

Supporting Information

for

A Formal [3+2] Annulation Reaction of Propargyl Sulfonium Compounds and *N*-Ylides: Access to Pyrrolo[2,1-*a*]quinolines, Pyrrolo[2,1-*a*]phthalazines and Indolizines

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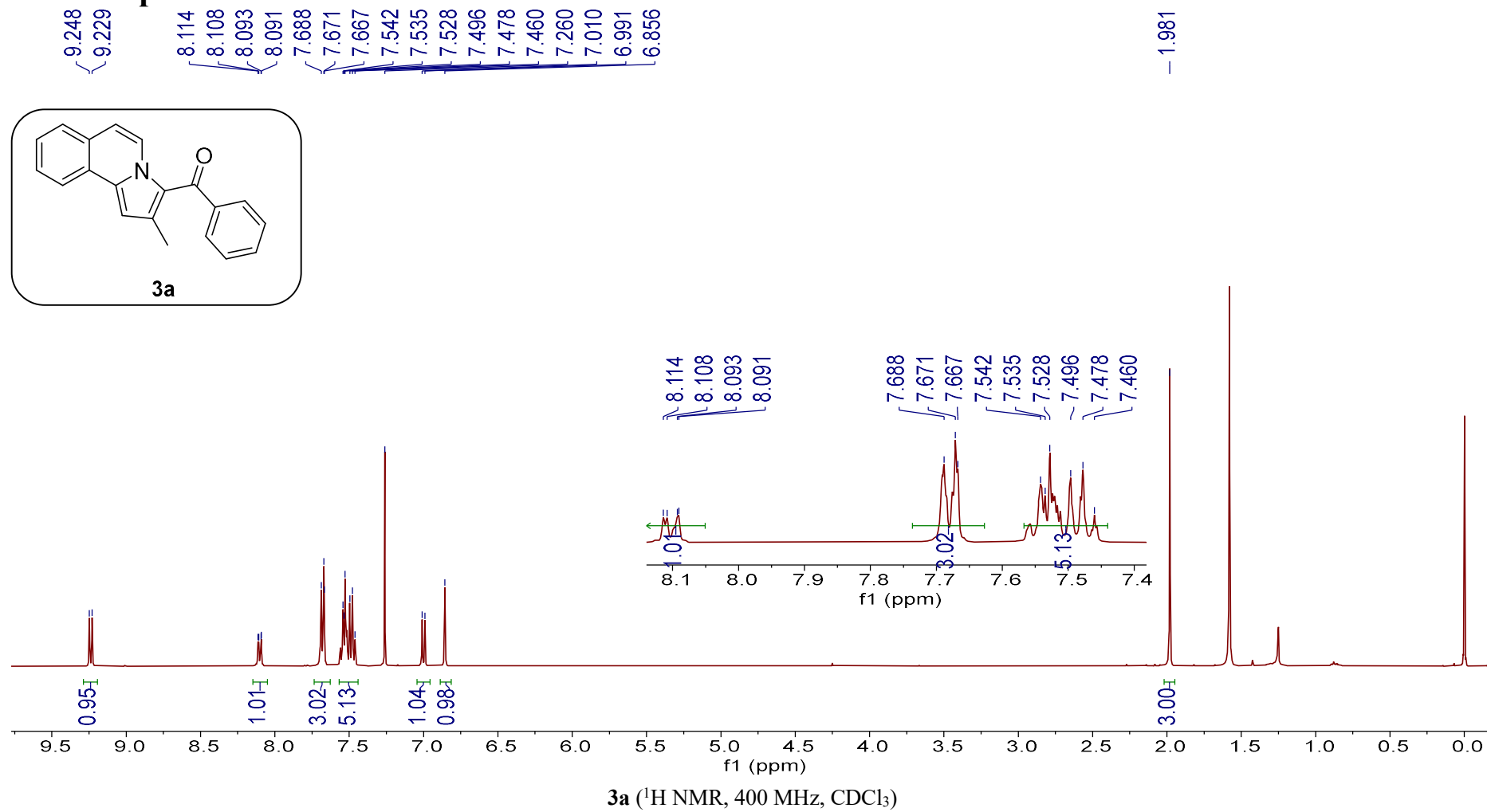
