

Supporting Information

A Facile access to functionalized indenenes and fused quinolines by regioselective 5-*enolexo*-dig Michael addition and cyclization reaction

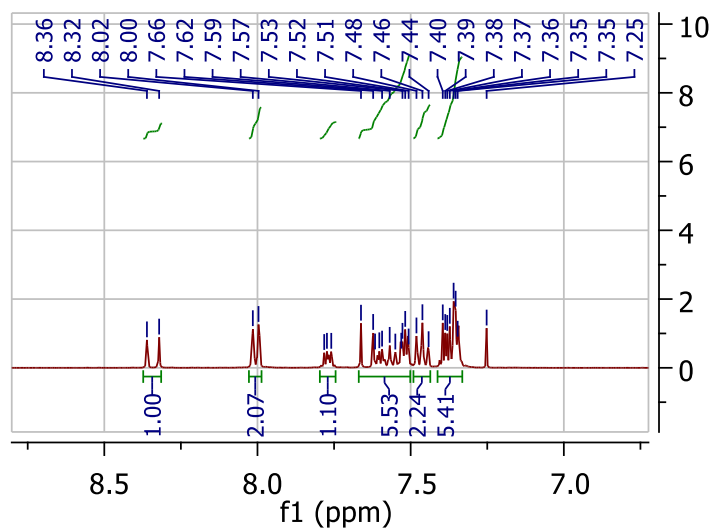
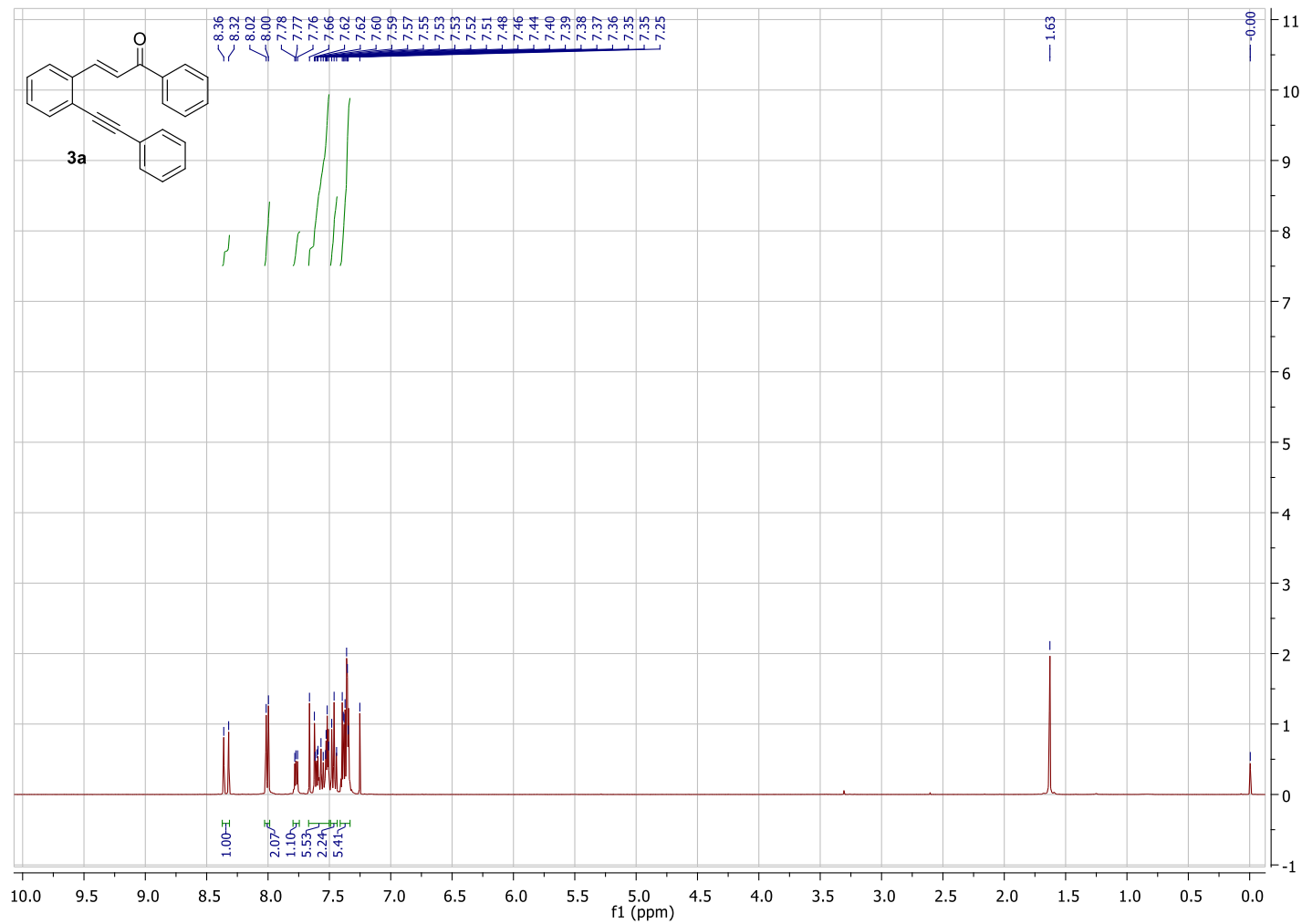
Tohasib Yusub Chaudhari,^a Sandeep K. Ginotra^b and Vibha Tandon^{*a}

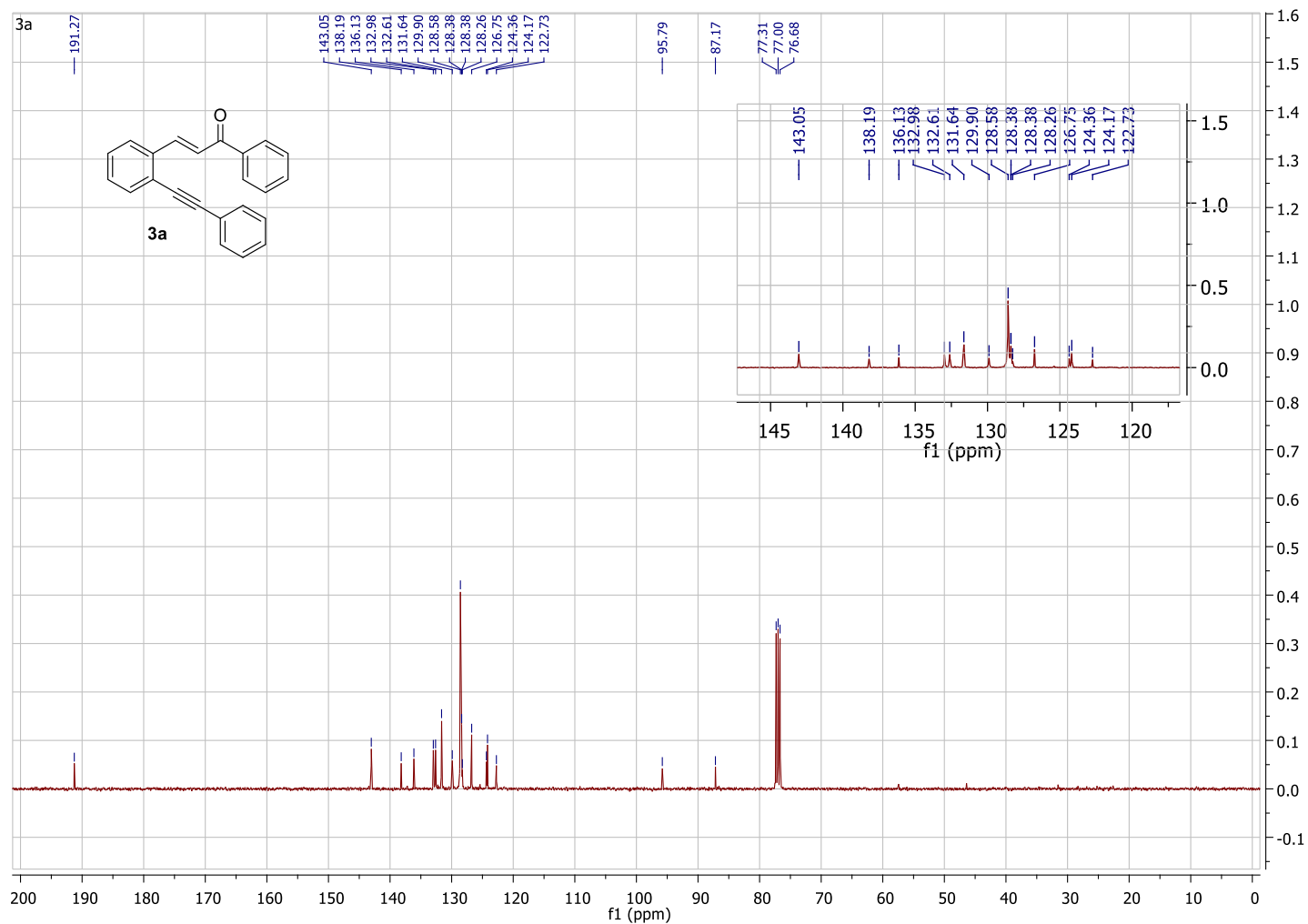
^aSpecial Centre for Molecular Medicine, Jawaharlal Nehru University, New Delhi-110067

^bDepartment of Chemistry, University of Delhi, New Delh-110007

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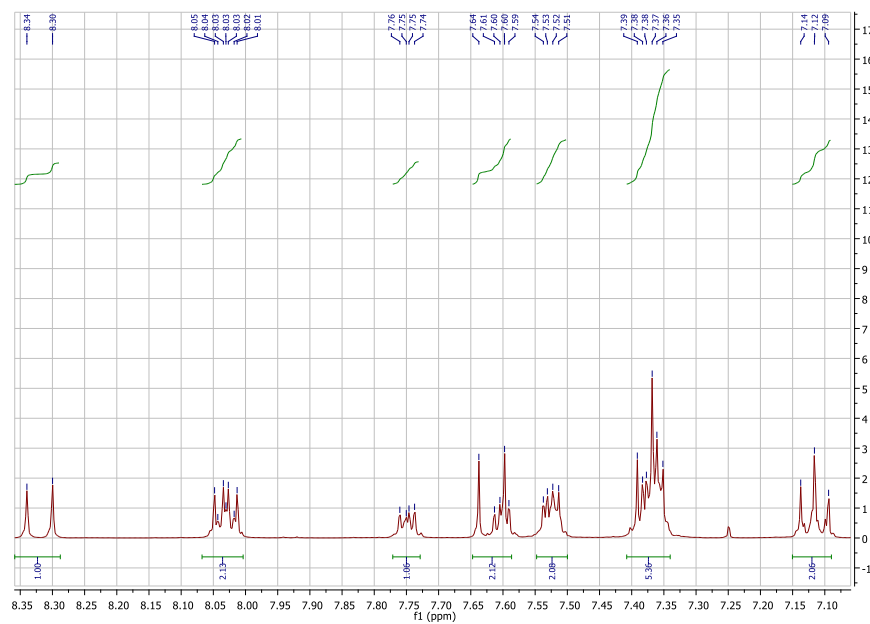
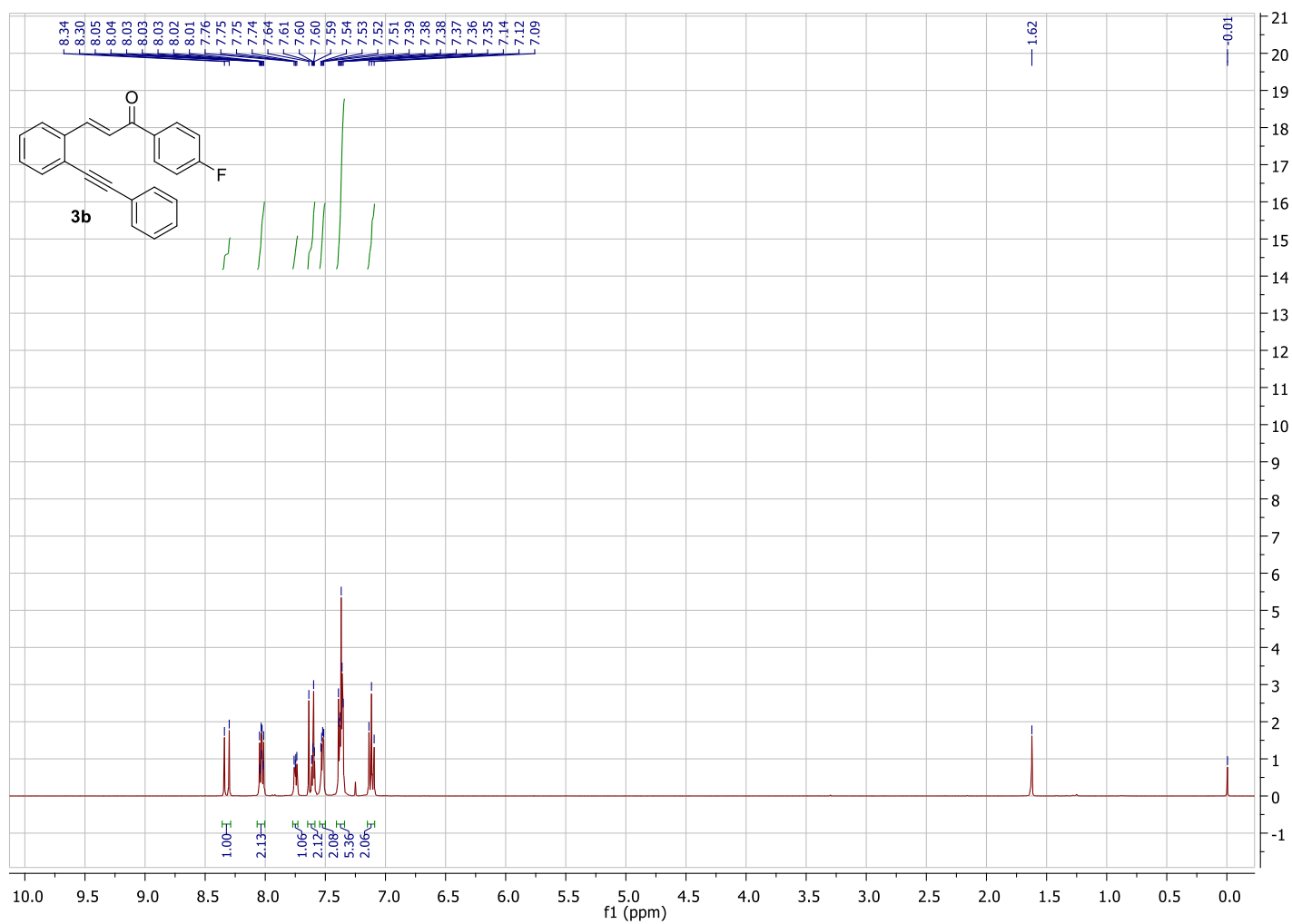
1. ^1H , ^{13}C NMR and HRMS spectra of chalcone substrates 3a-o

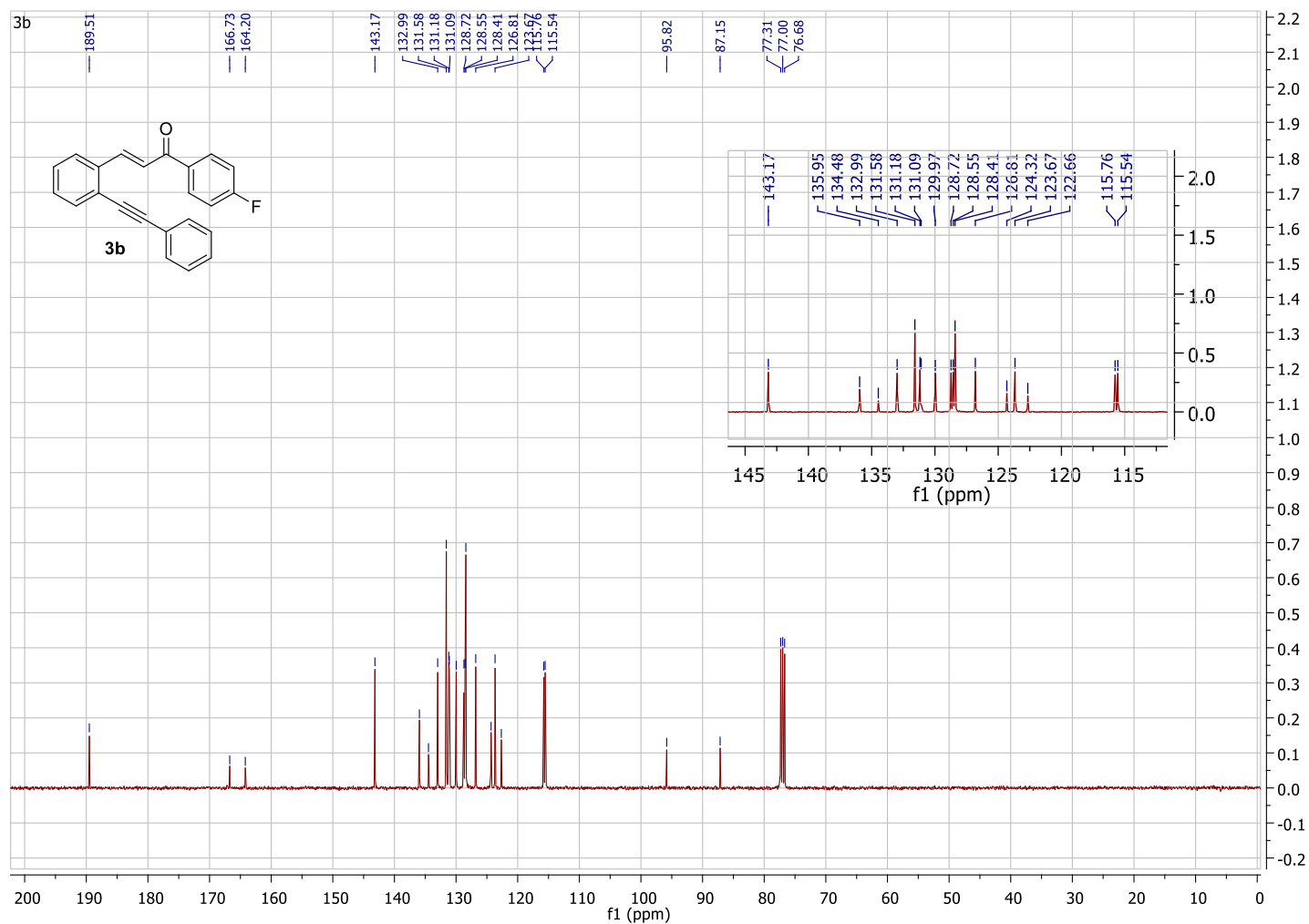




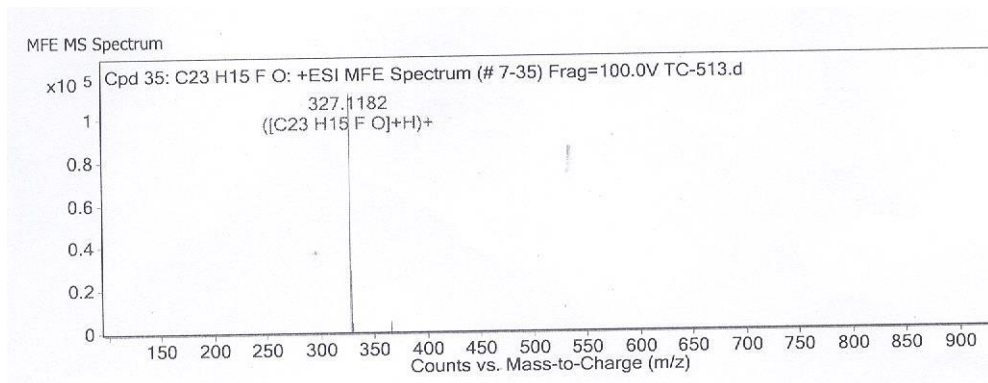
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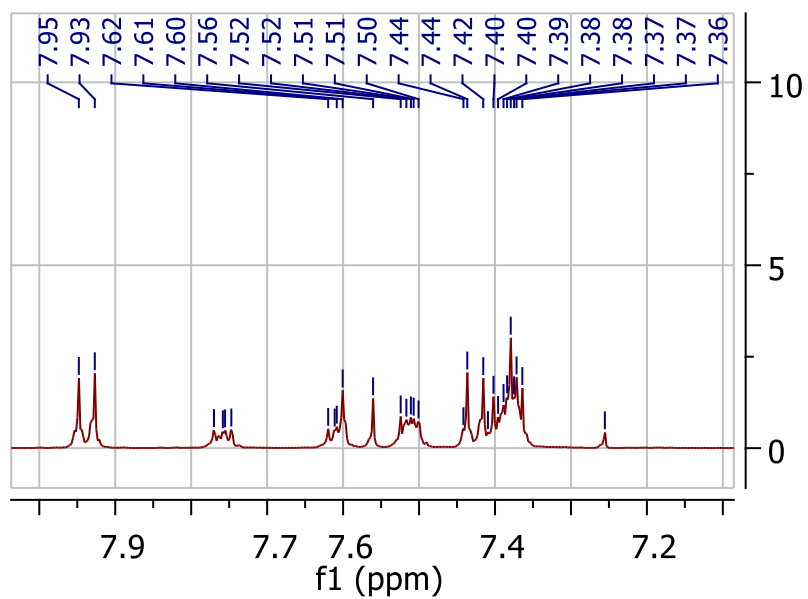
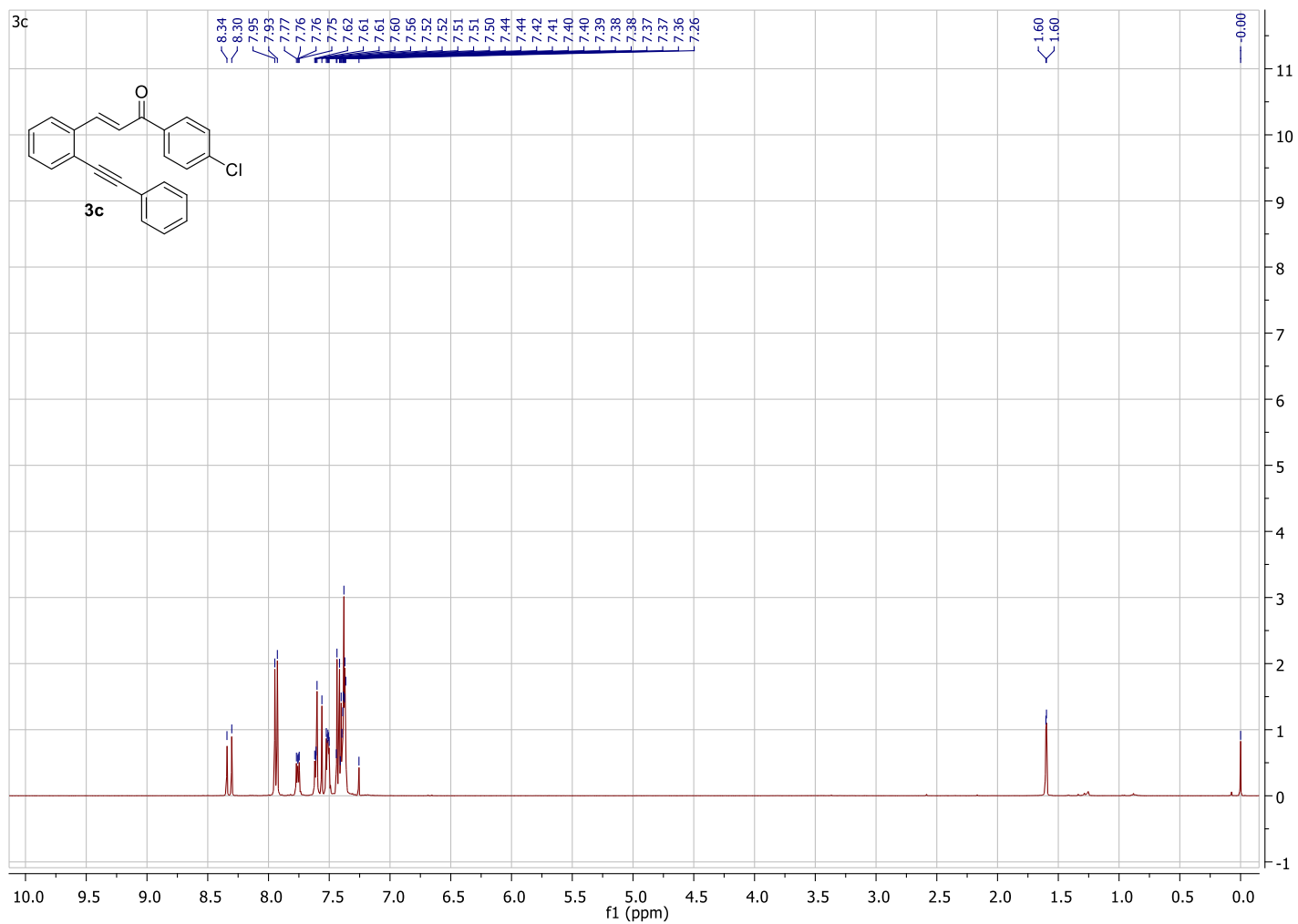


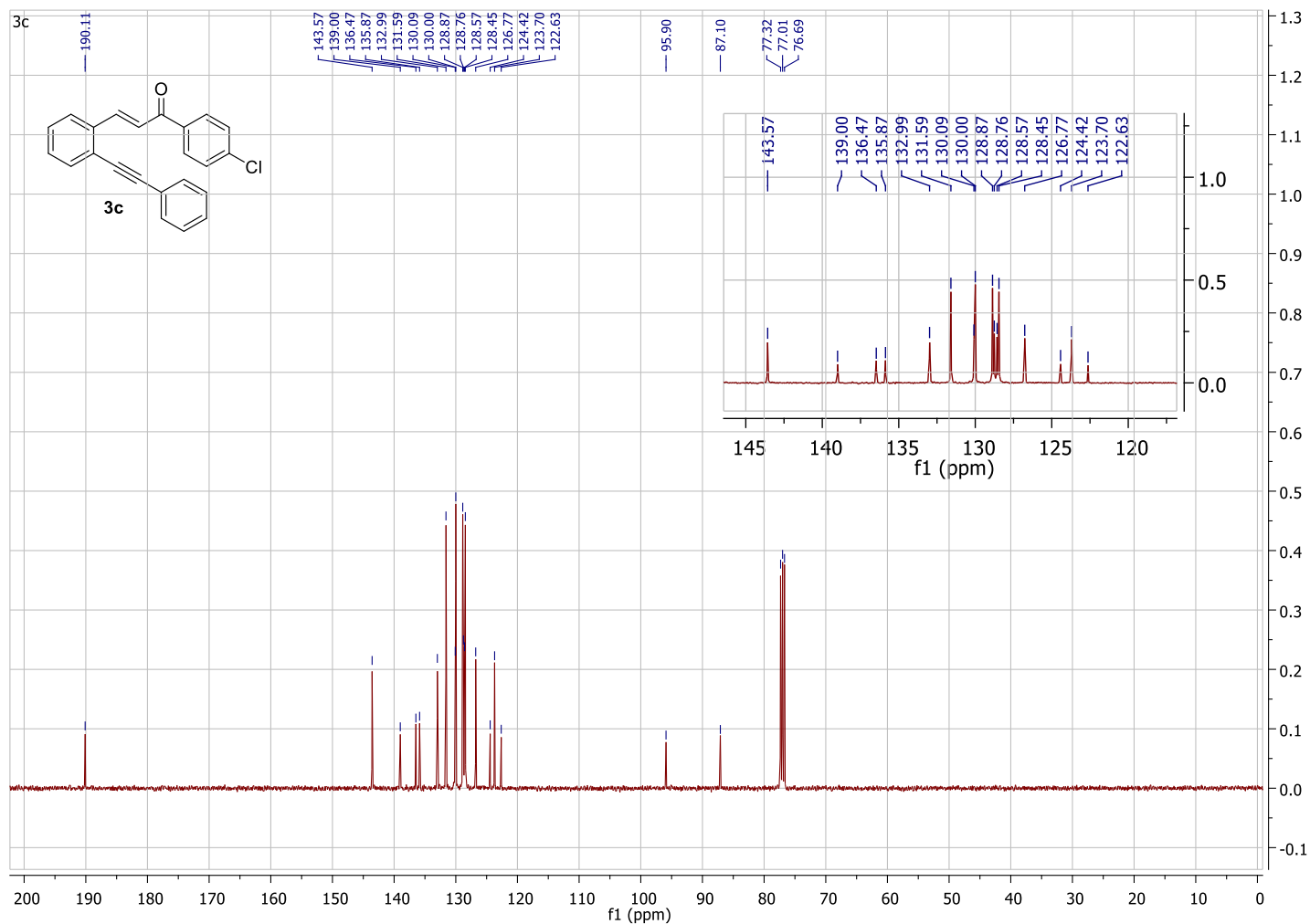




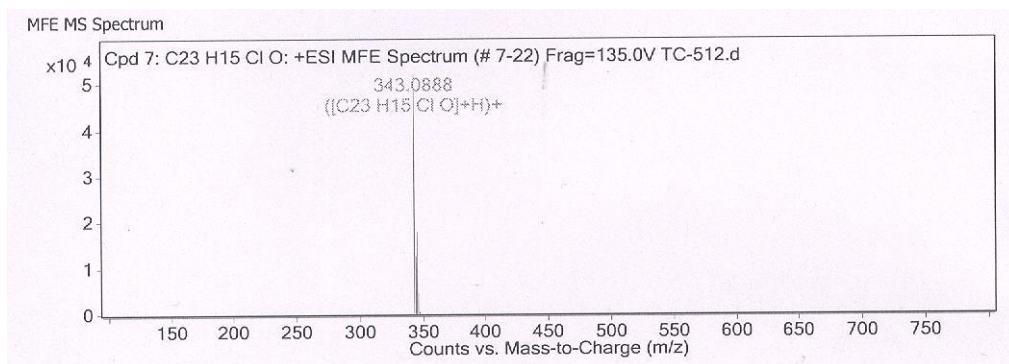
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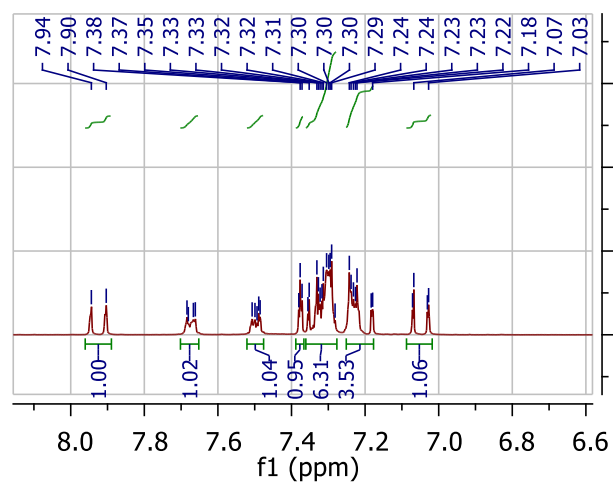
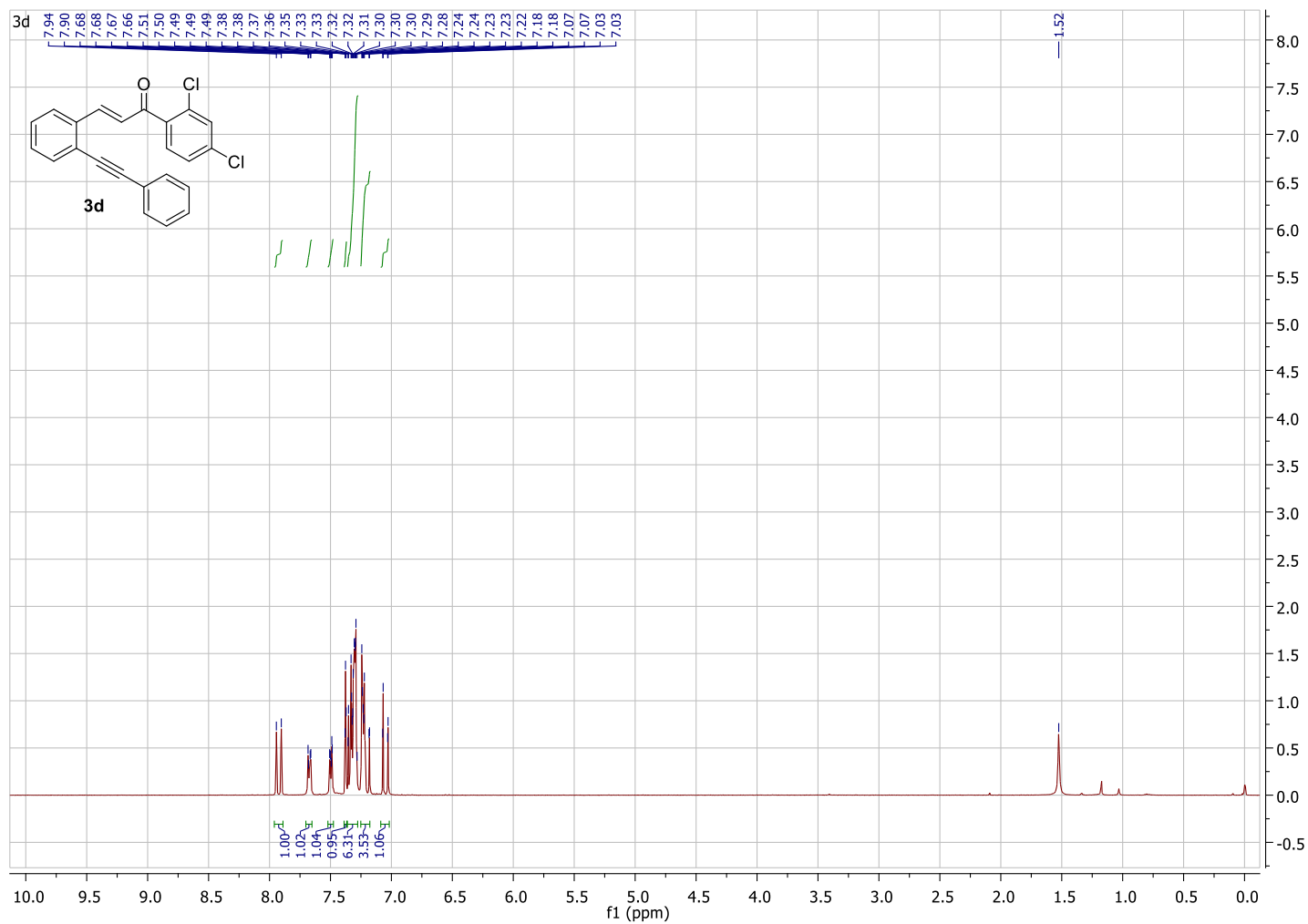


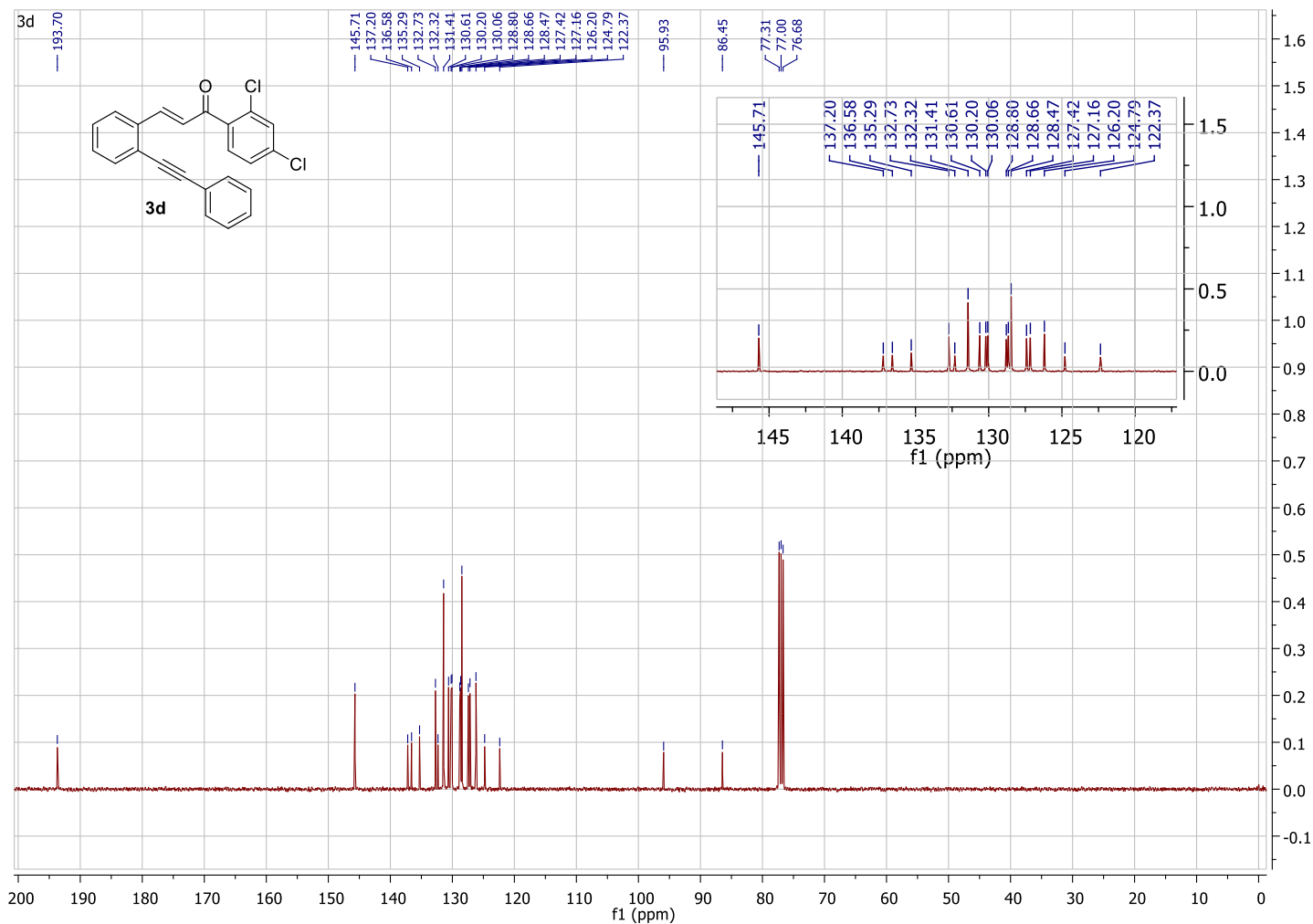




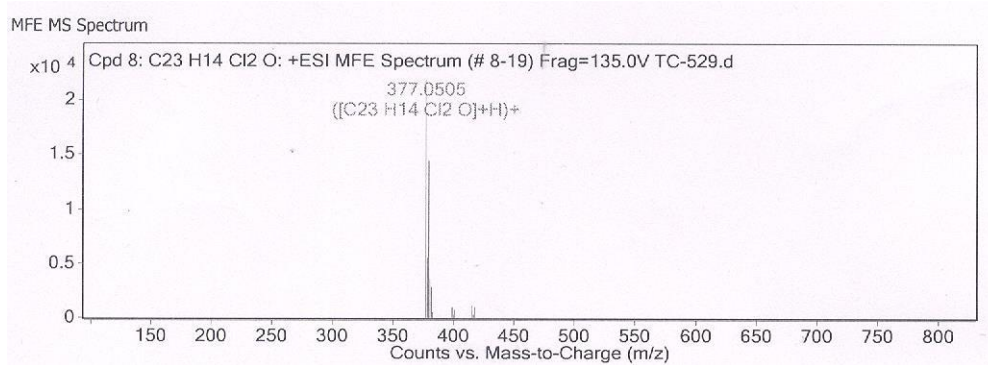
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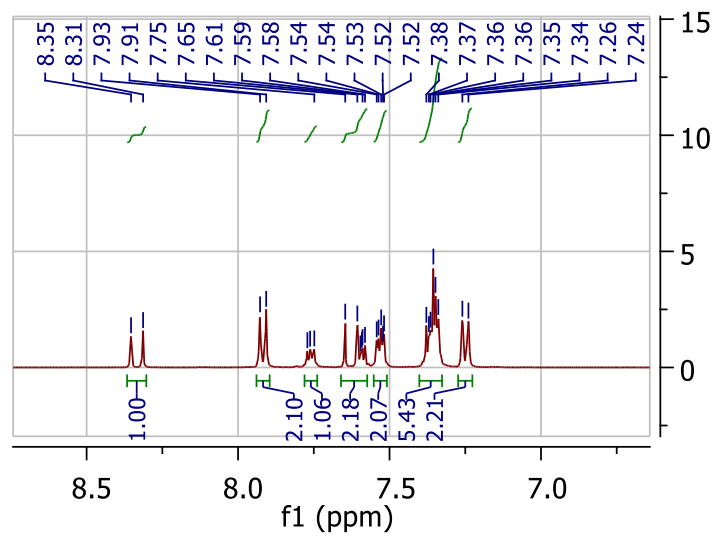
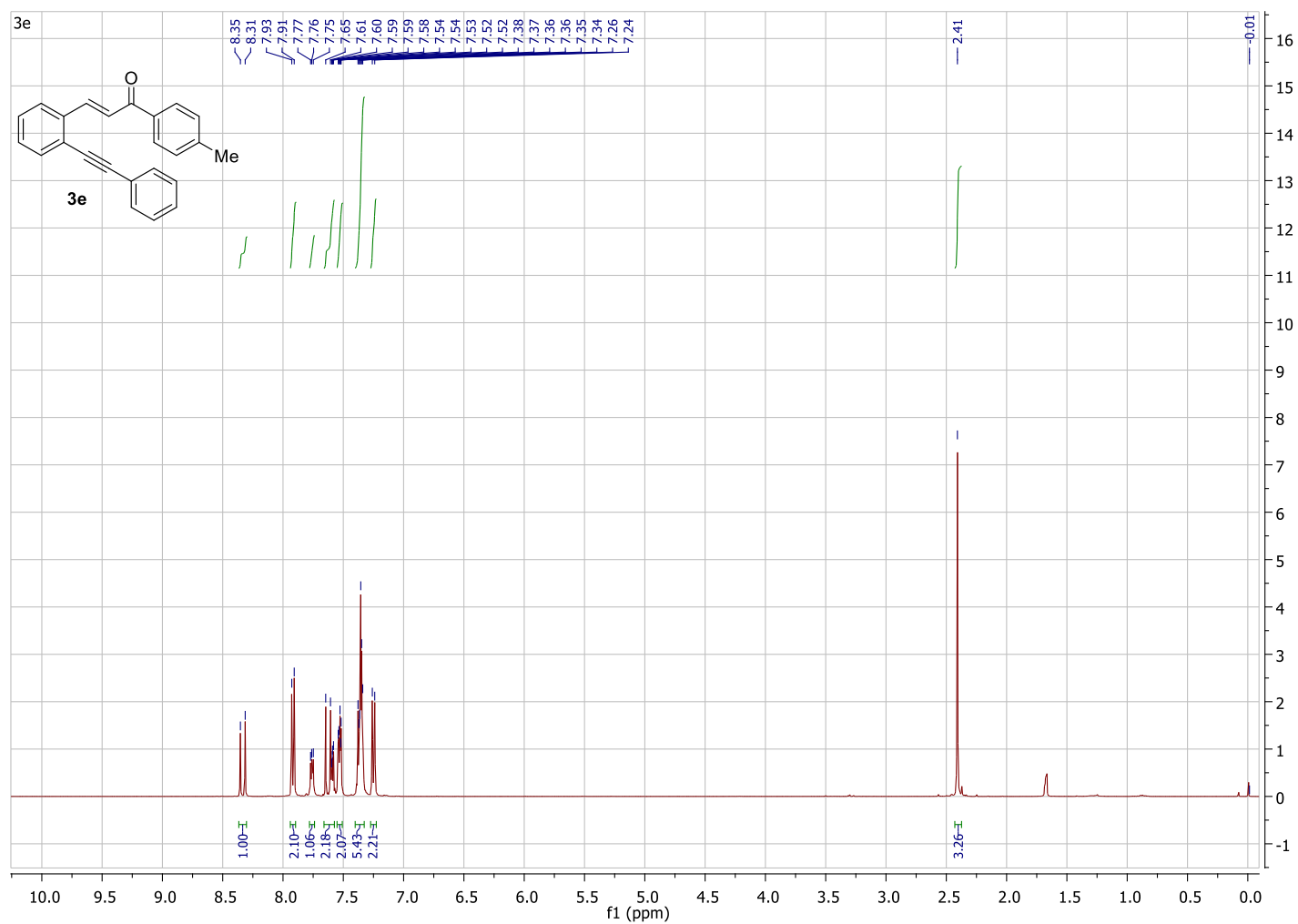


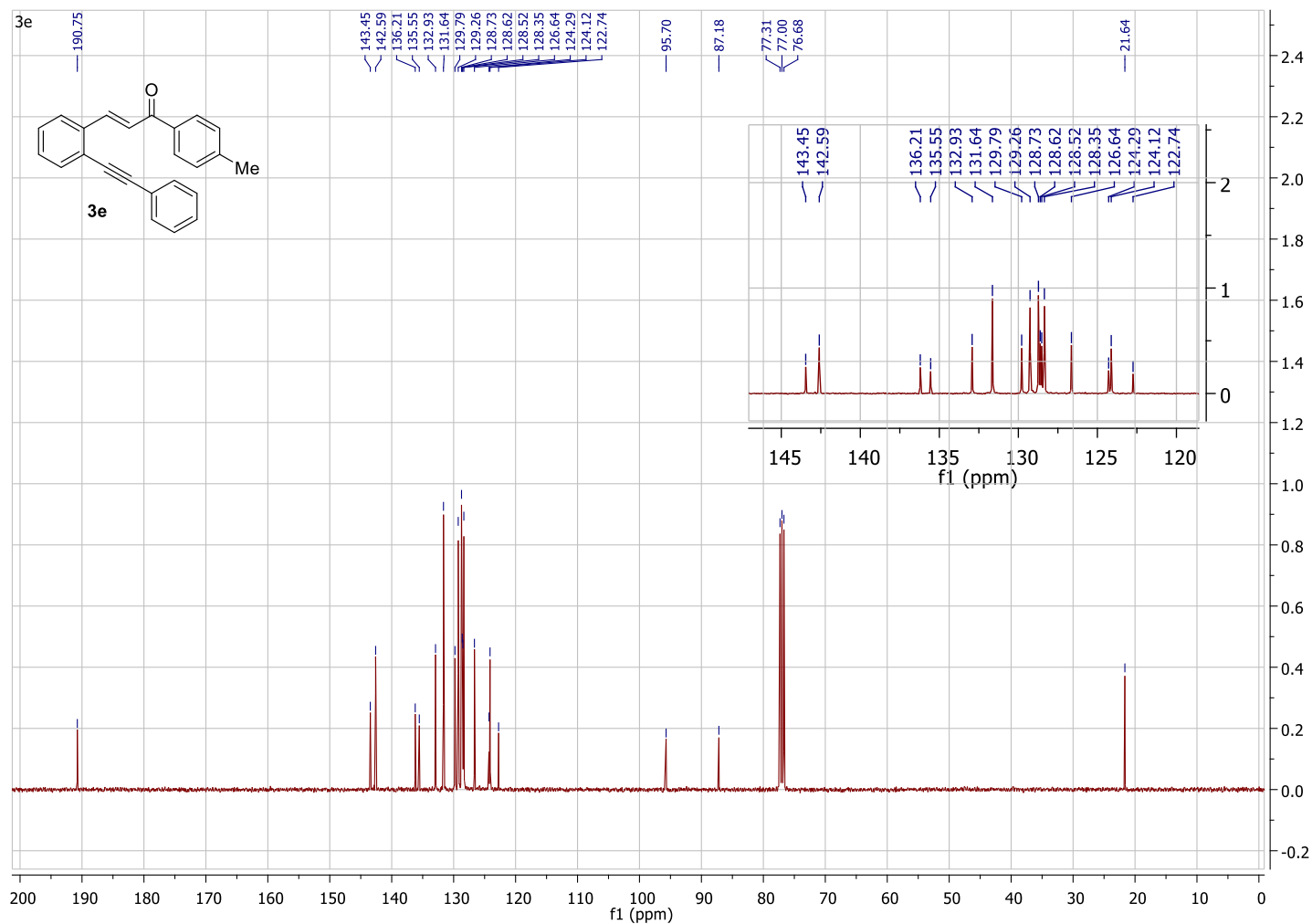




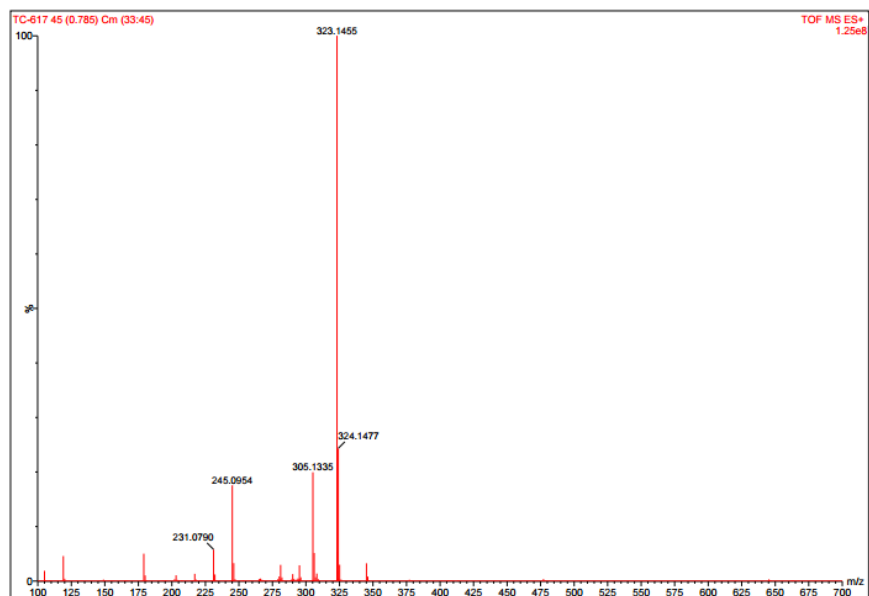
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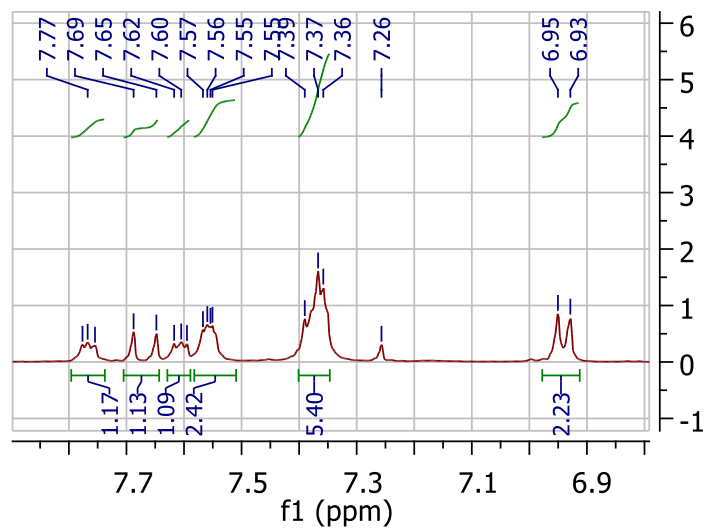
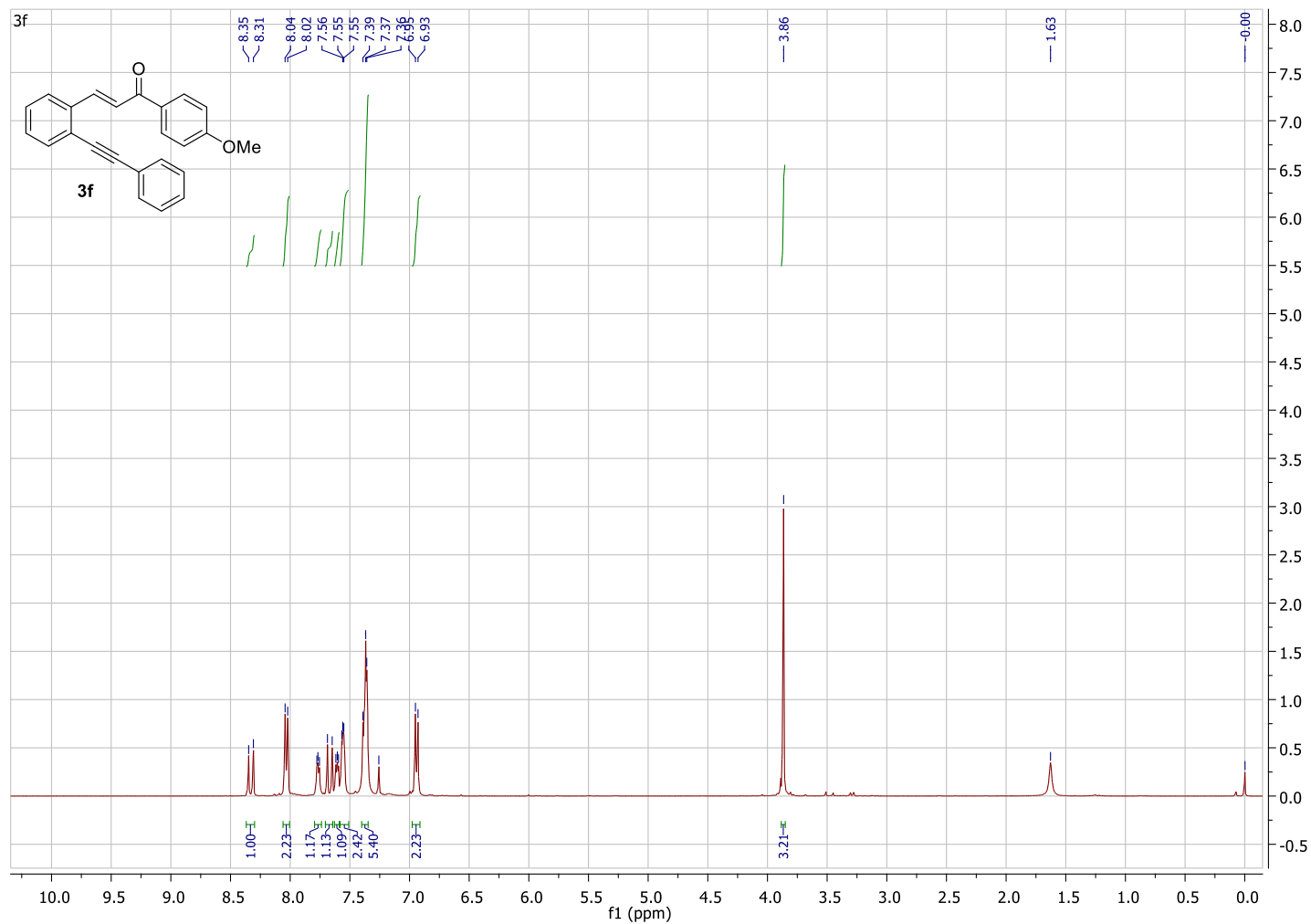


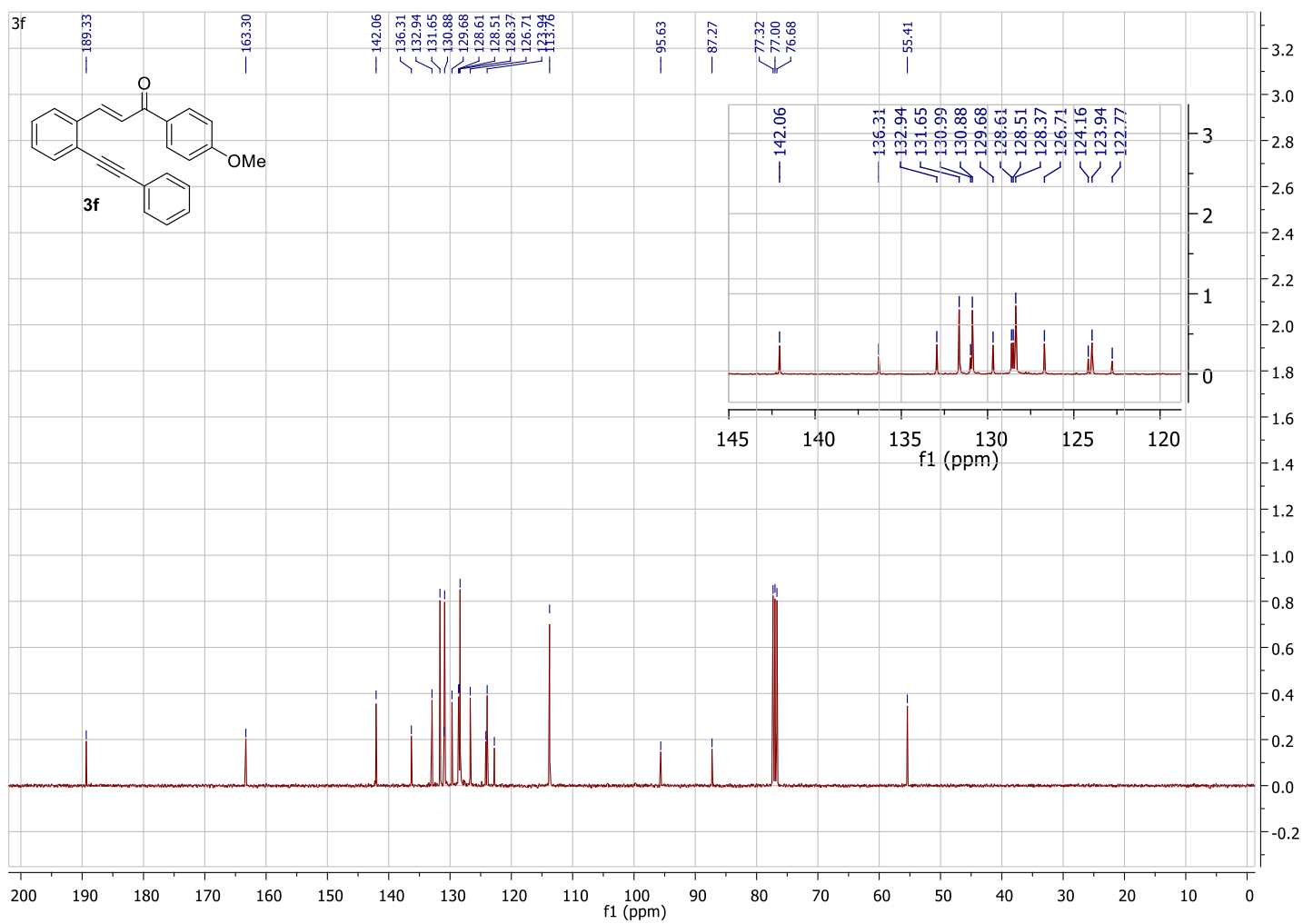




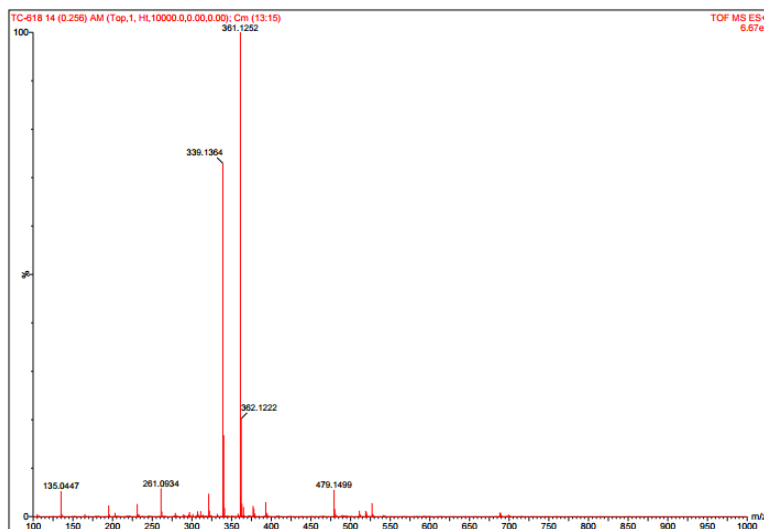
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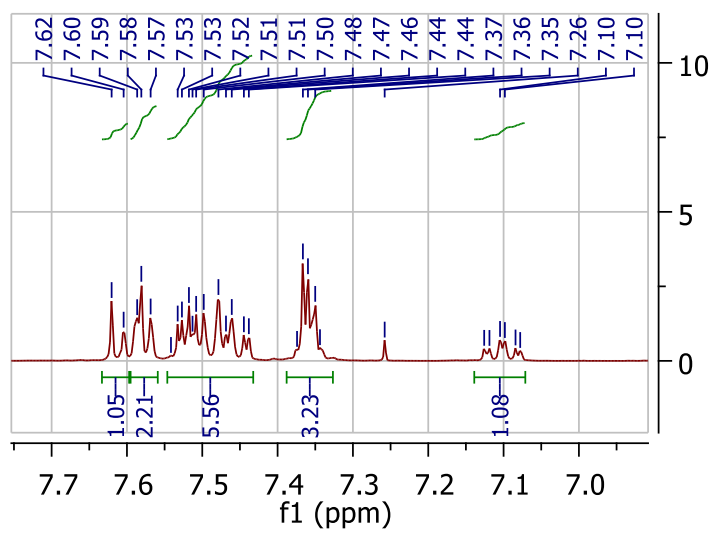
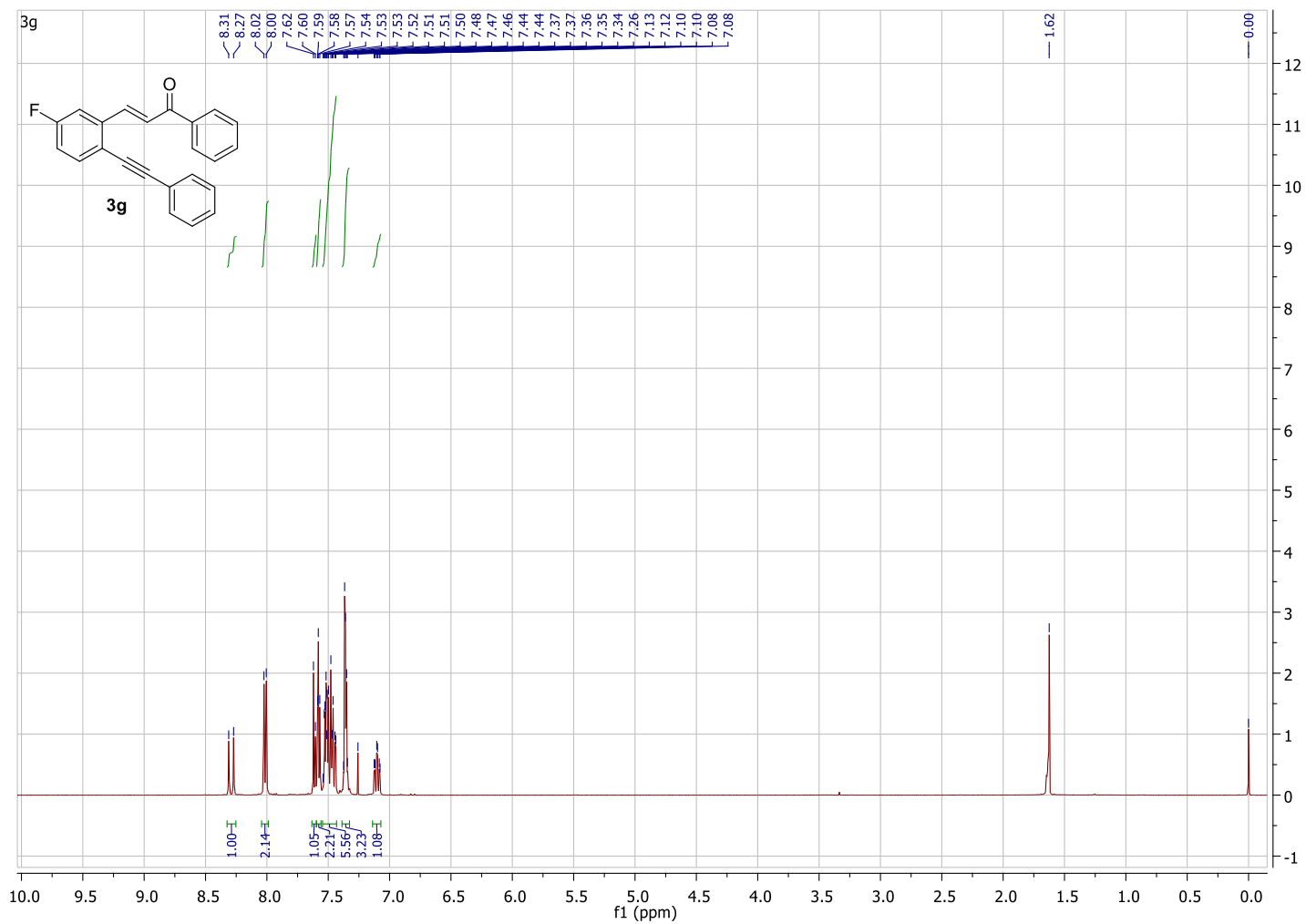


