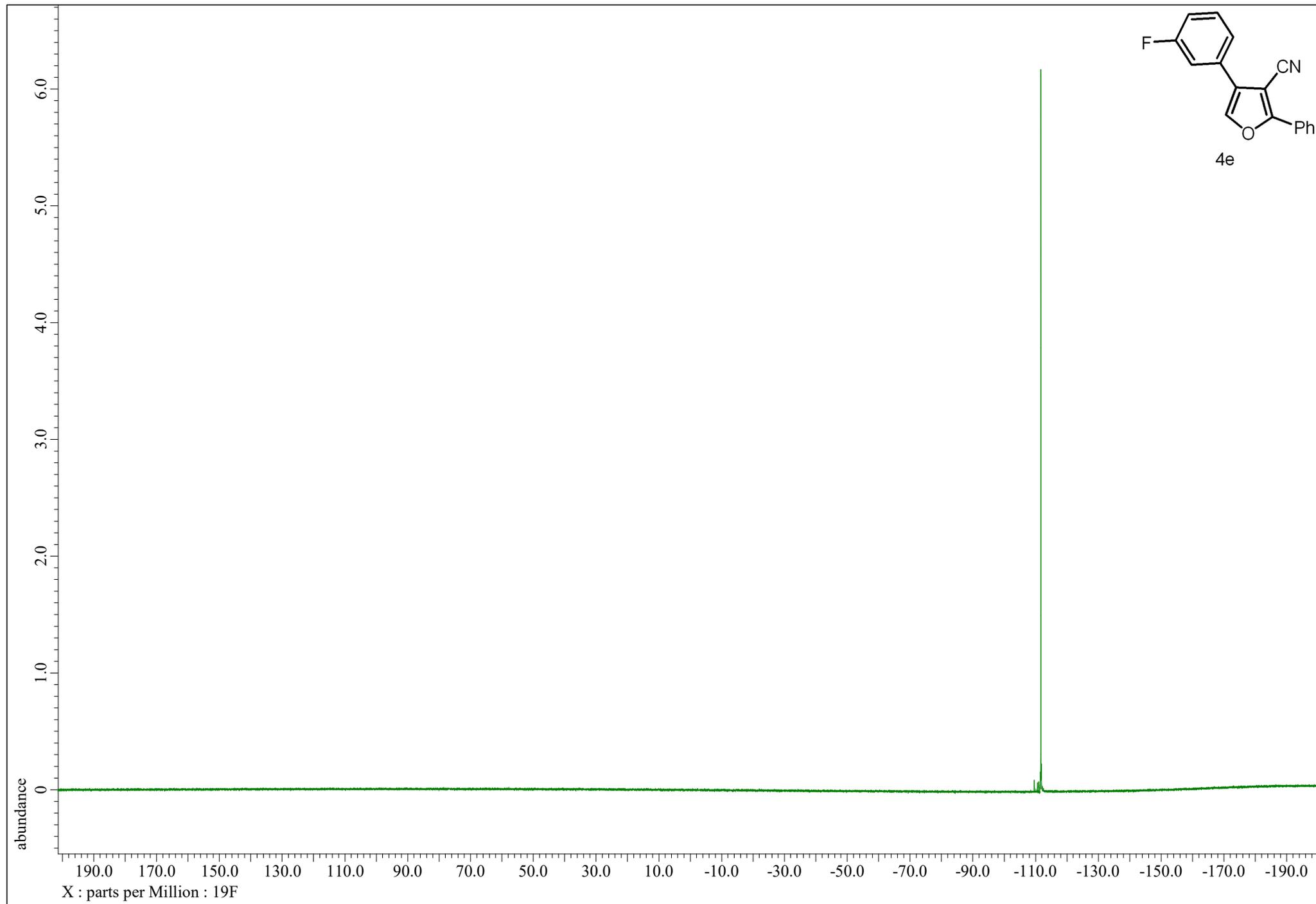
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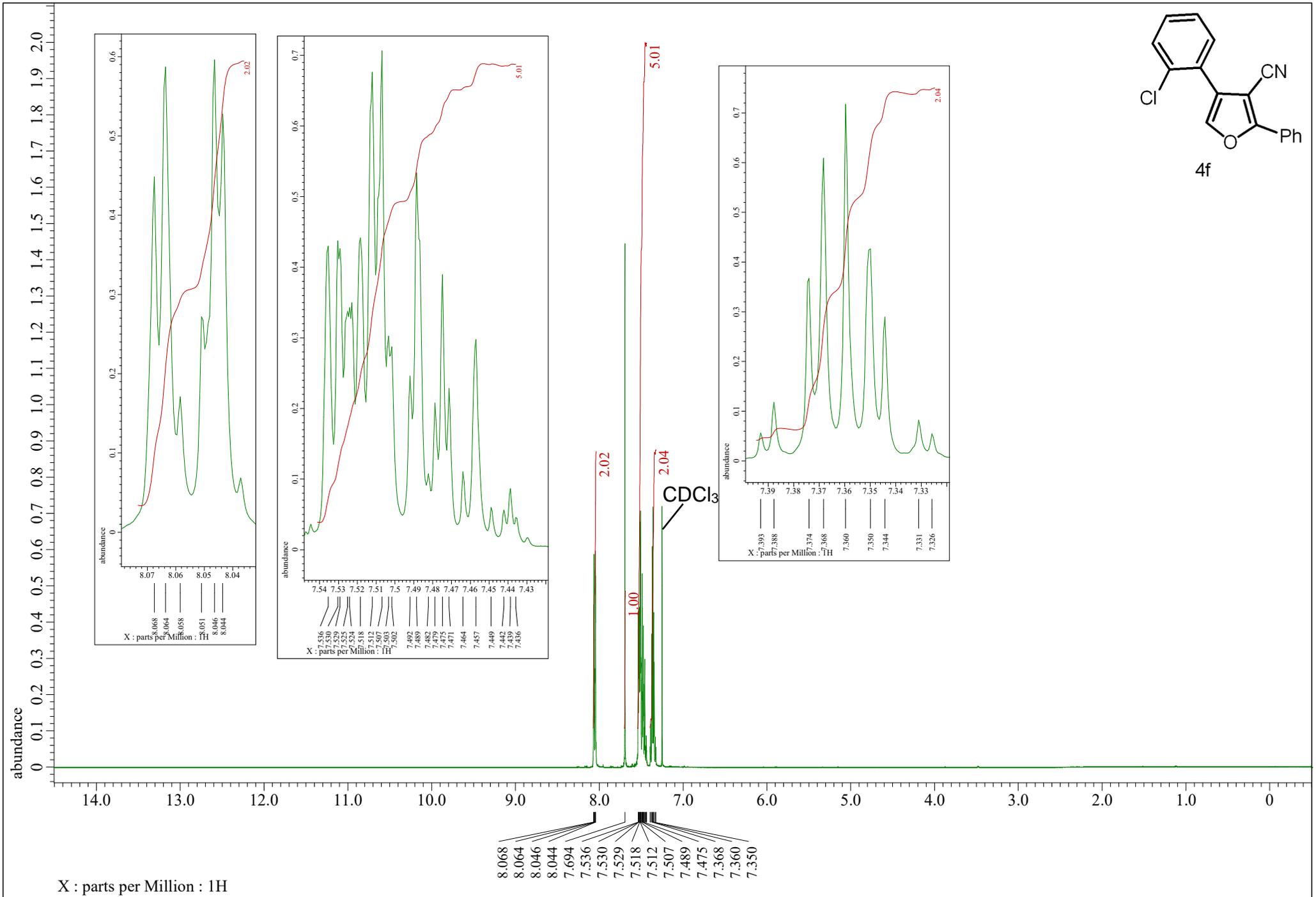
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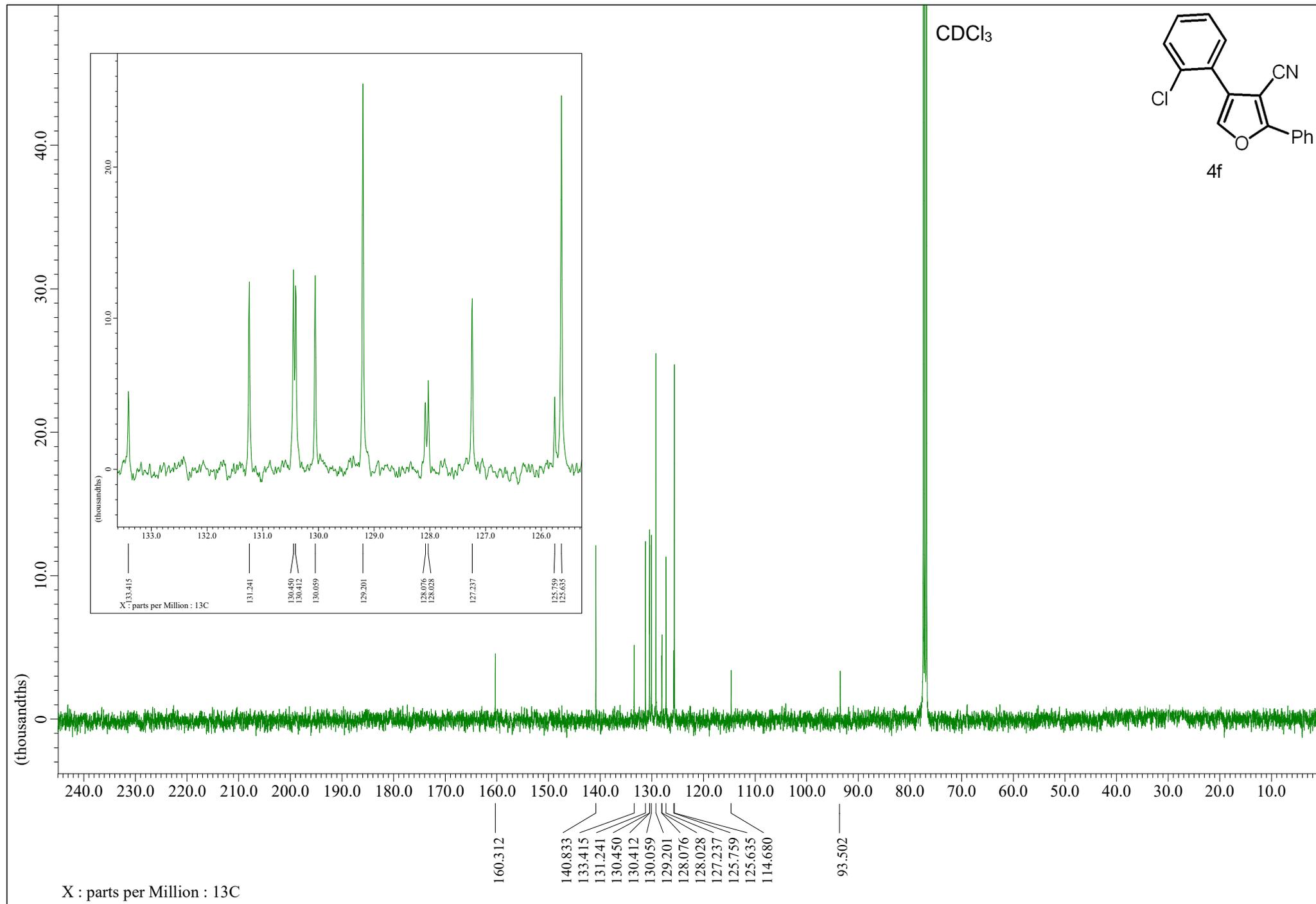


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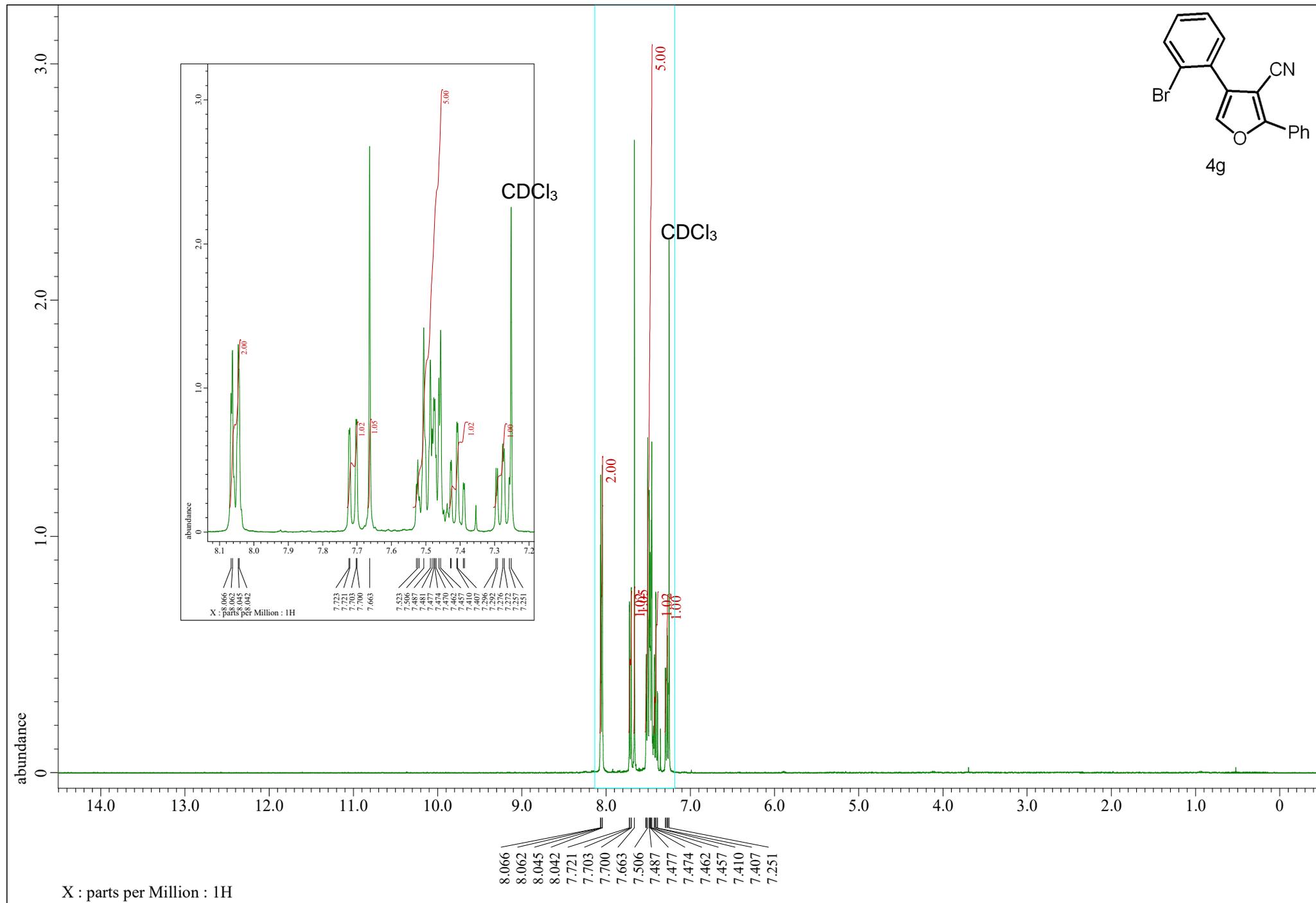


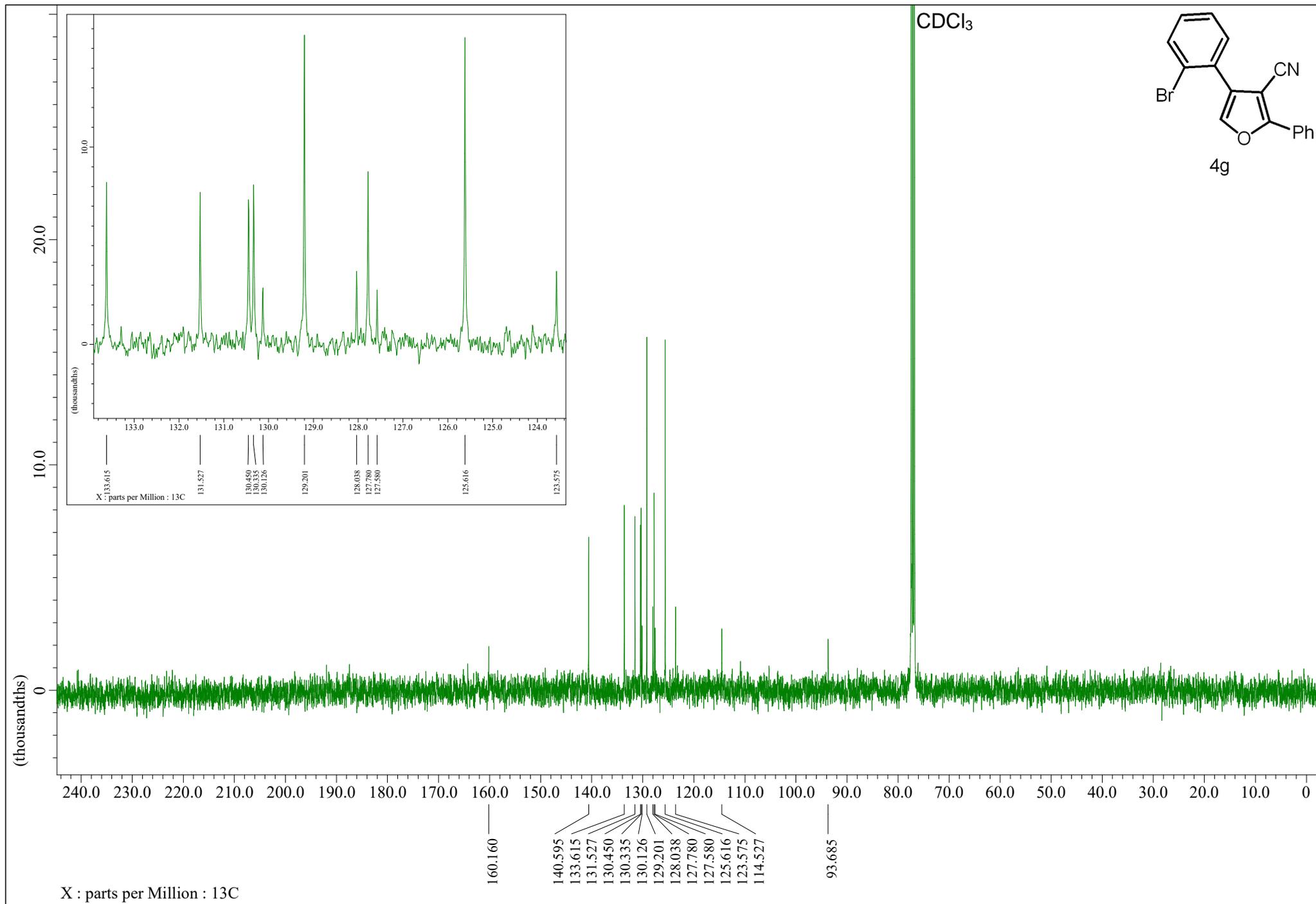
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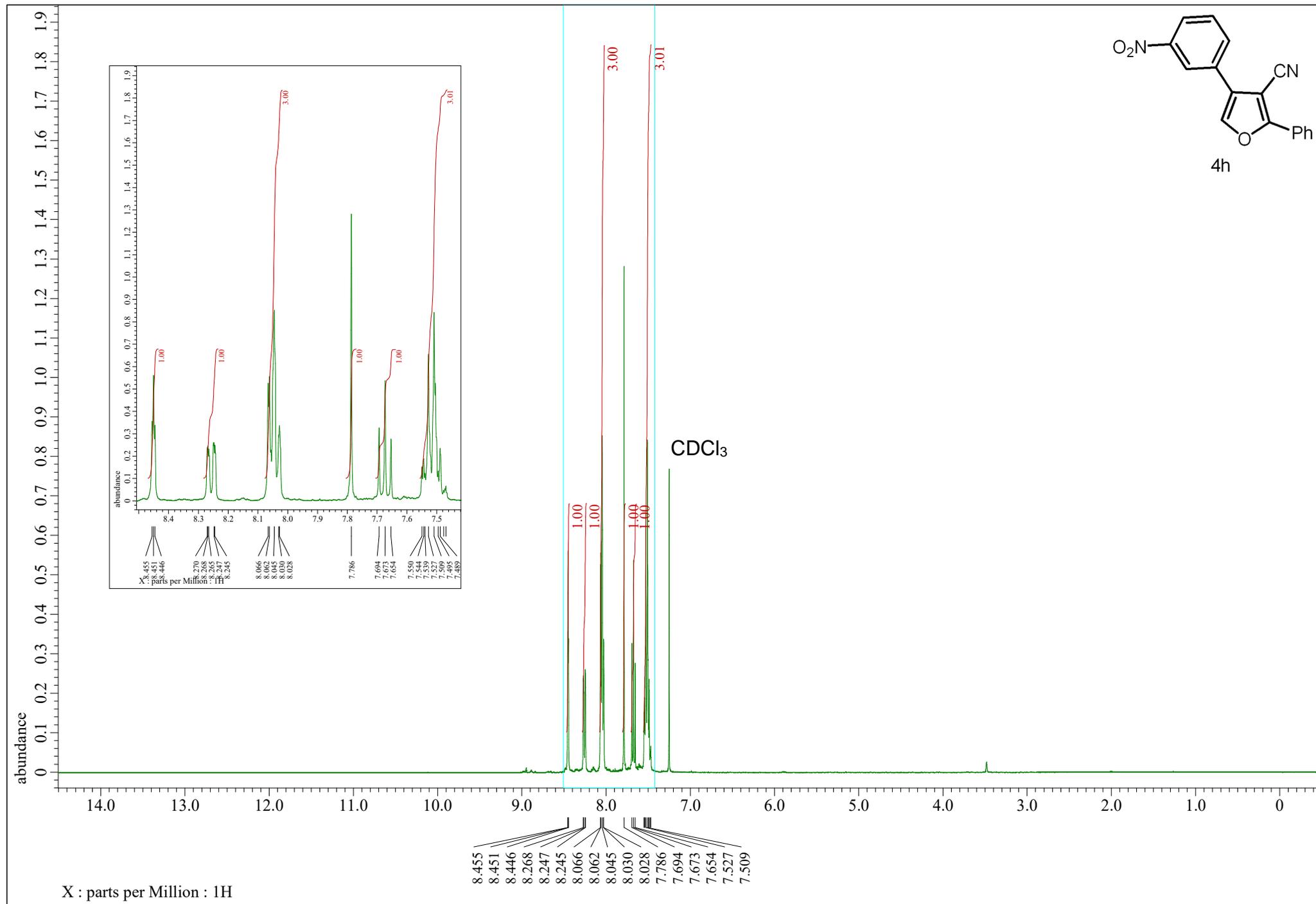


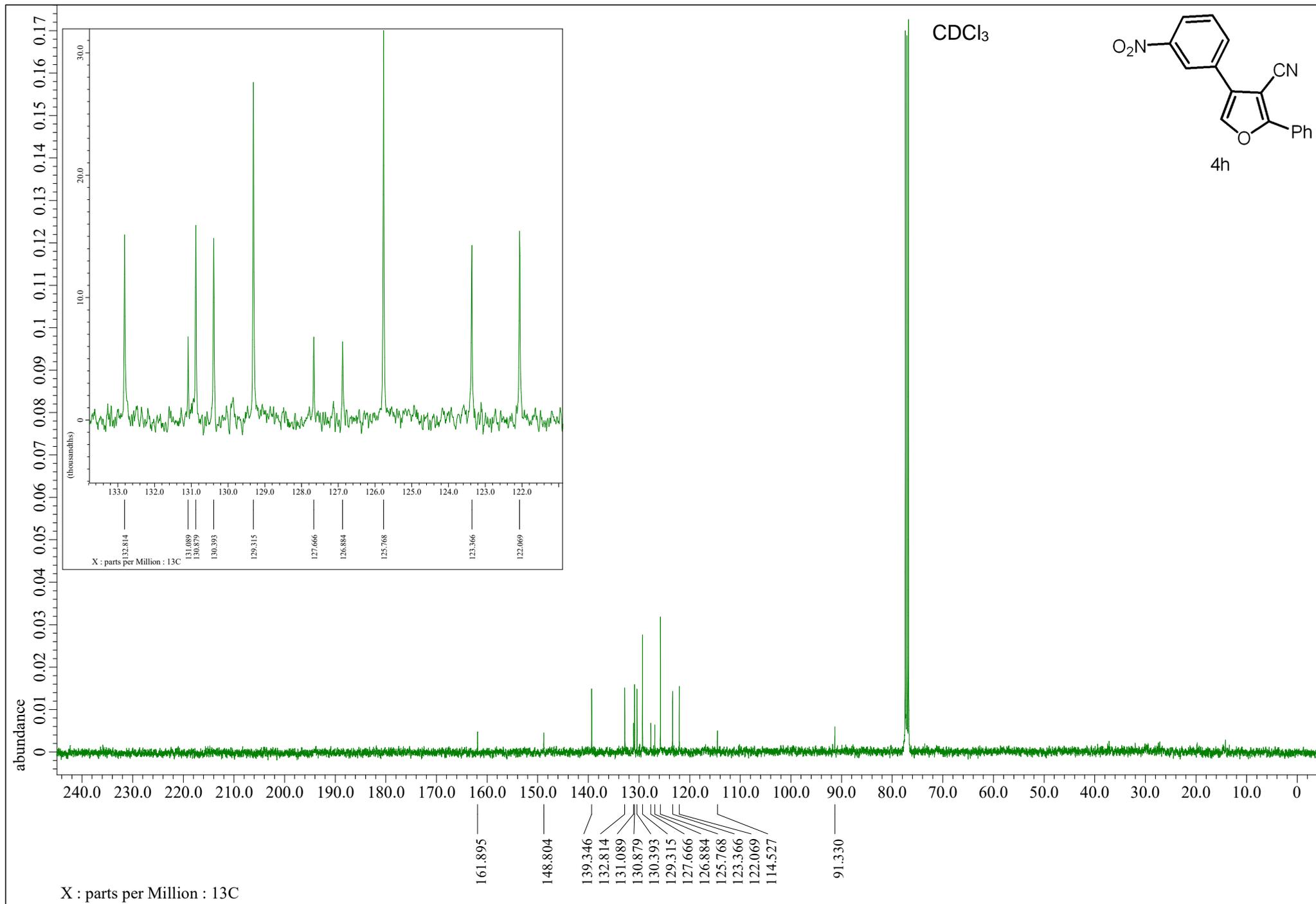
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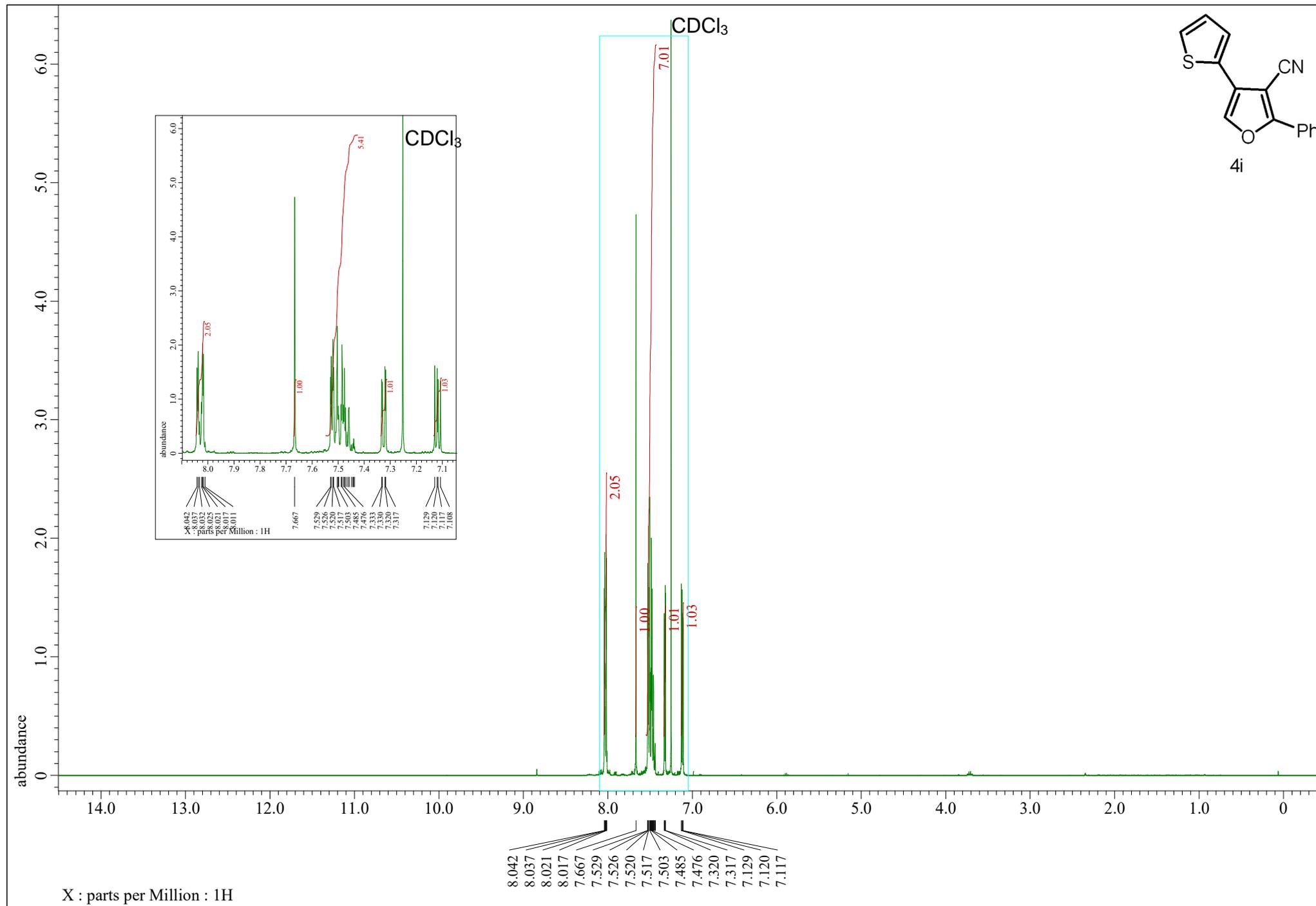


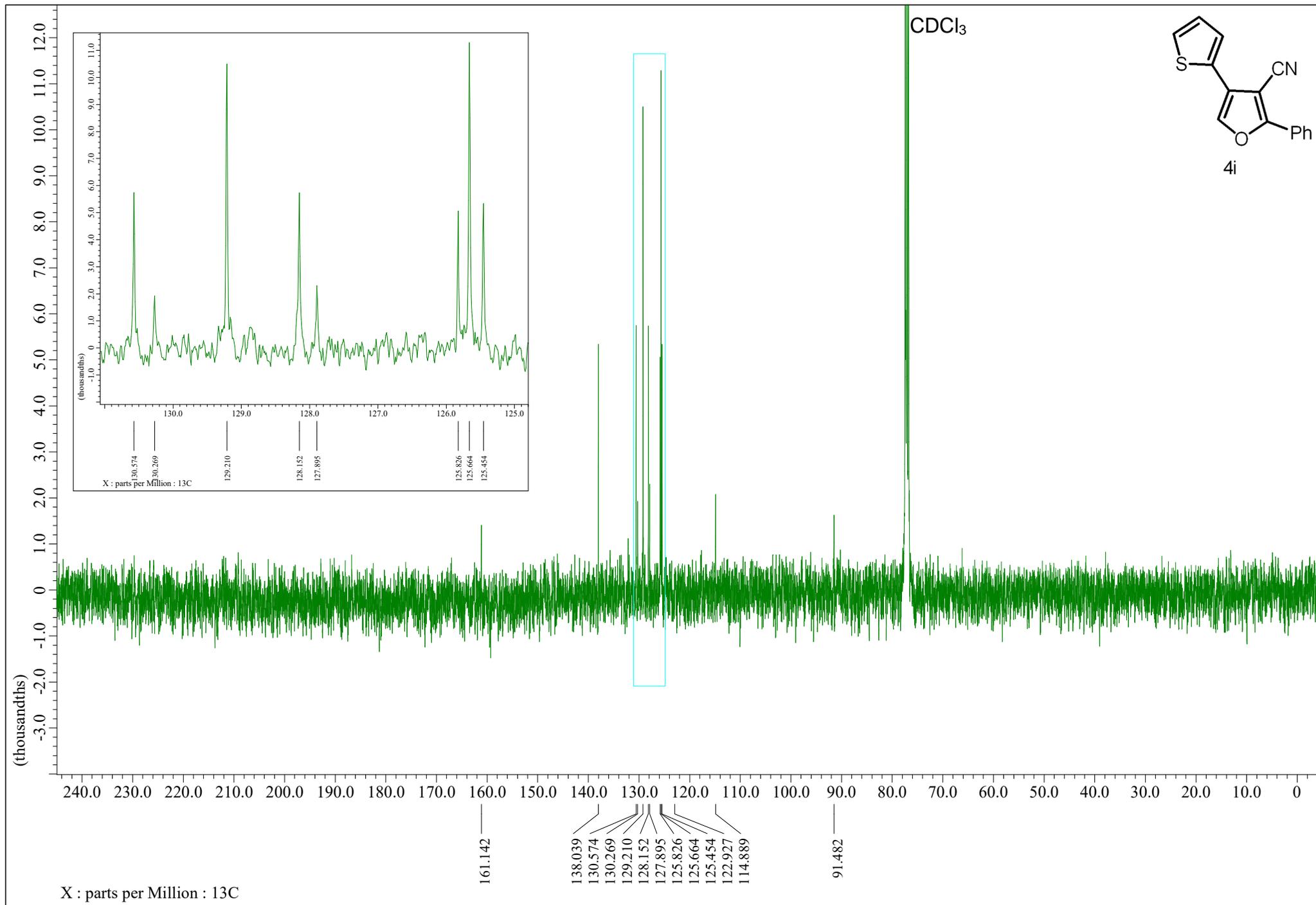
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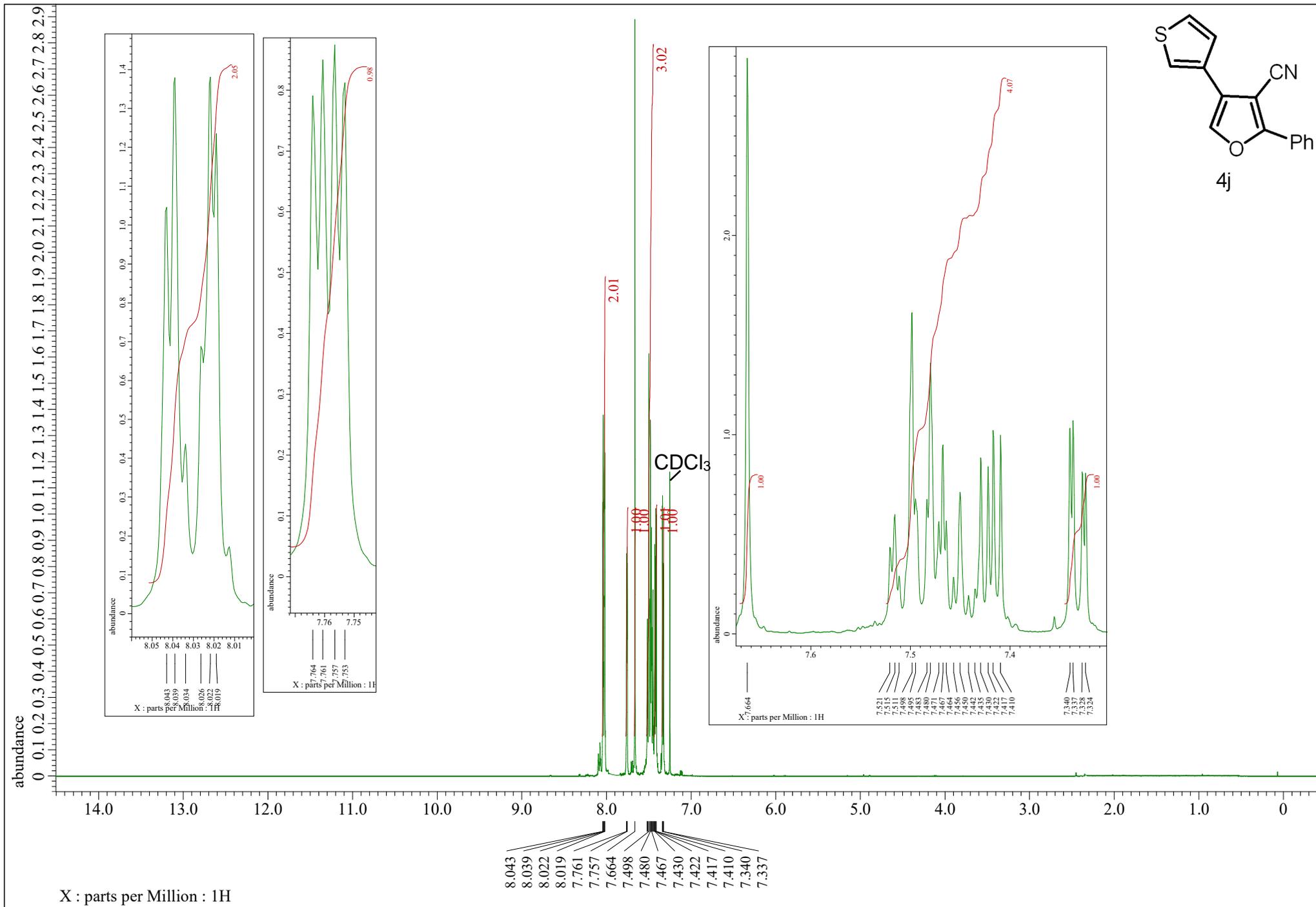