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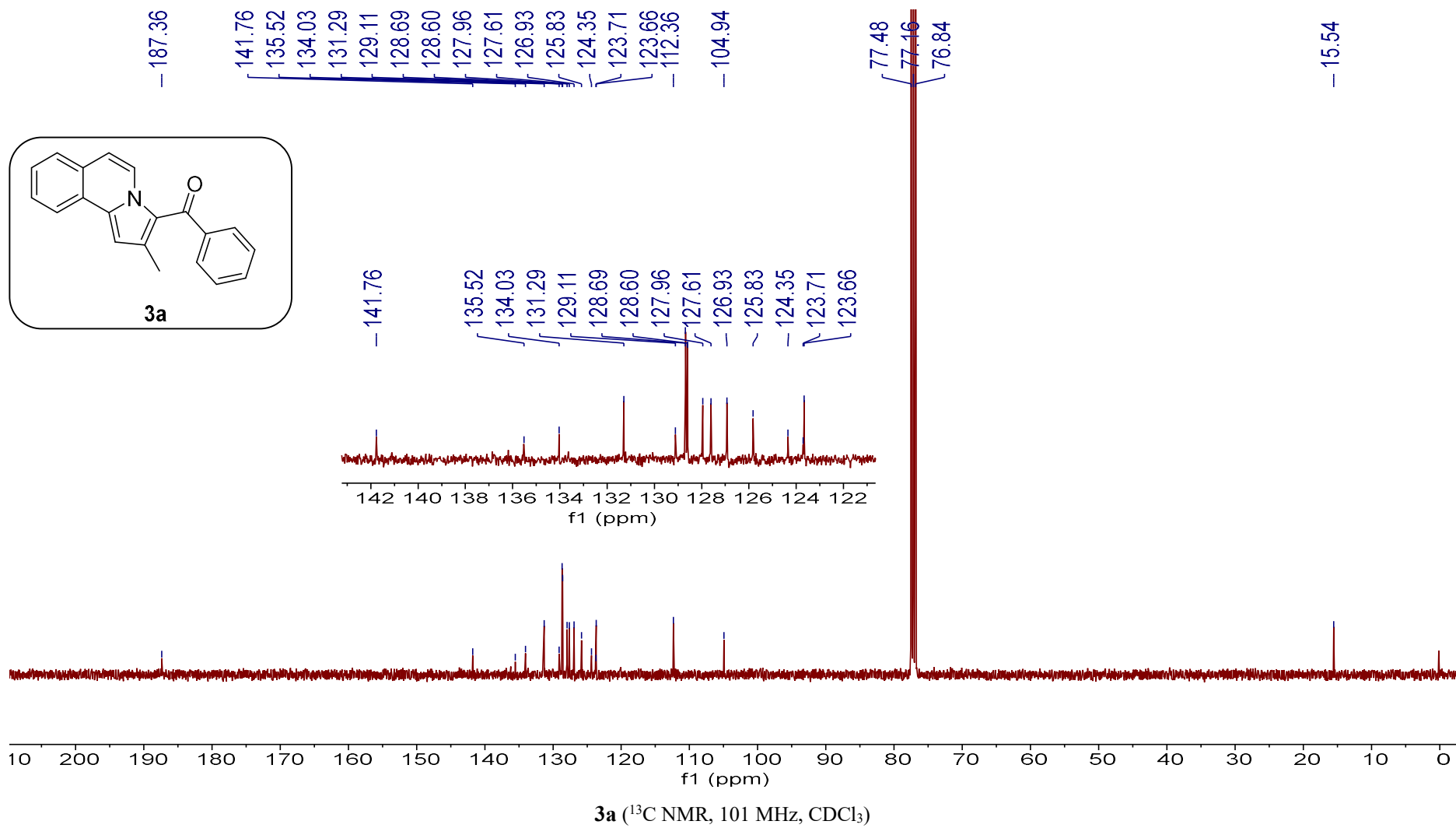
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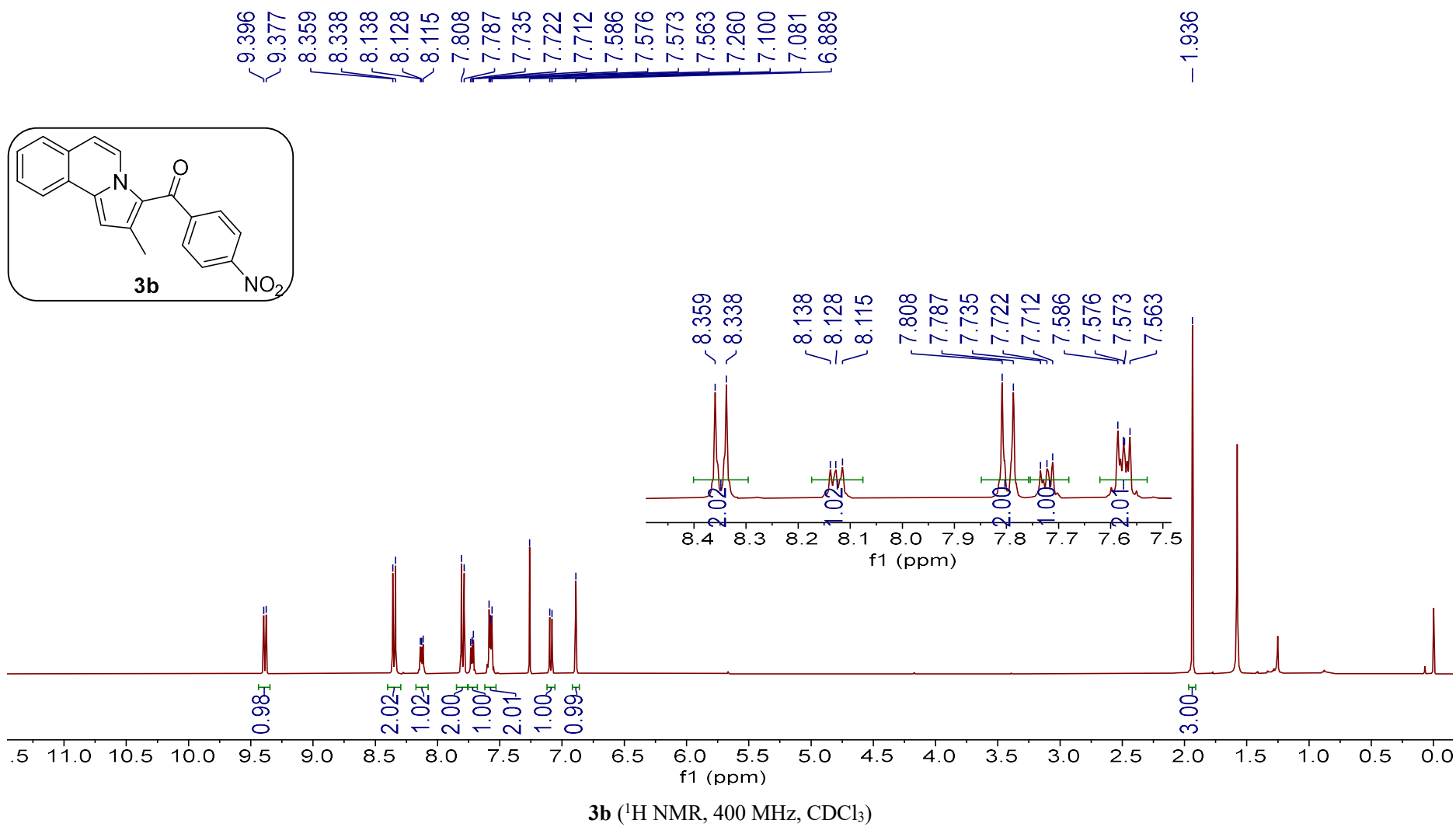