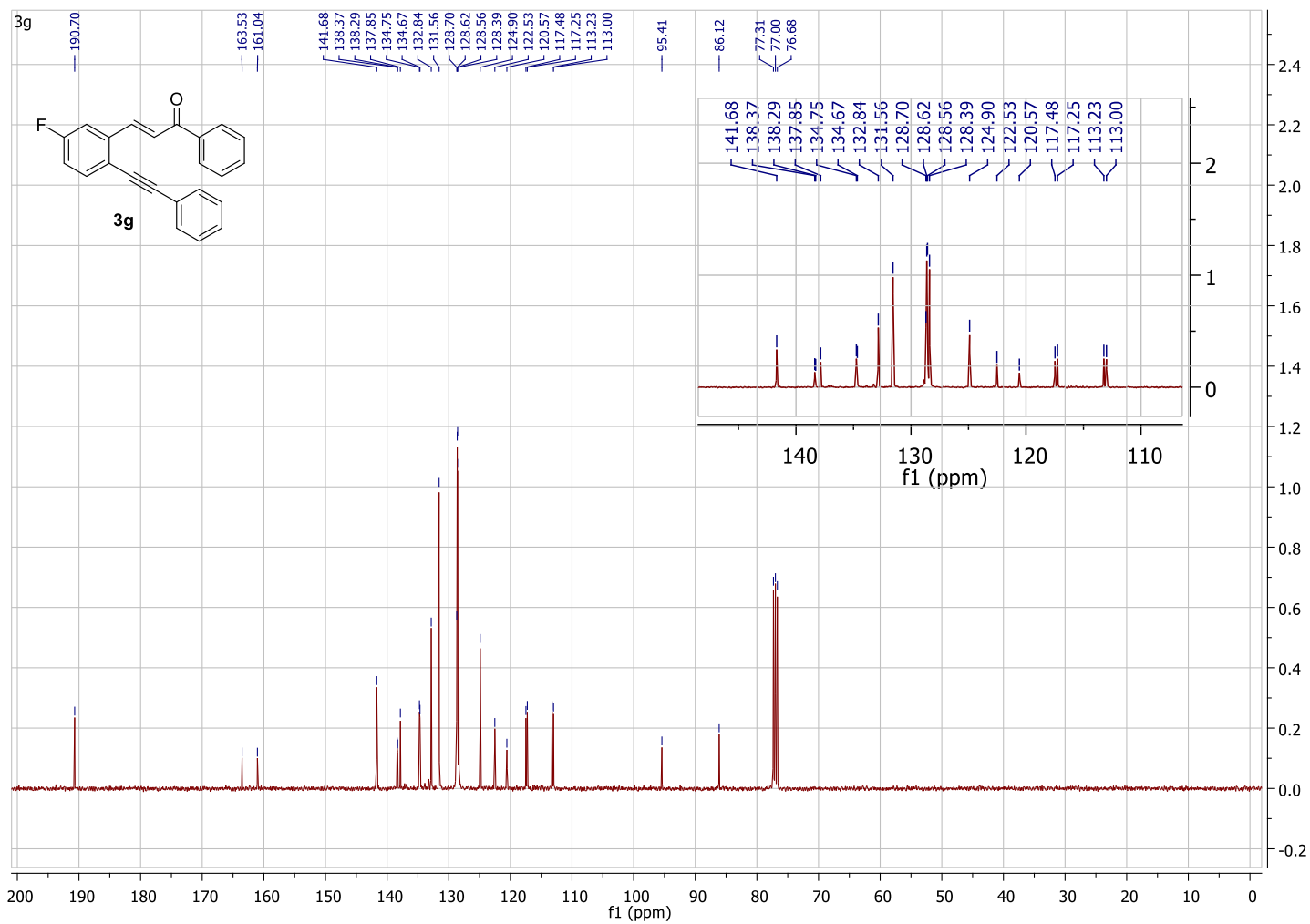




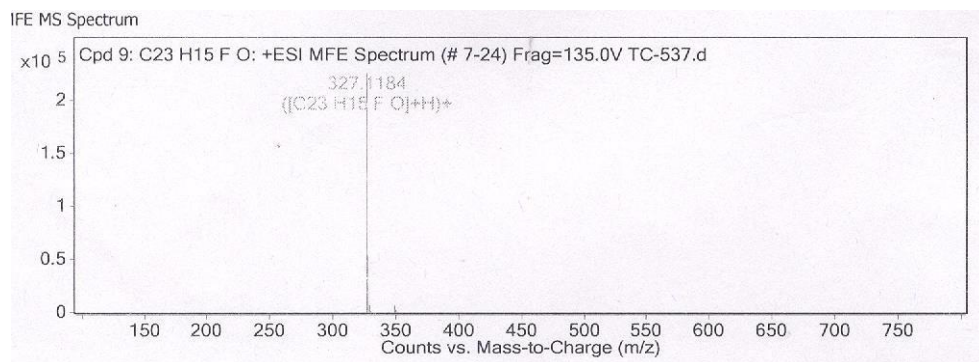
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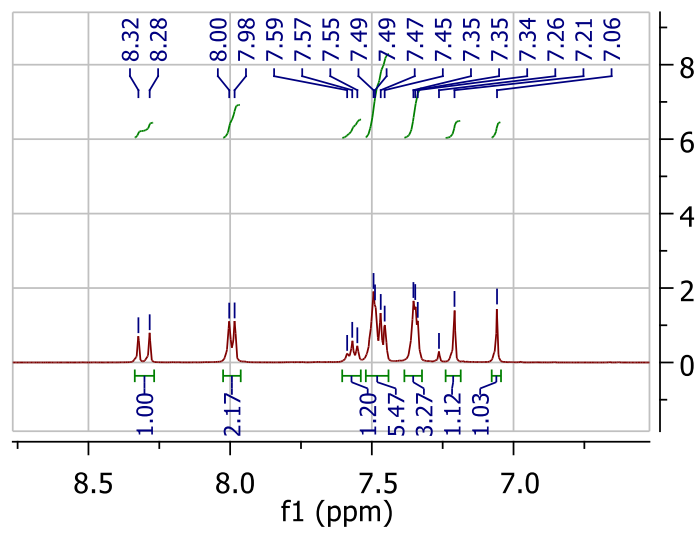
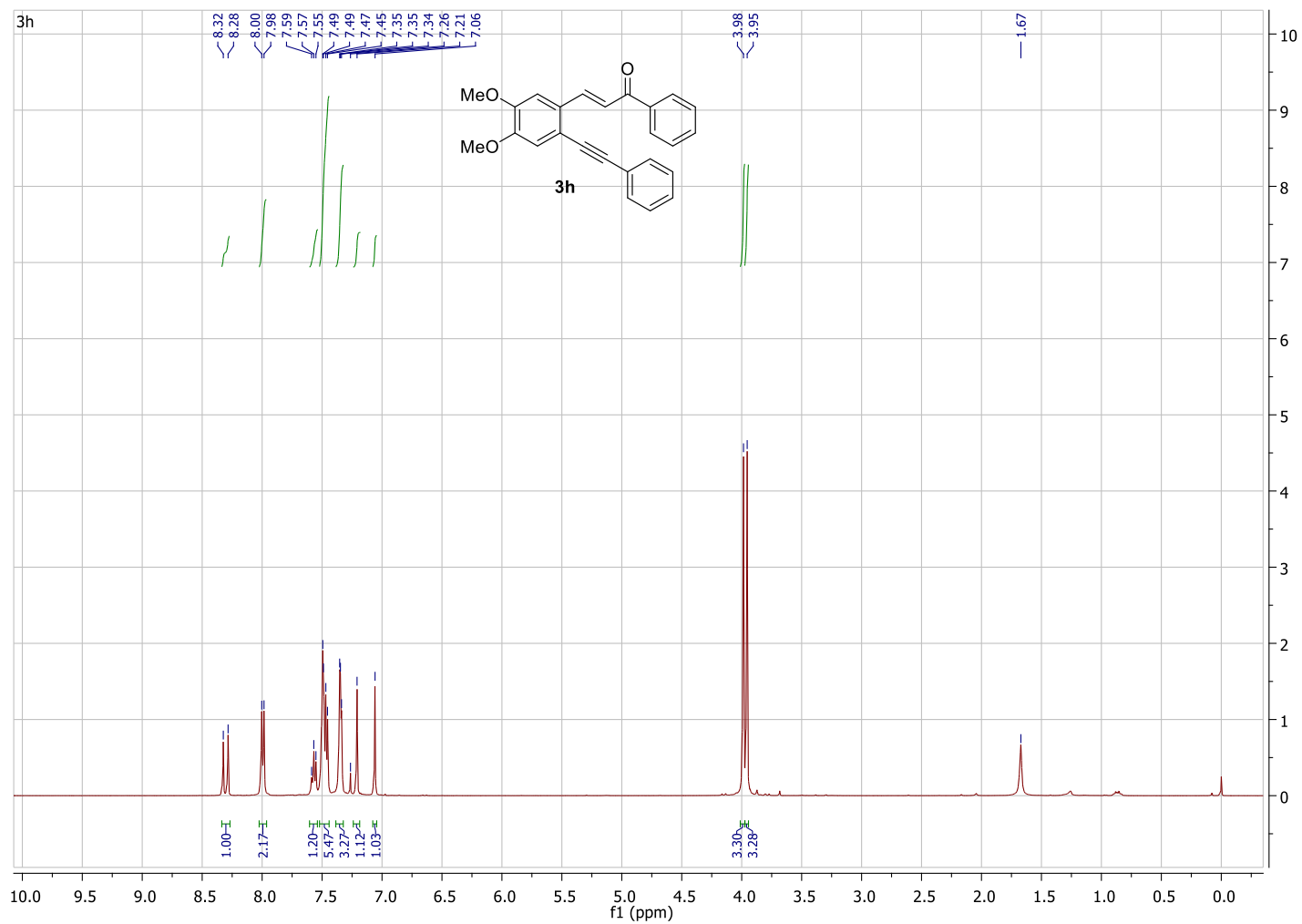


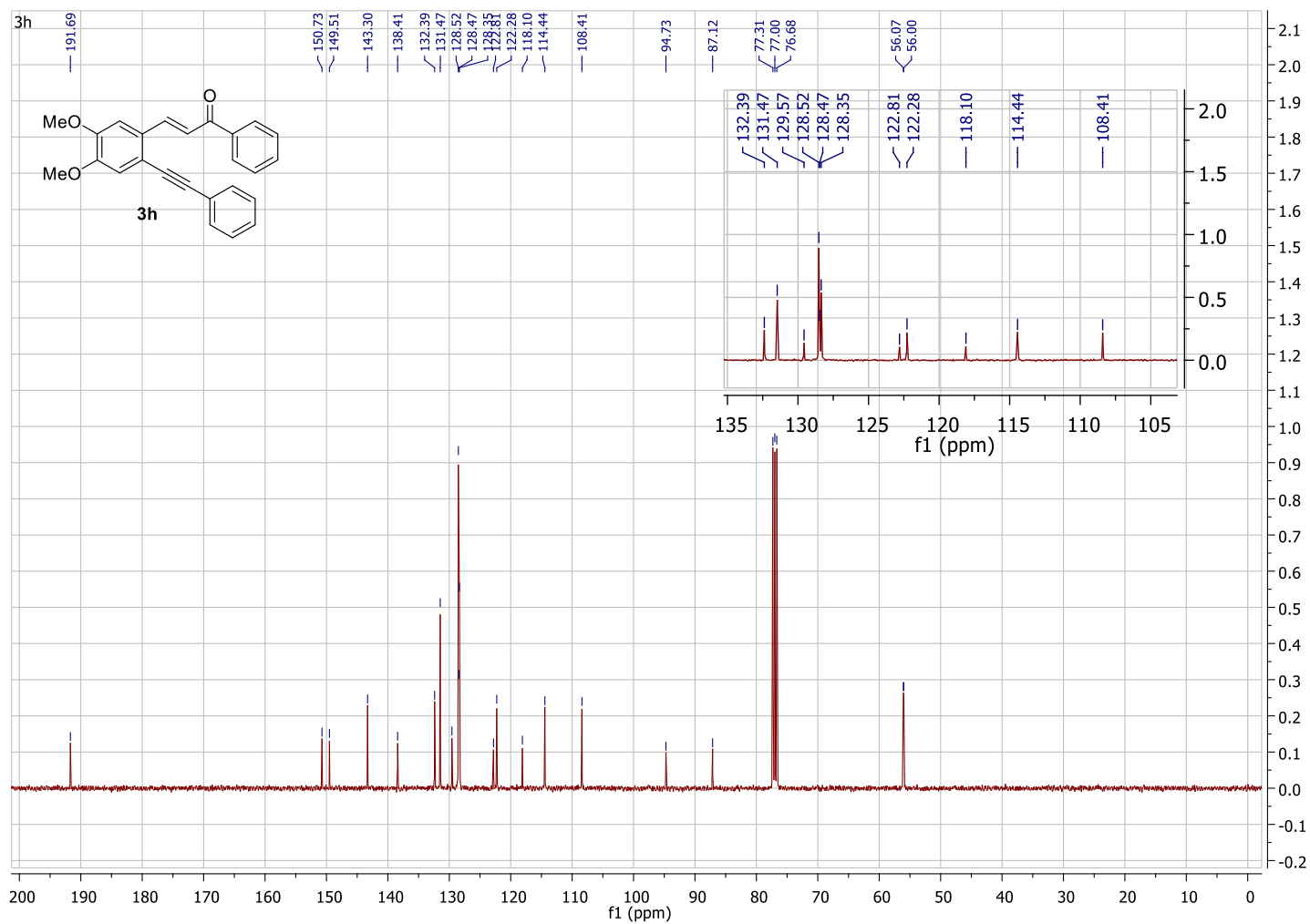




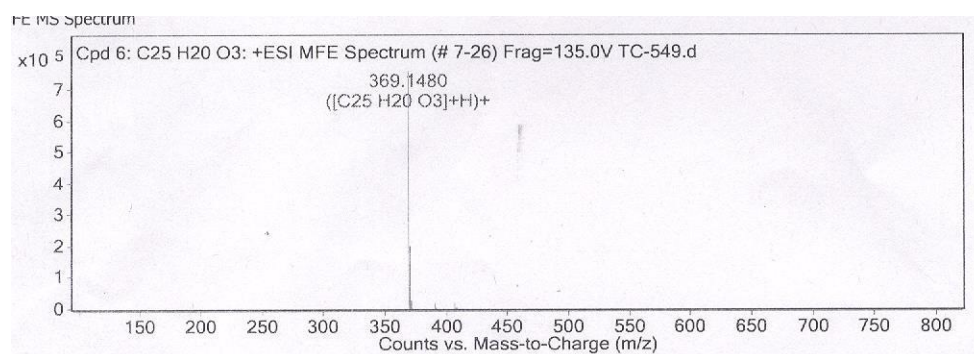
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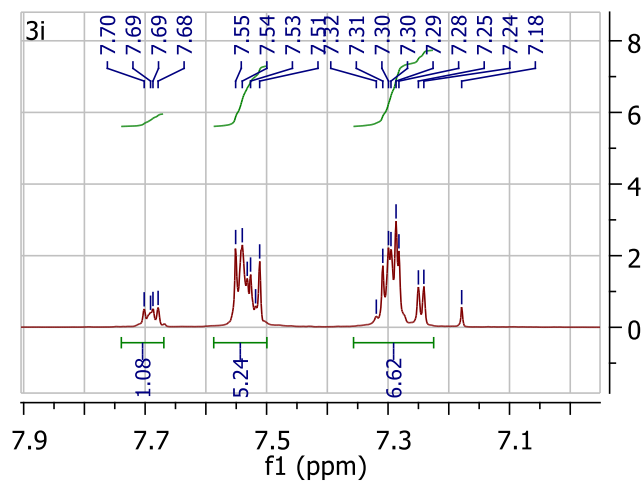
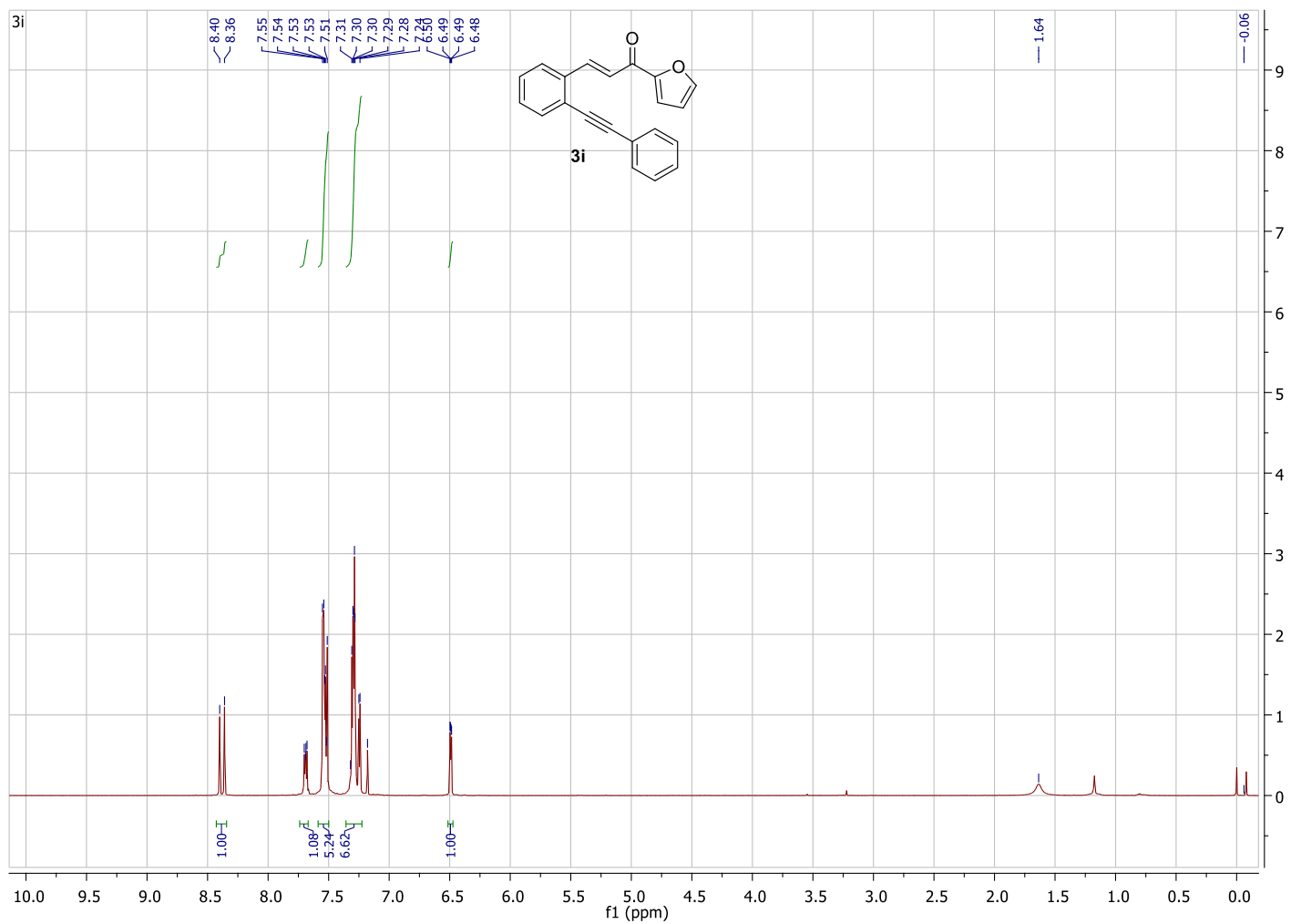


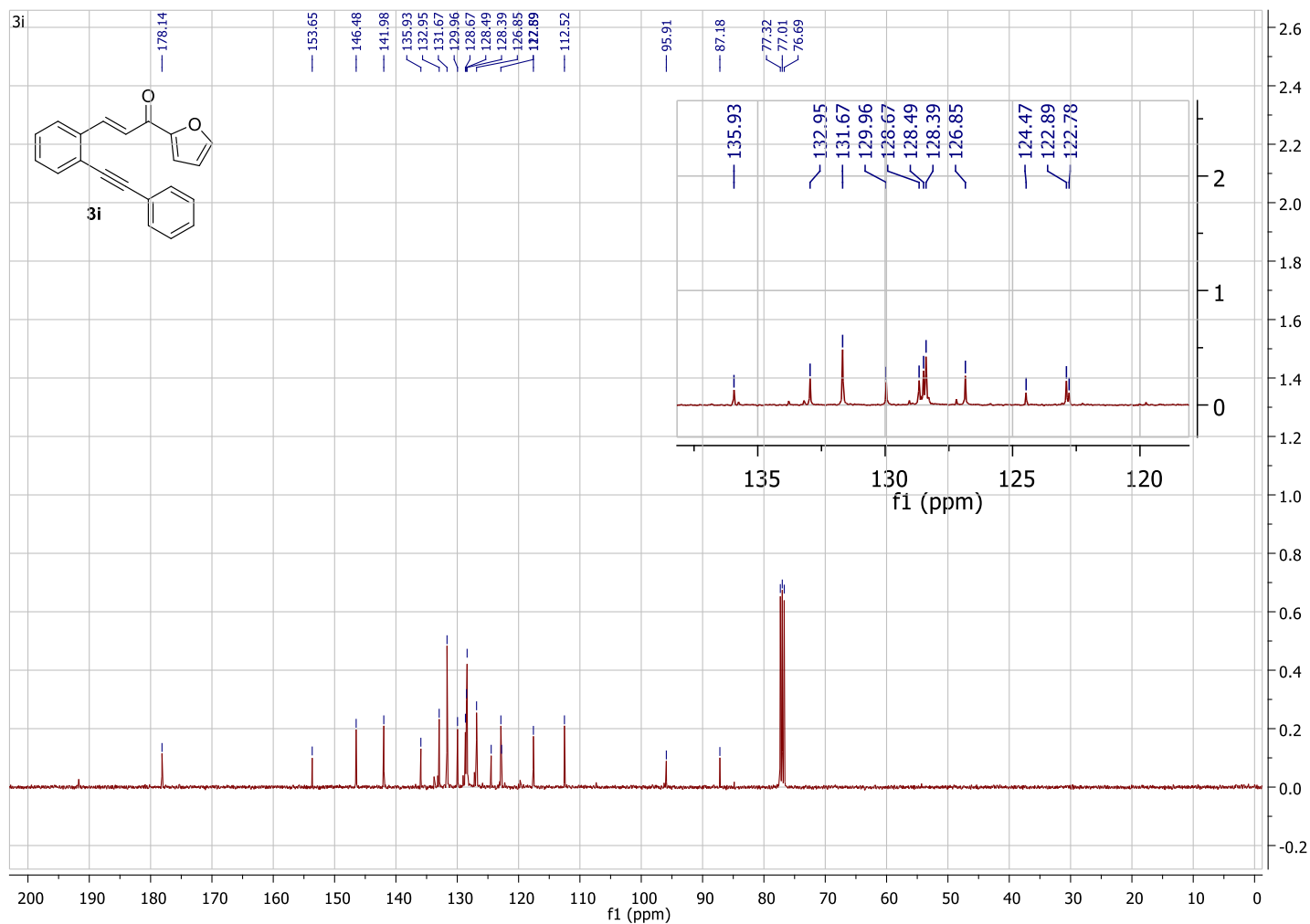




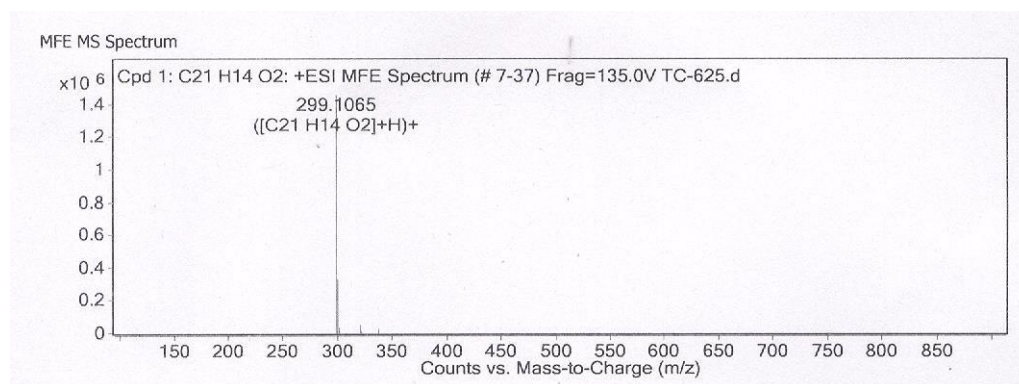
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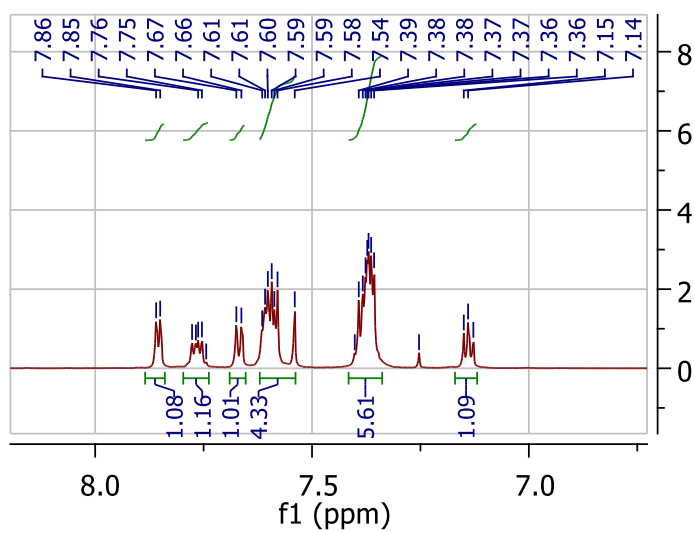
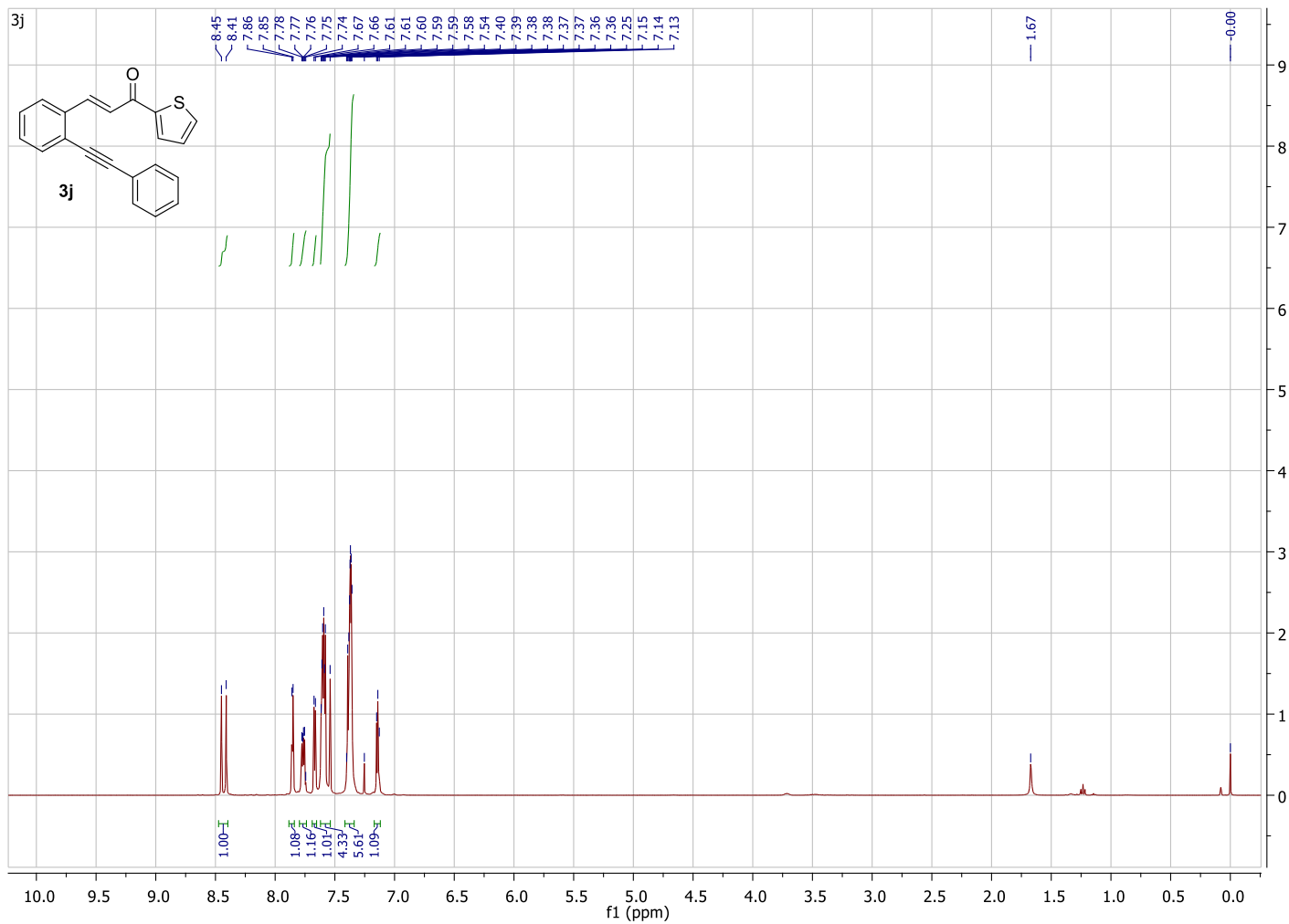


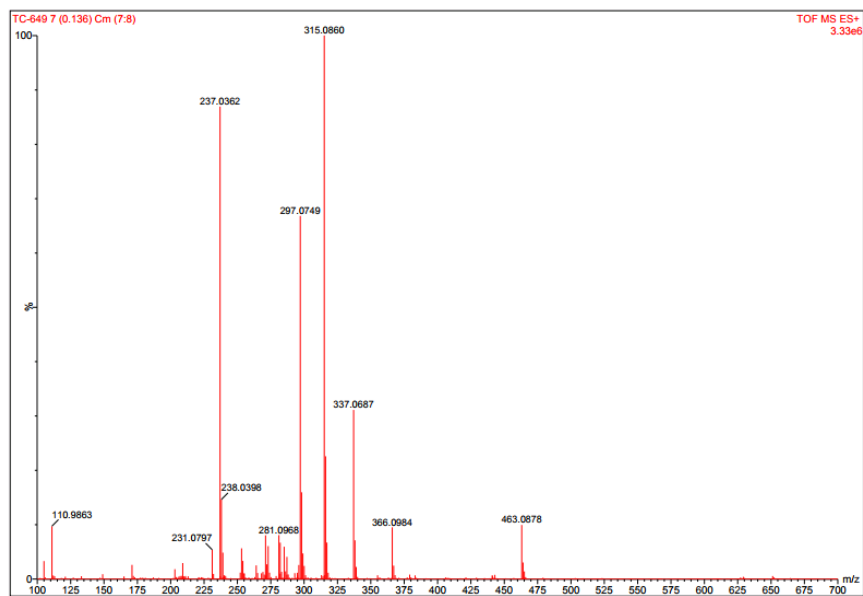
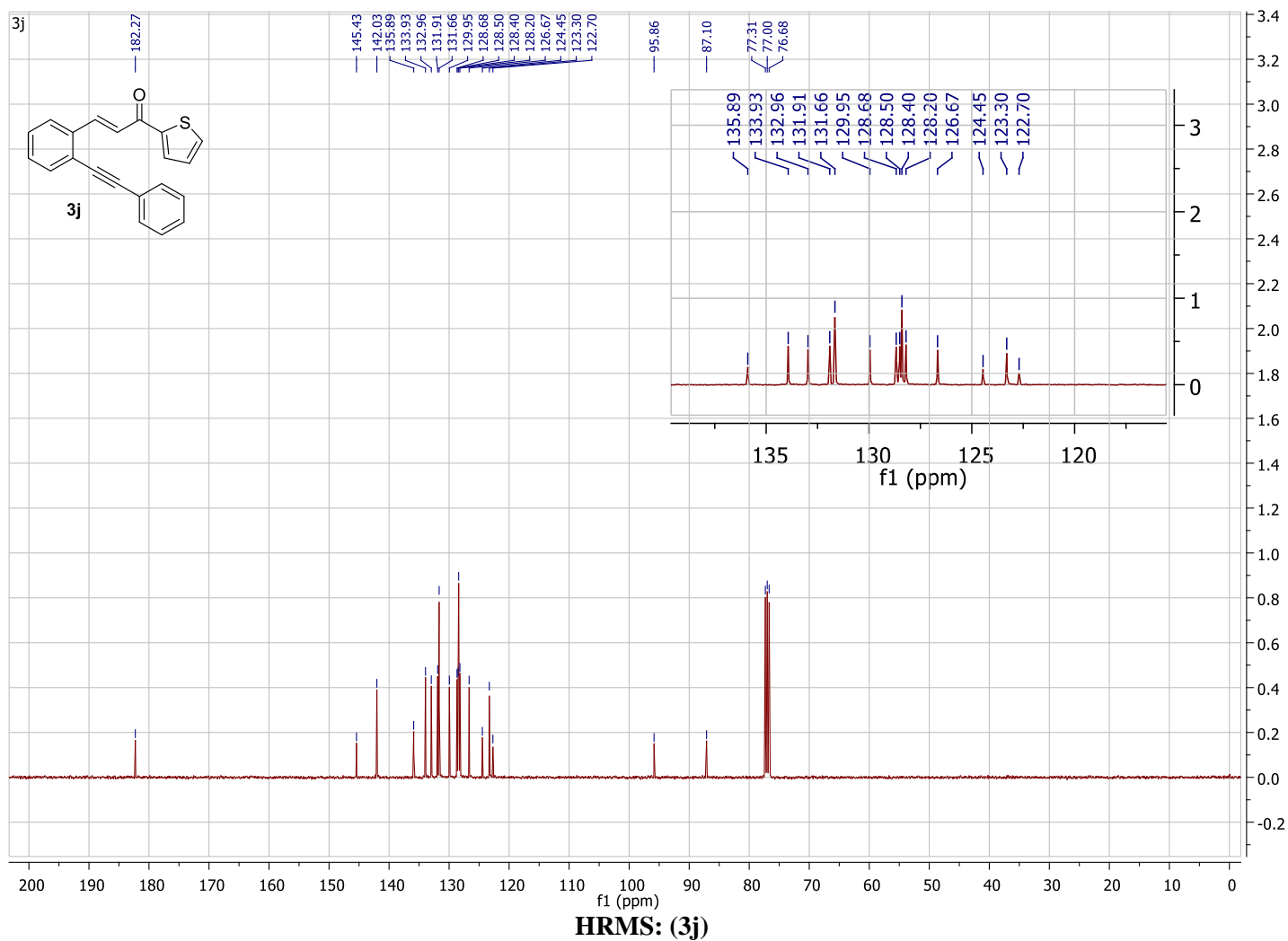


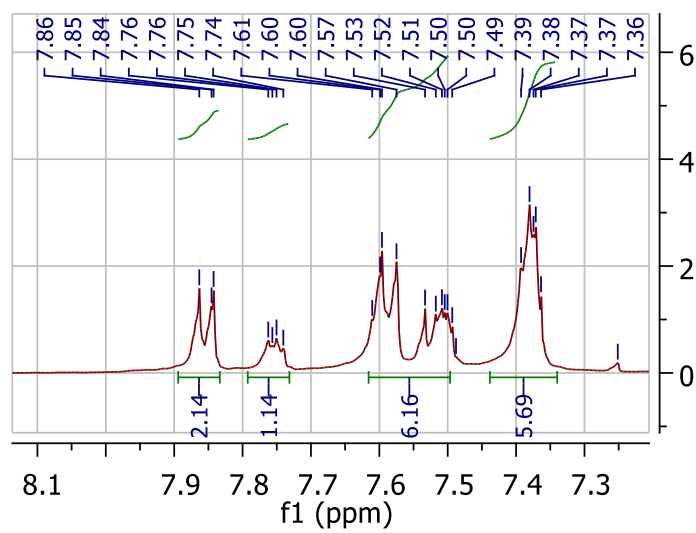
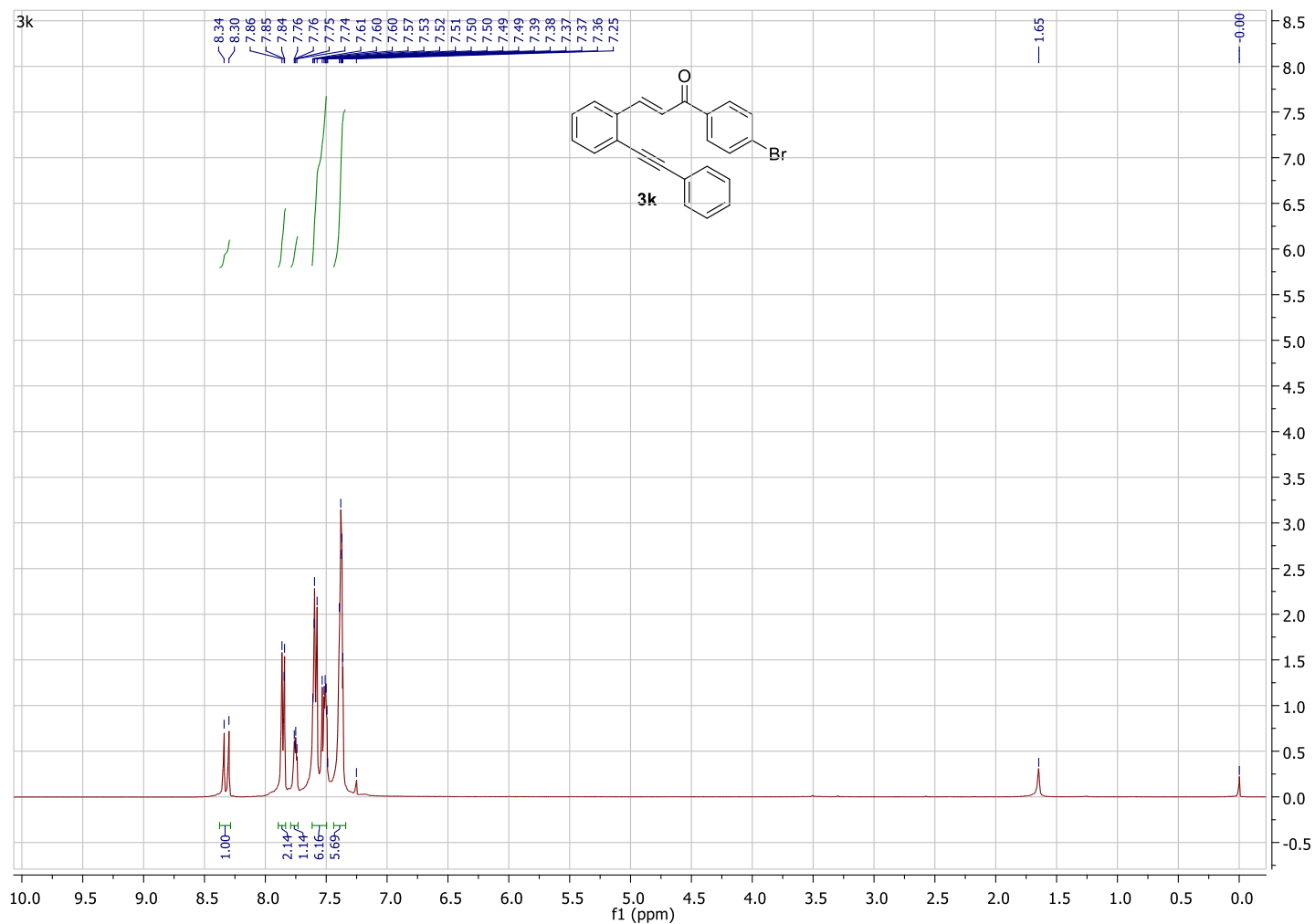


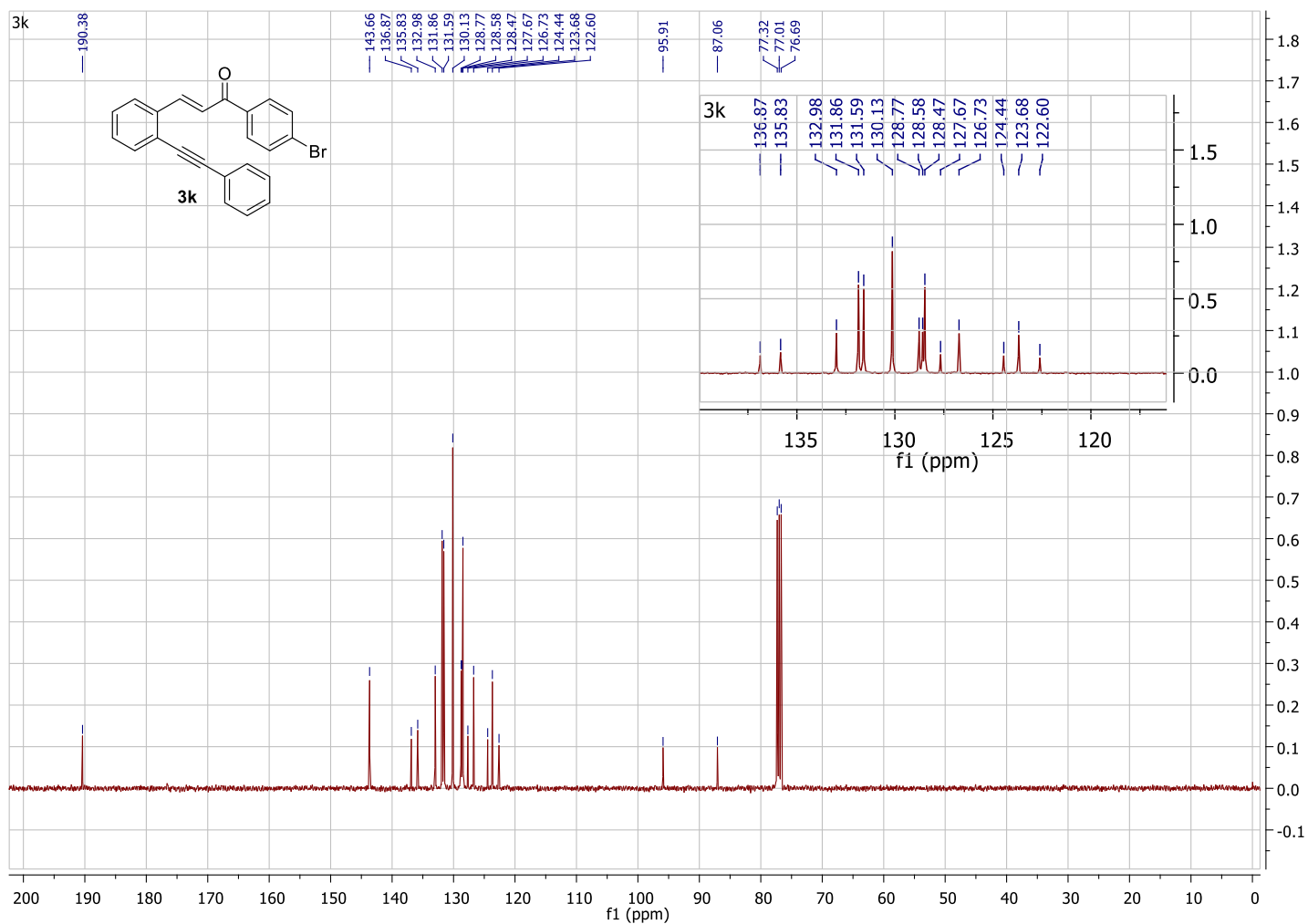
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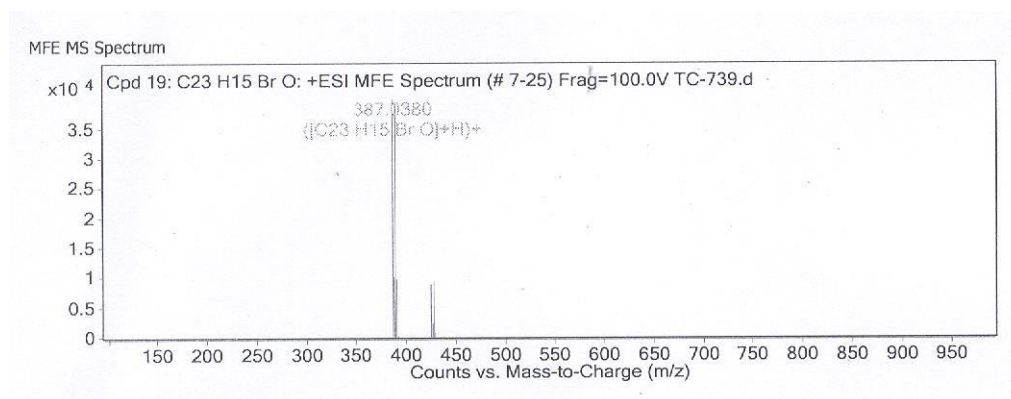


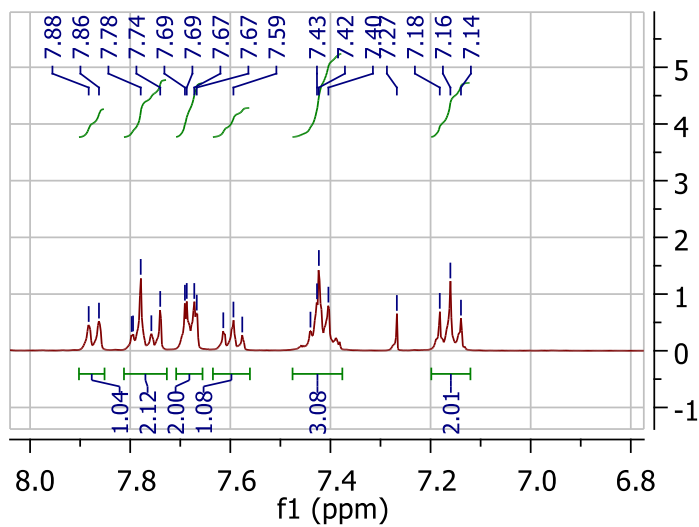
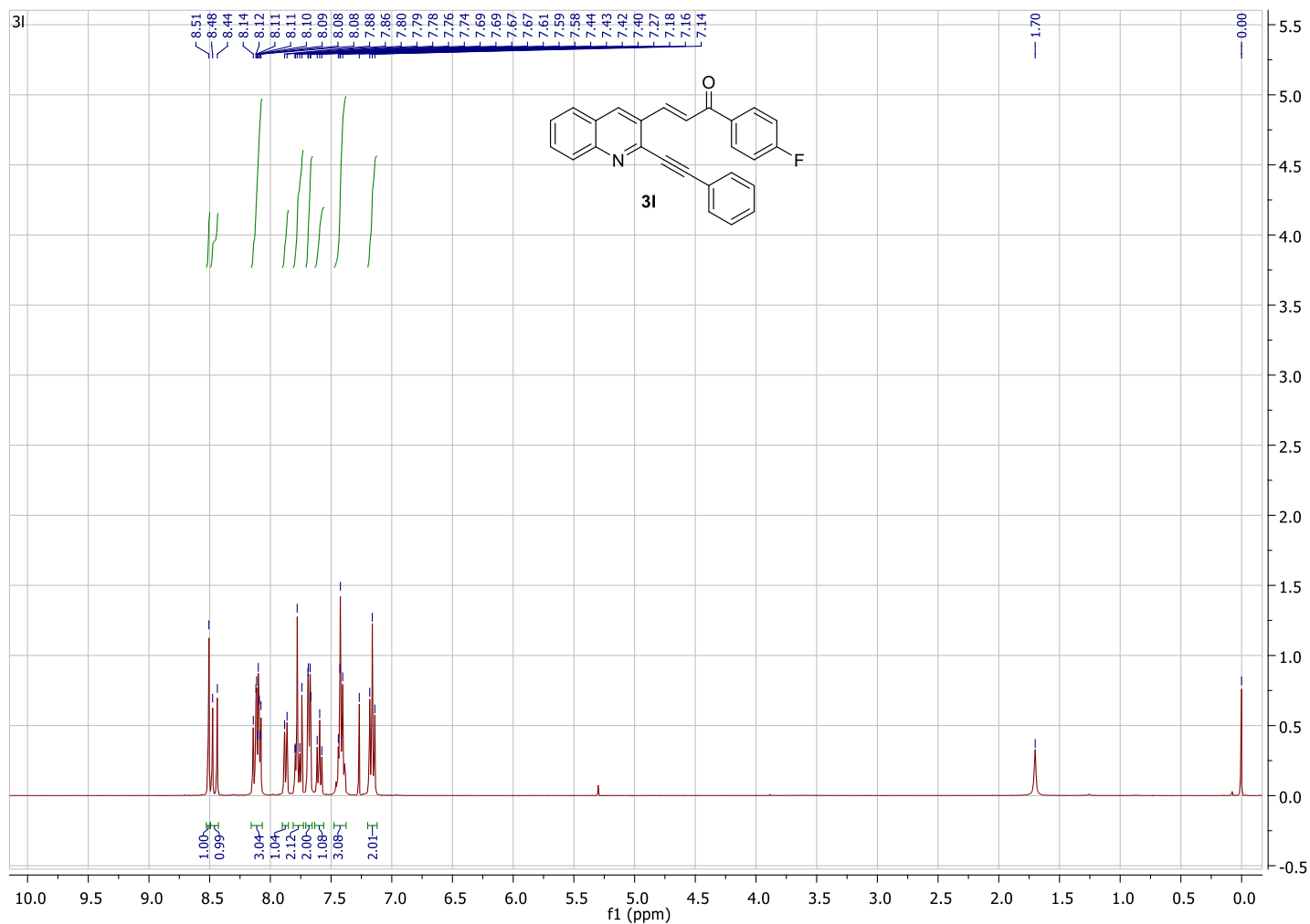


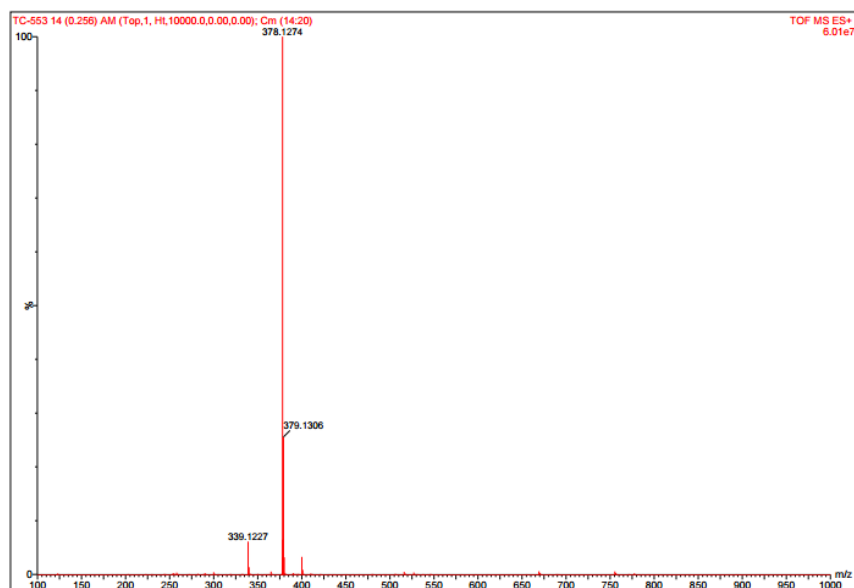
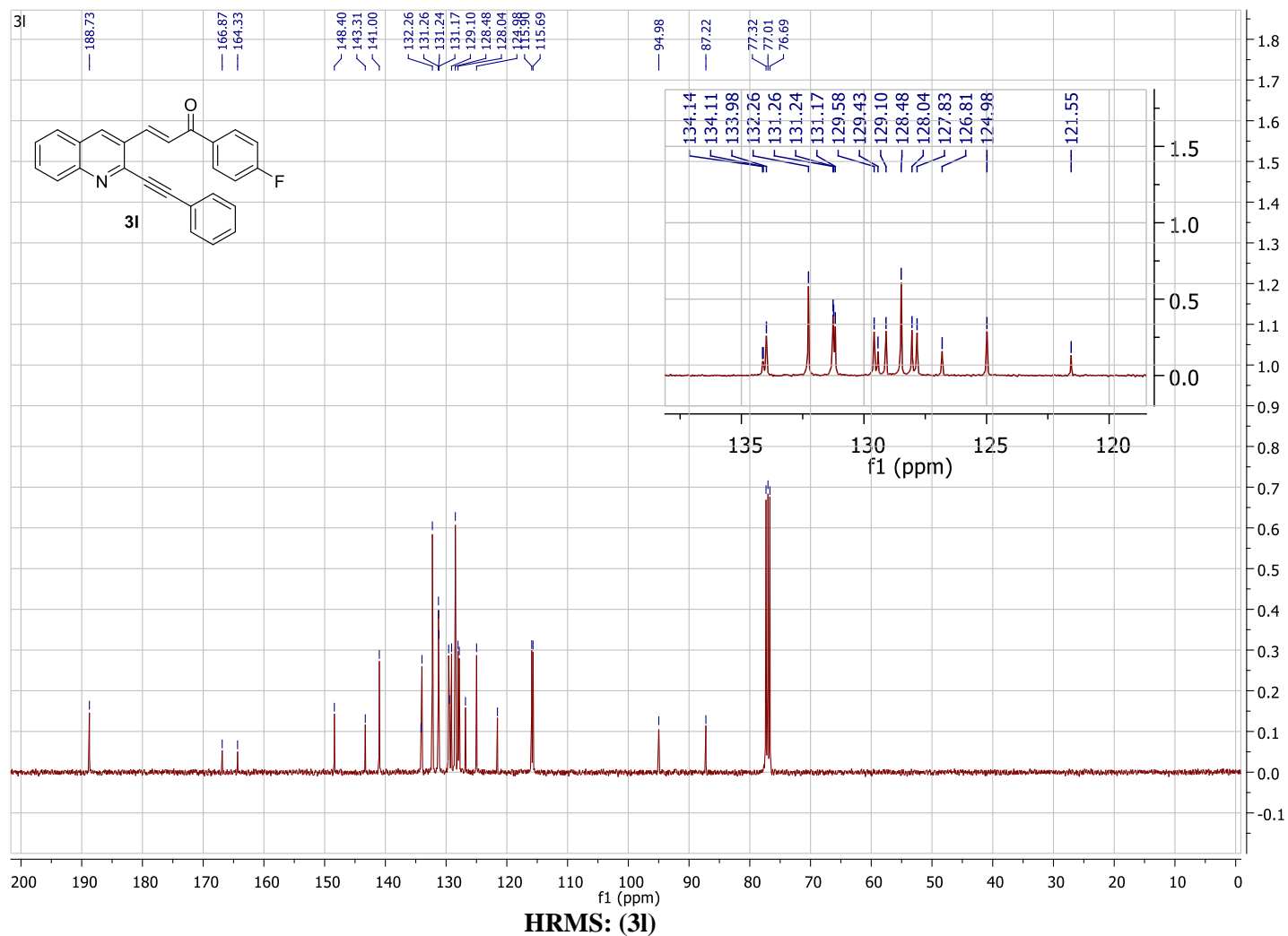


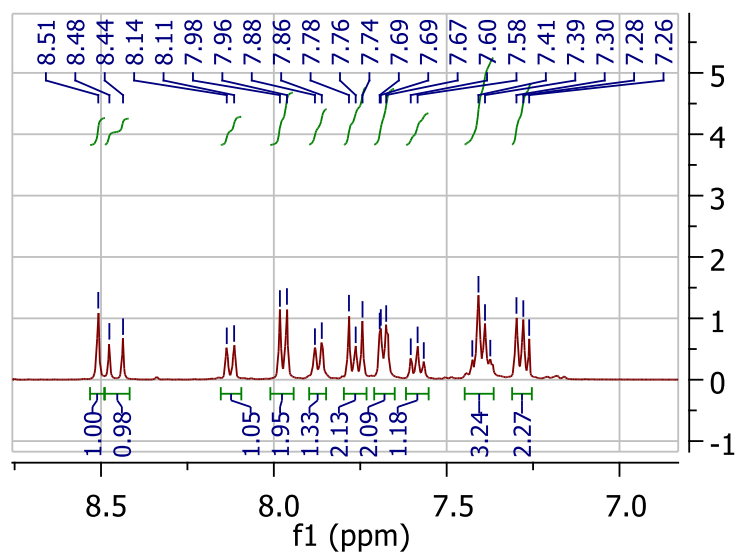
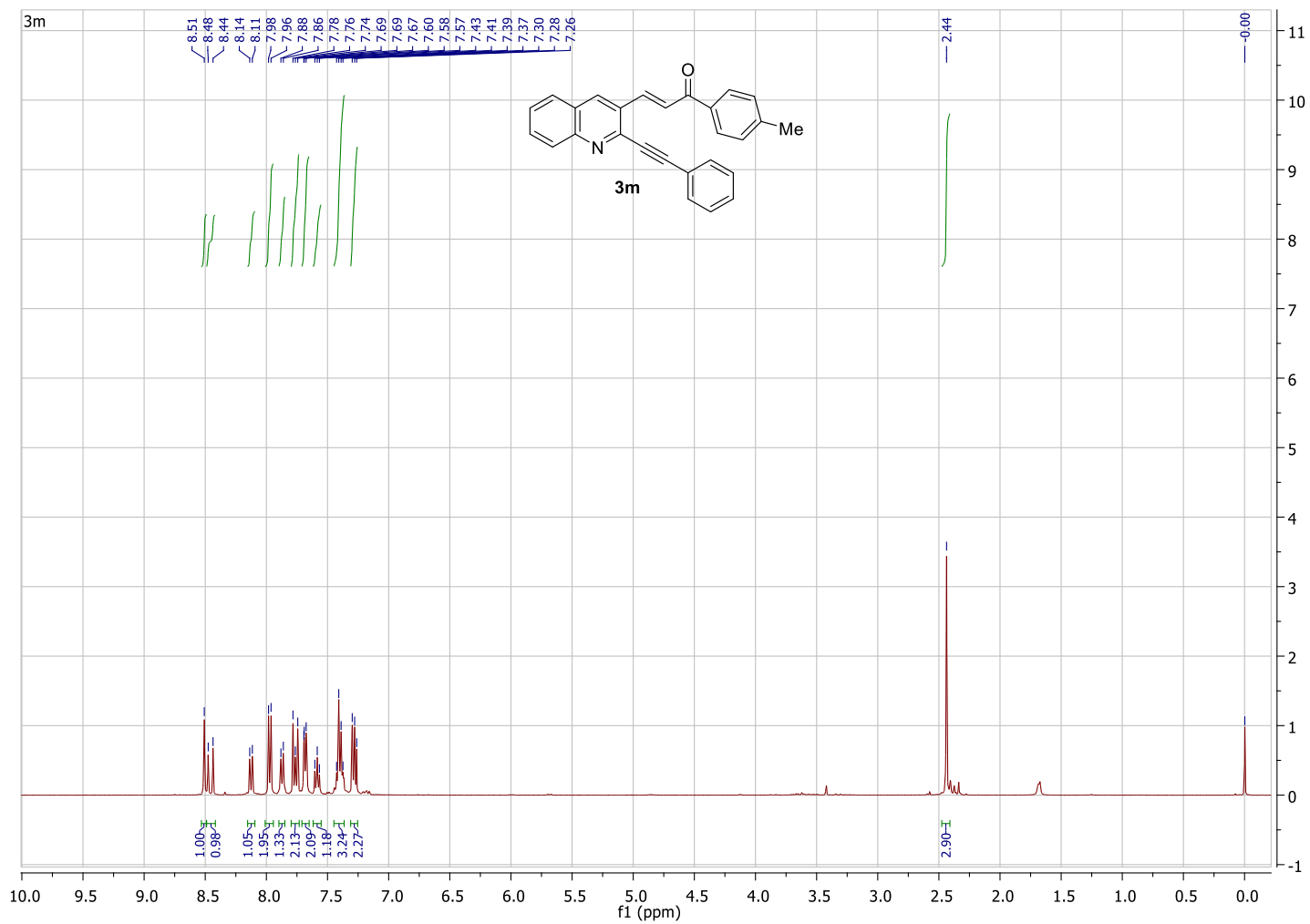


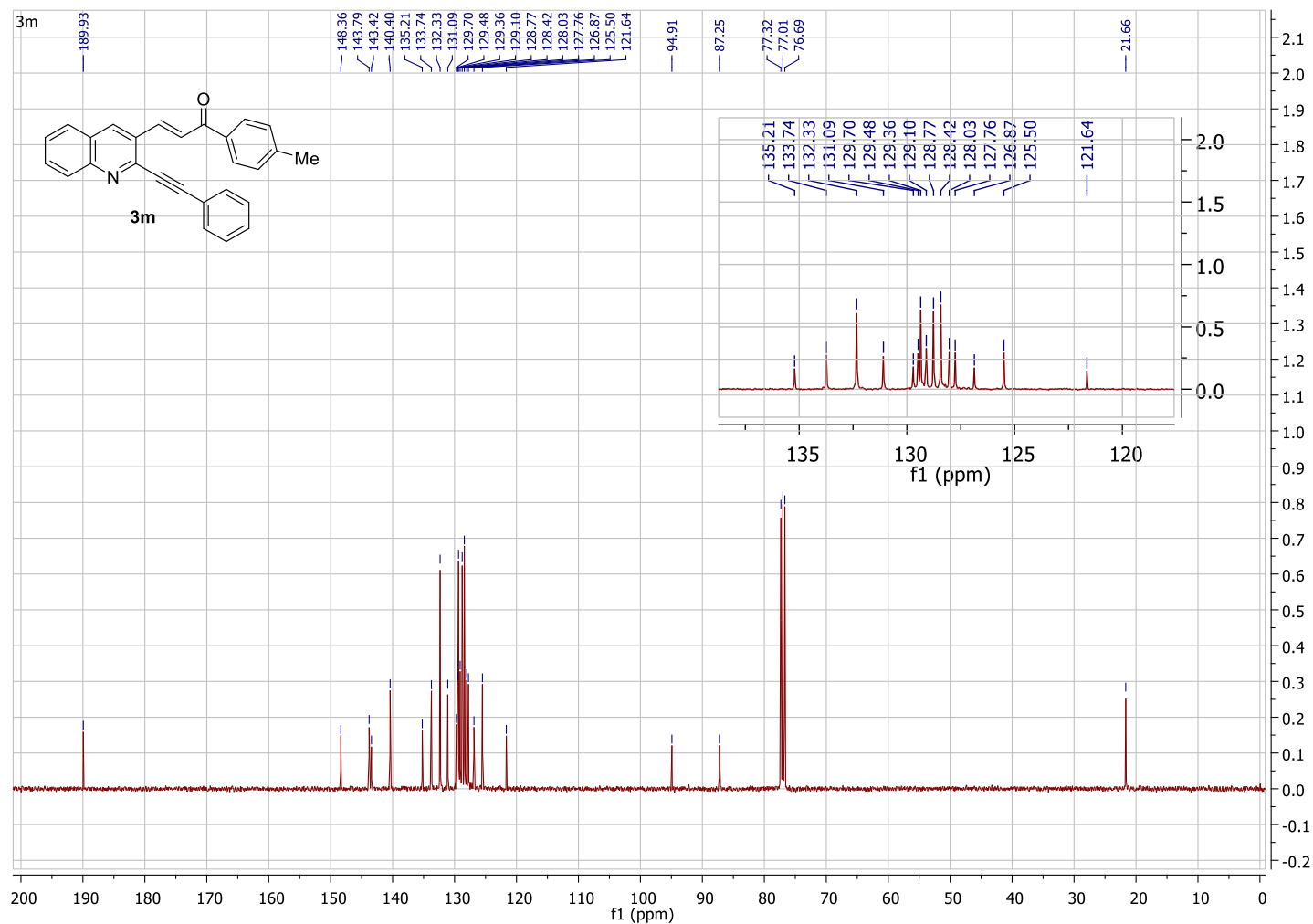
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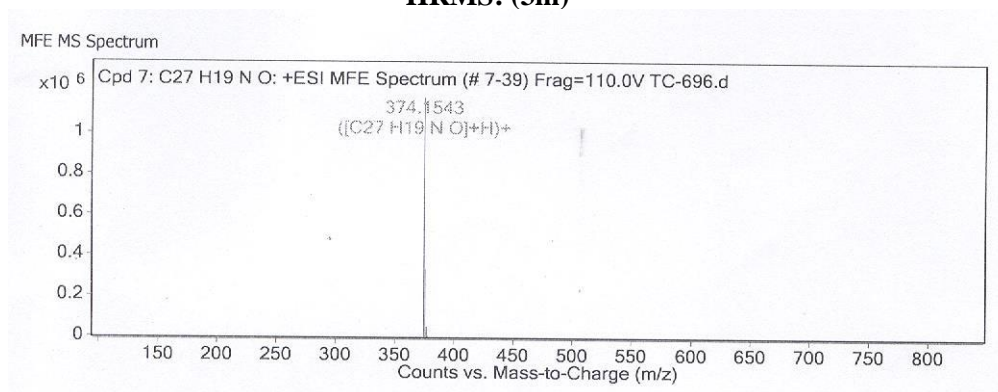


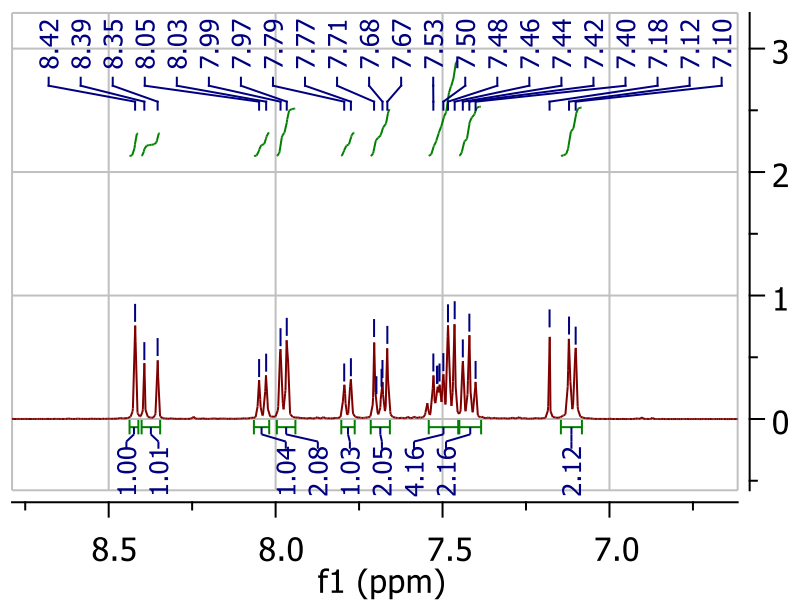
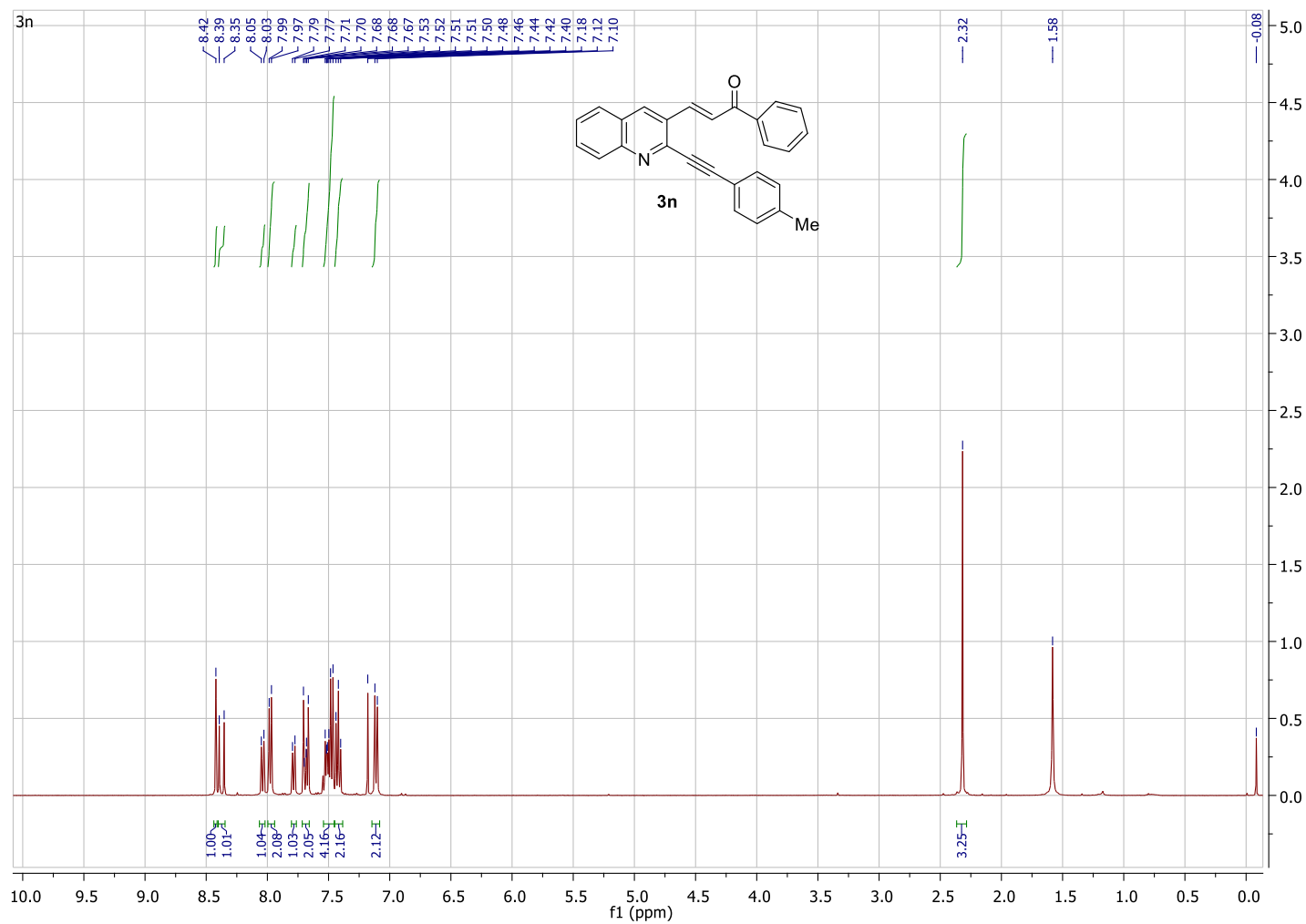