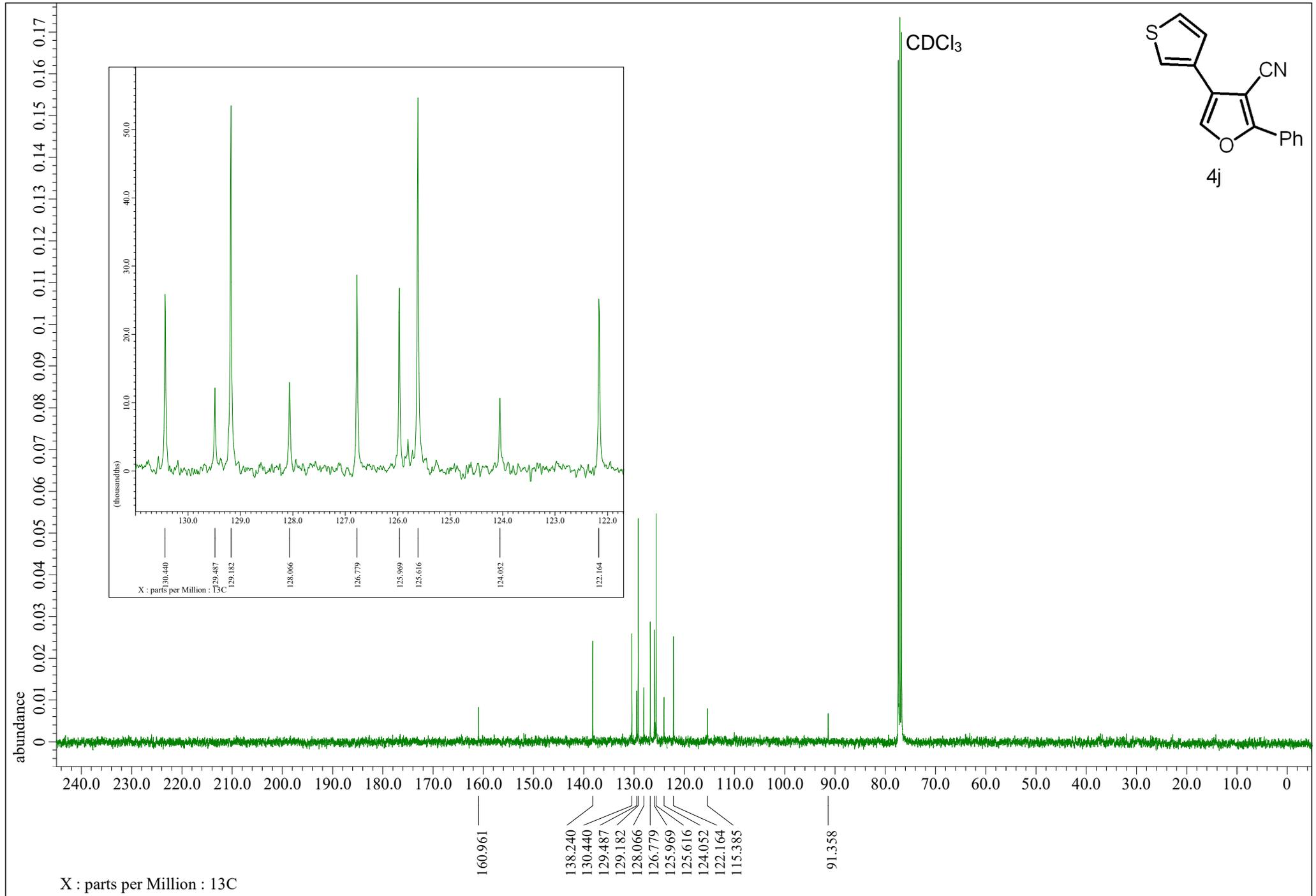
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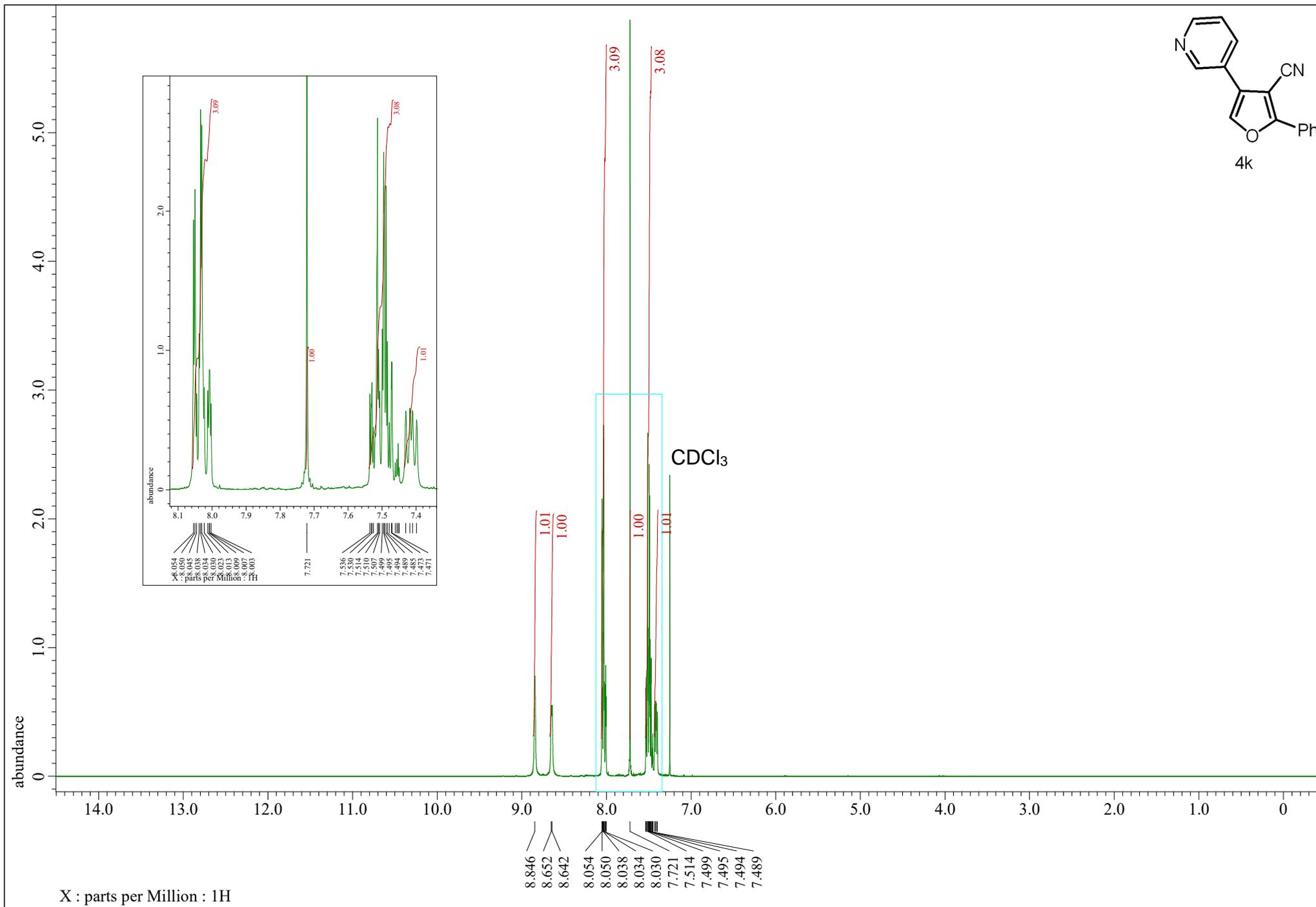
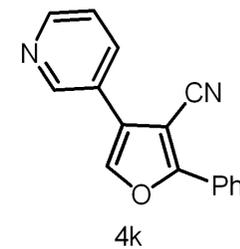


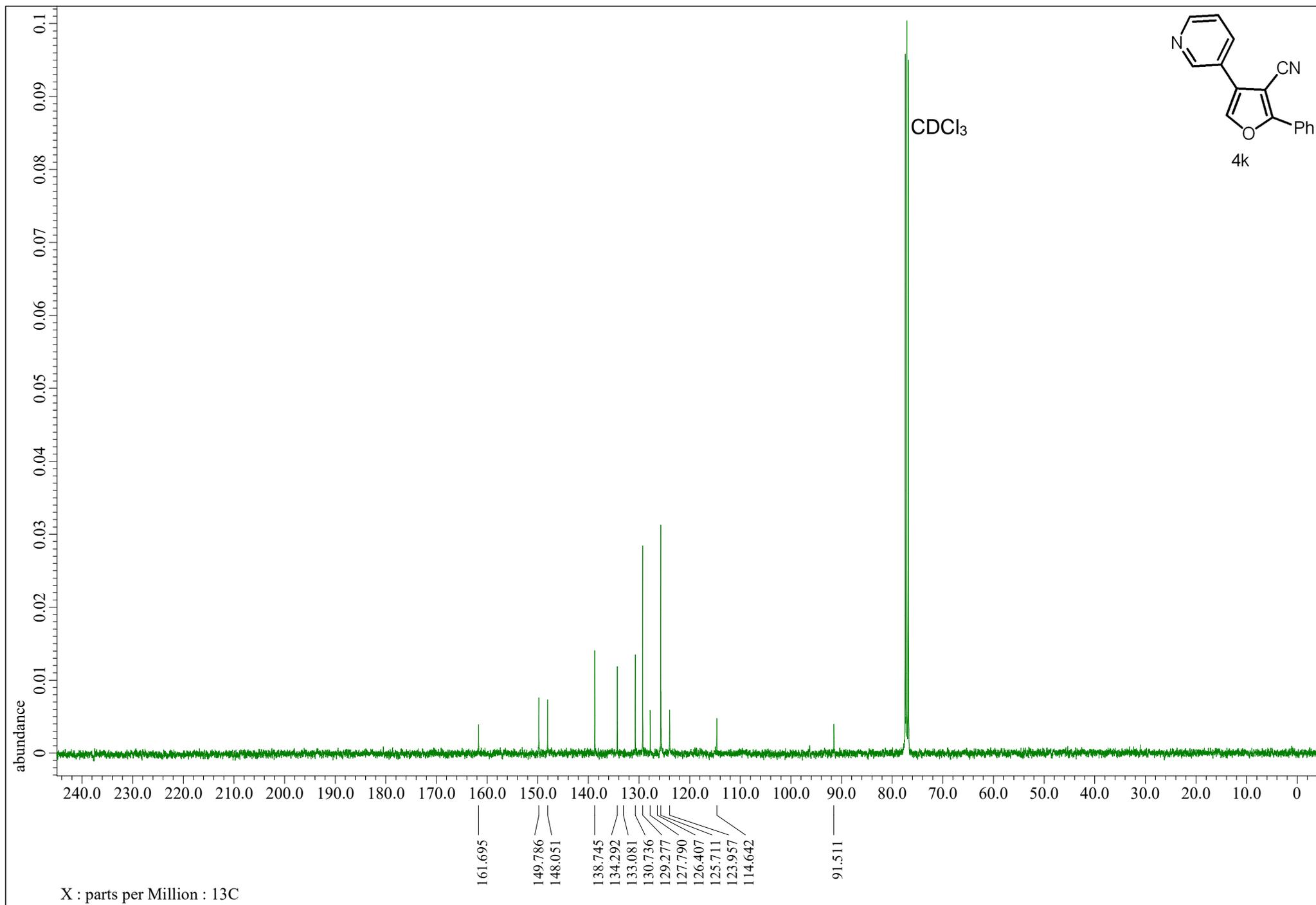
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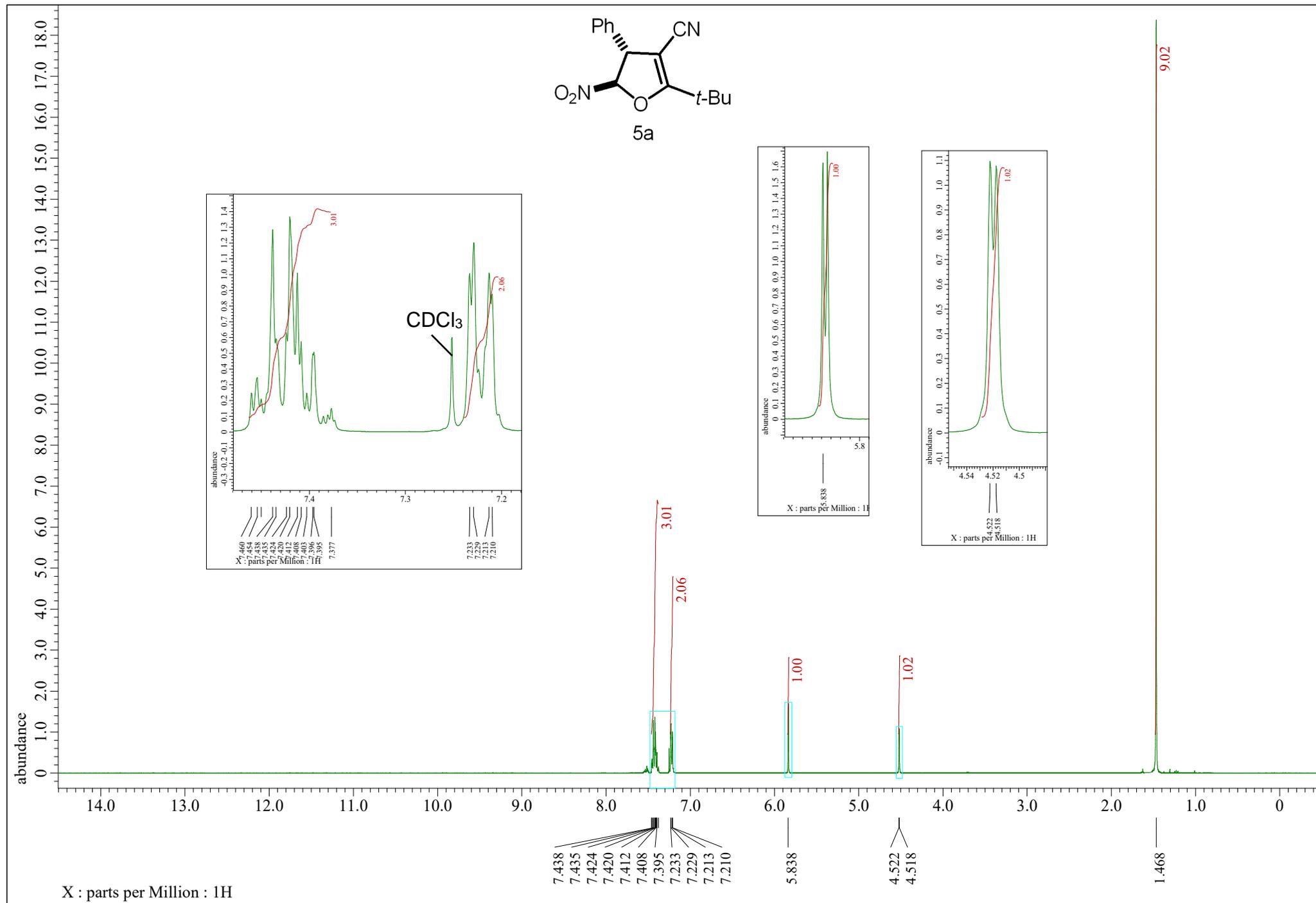




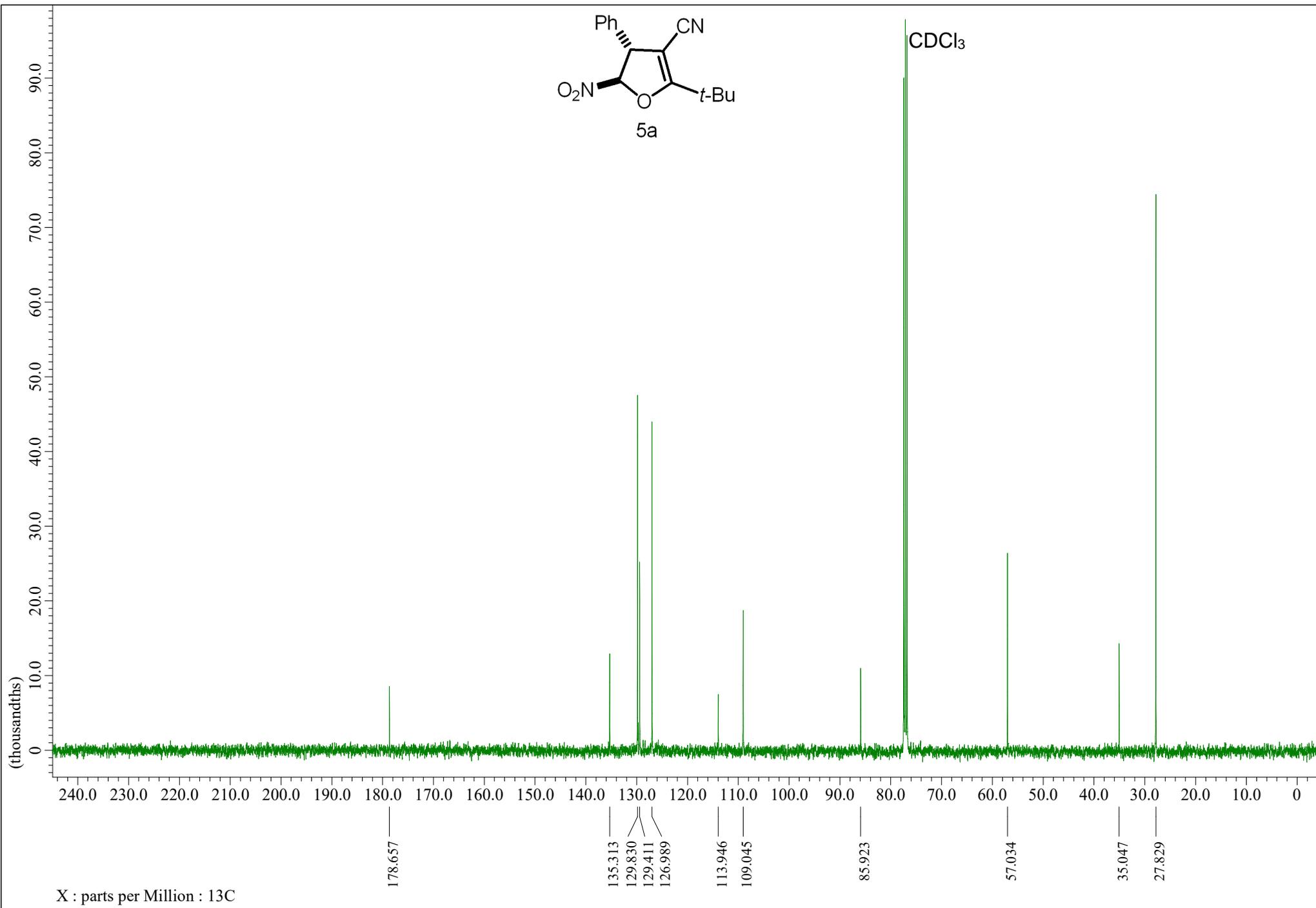
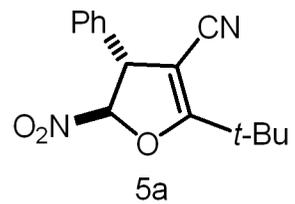
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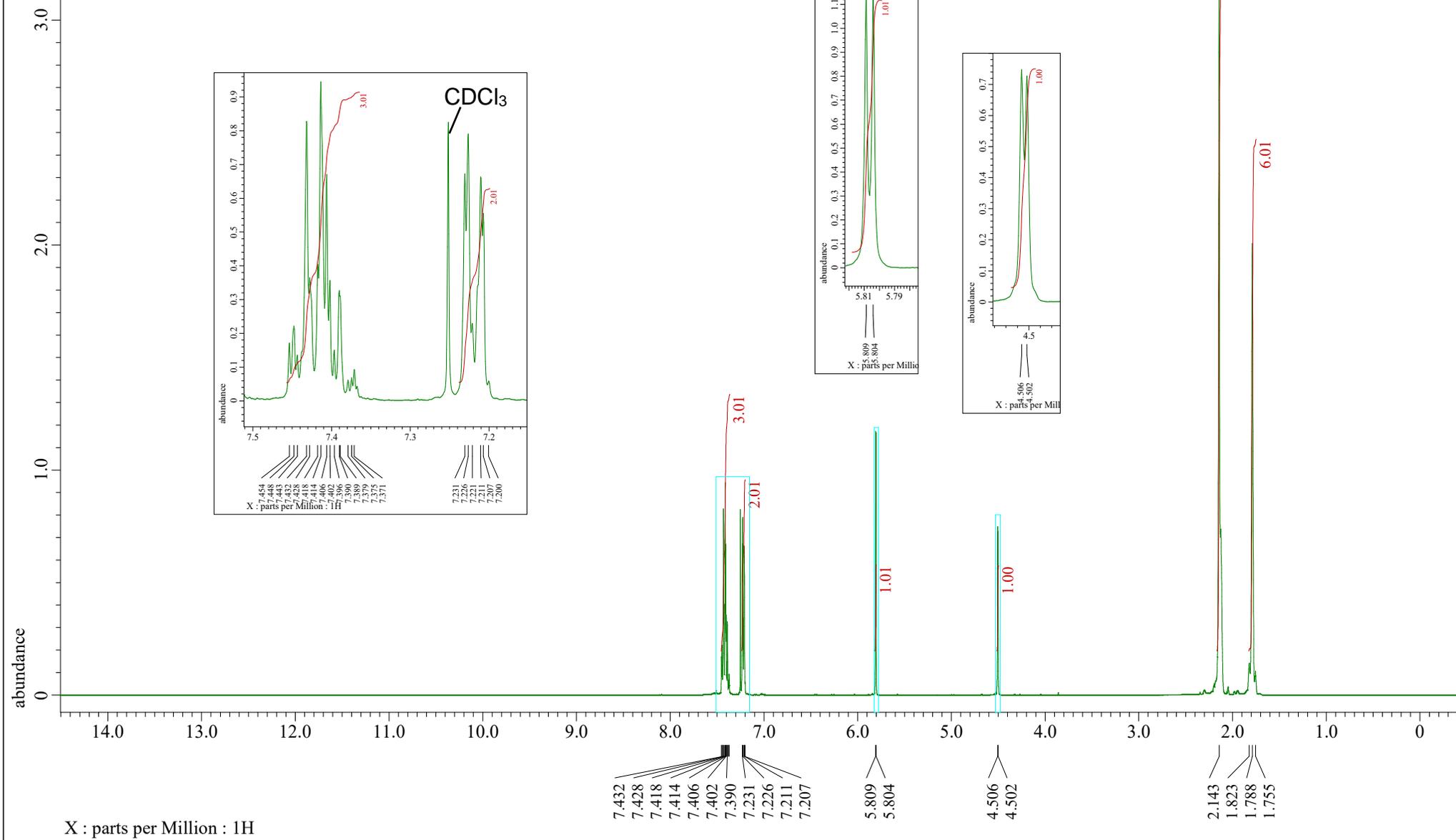
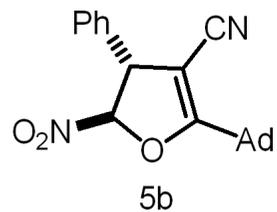


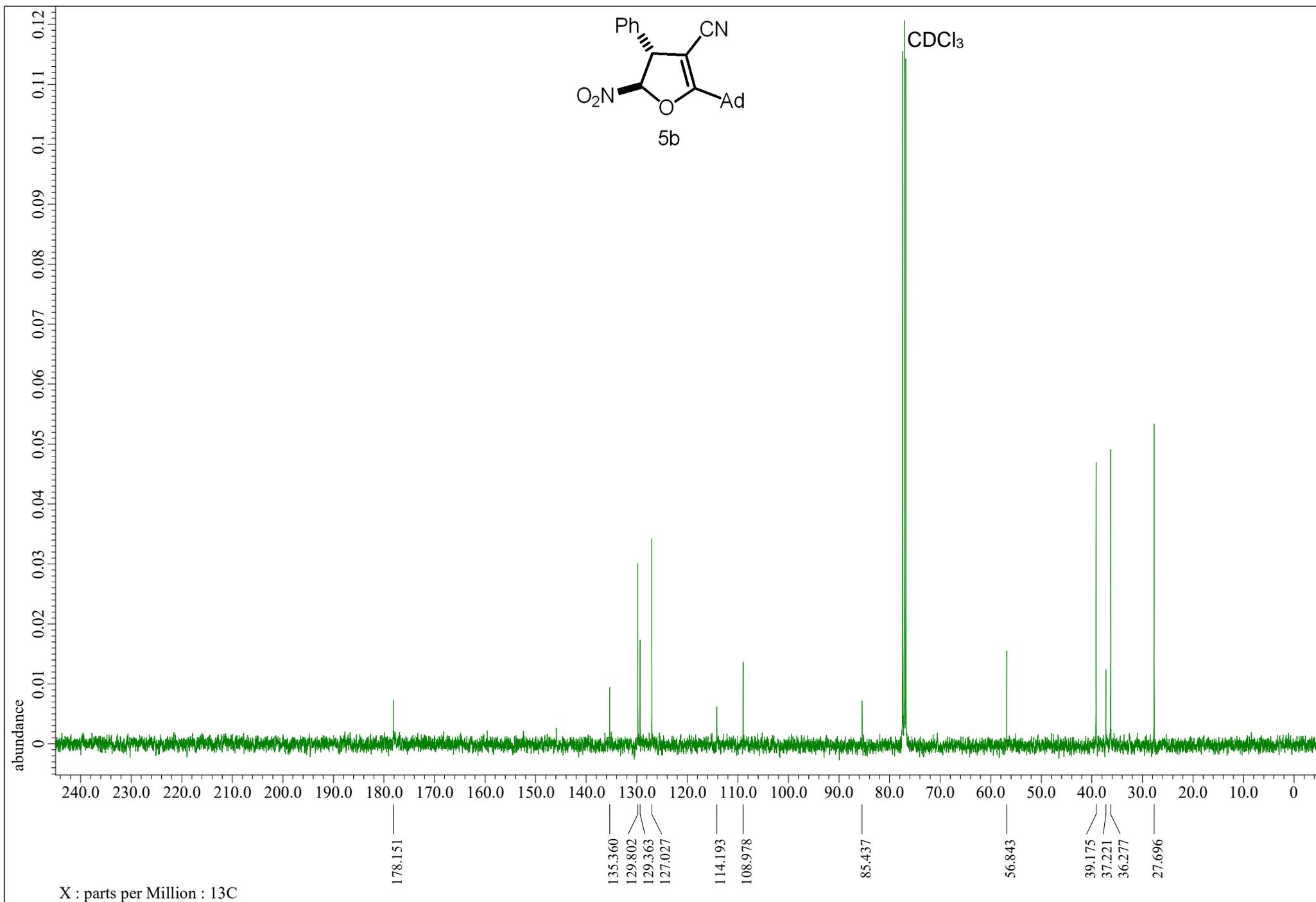
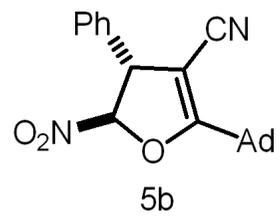


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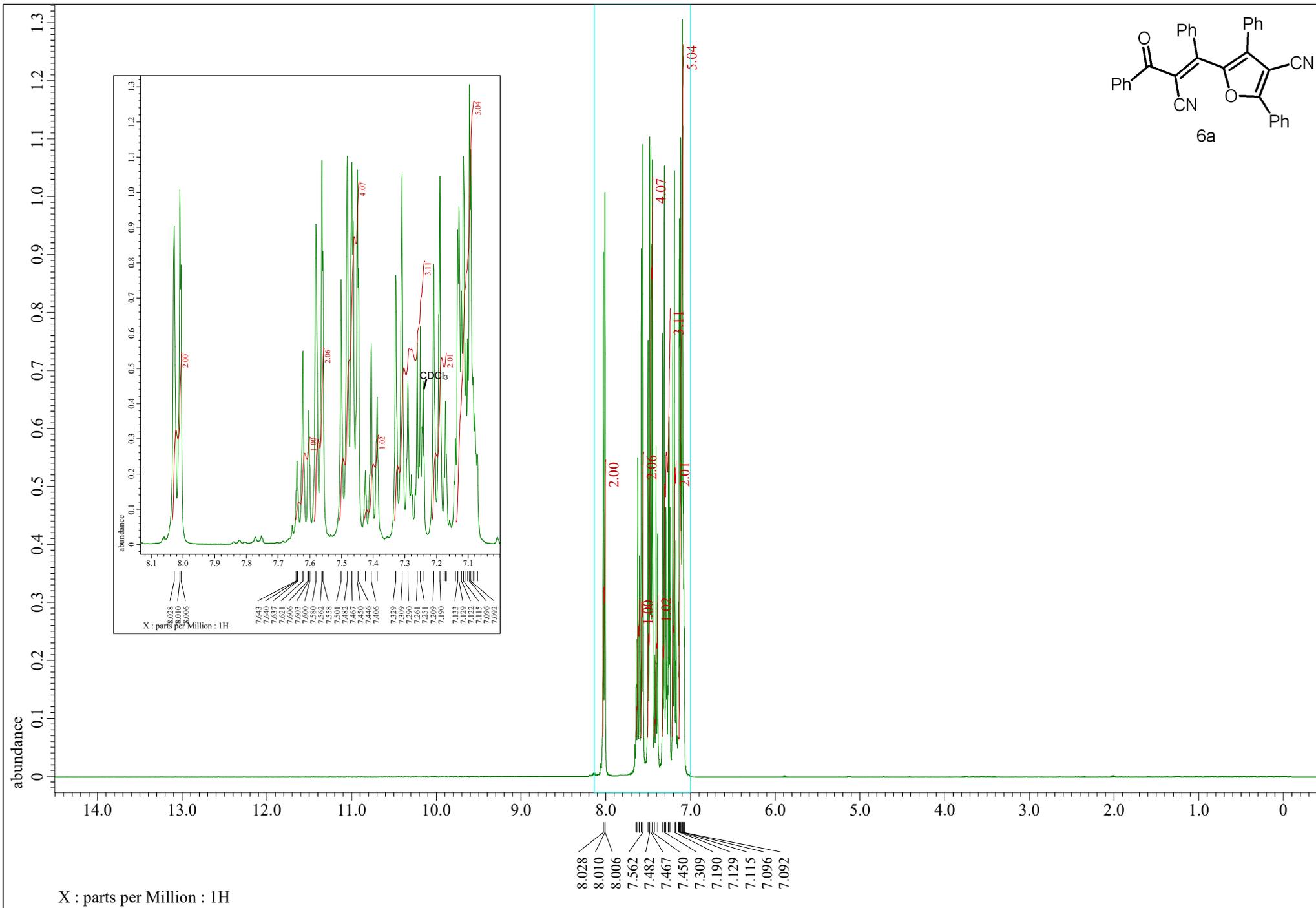


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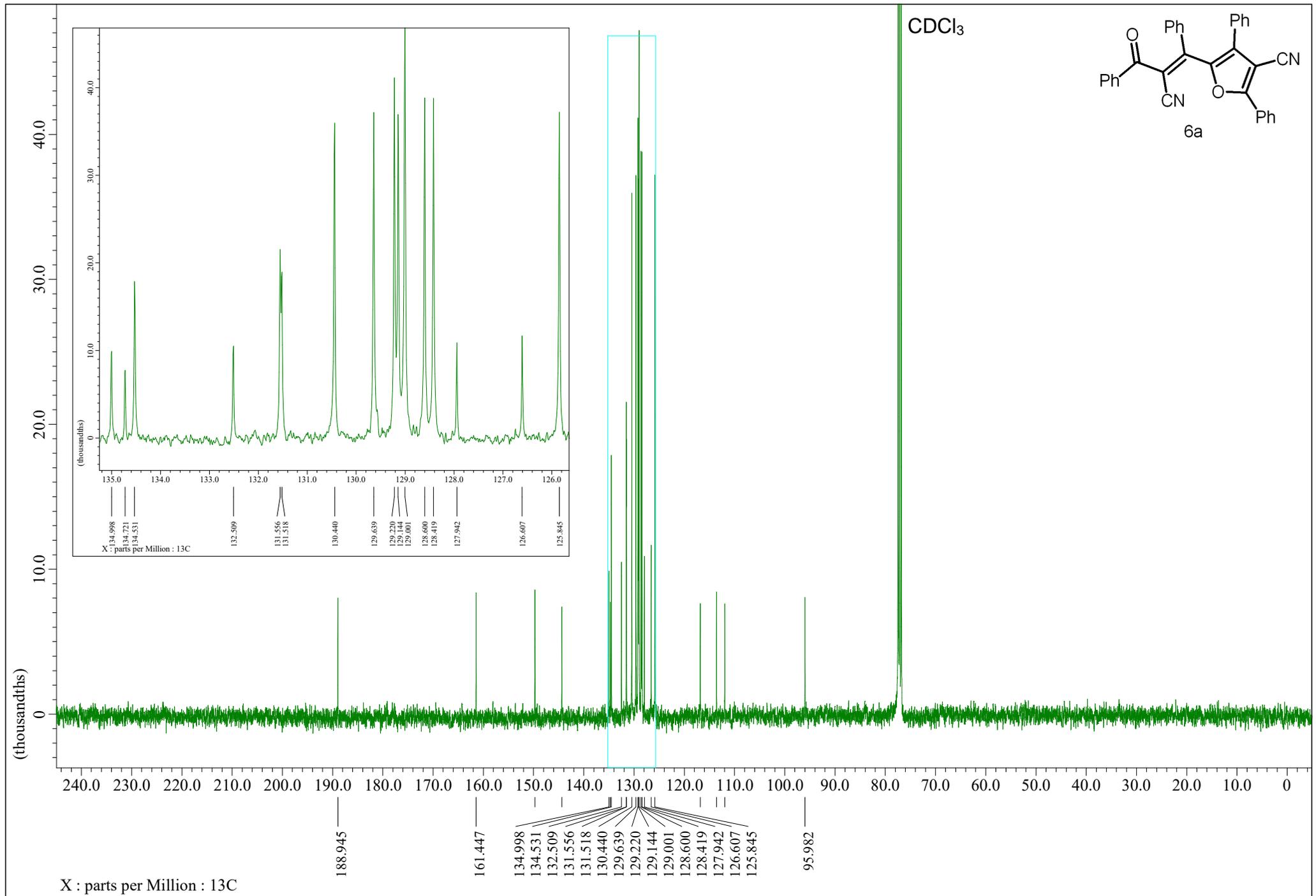