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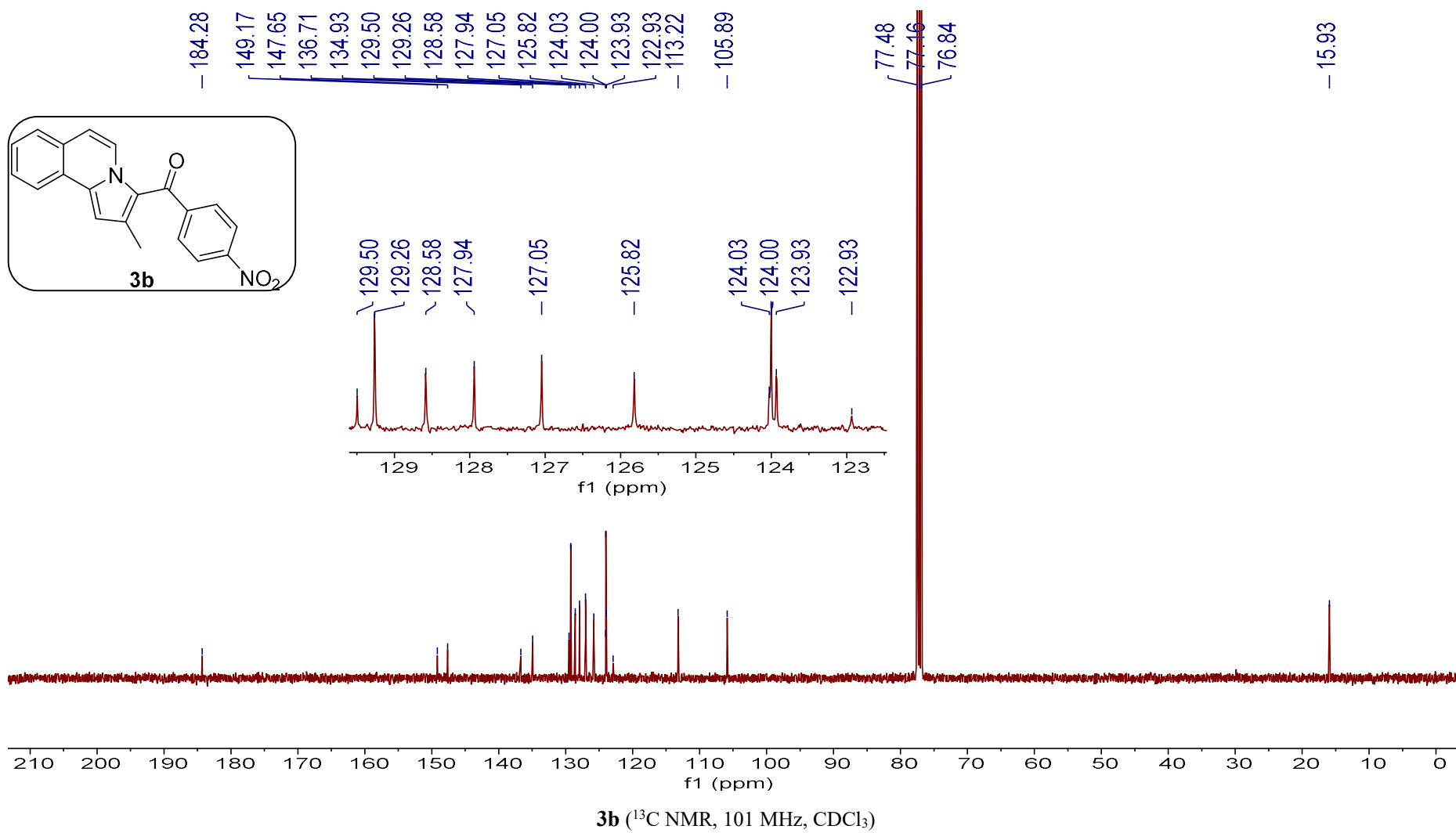
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