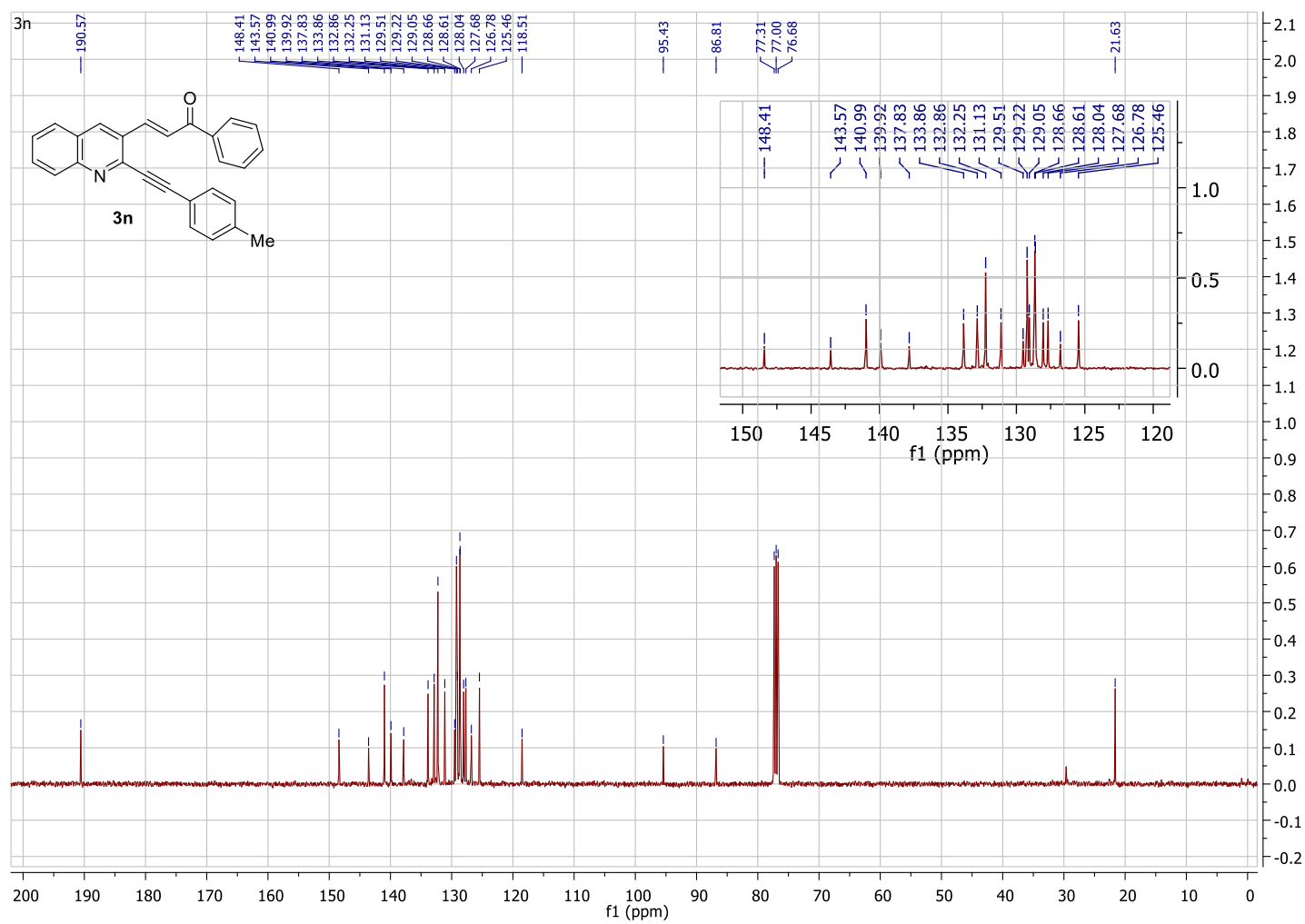




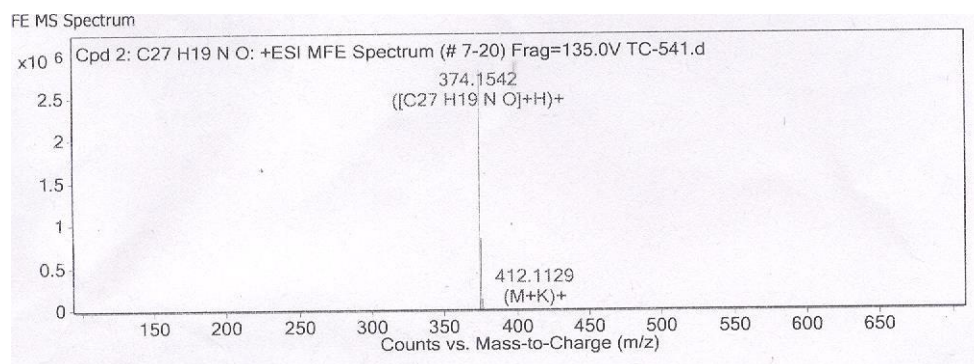
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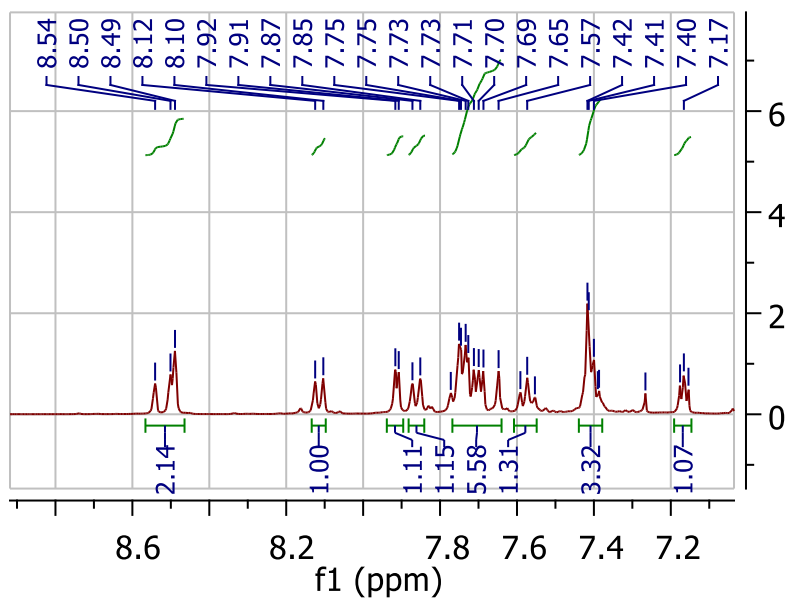
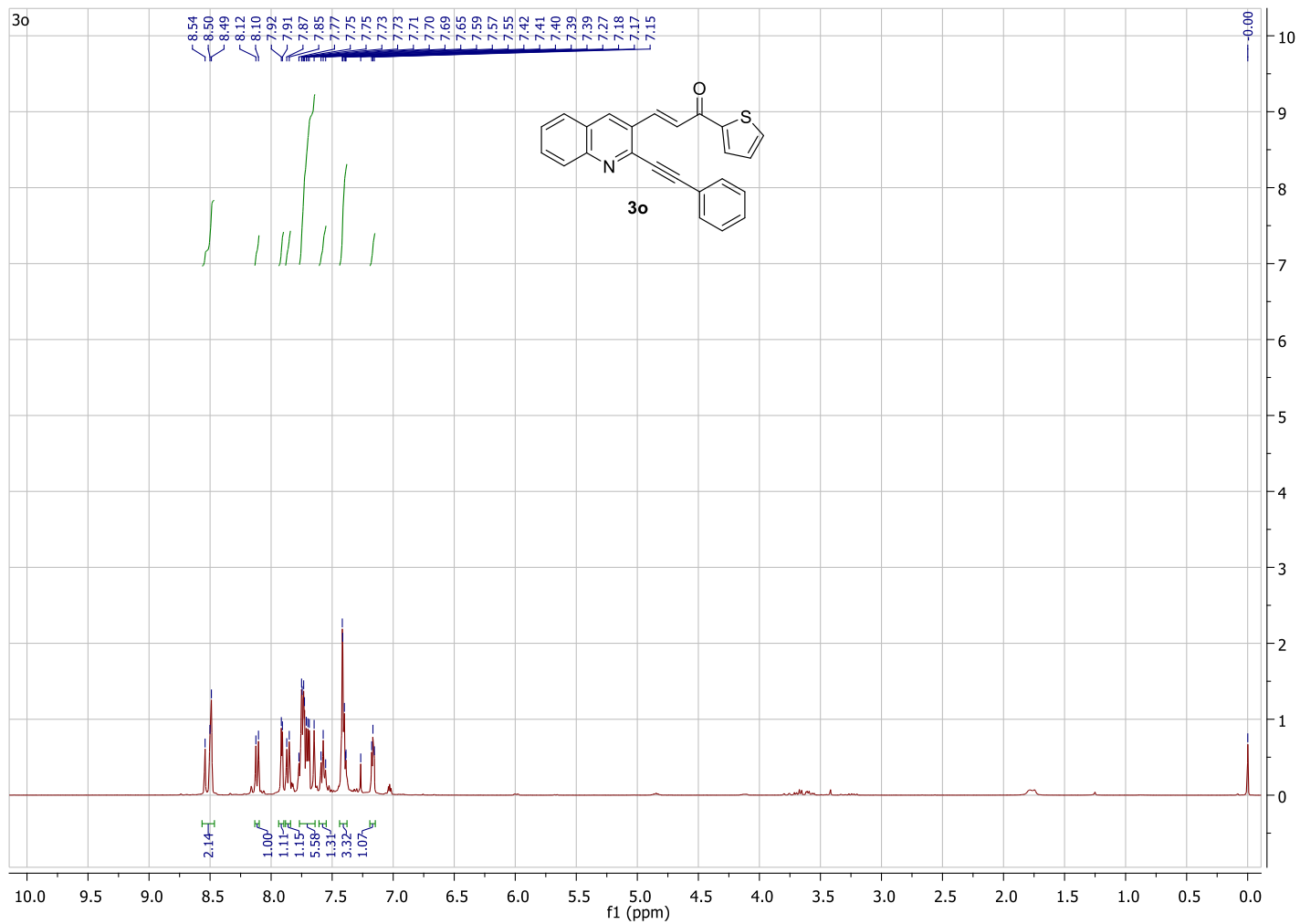




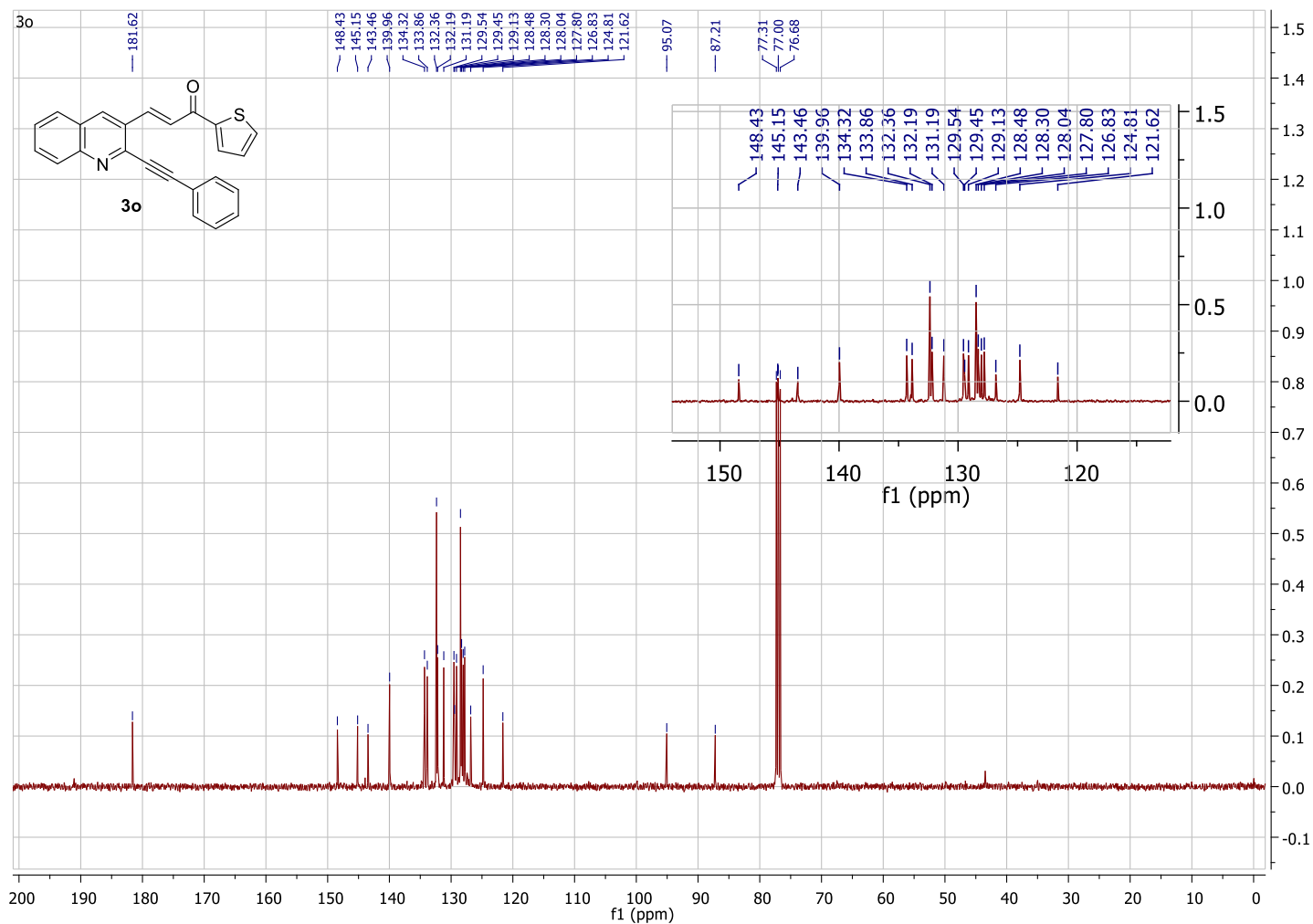


HRMS: (3n)



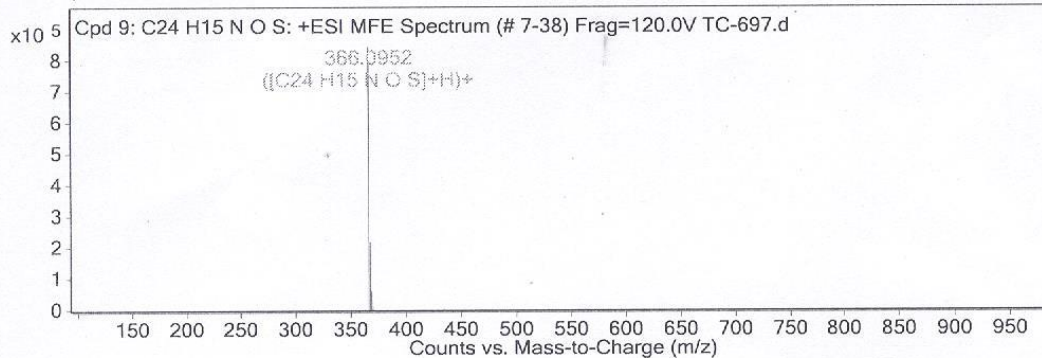


S30

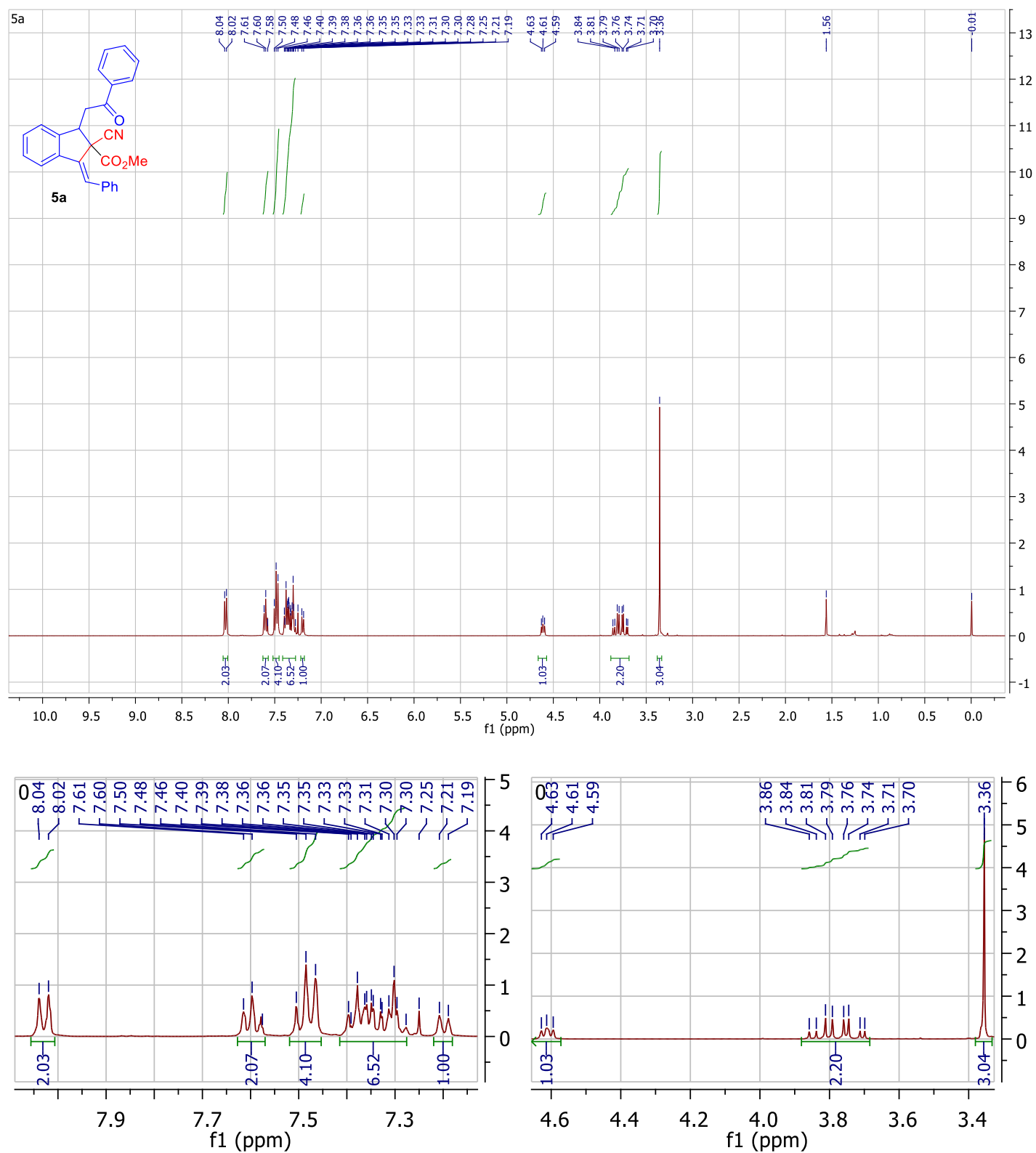


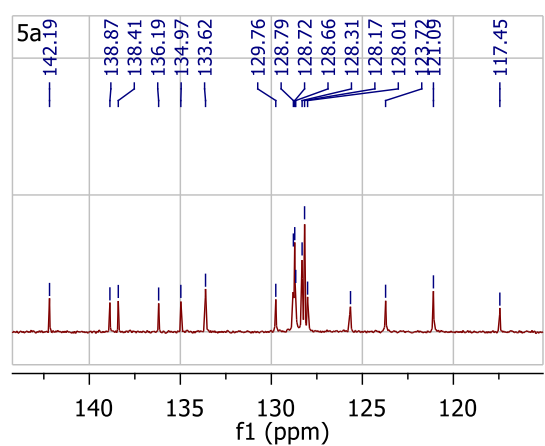
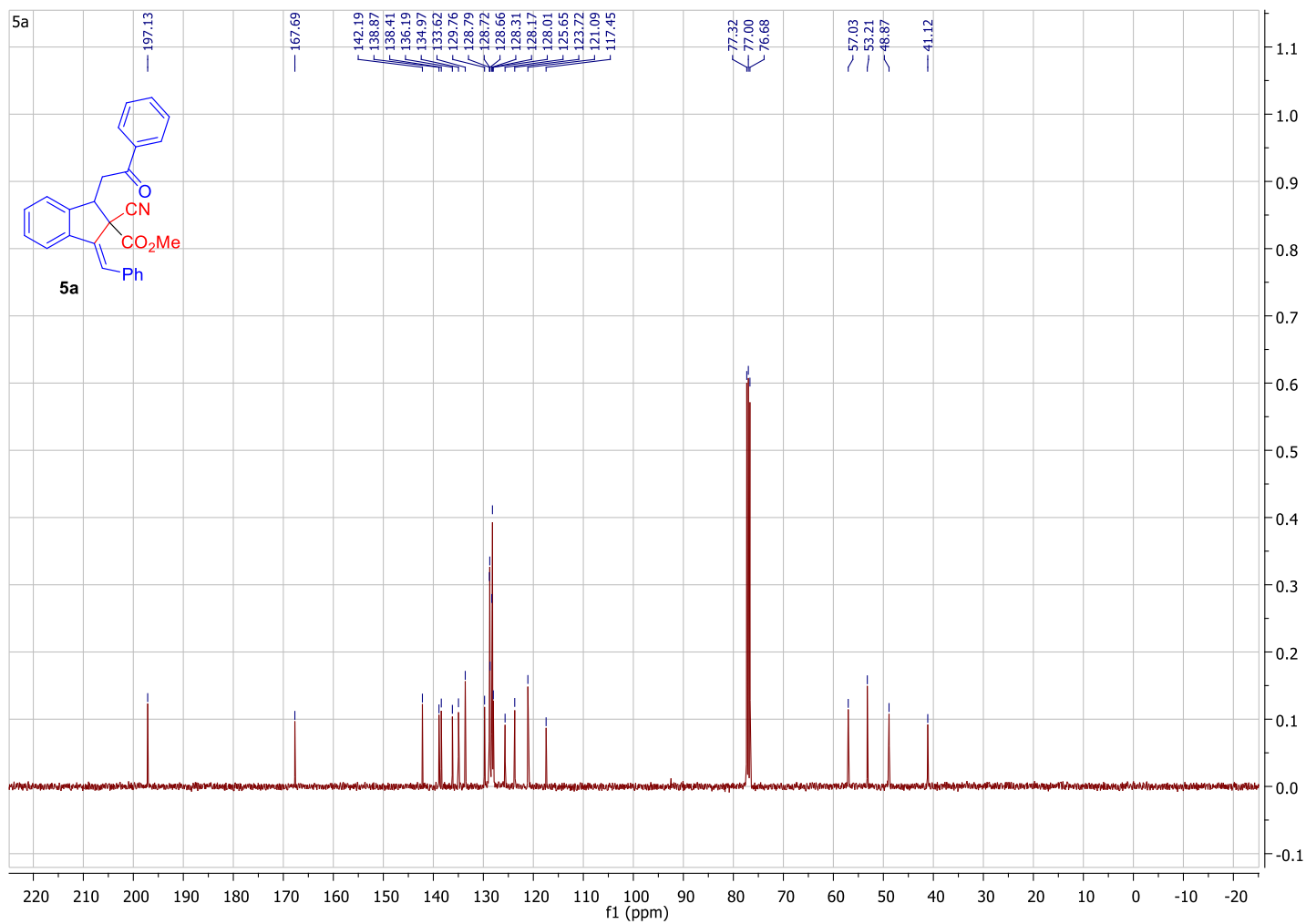
HRMS: (3o)

MFE MS Spectrum



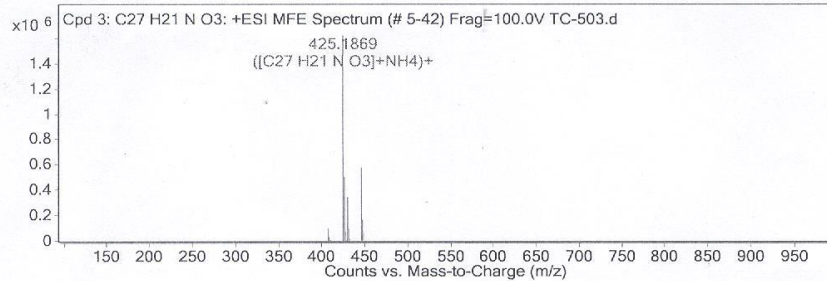
2. ^1H , ^{13}C NMR and HRMS spectra of compounds 3a-7h and 8:

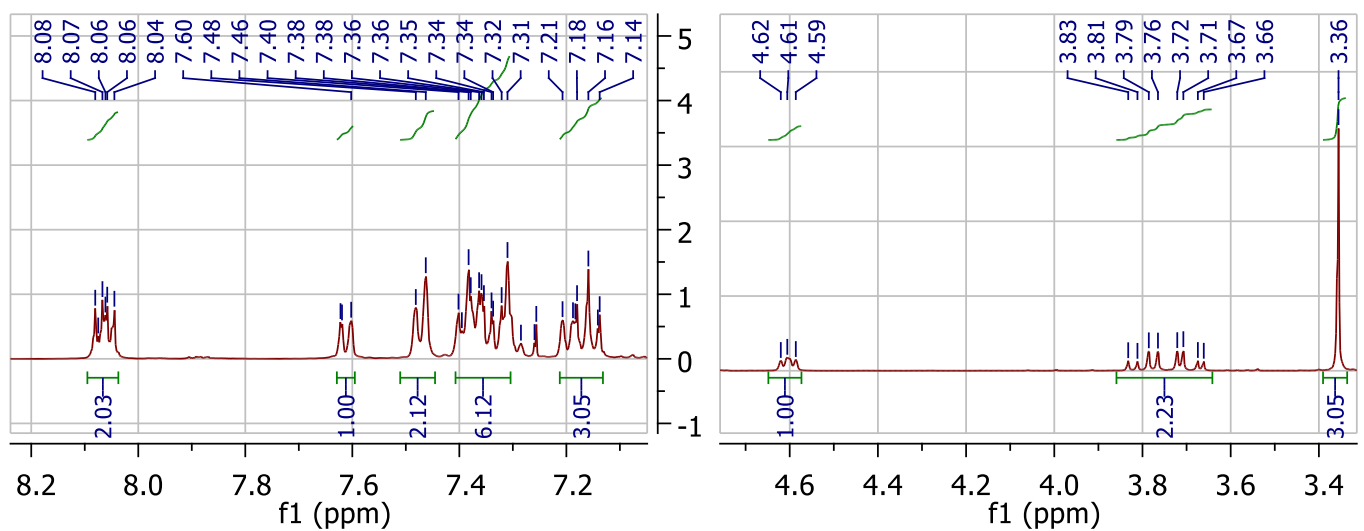
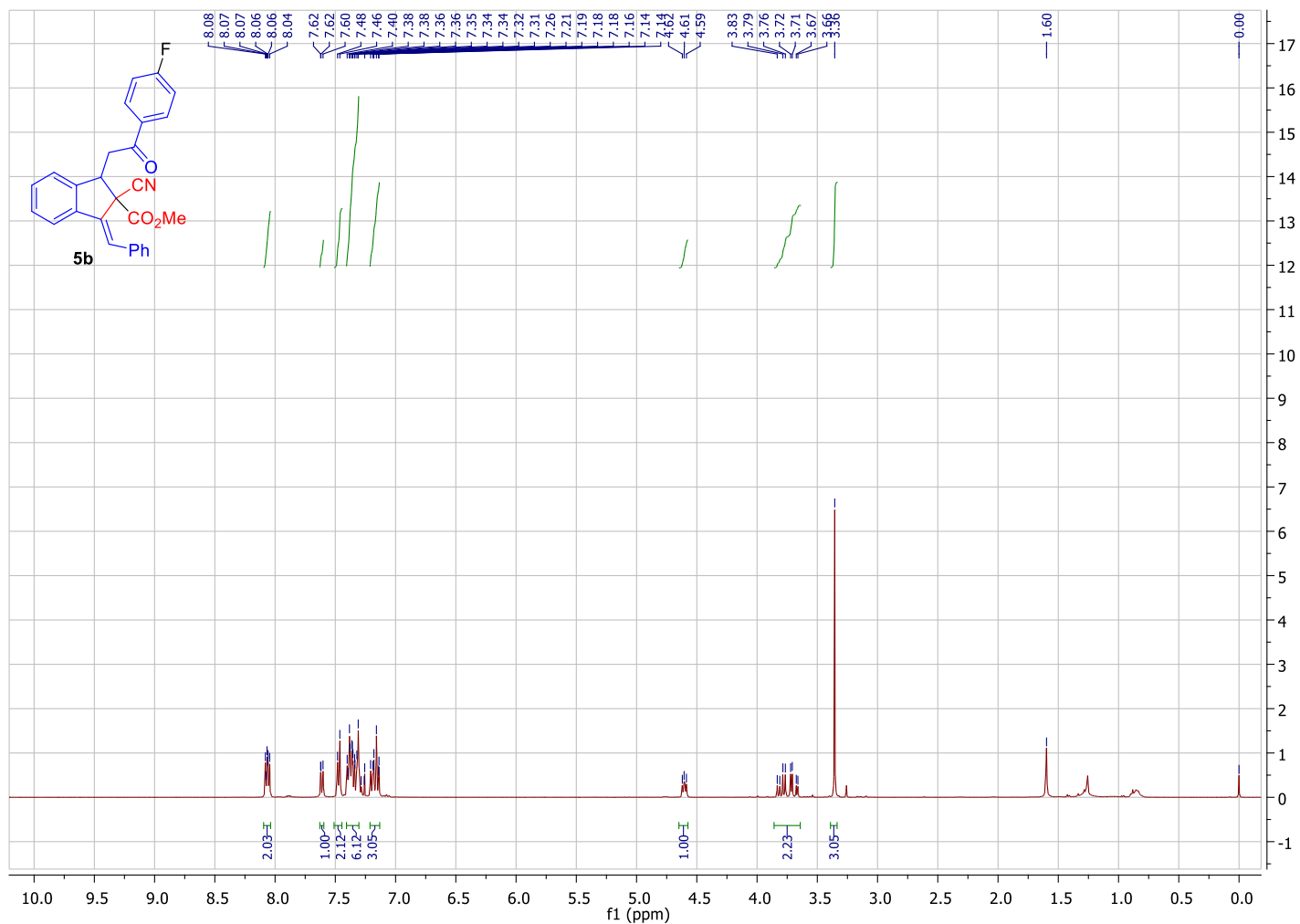


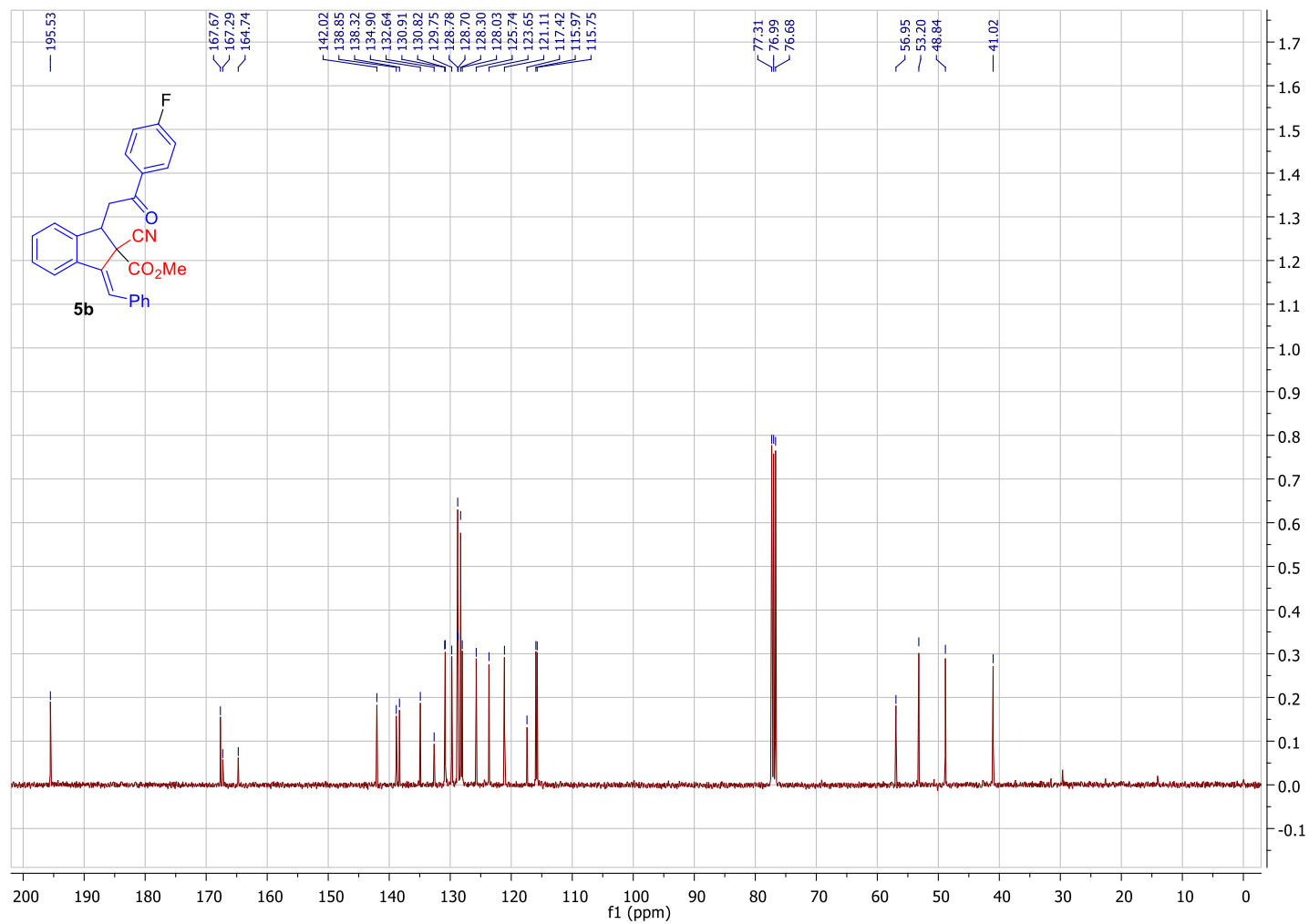


HRMS: (5a)

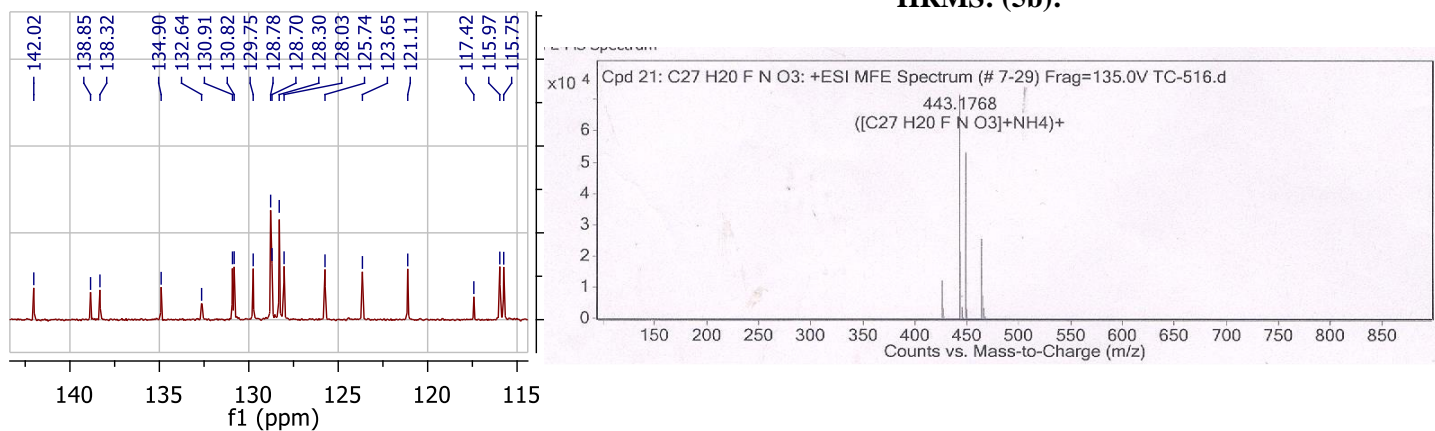
MFE MS Spectrum

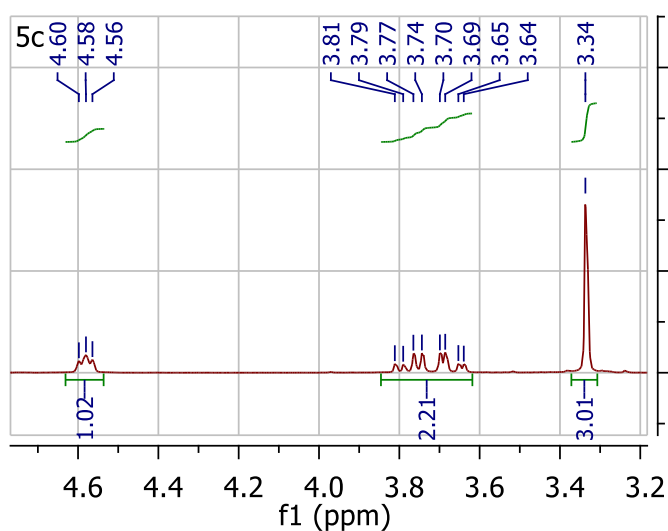
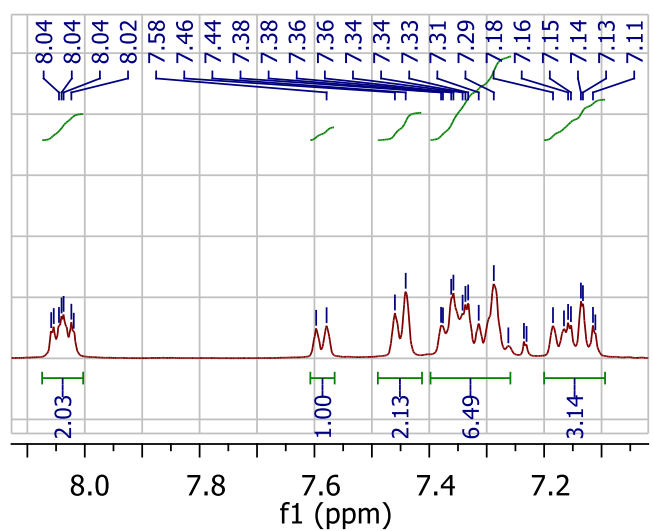
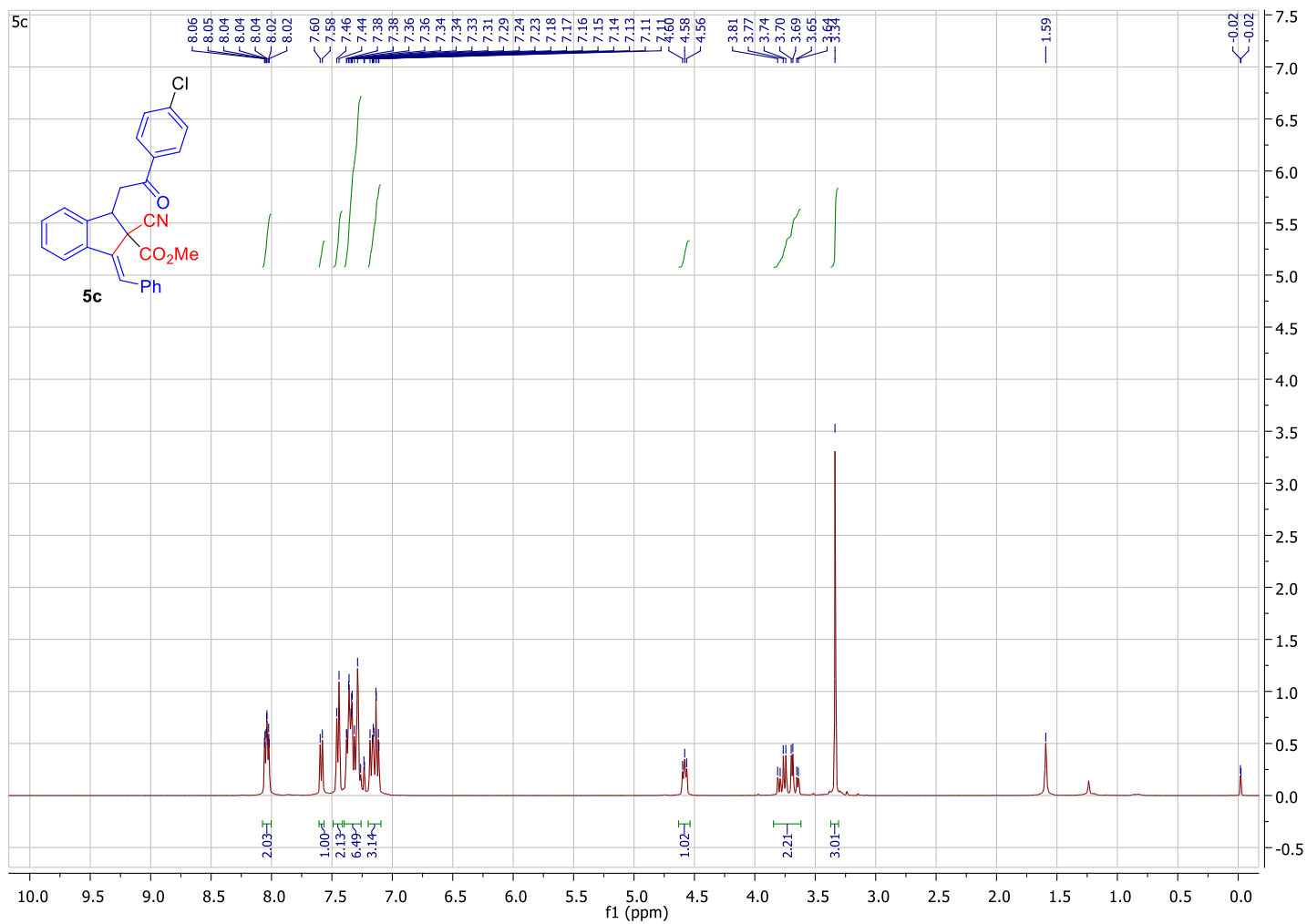


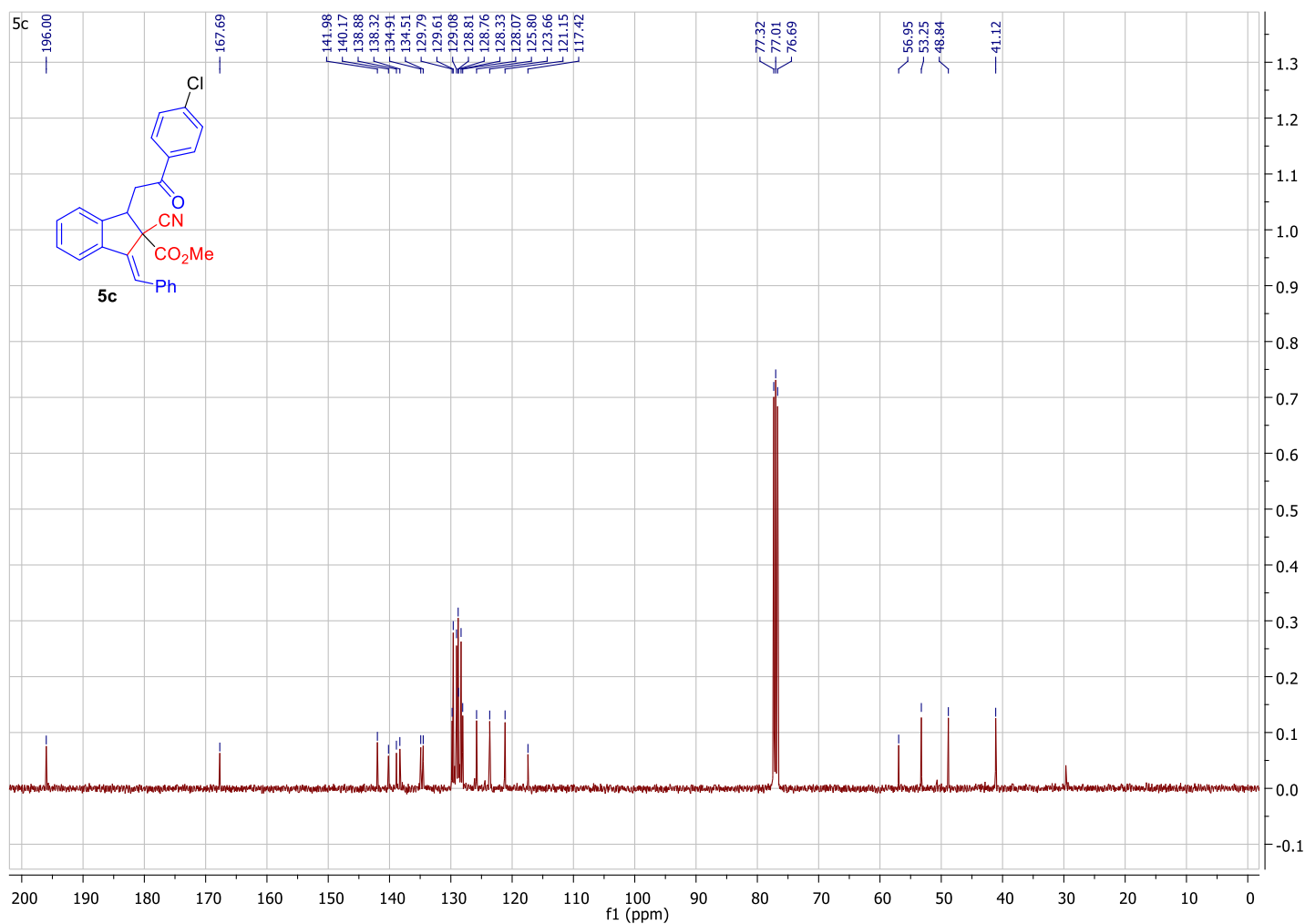




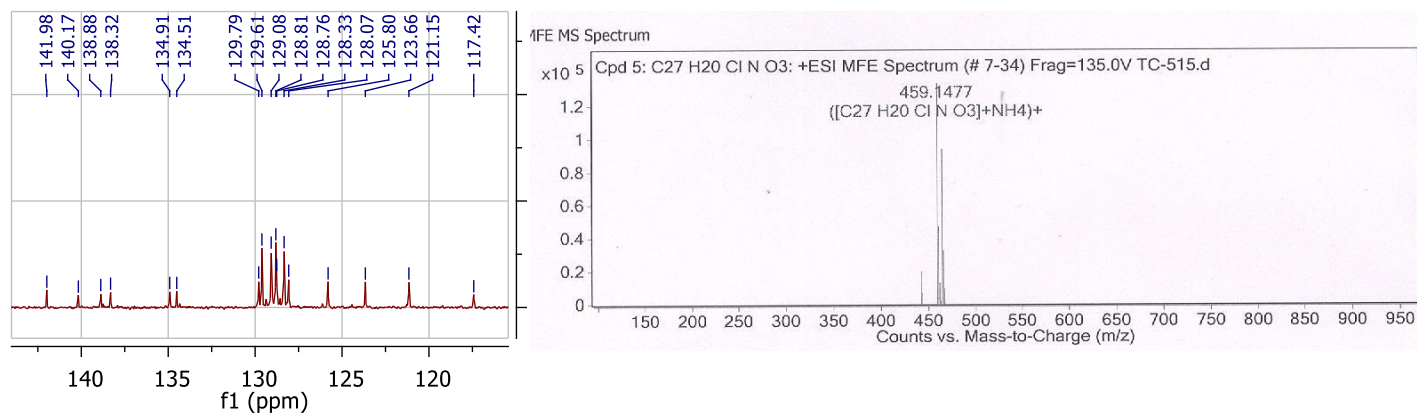
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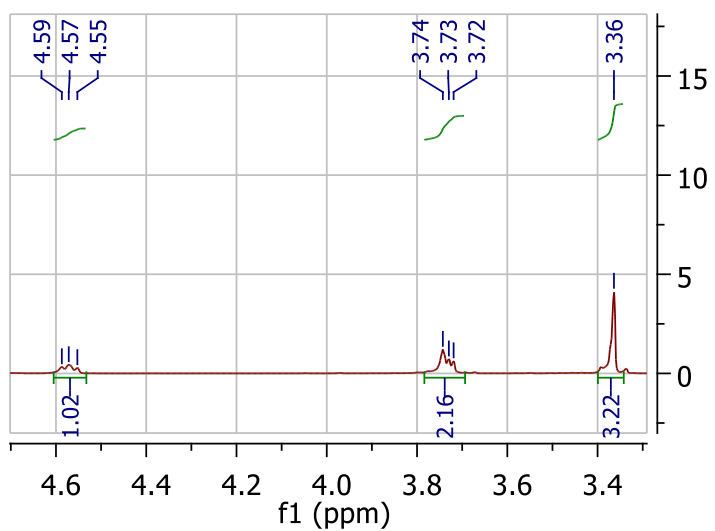
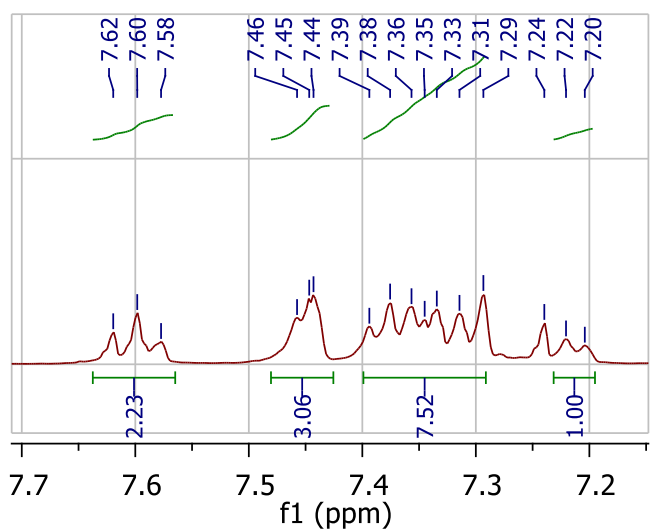
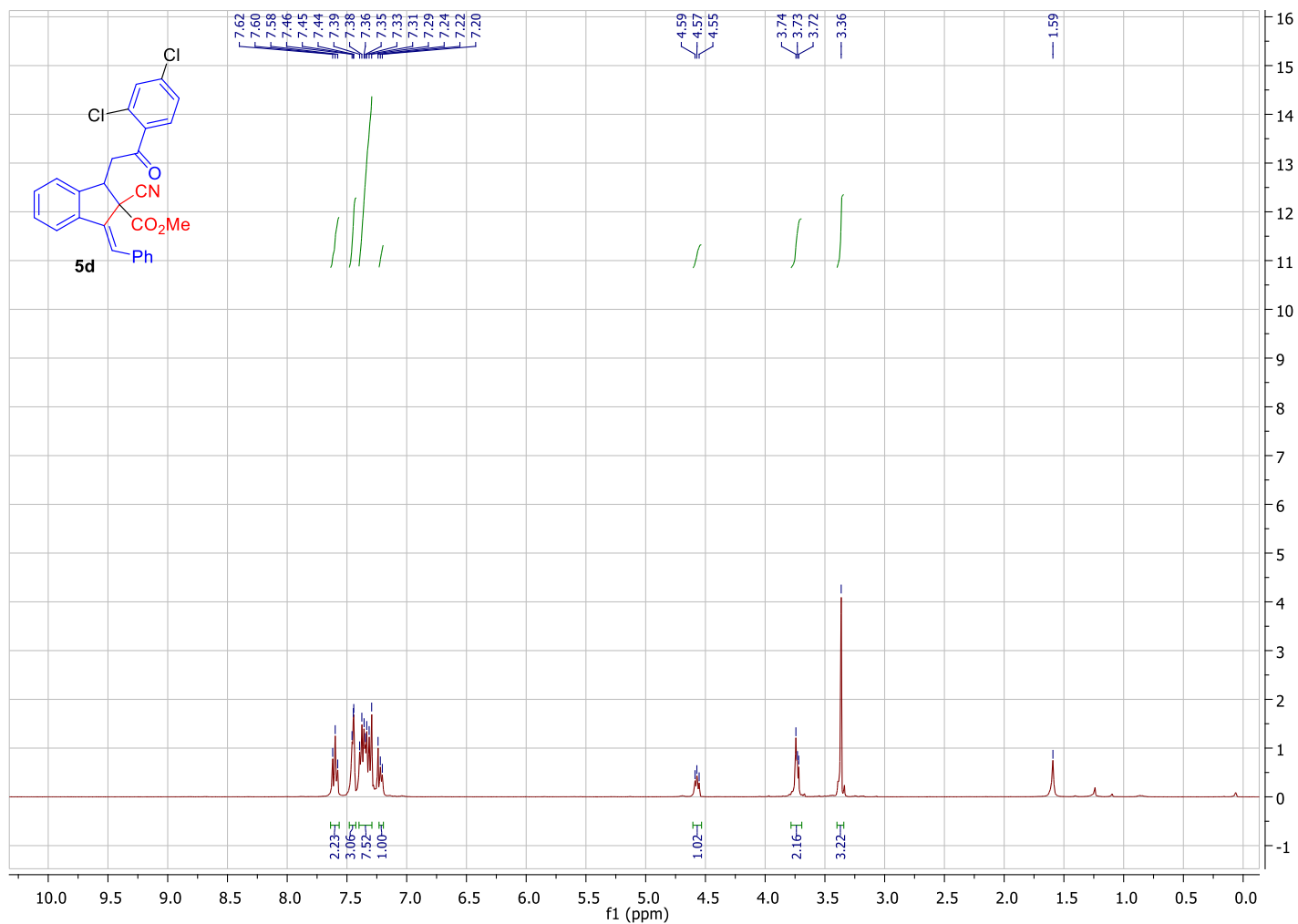


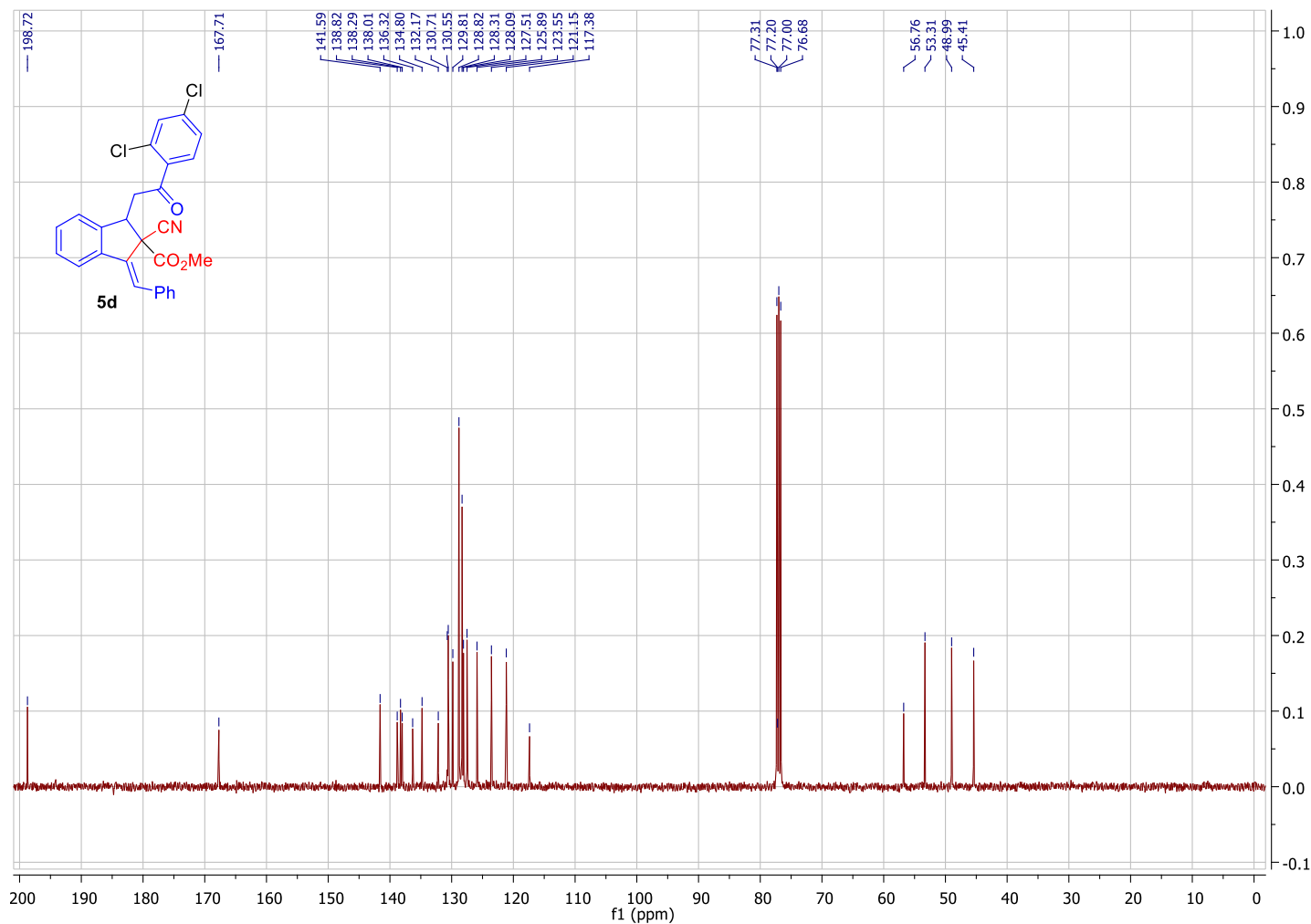




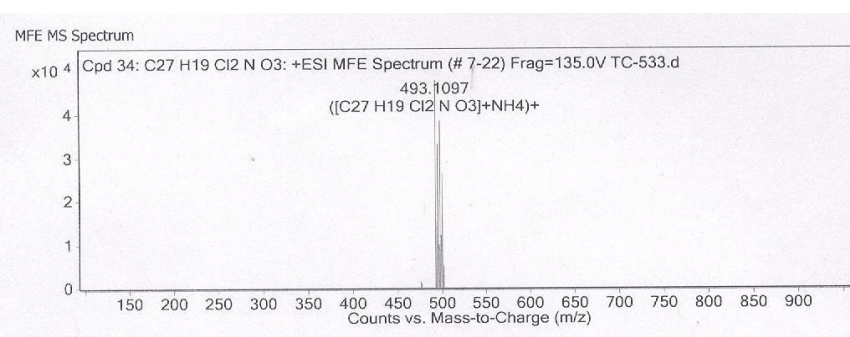
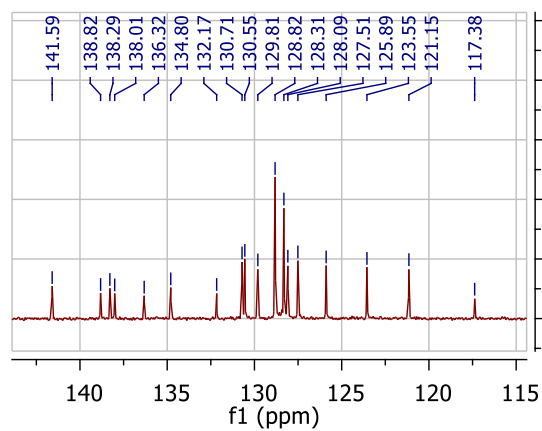
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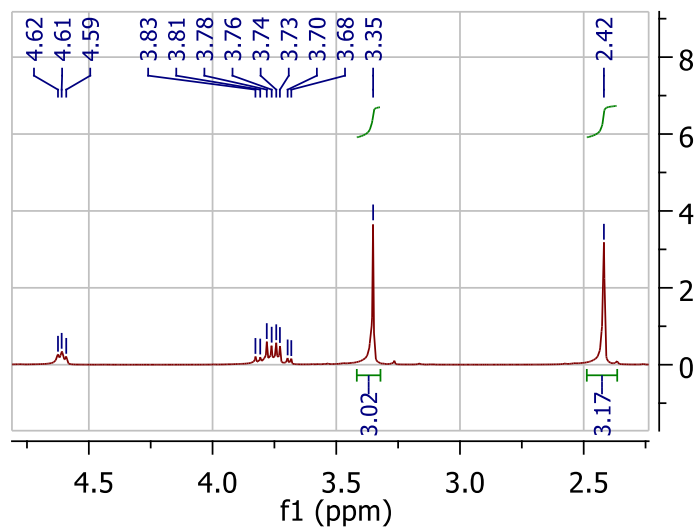
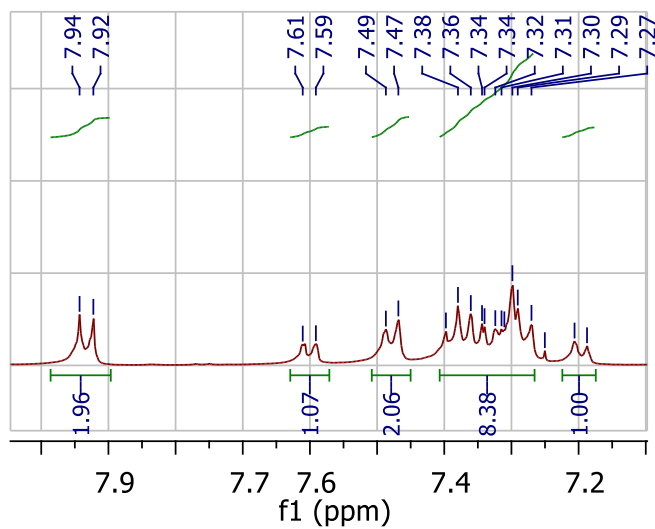
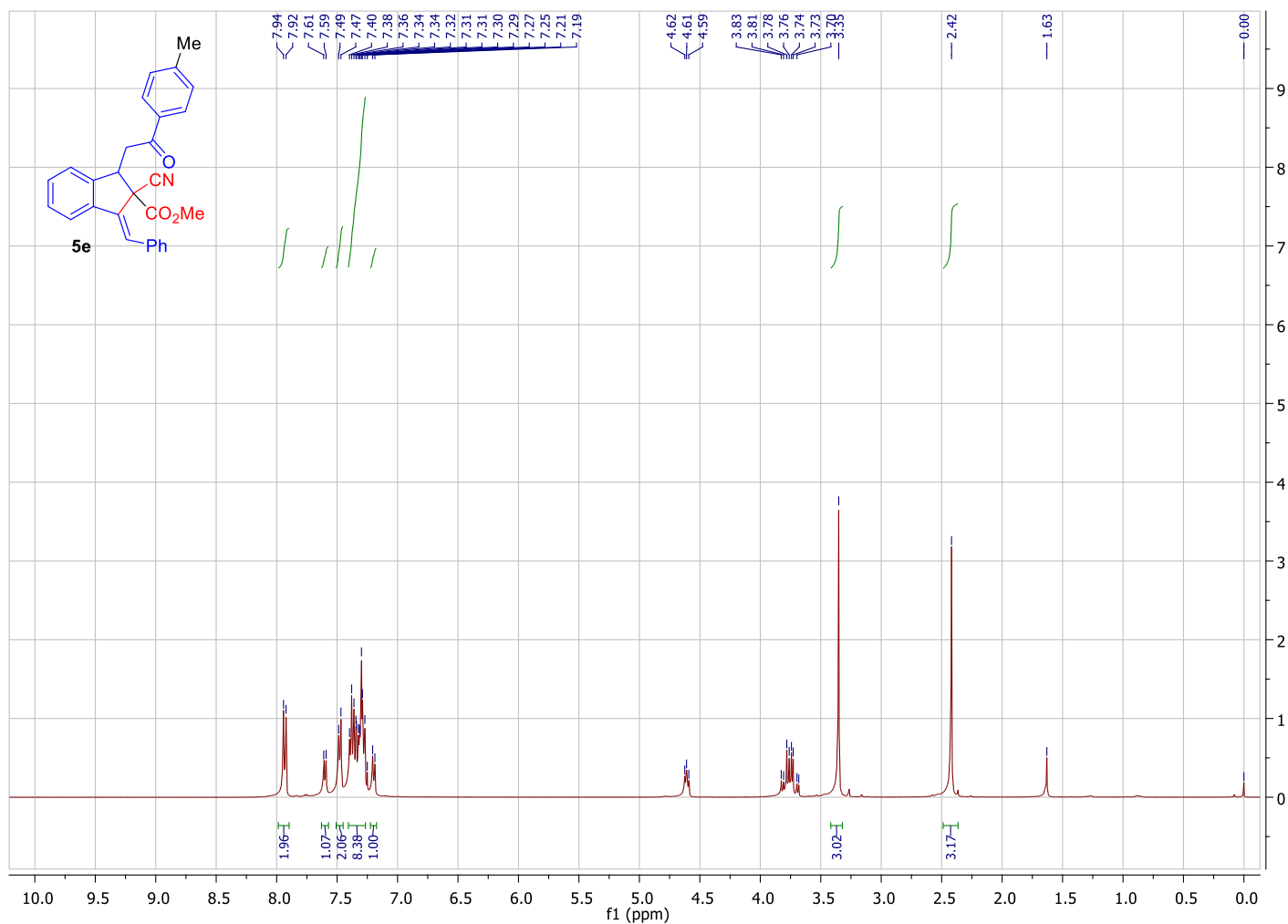


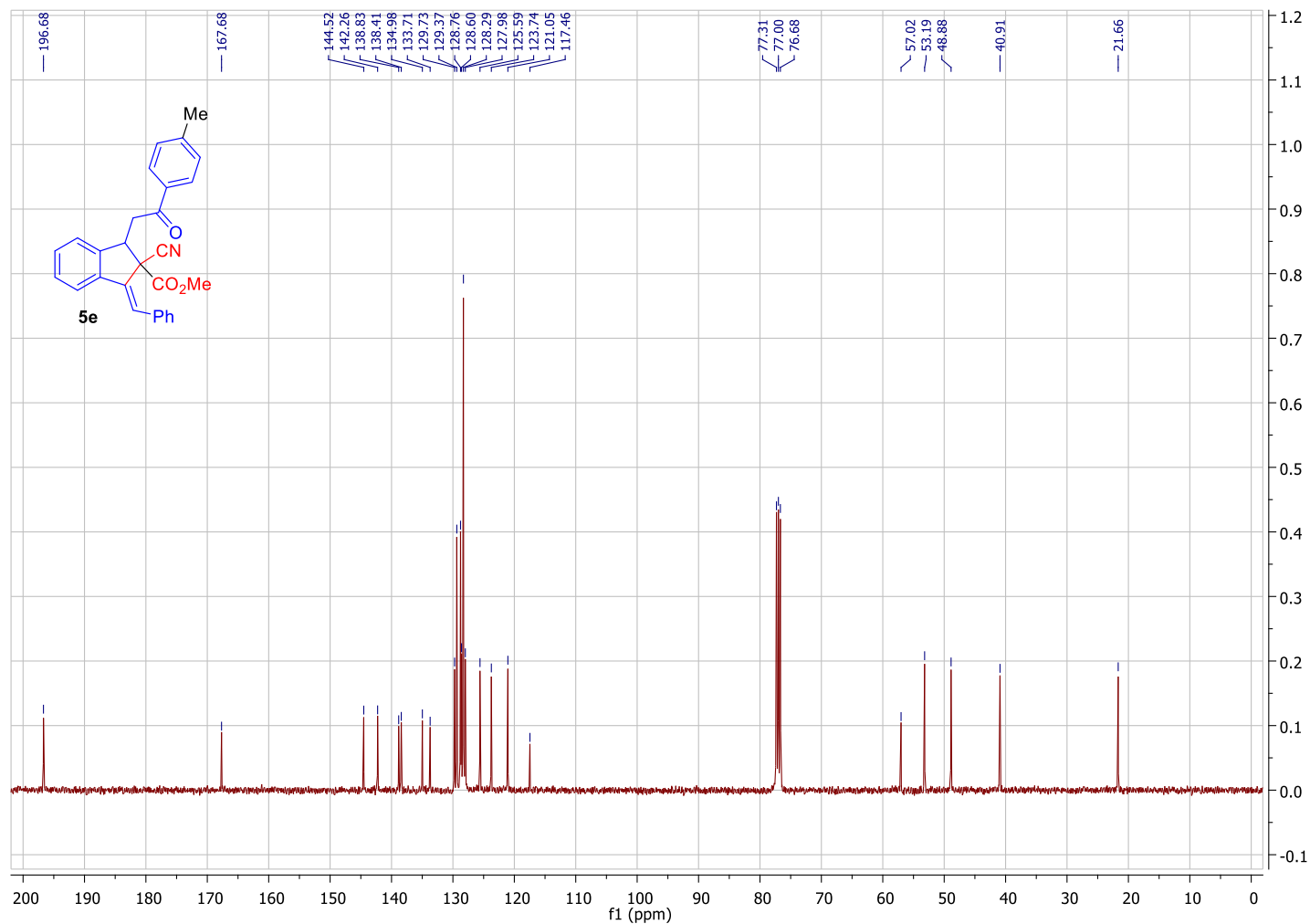




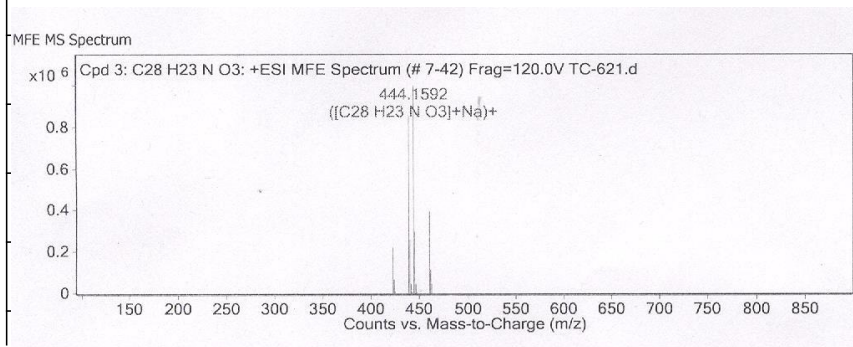
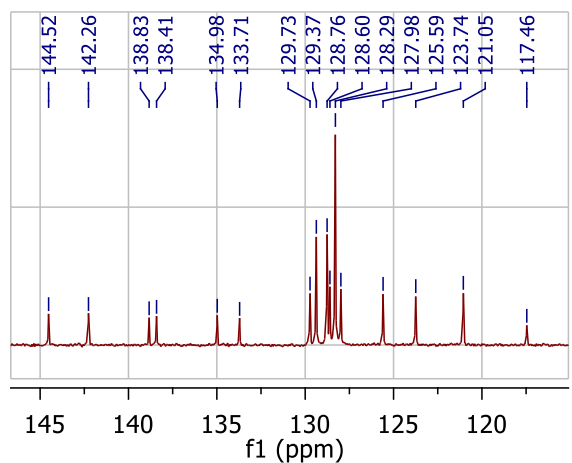
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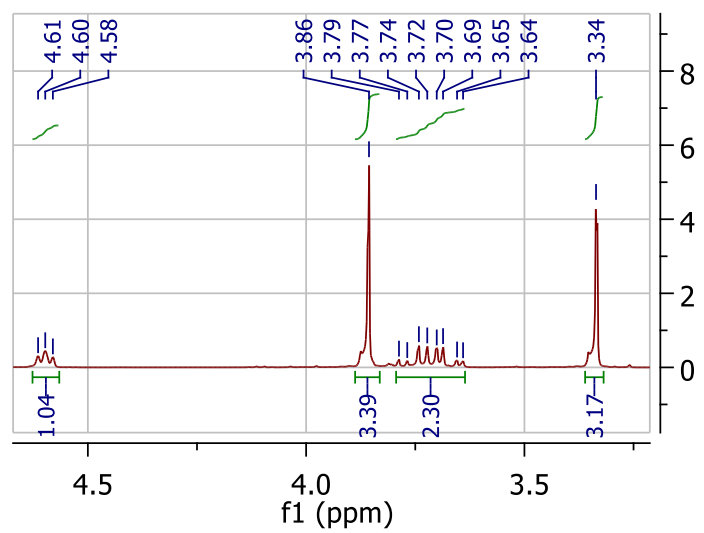
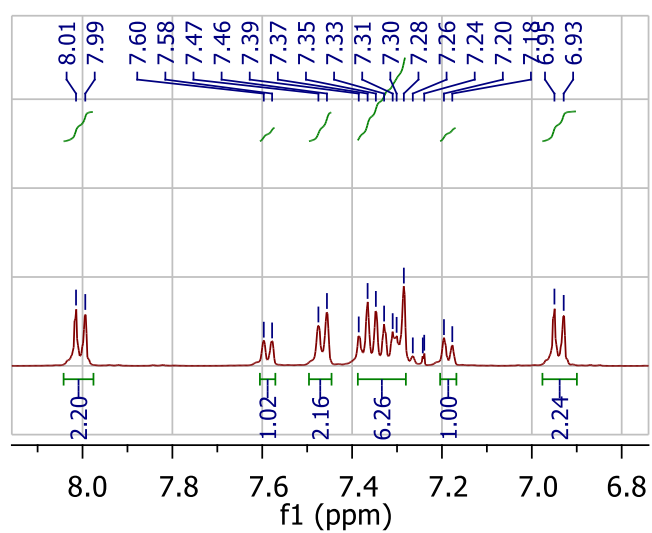
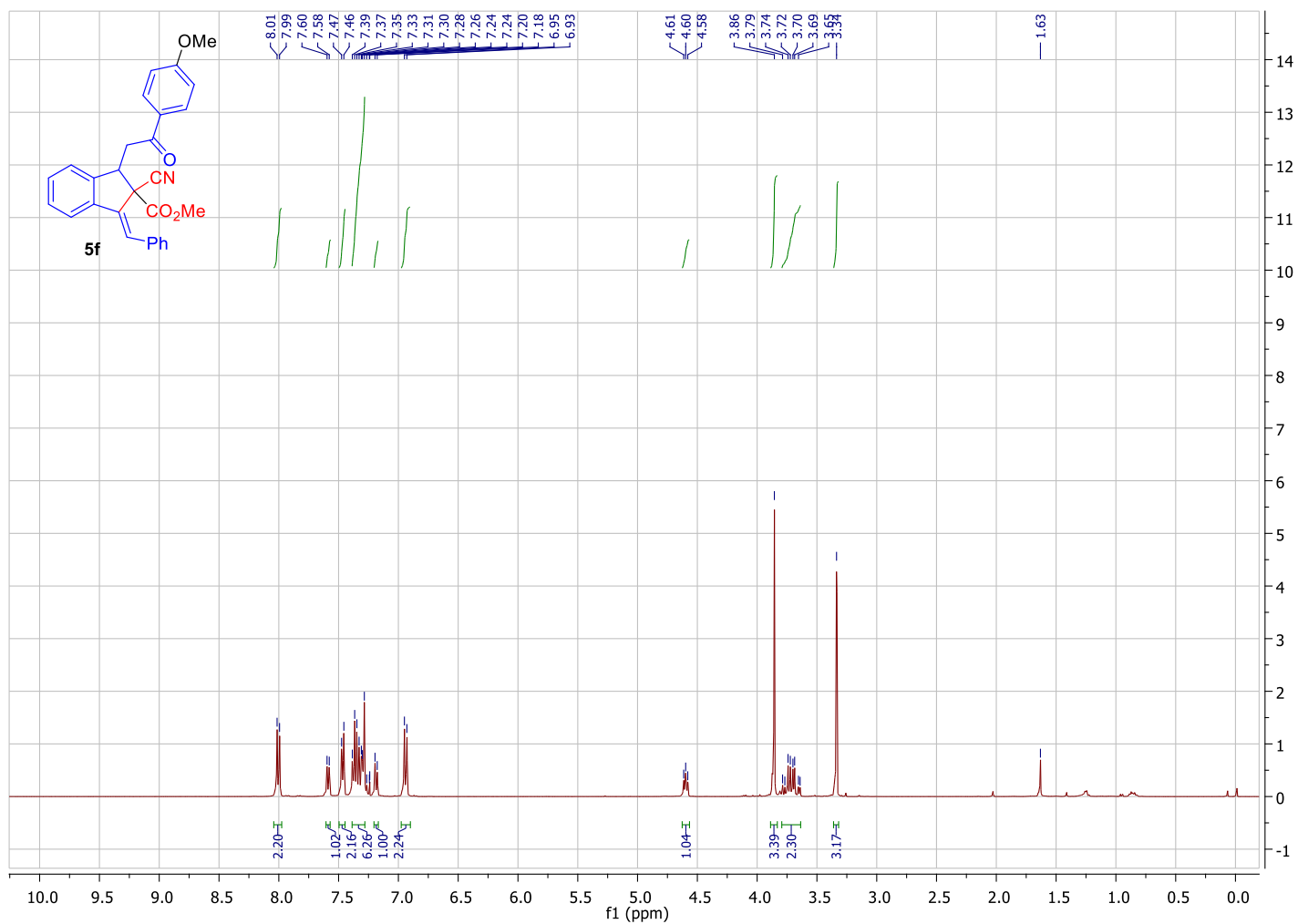