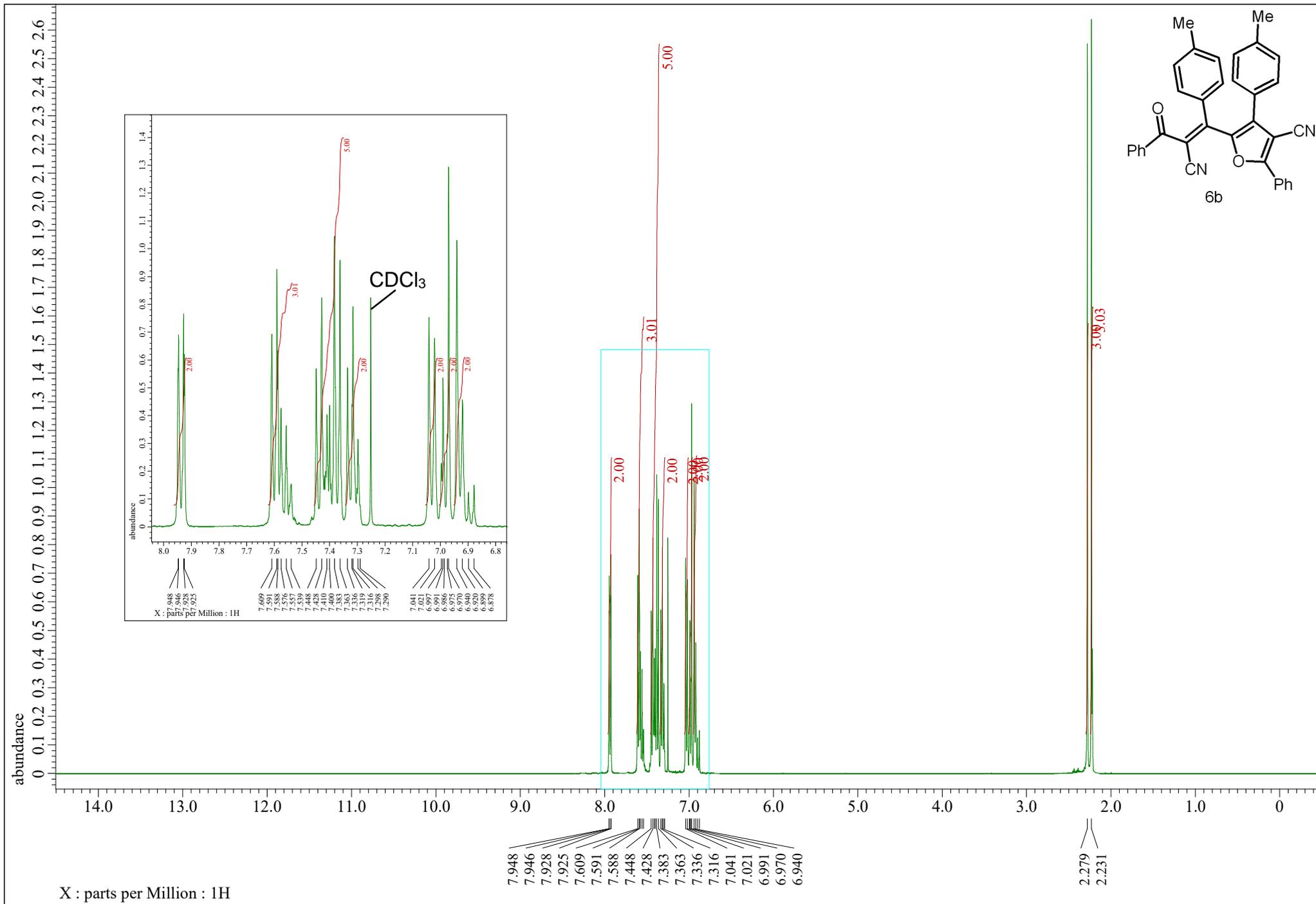
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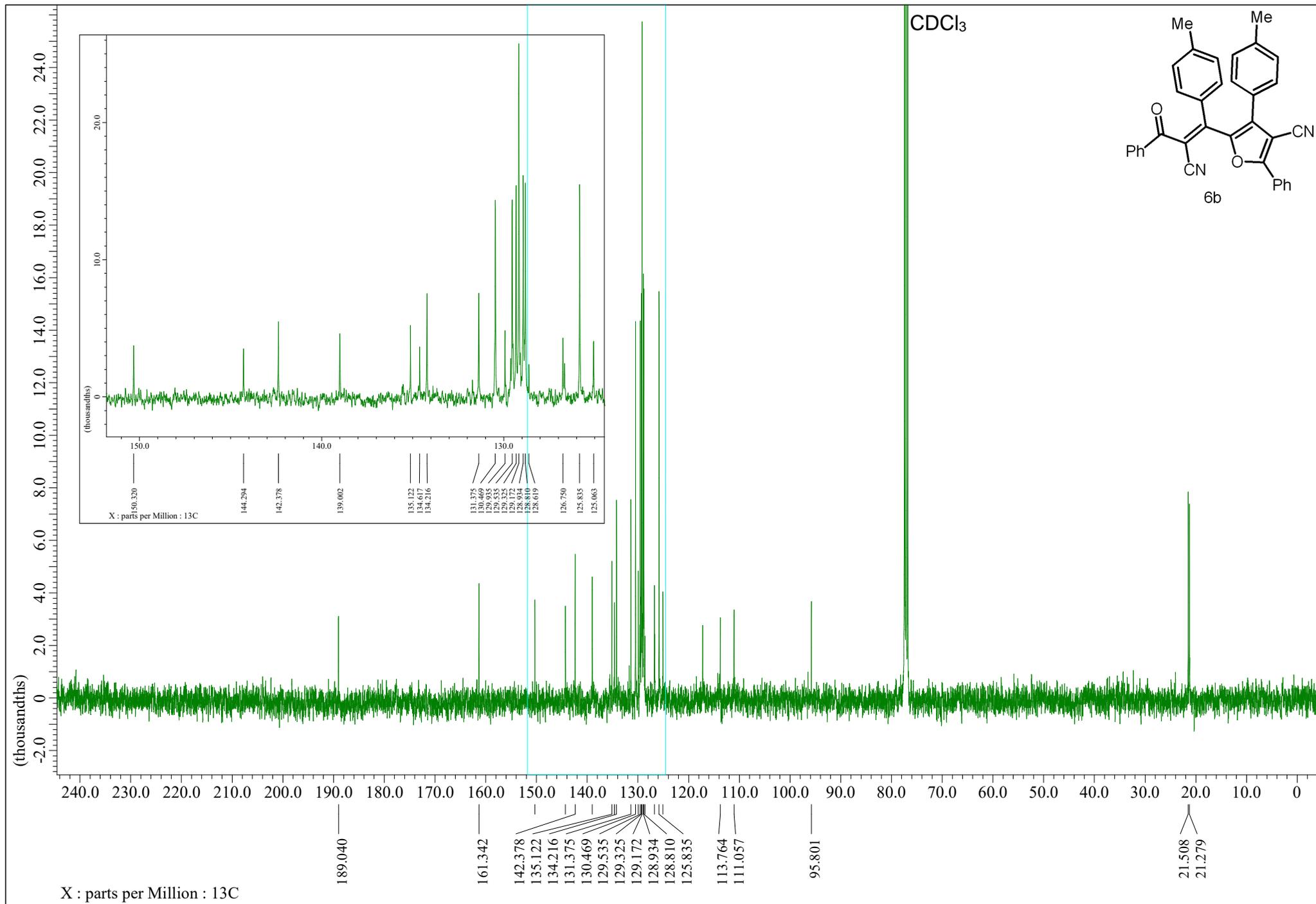


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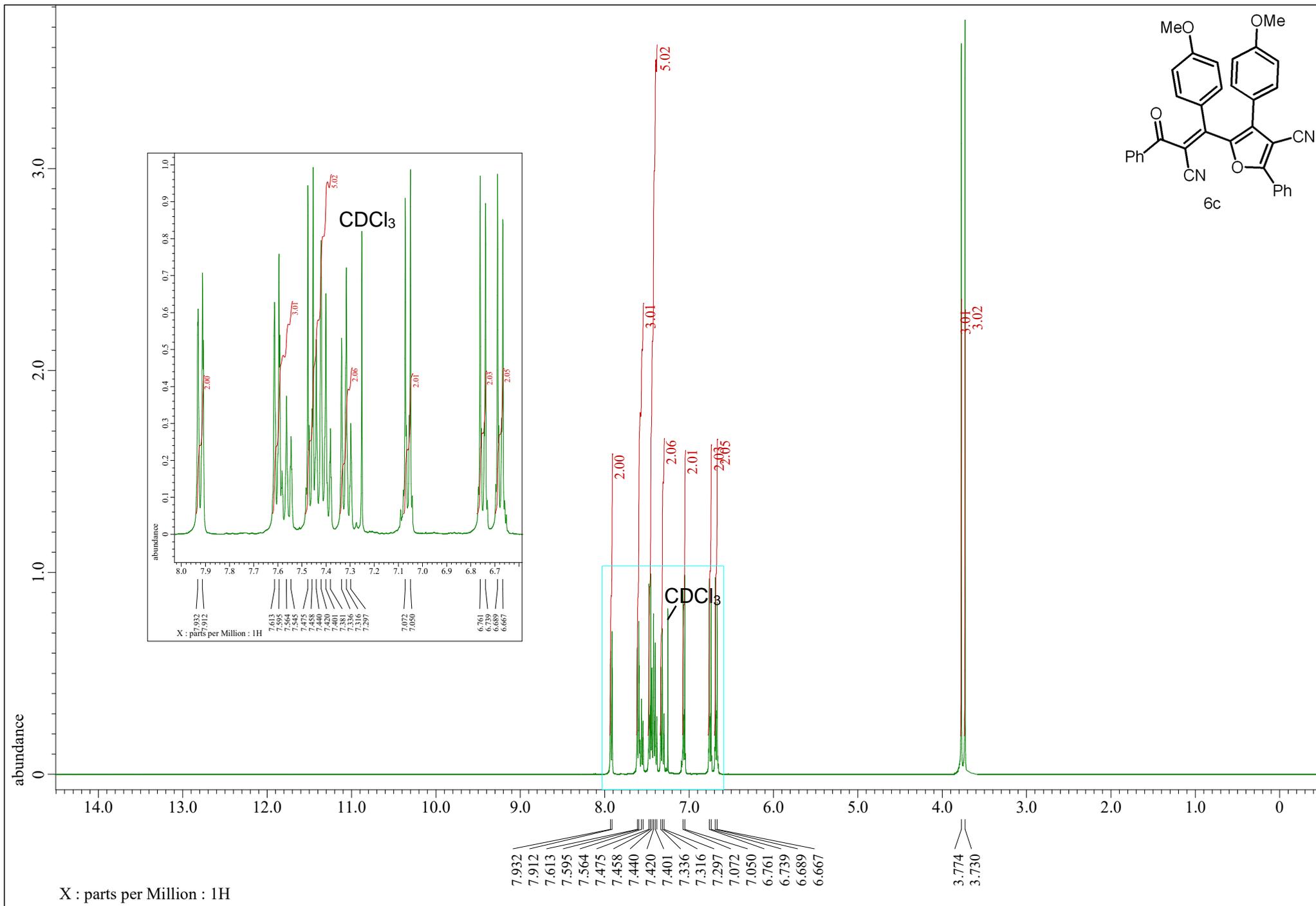


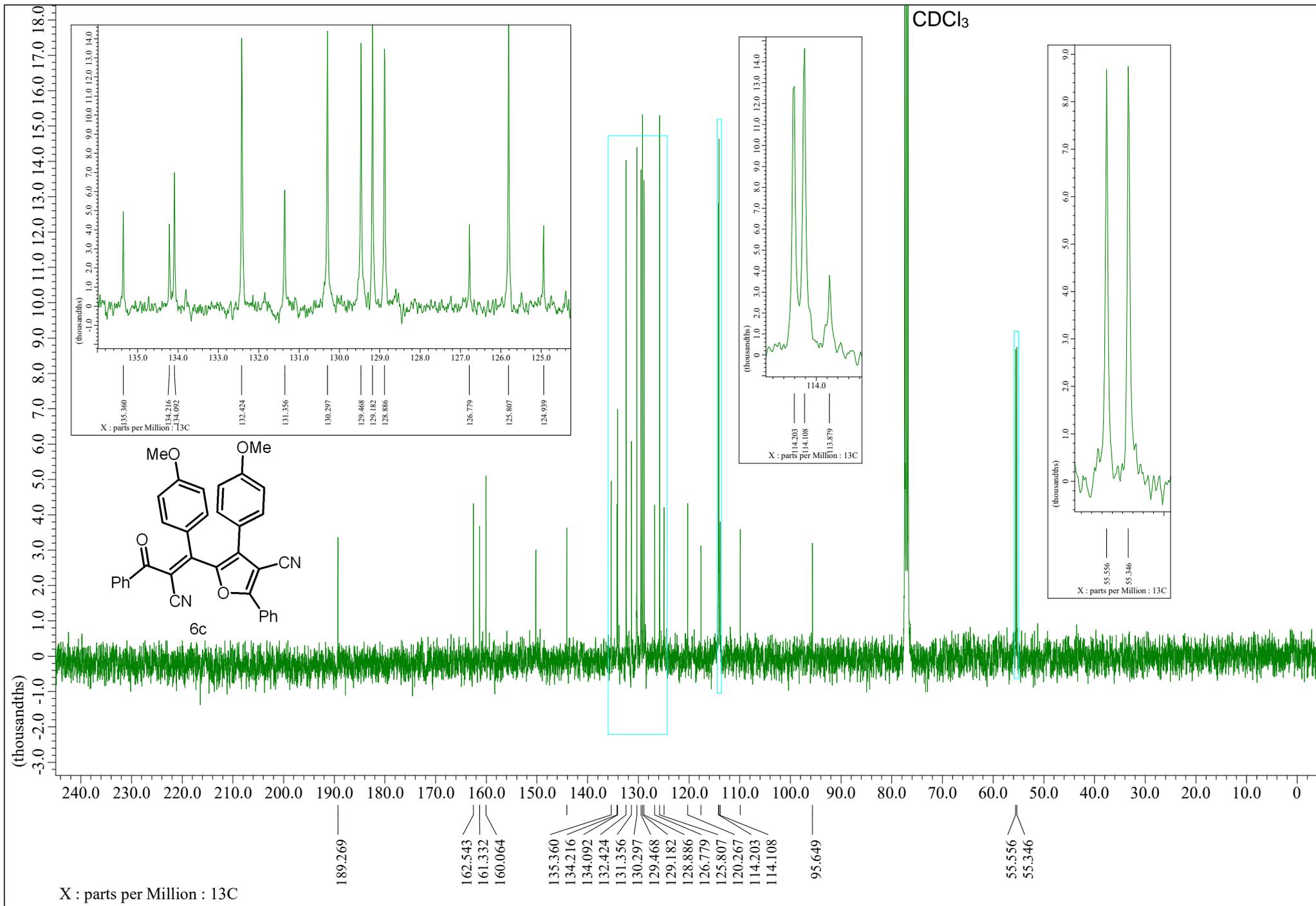
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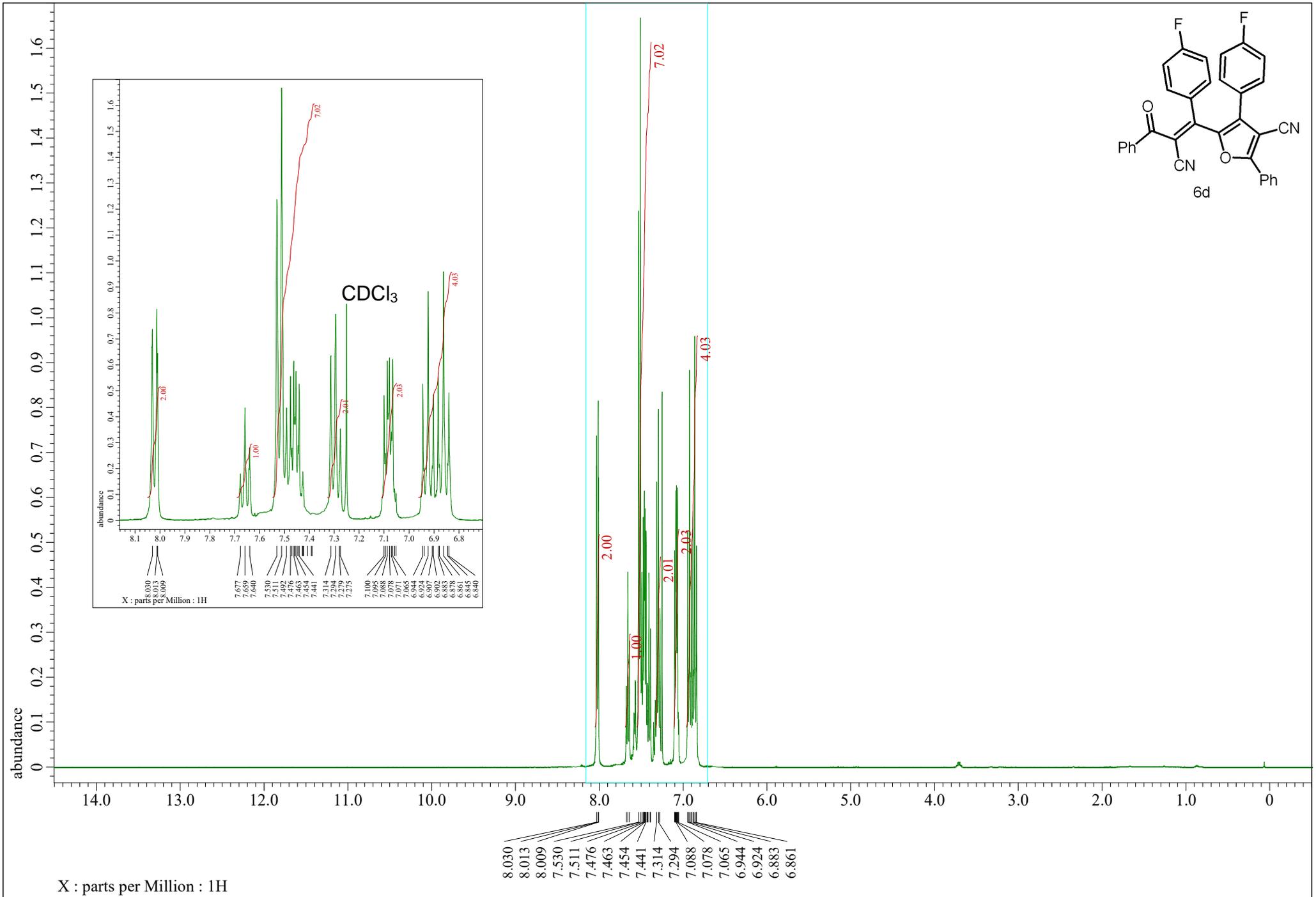


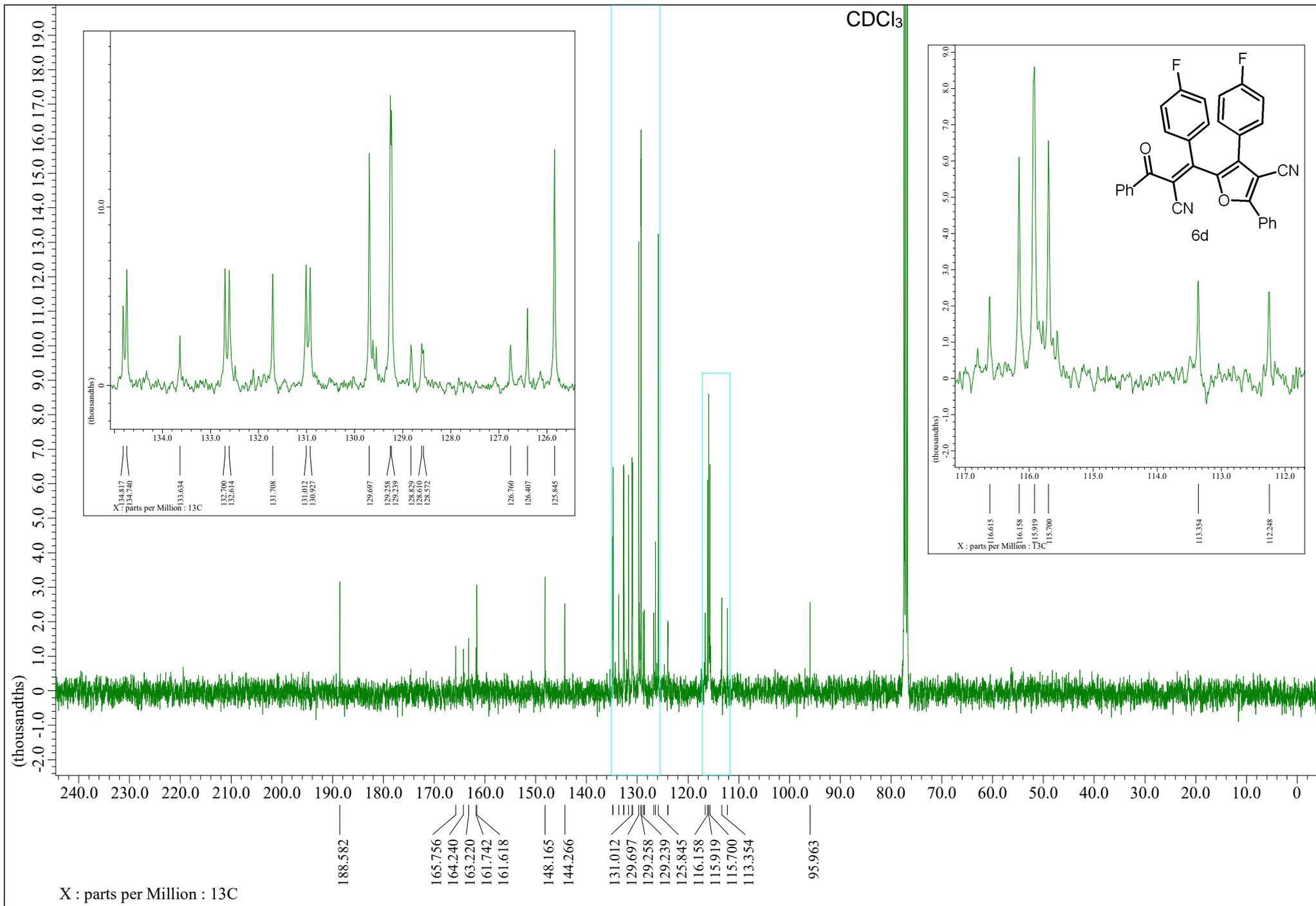
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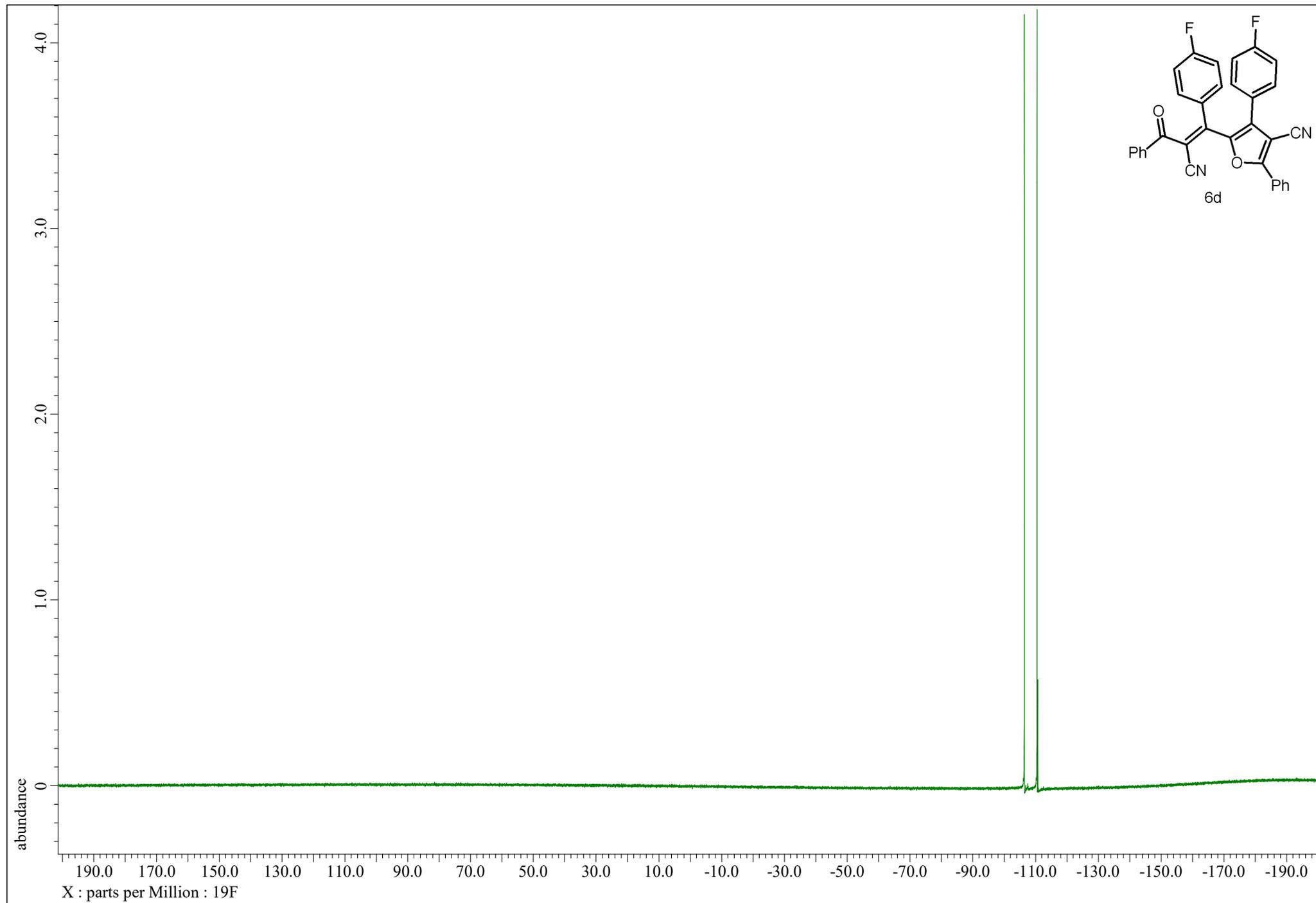


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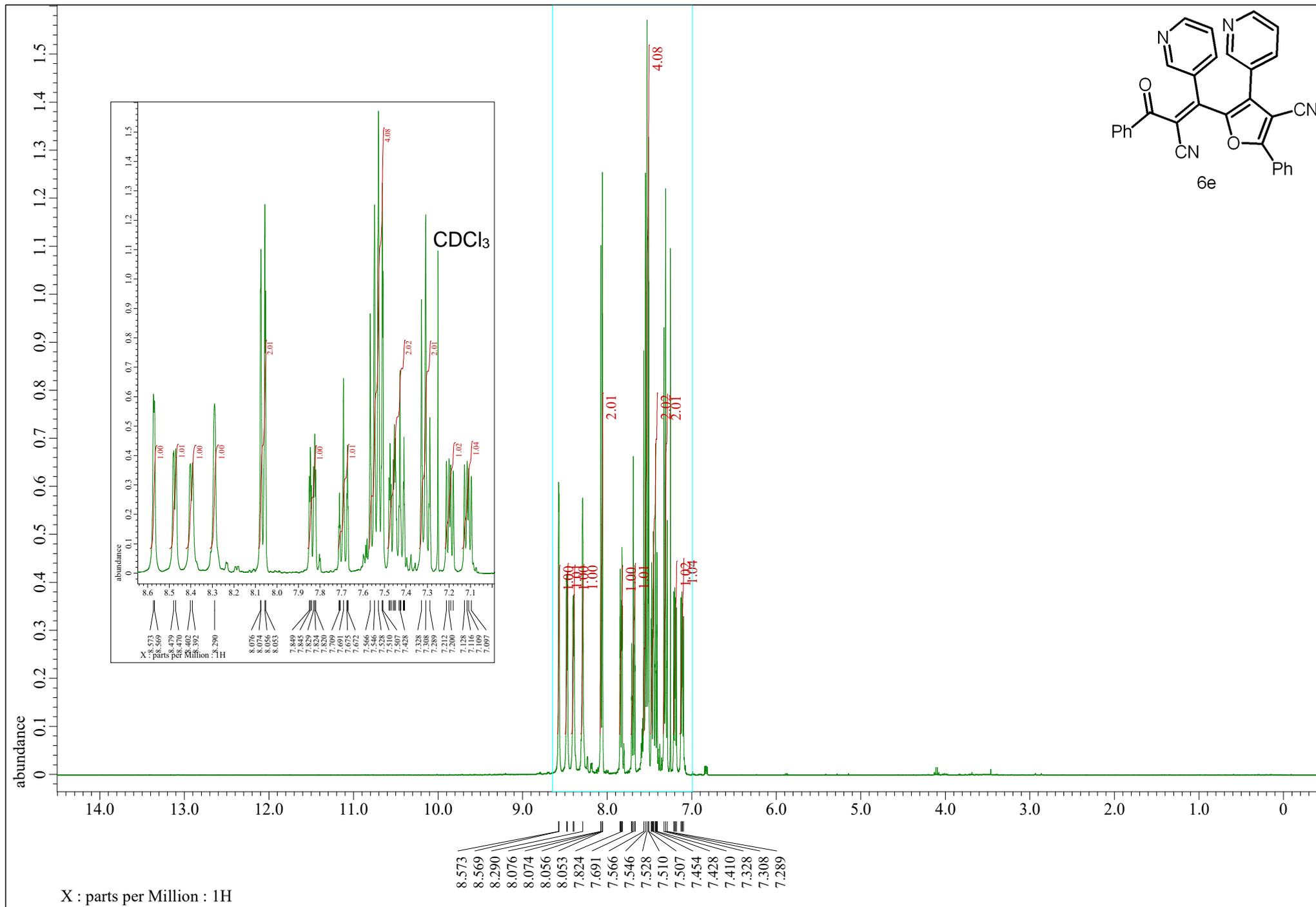


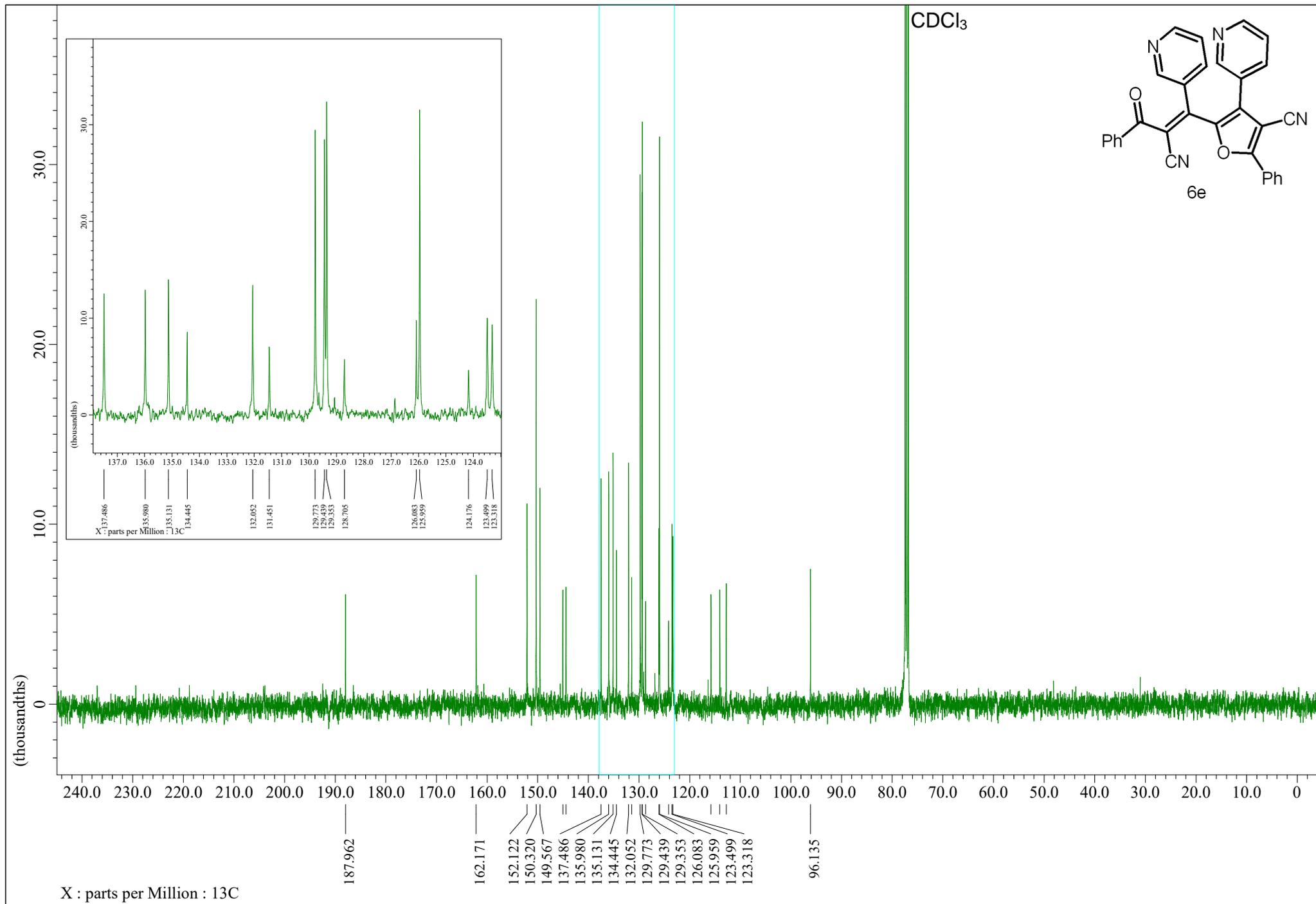


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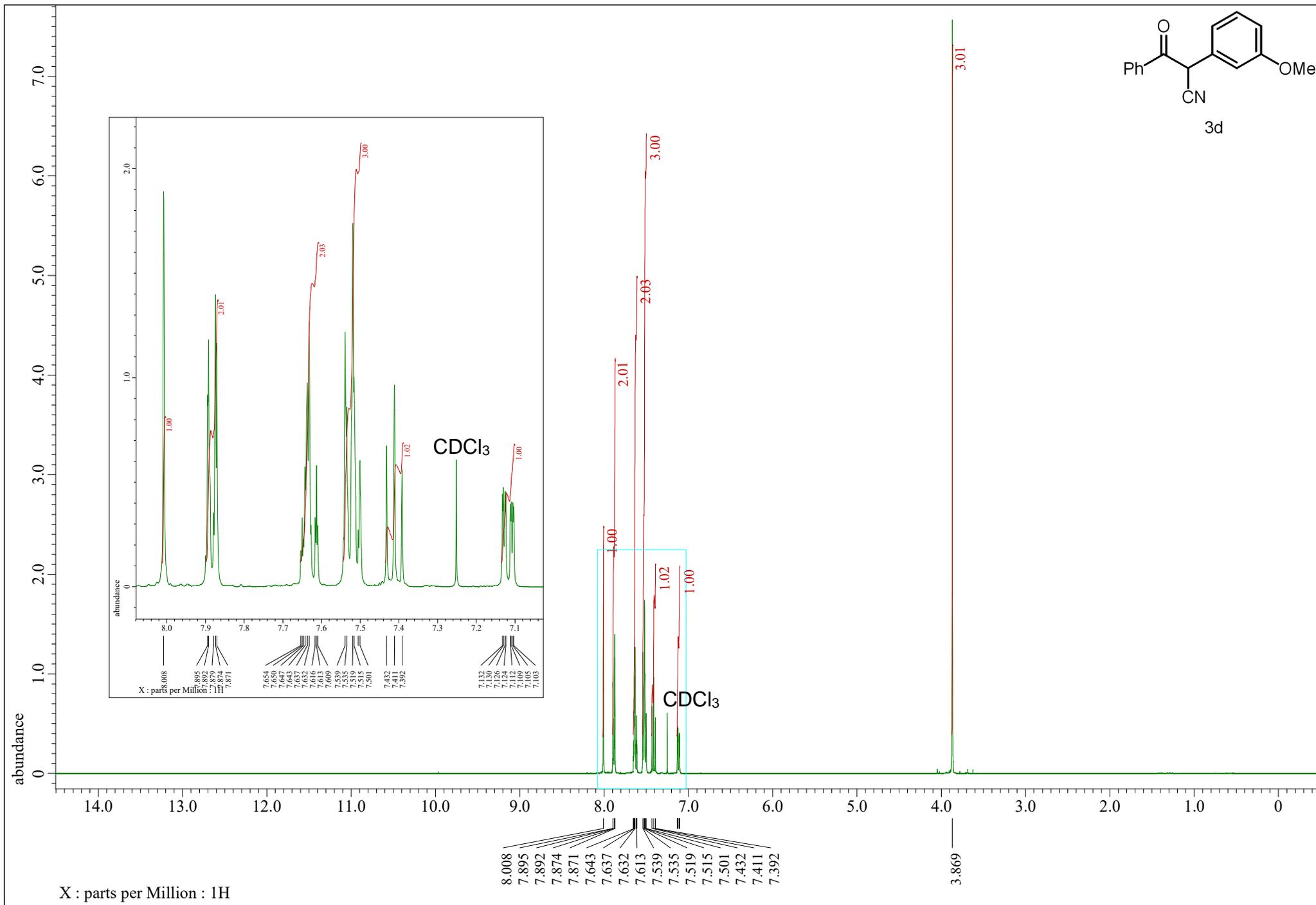
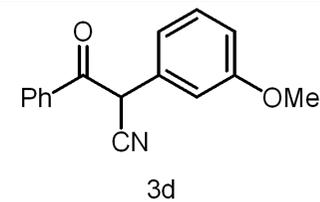