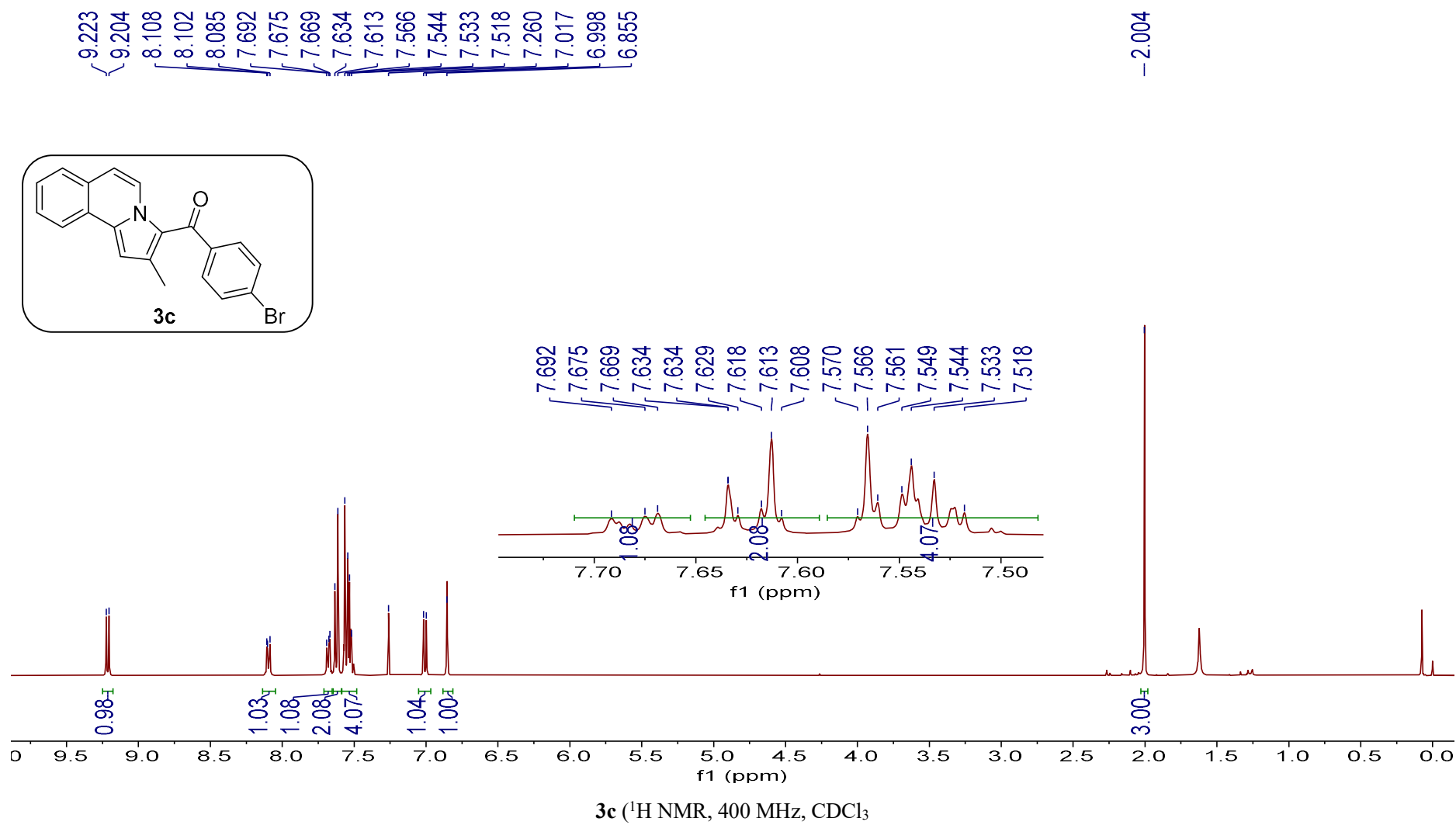
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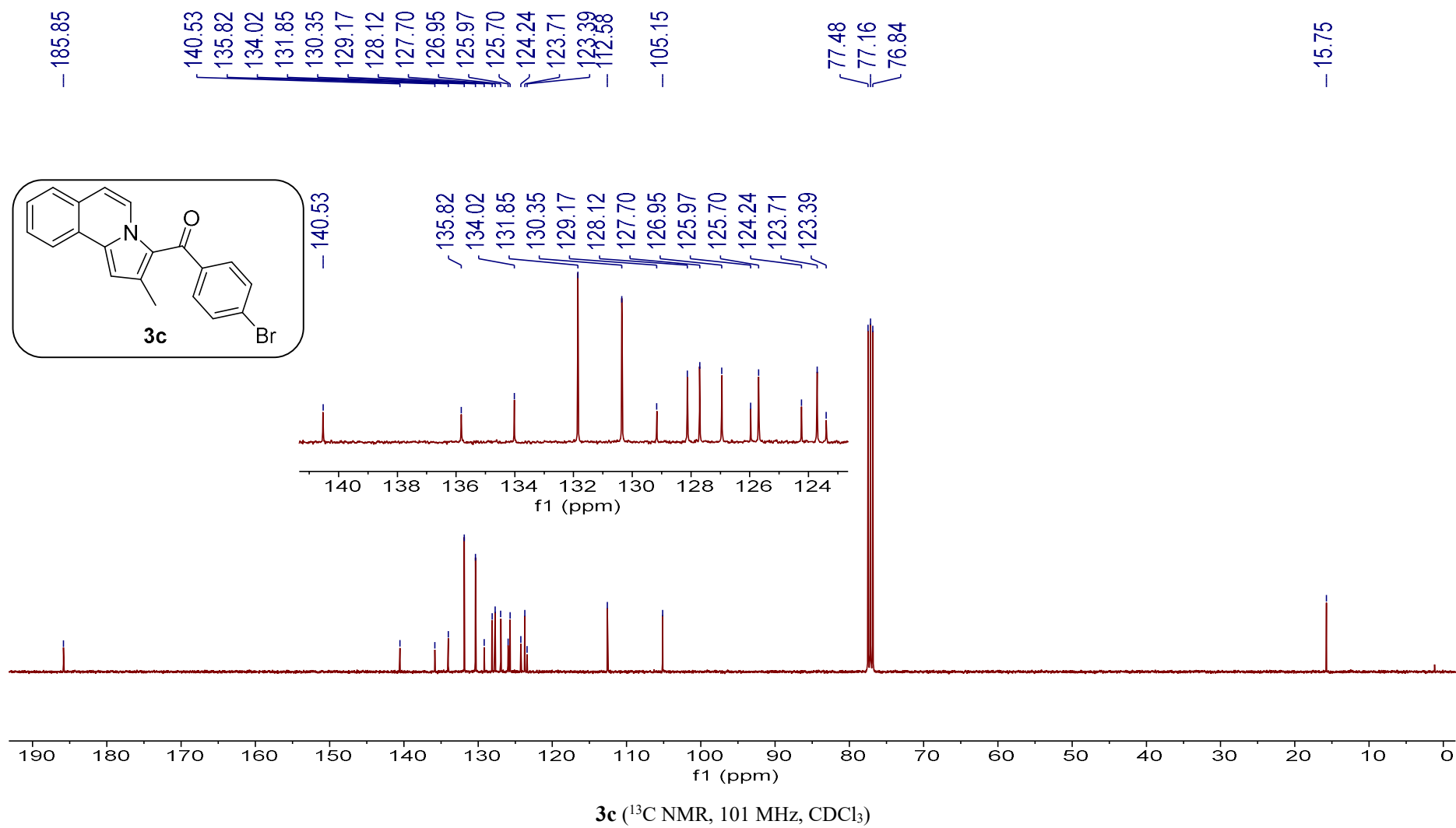