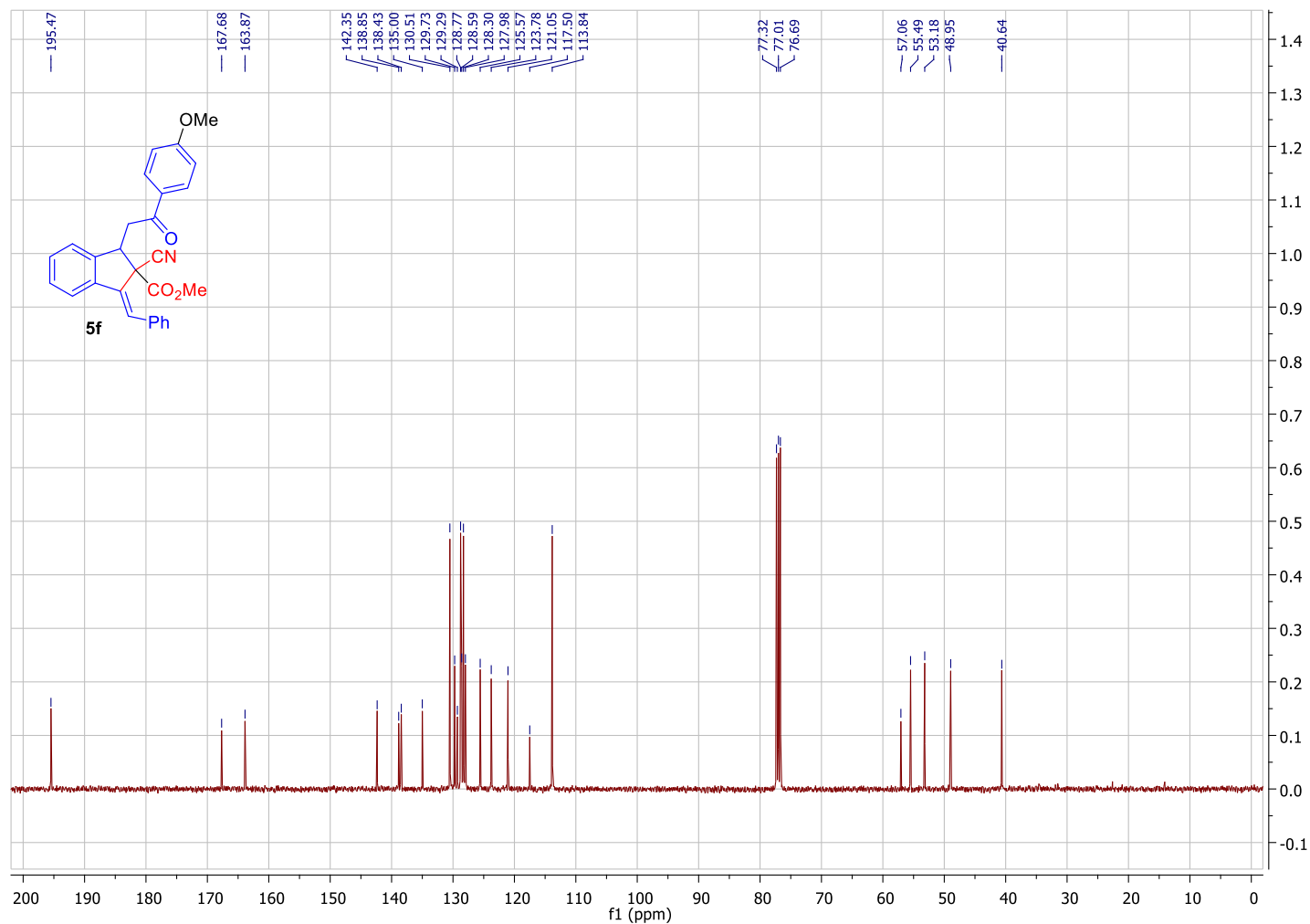




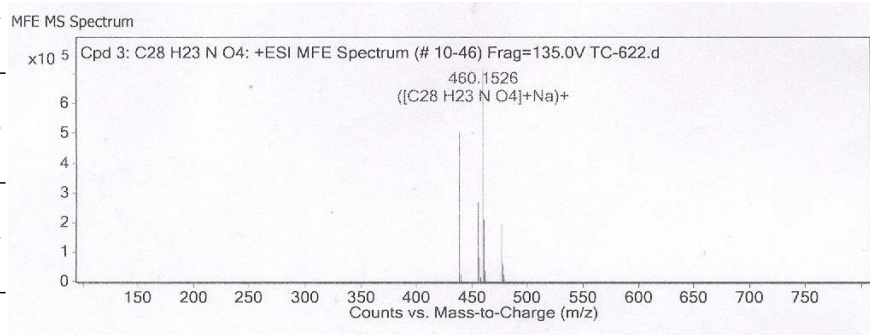
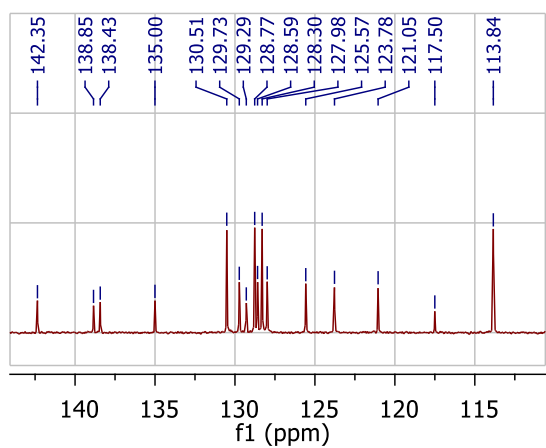
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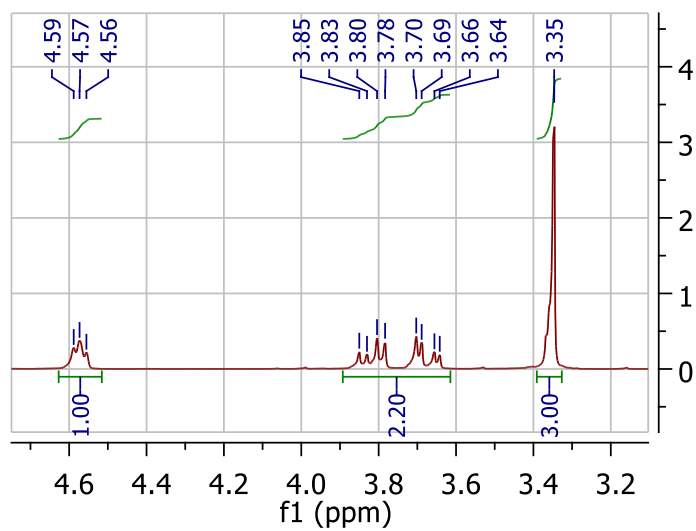
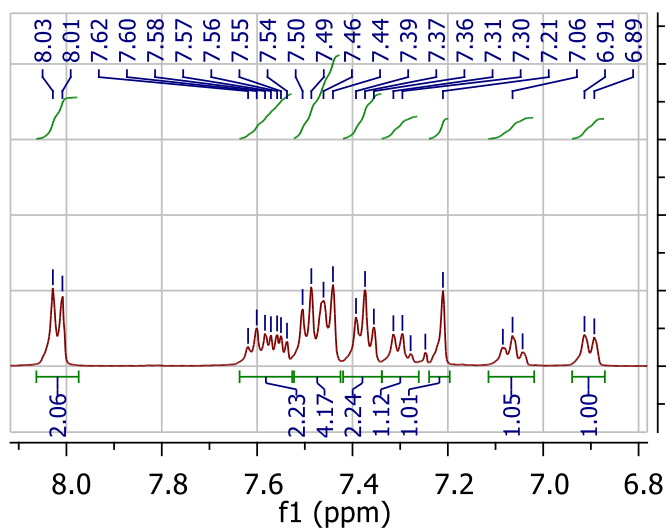
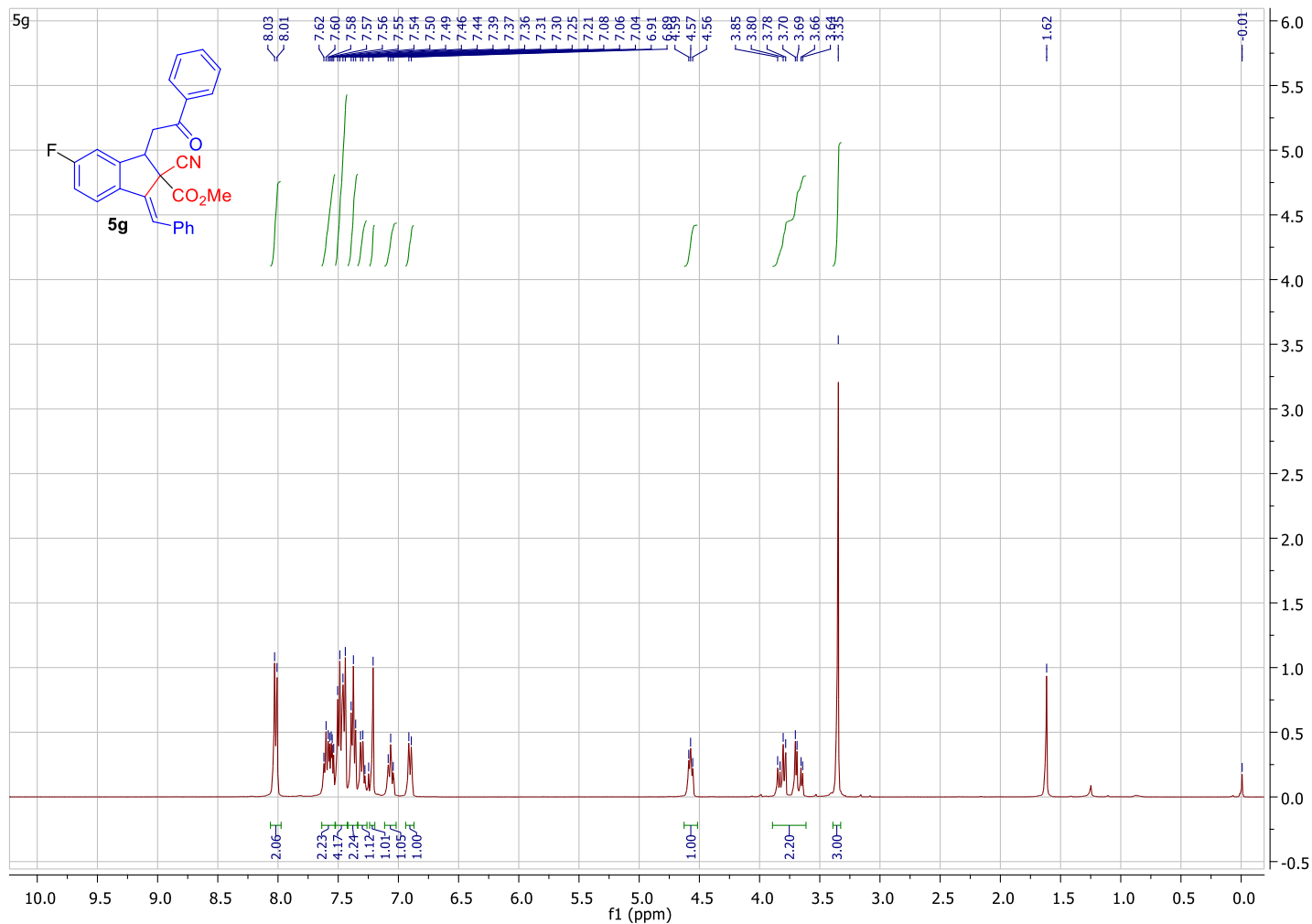


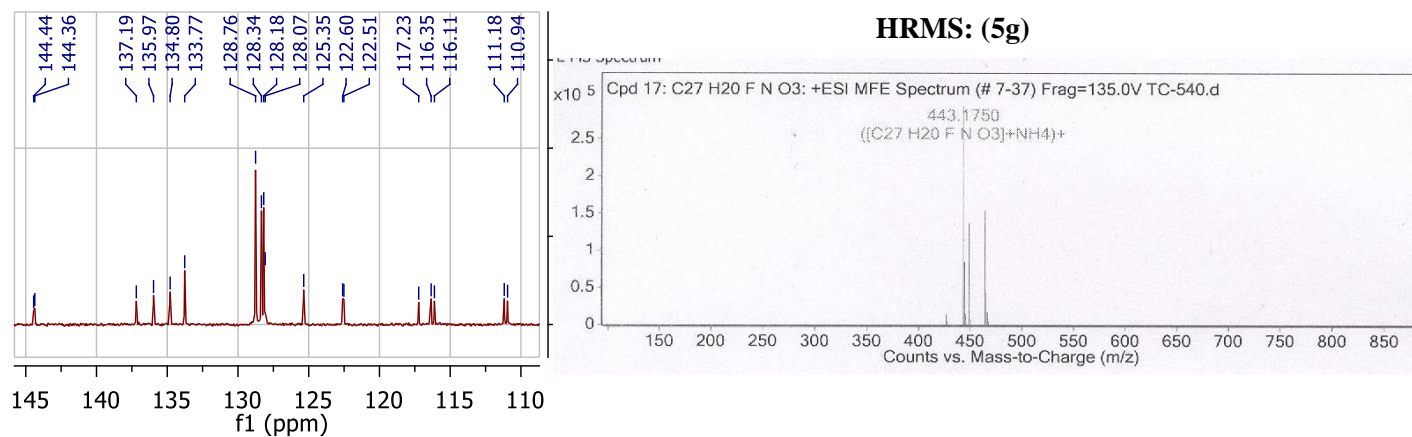
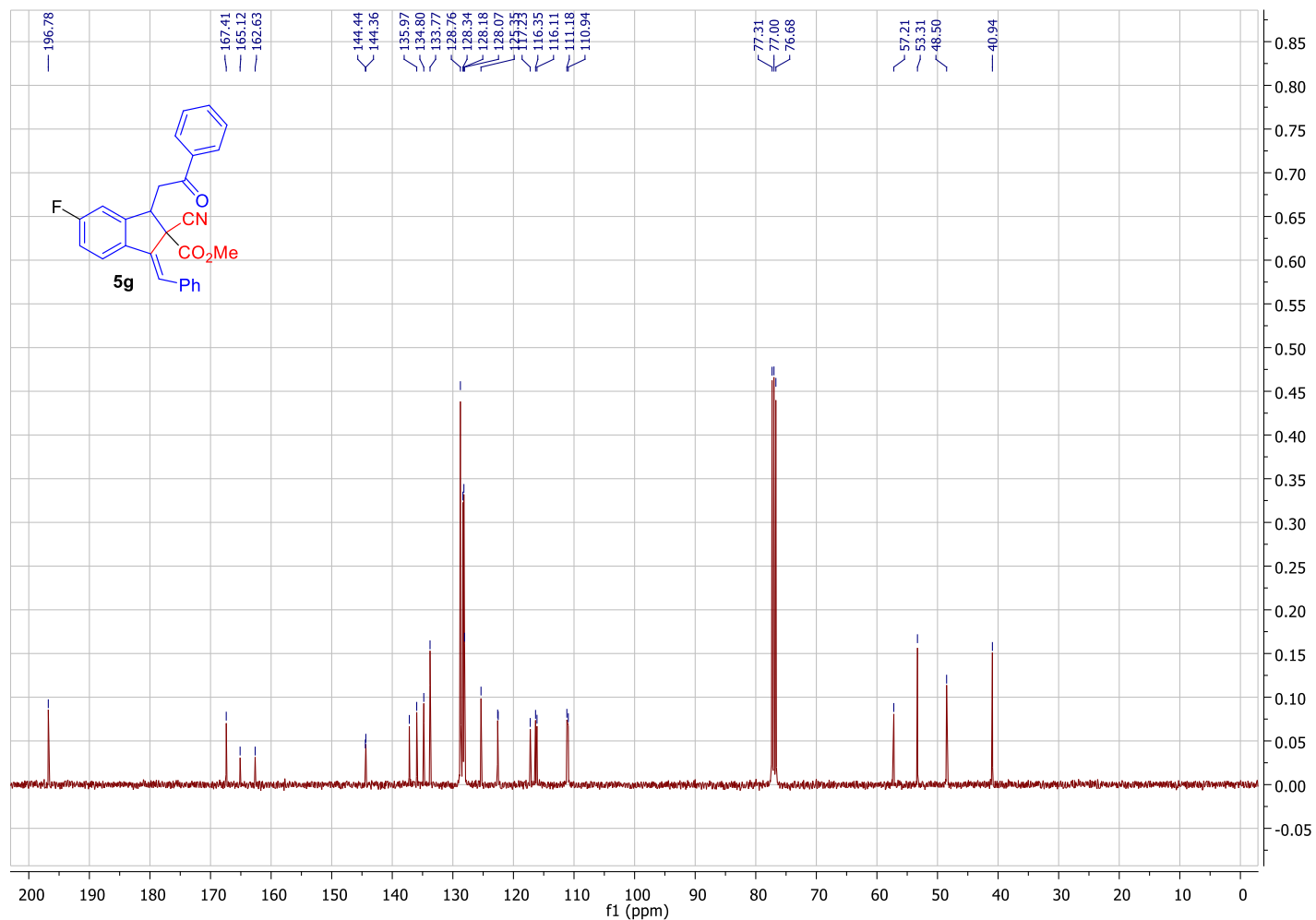


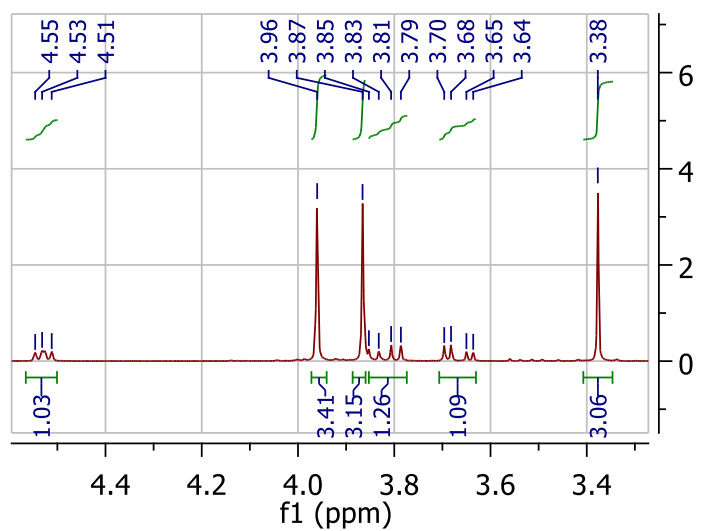
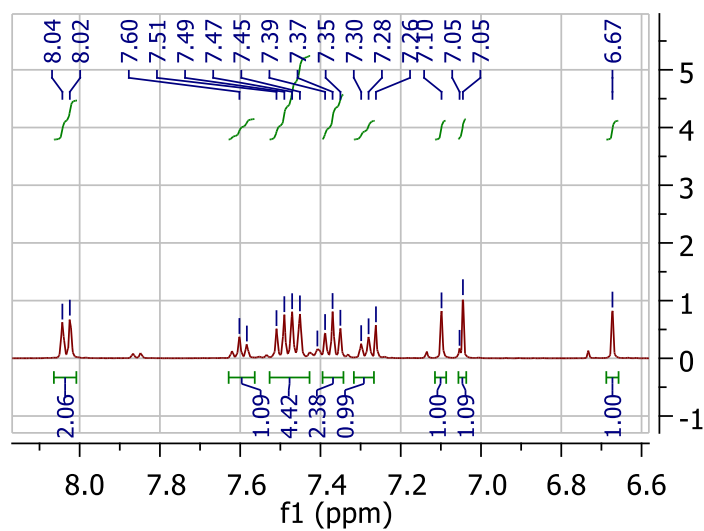
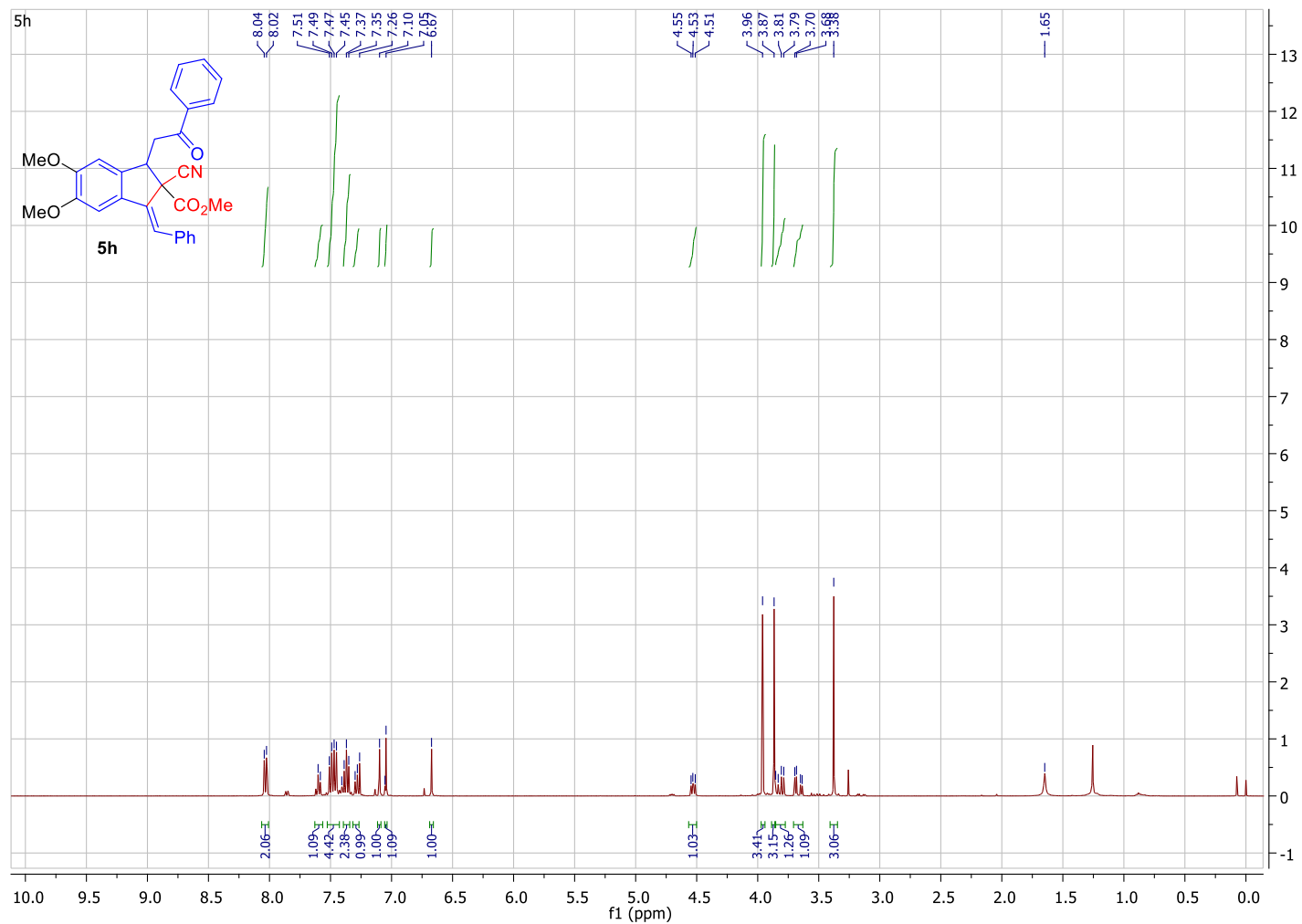


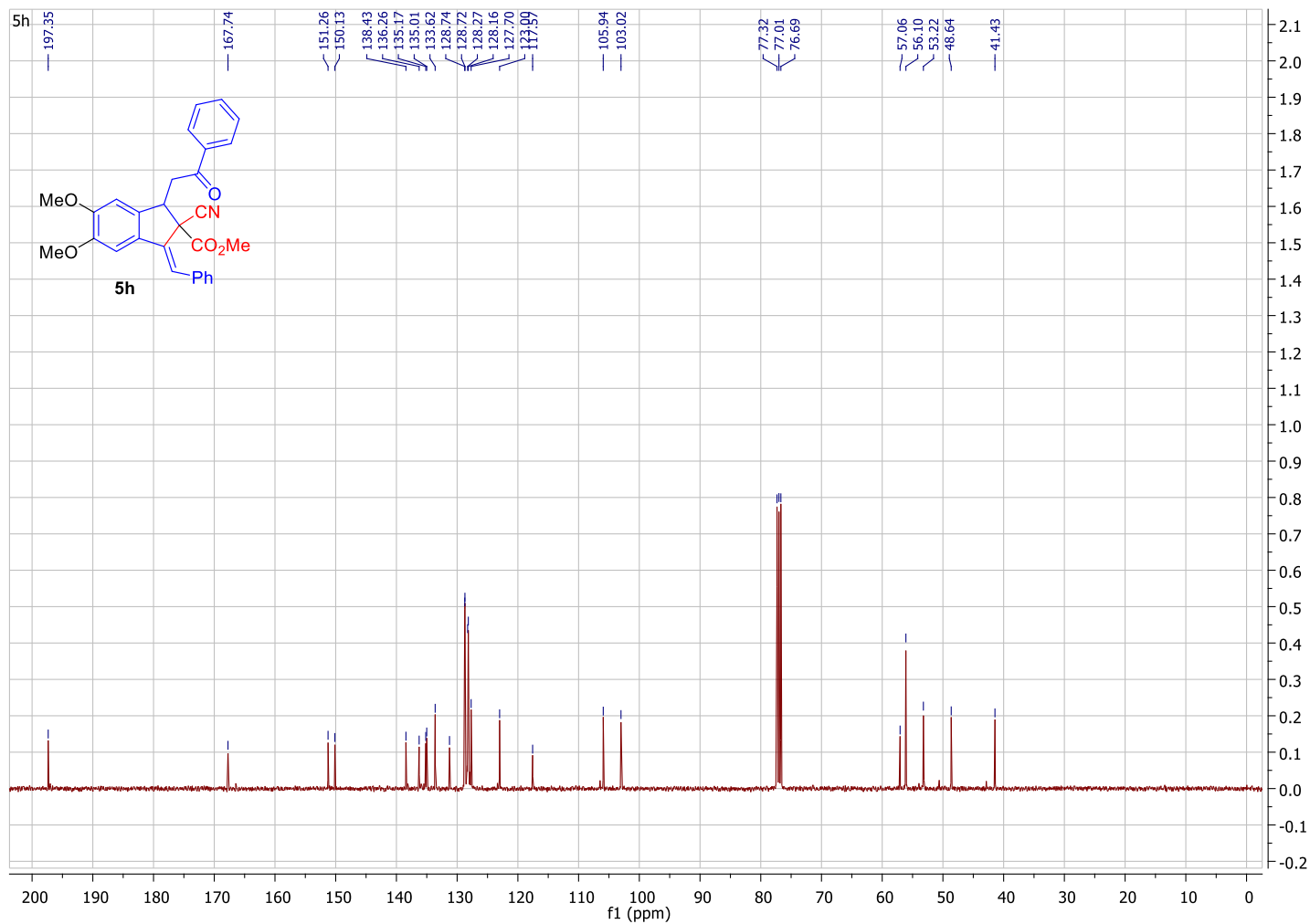
HRMS: (5f)



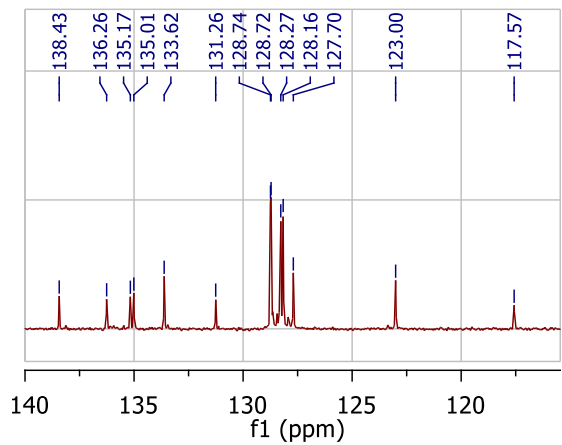




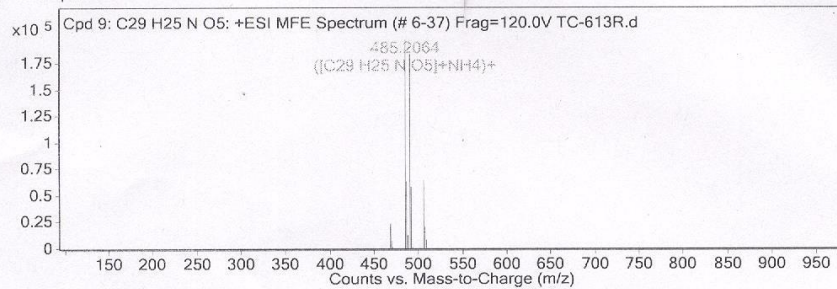


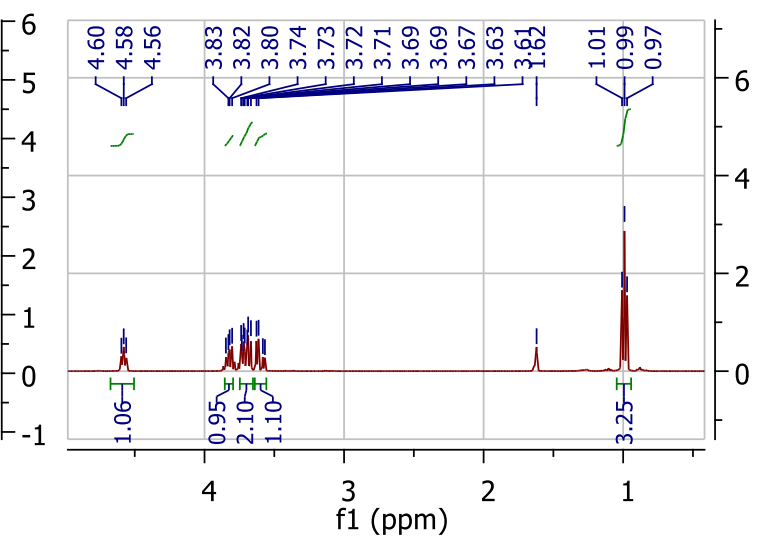
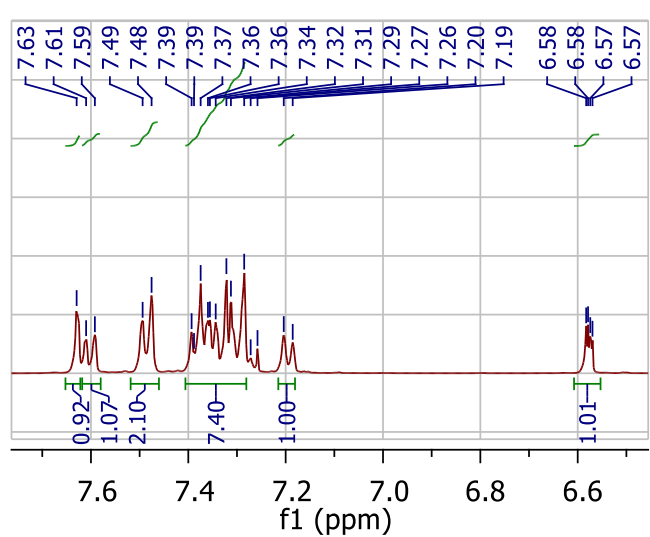
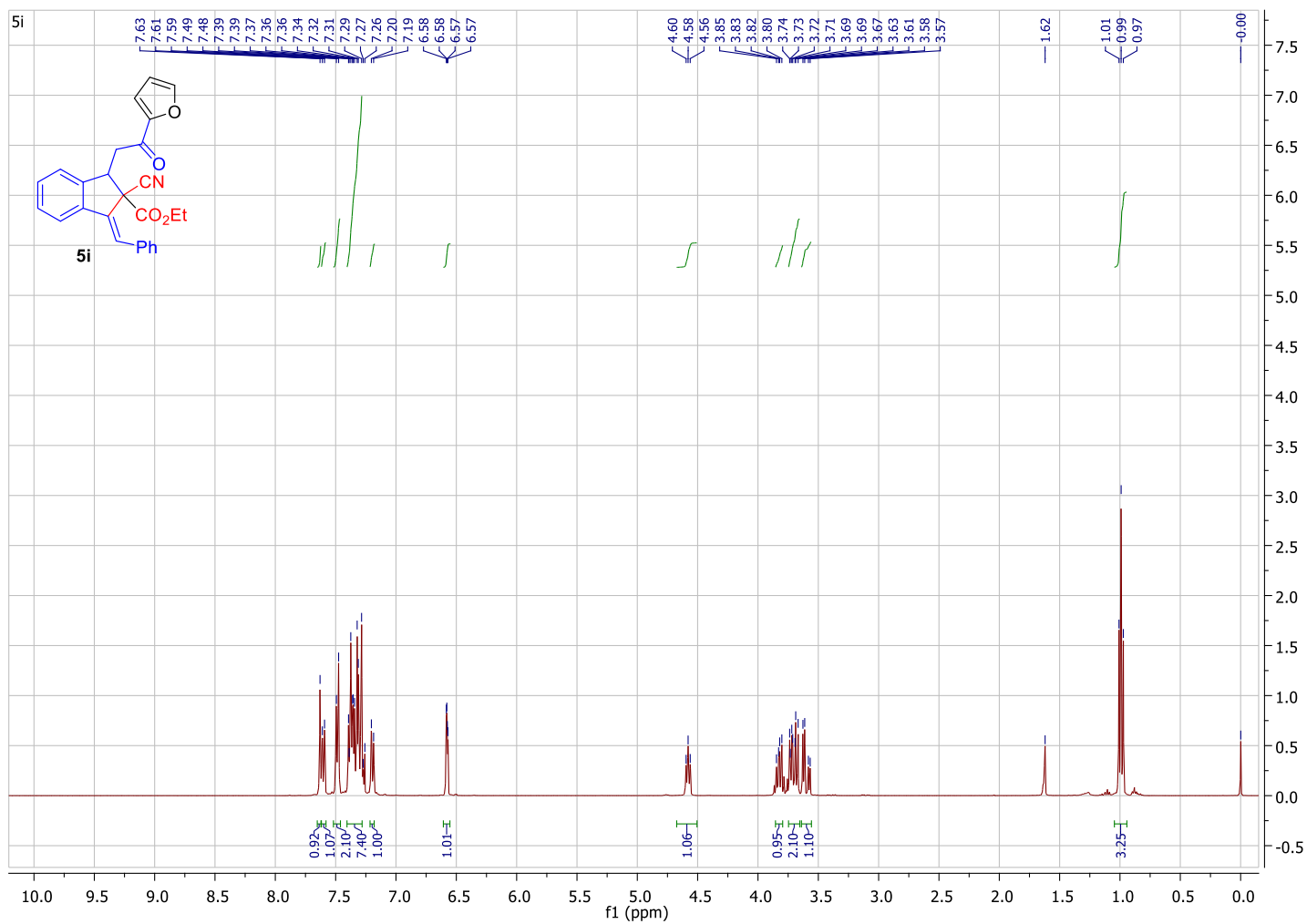


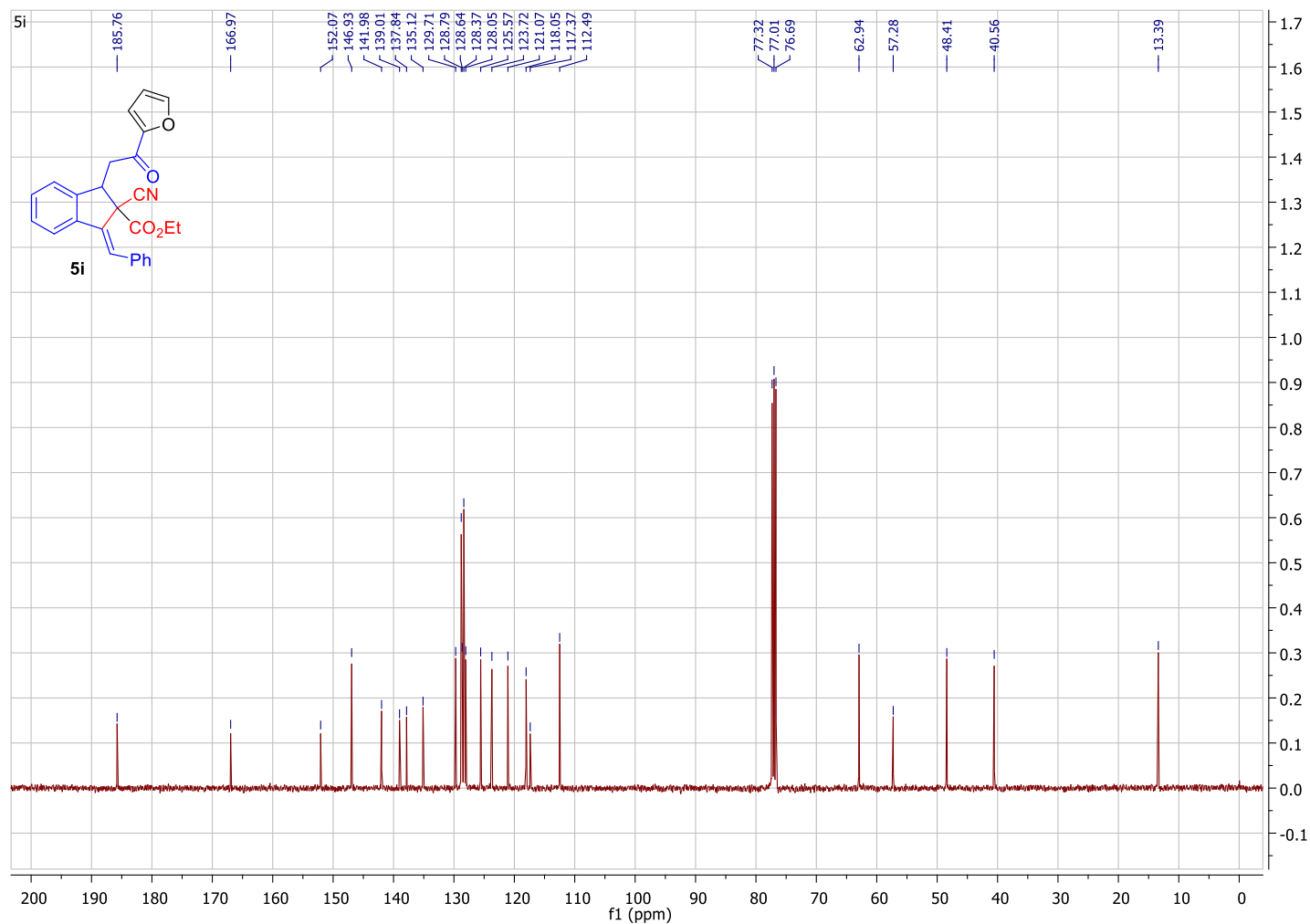
HRMS: (5h)



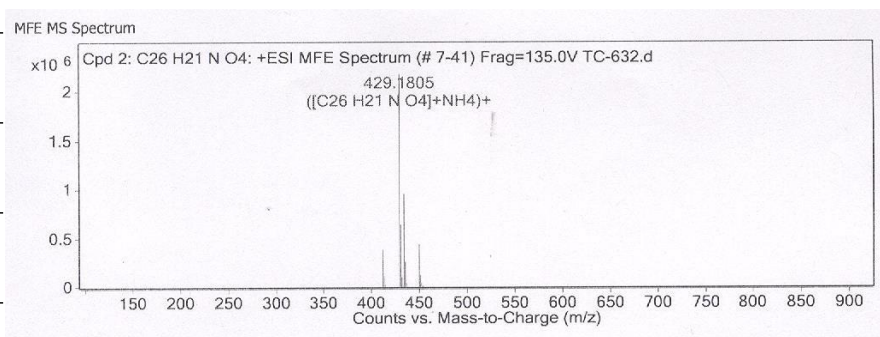
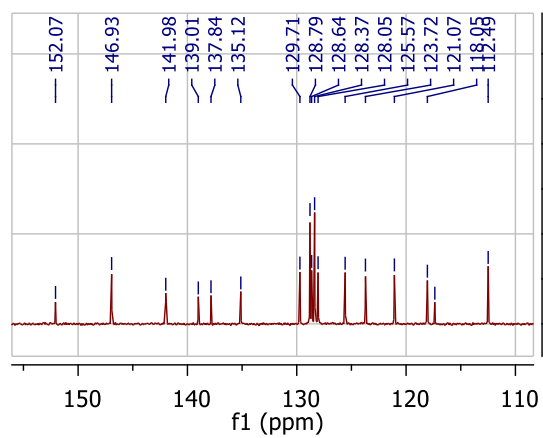
MFE MS Spectrum

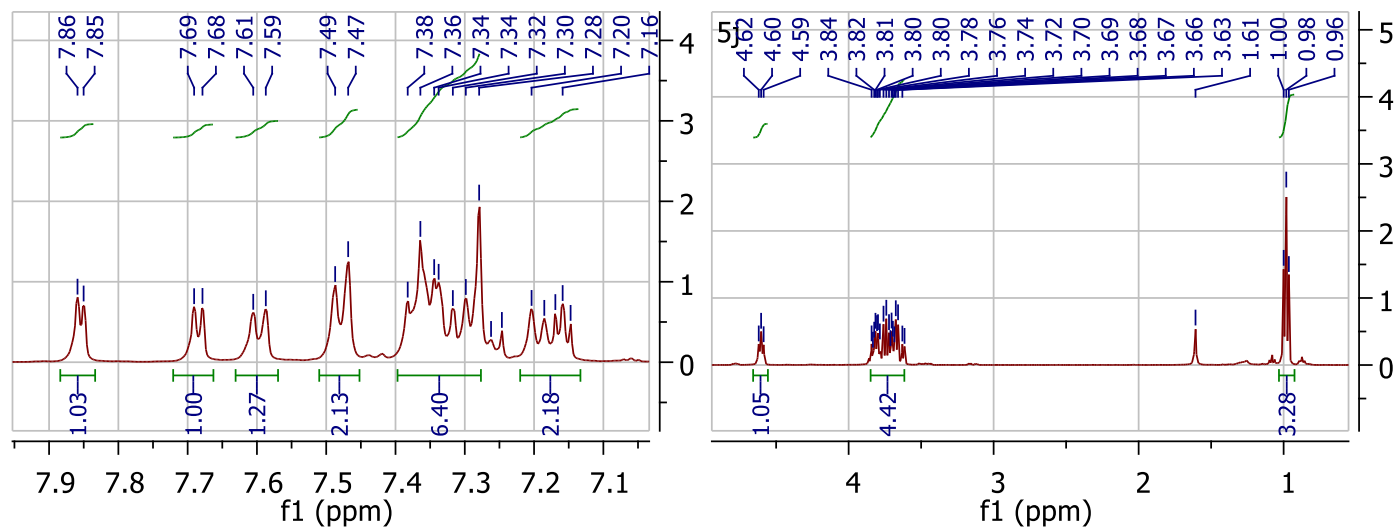
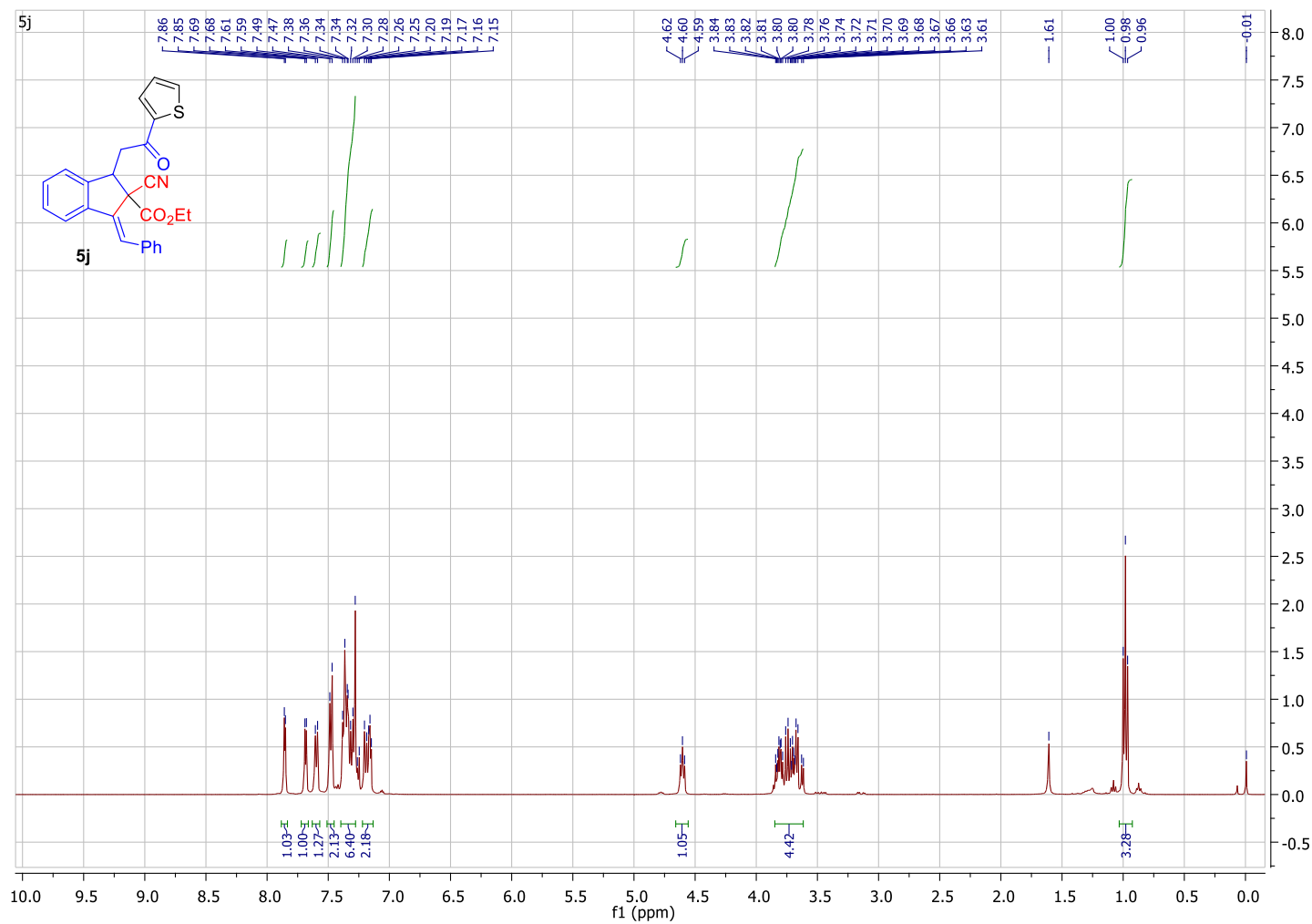


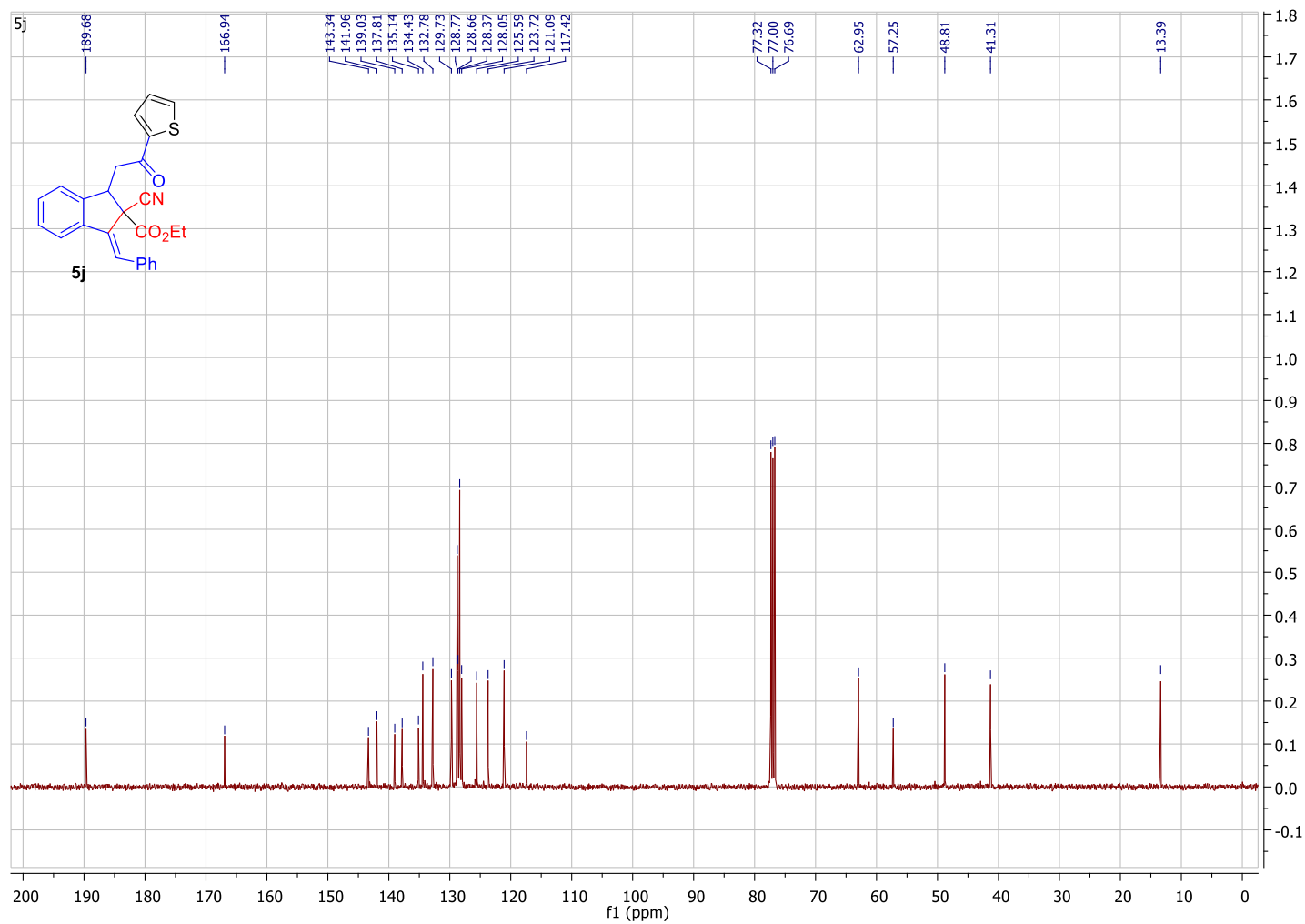




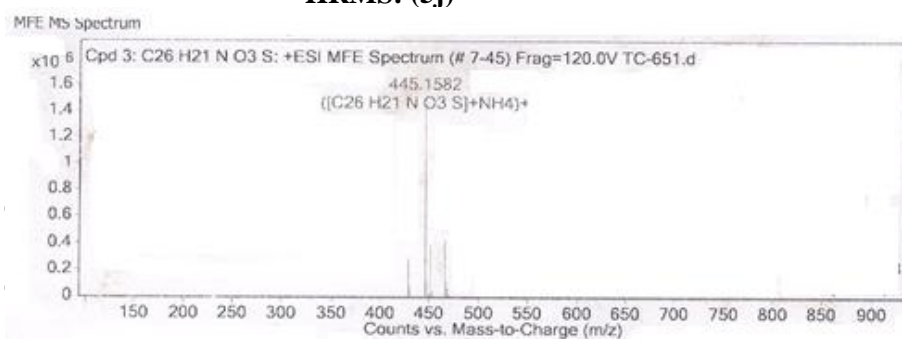
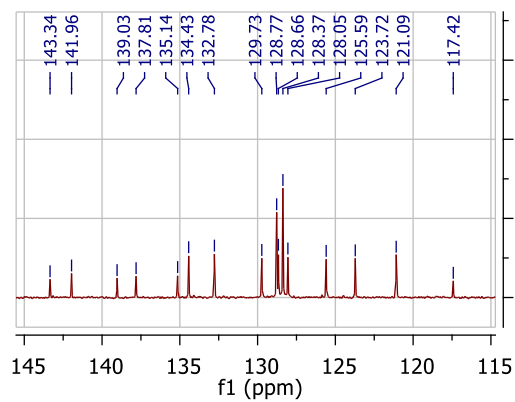
HRMS: (5i)

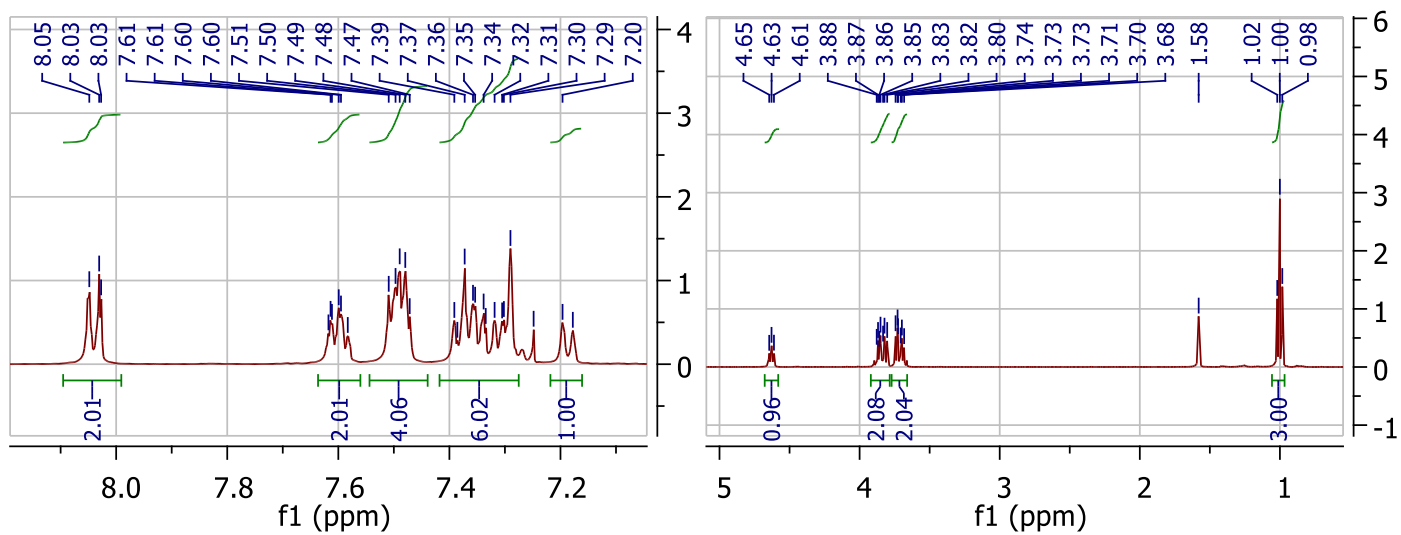
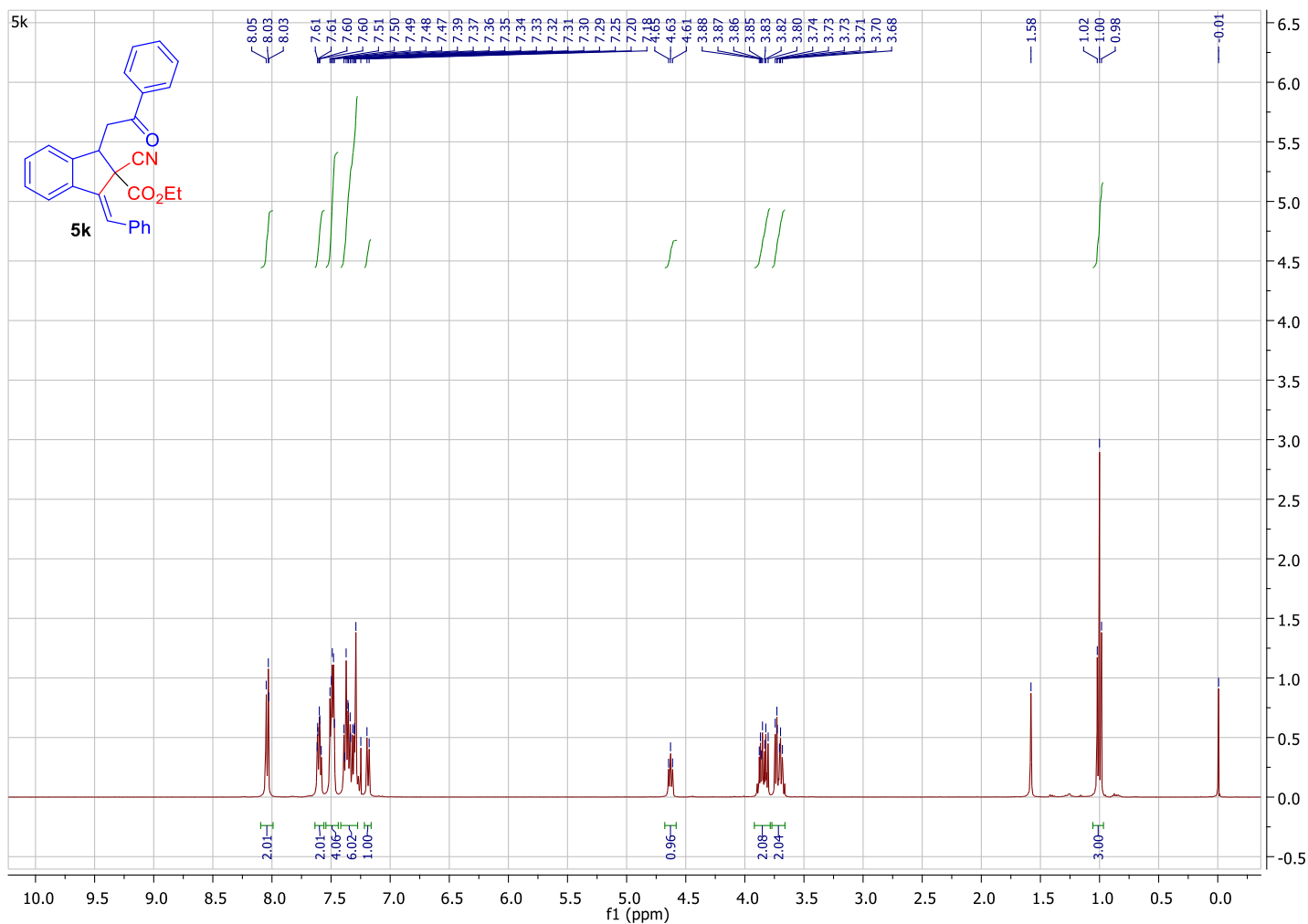


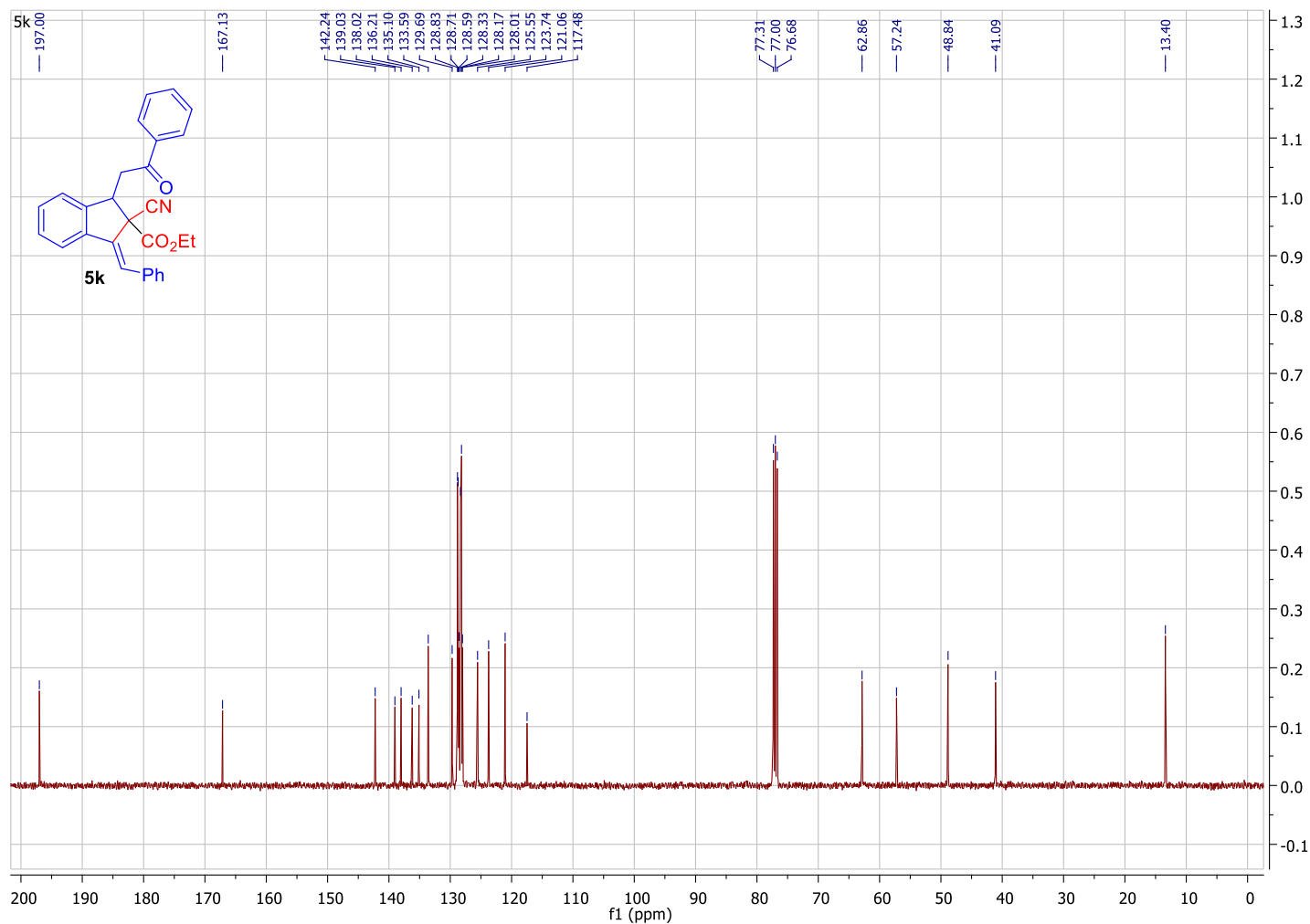




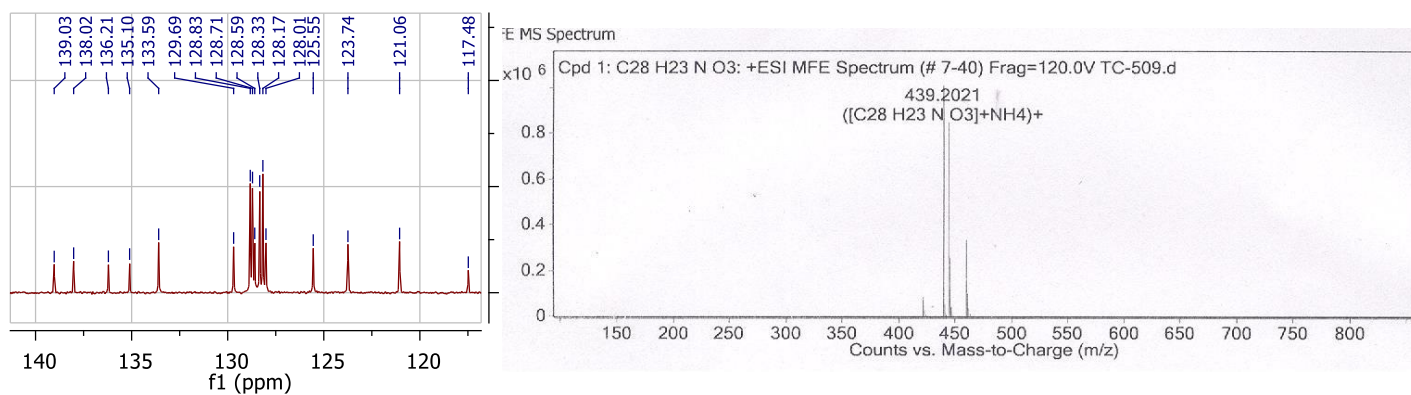
HRMS: (5j)