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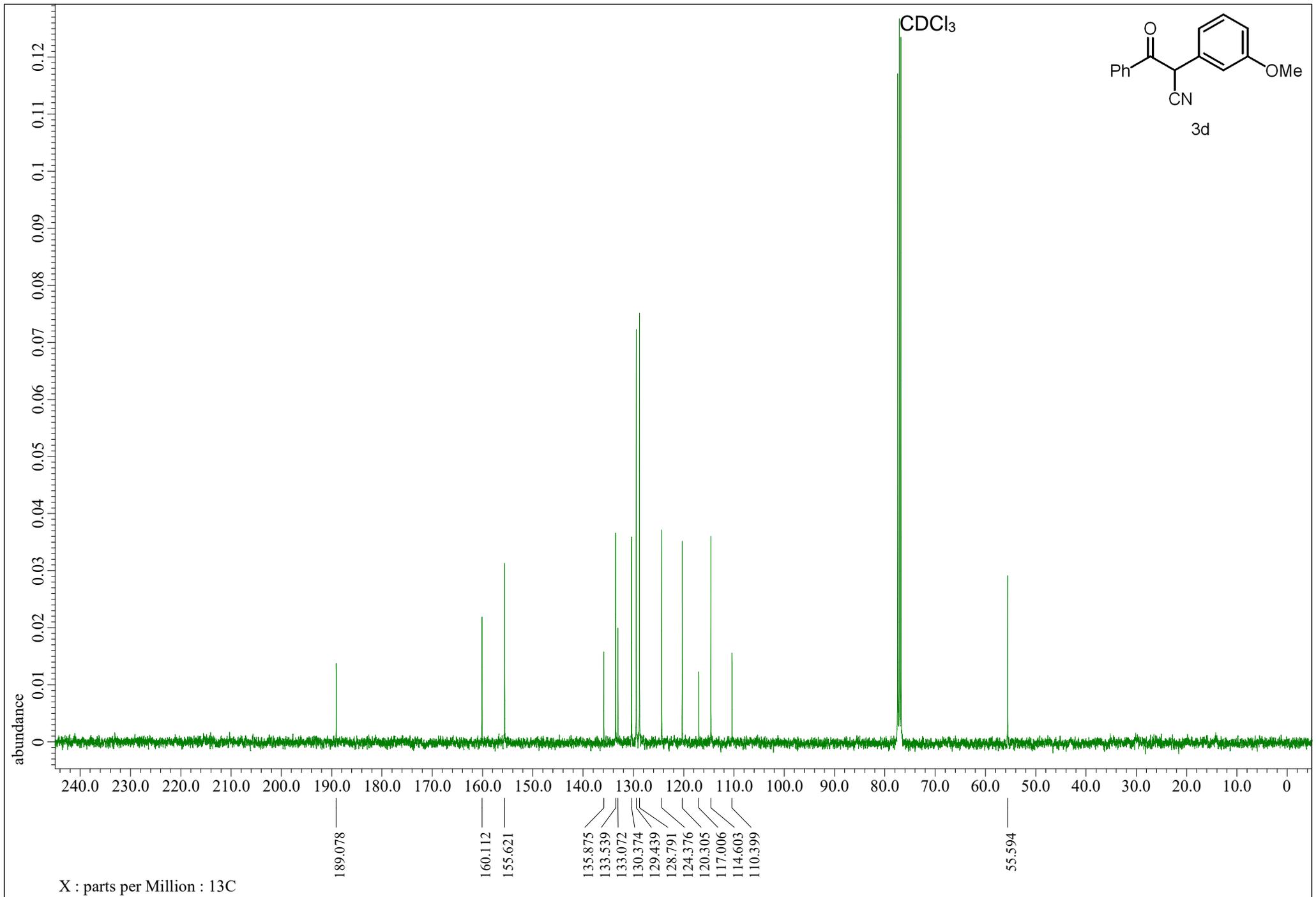




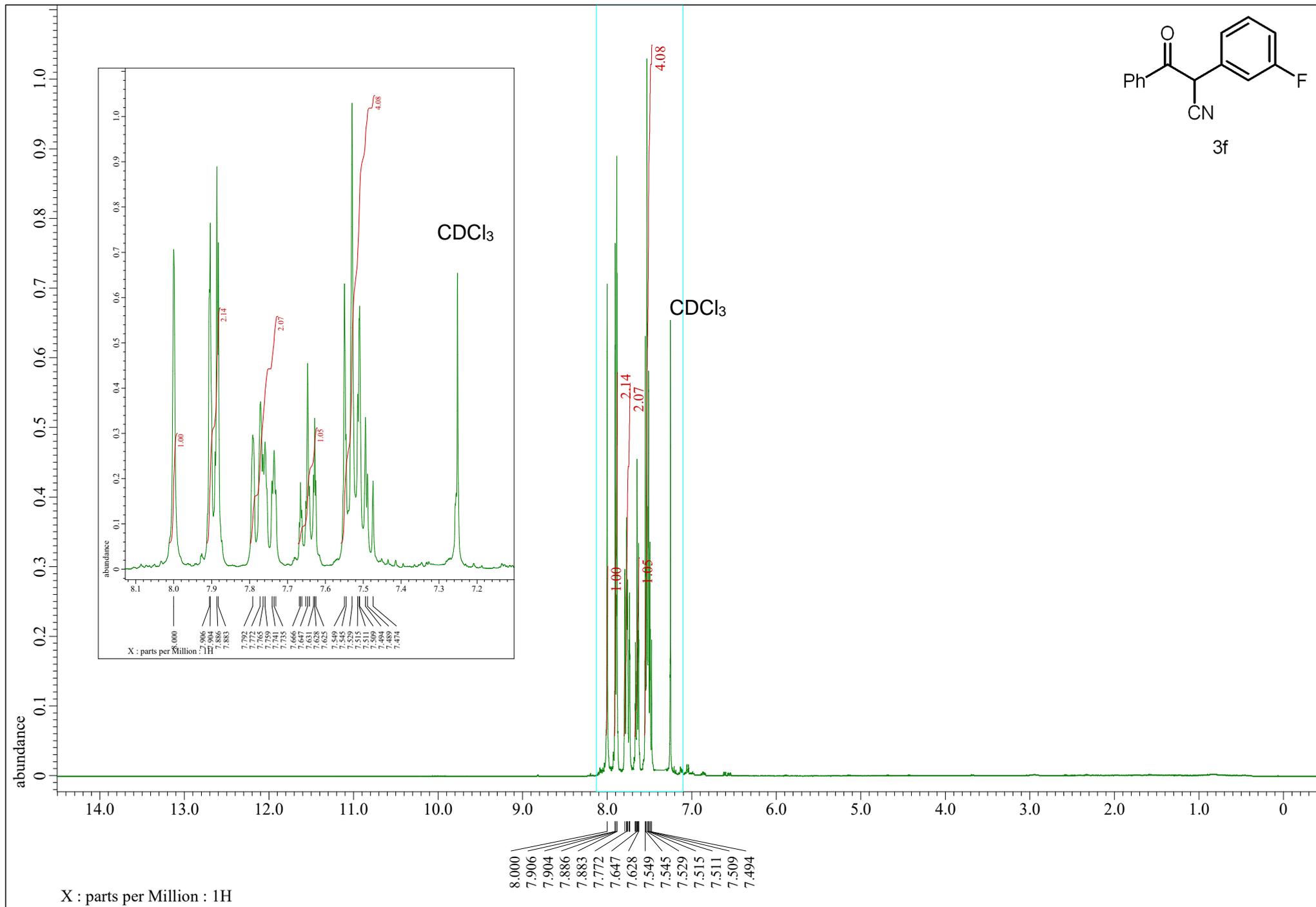
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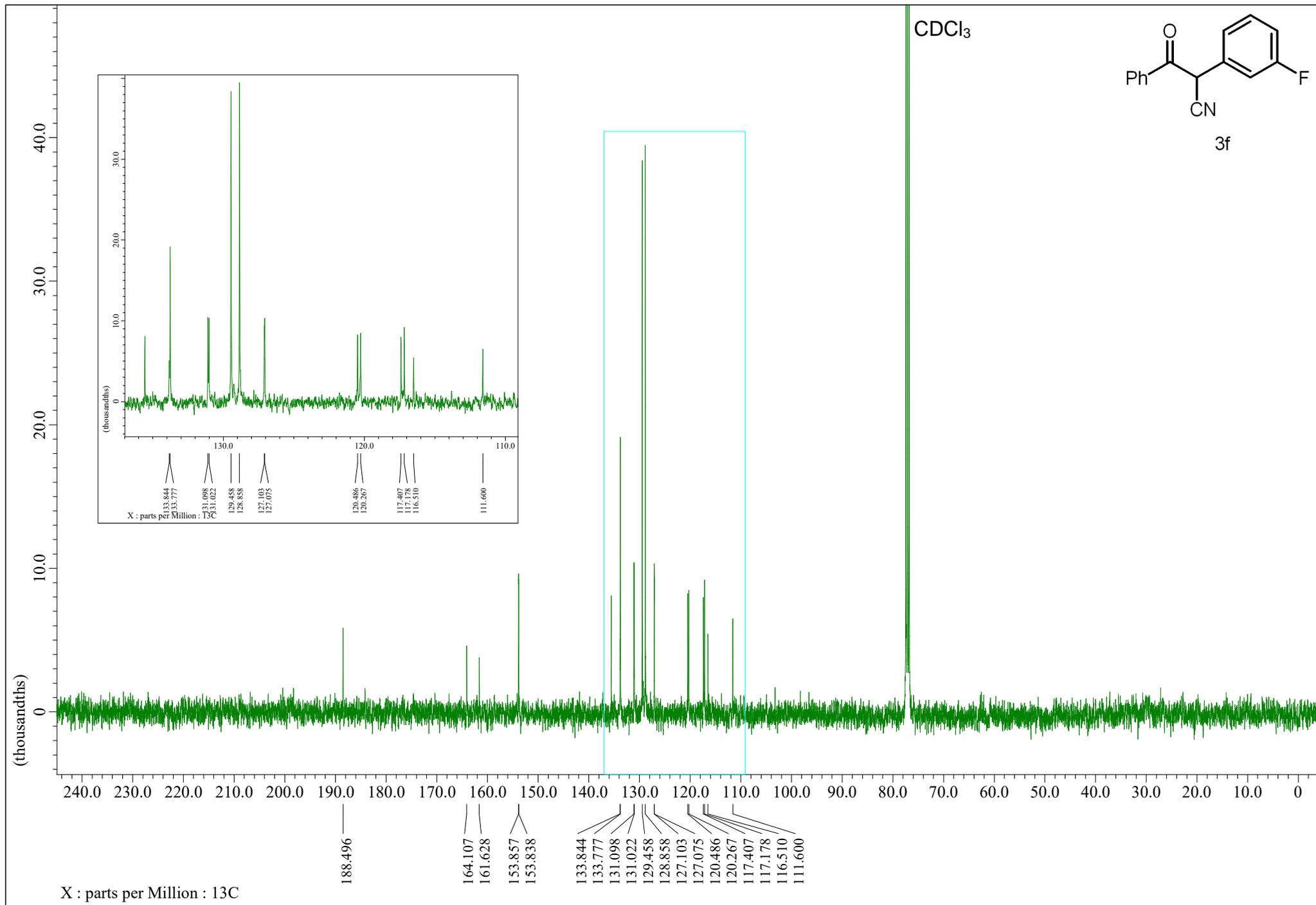


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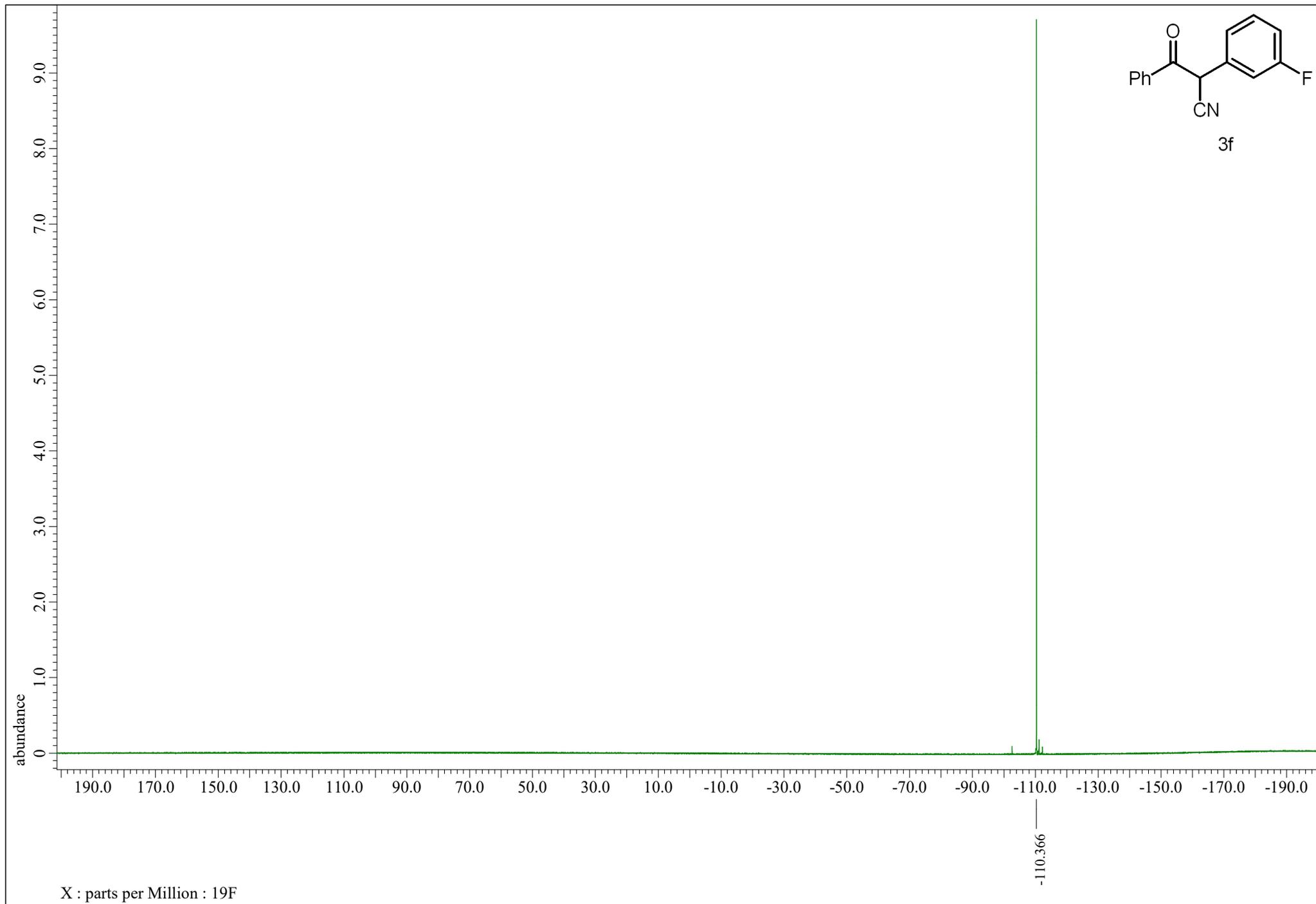


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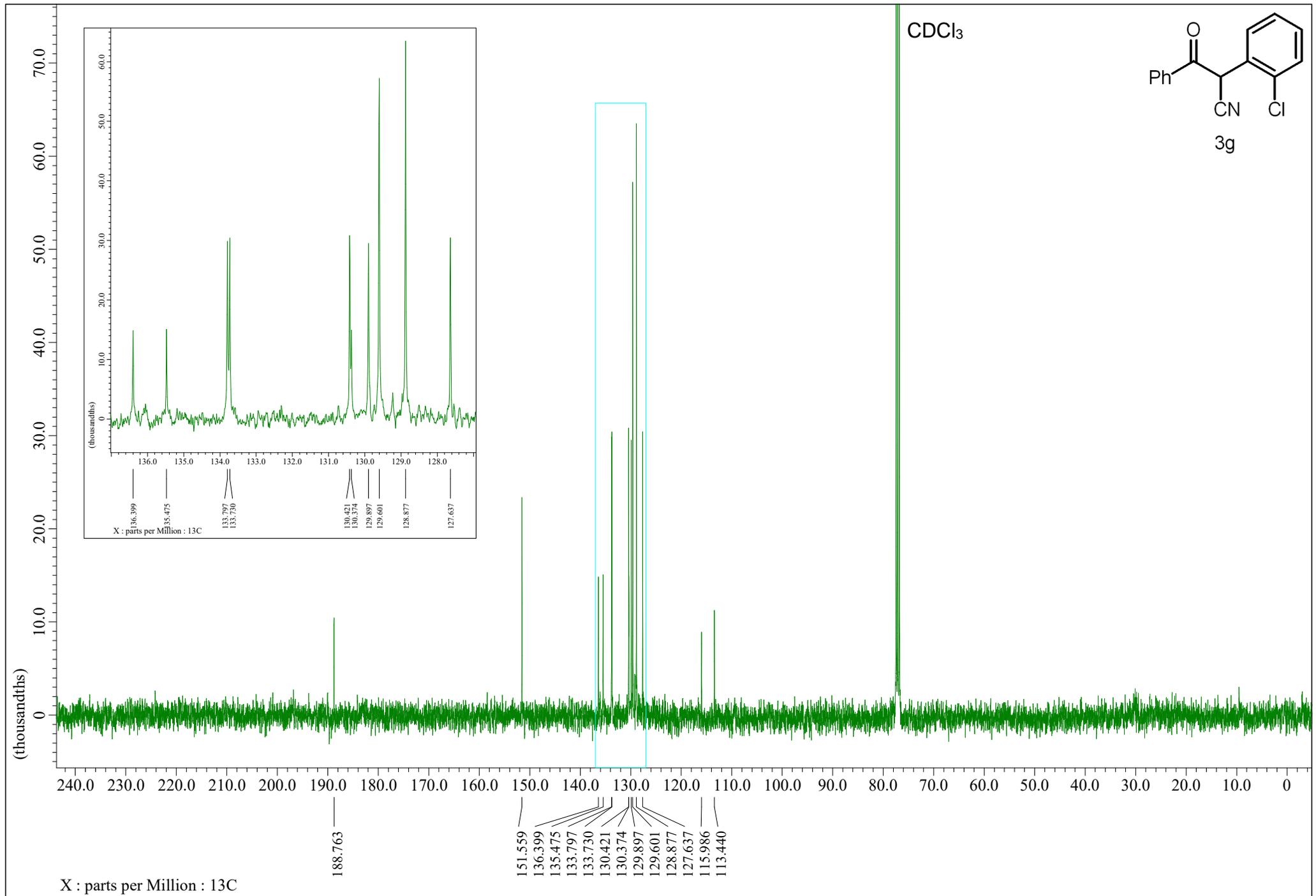


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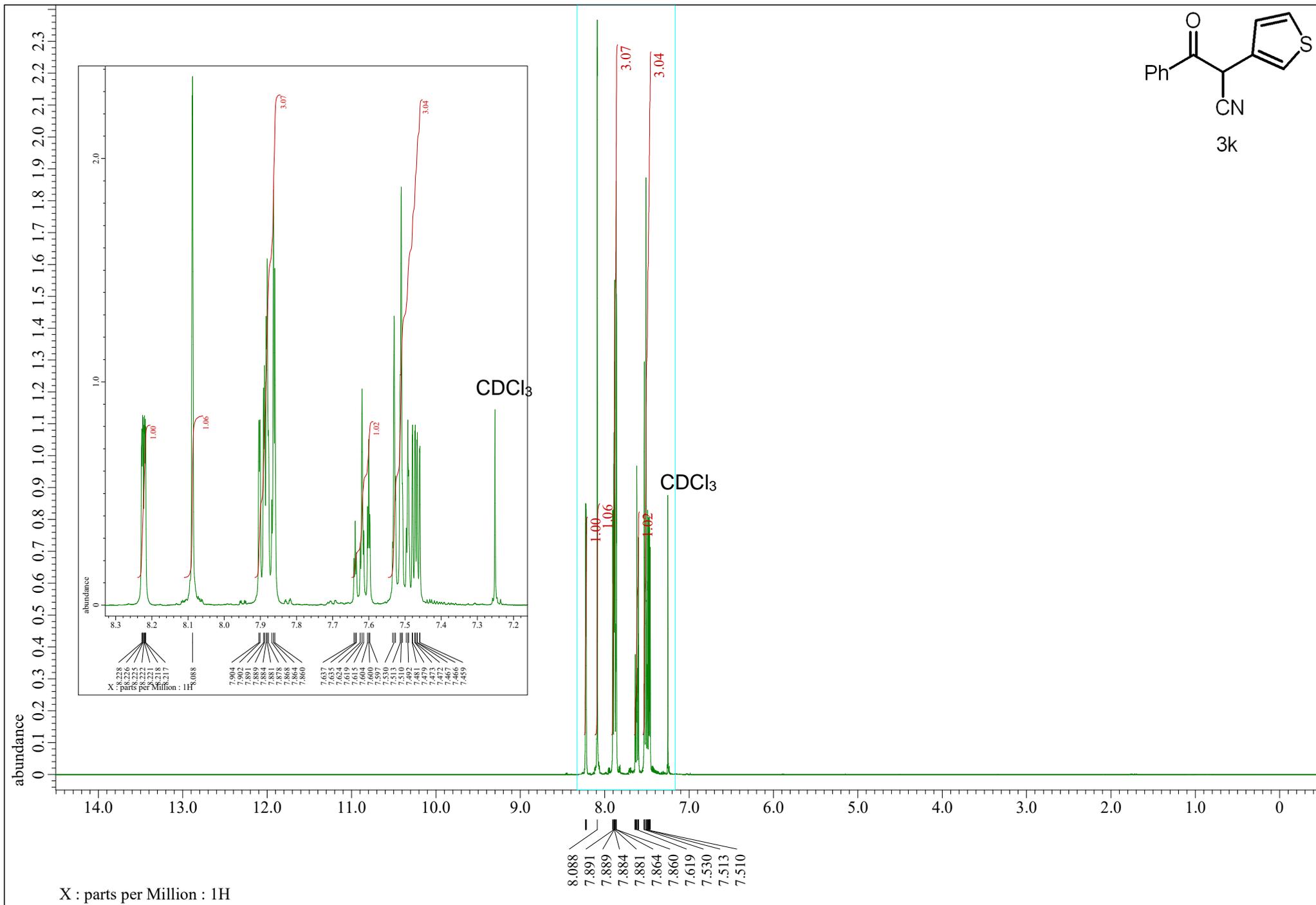


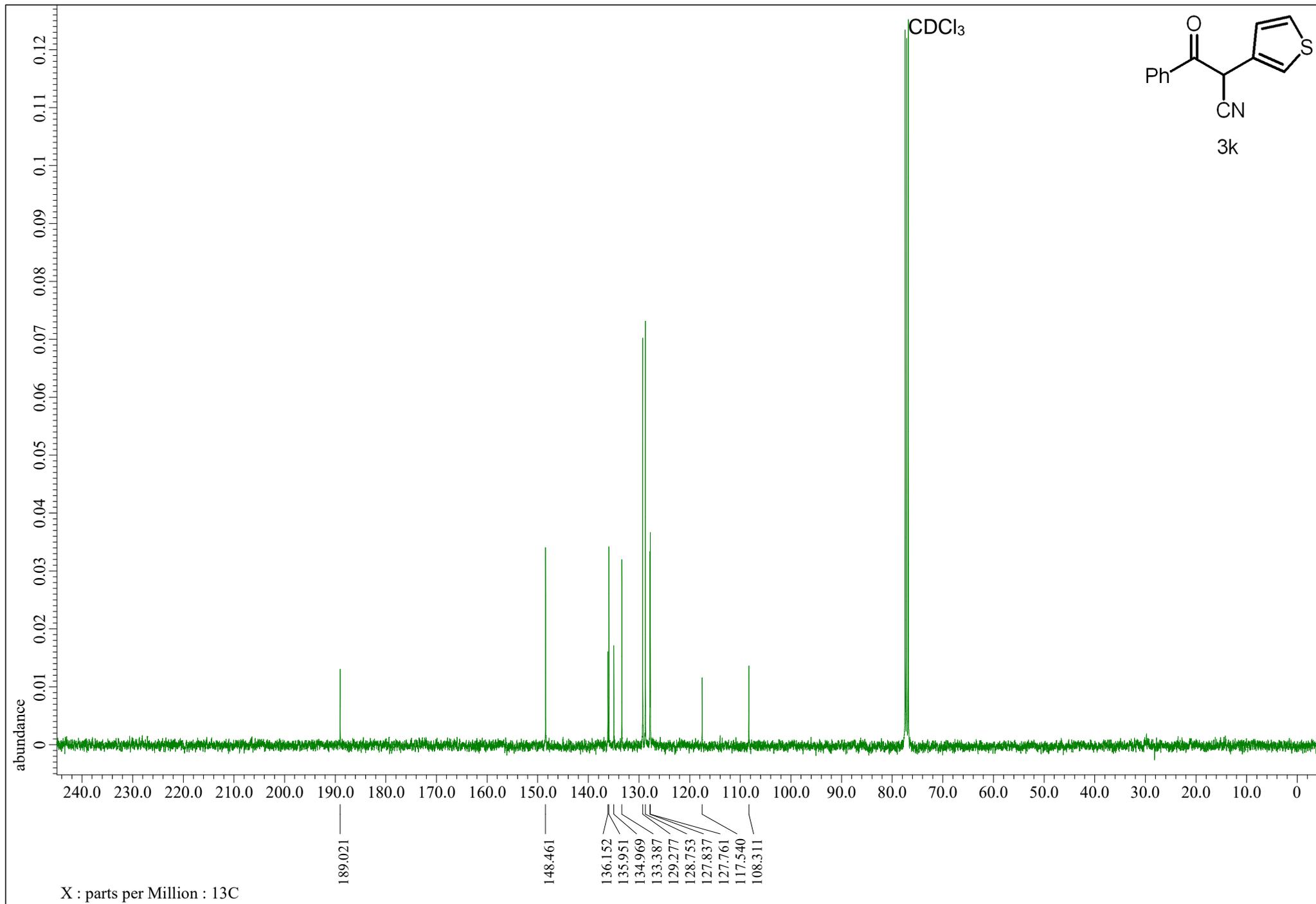


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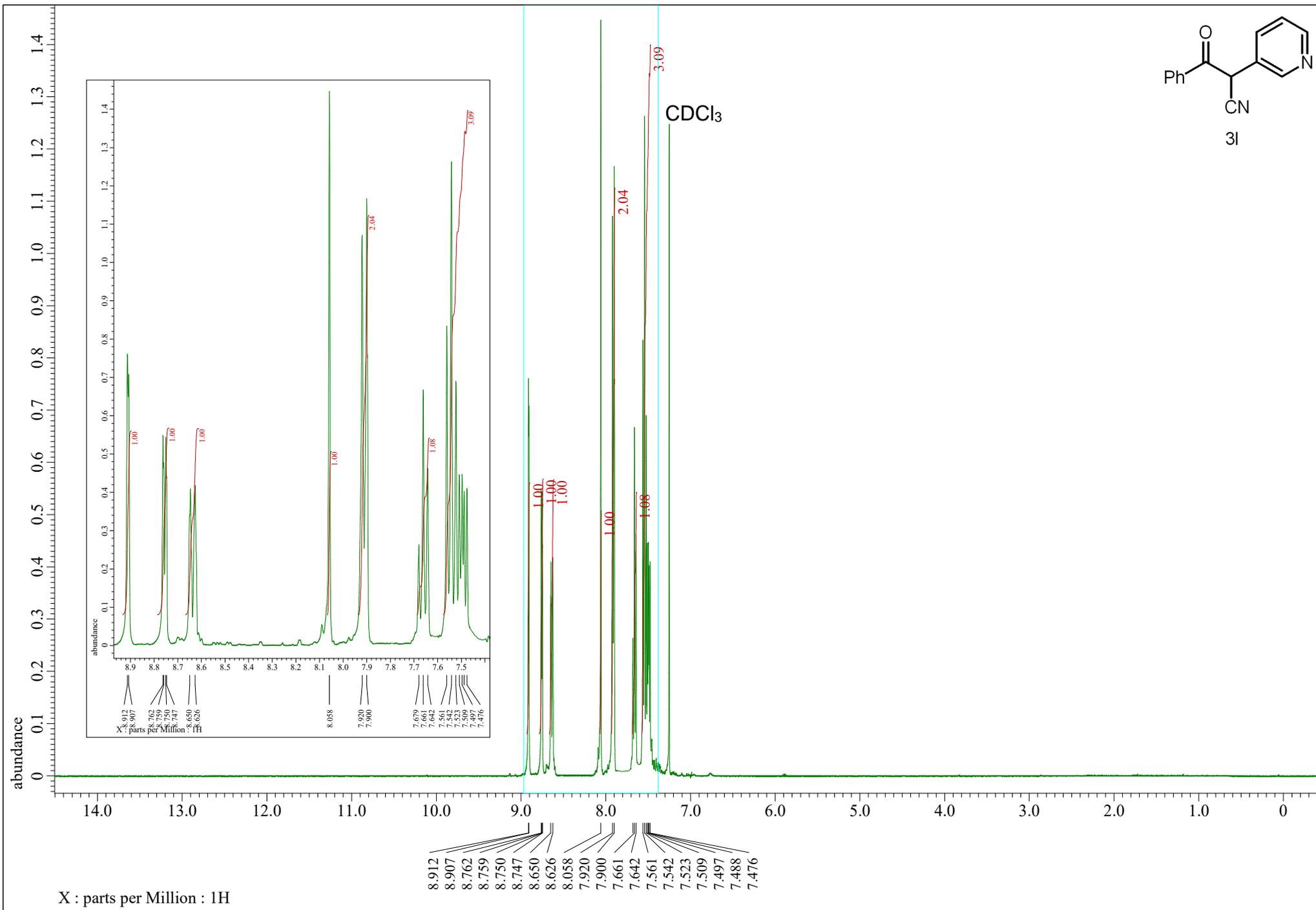
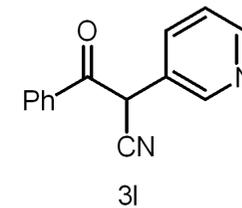


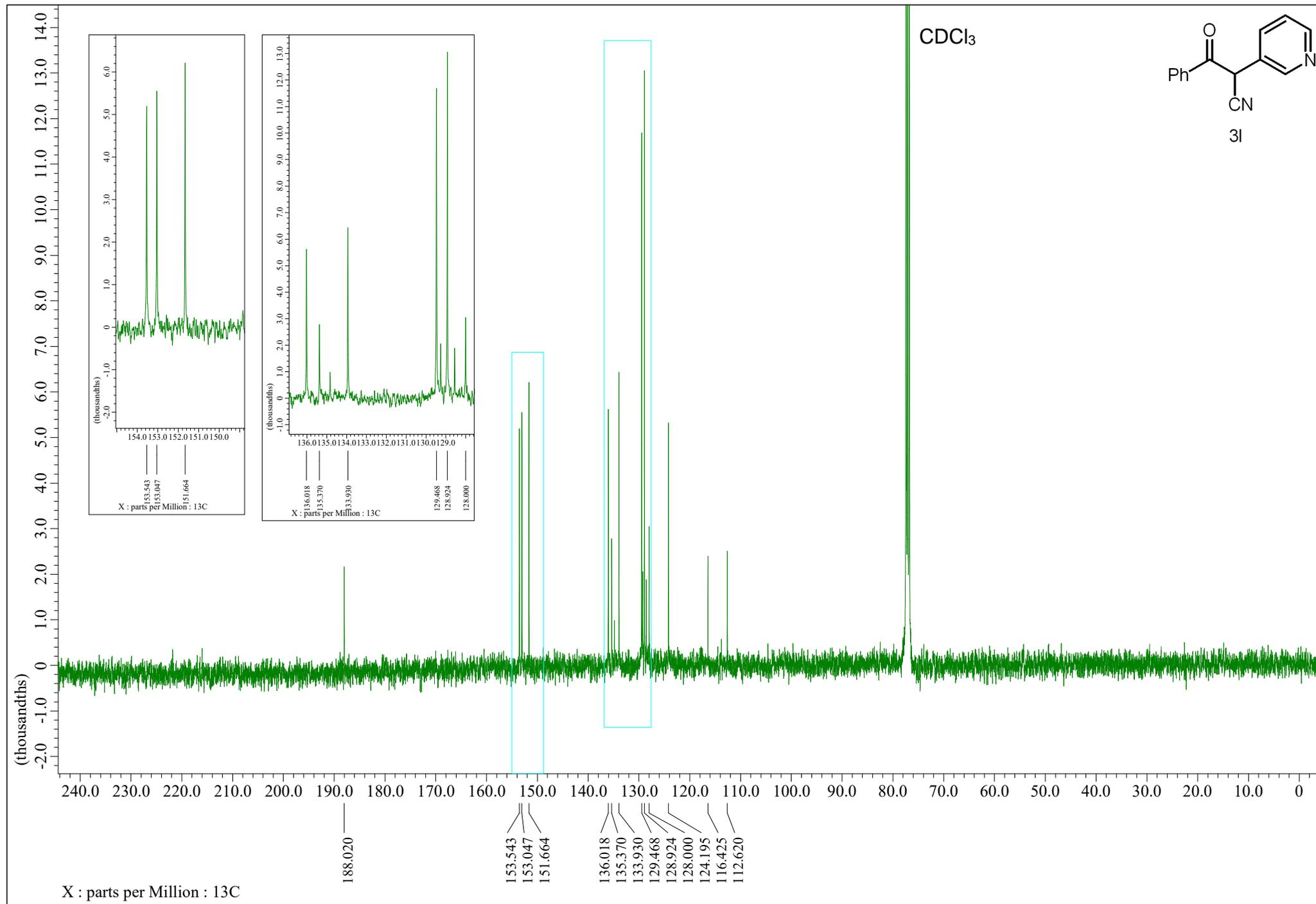
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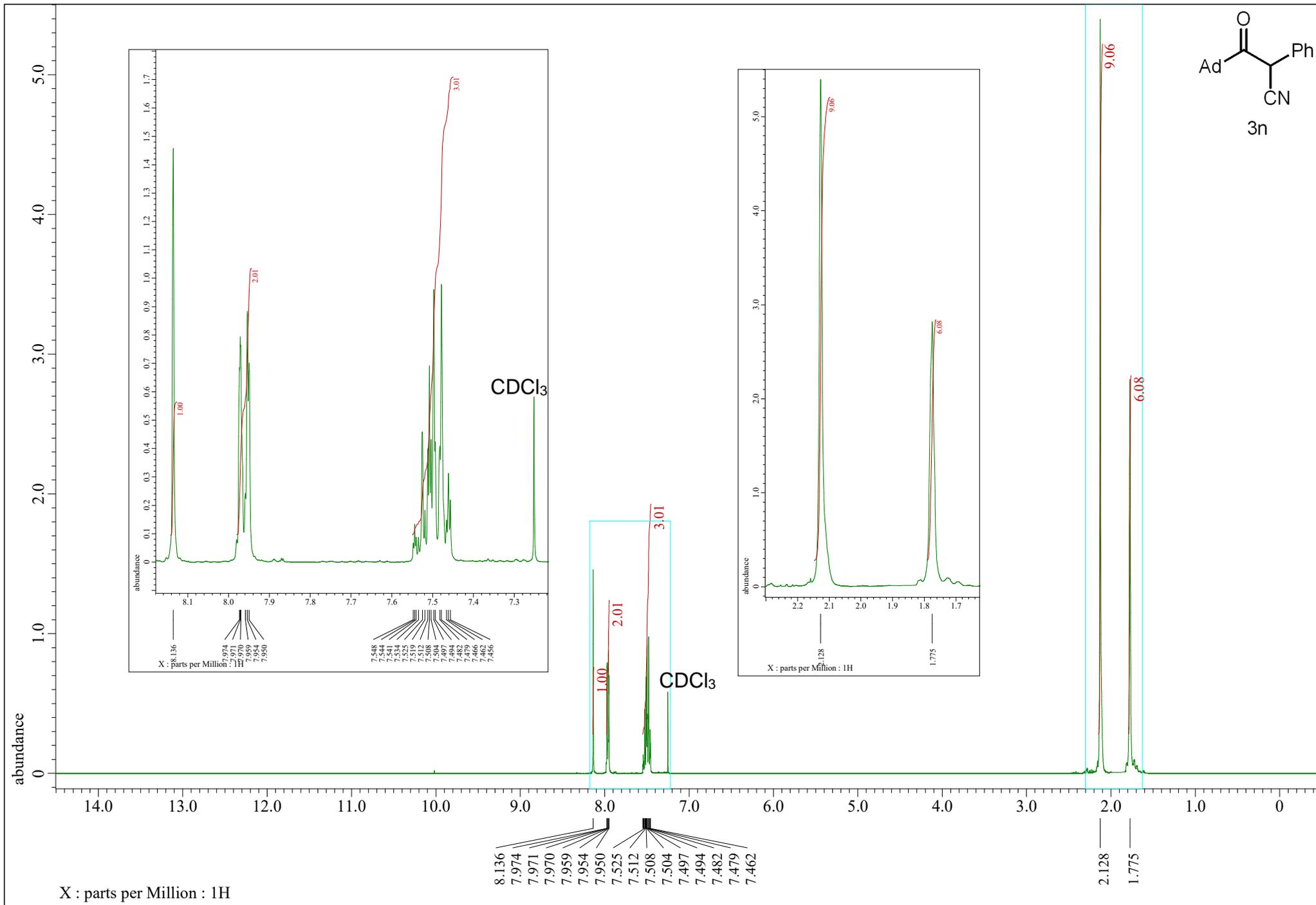