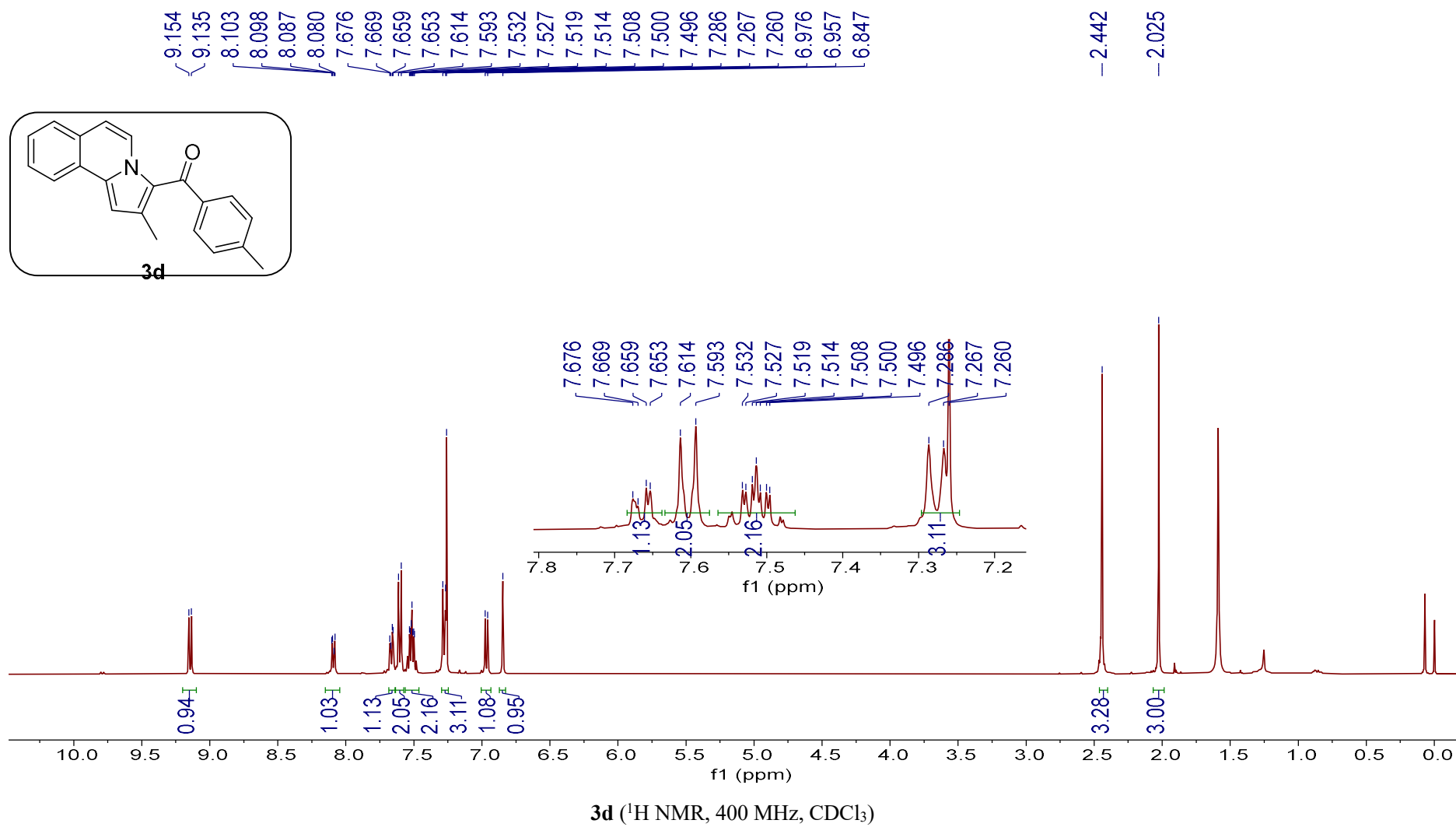


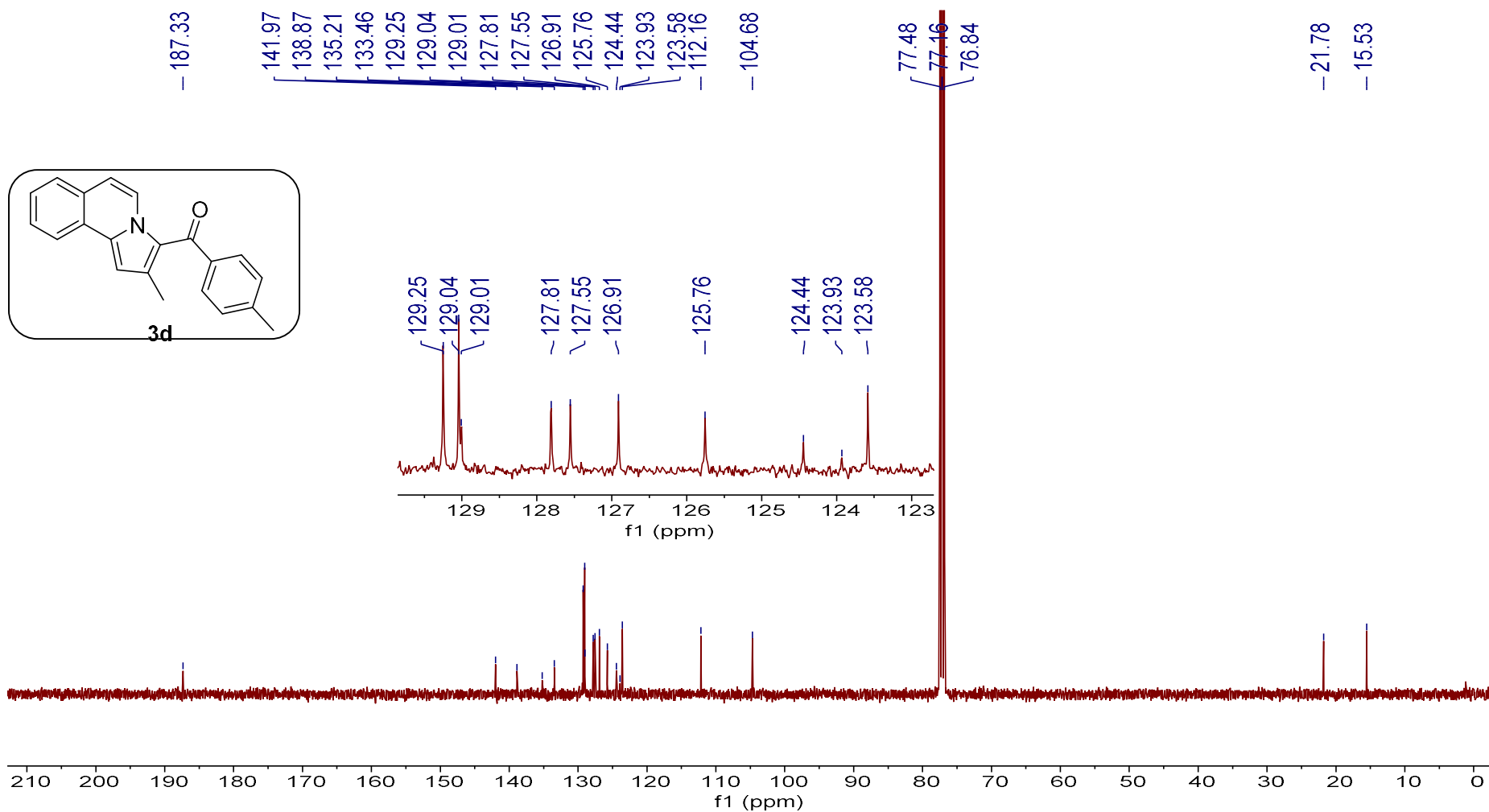




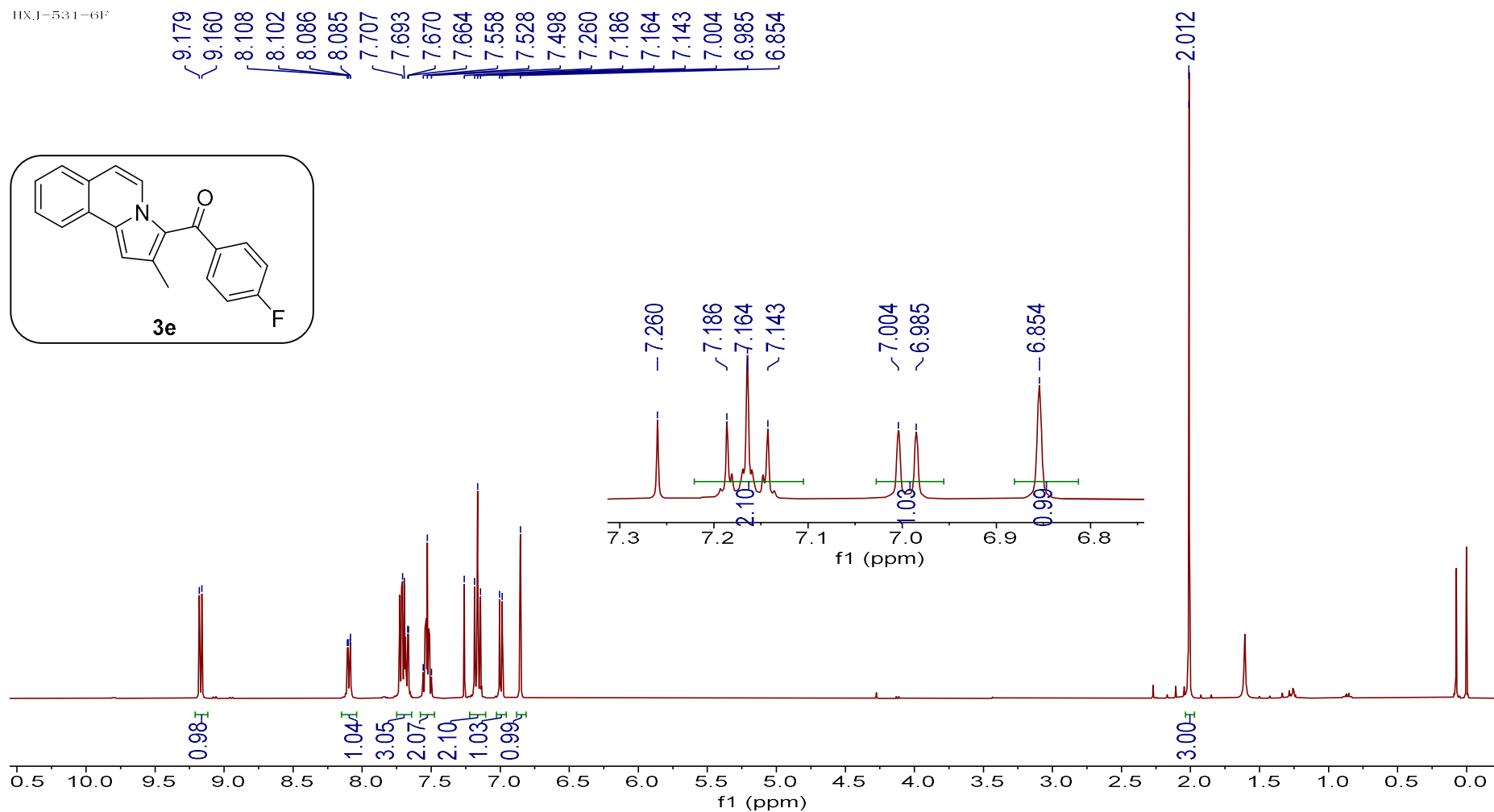
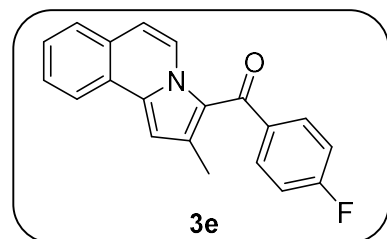