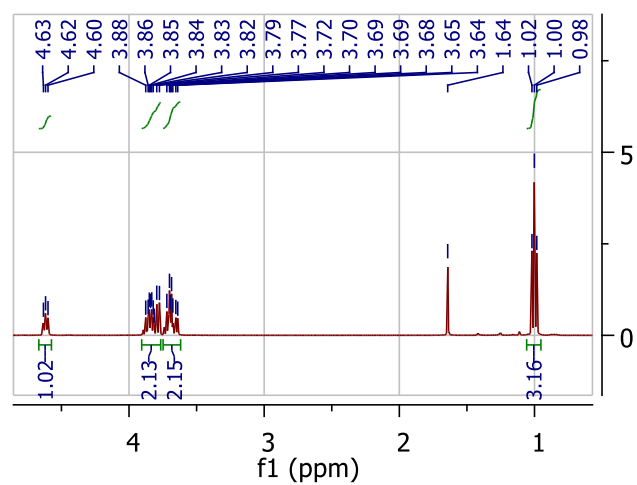
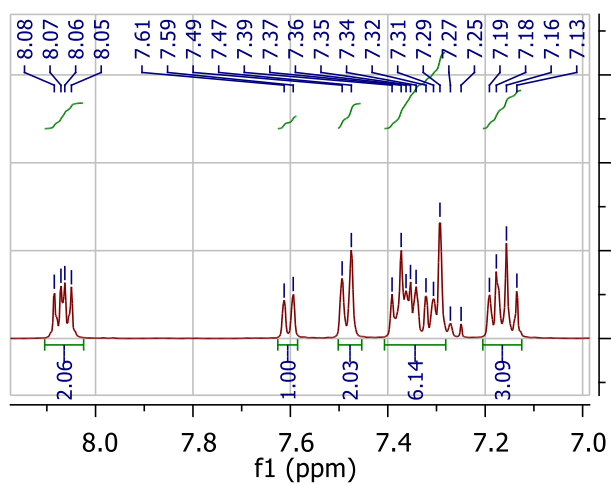
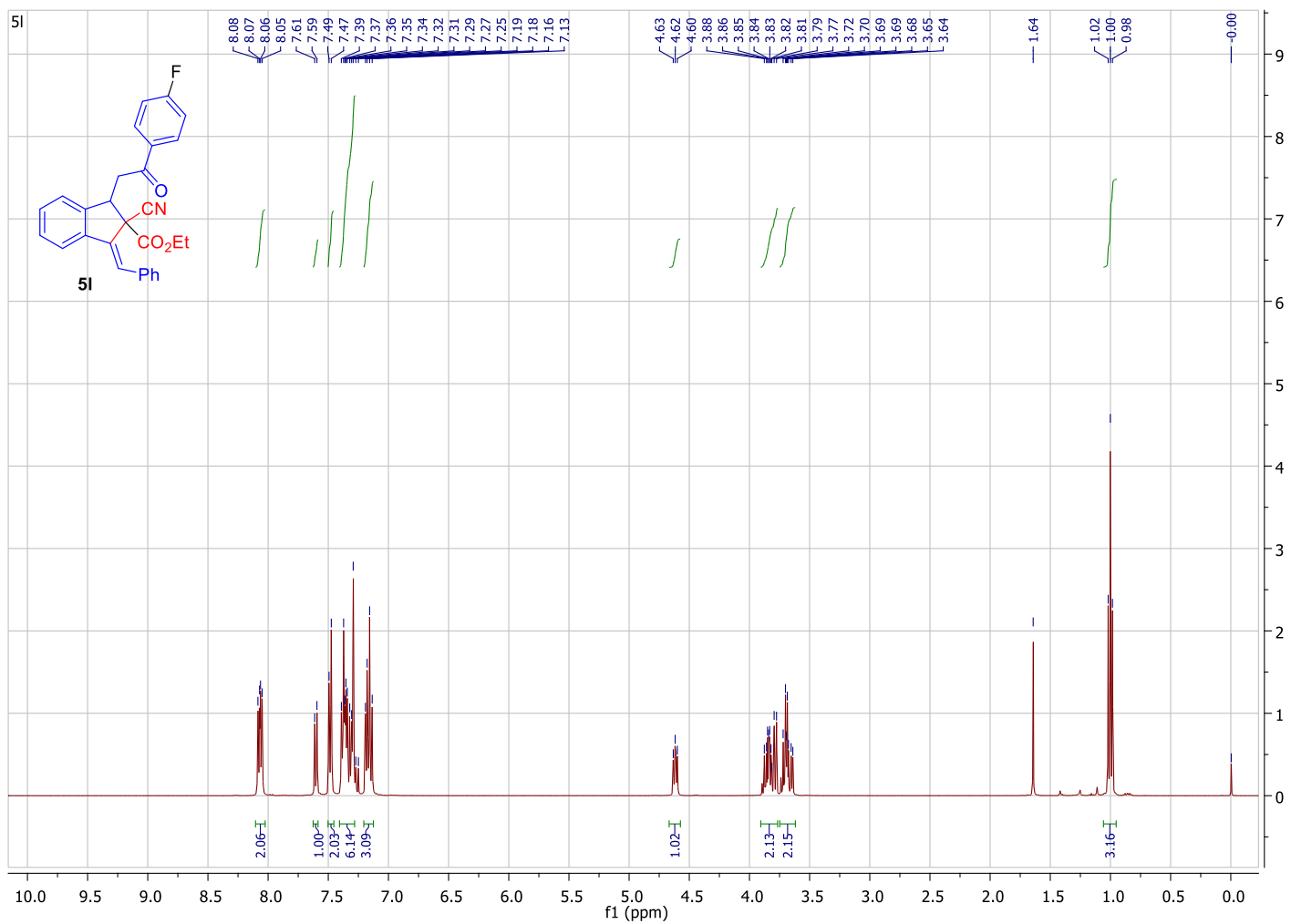


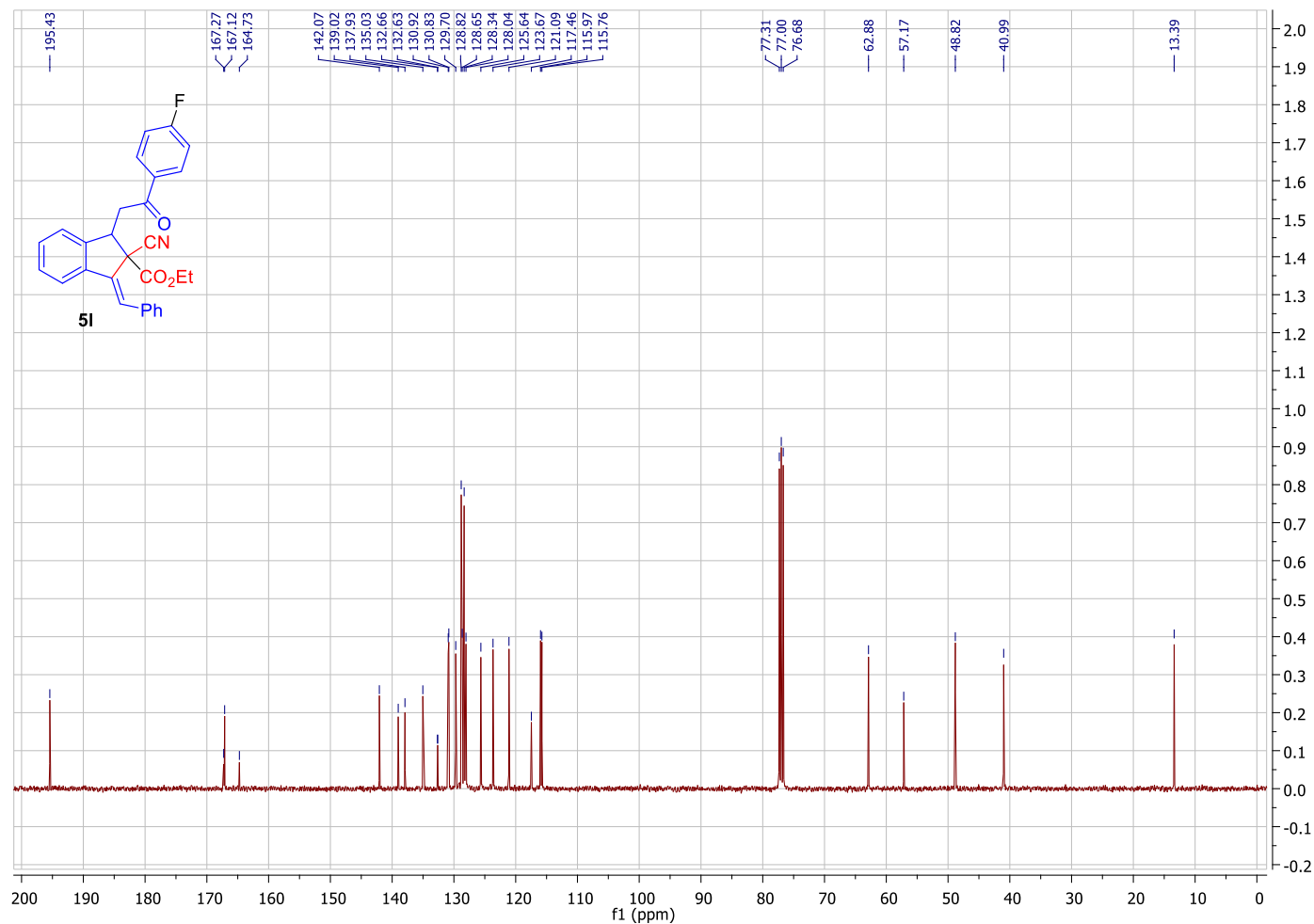




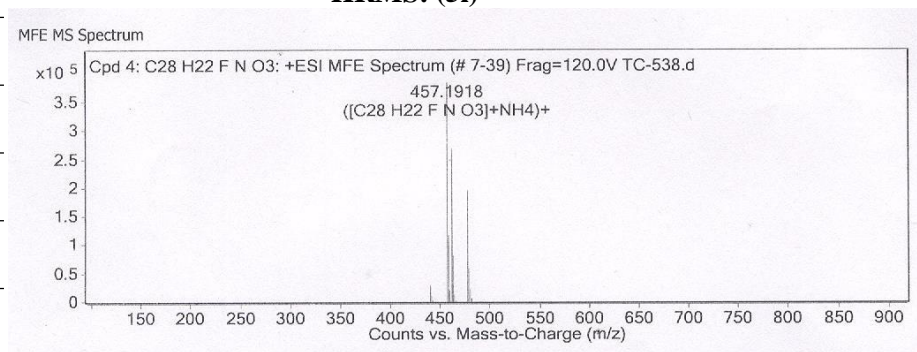
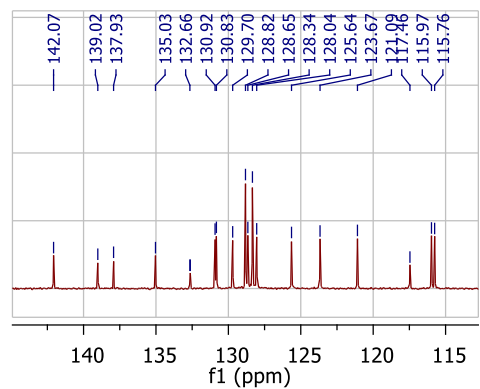
HRMS: (5k)

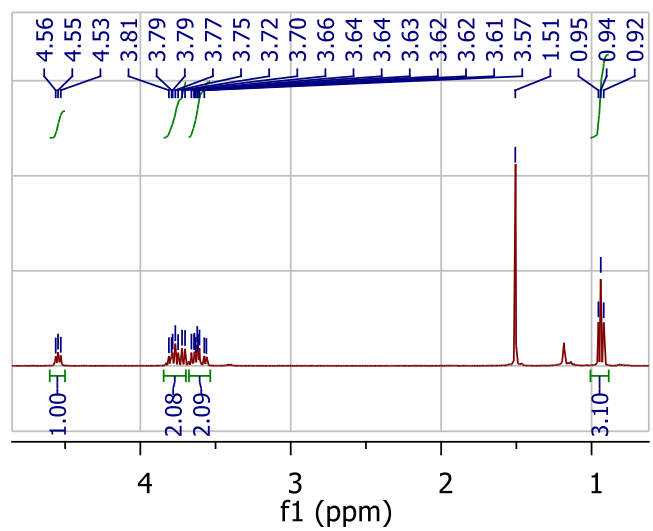
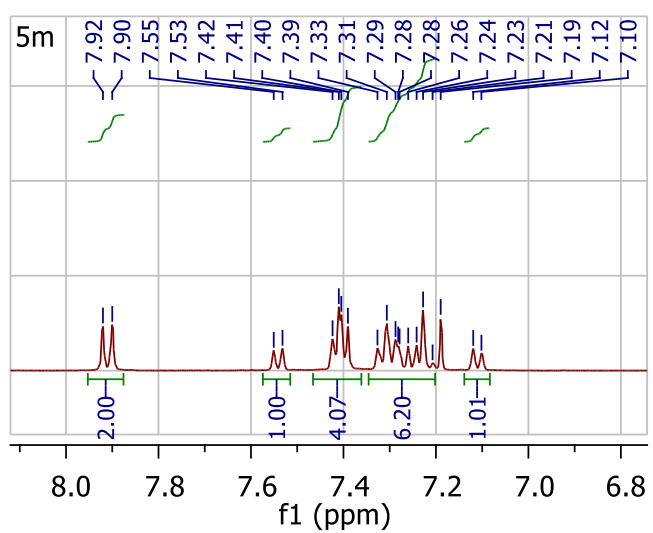
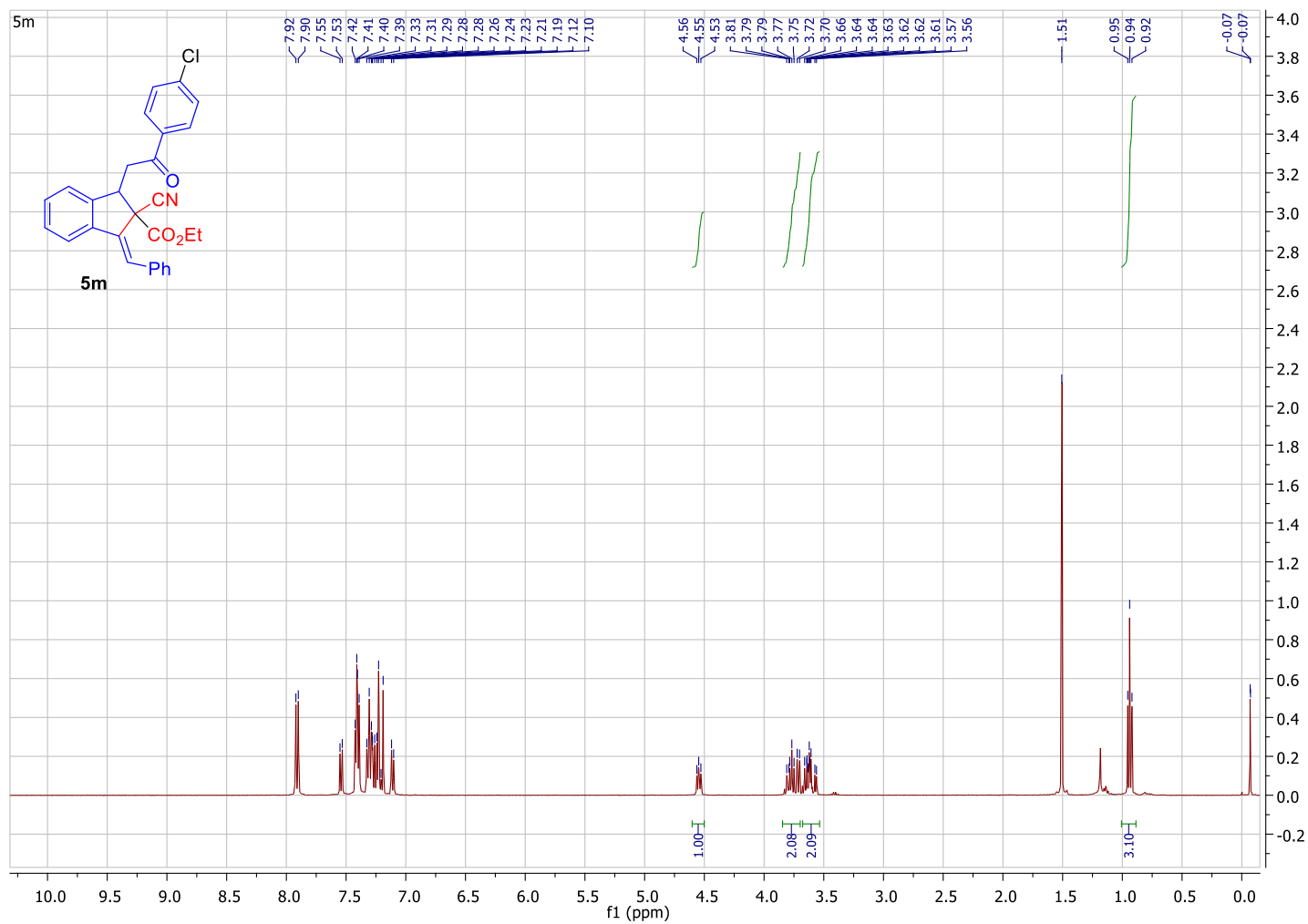


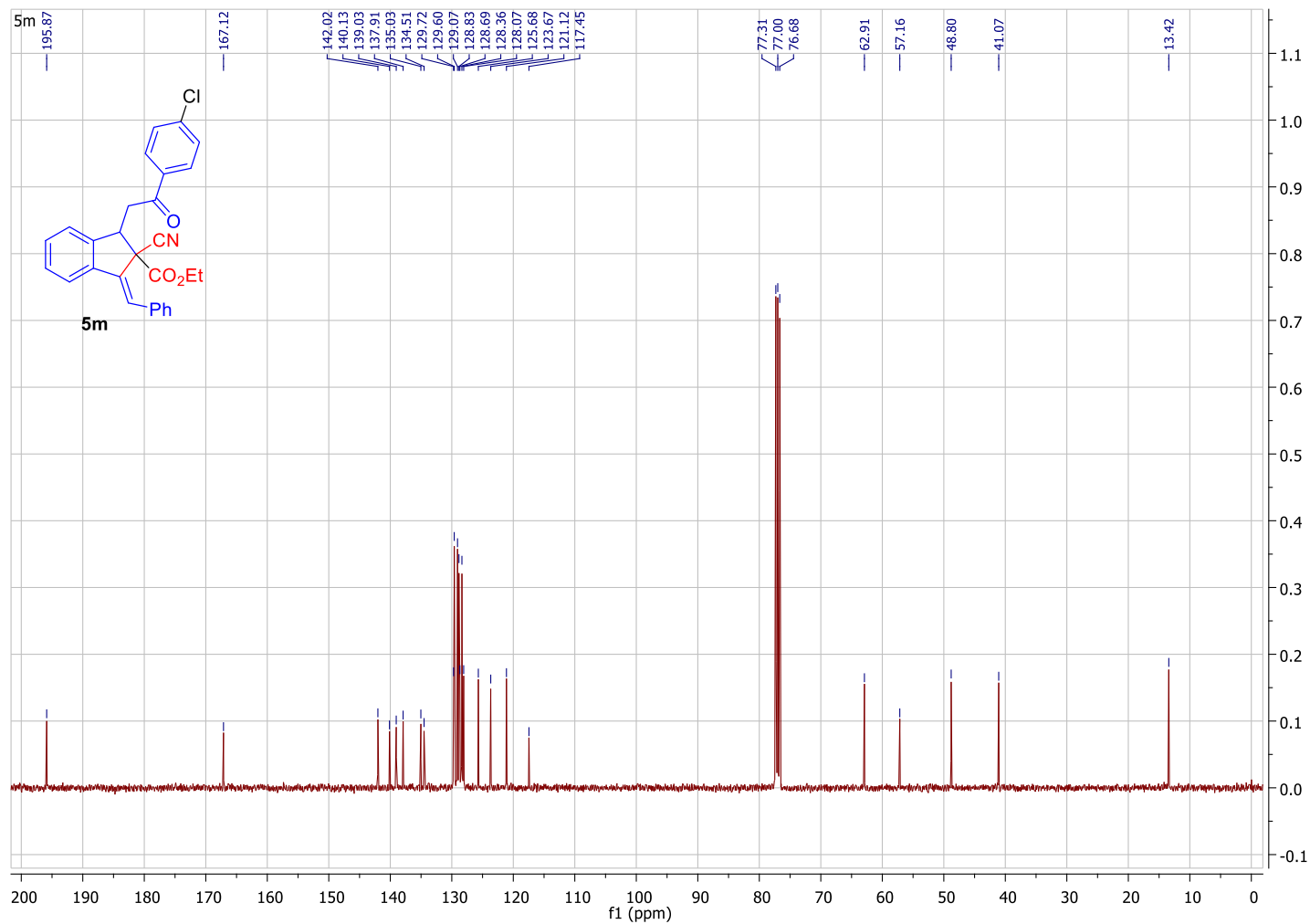




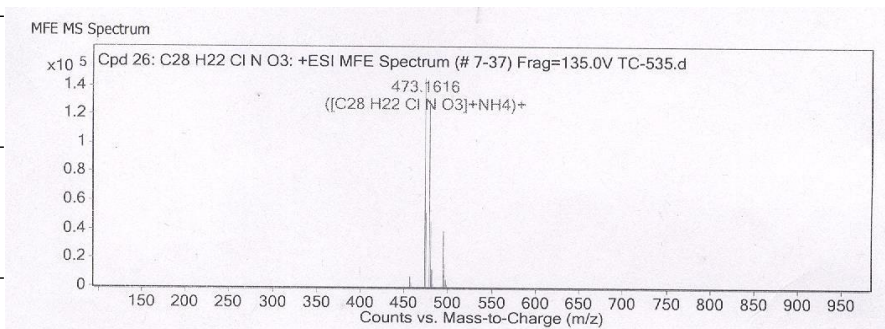
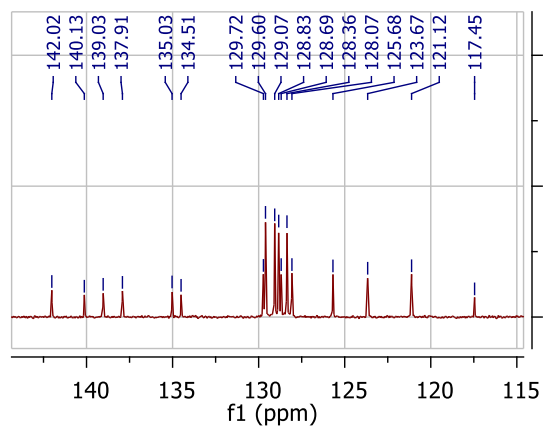
HRMS: (51)

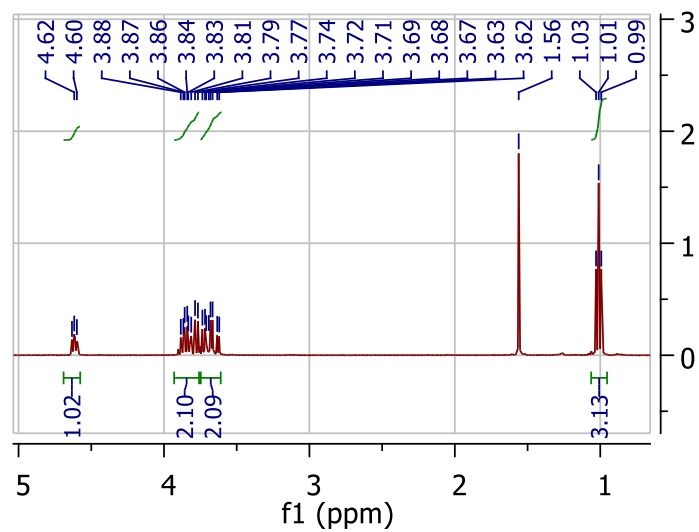
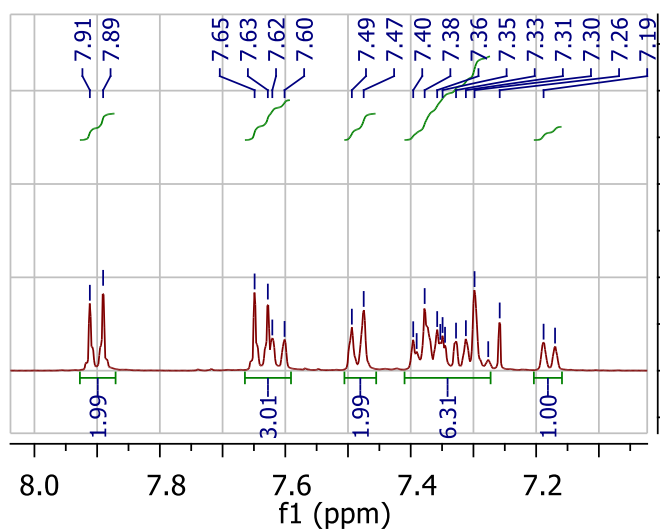
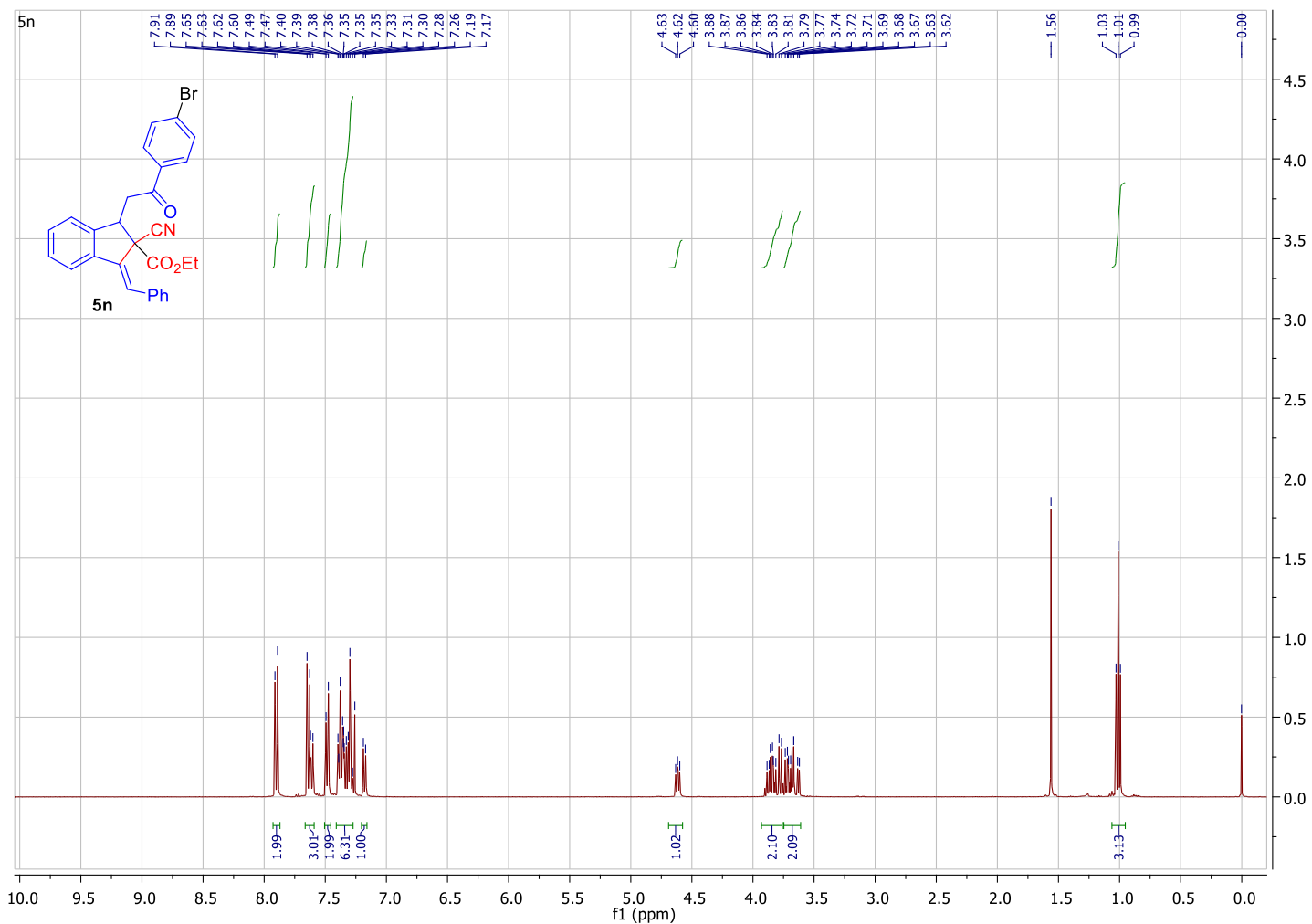


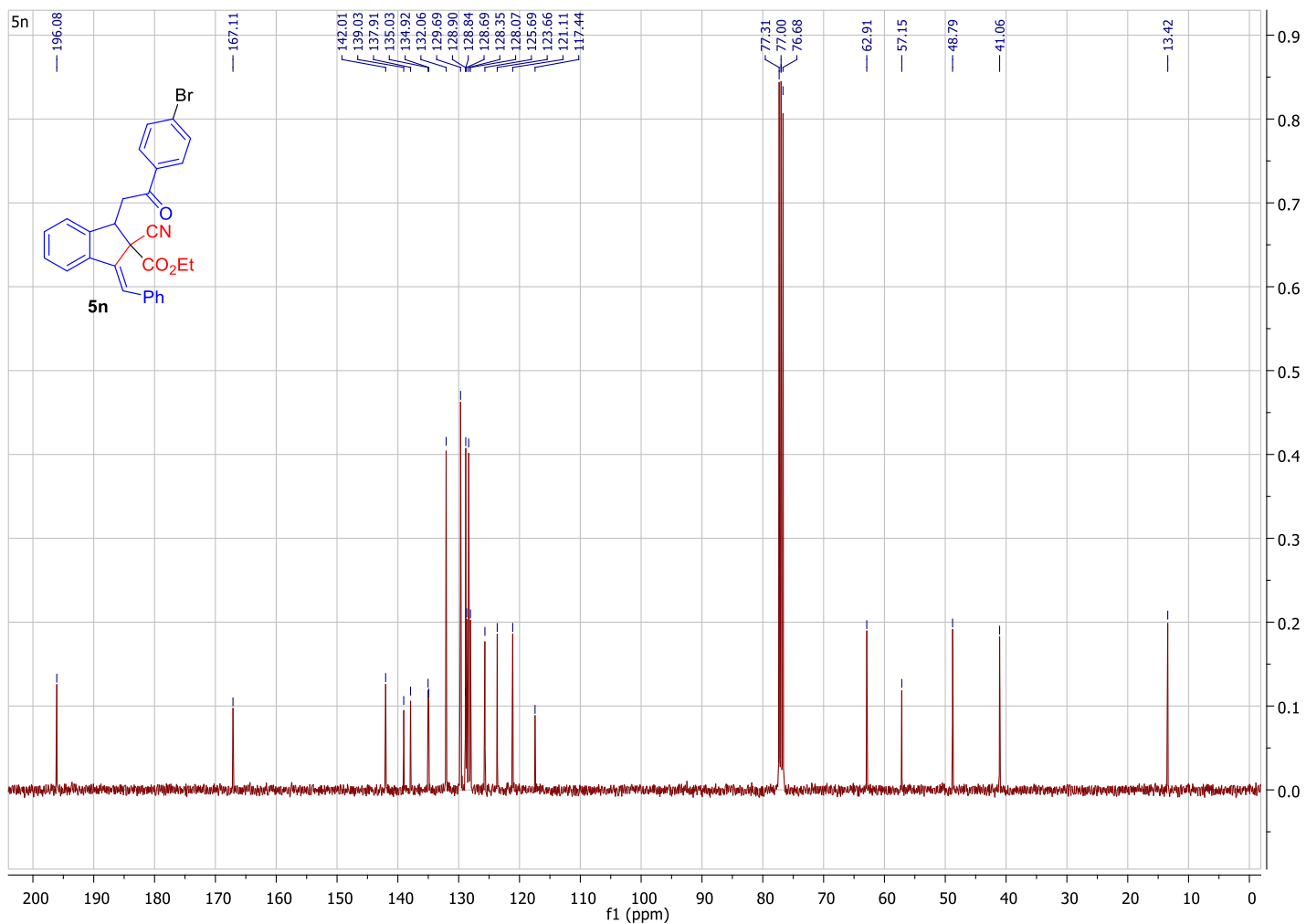




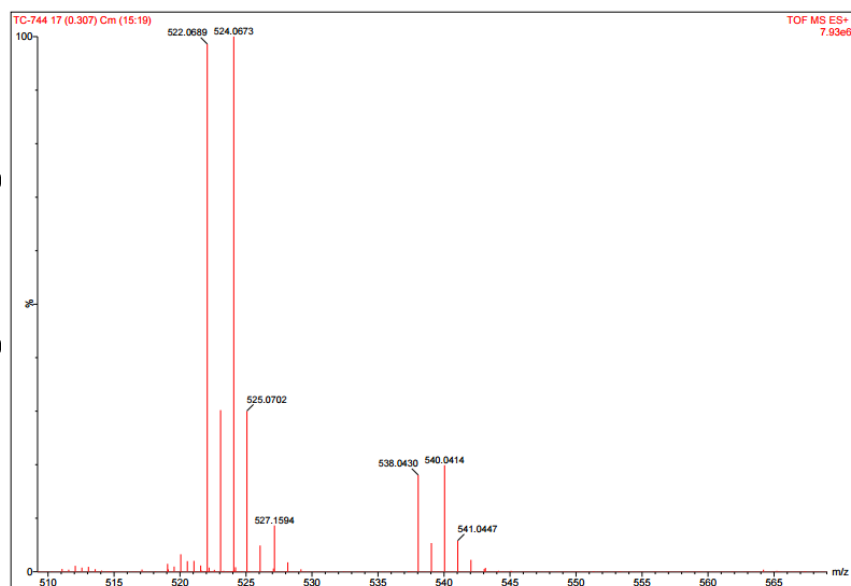
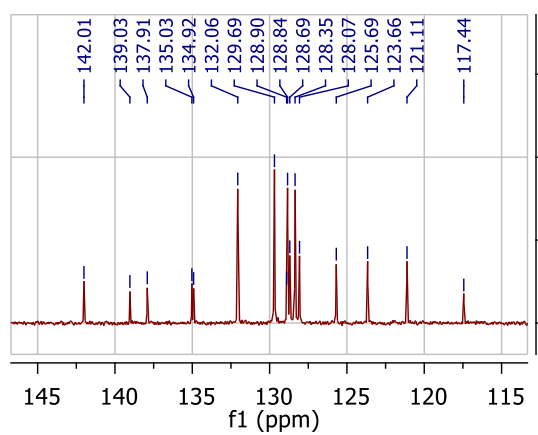
HRMS: (5m)

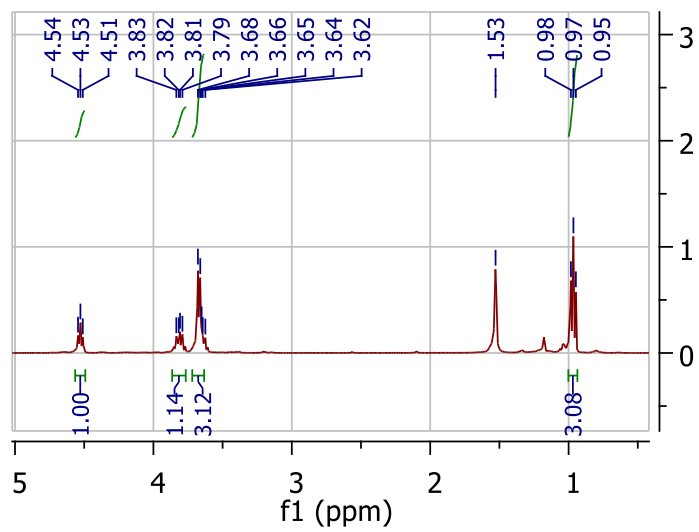
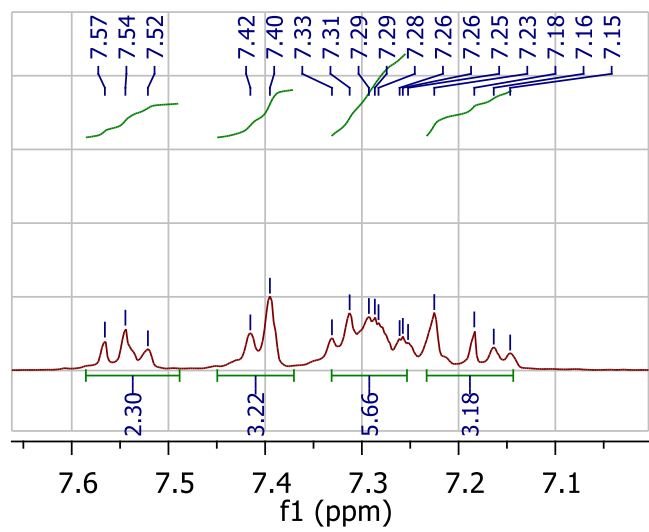
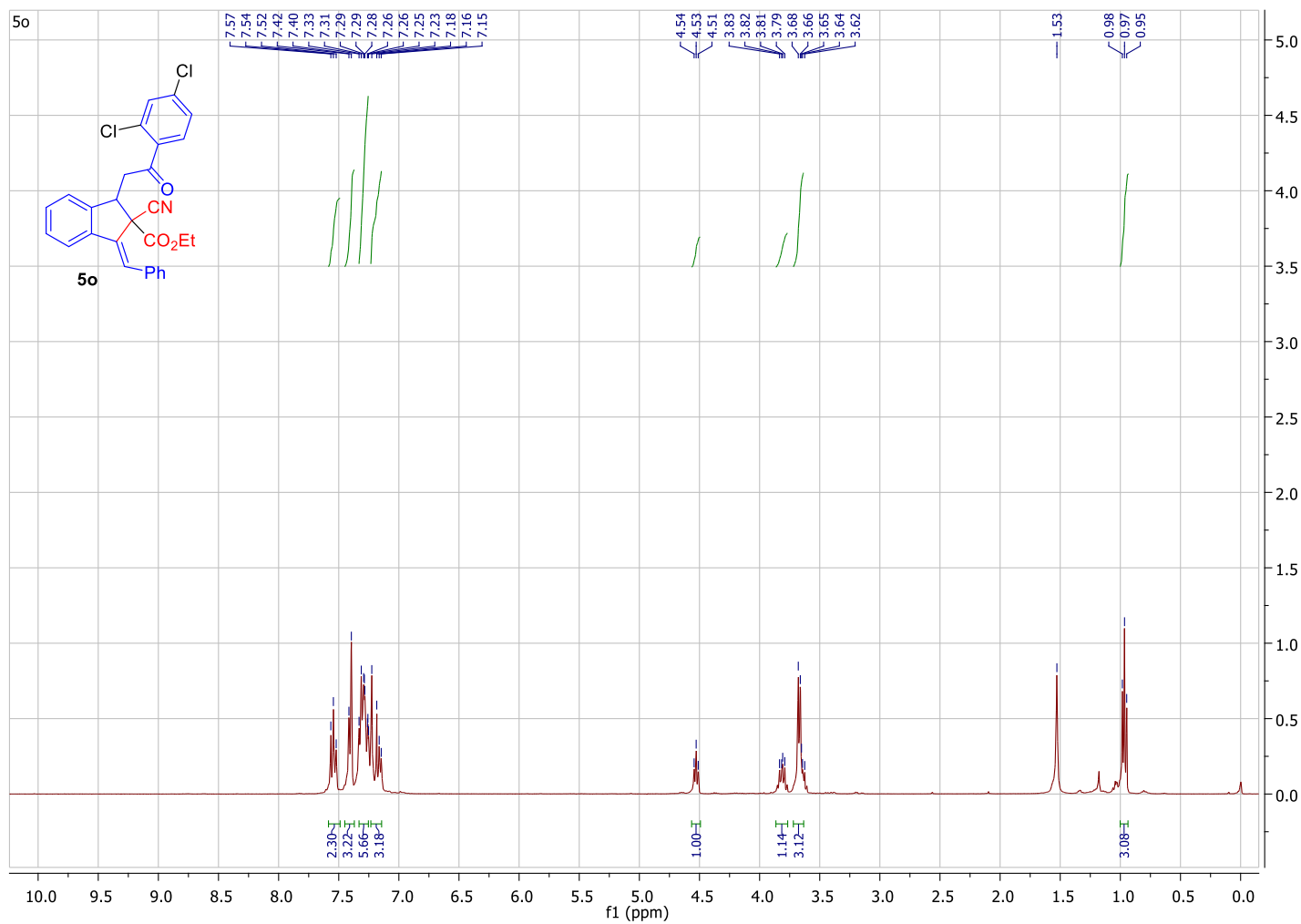


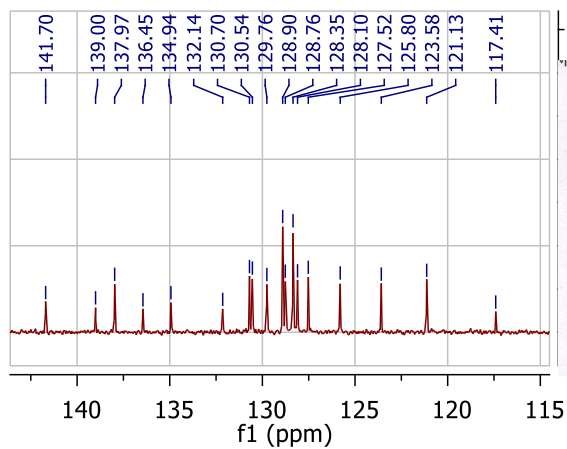
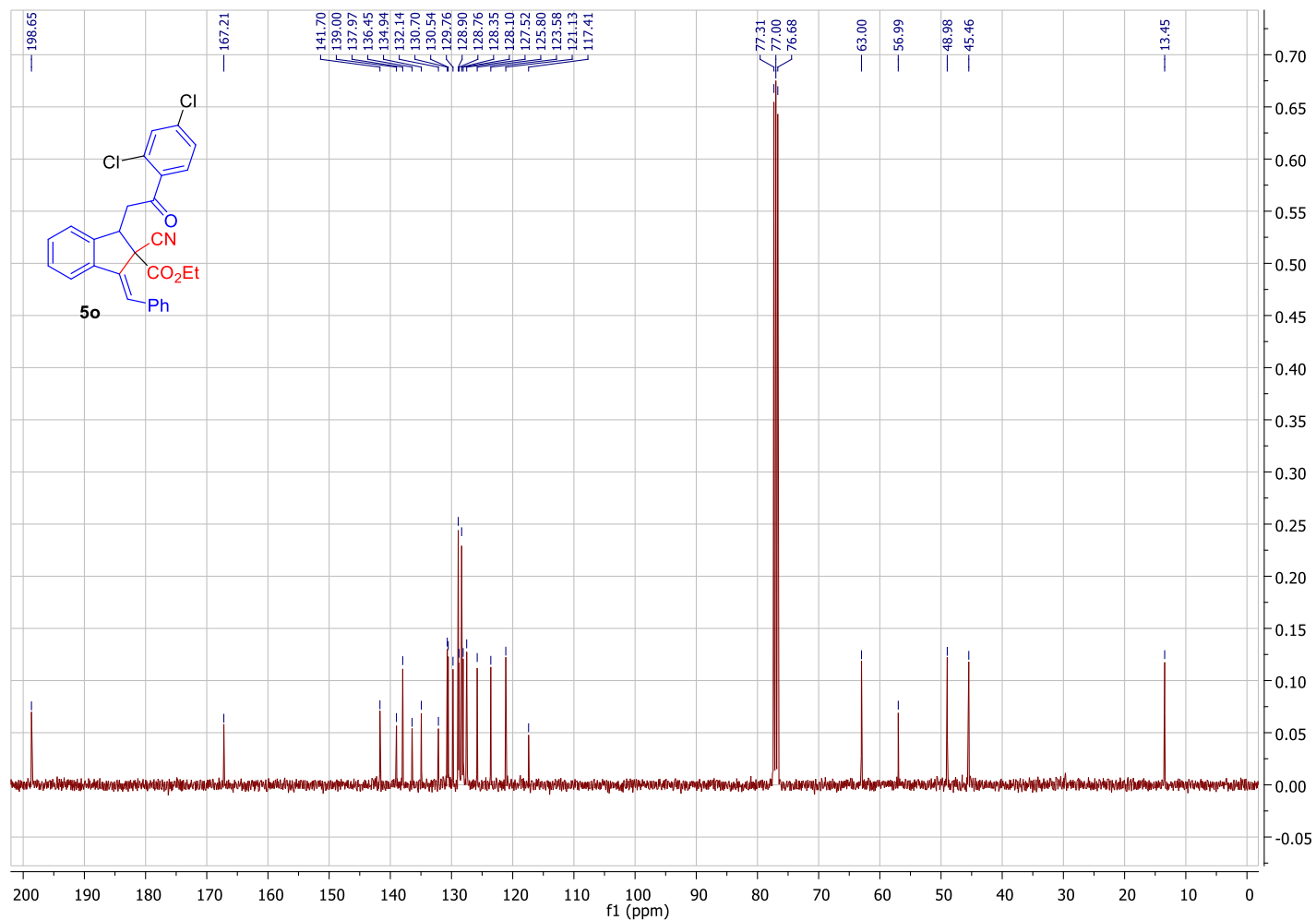




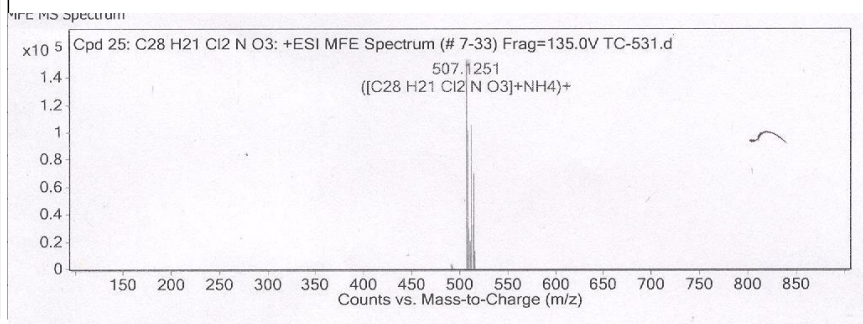
HRMS: (3n):

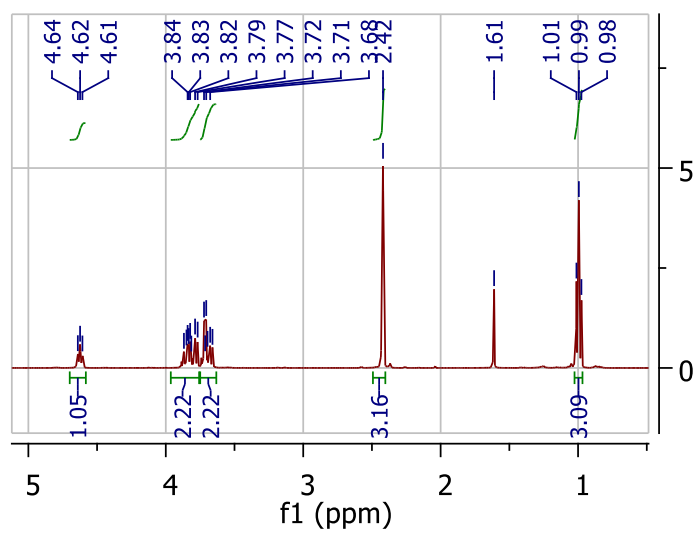
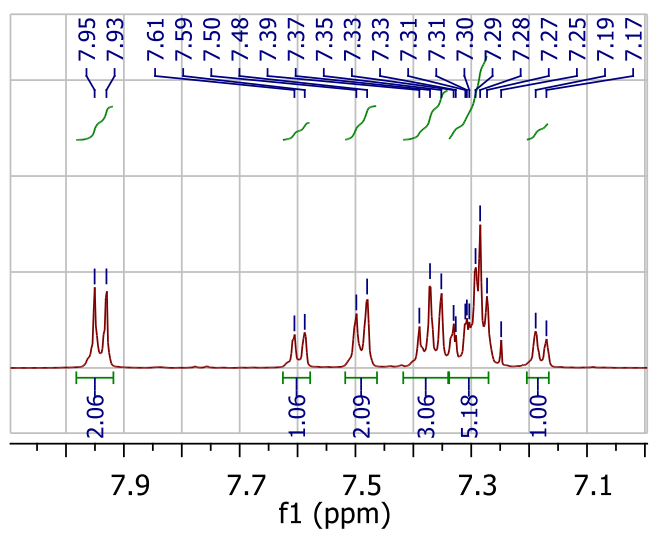
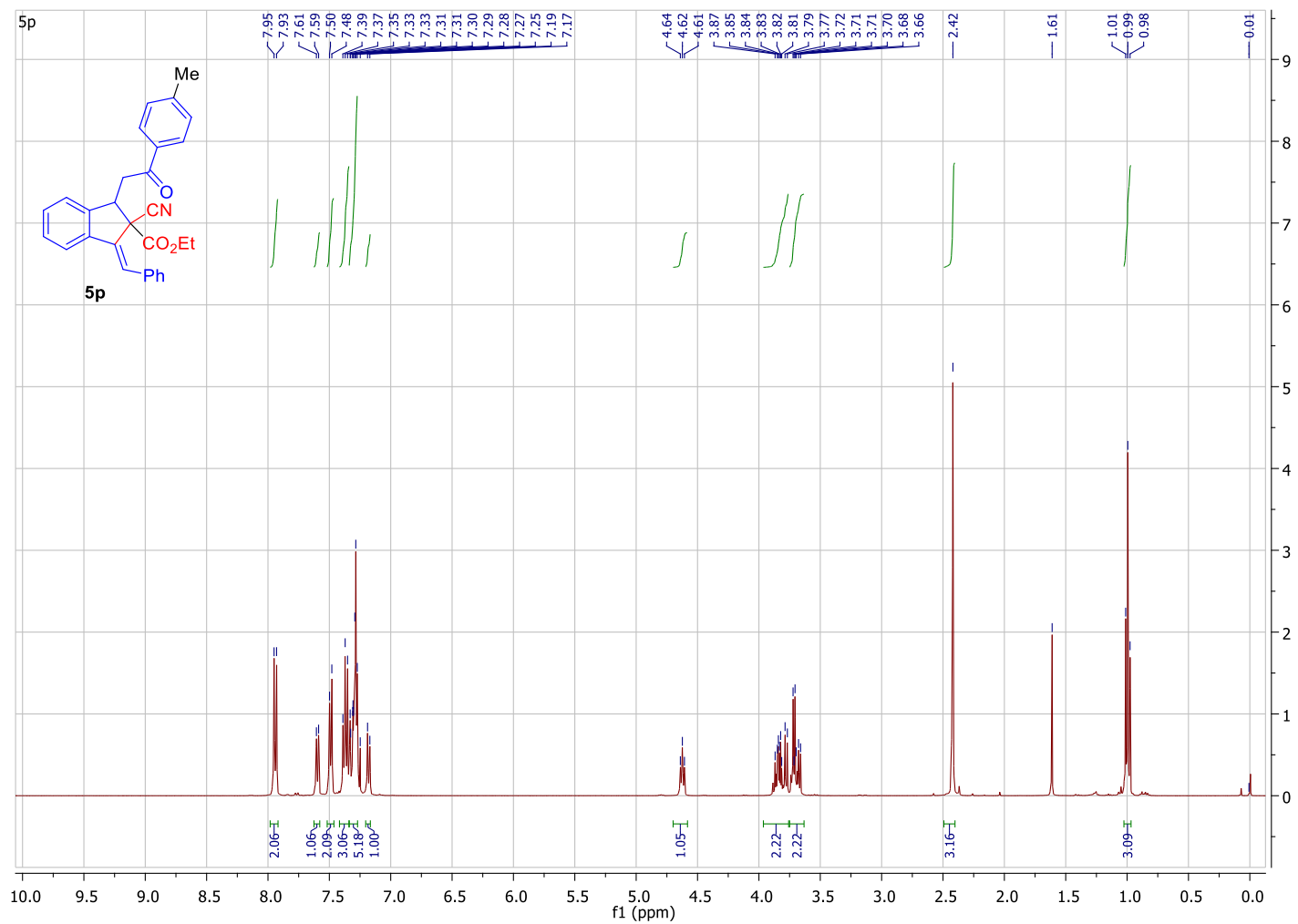


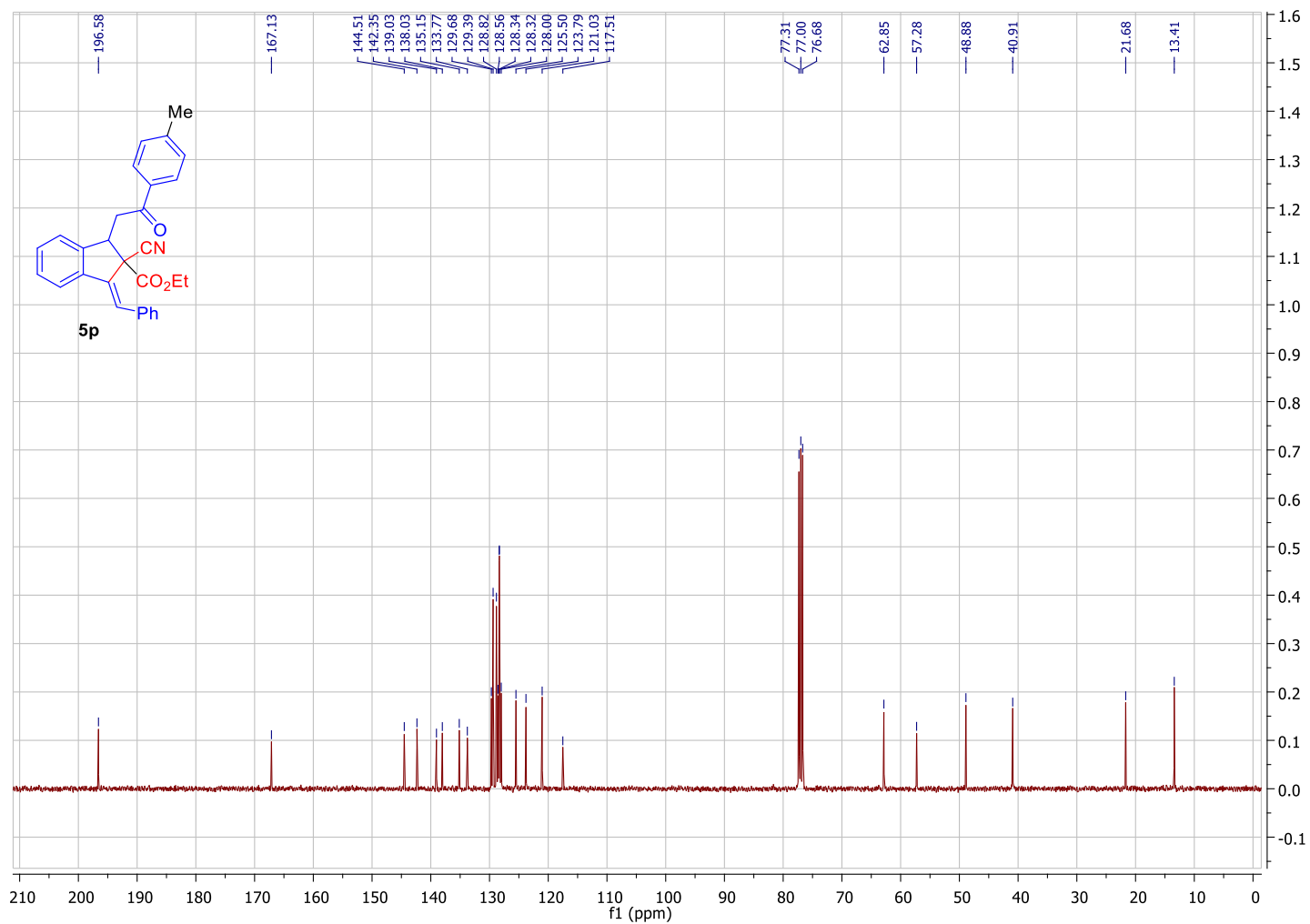




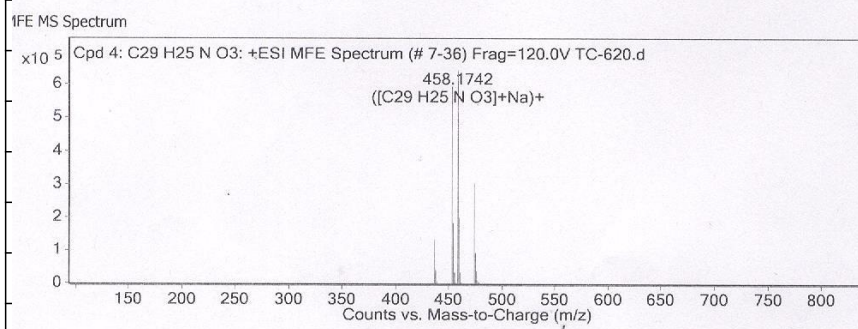
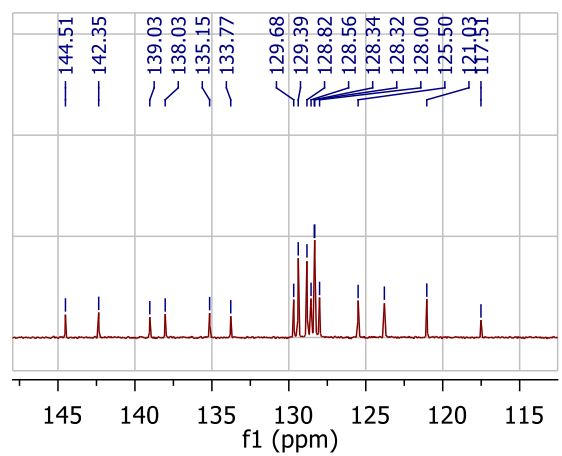
HRMS: (5o)

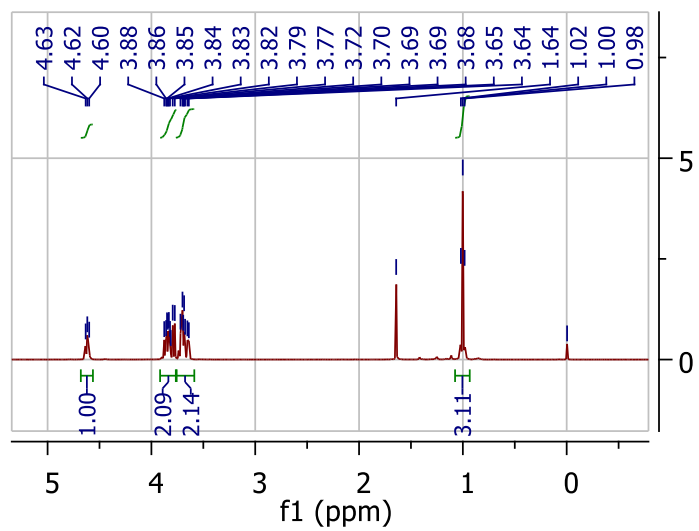
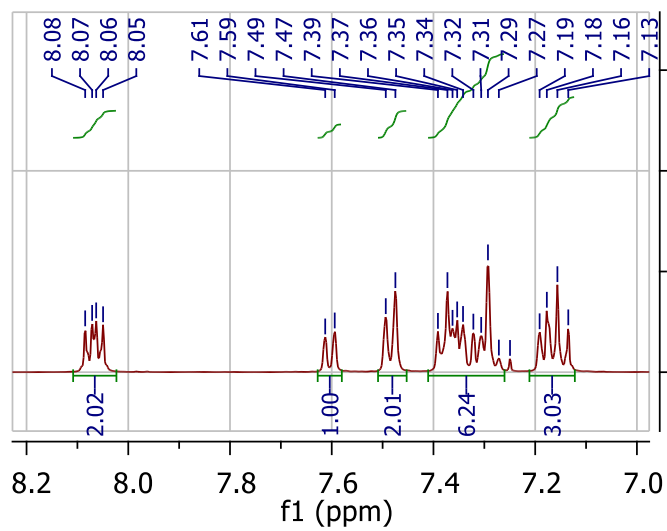
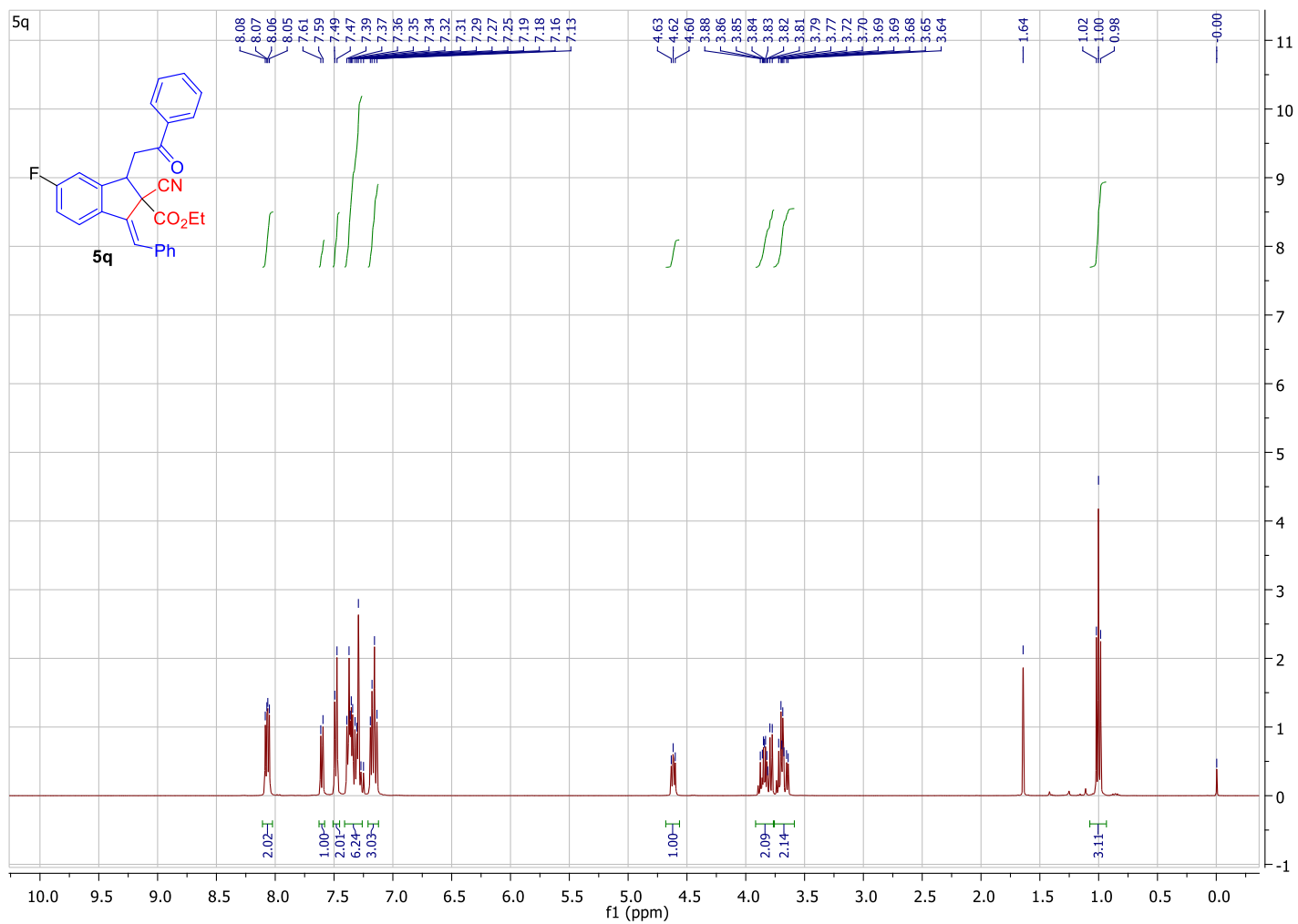


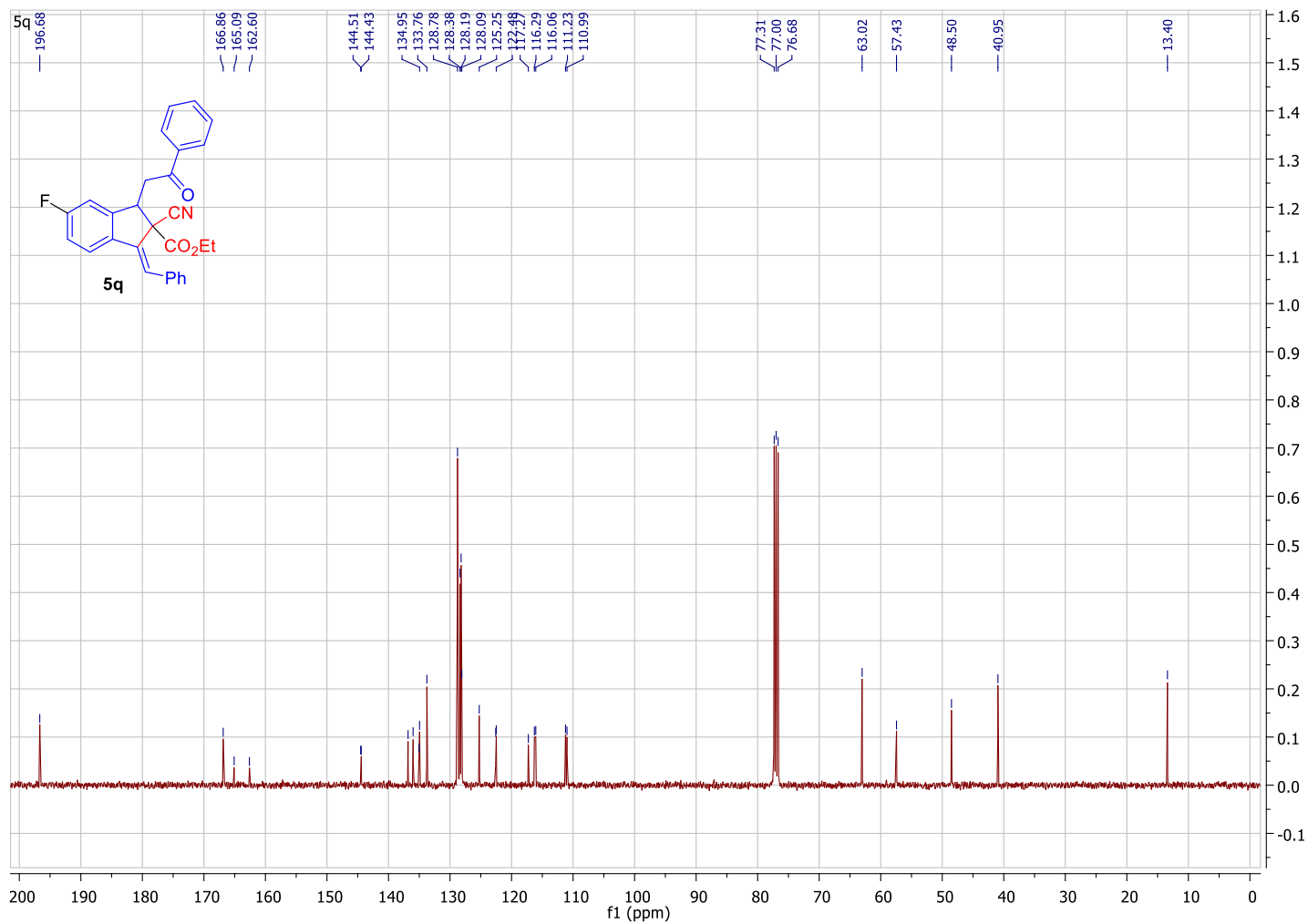




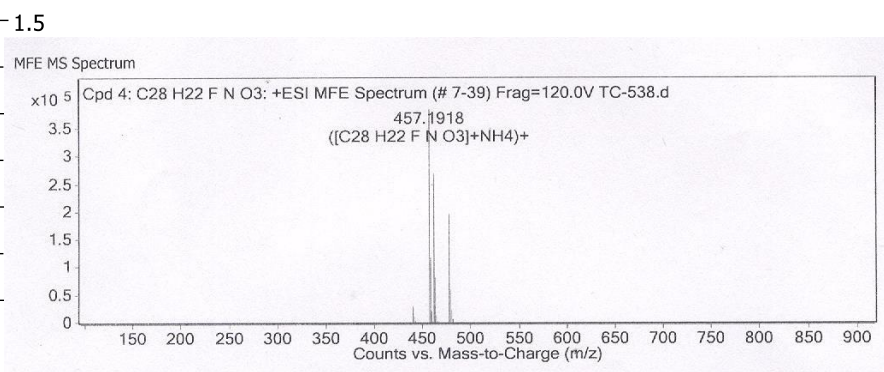
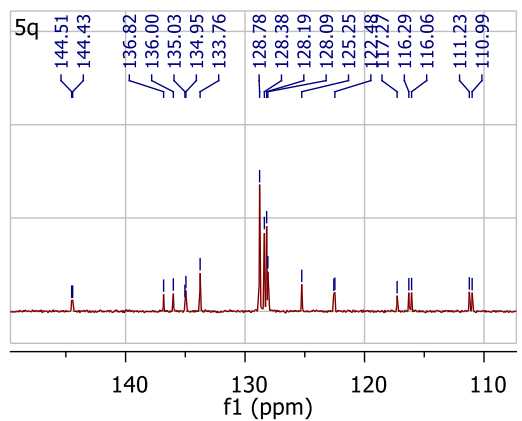
HRMS: (5p)