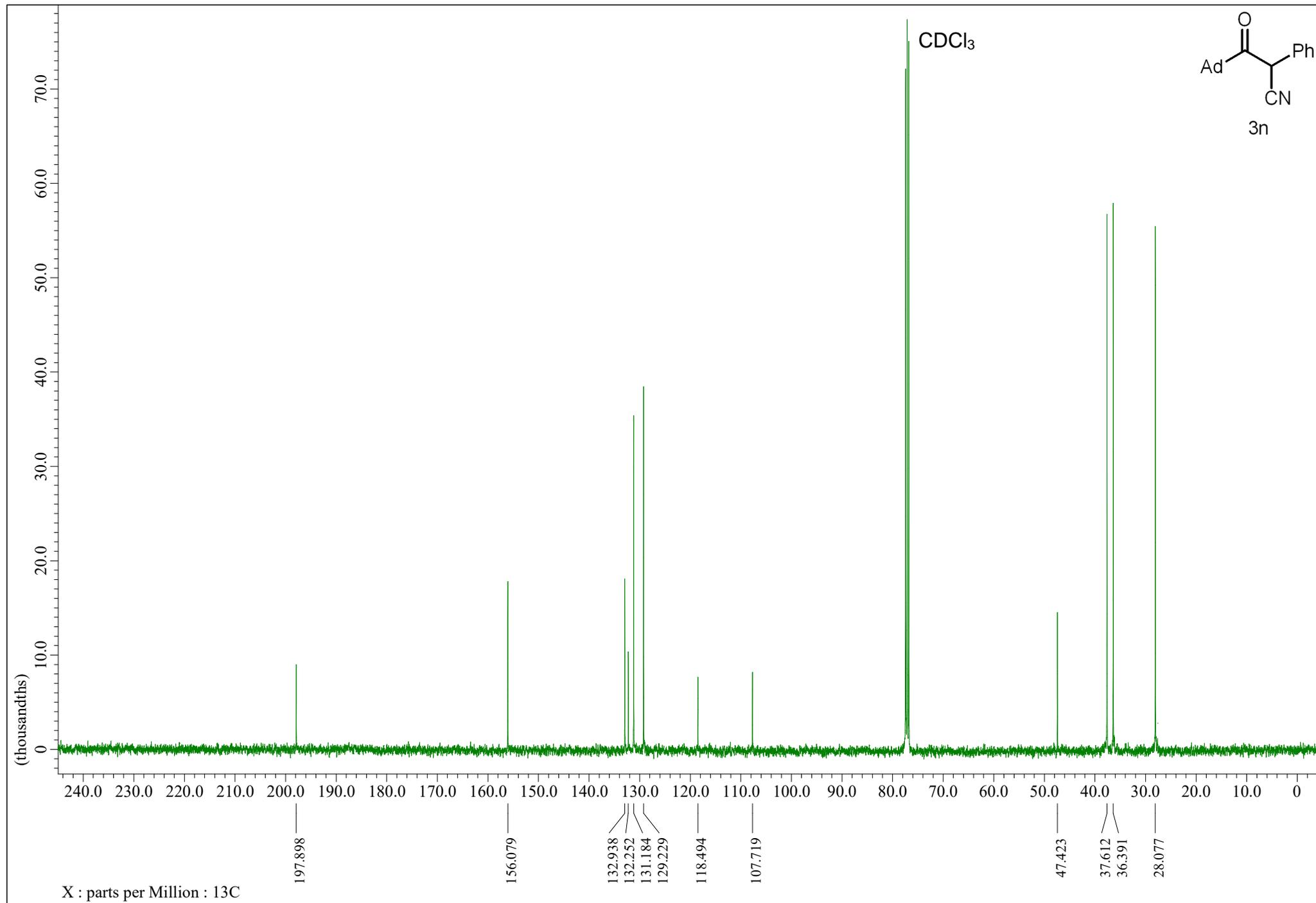
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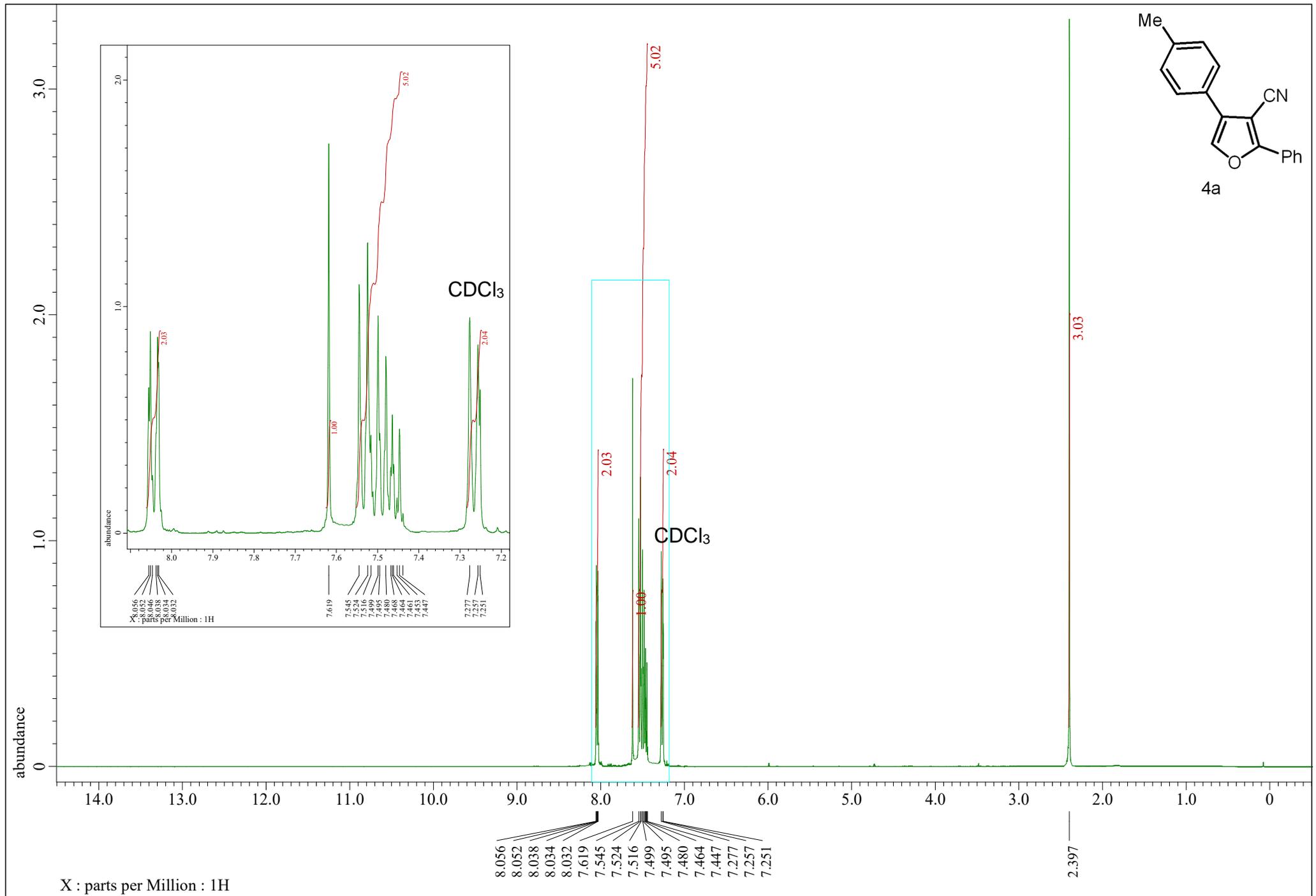


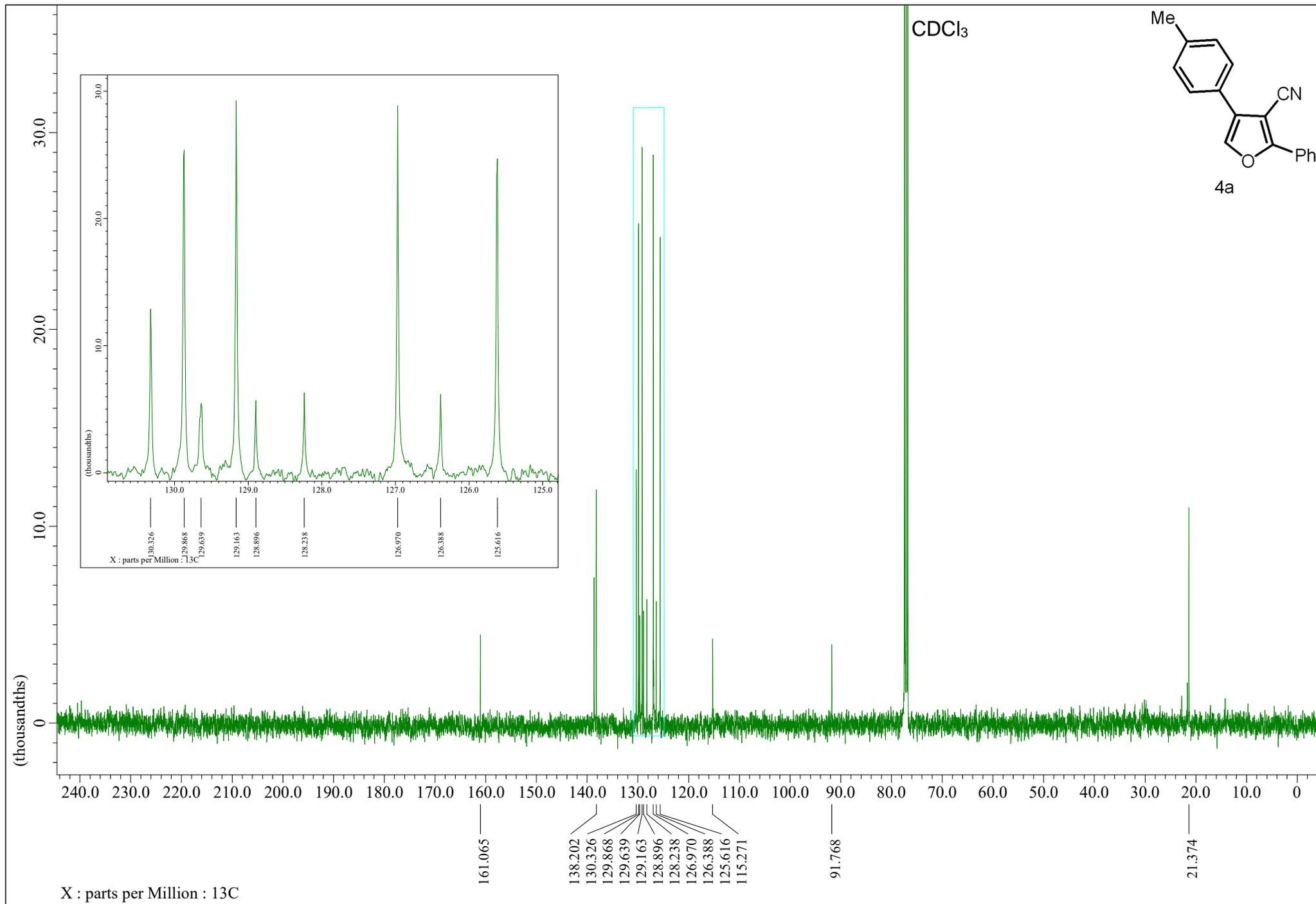
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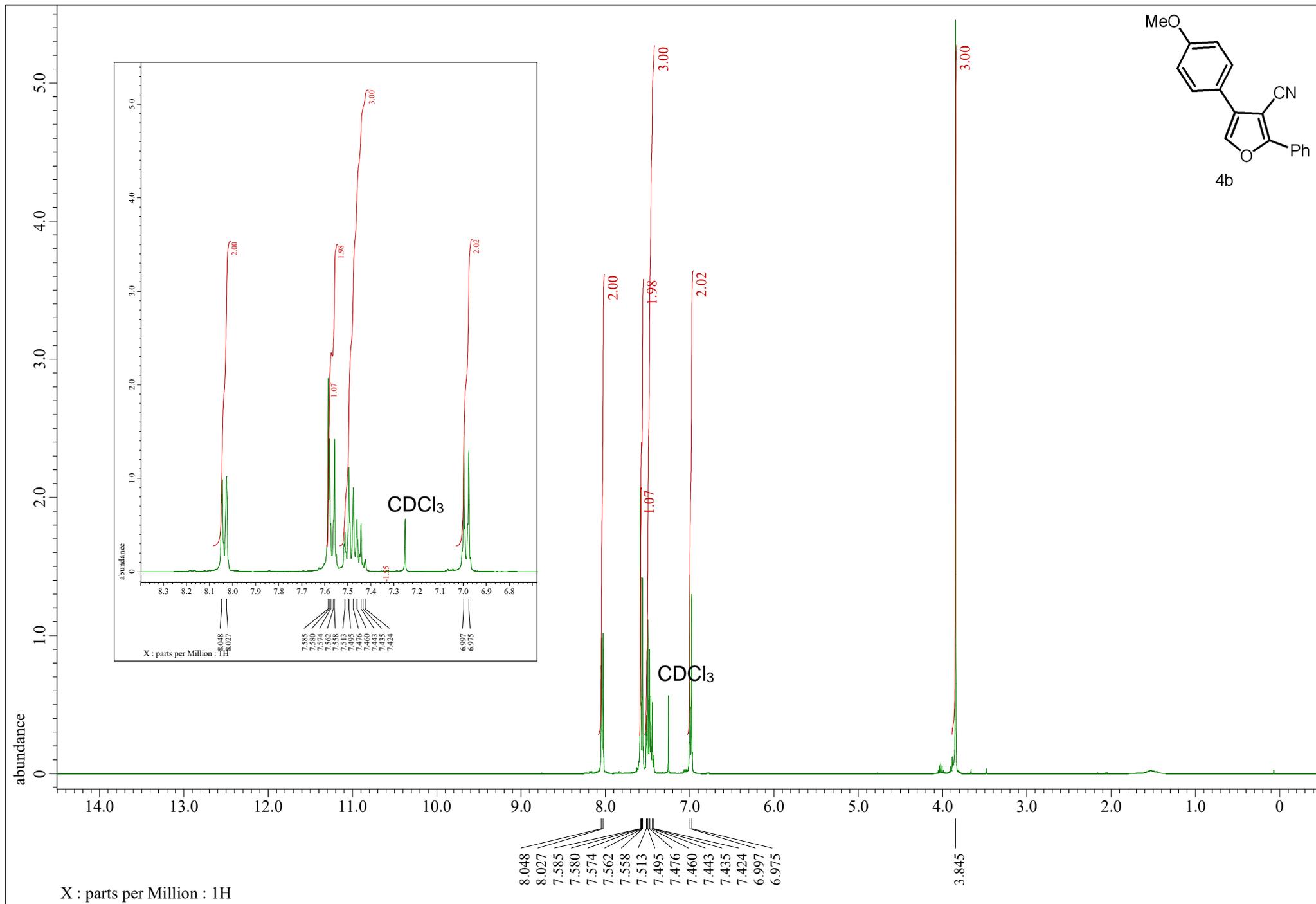


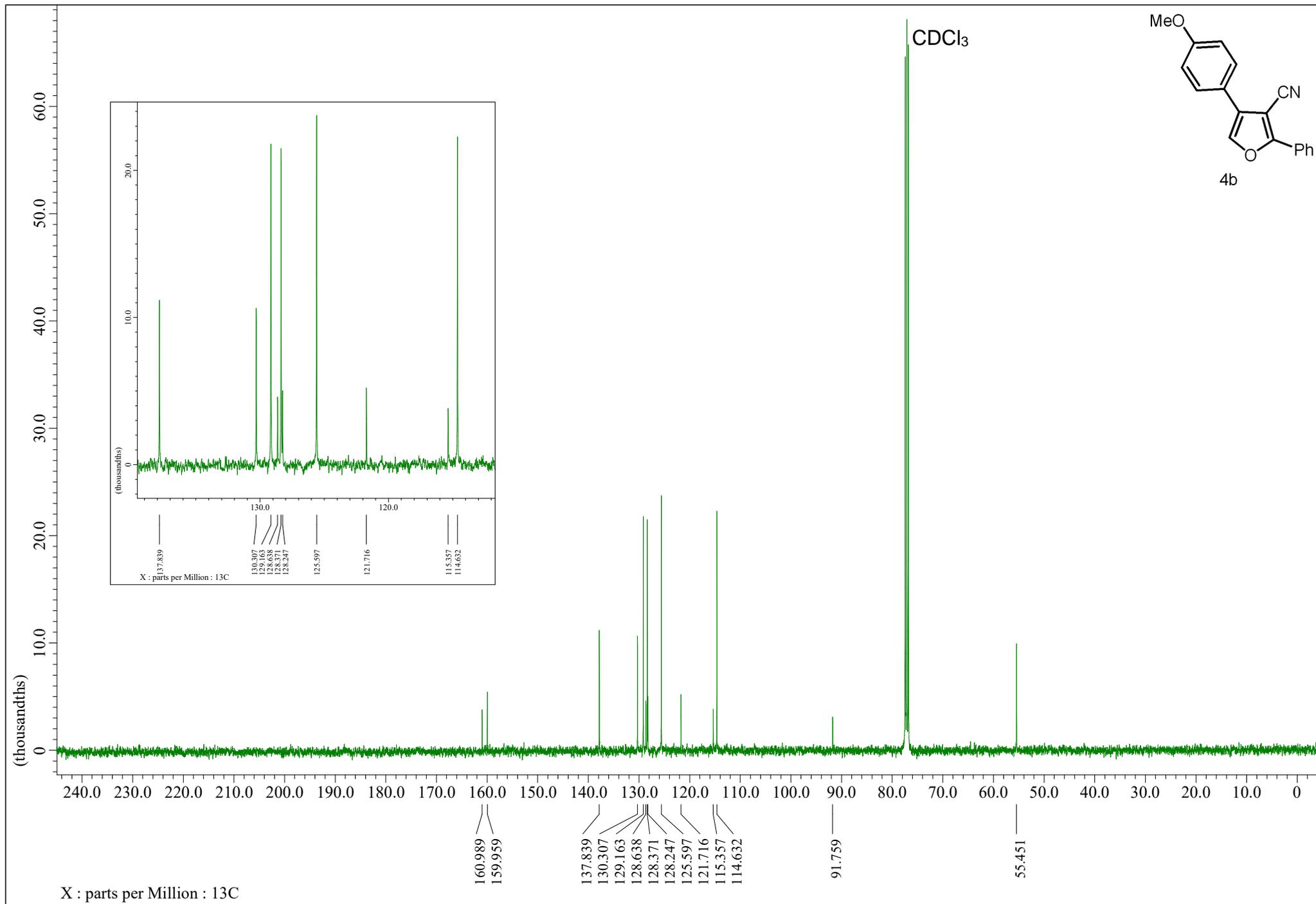
<sup>1</sup>H NMR



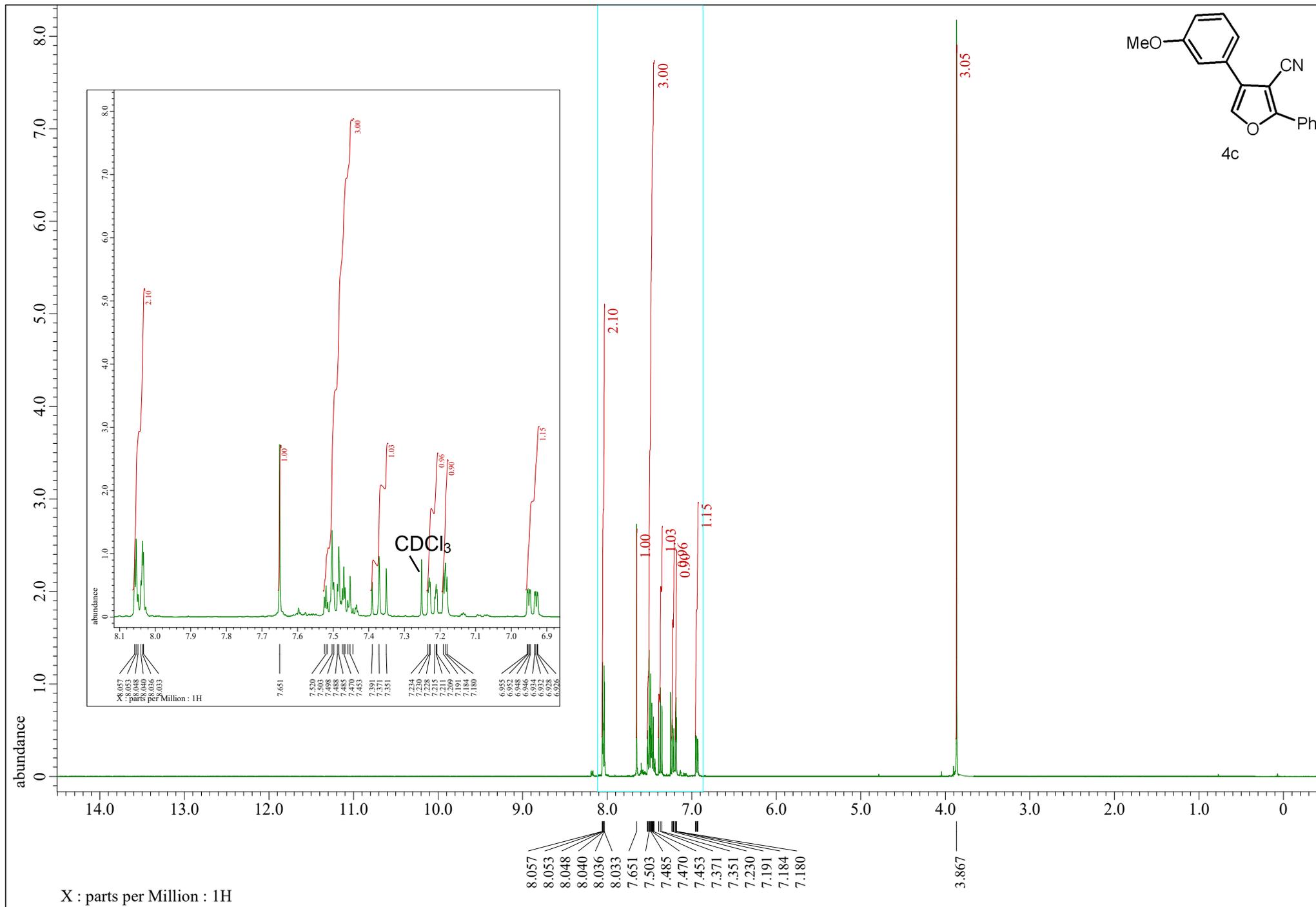


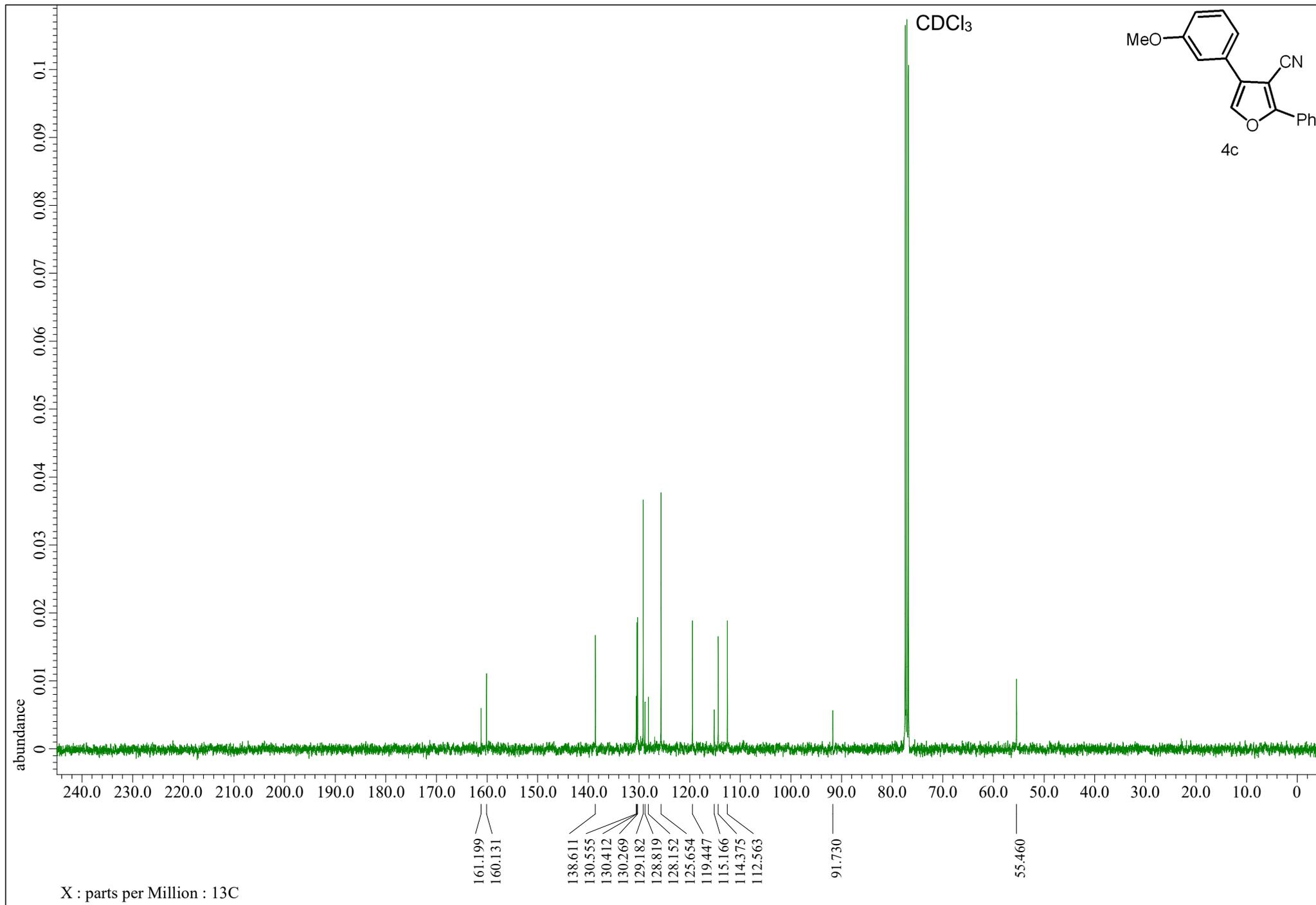
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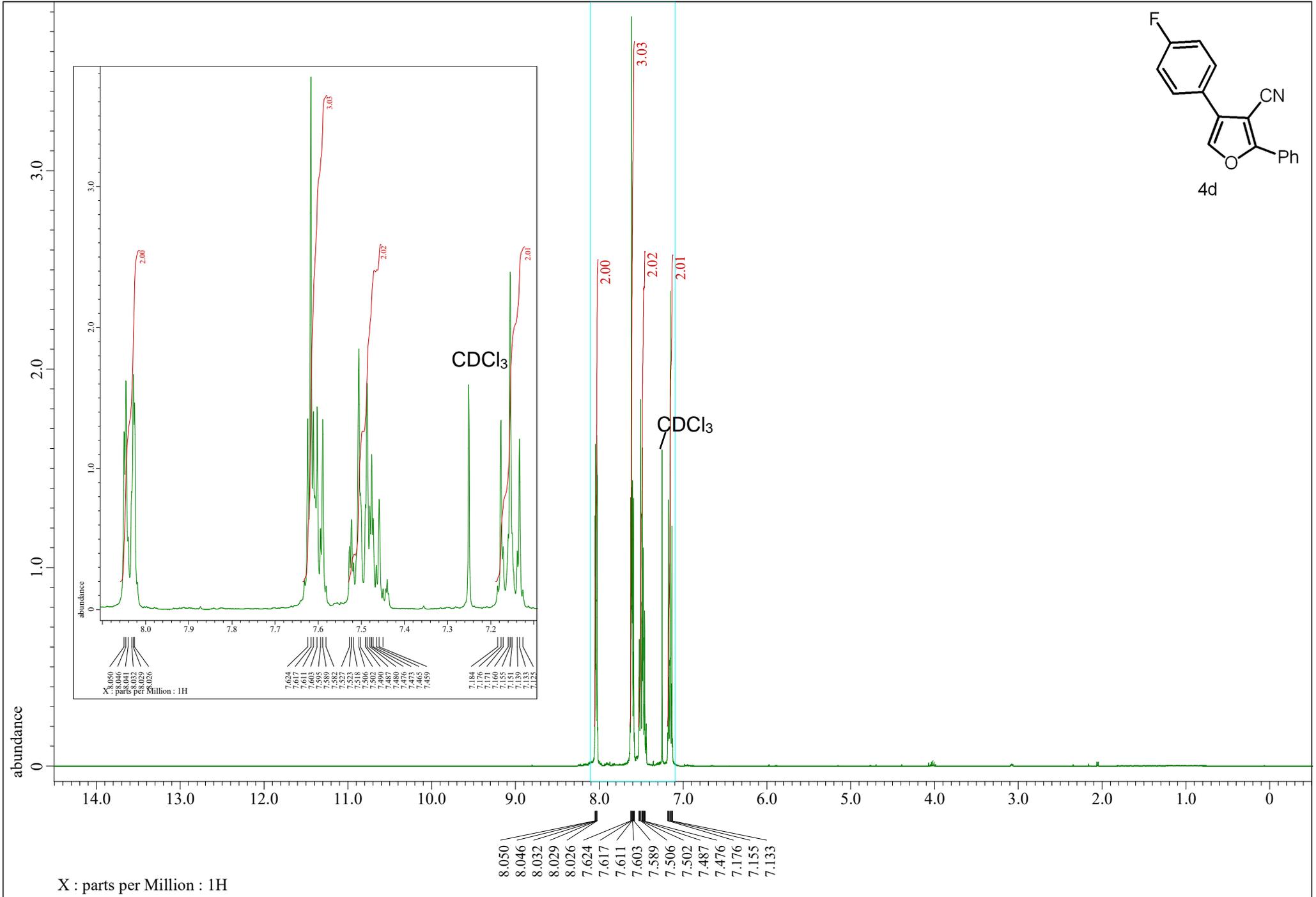


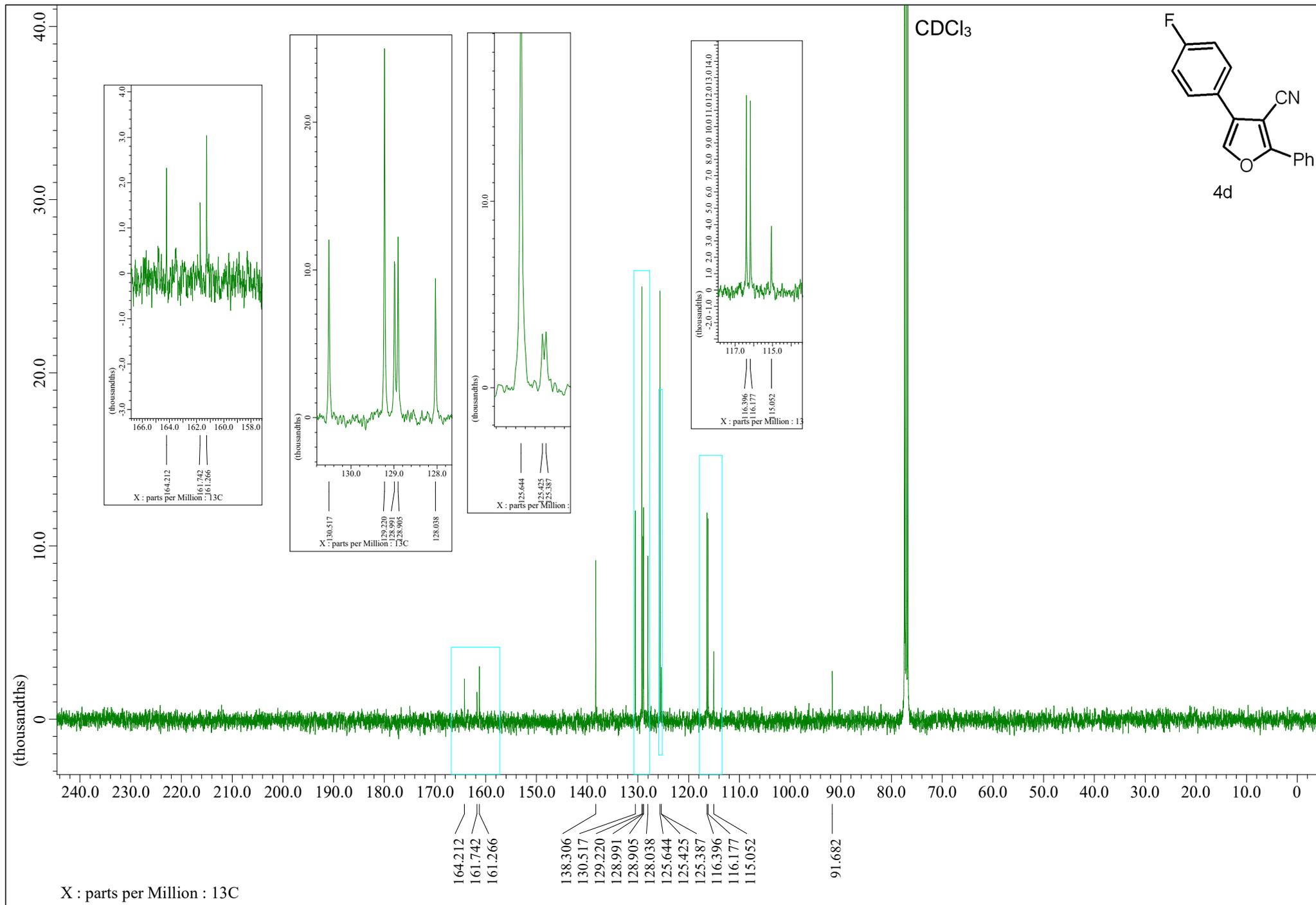
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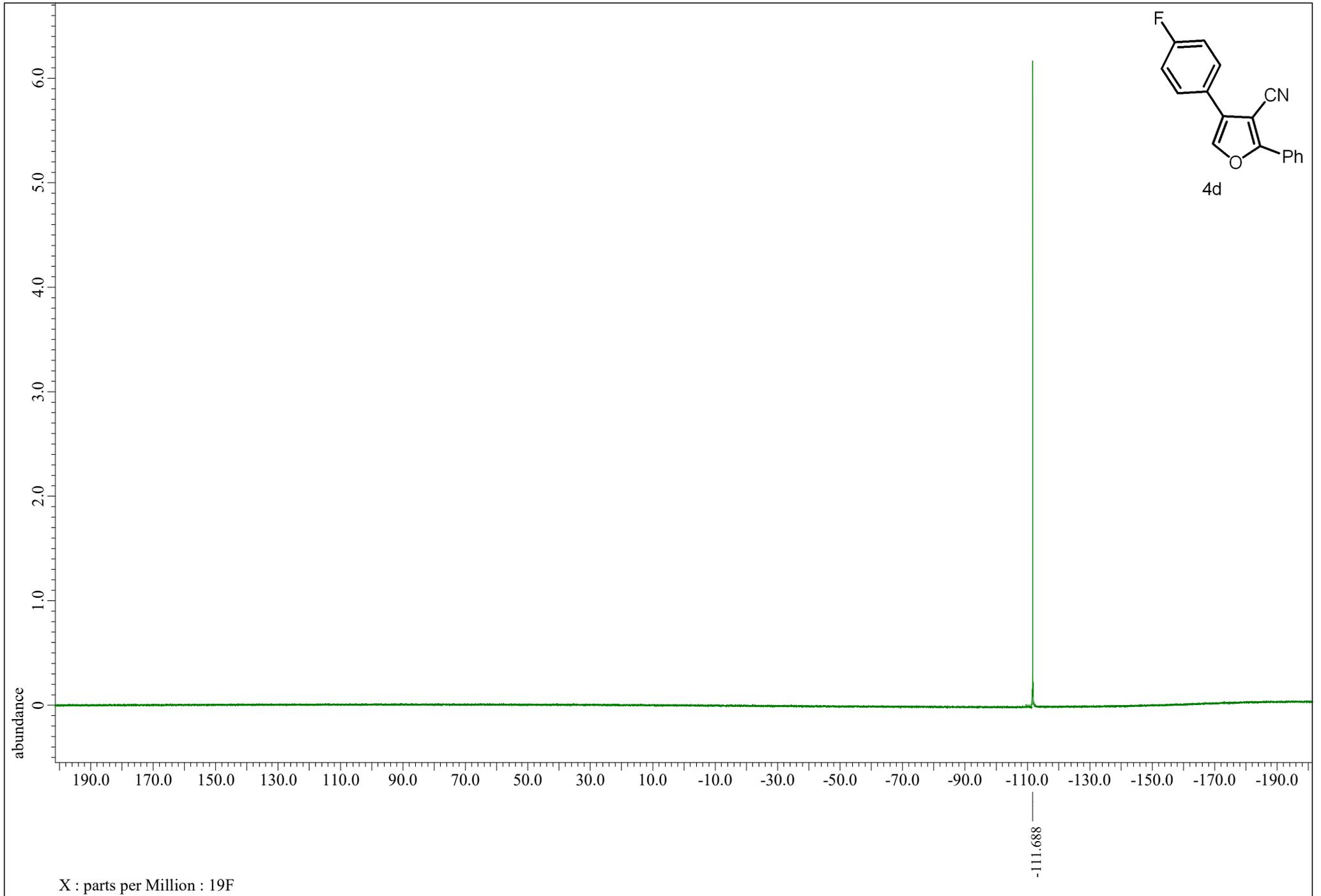