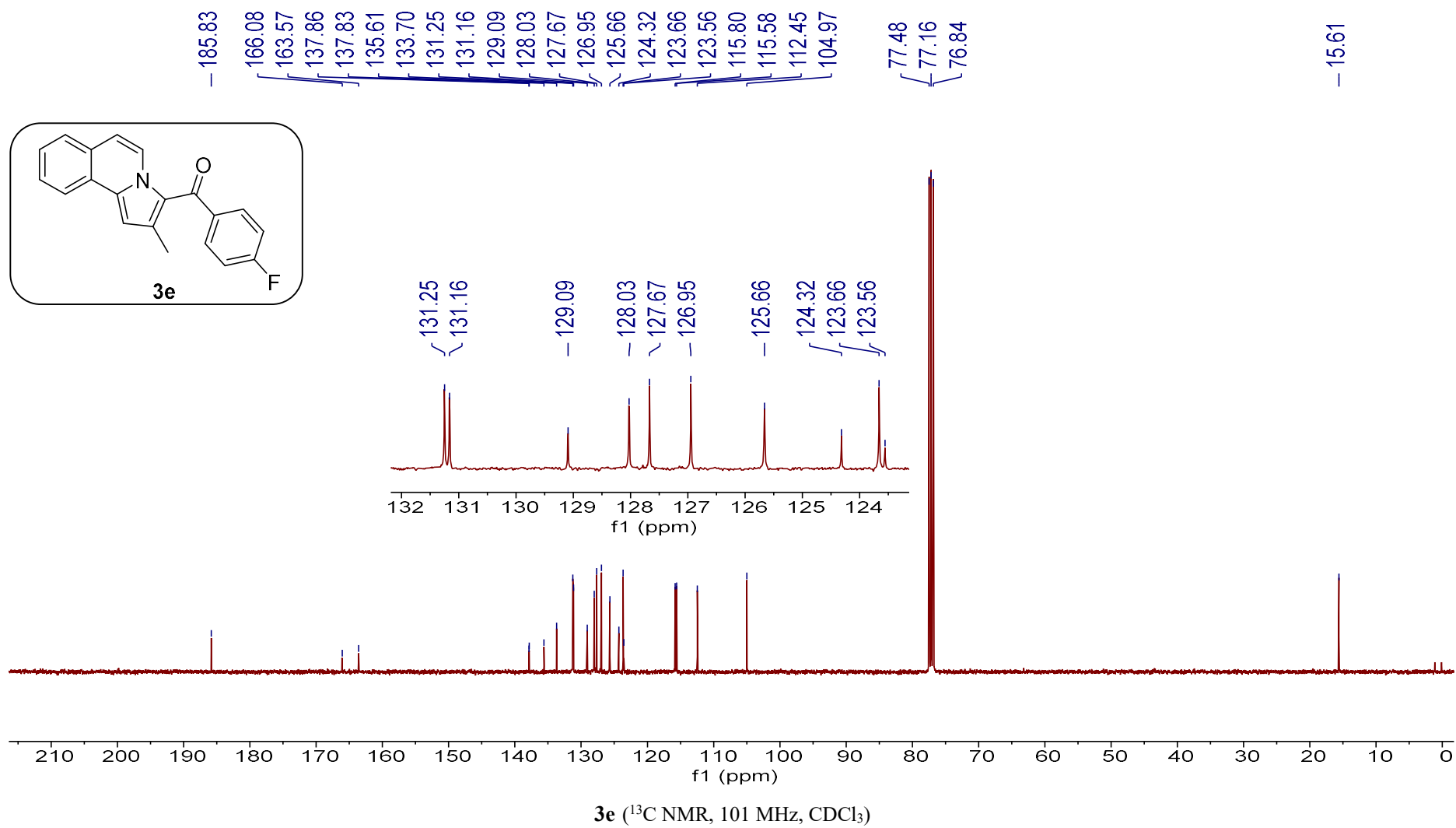


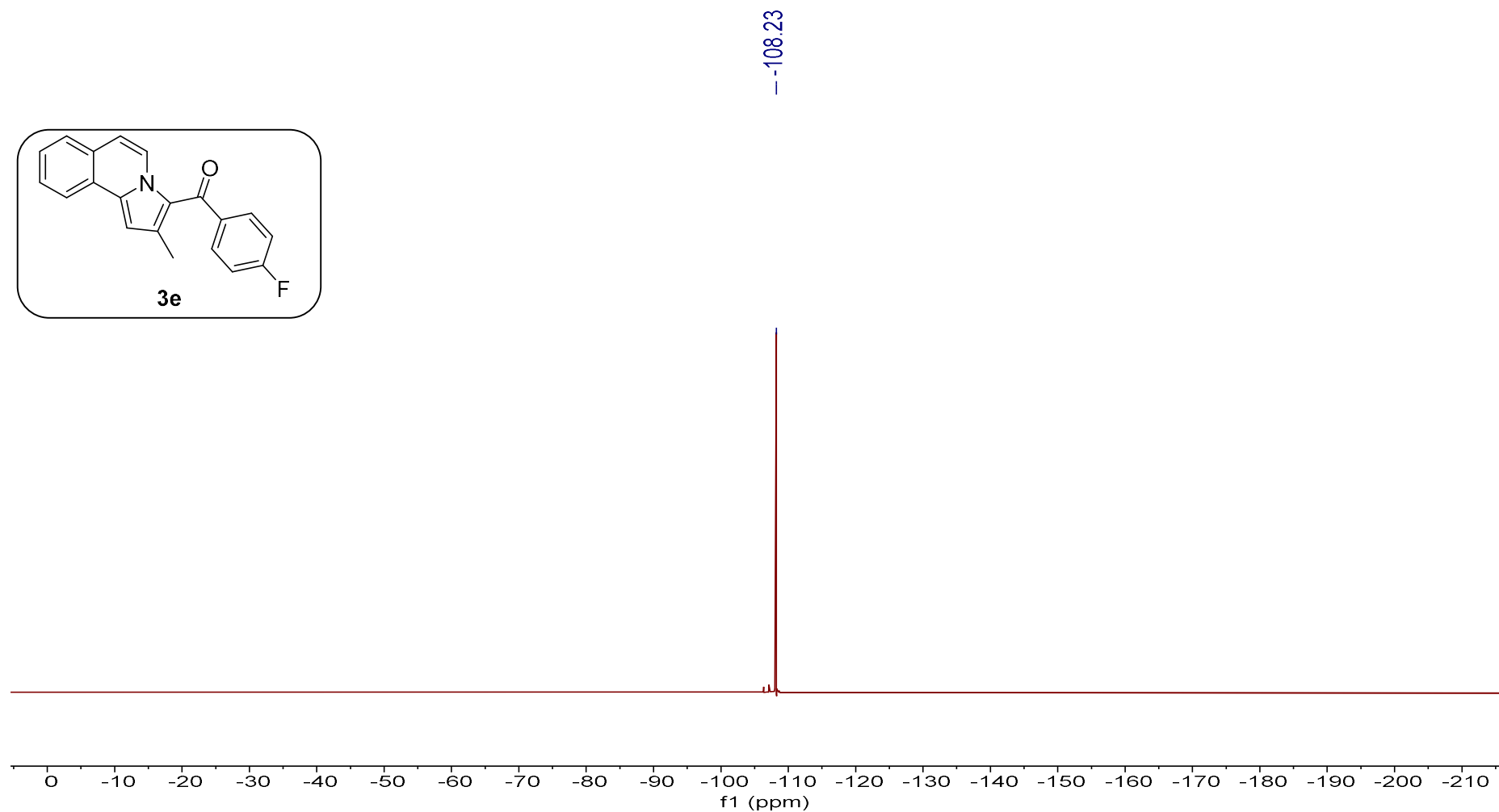
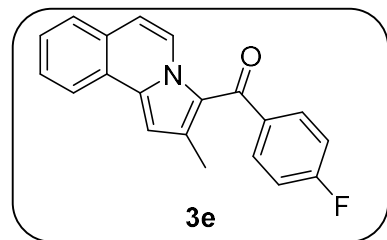


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