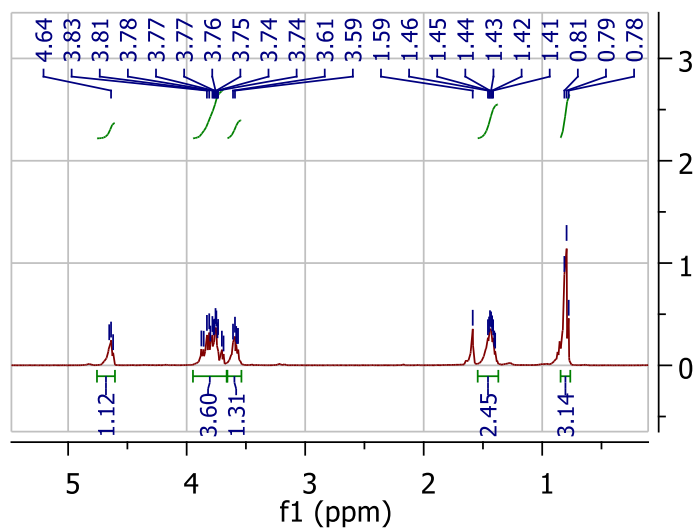
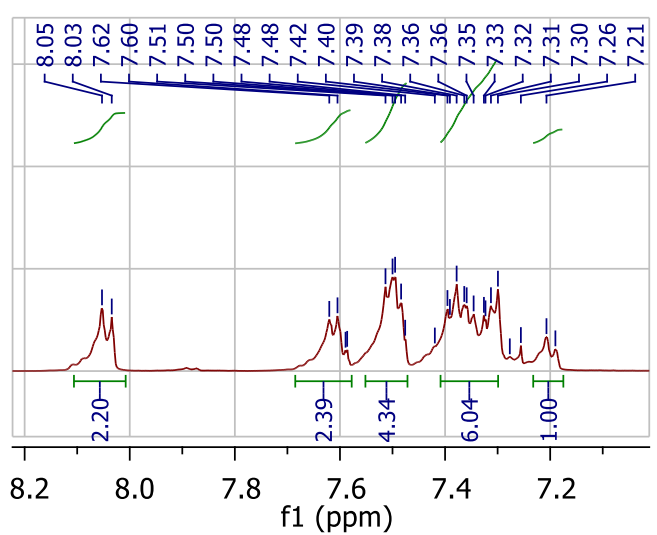
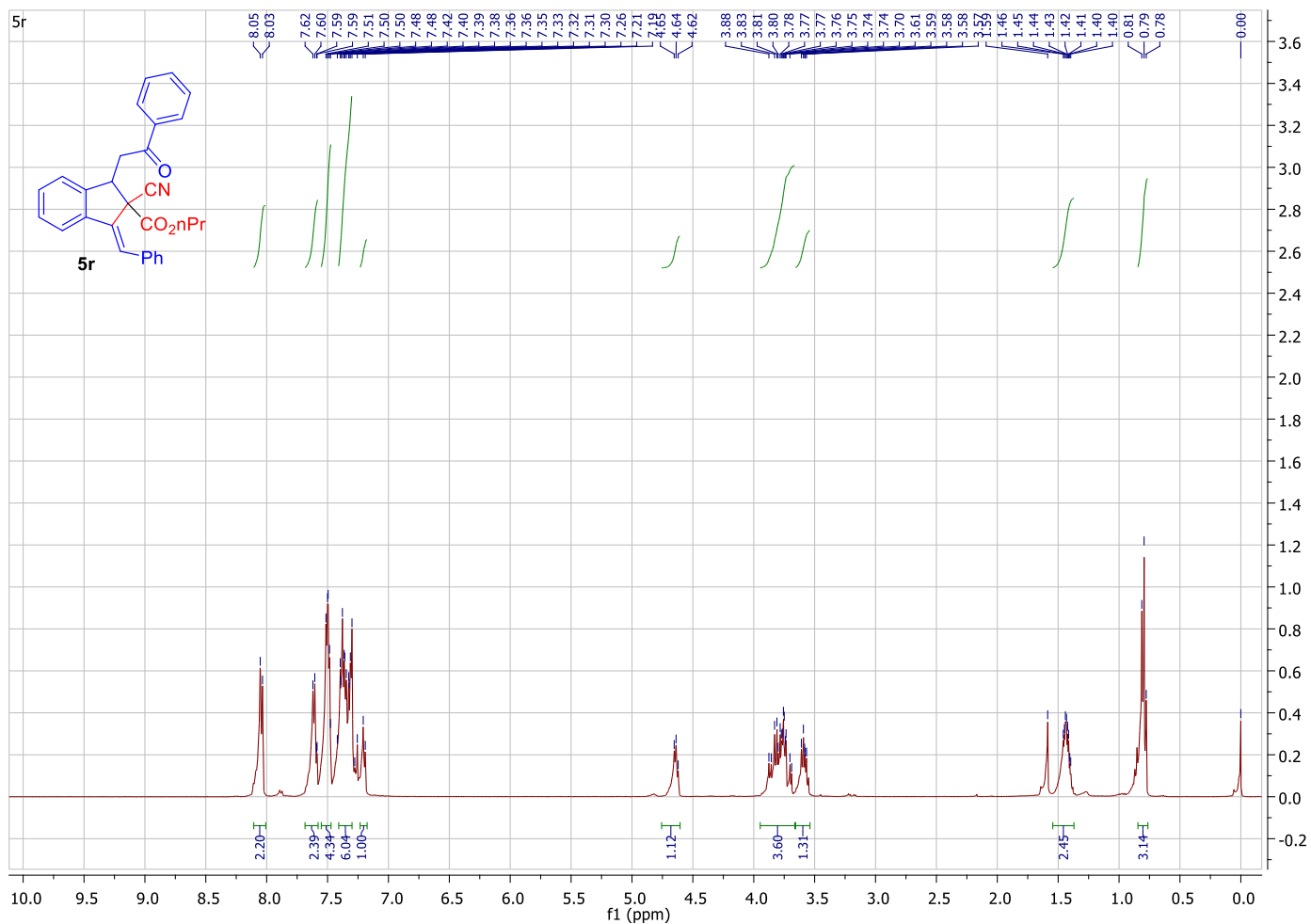


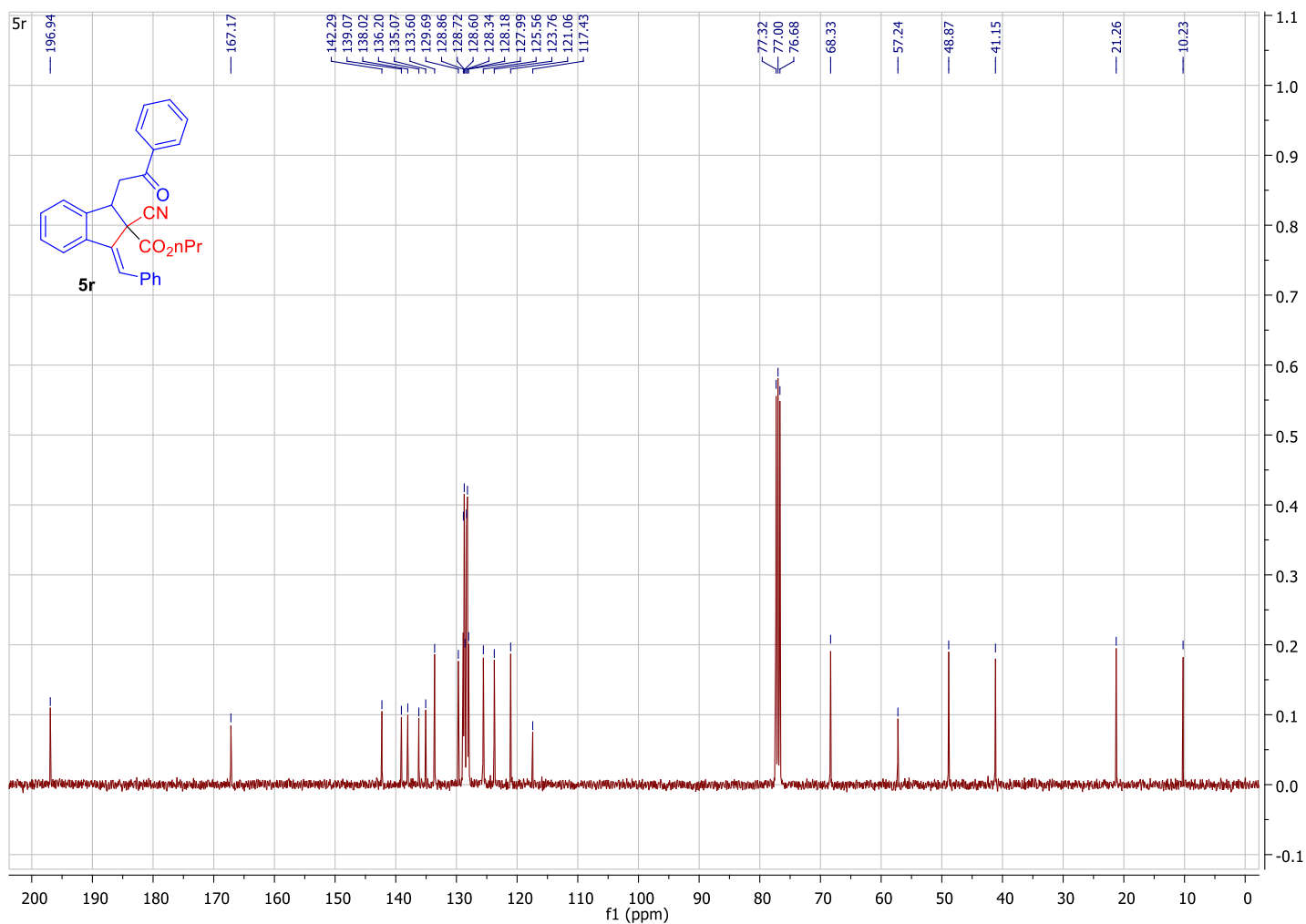




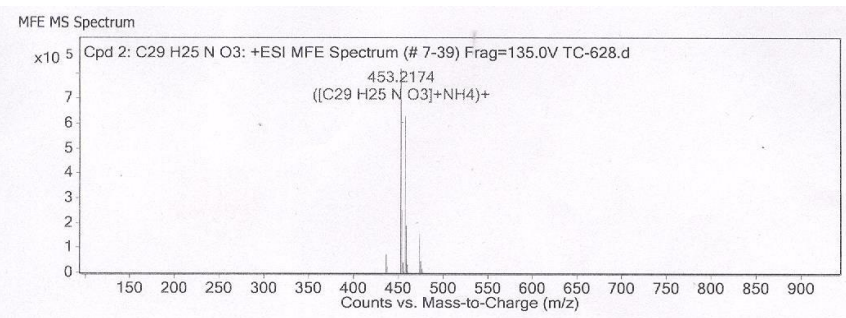
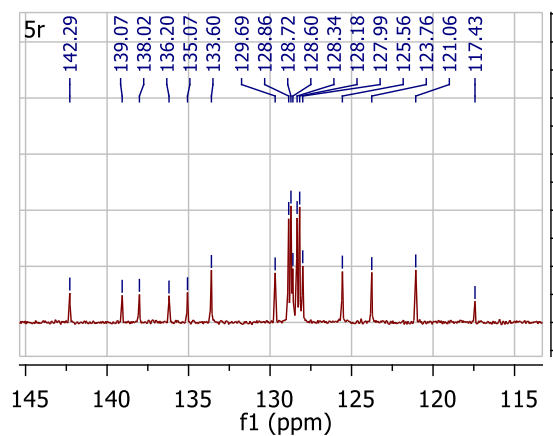
HRMS: (5q)

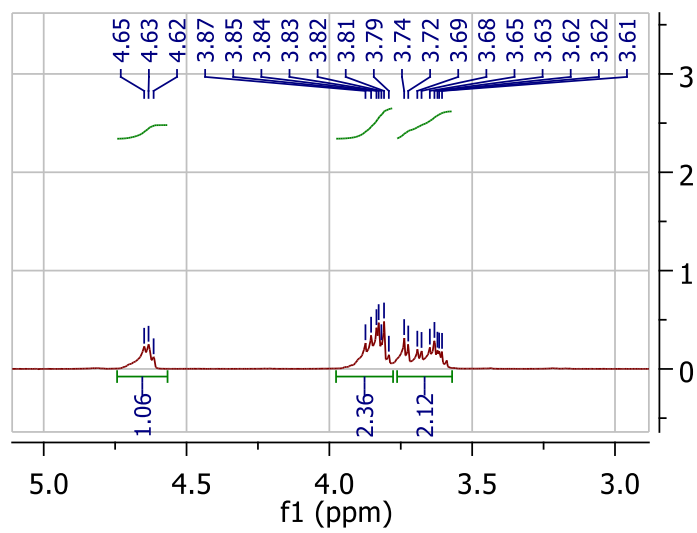
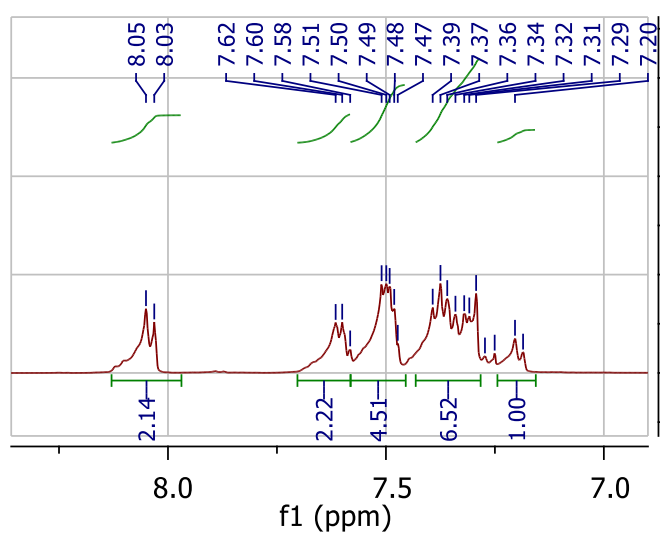
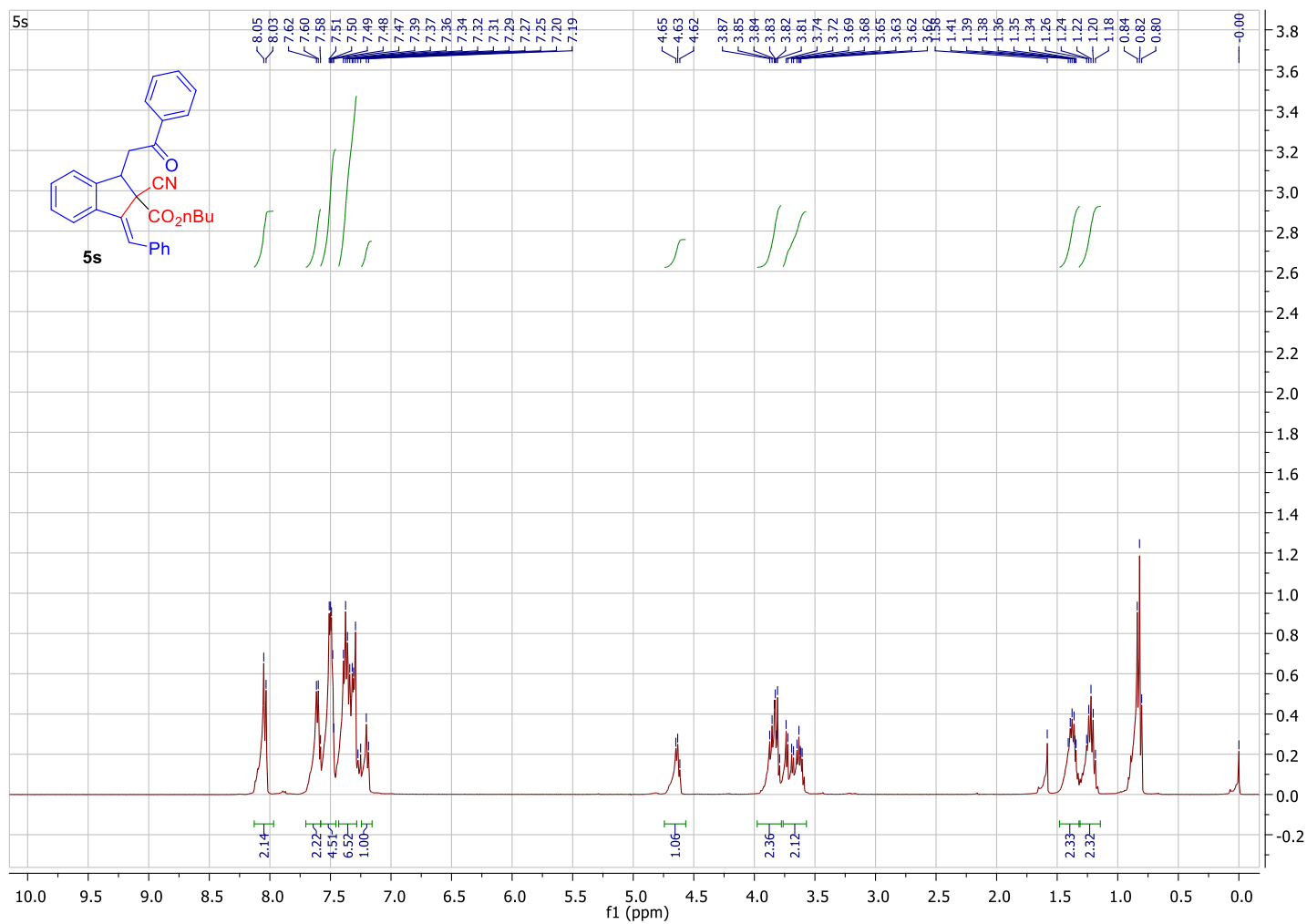


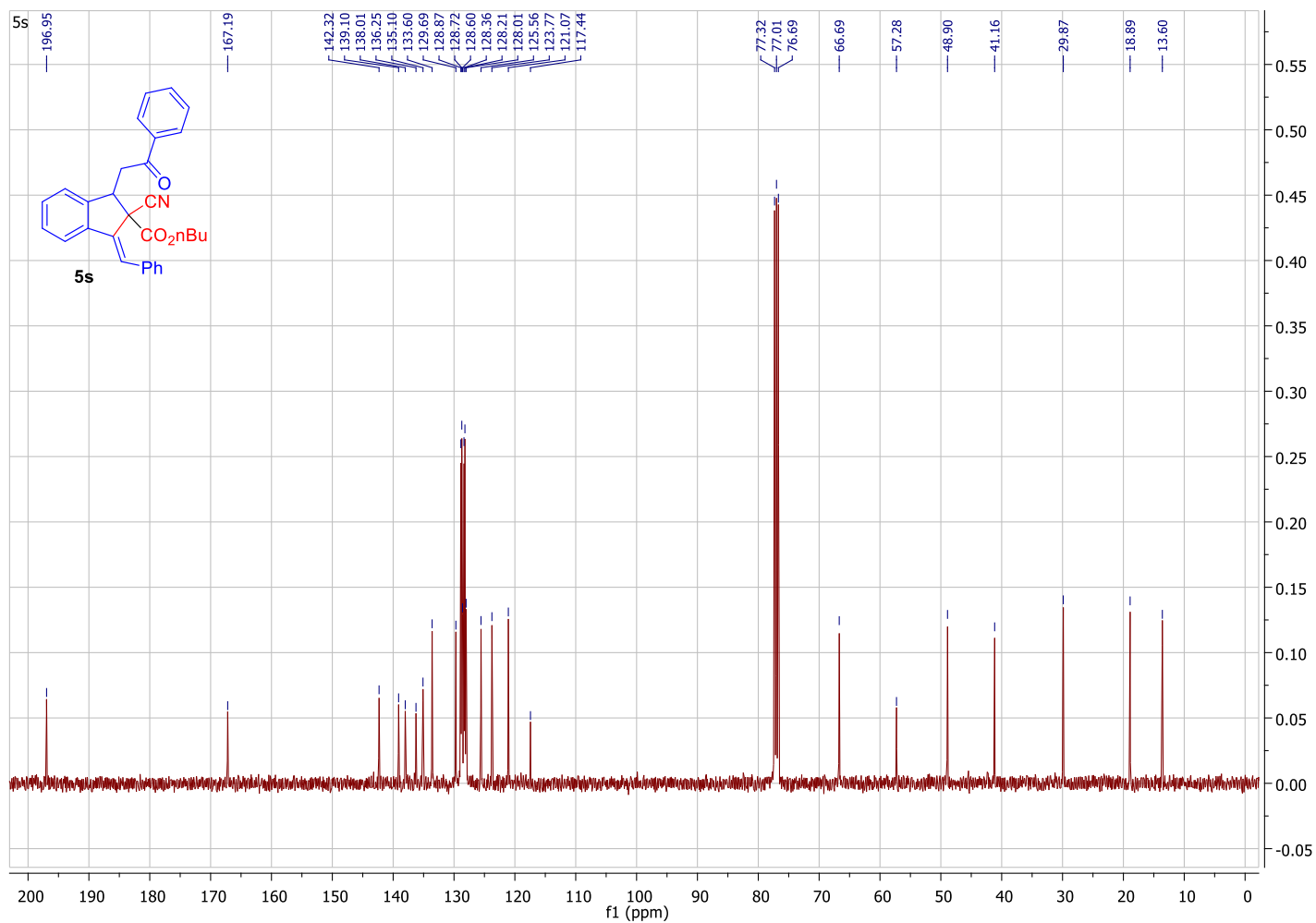




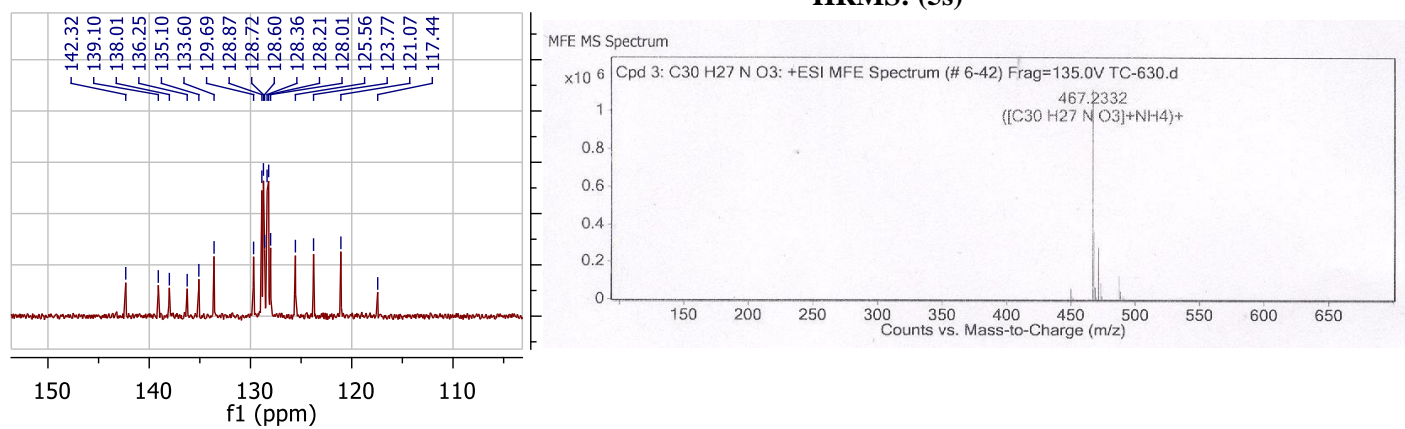
HRMS: (5r)

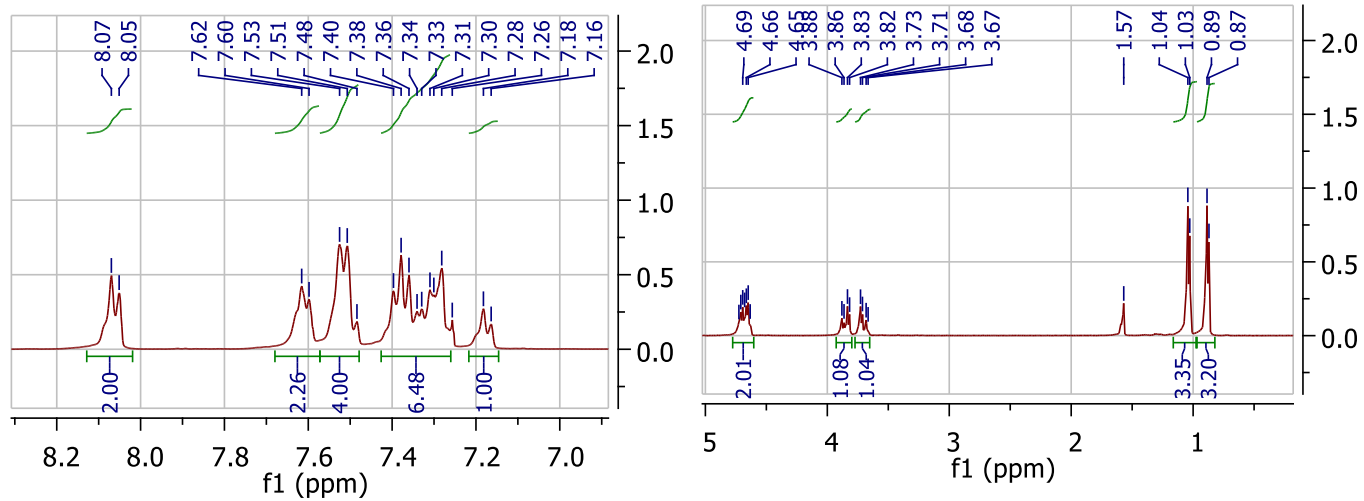
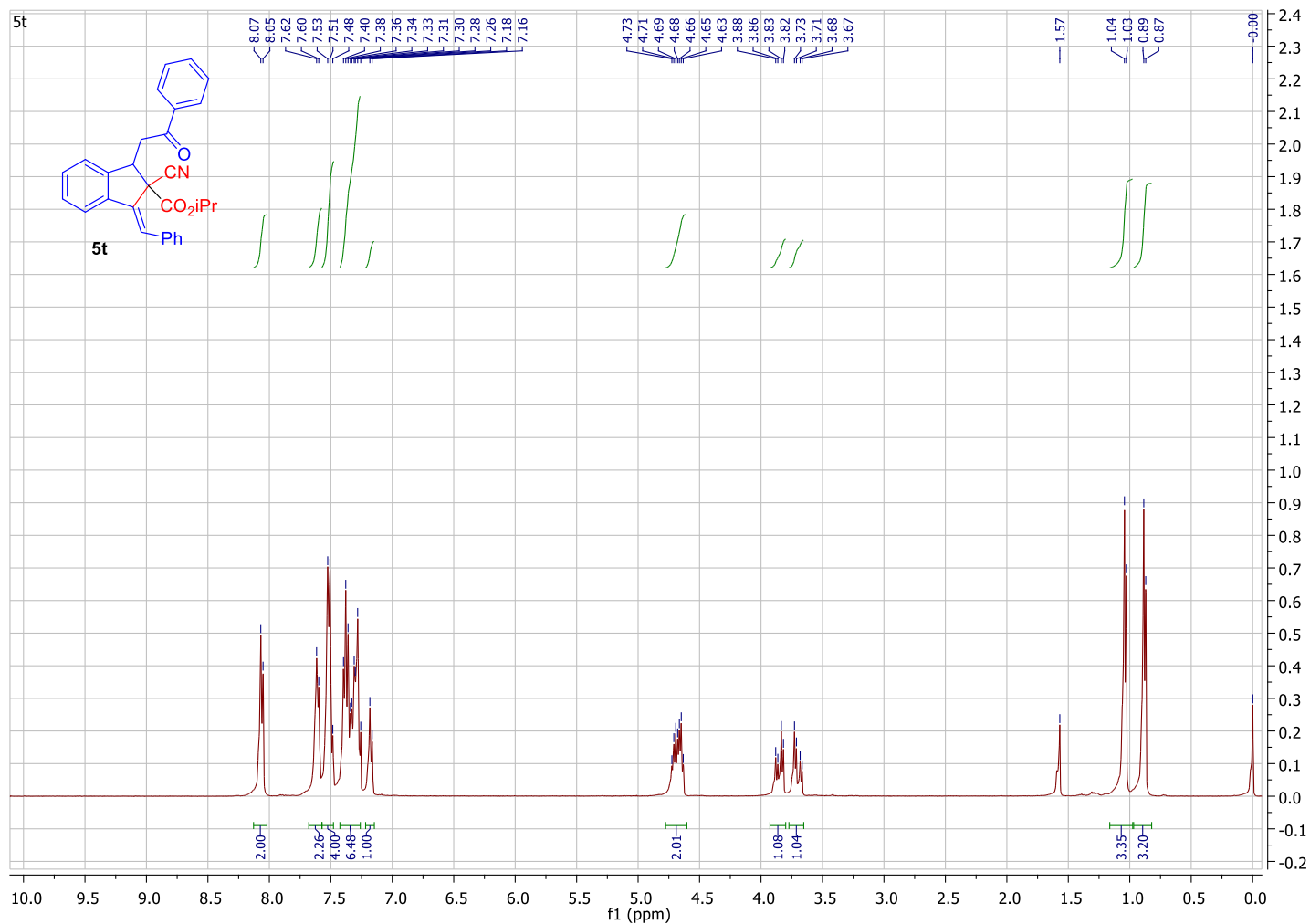


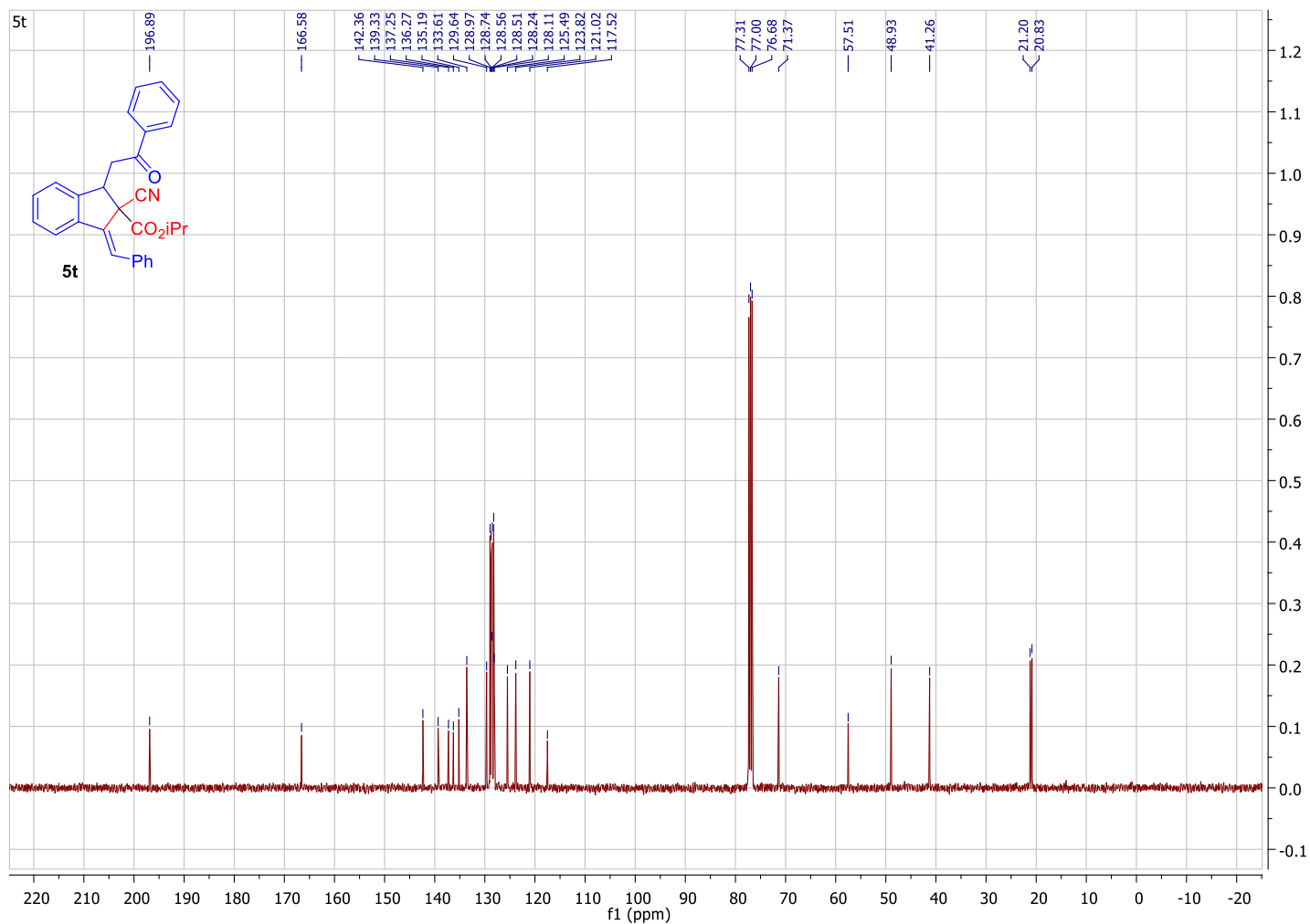




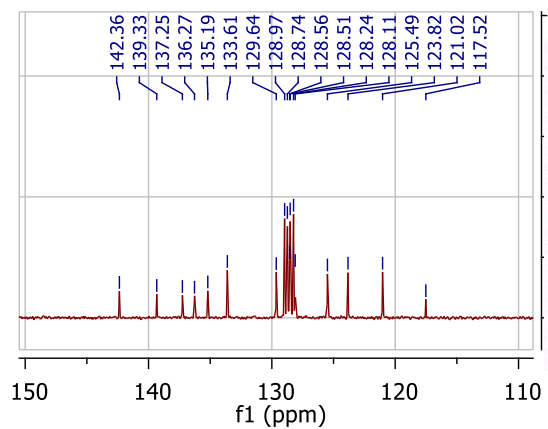
HRMS: (5s)



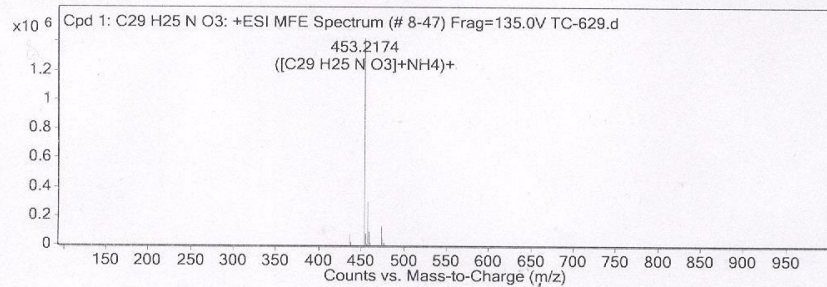


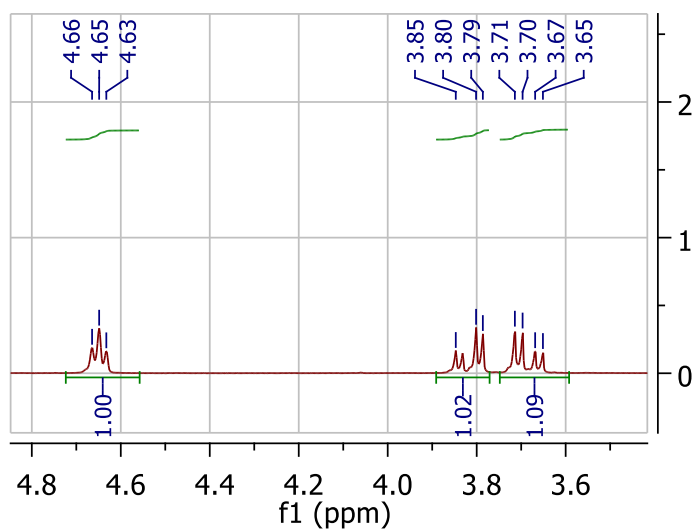
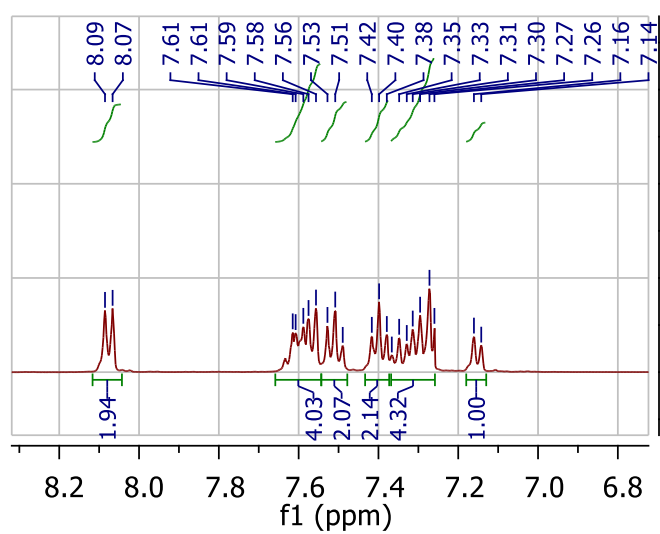
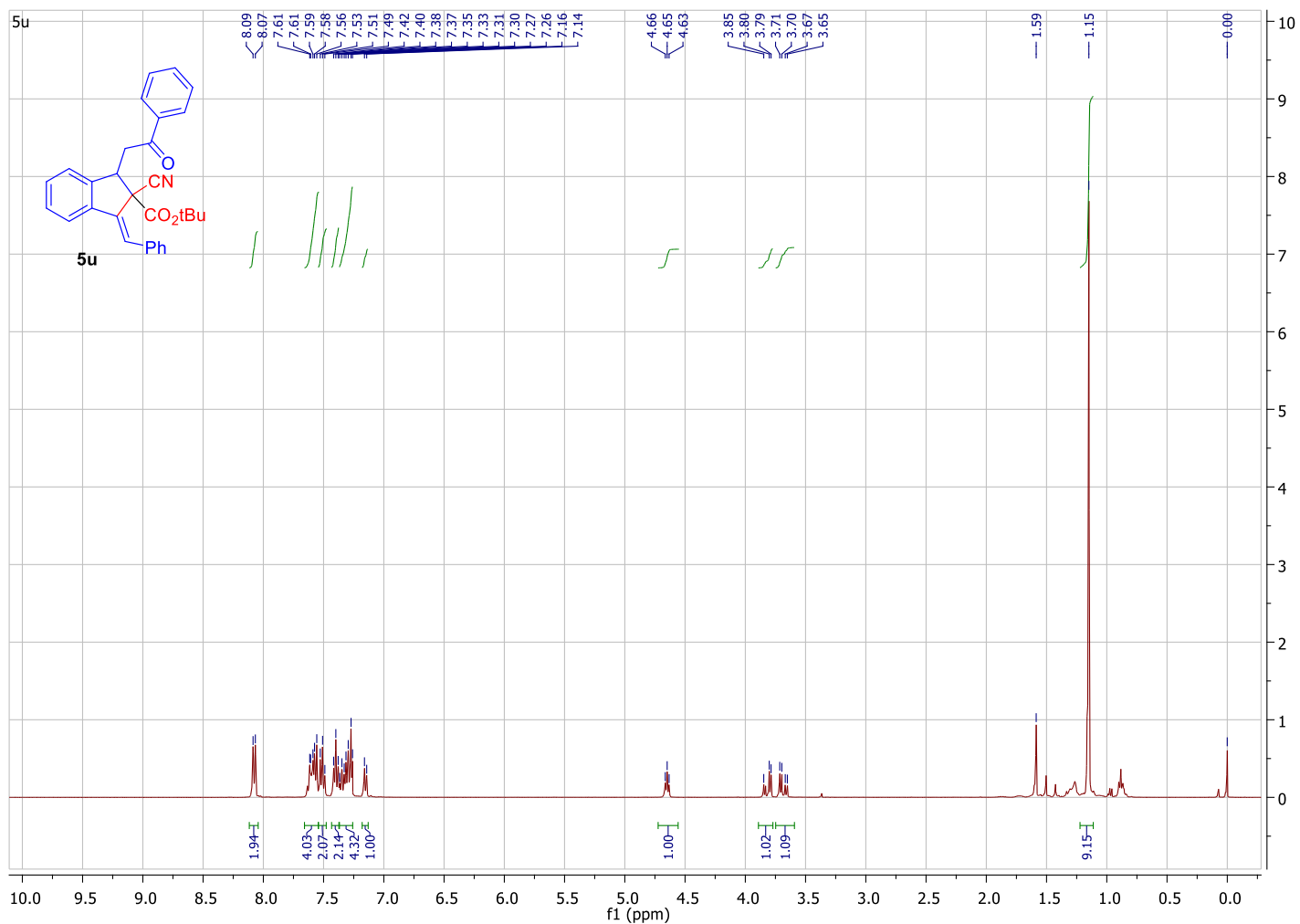


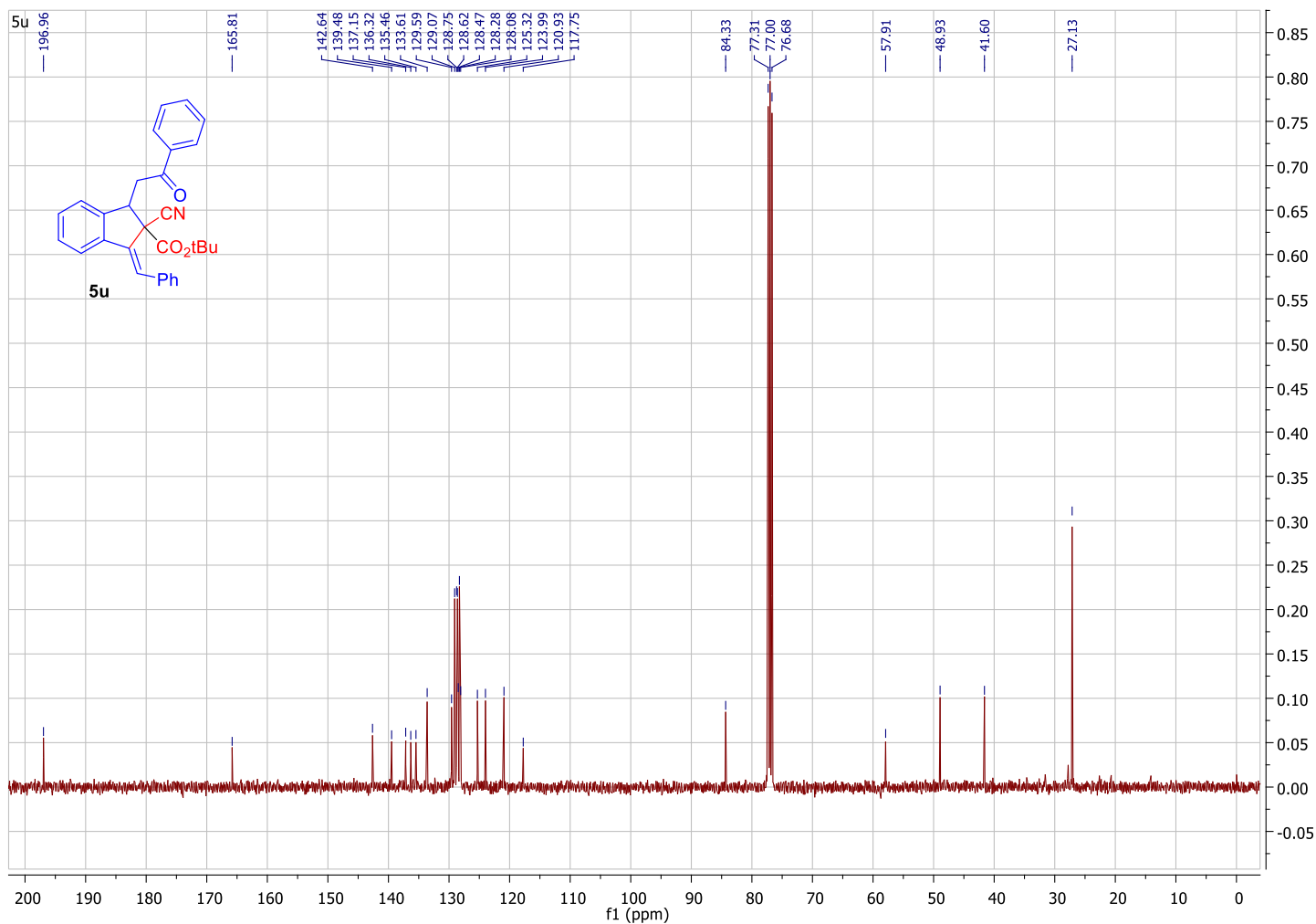
HRMS: (5t)



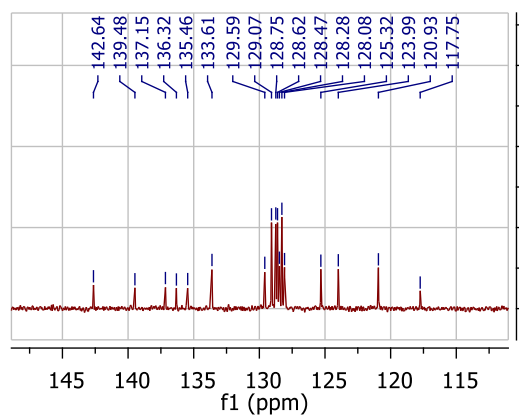
MFE MS Spectrum







HRMS: (5u)

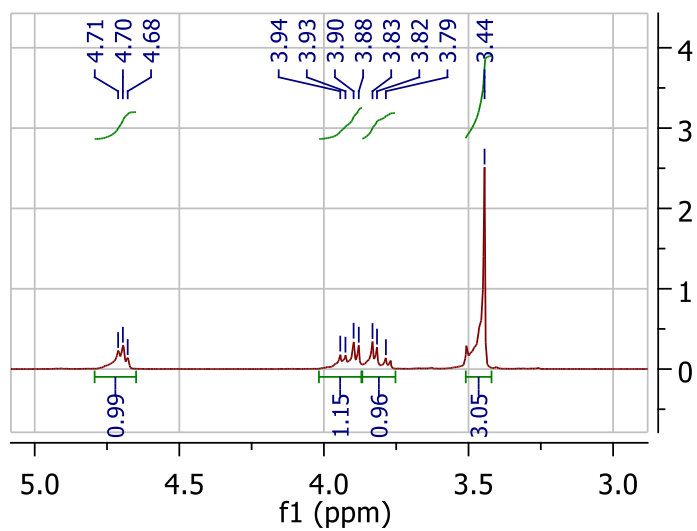
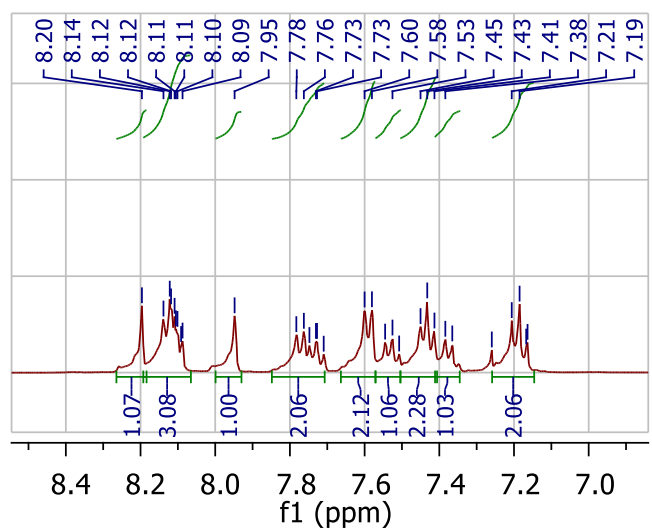
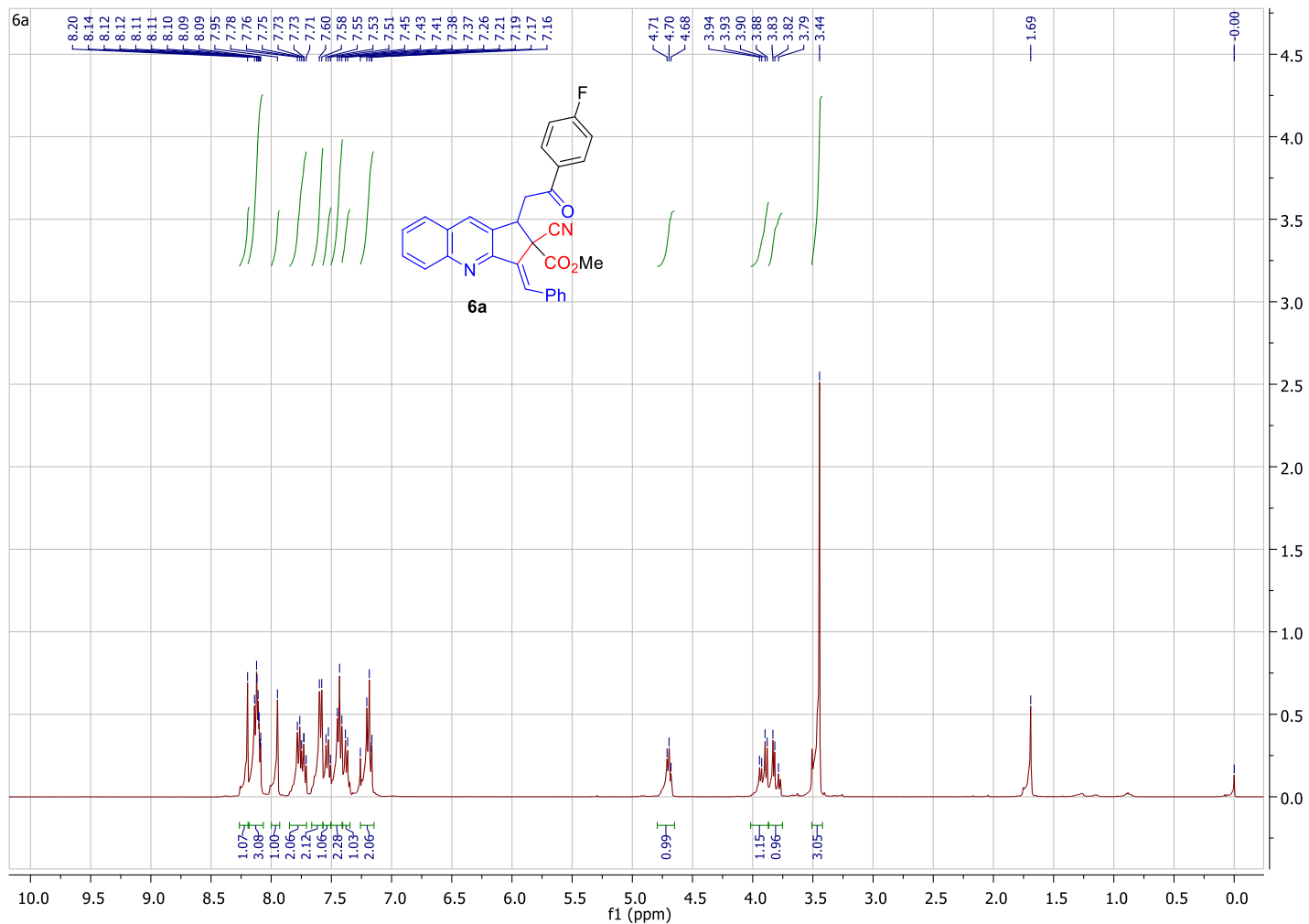


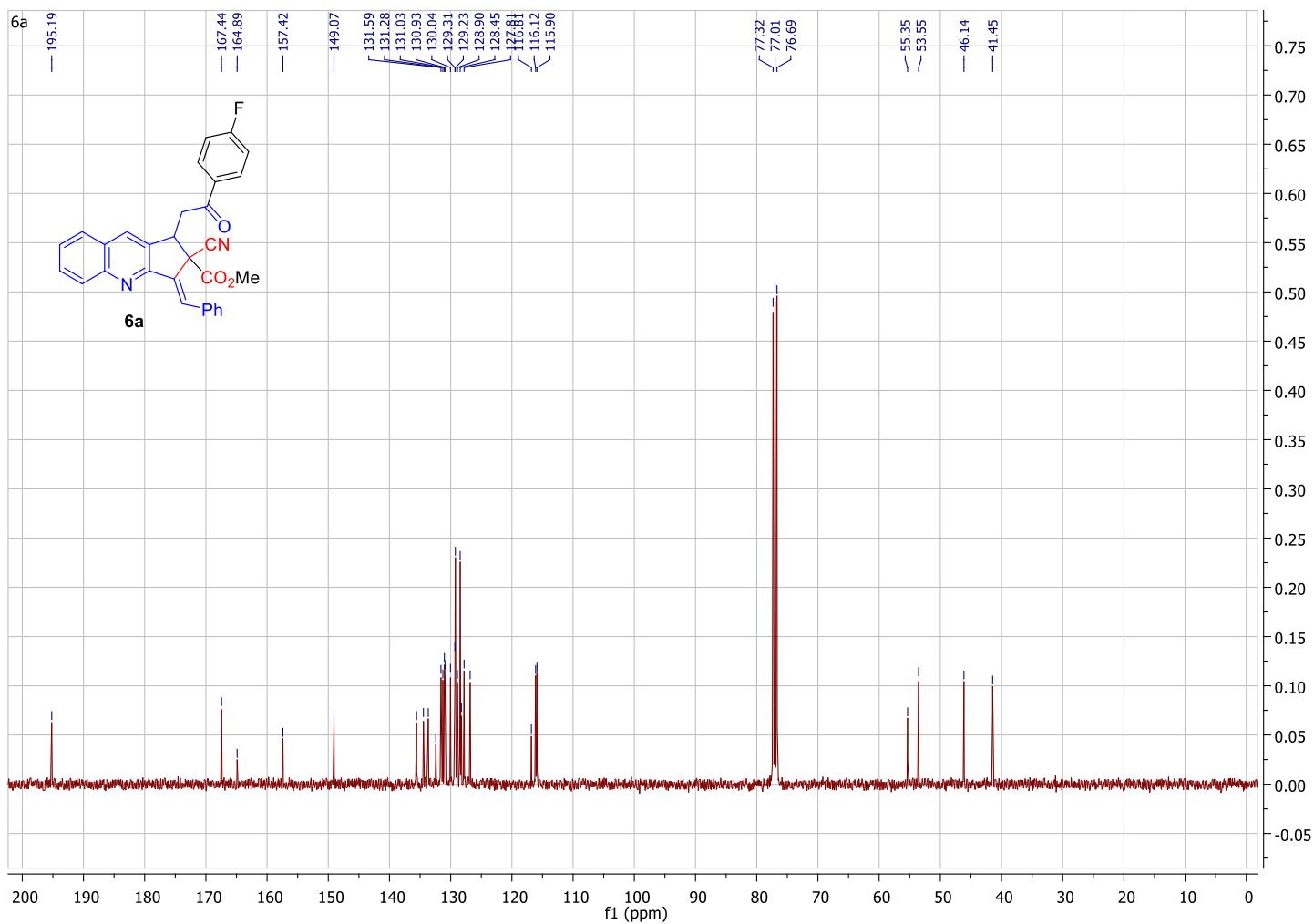
MFE MS Spectrum

x10⁵ Cpd 4: C₃₀ H₂₇ N O₃: +ESI MFE Spectrum (# 6-42) Frag=135.0V TC-637.d

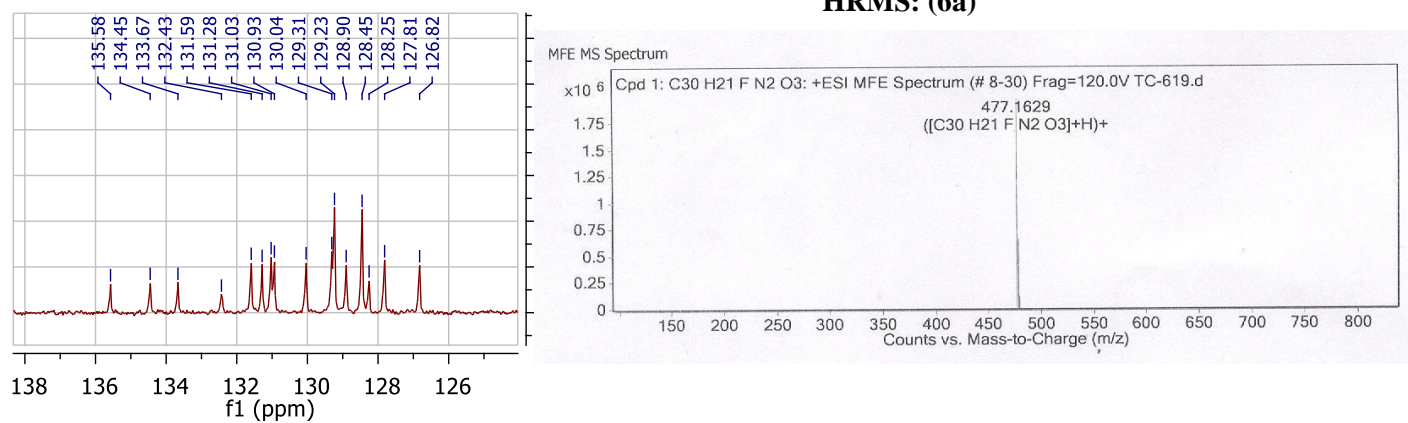
472.1872
([C₃₀ H₂₇ N O₃]+Na)⁺

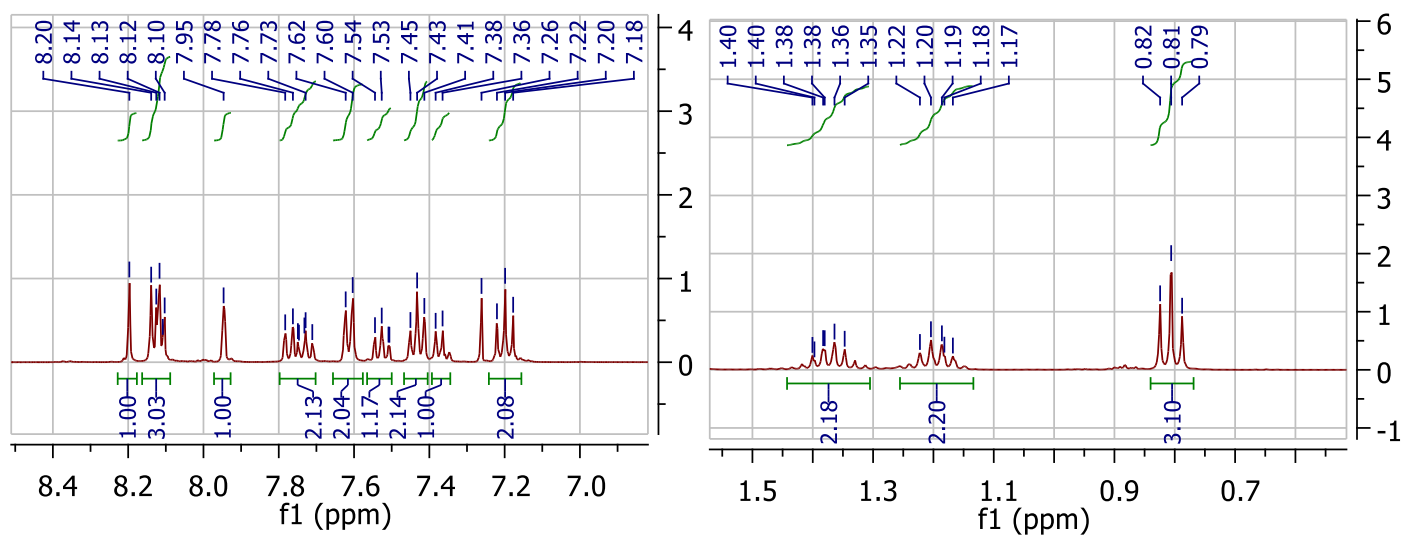
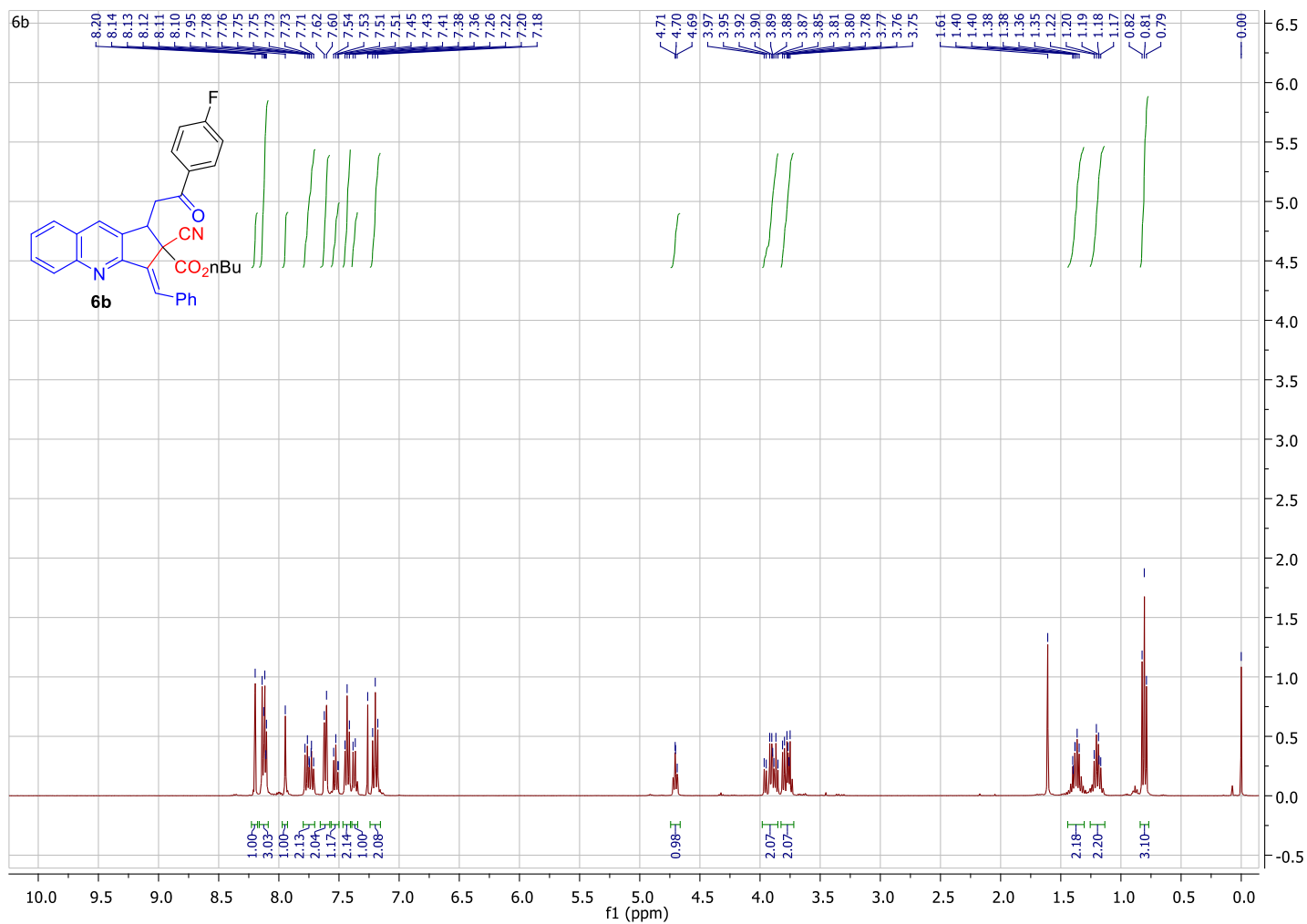
Counts vs. Mass-to-Charge (m/z)

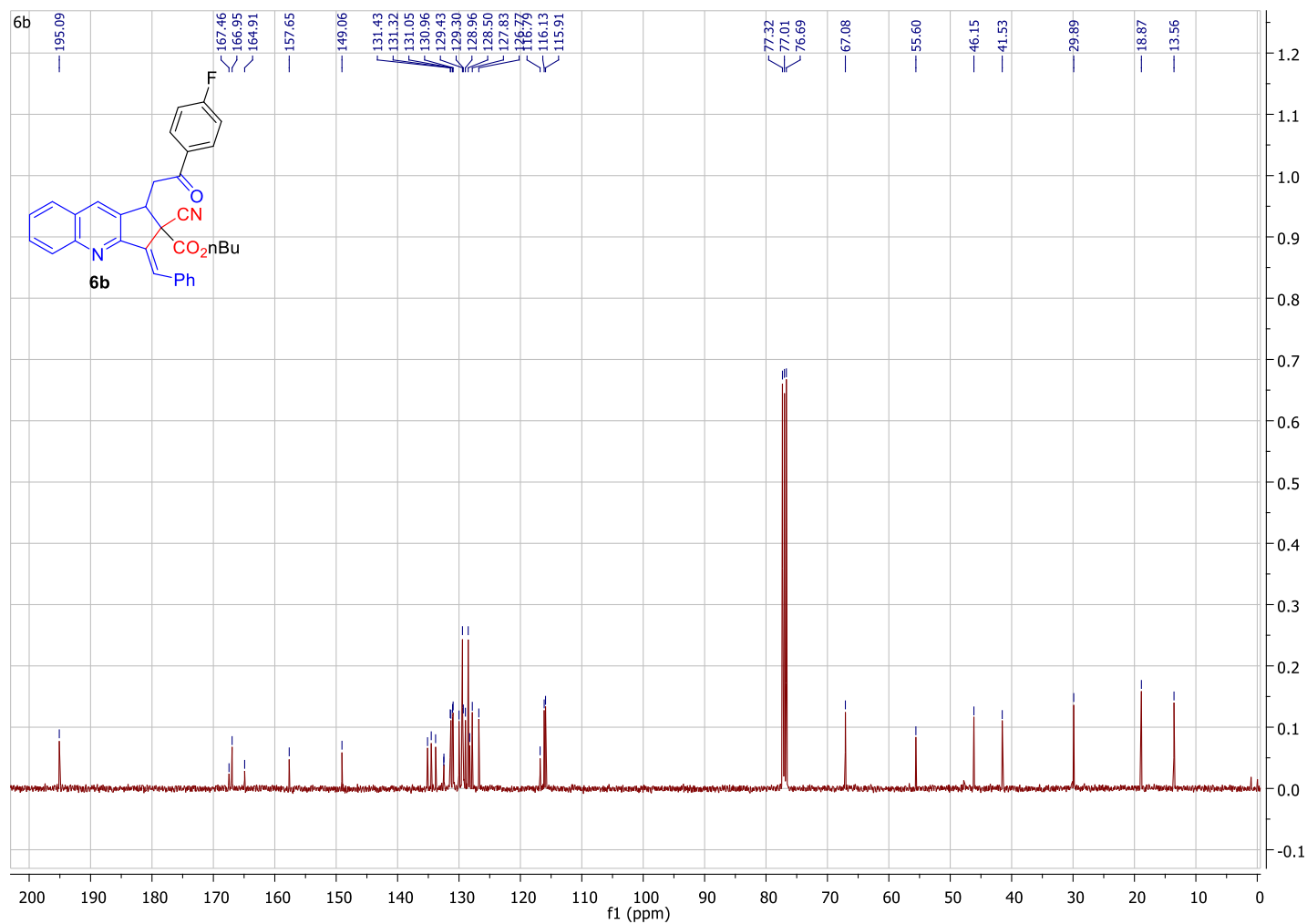




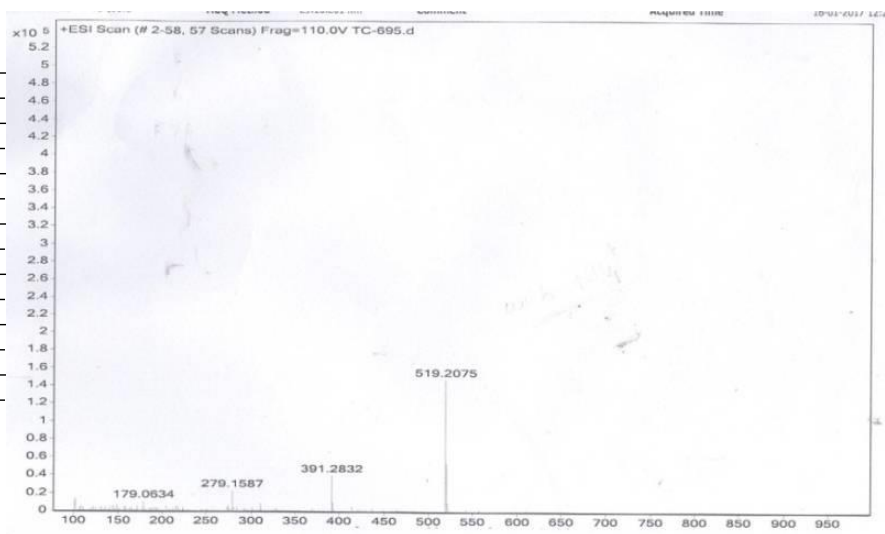
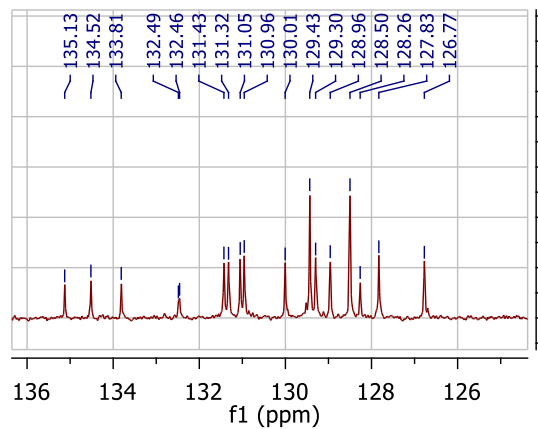
HRMS: (6a)