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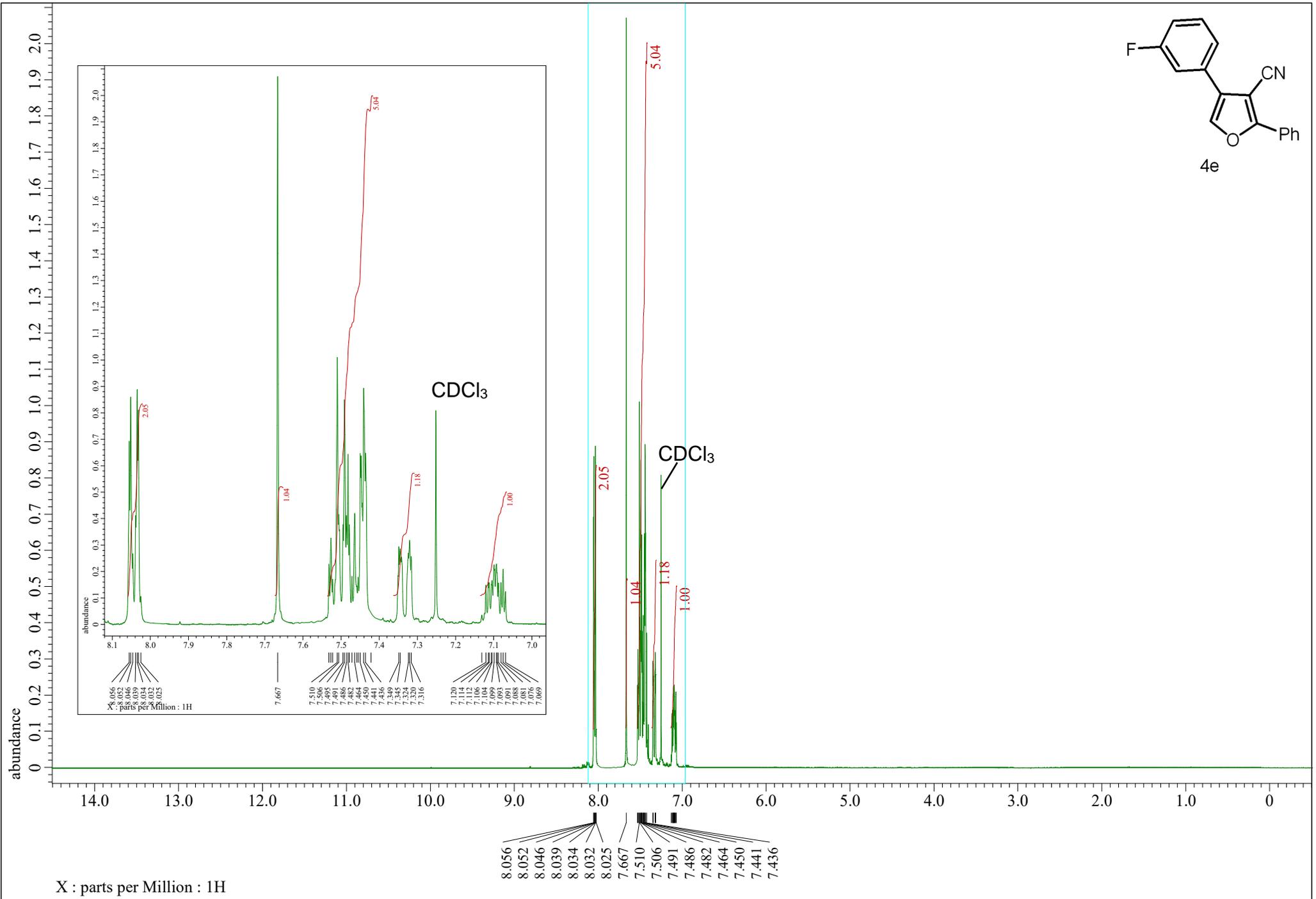
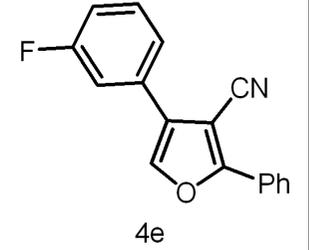




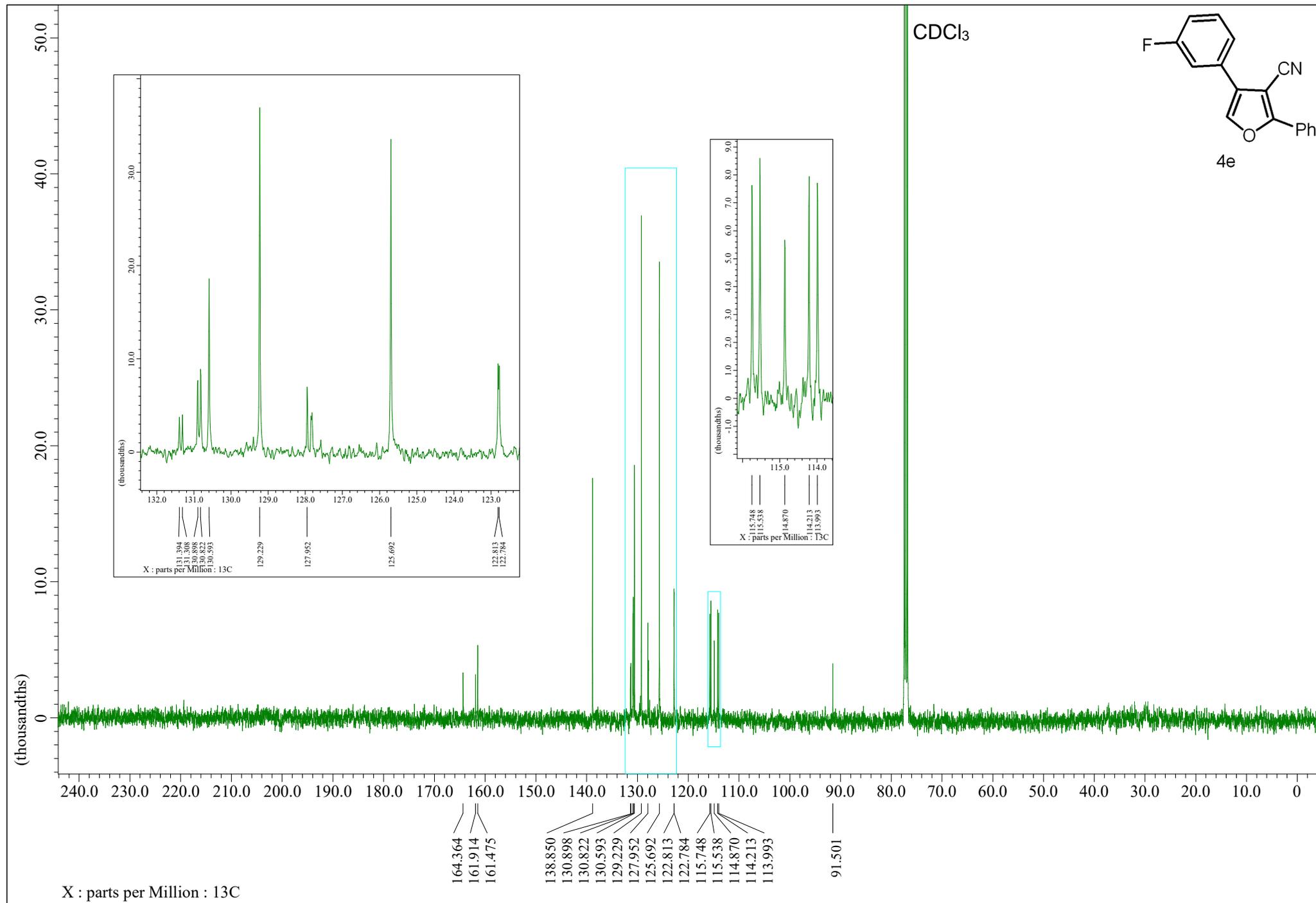
<sup>19</sup>F NMR



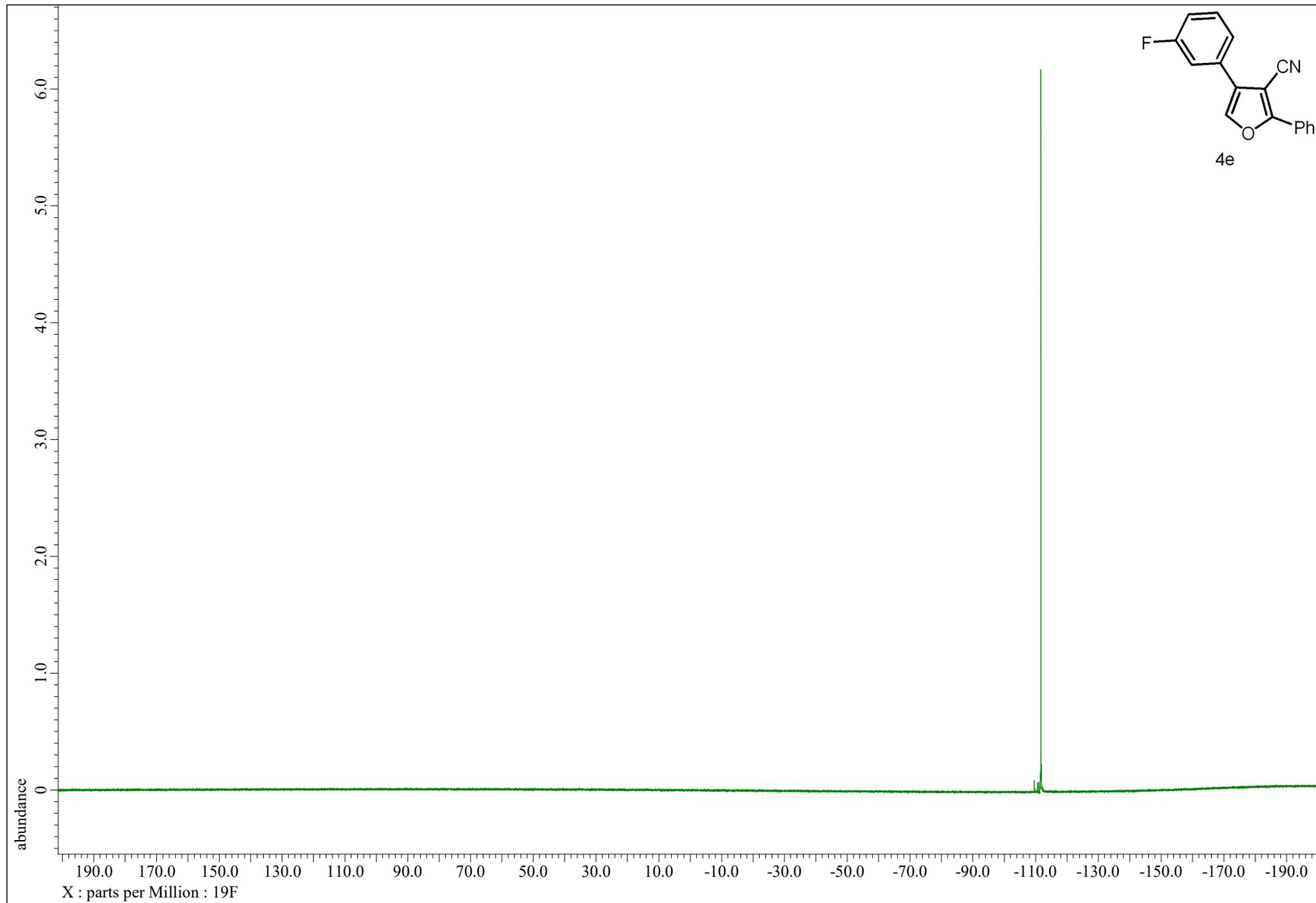
<sup>1</sup>H NMR



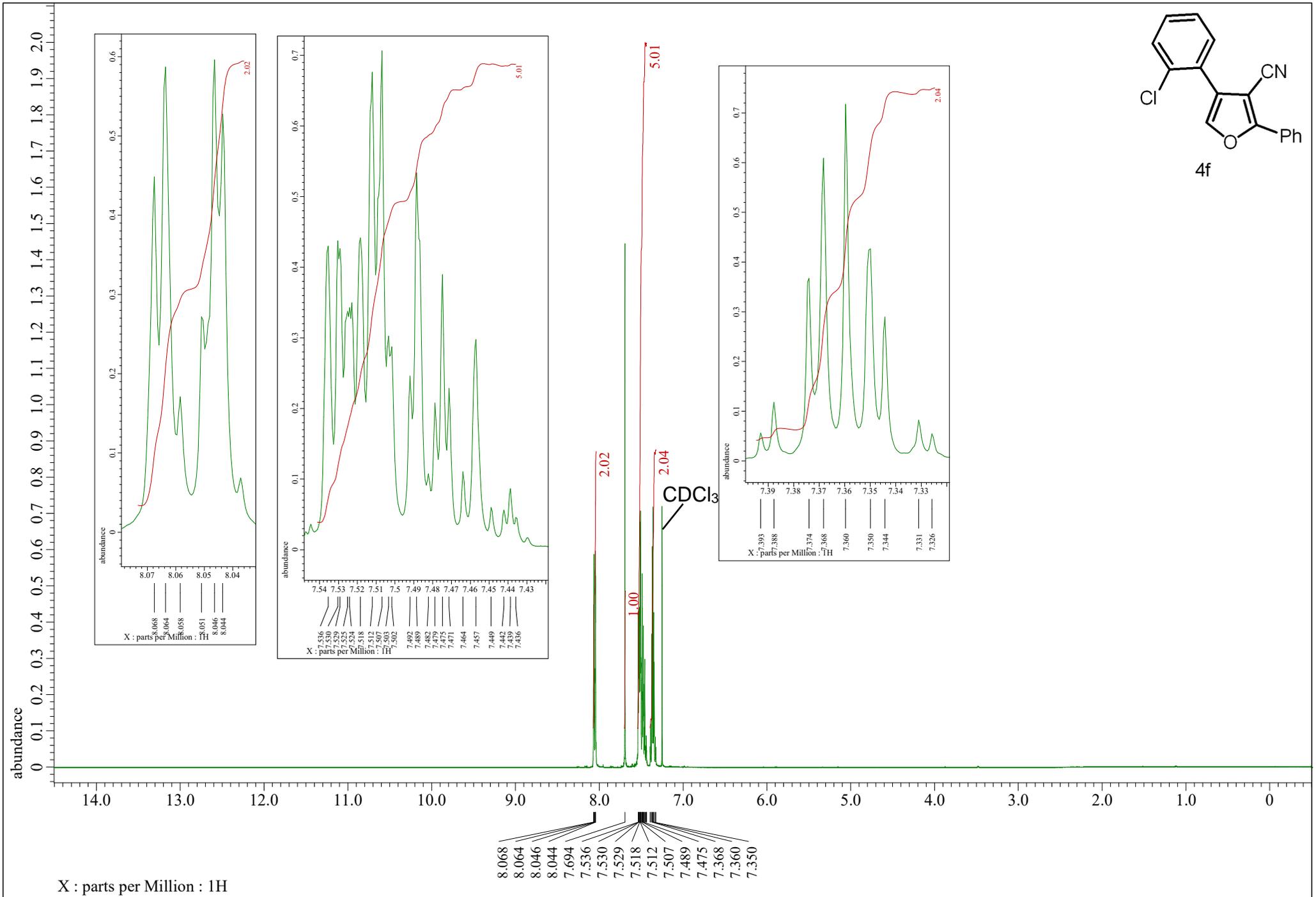
<sup>13</sup>C NMR

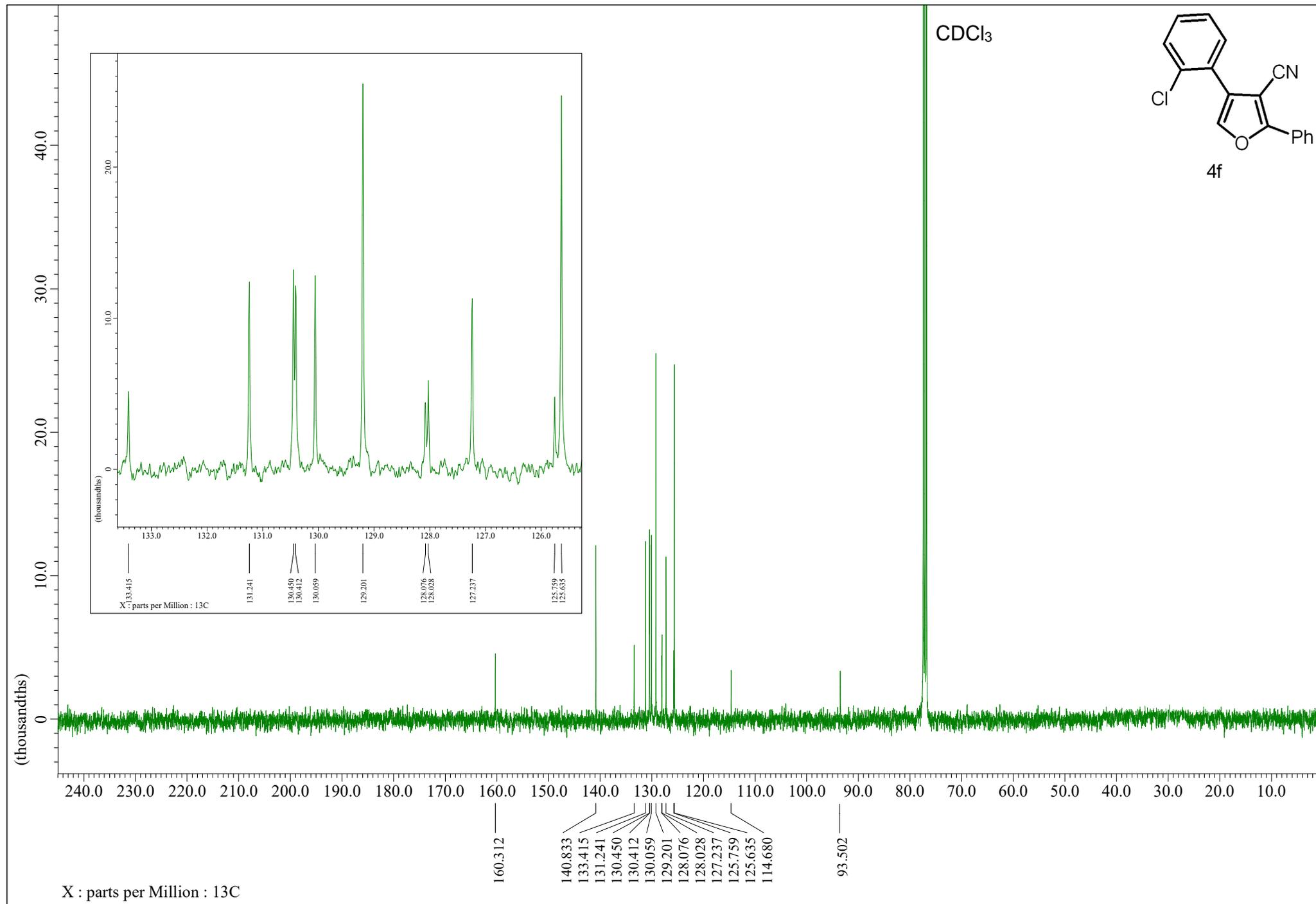


<sup>19</sup>F NMR

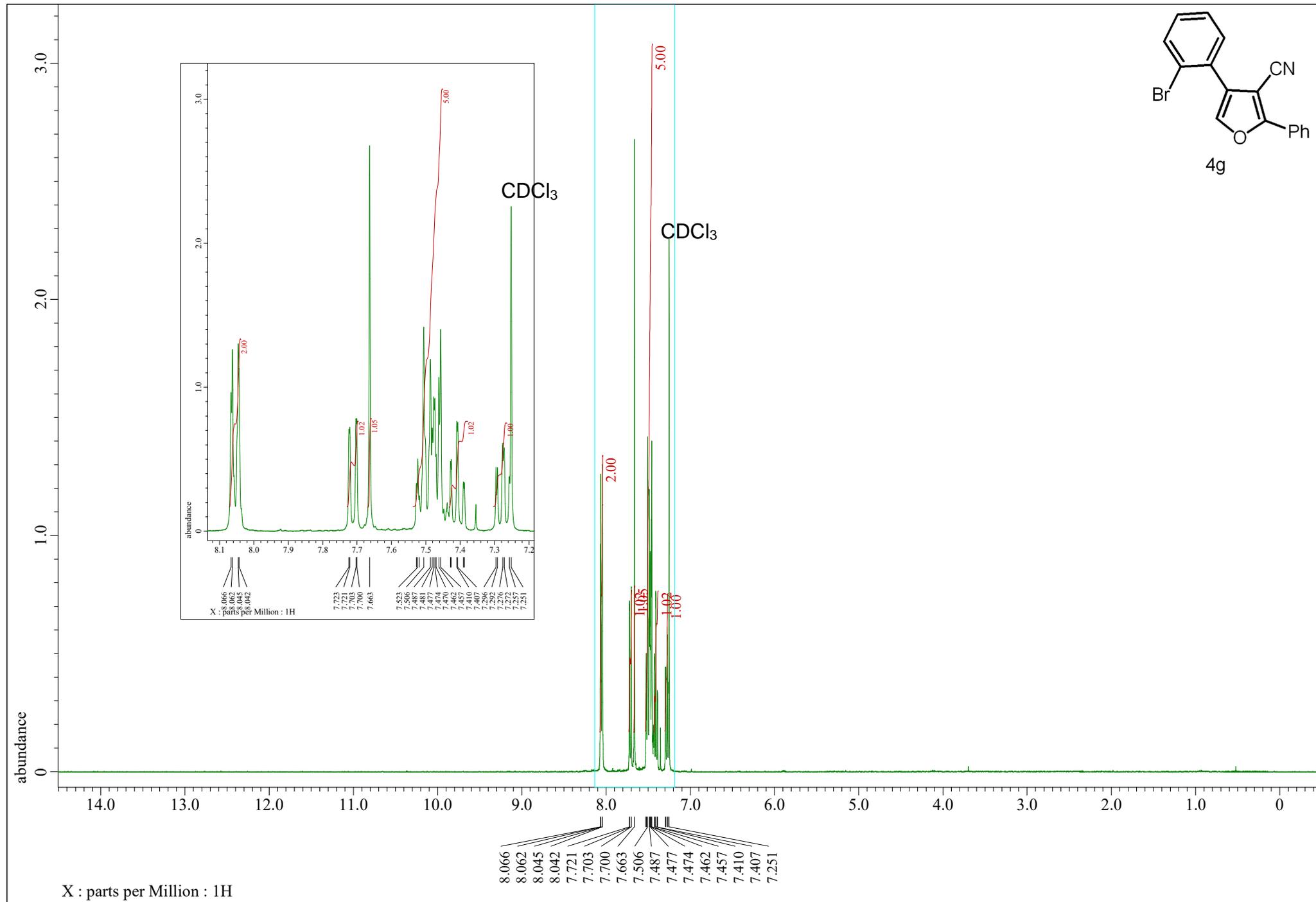


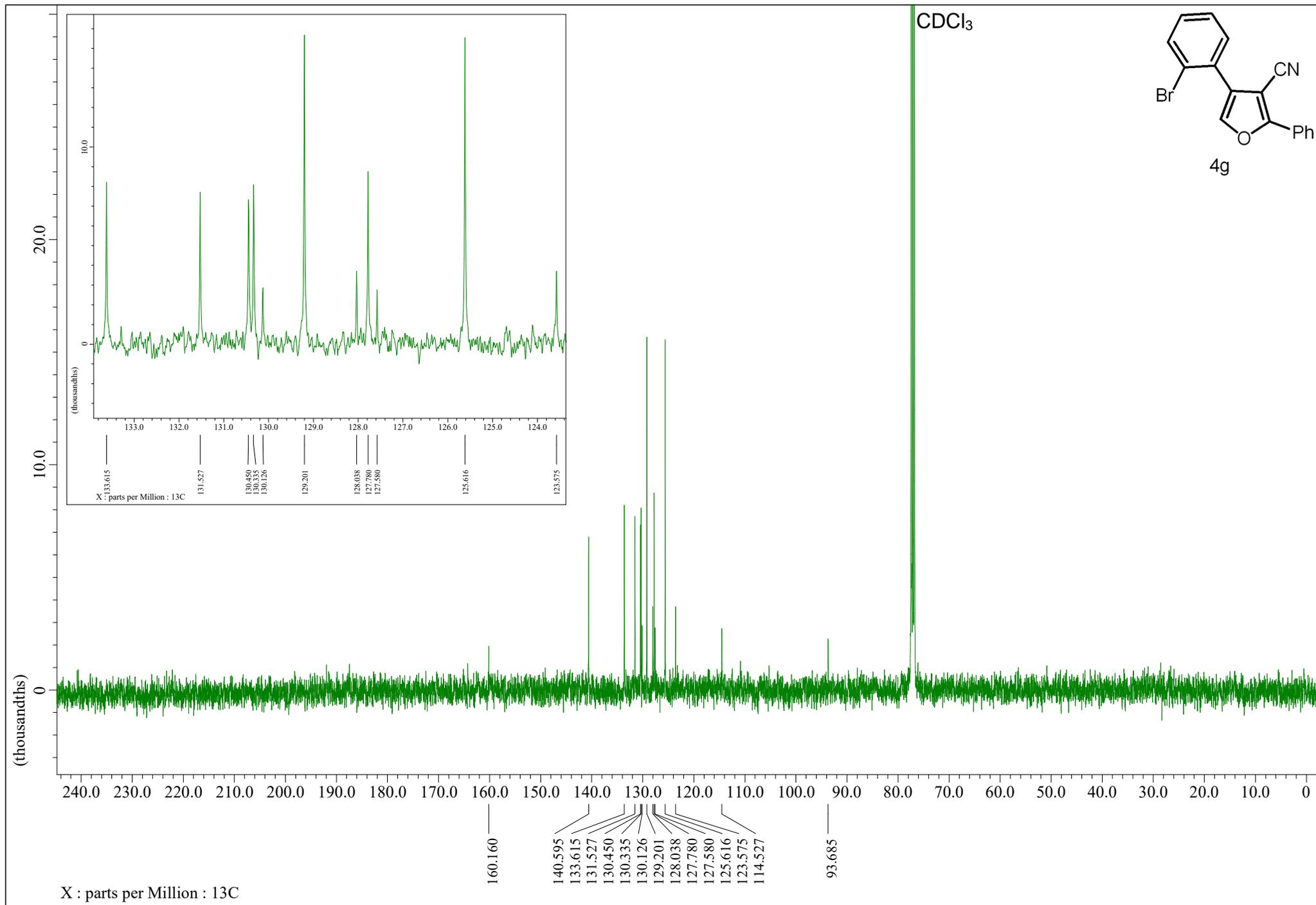
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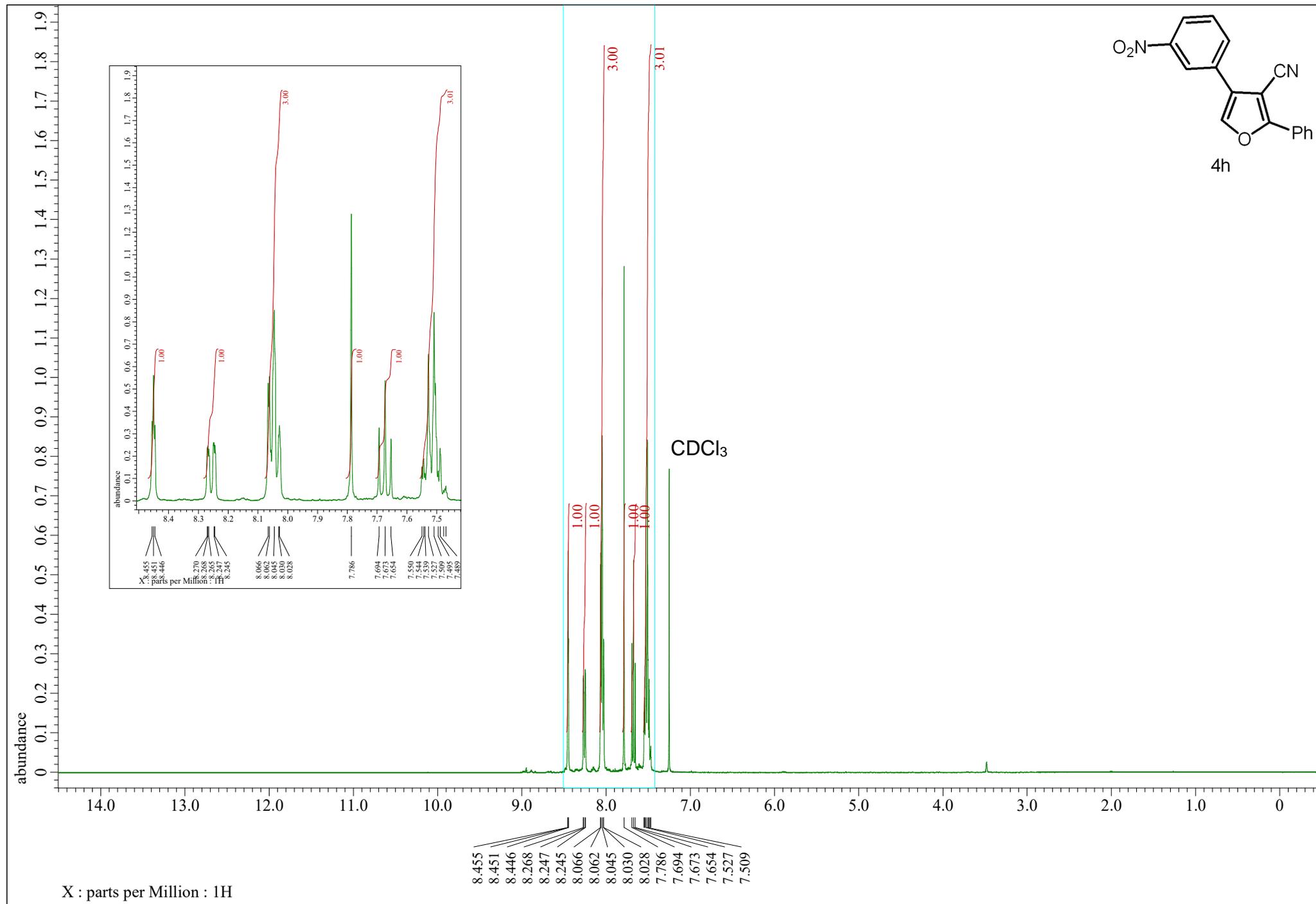


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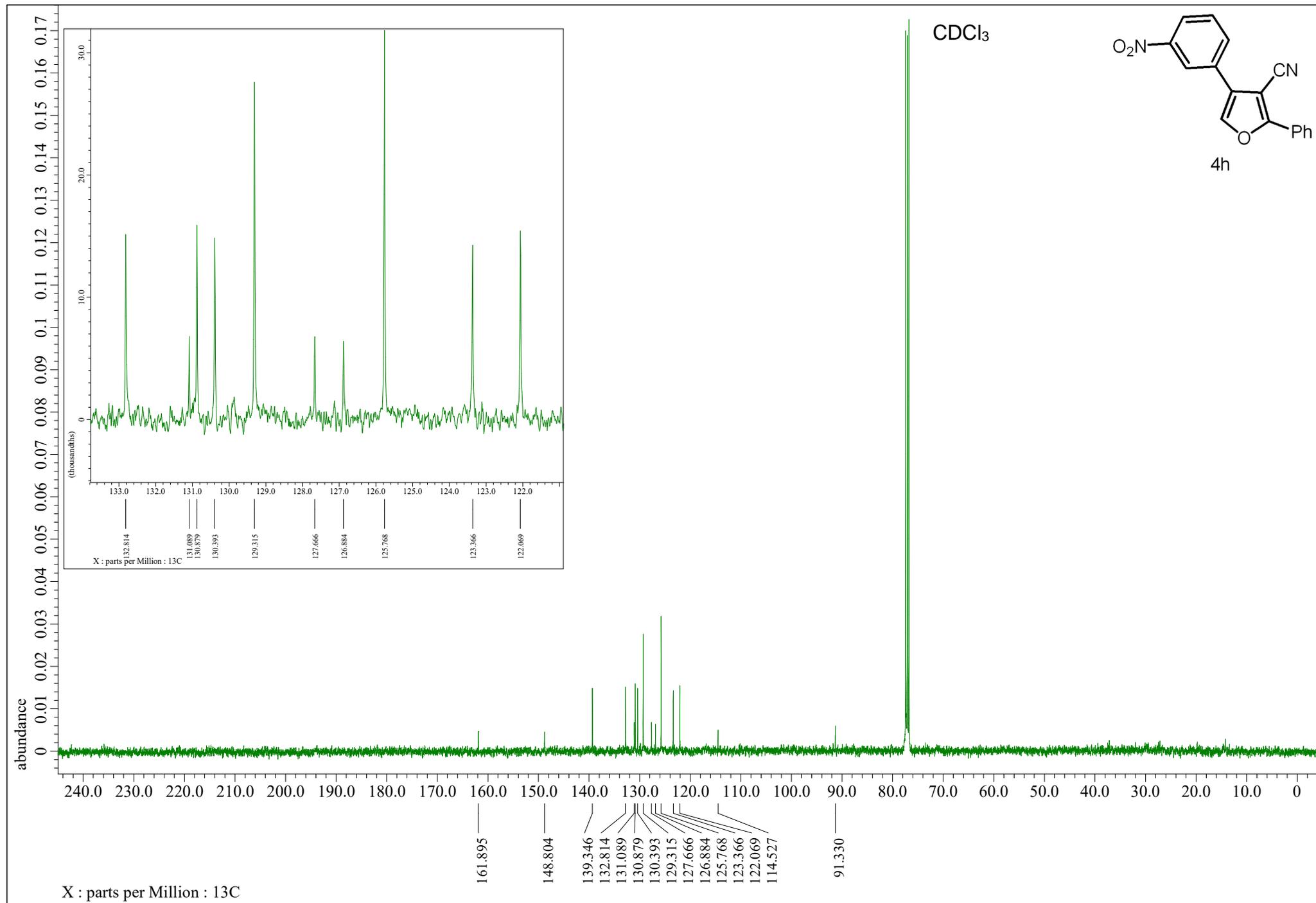




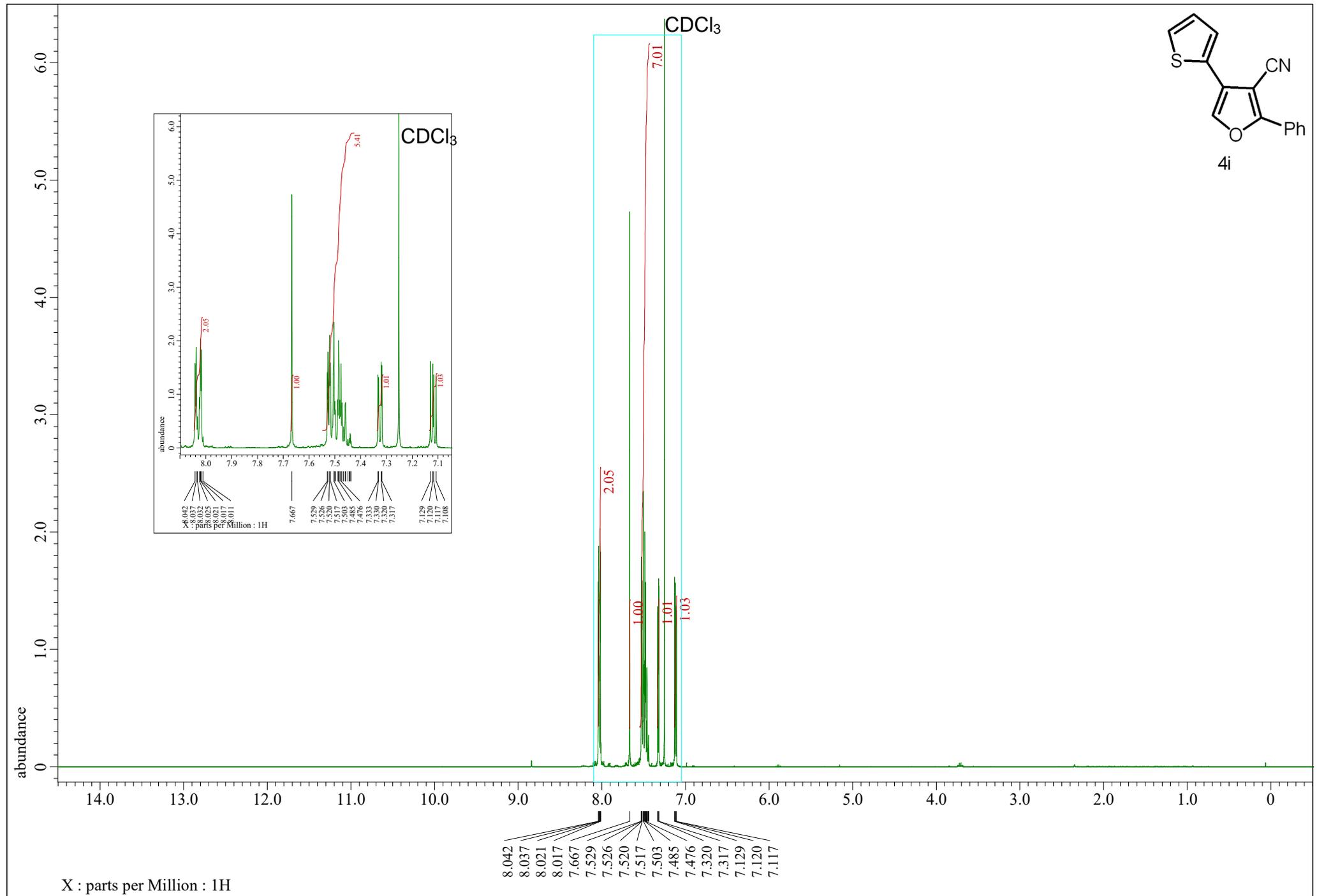
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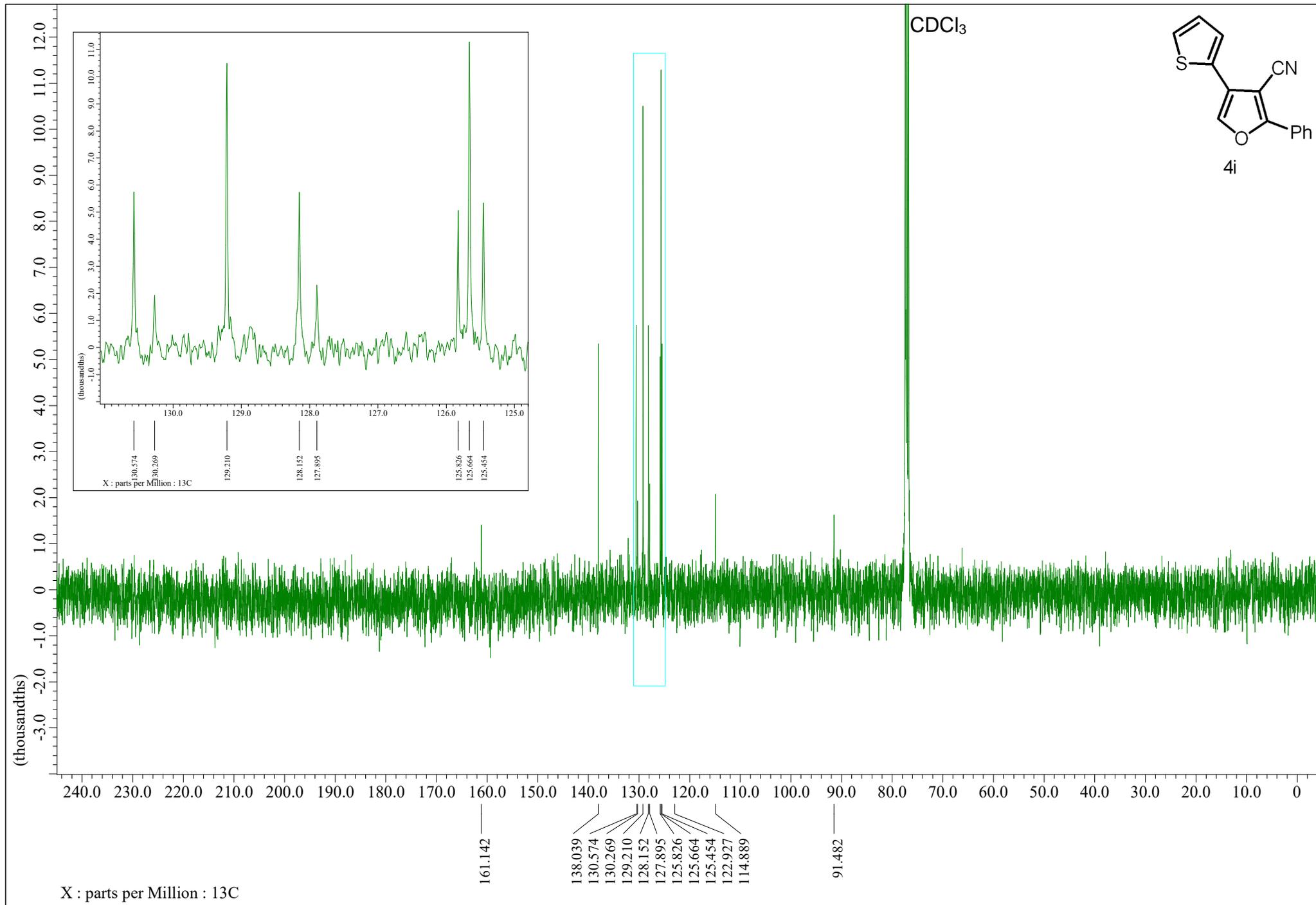


X : parts per Million : <sup>1</sup>H

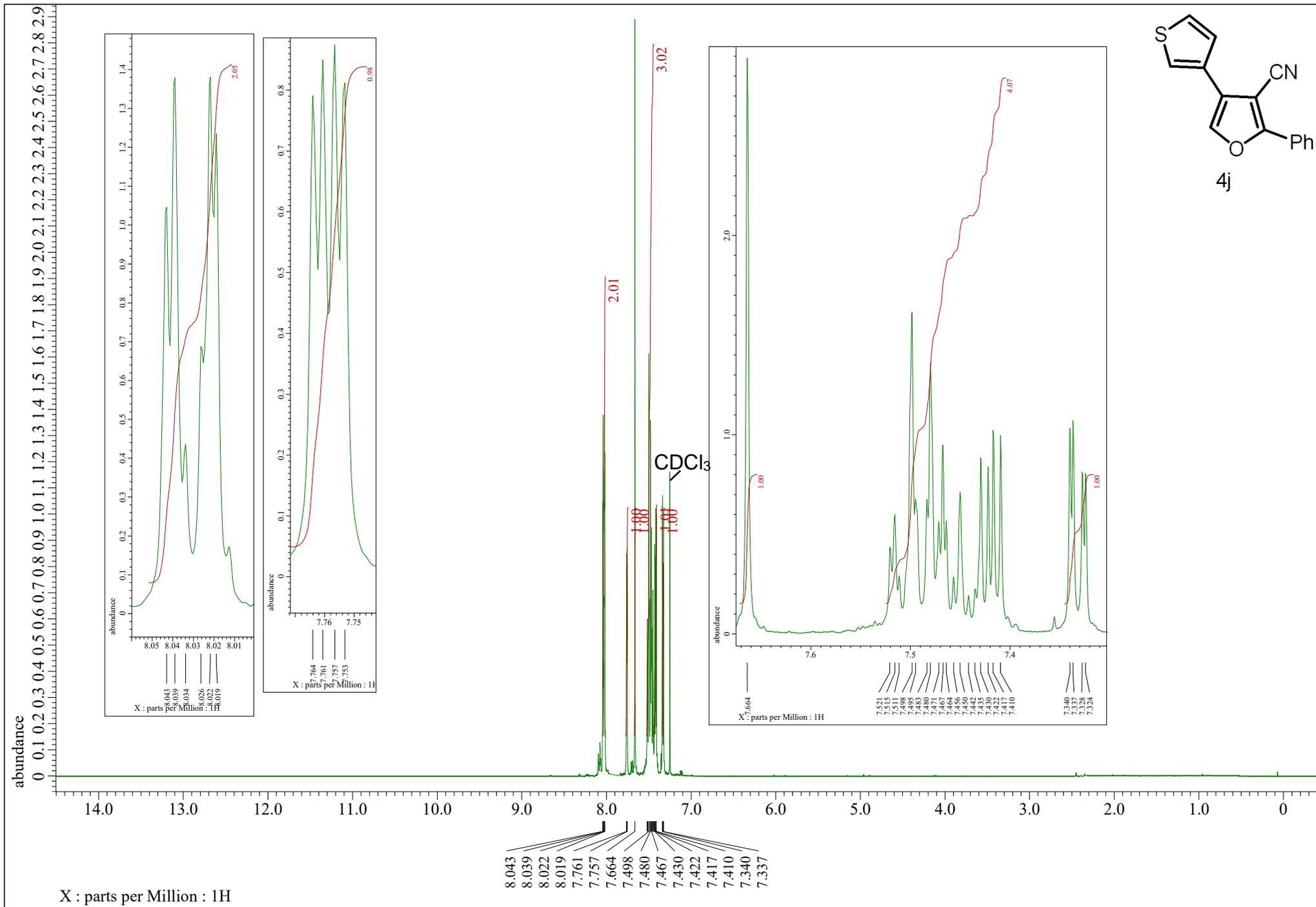


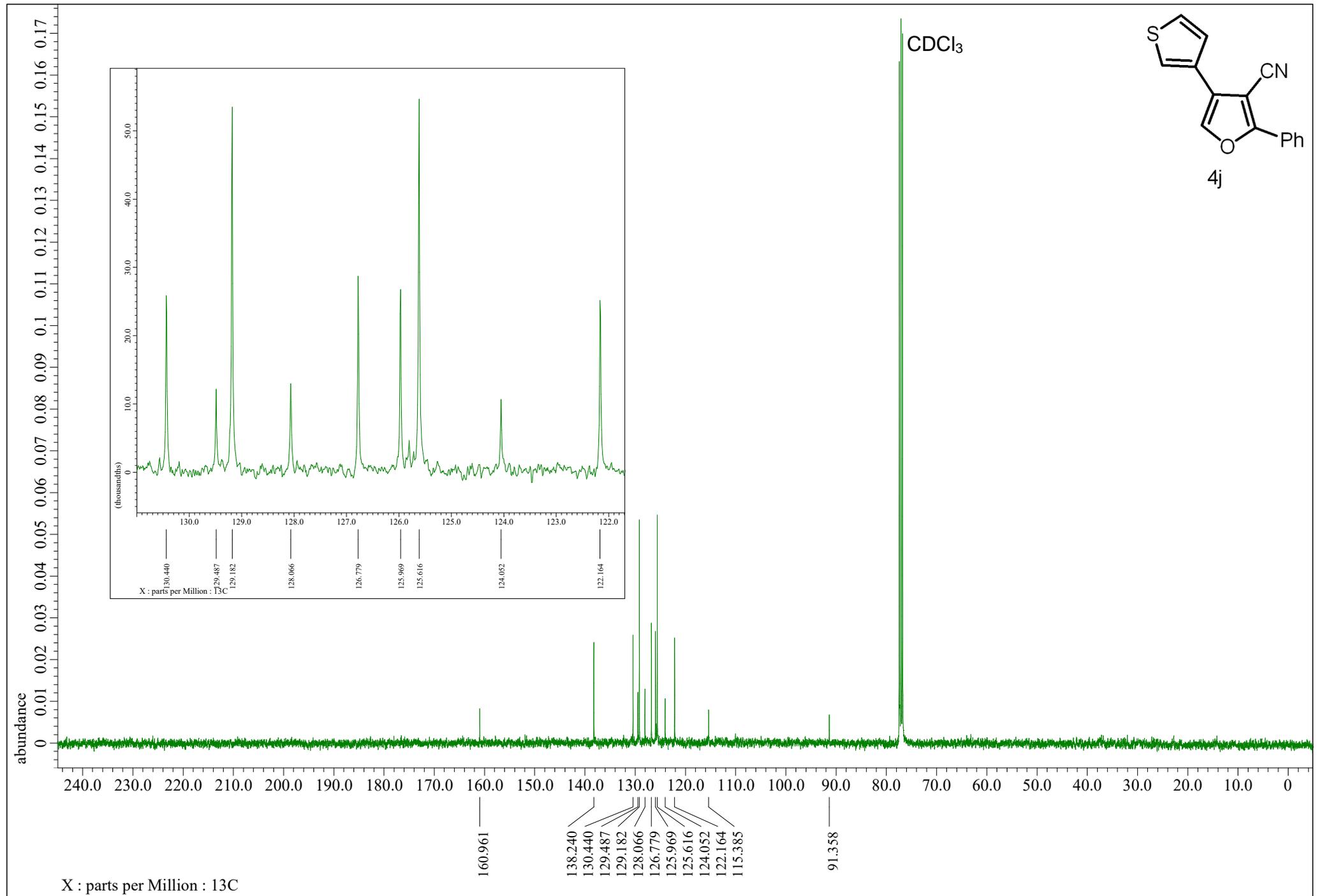
<sup>1</sup>H NMR



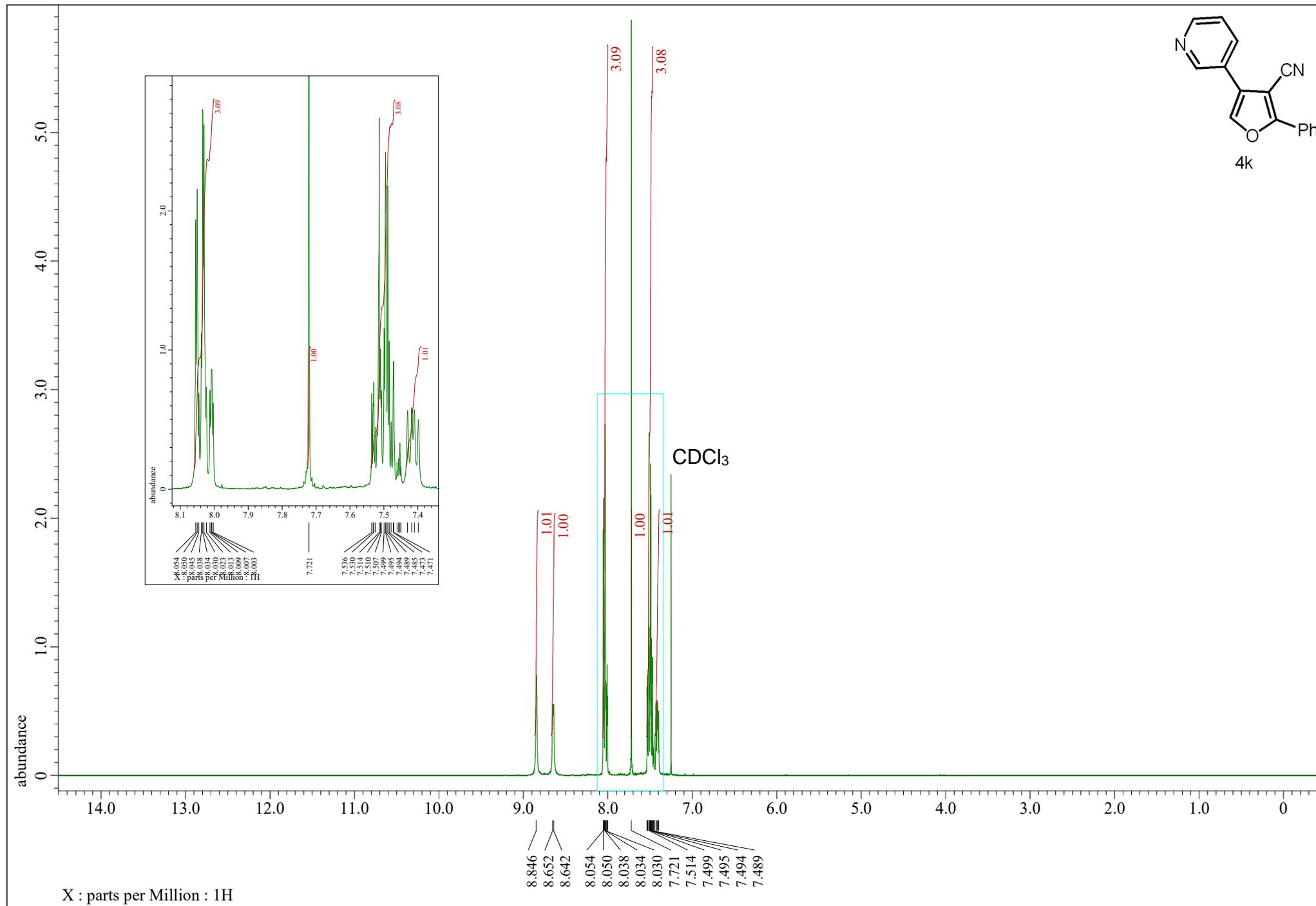
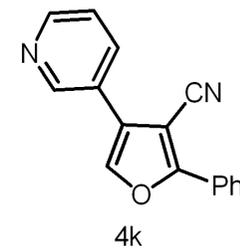


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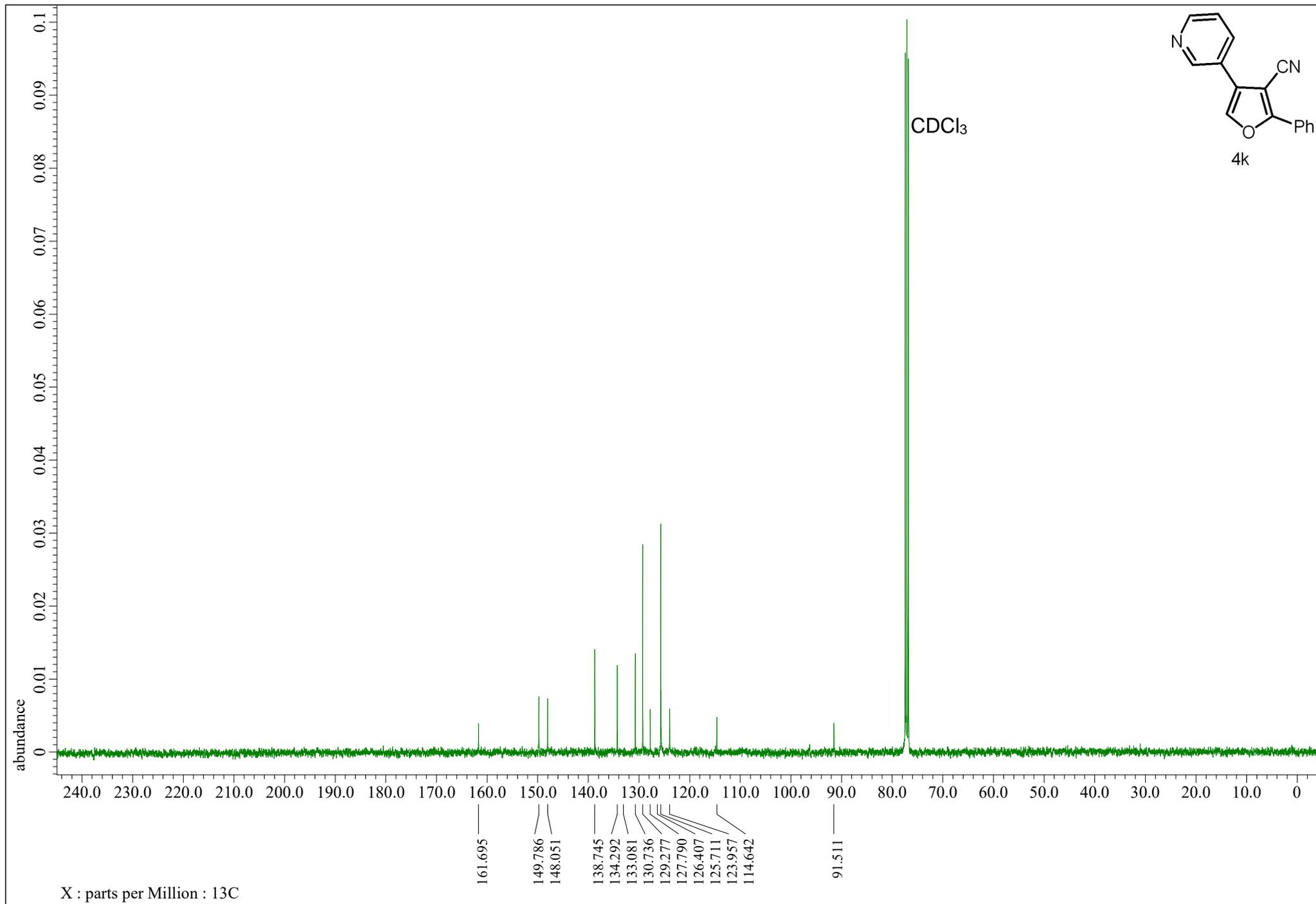


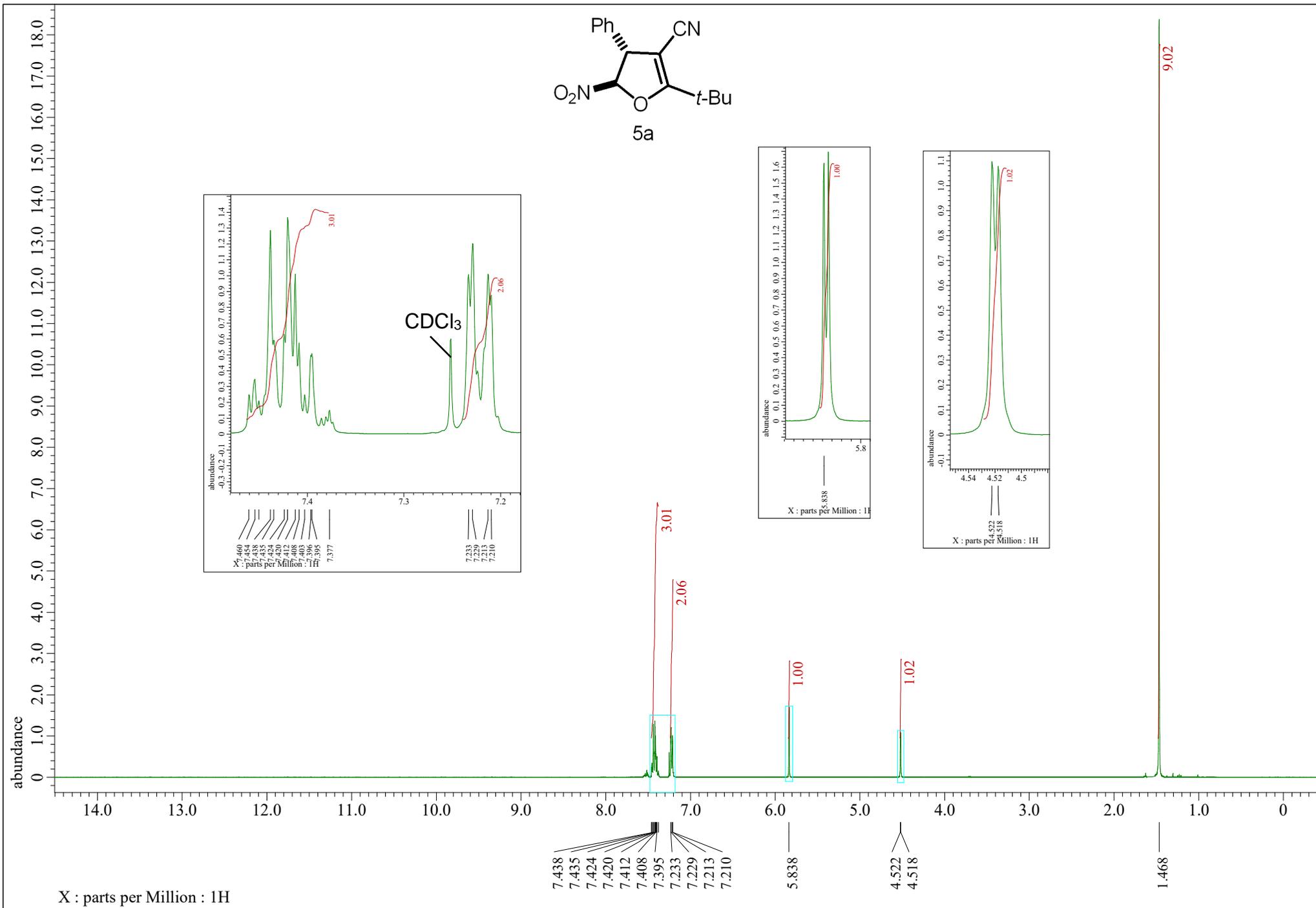
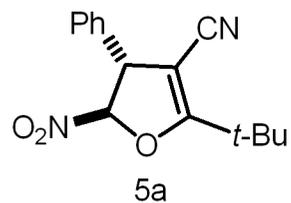


<sup>1</sup>H NMR

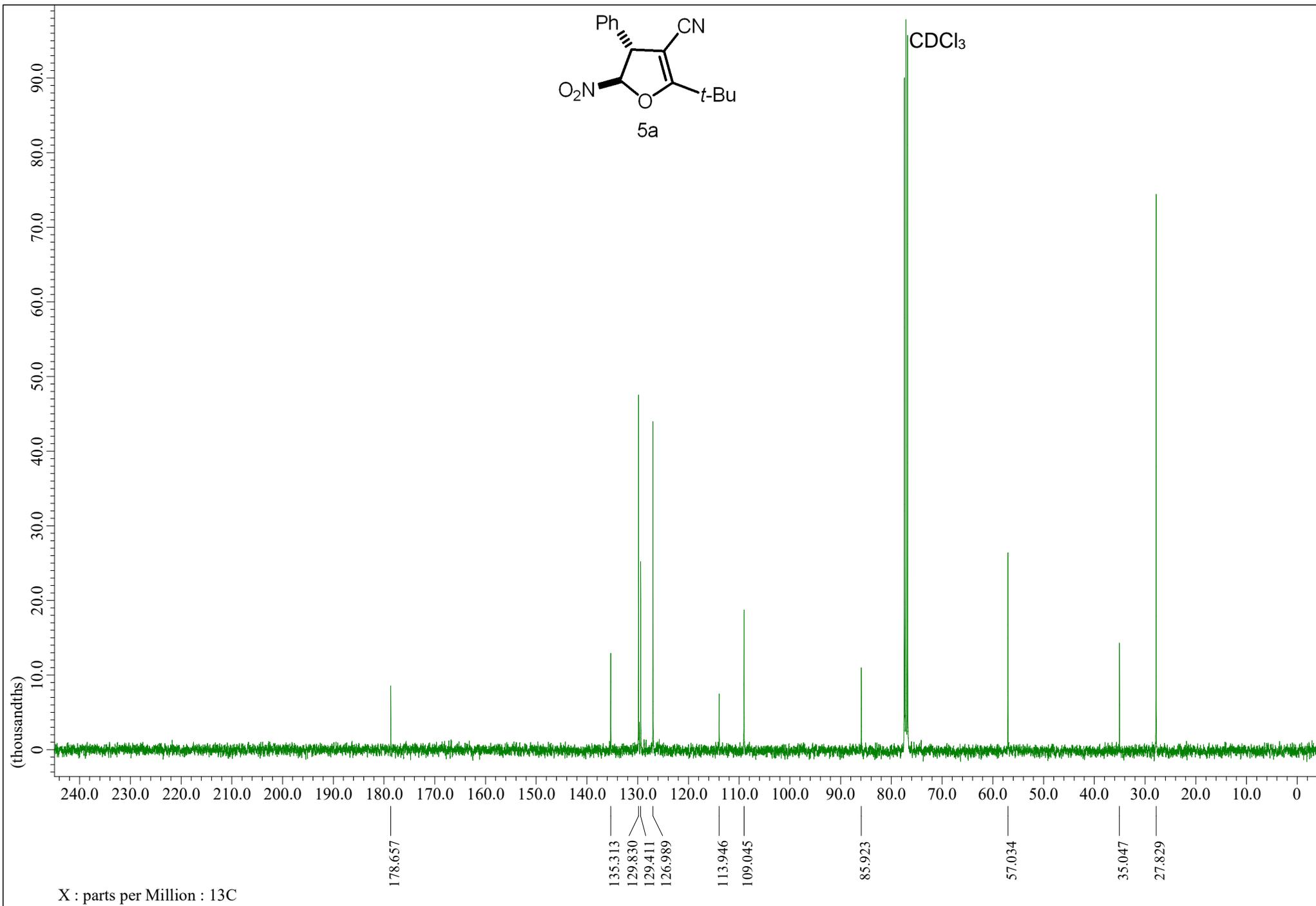
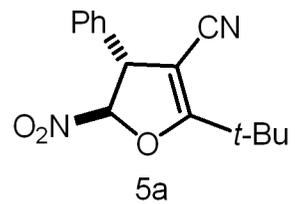


<sup>13</sup>C NMR

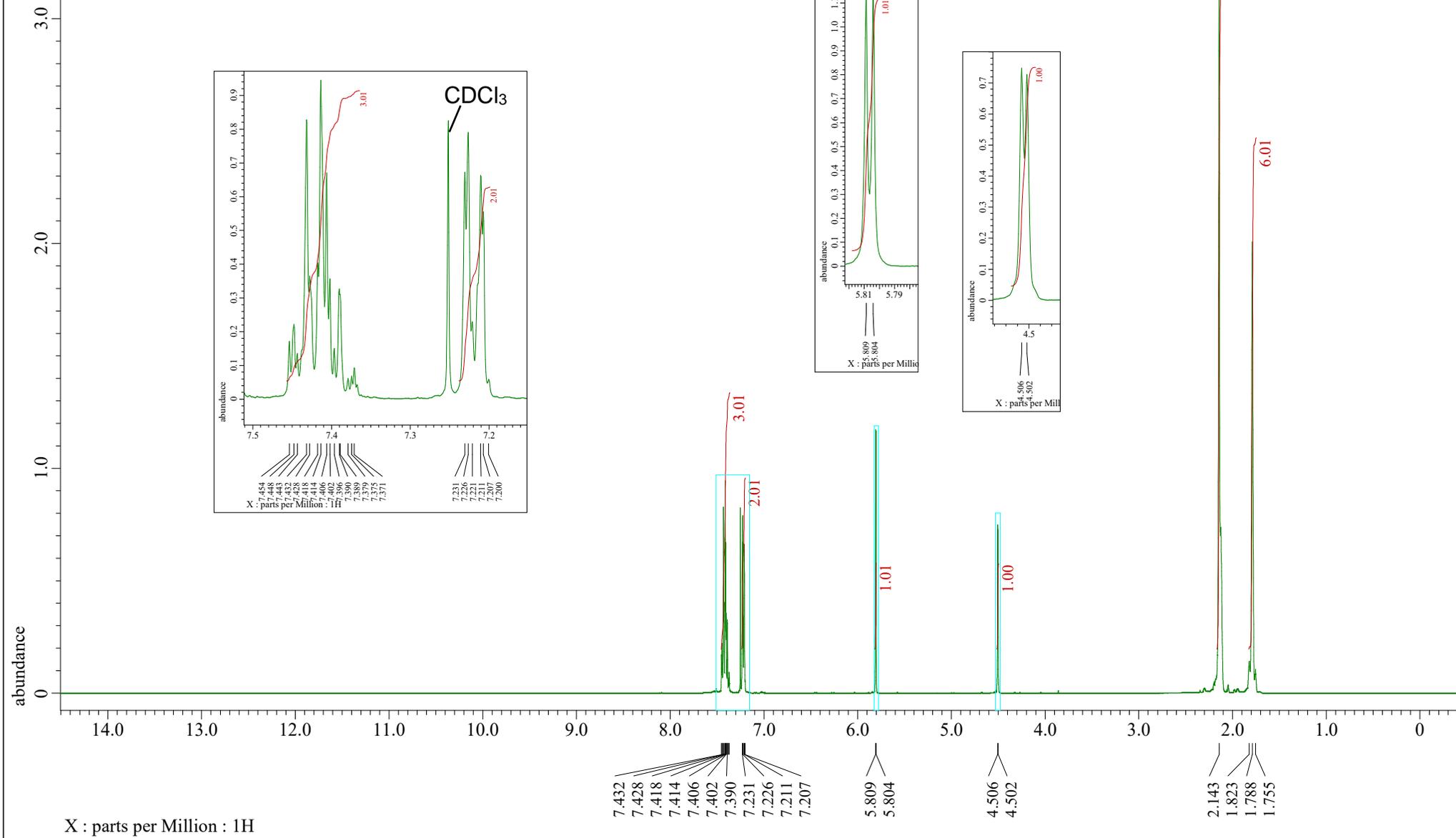
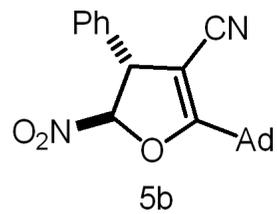