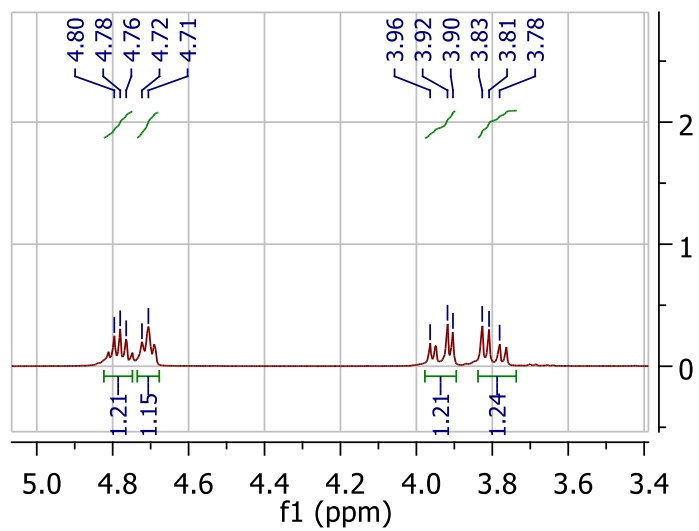
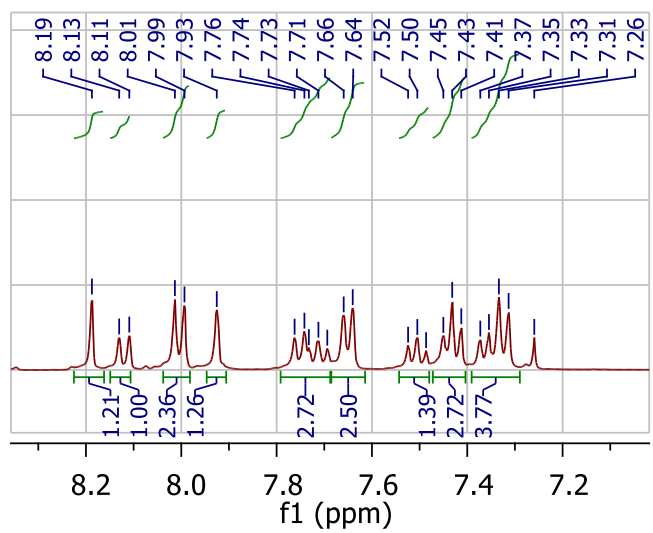
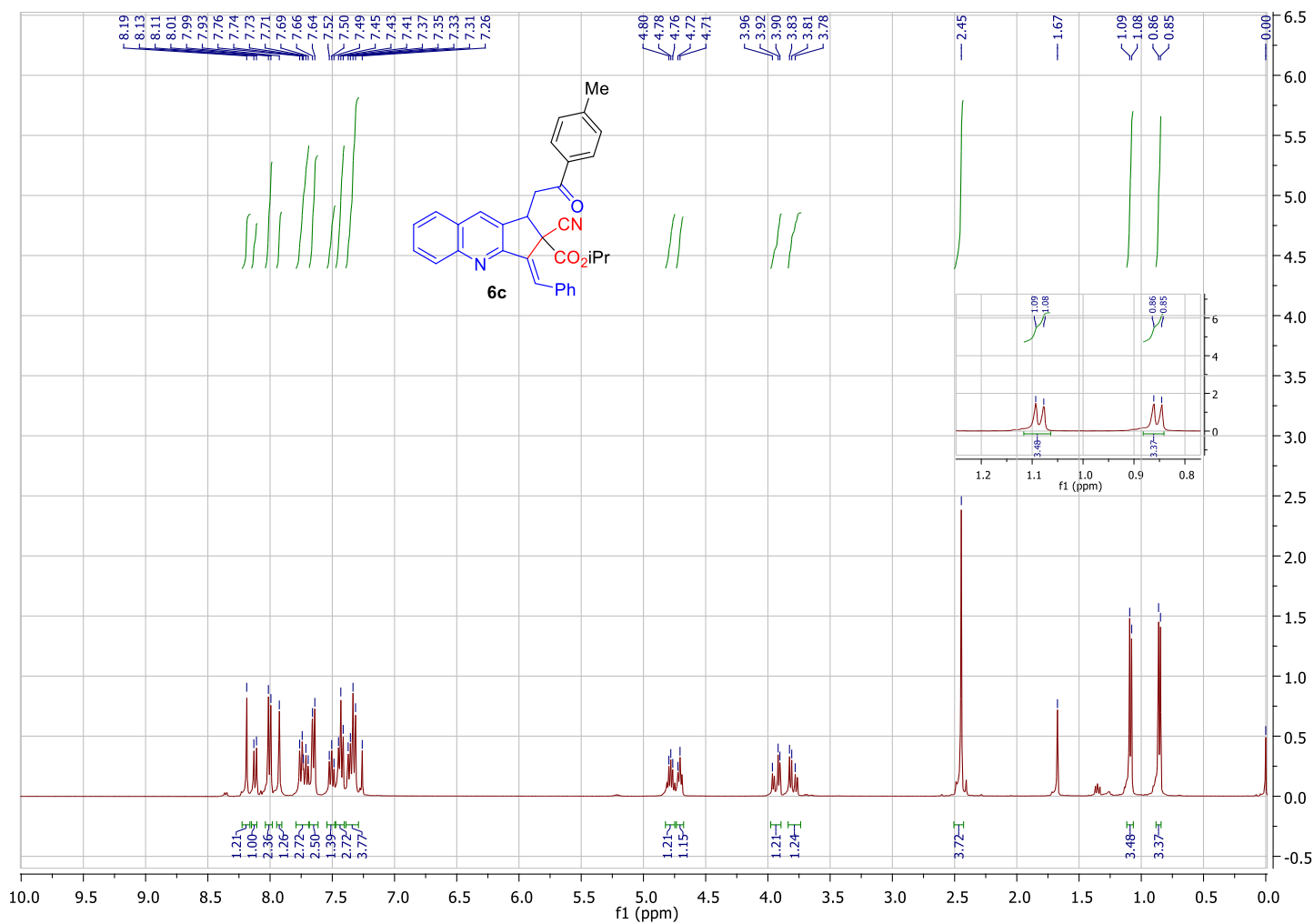


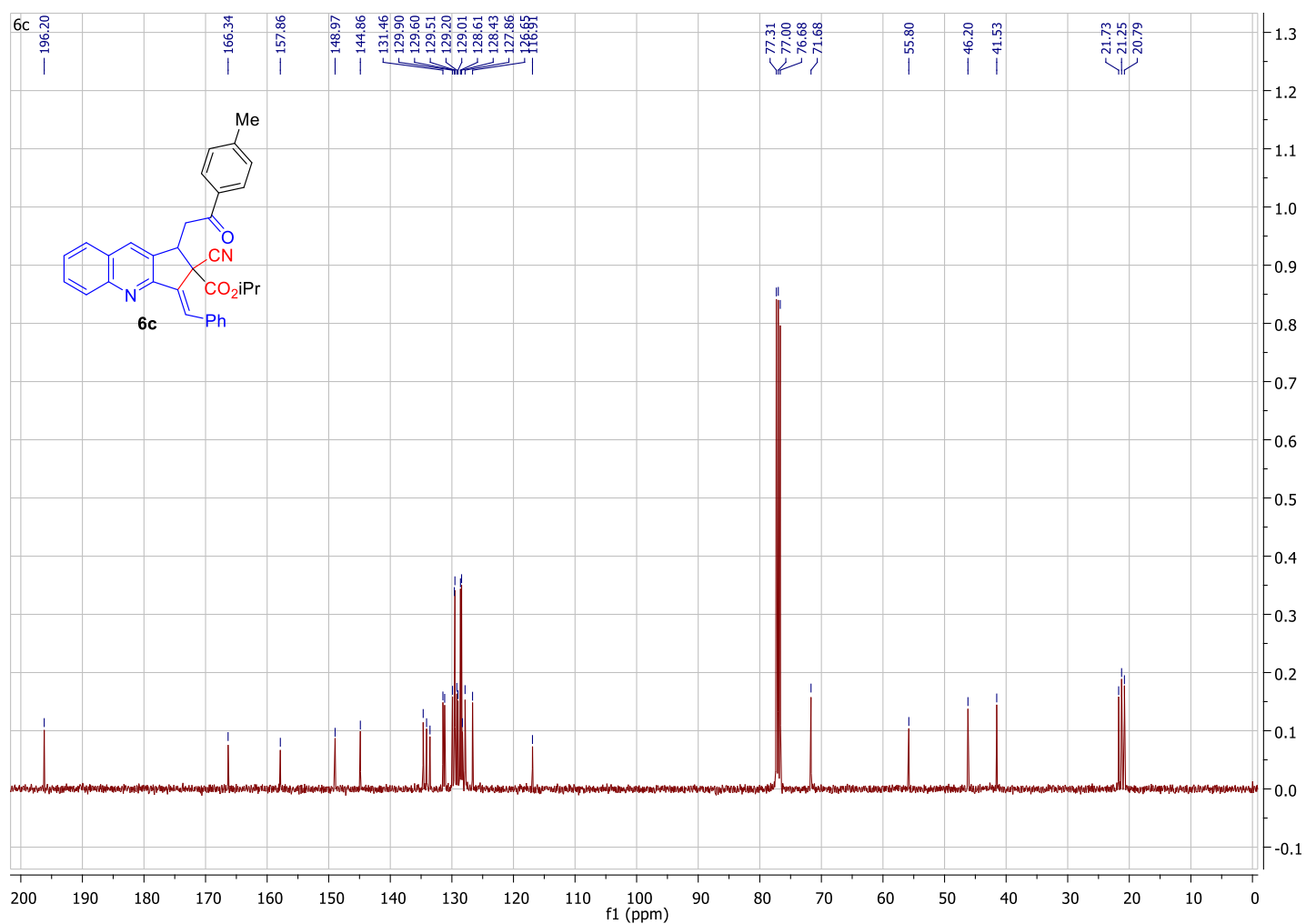




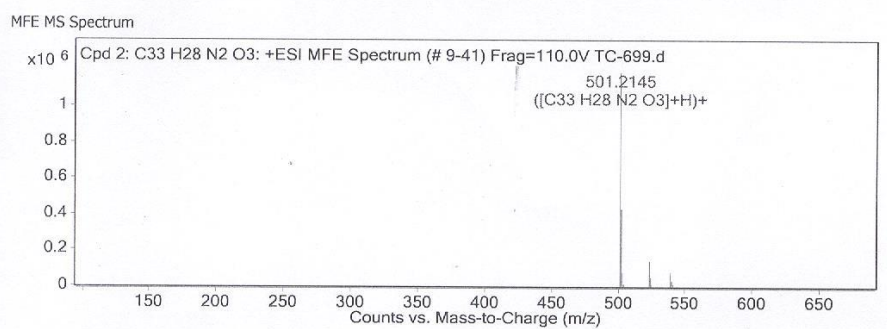
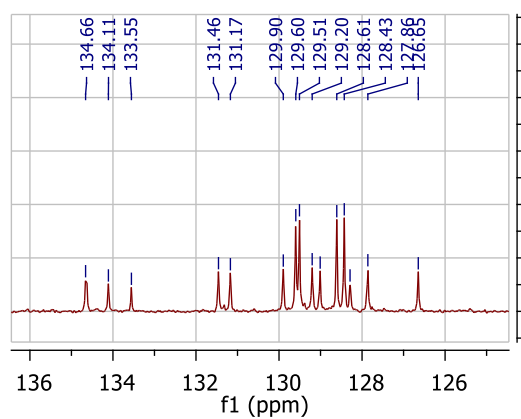
HRMS: (6b)

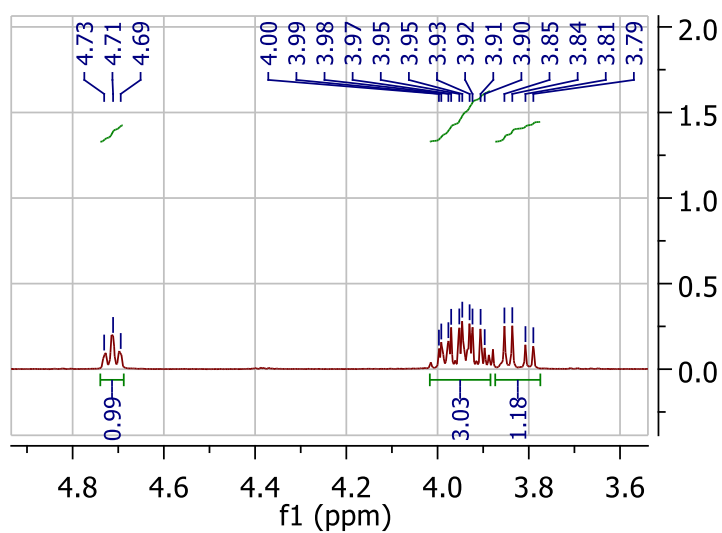
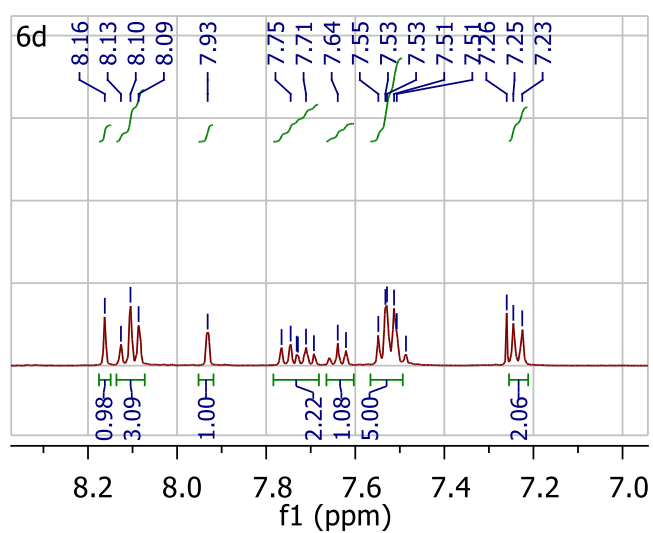
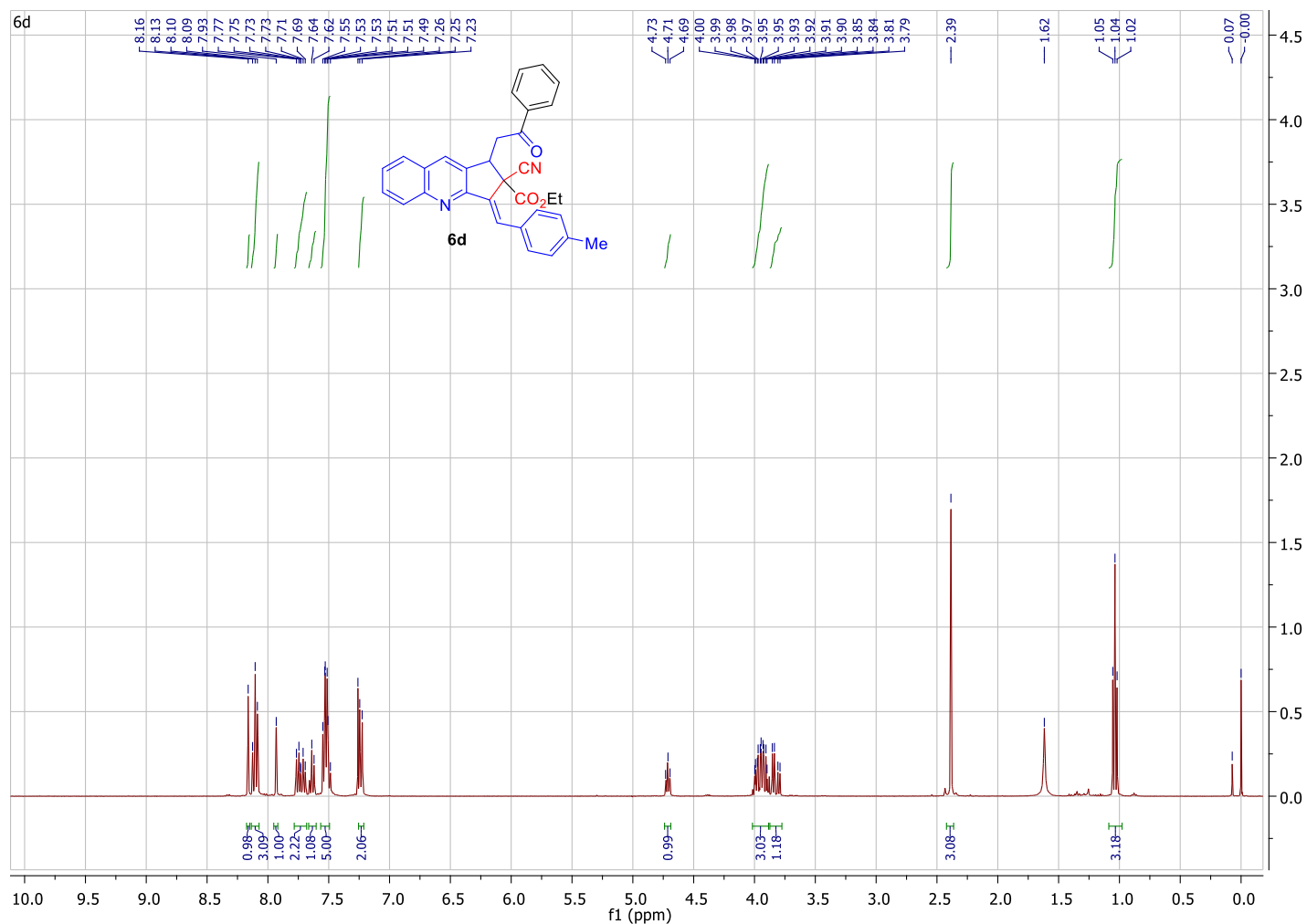


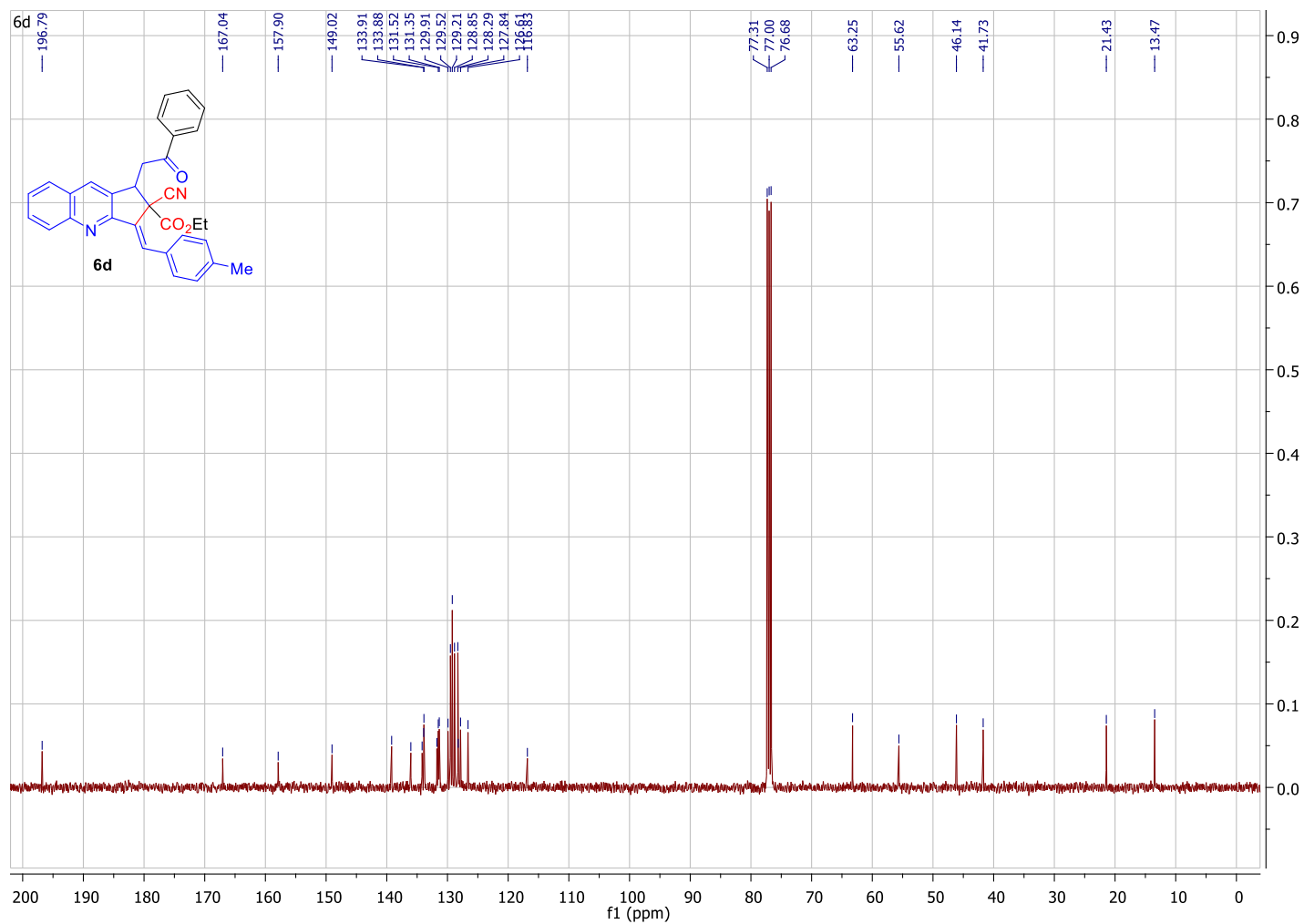




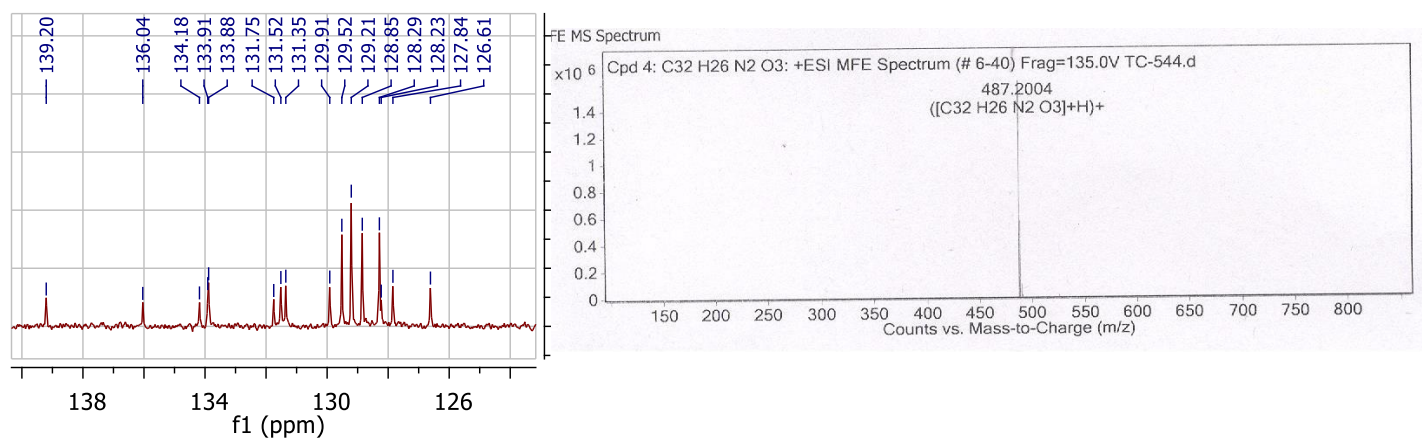
HRMS: (6c)

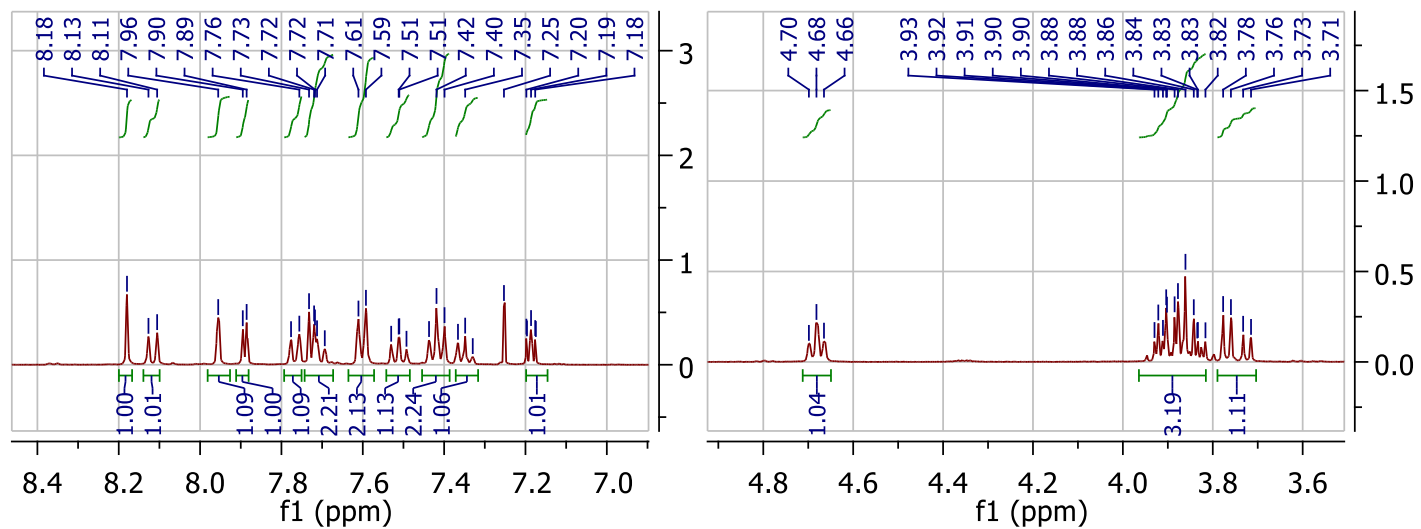
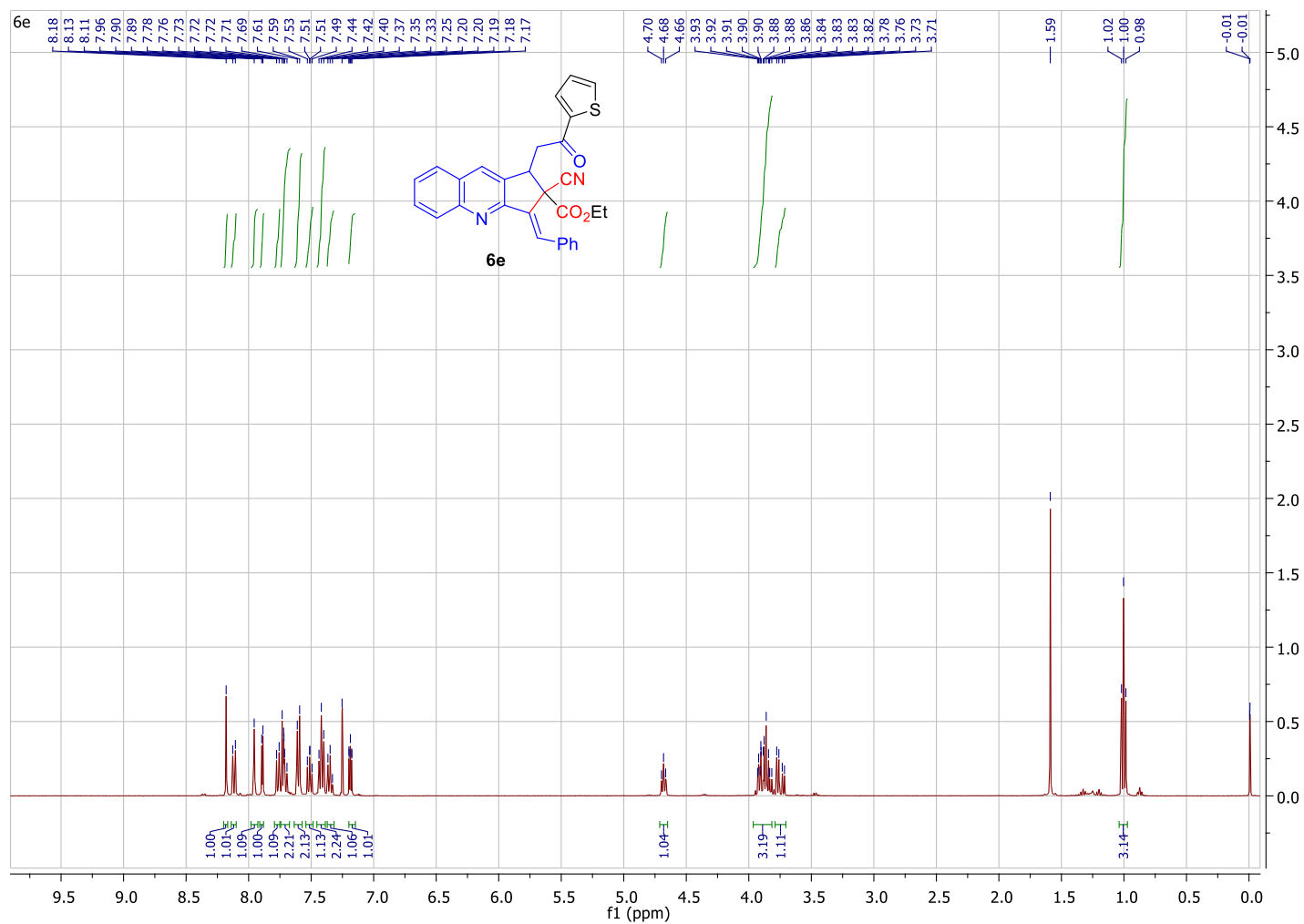


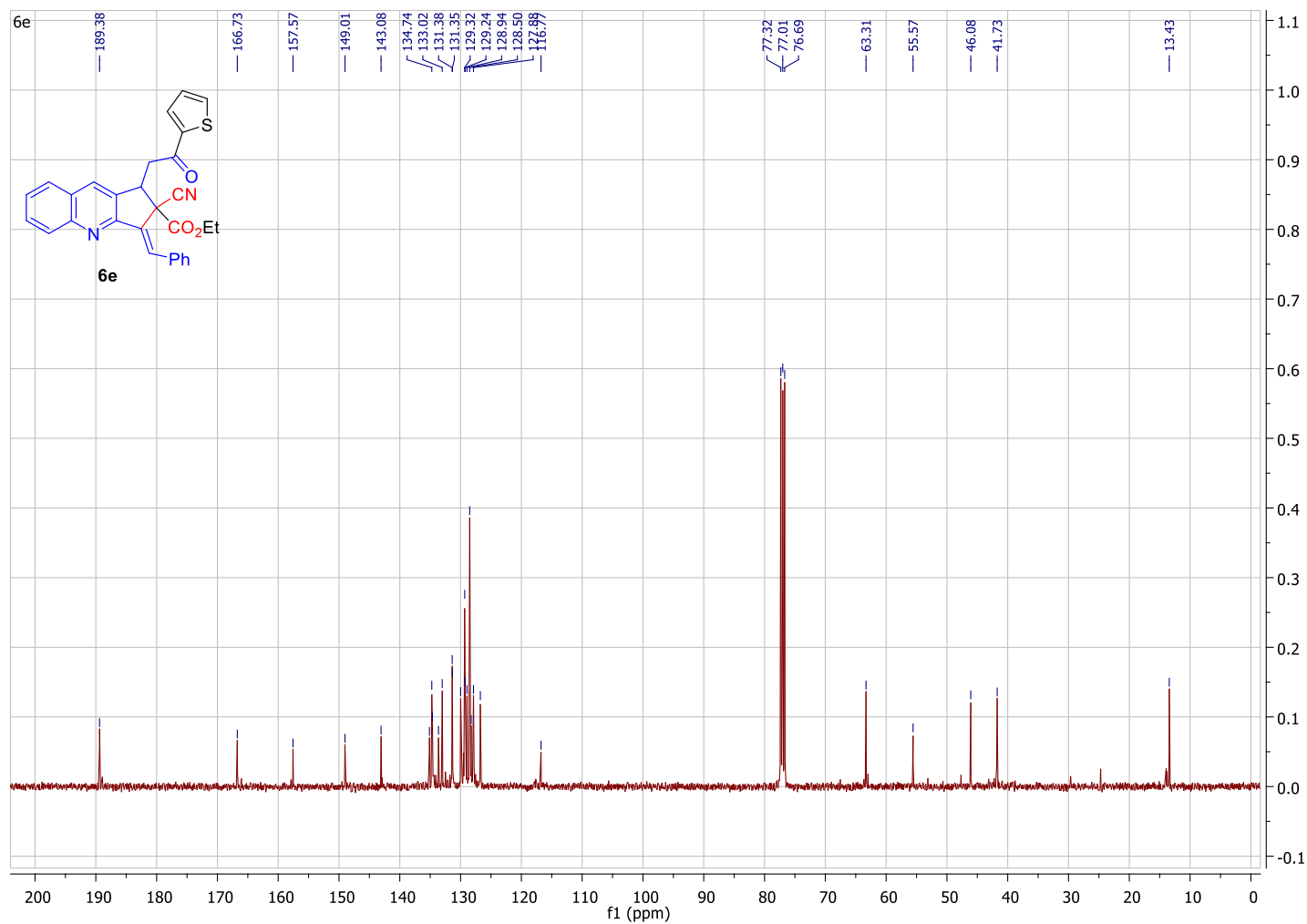




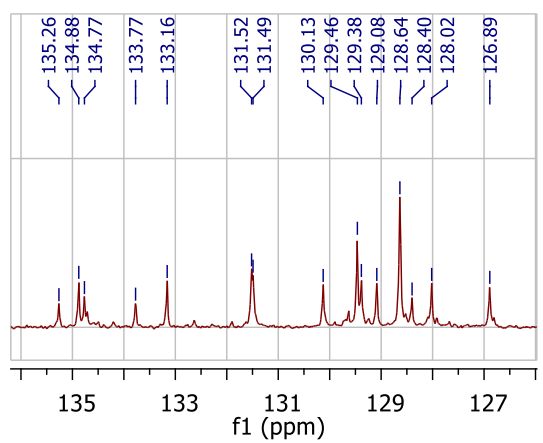
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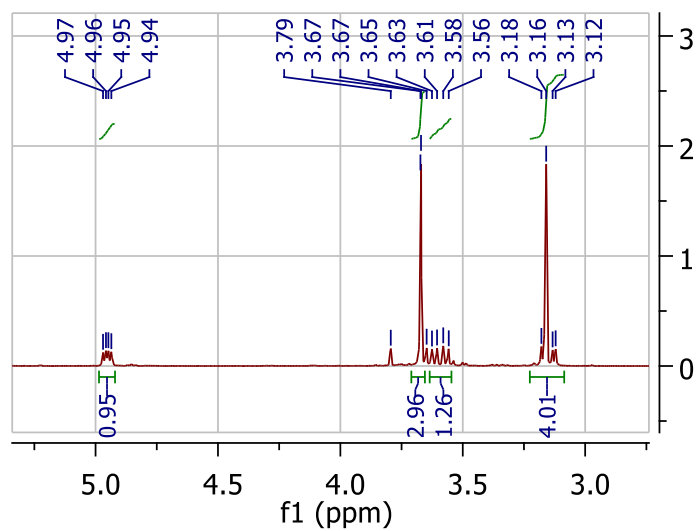
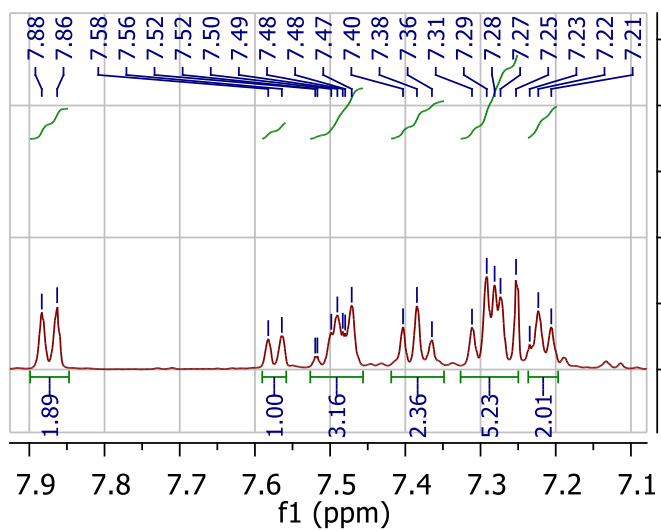
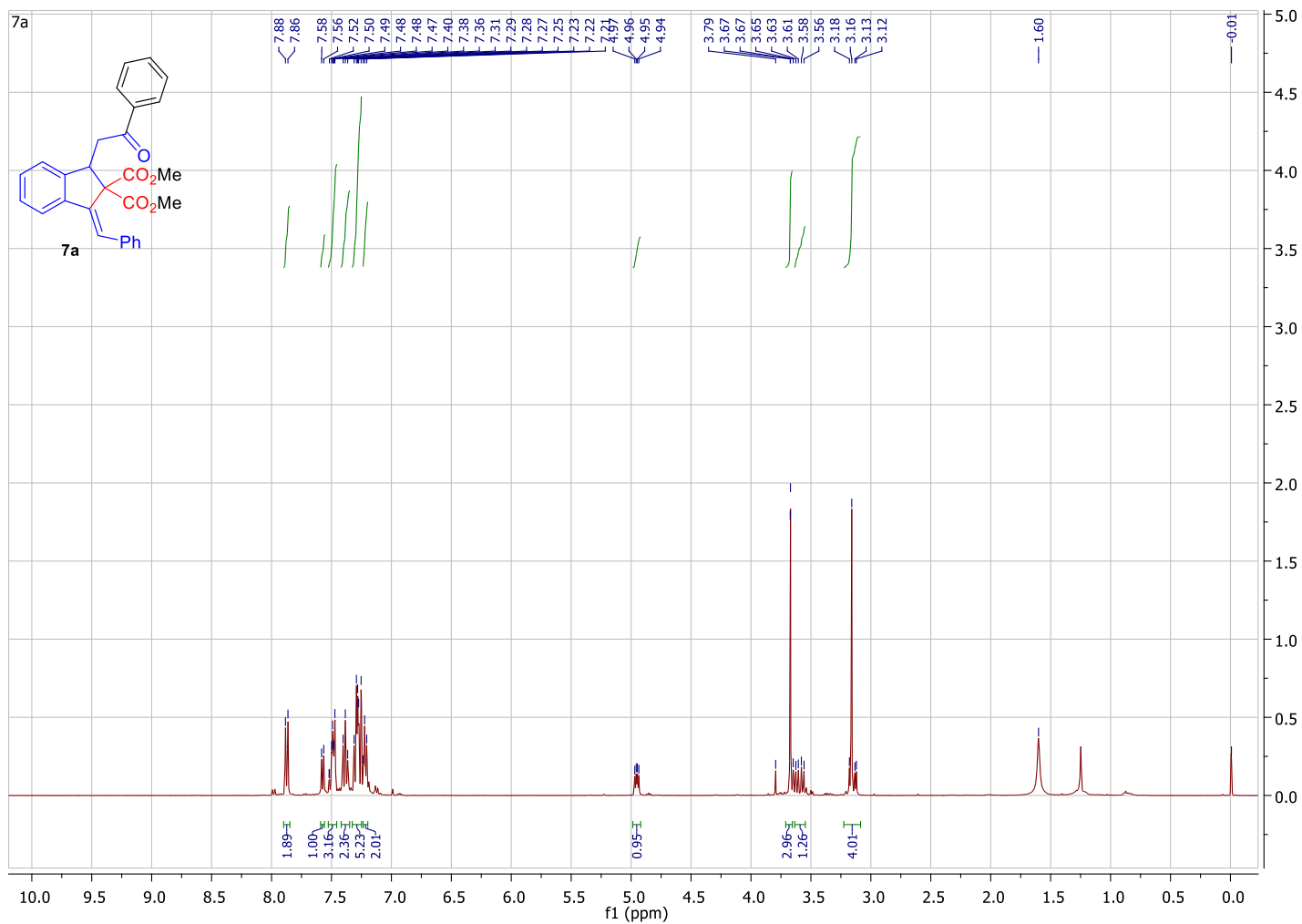


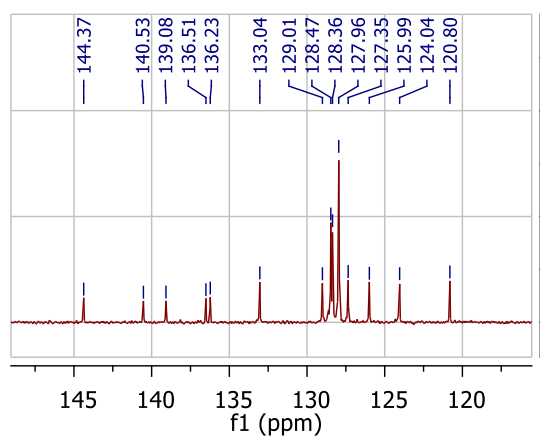
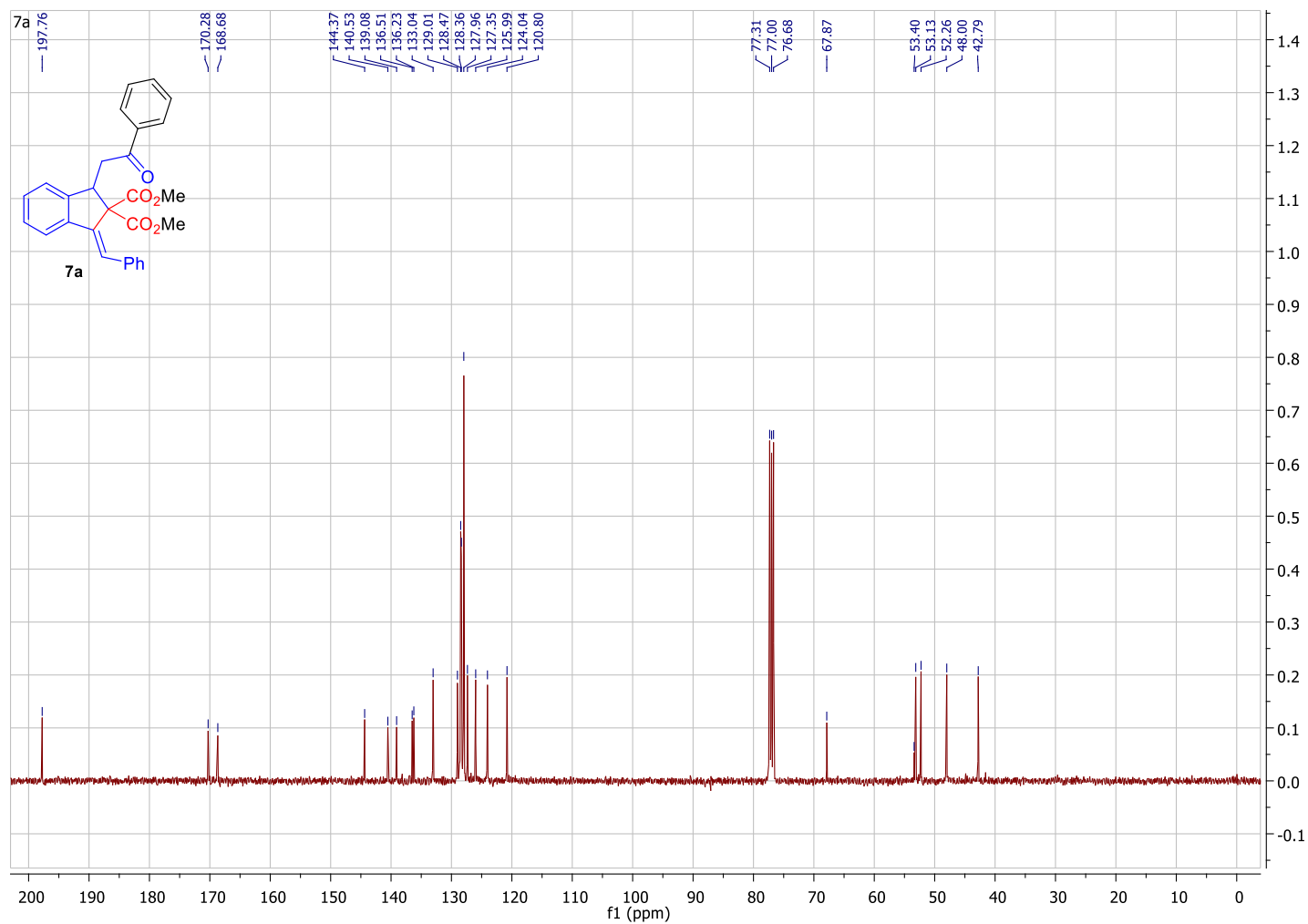




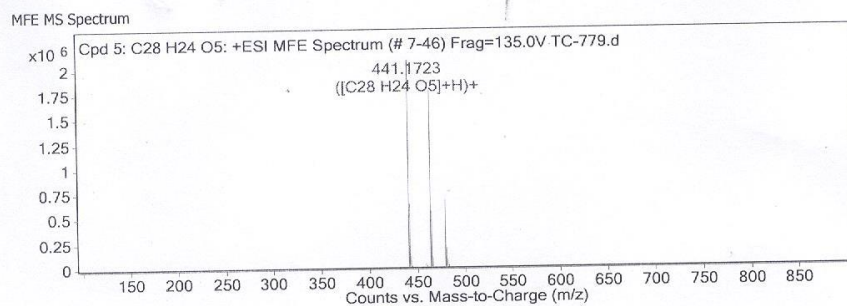
HRMS: (6e)

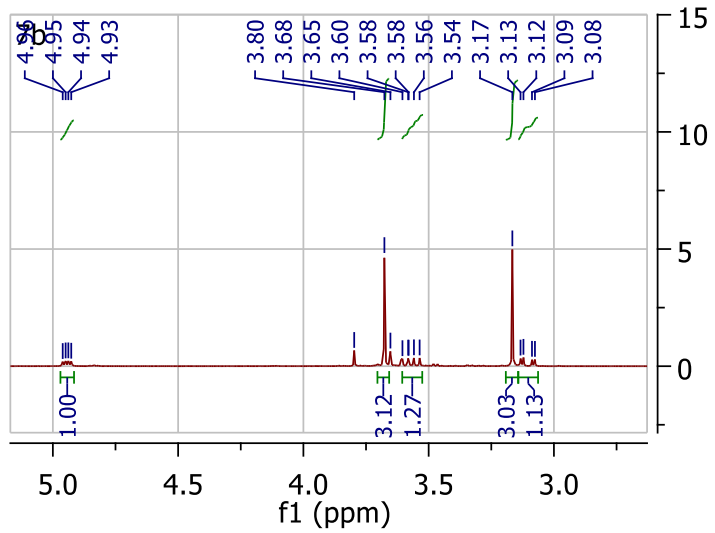
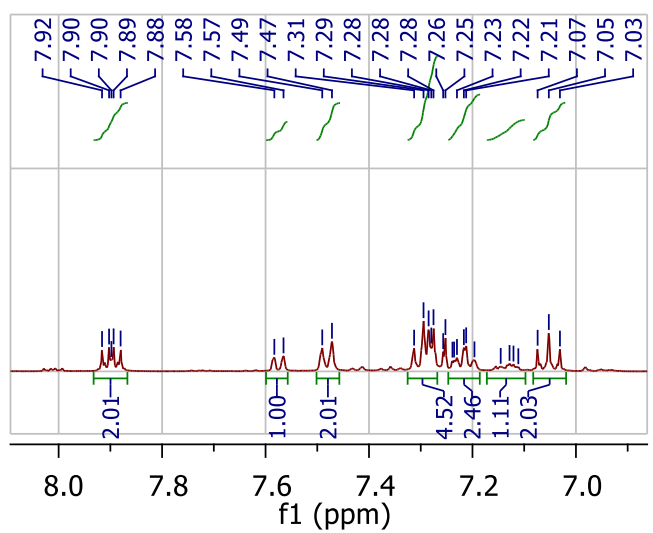
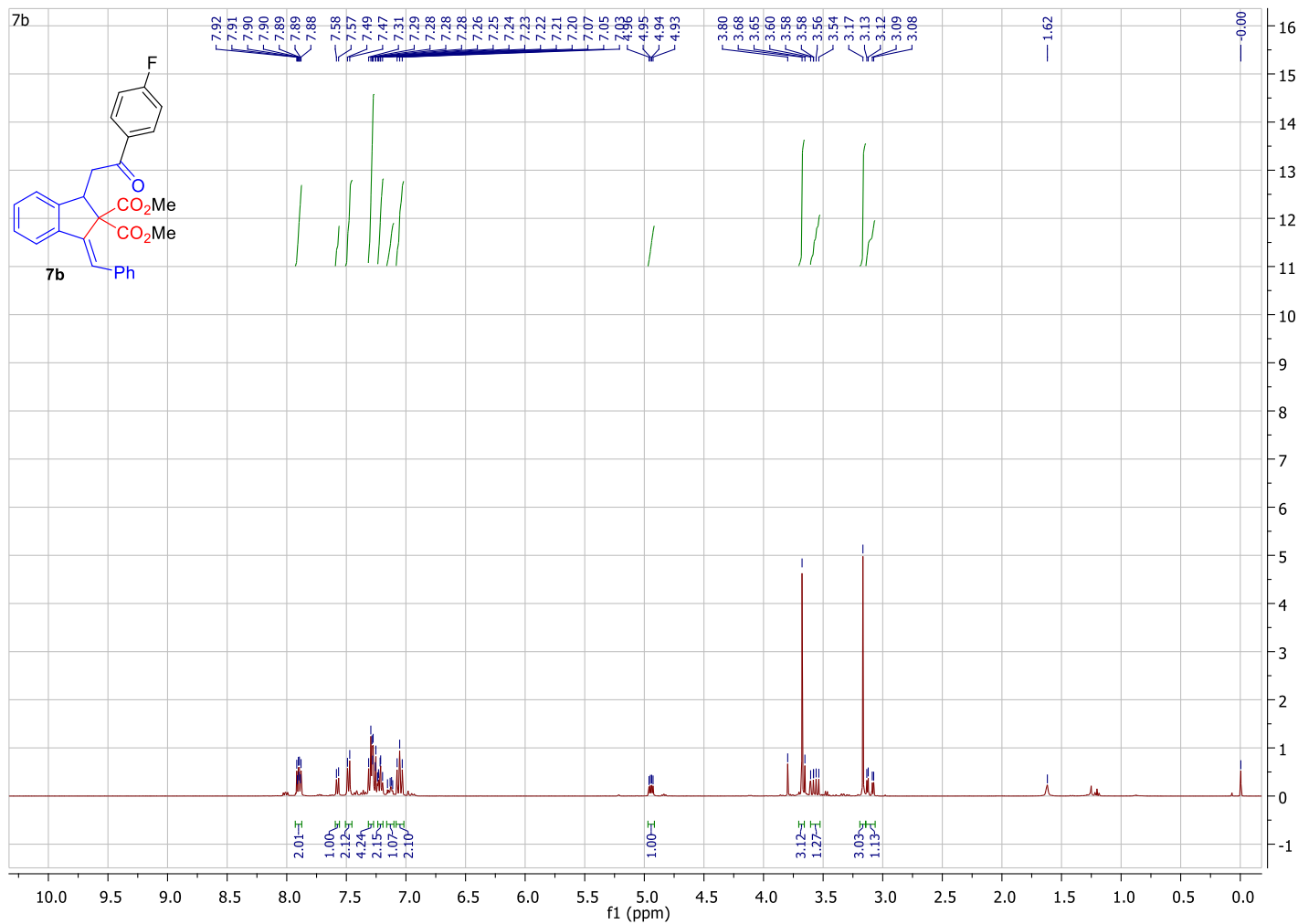


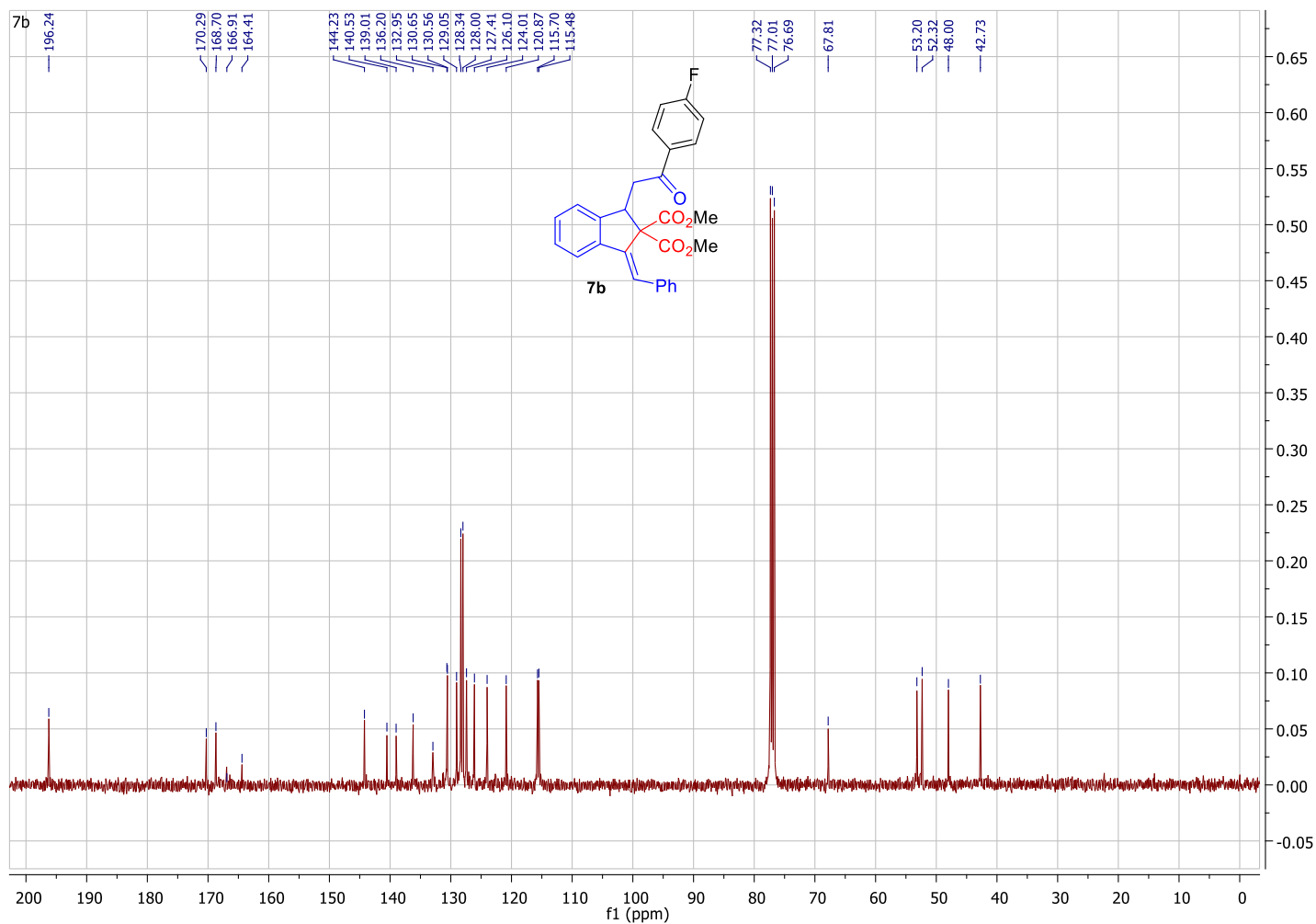




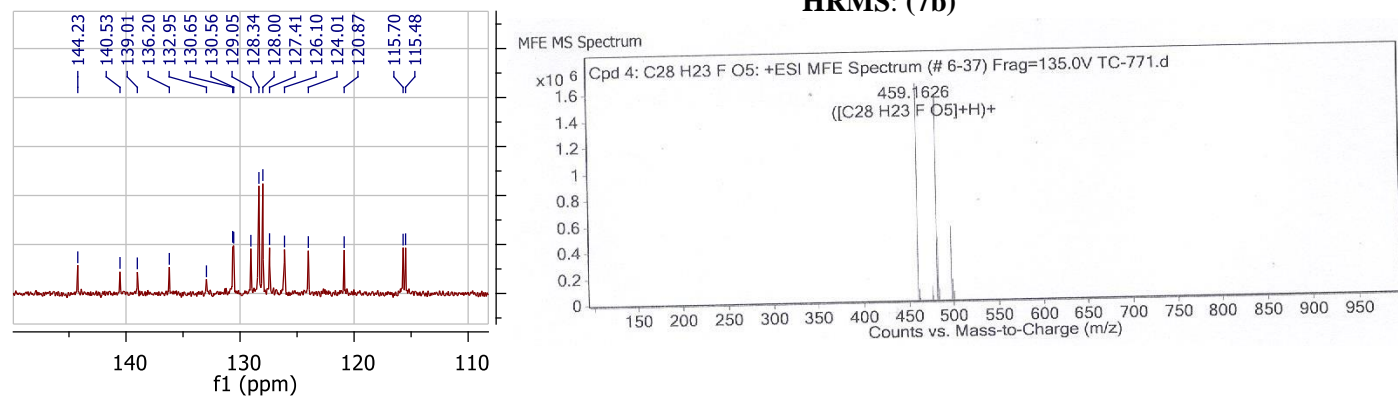
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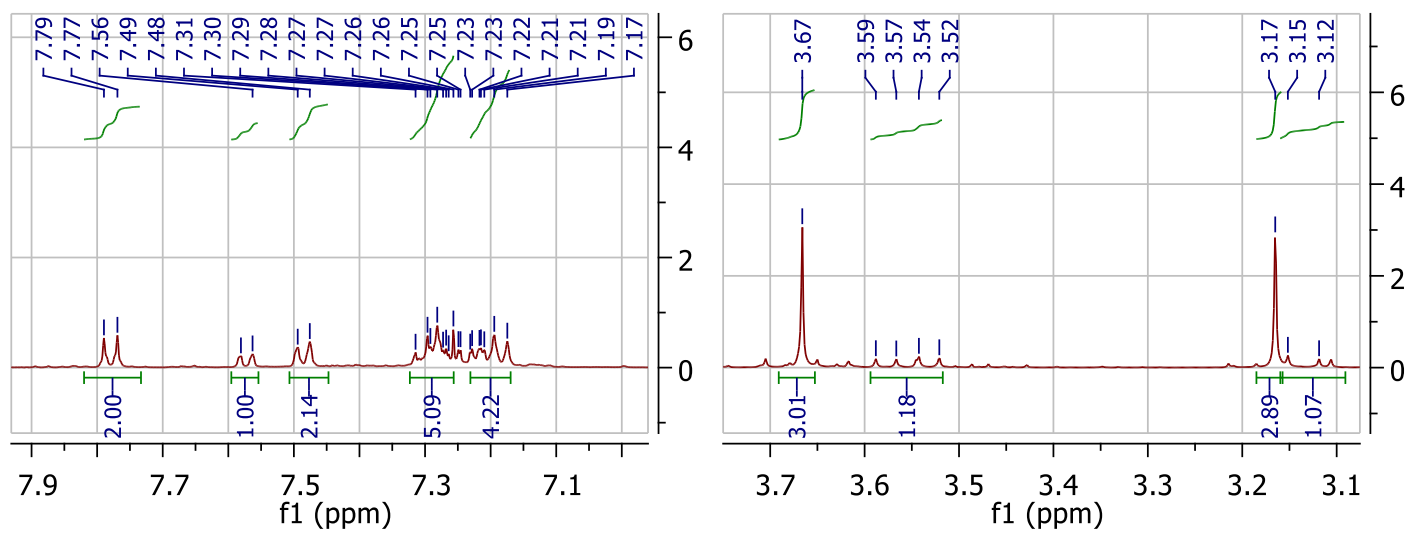
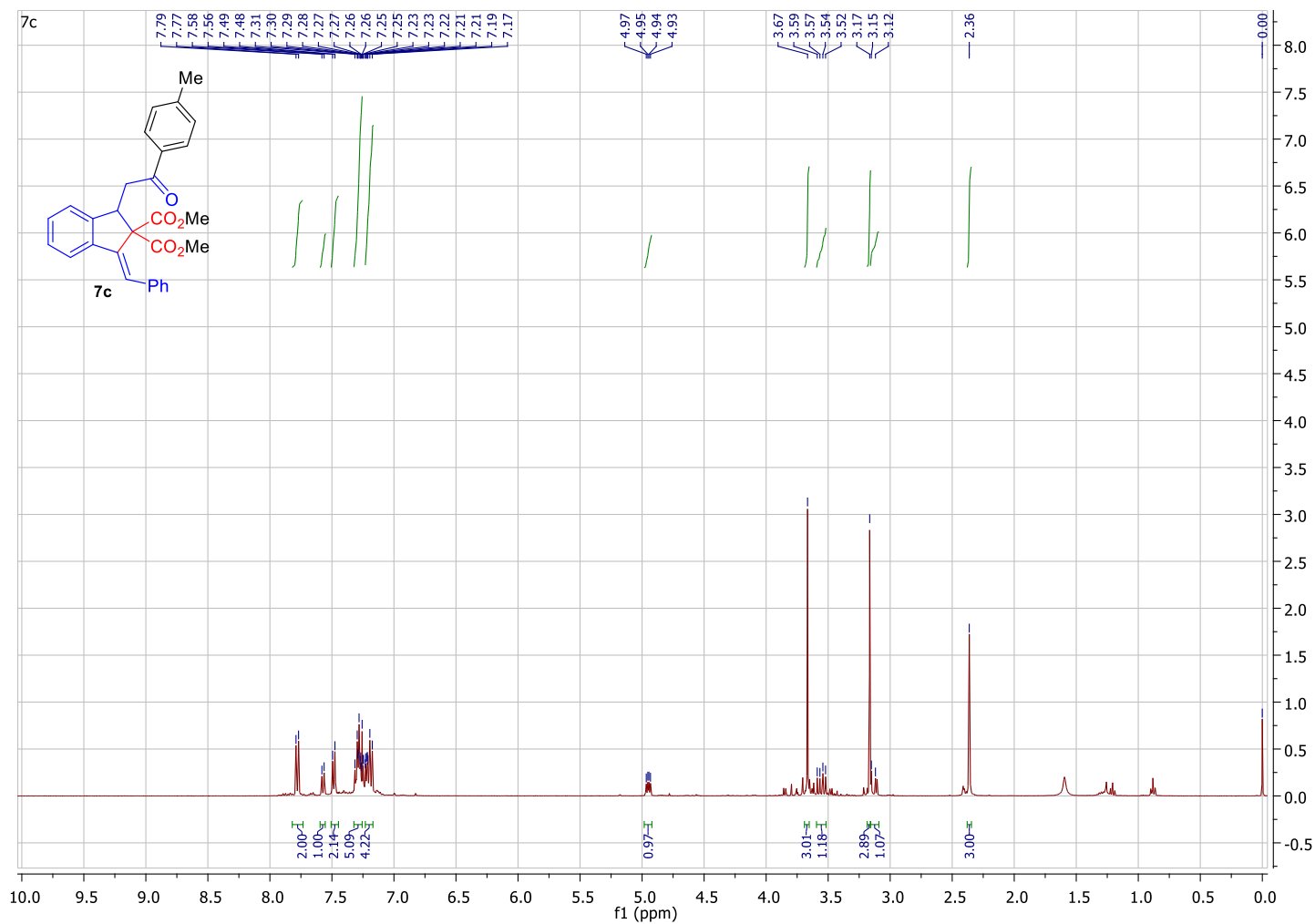


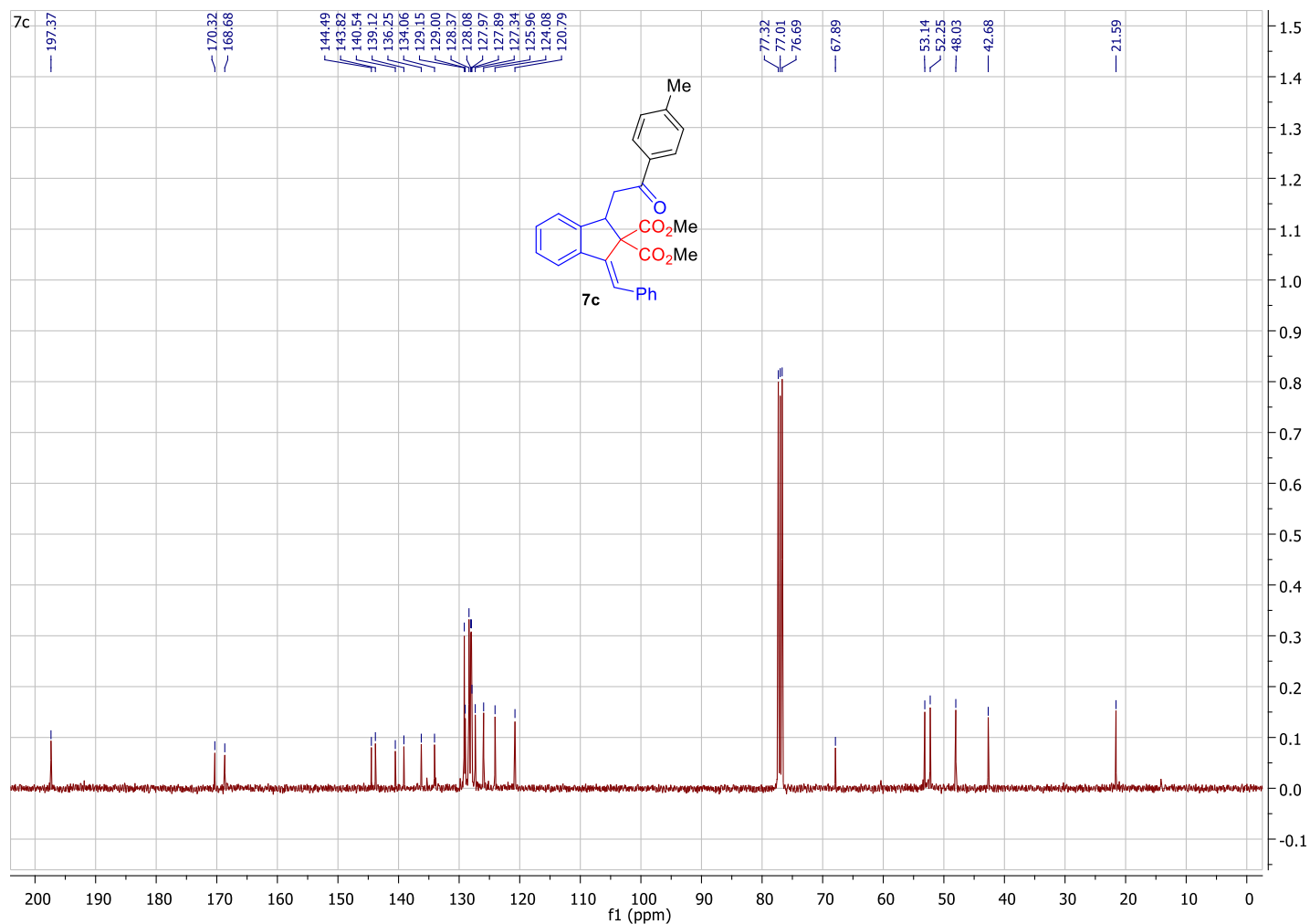




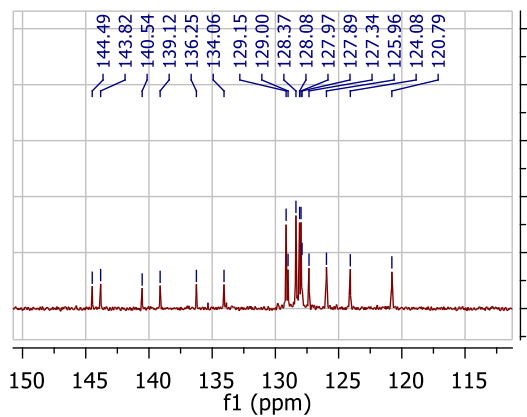
HRMS: (7b)



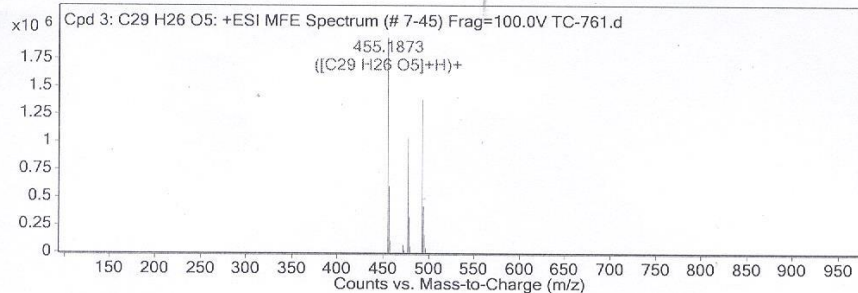


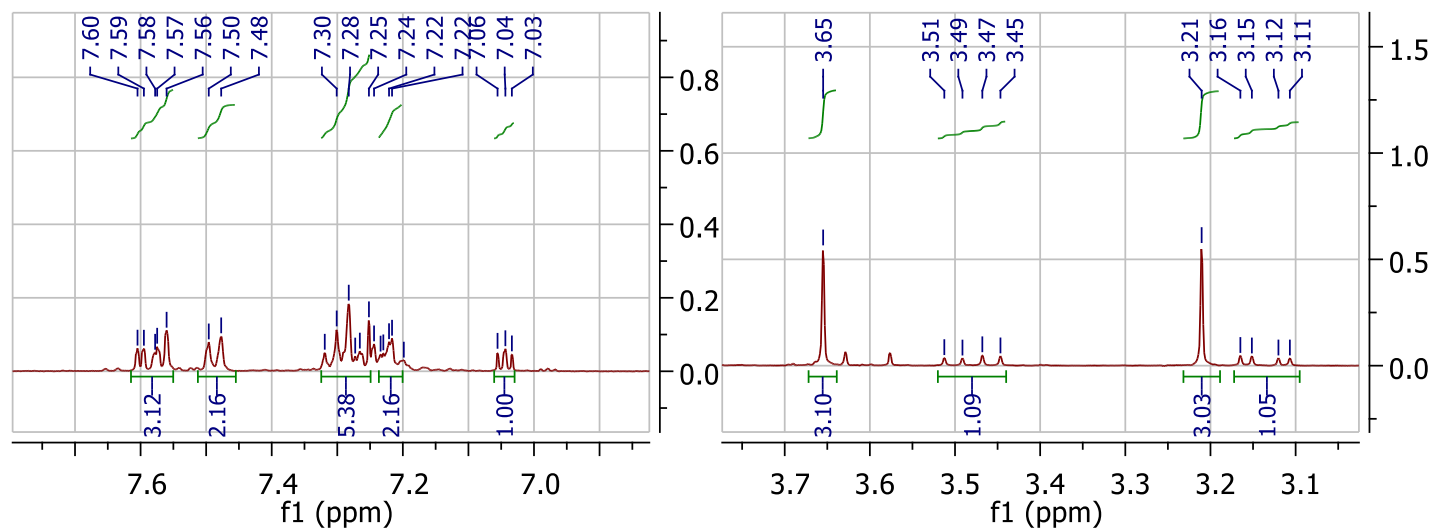
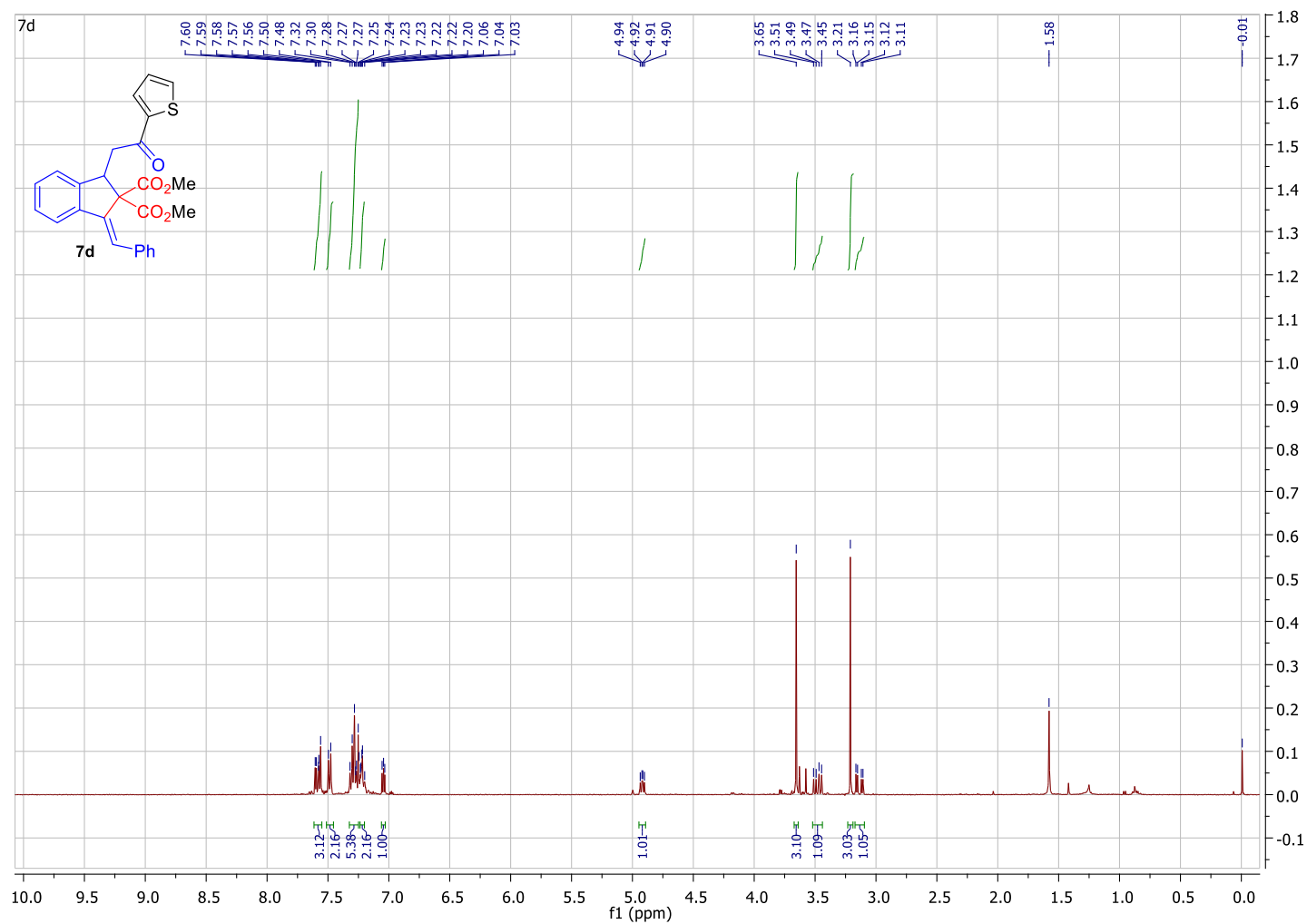