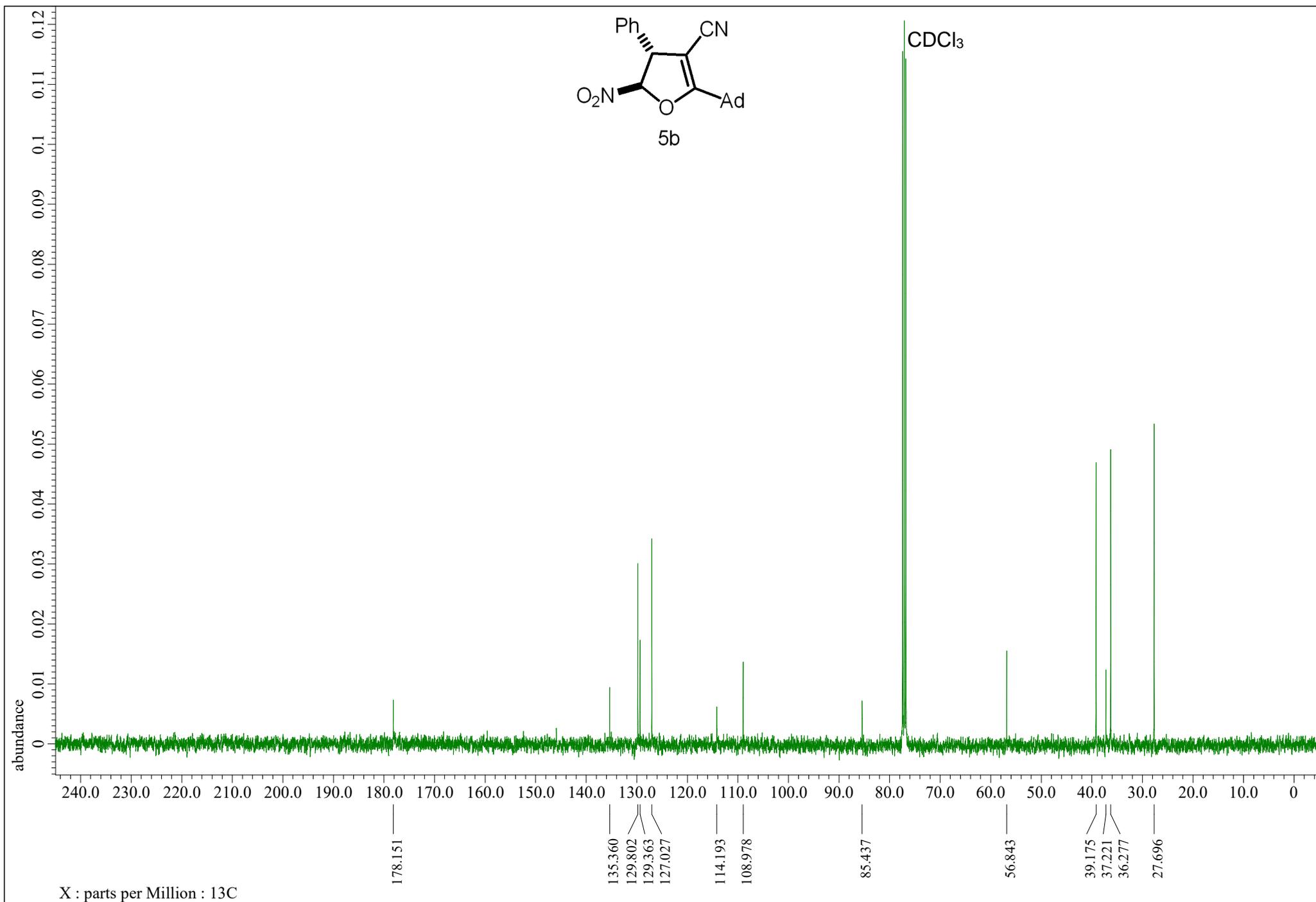
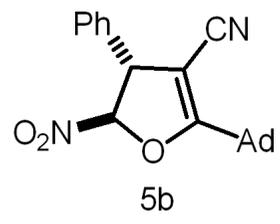
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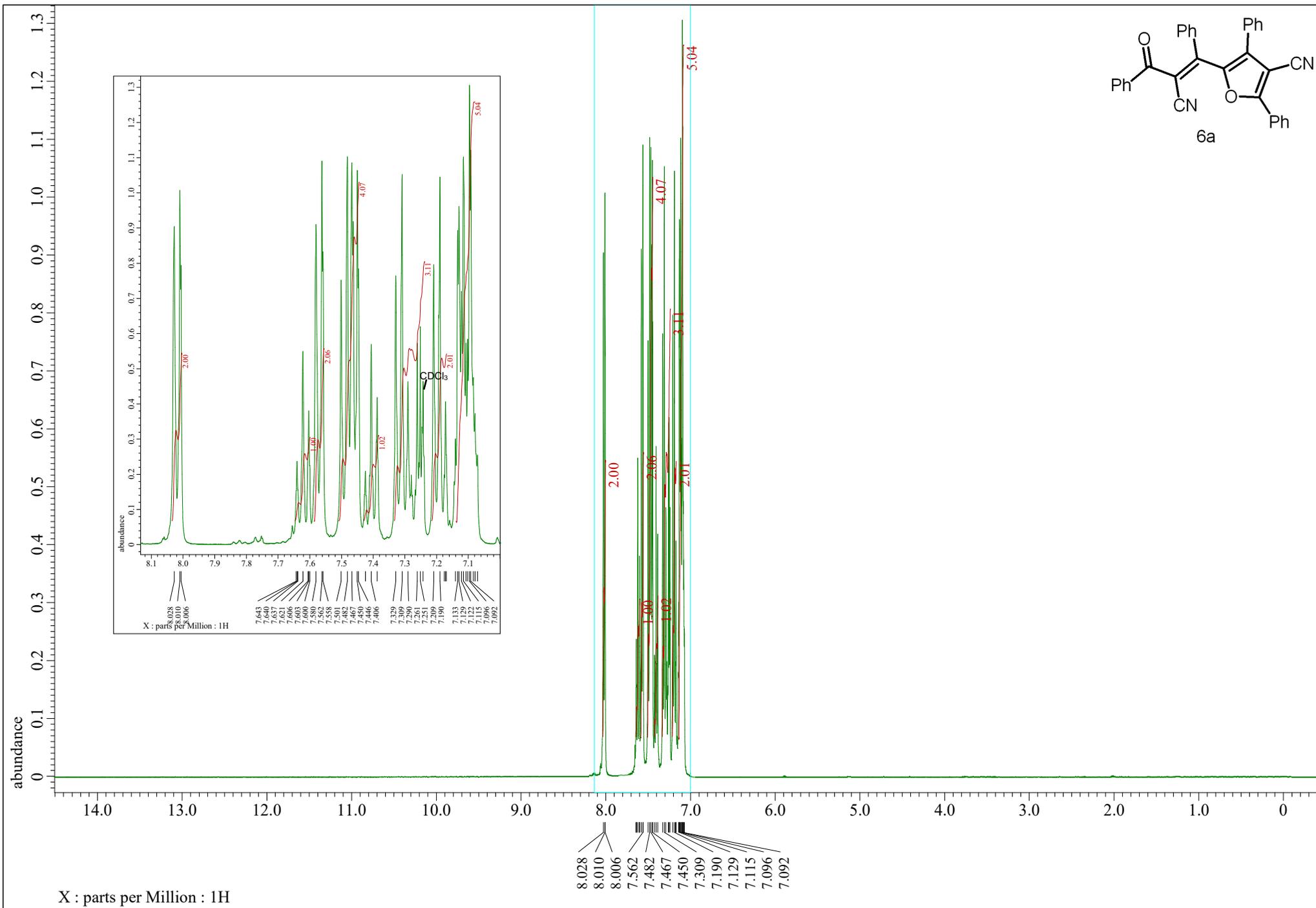
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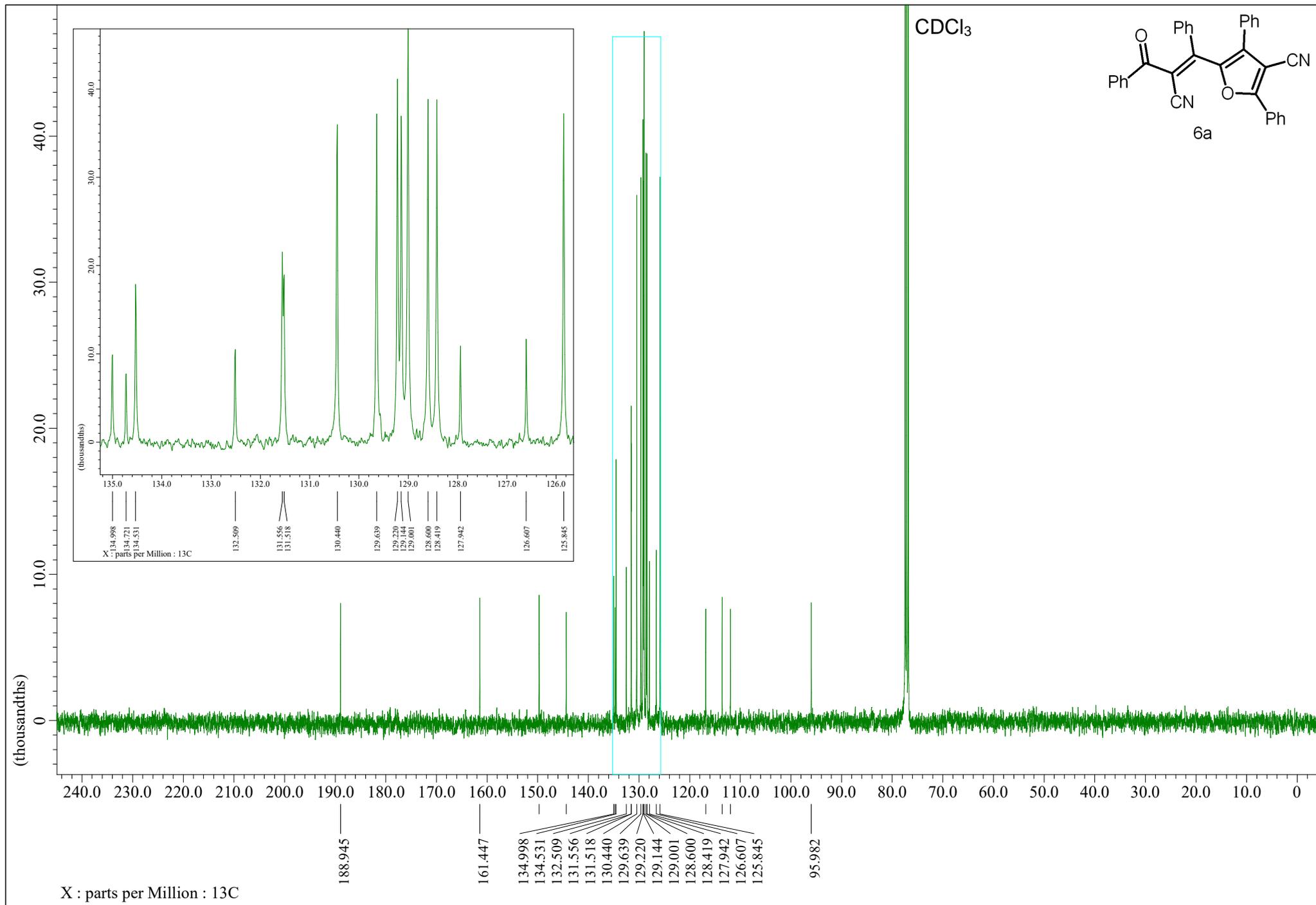
X : parts per Million : 1H



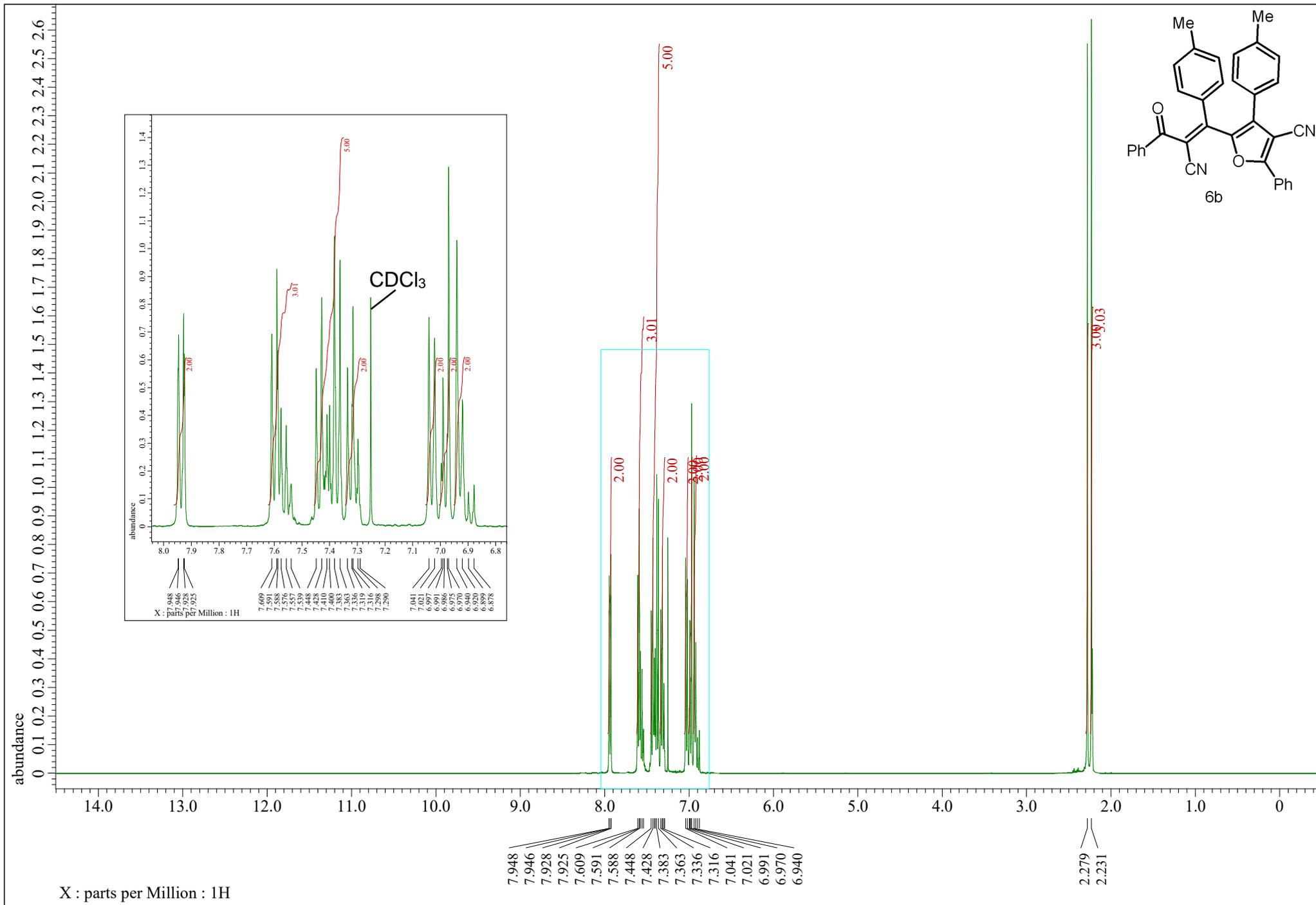
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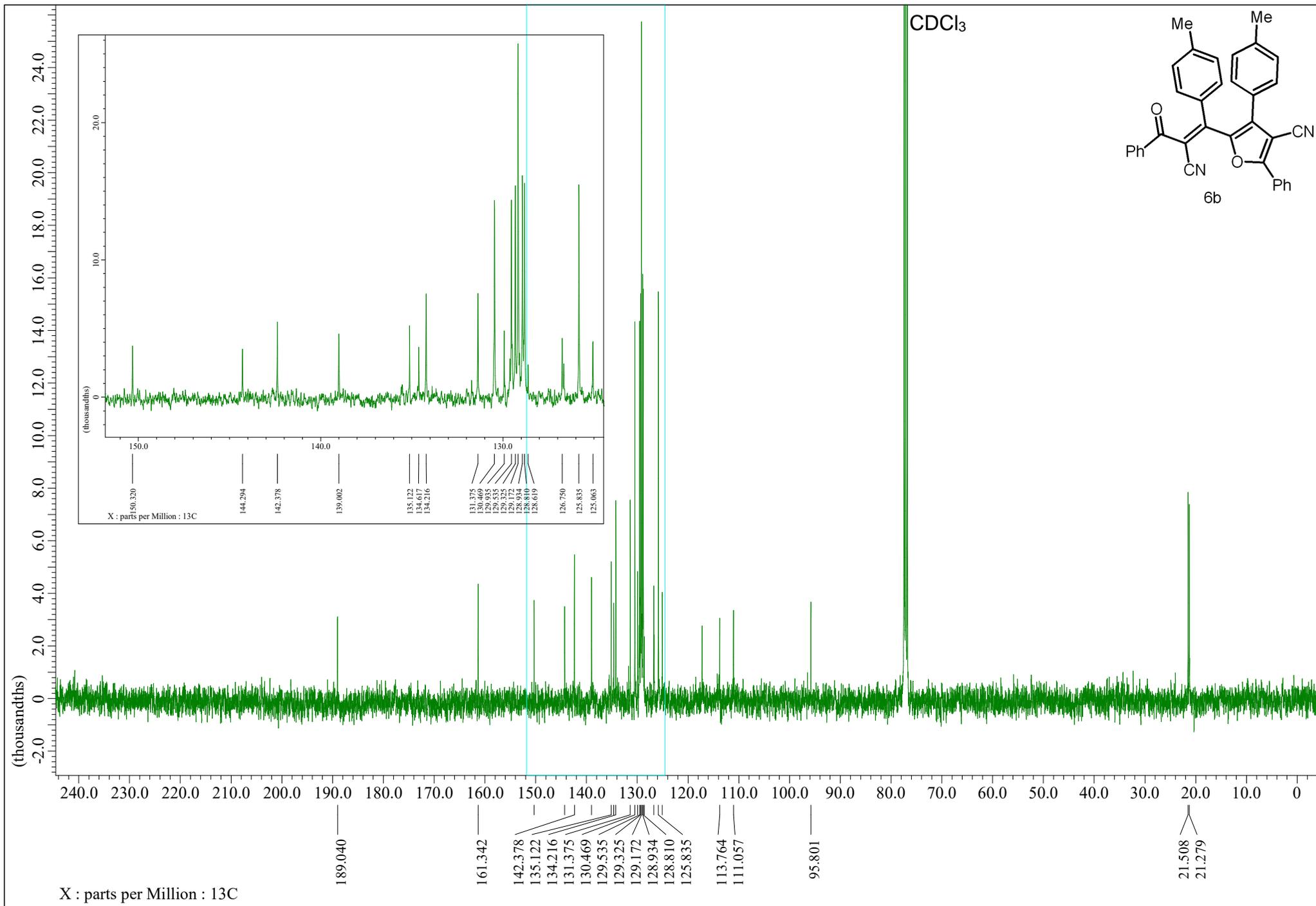


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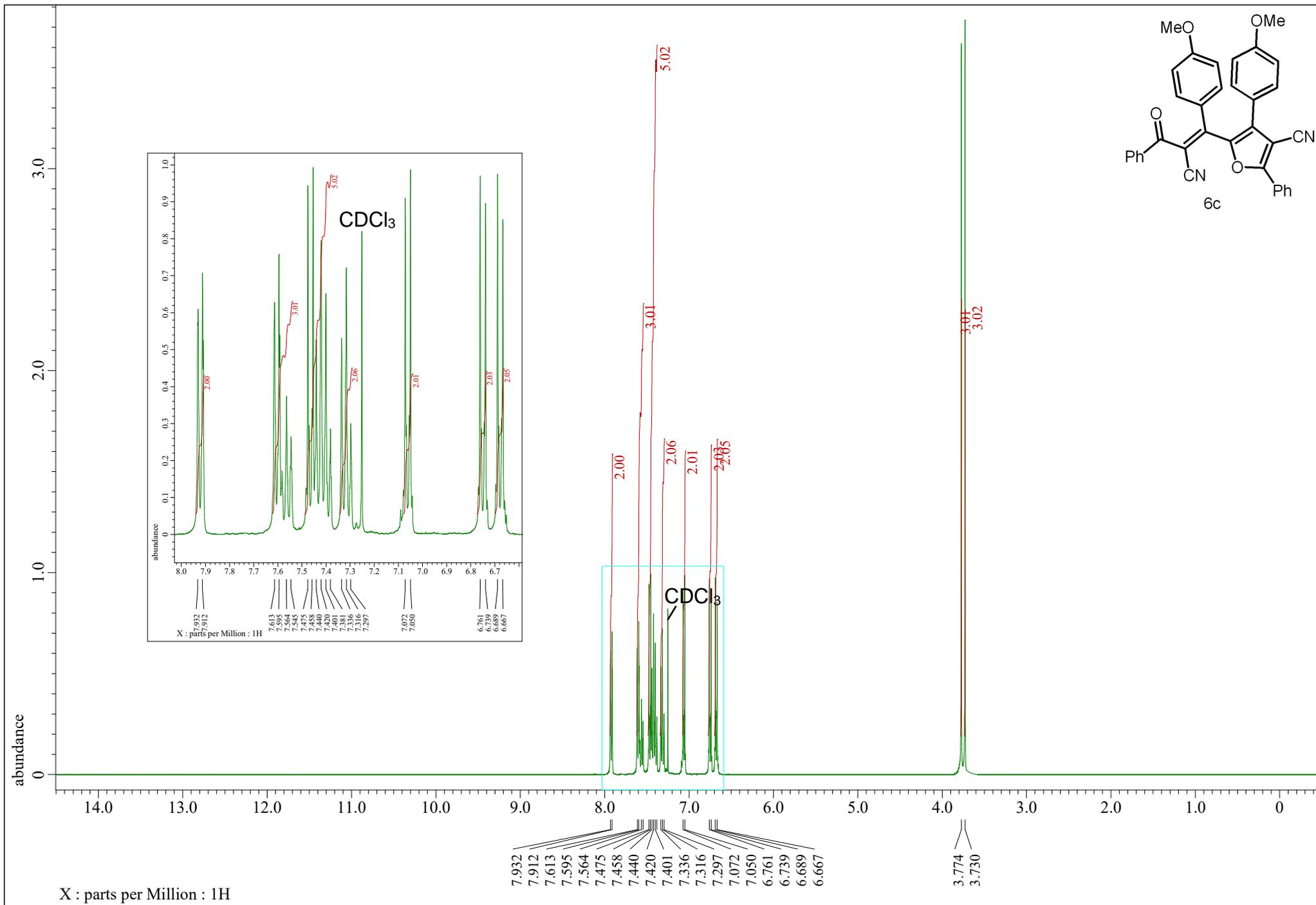


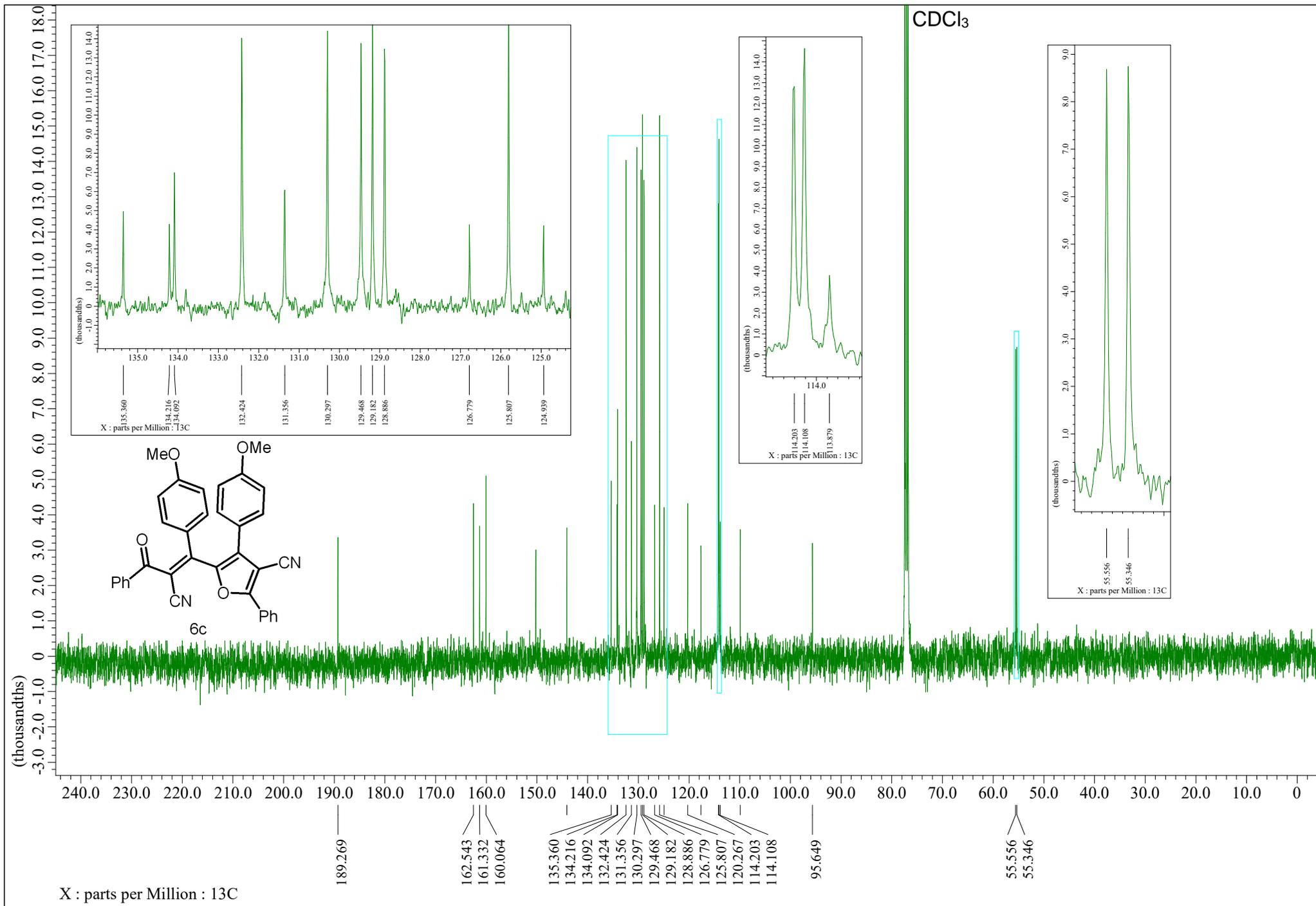
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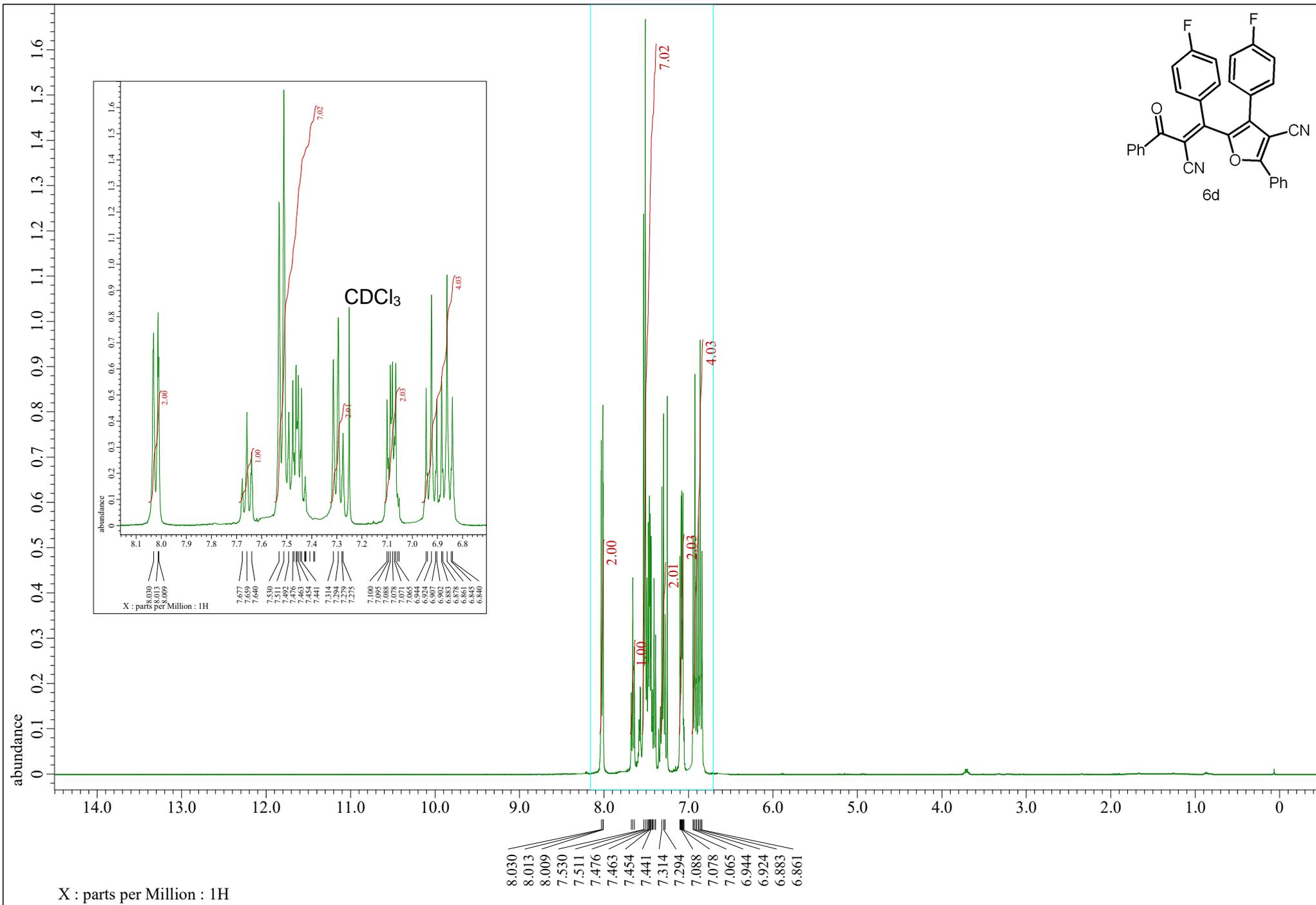


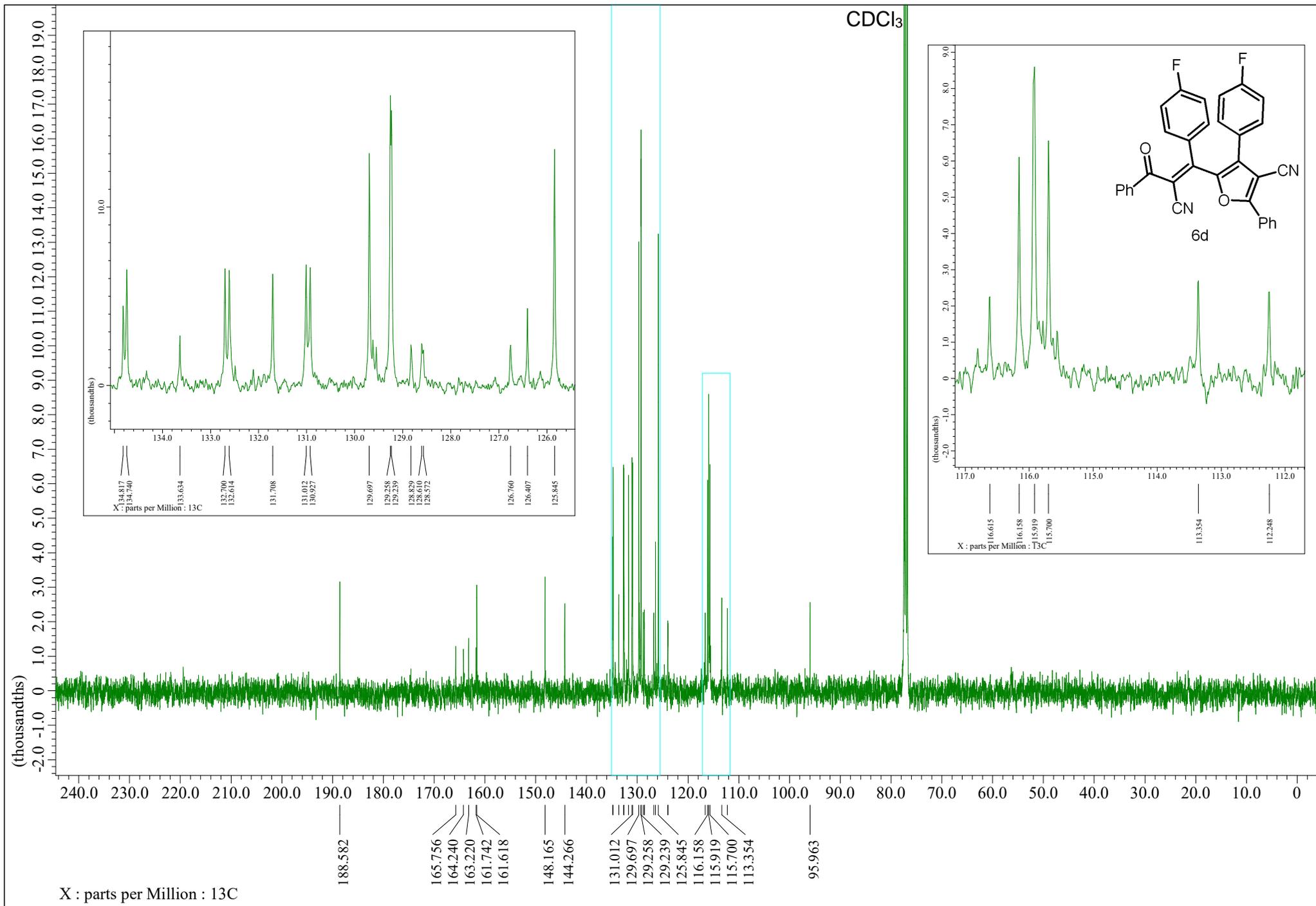
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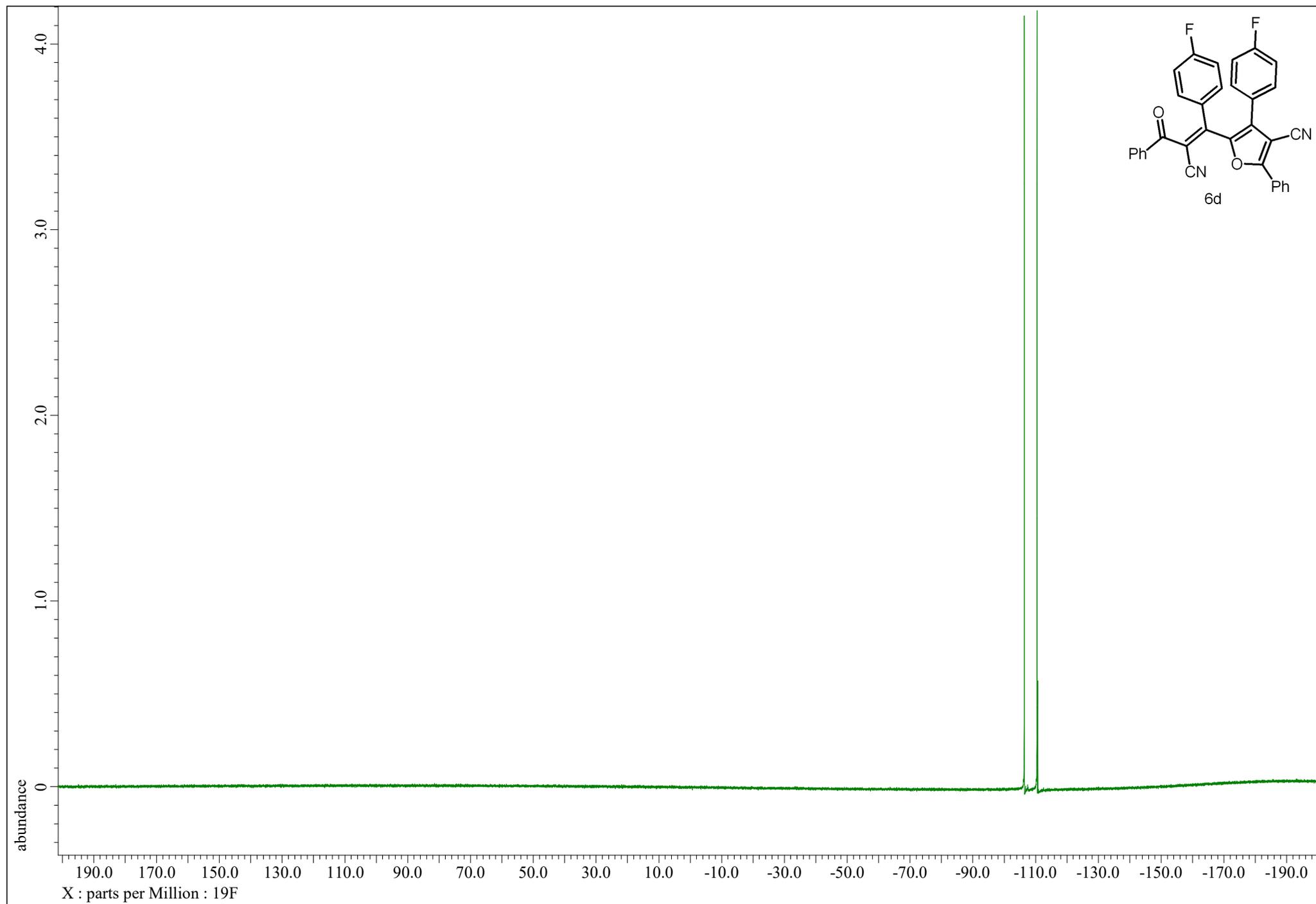


<sup>1</sup>H NMR

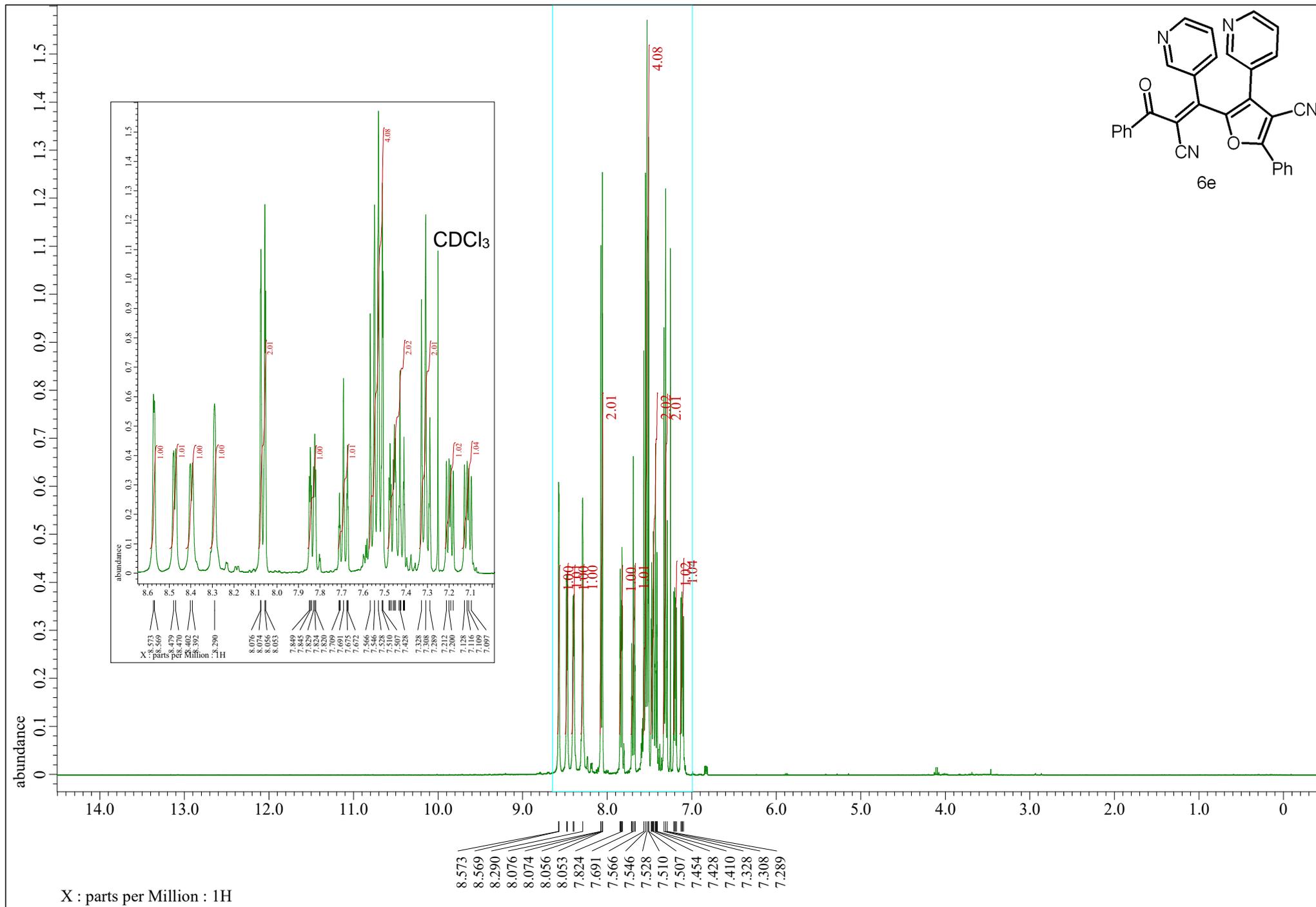




<sup>19</sup>F NMR



<sup>1</sup>H NMR



<sup>13</sup>C NMR