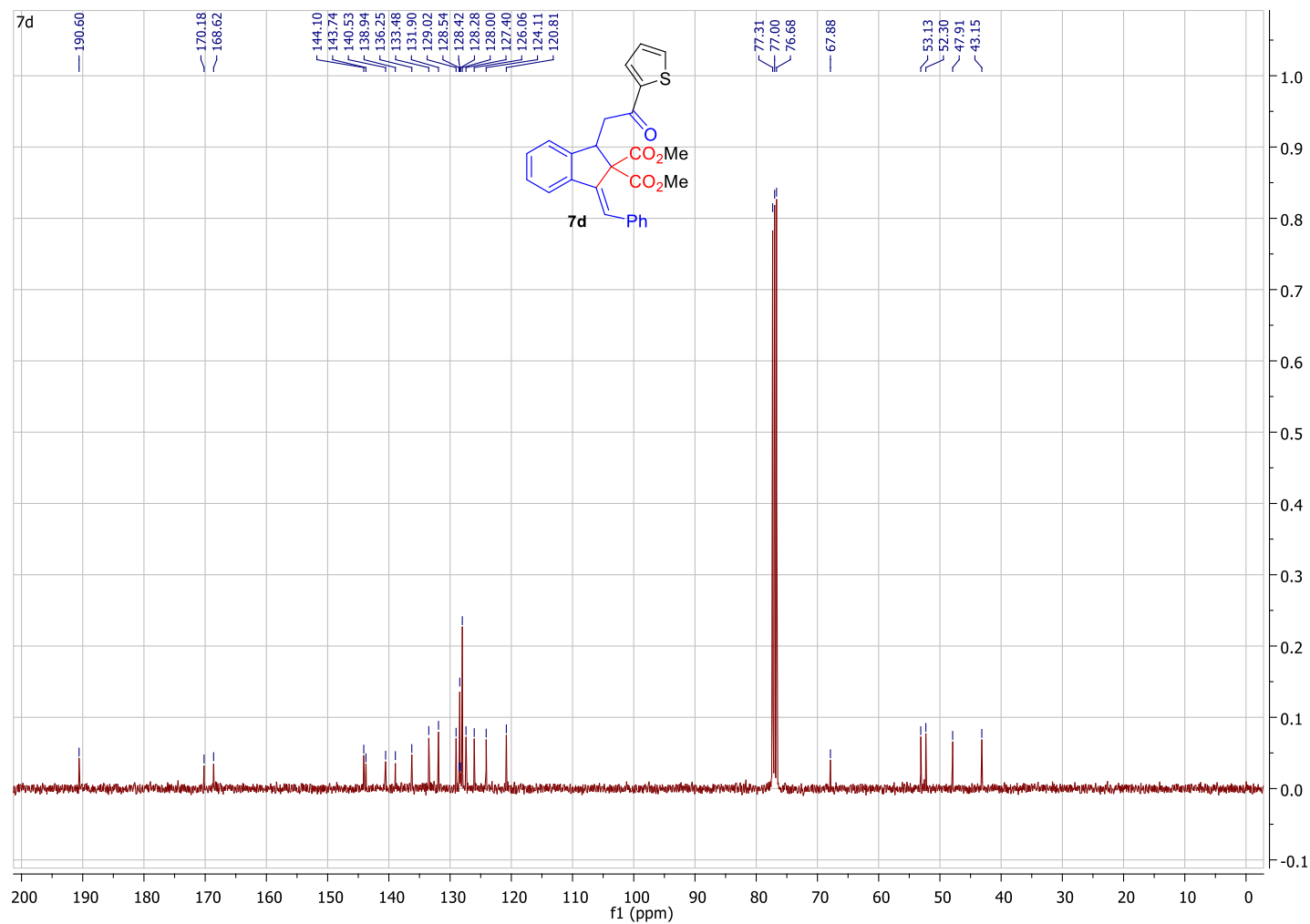
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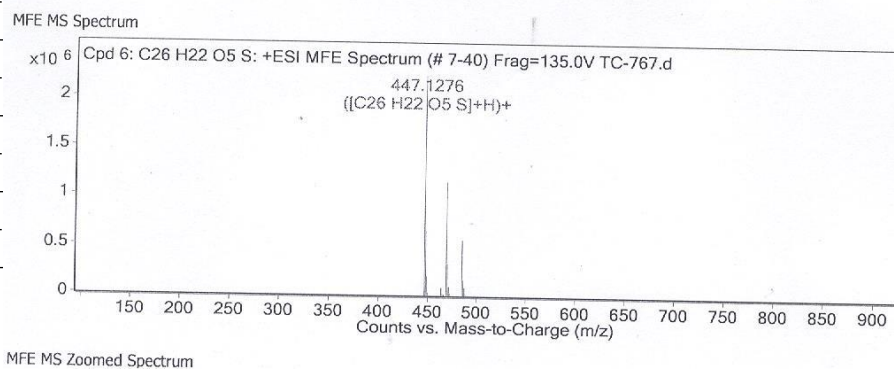
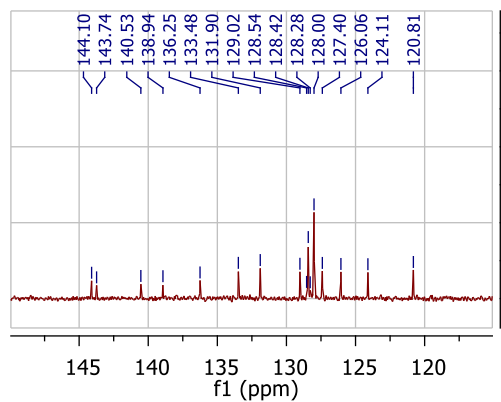
MFE MS Spectrum

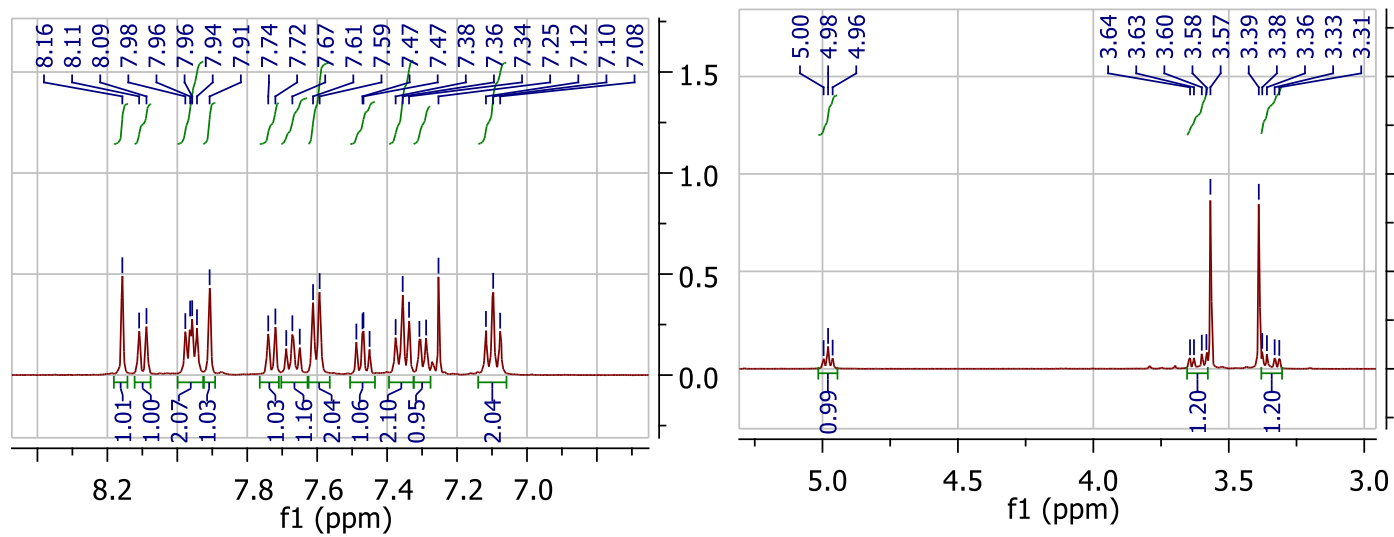
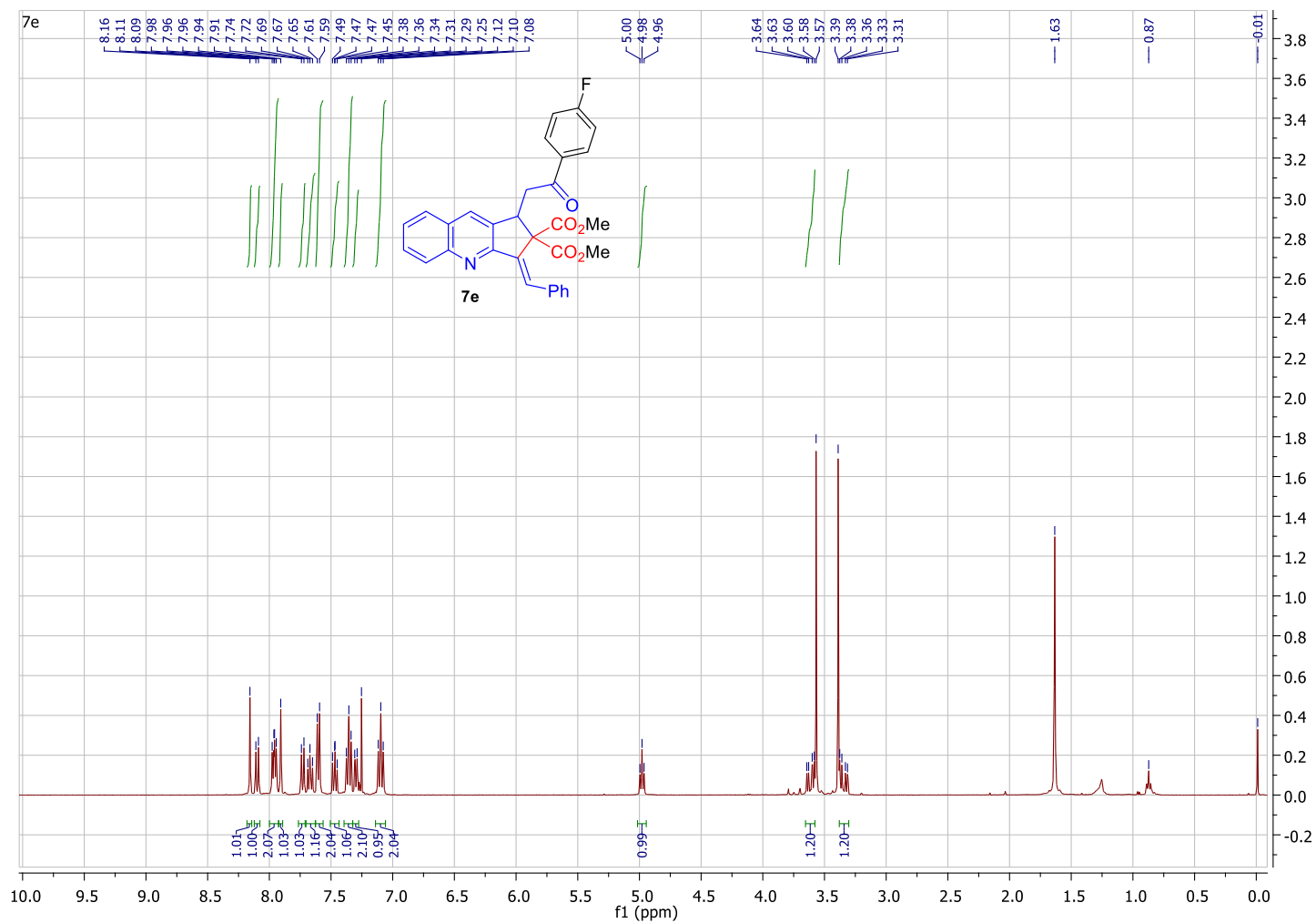


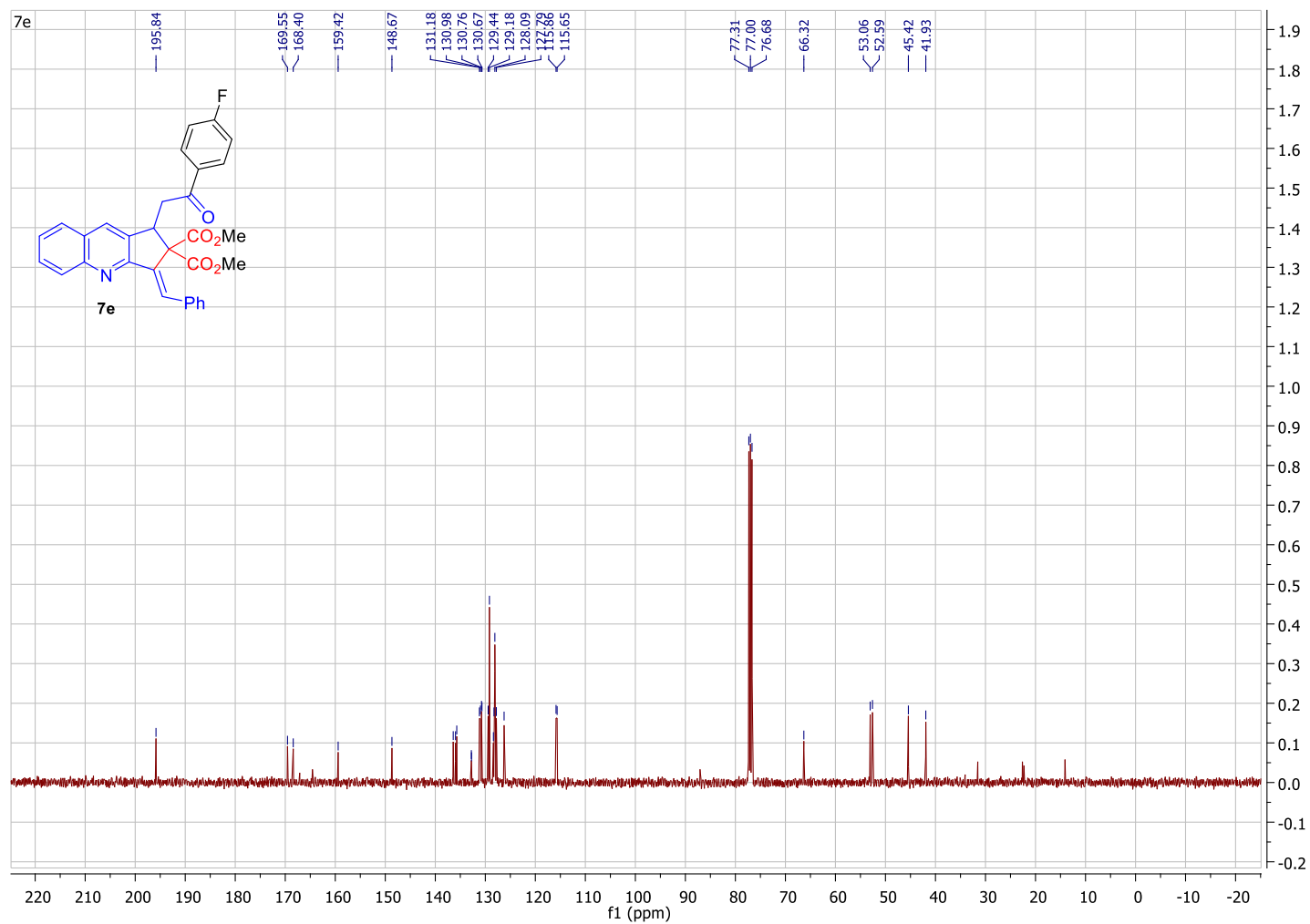




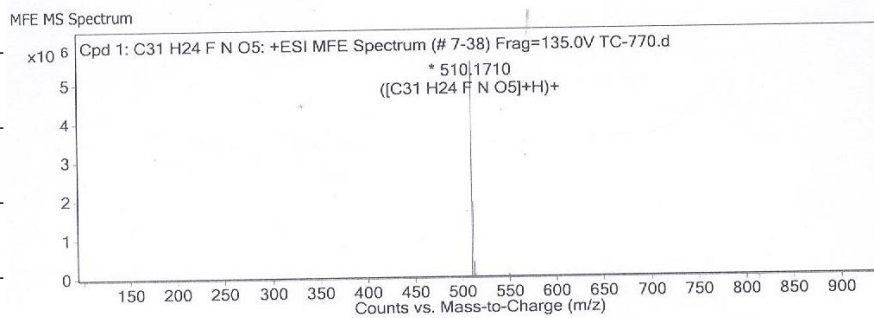
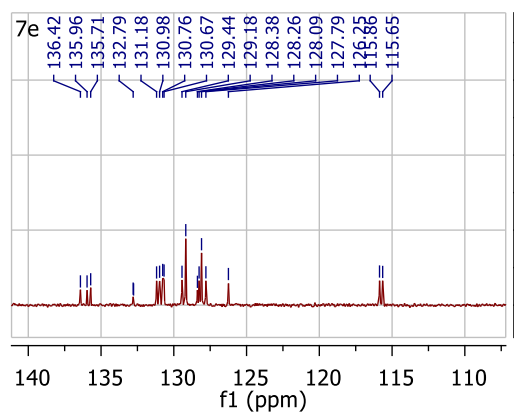
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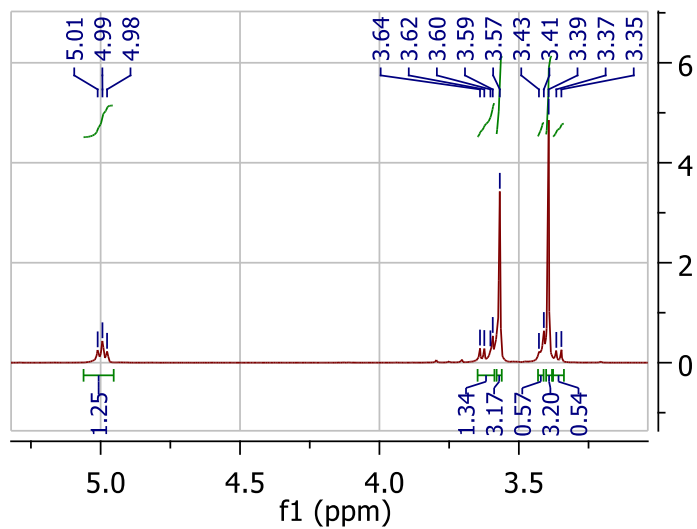
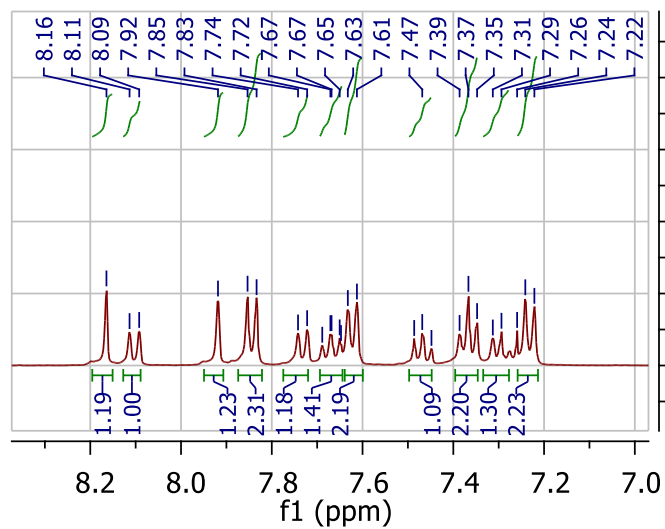
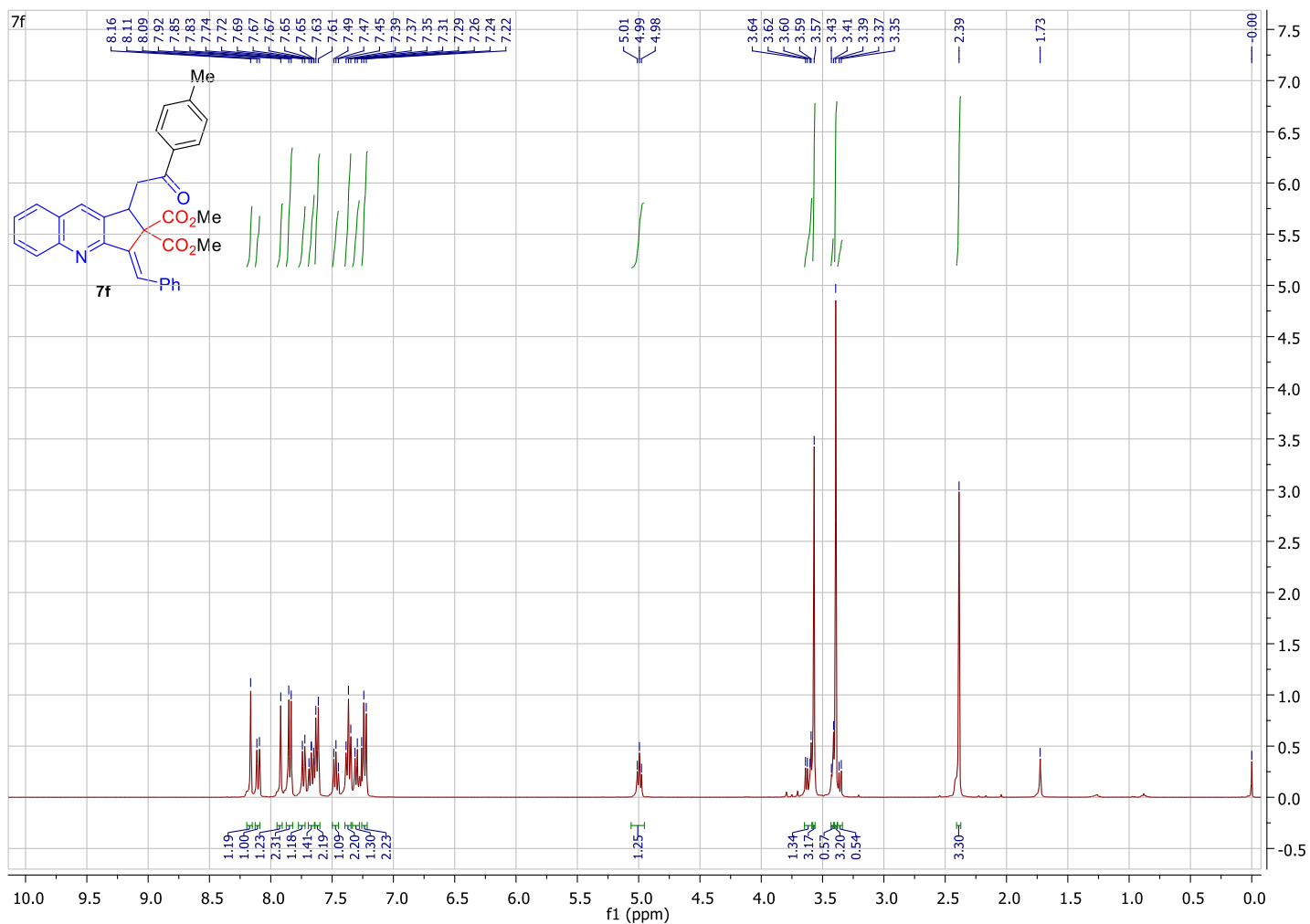


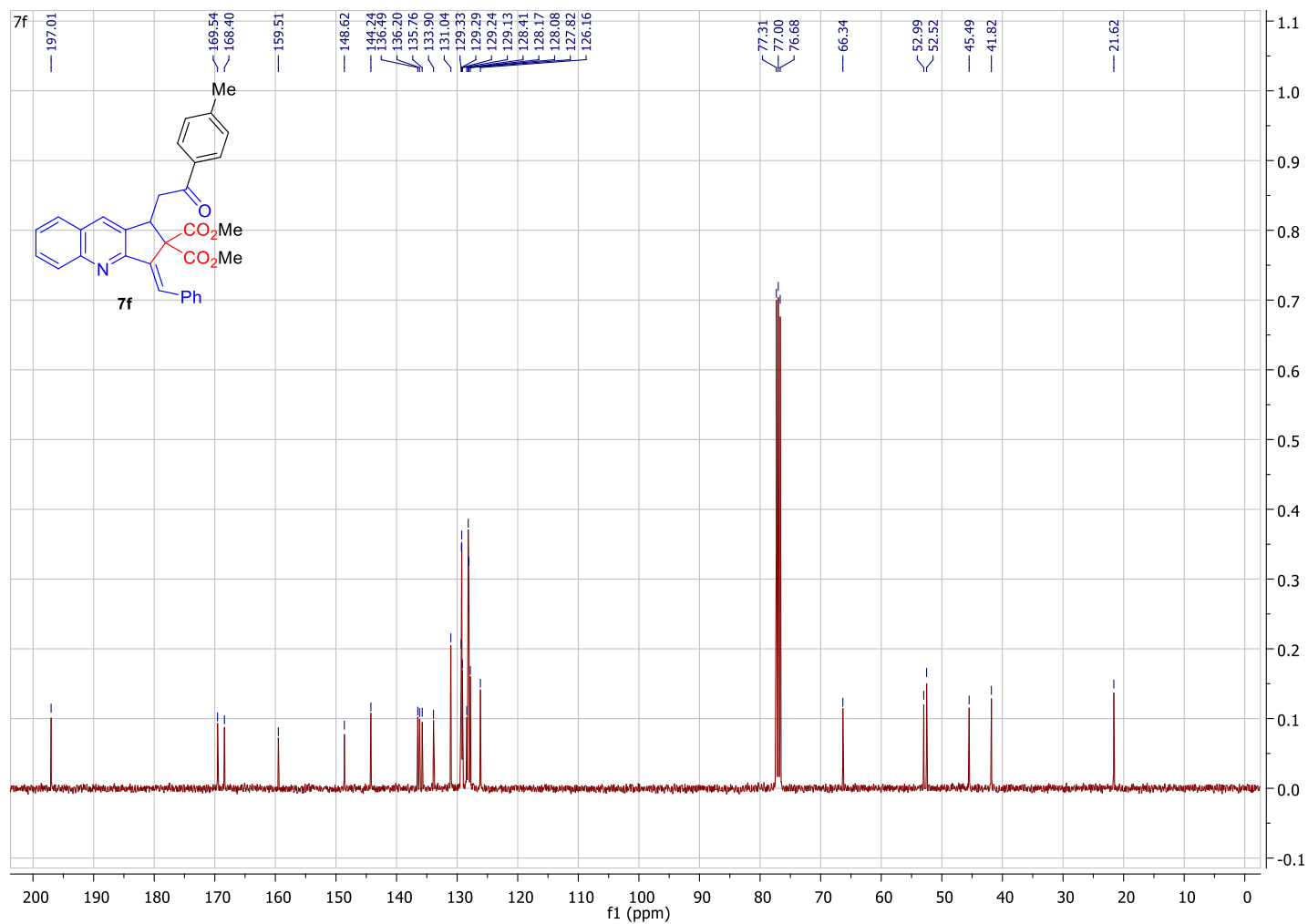




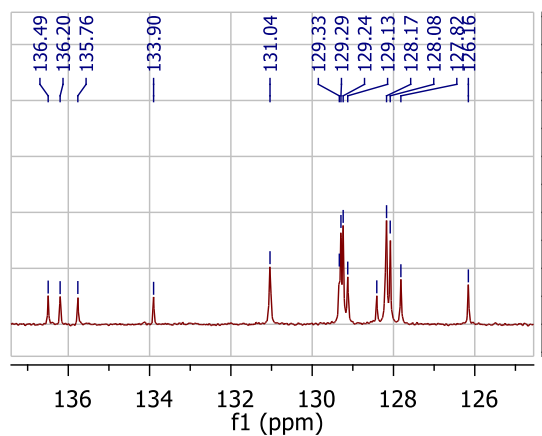
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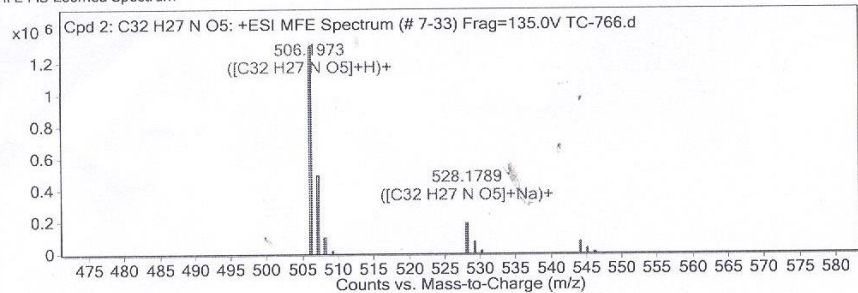


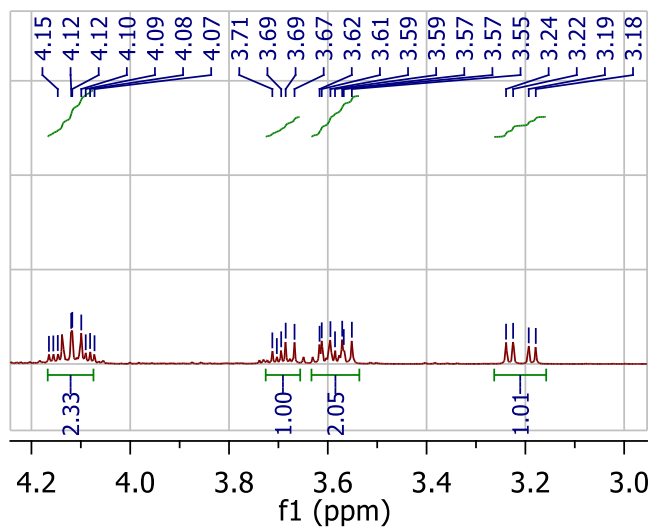
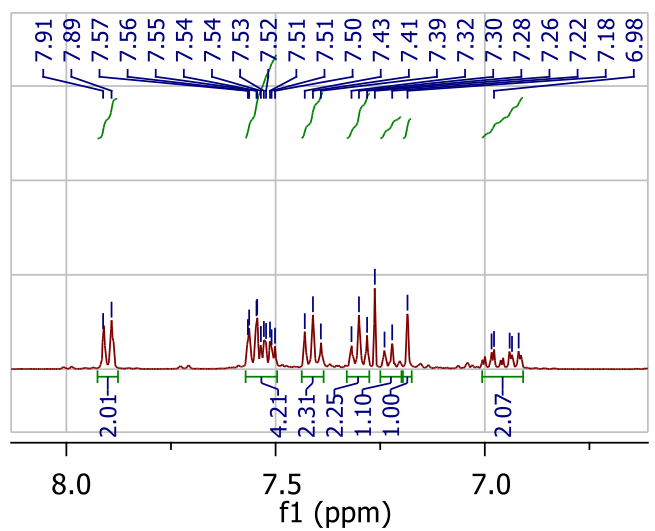
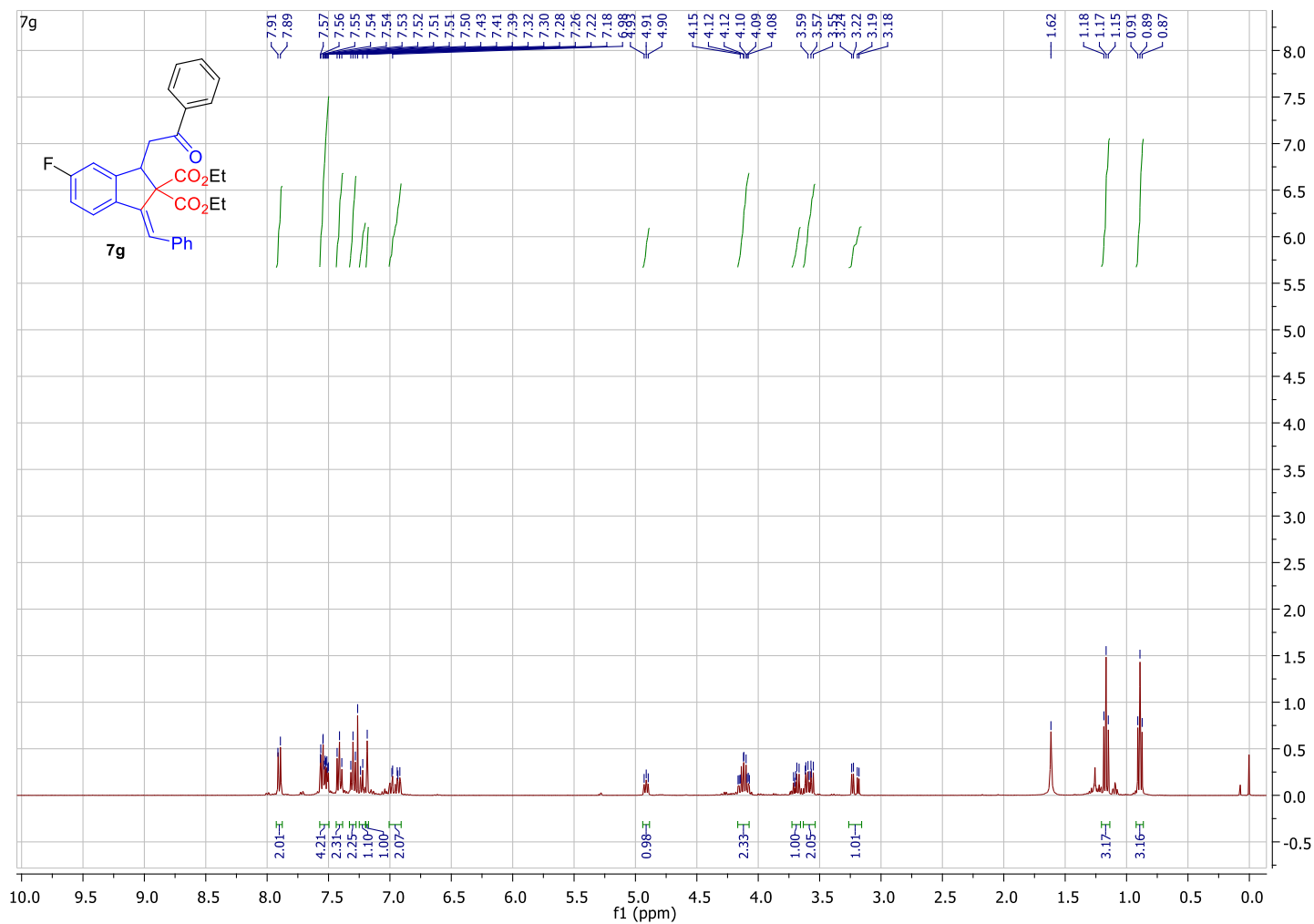


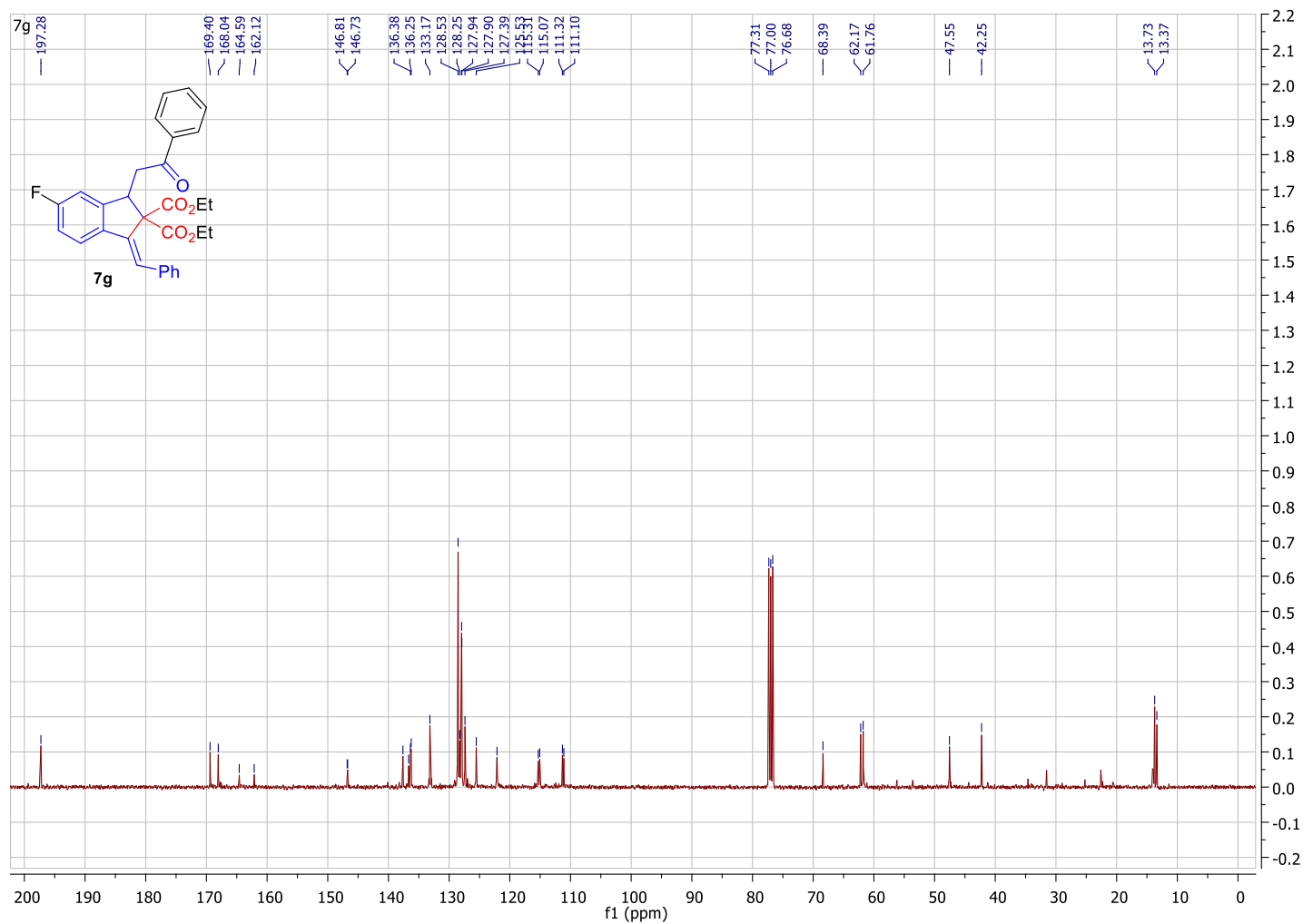
HRMS: (7f)



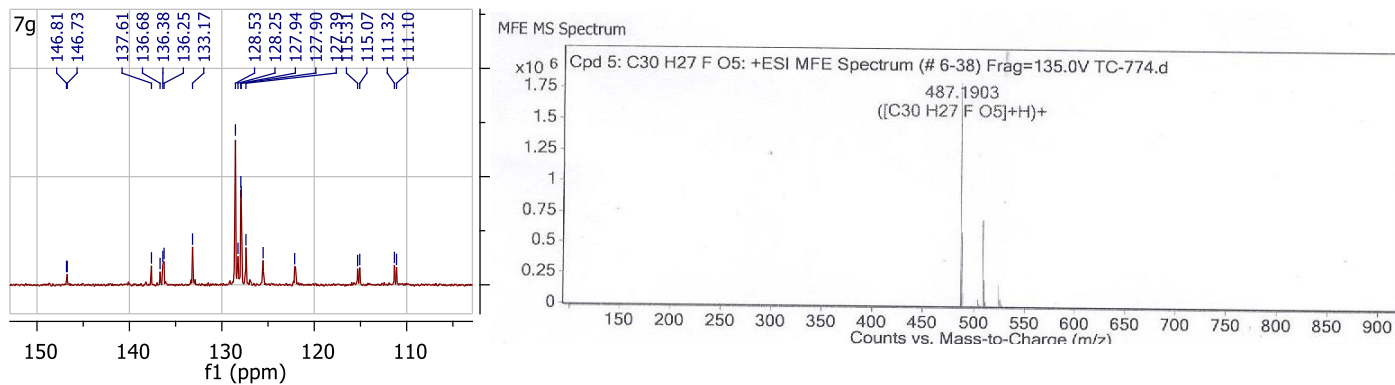
MFE MS Zoomed Spectrum

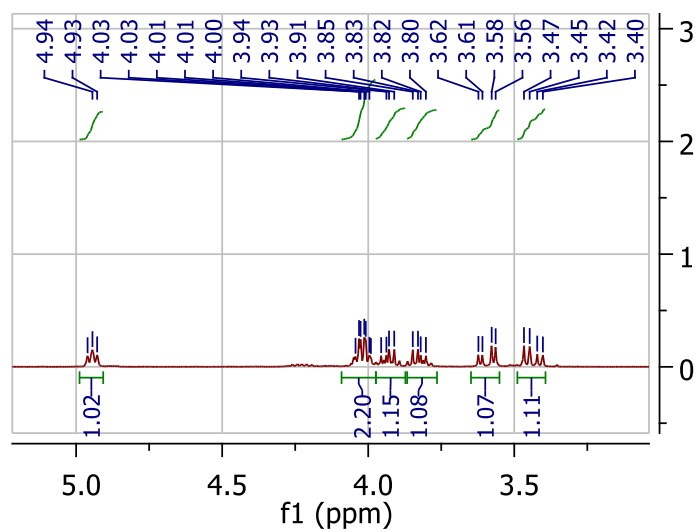
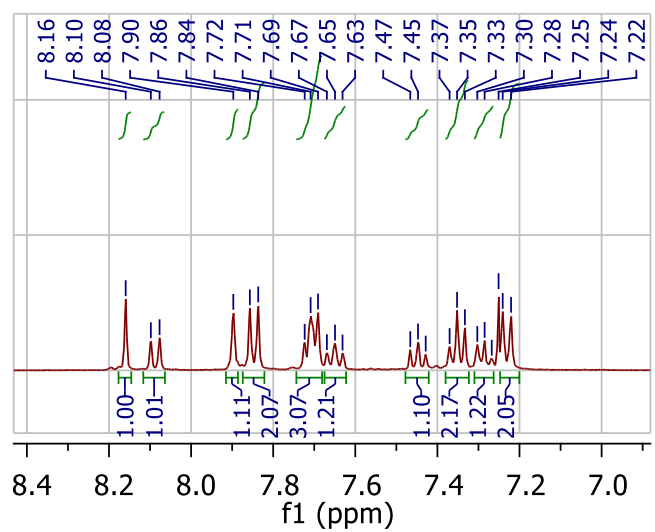
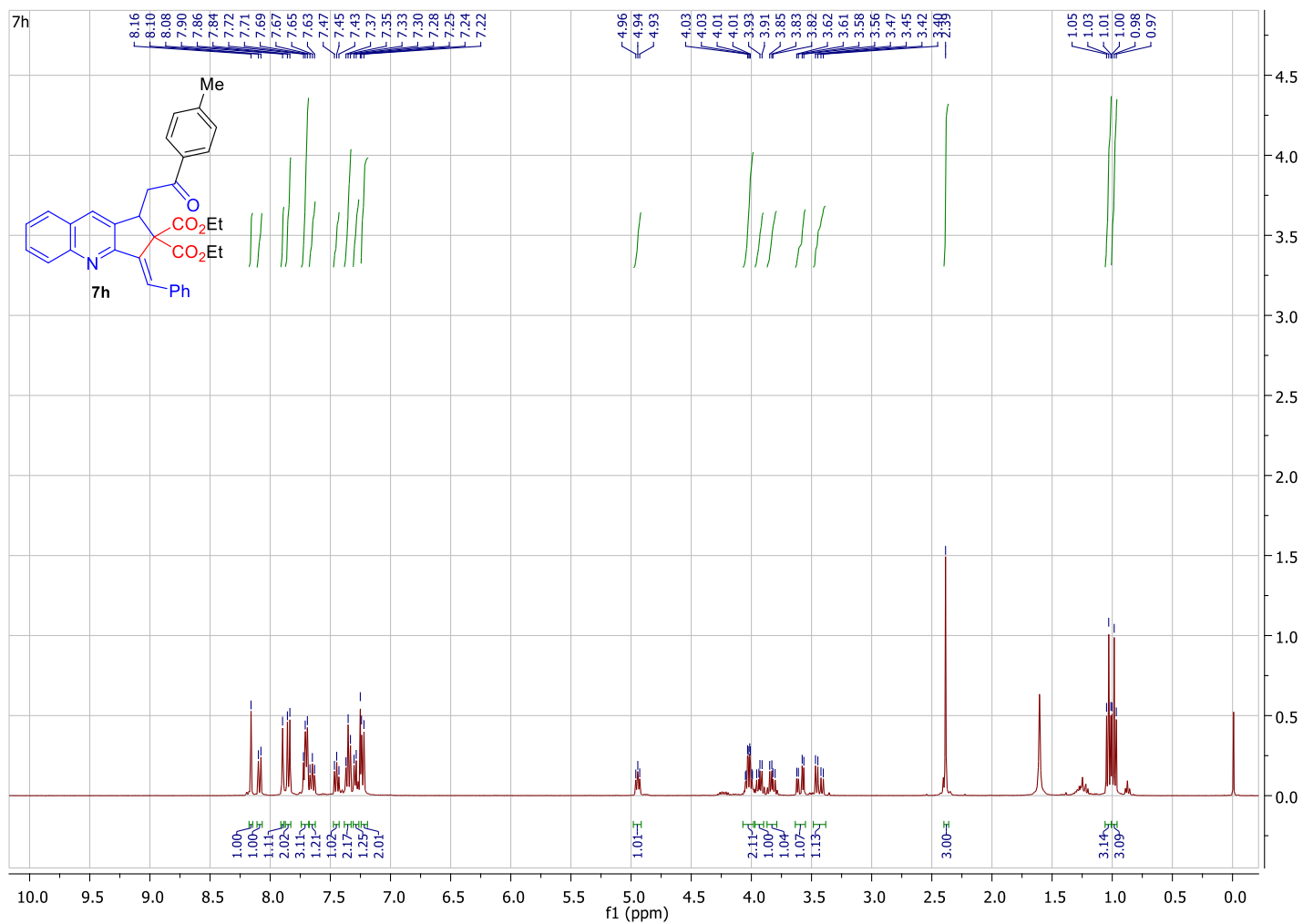


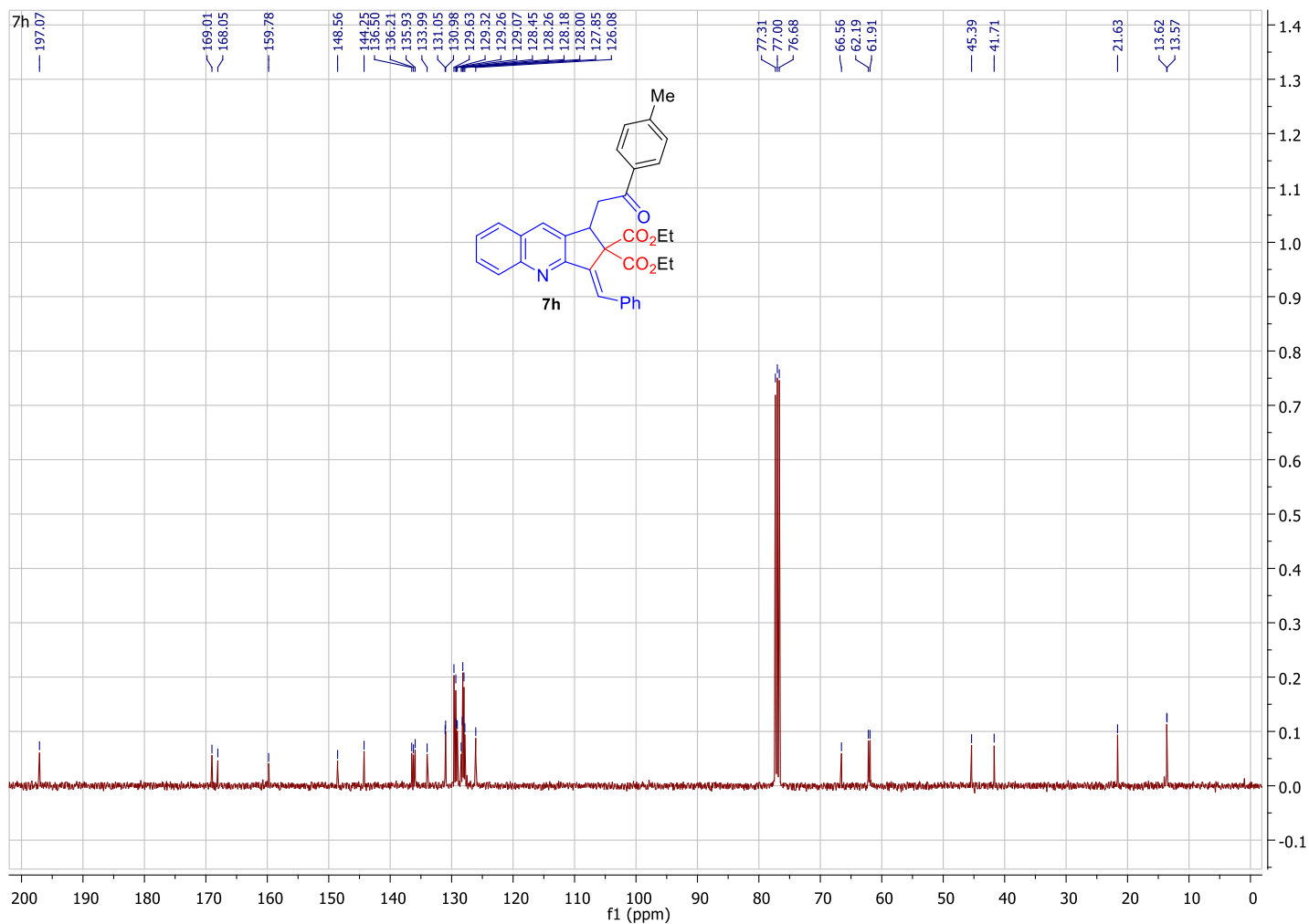




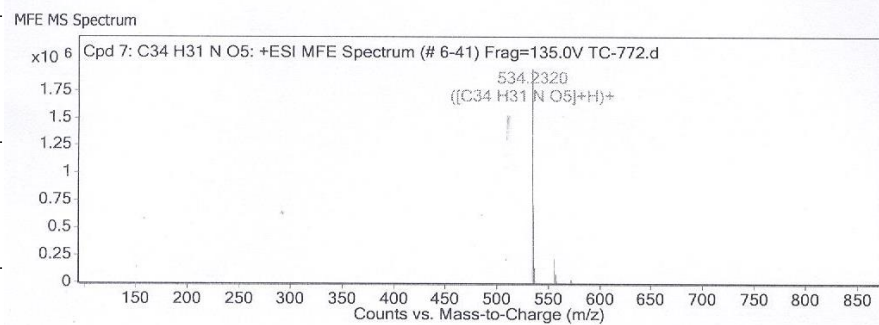
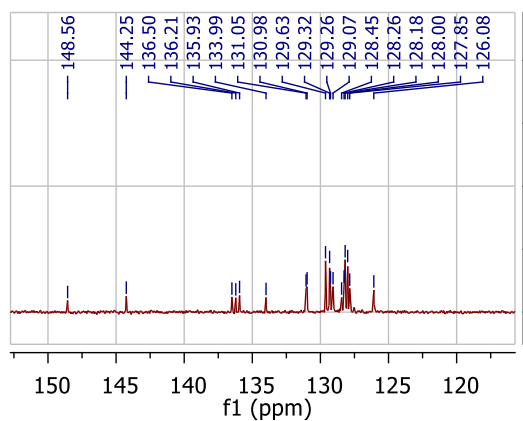
HRMS: (7g)

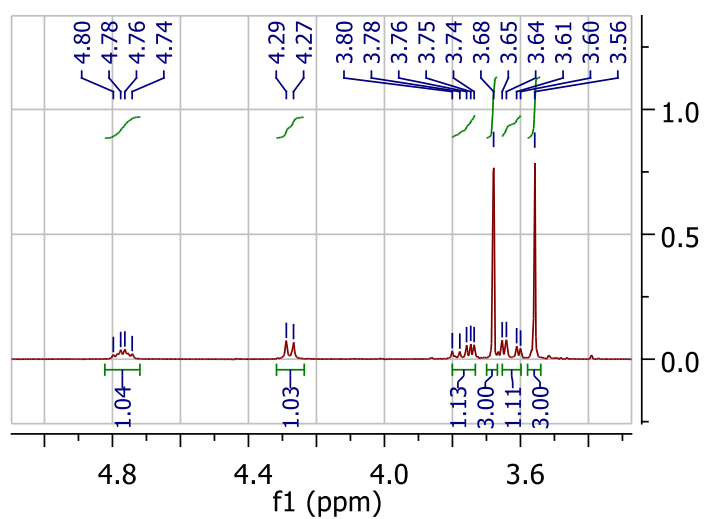
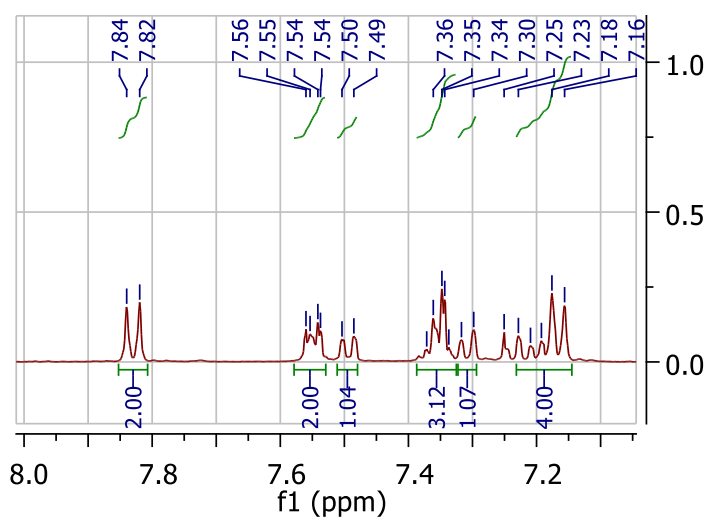
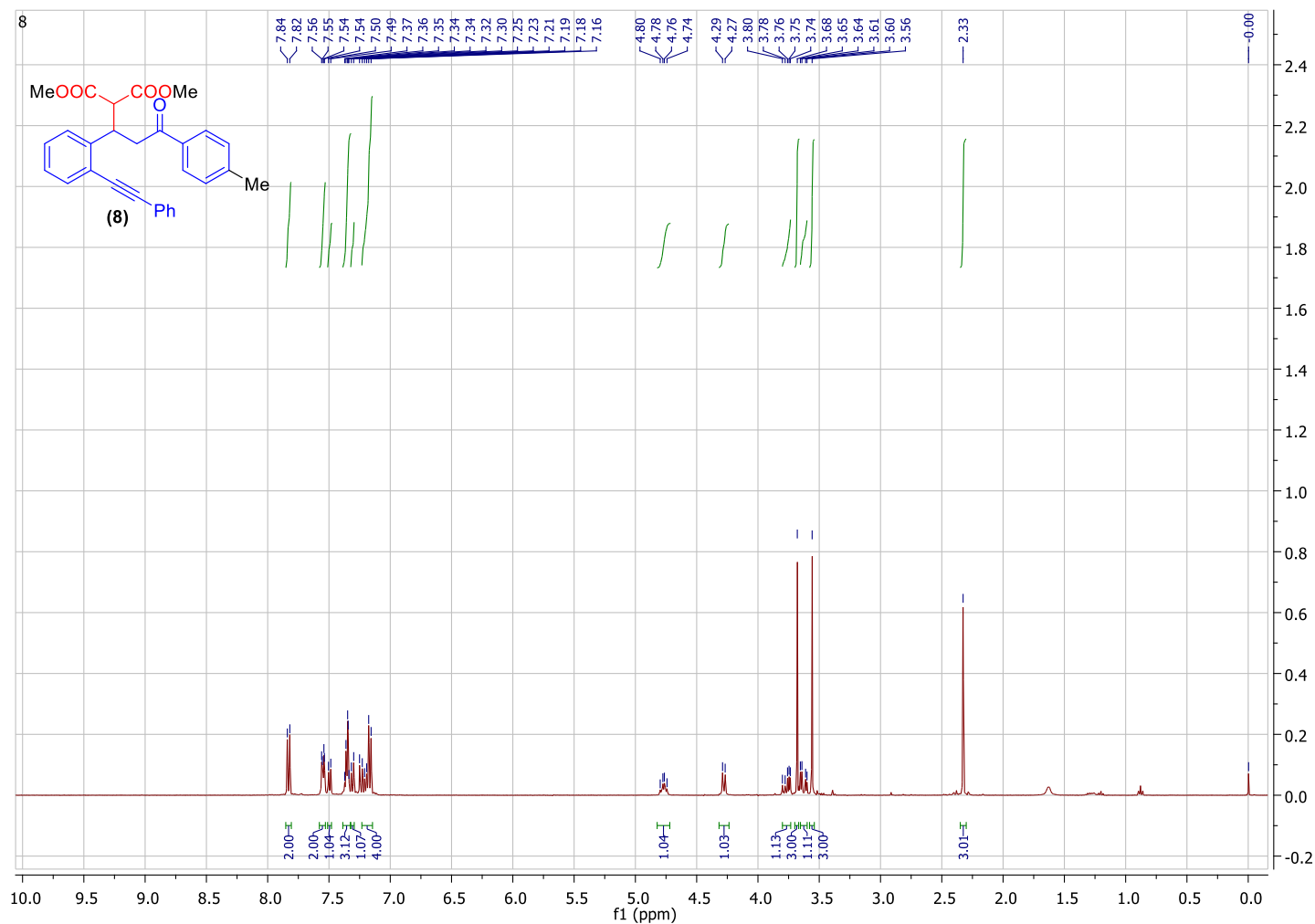


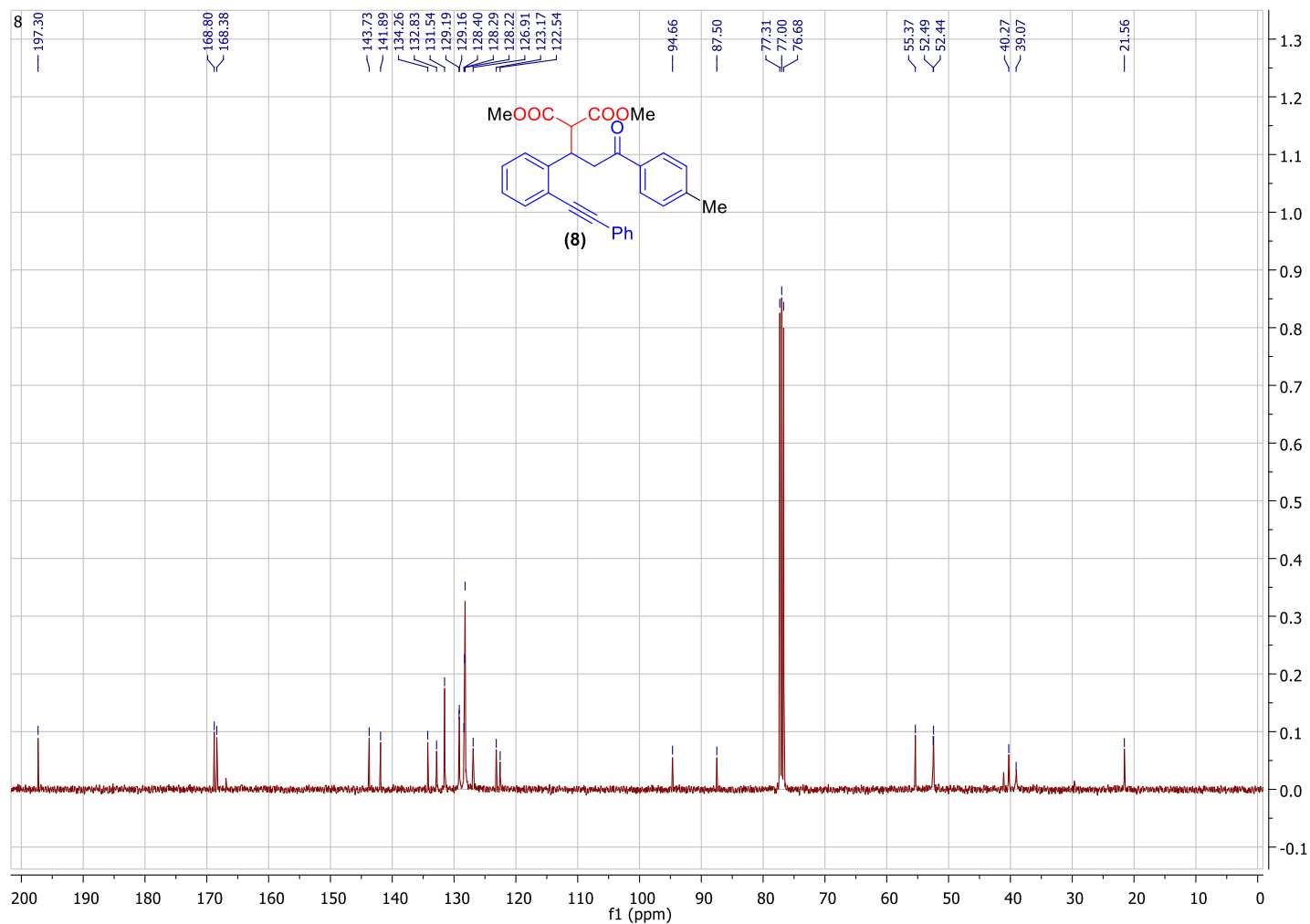




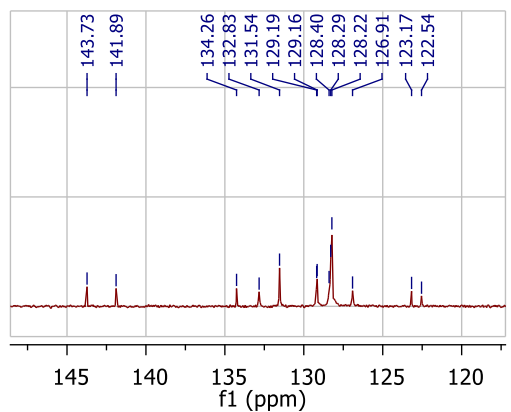
HRMS: 7h



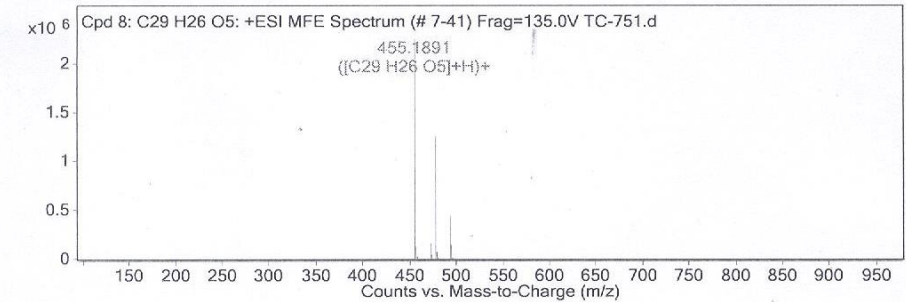




HRMS: (8)



MFE MS Spectrum



3. X-ray crystal structure data of (5a)

The single crystal X-ray data ^[S1] of the given compound was collected on an Oxford Xcalibur CCD diffractometer using graphite monochromated MoK α -radiation ($\lambda = 0.71073 \text{ \AA}$) at 293(2) K. The multi-scan correction was applied to it. The structure was solved by the direct method using SIR-92 and refined by full matrix least-square refinement technique on F^2 using SHELXL97.² The hydrogen atoms were placed into the calculated position and included in the last cycle of the refinement. All the calculations were done using WinGX software package.³ The main crystallographic data and structural refinement details of **5a** is given in Table S1. Atomic coordinates, bond lengths, bond angles, and thermal parameters for compound **5a** have been deposited at the Cambridge Crystallographic Data Centre (CCDC, deposit no. 1526254)

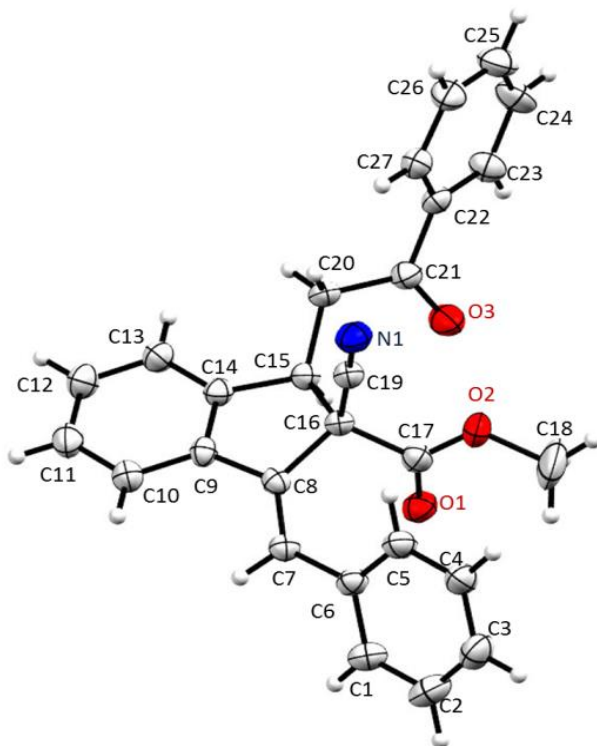


Fig. 1s. X-ray crystallographic ORTEP diagram of compound **5a**

Table S1. Crystal data and structure refinement for 5a.

Empirical Formula	C ₂₇ H ₂₁ NO ₃
Formula Weight	407.45
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	<i>Fdd2</i>
a [Å]	37.951(3)
b [Å]	24.111(2)
c [Å]	9.5003(6)
α [°]	90.00
β [°]	90.00
λ [°]	90.00
Volume [Å ³]	8694.4 (11)
Z	16
Density (calculated) [Mg/m ³]	1.245
Absorption coefficient [mm ⁻¹]	0.081
F(000)	3424
Crystal size [mm ³]	0.28 x 0.19x 0.12

Theta range for data collection [°]	3.36 to 25.00
Index ranges	-44 ≤ h ≤ 44, -28 ≤ k ≤ 28, -11 ≤ l ≤ 11
Reflections collected / unique	25627 / 3819
R(int)	0.1343
Completeness of Theta at 25 °C (%)	99.8
Refinement method	Full-matrix least square on F ²
Data/ restraints/ parameters	3819/1/280
Goodness-of-fit on F ²	1.031
Final R indices [I>2sigma (I)] ^{a,b}	R ₁ = 0.0660, ^w R ₂ = 0.1385
R indices (all data)	R ₁ = 0.0947, ^w R ₂ = 0.1609
Largest diff. peak and hole [Å ⁻³]	0.197 and -0.152 e.Å ⁻³

$$^aR = \sum(|F_o| - |F_c|) / \sum |F_o| ; ^bR_w = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$$

References:

- 1.G.M. Sheldrick, *ActaCrystallogr.,Sect. A*, **1990**,46, 467.
- 2.G.M. Sheldrick, *SHELXL-97, Computer program for crystal structure refinement* University of Göttingen, Germany, **1997**.
- 3.L. J. Farrugia, WinGX Version 1.80.05, *An integrated system of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data*,Department of Chemistry, University of Glasgow (**1997-2009**).

[S1]. CCDC. 1526254 (**5a**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.