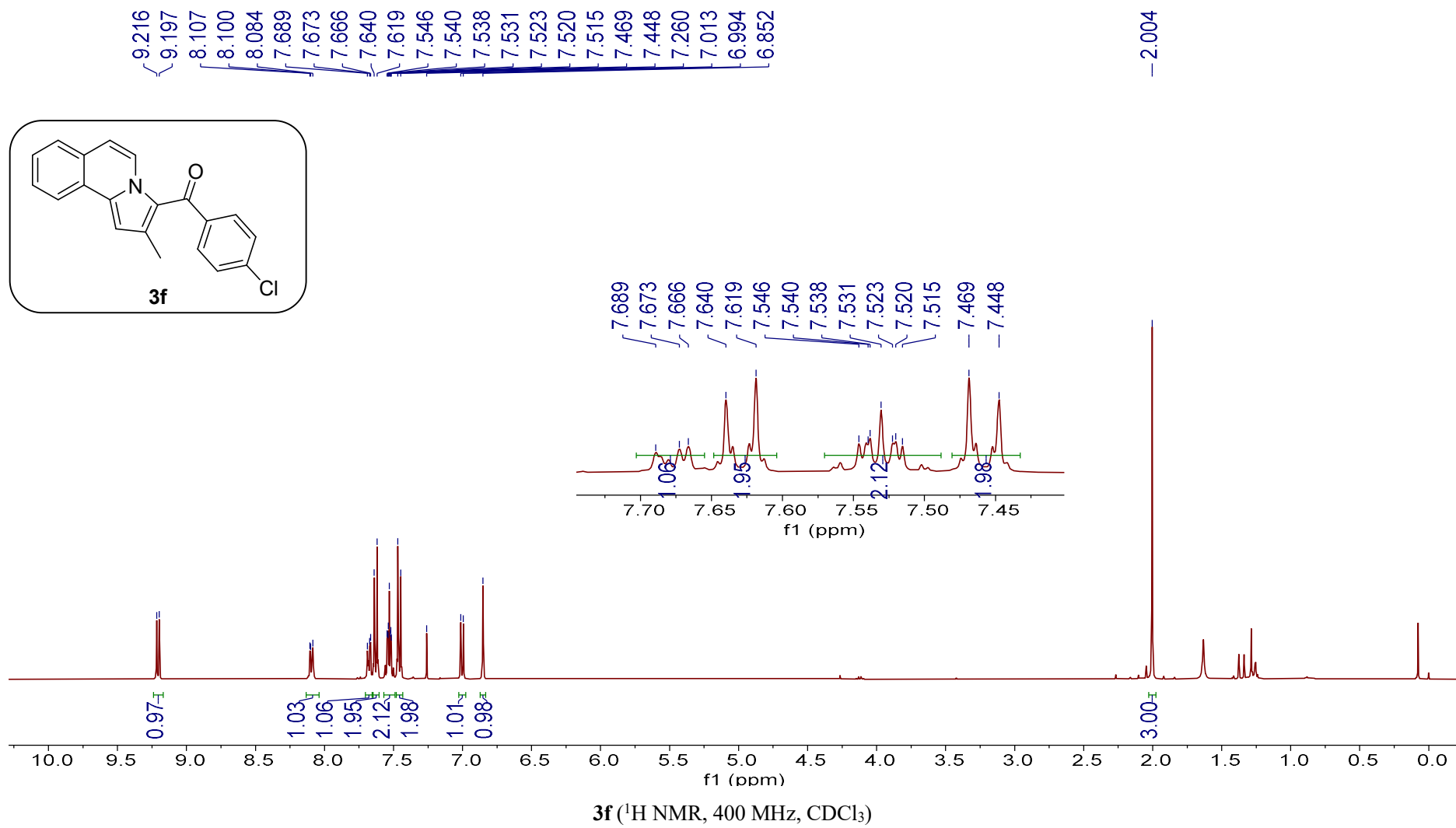


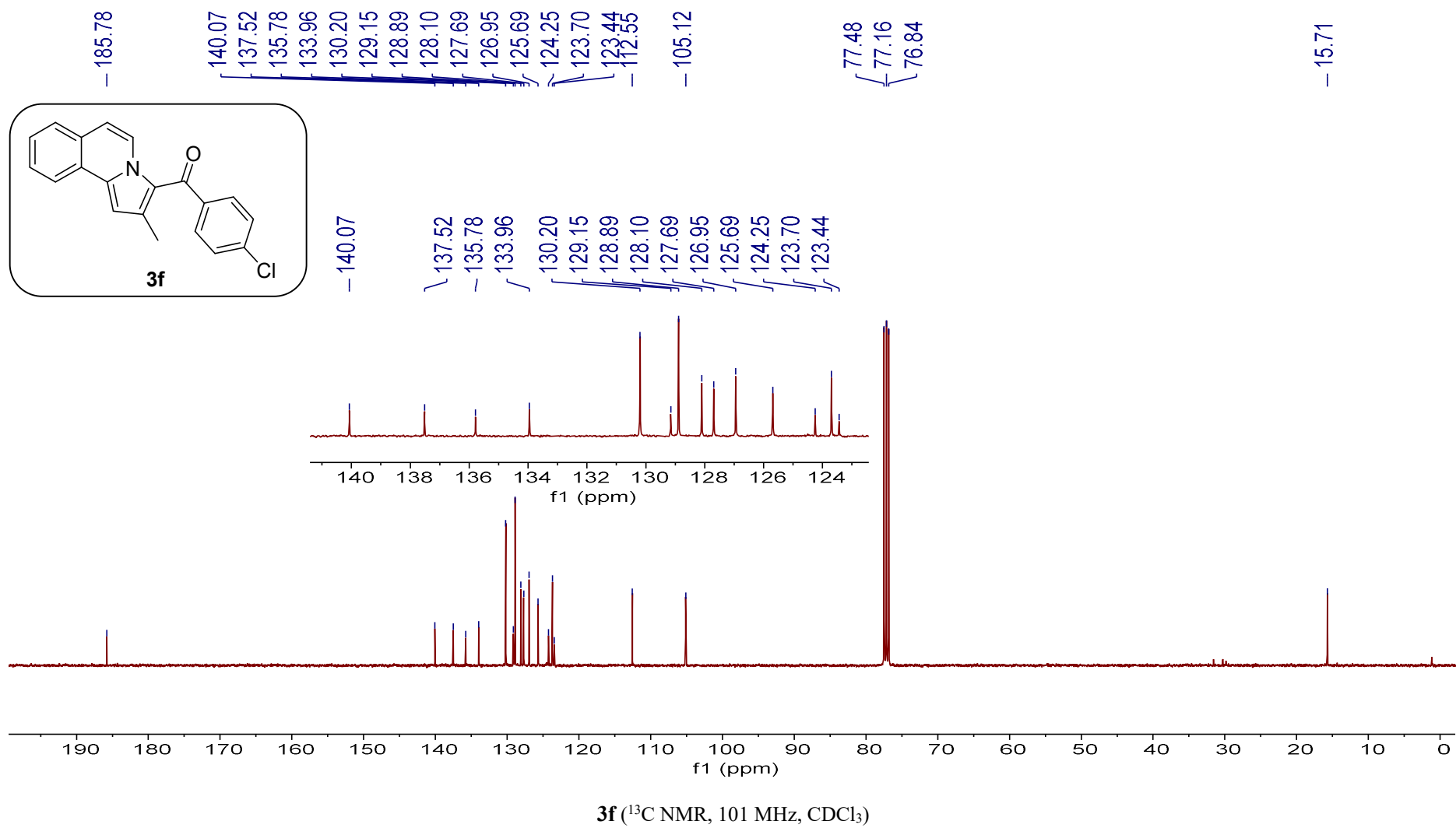
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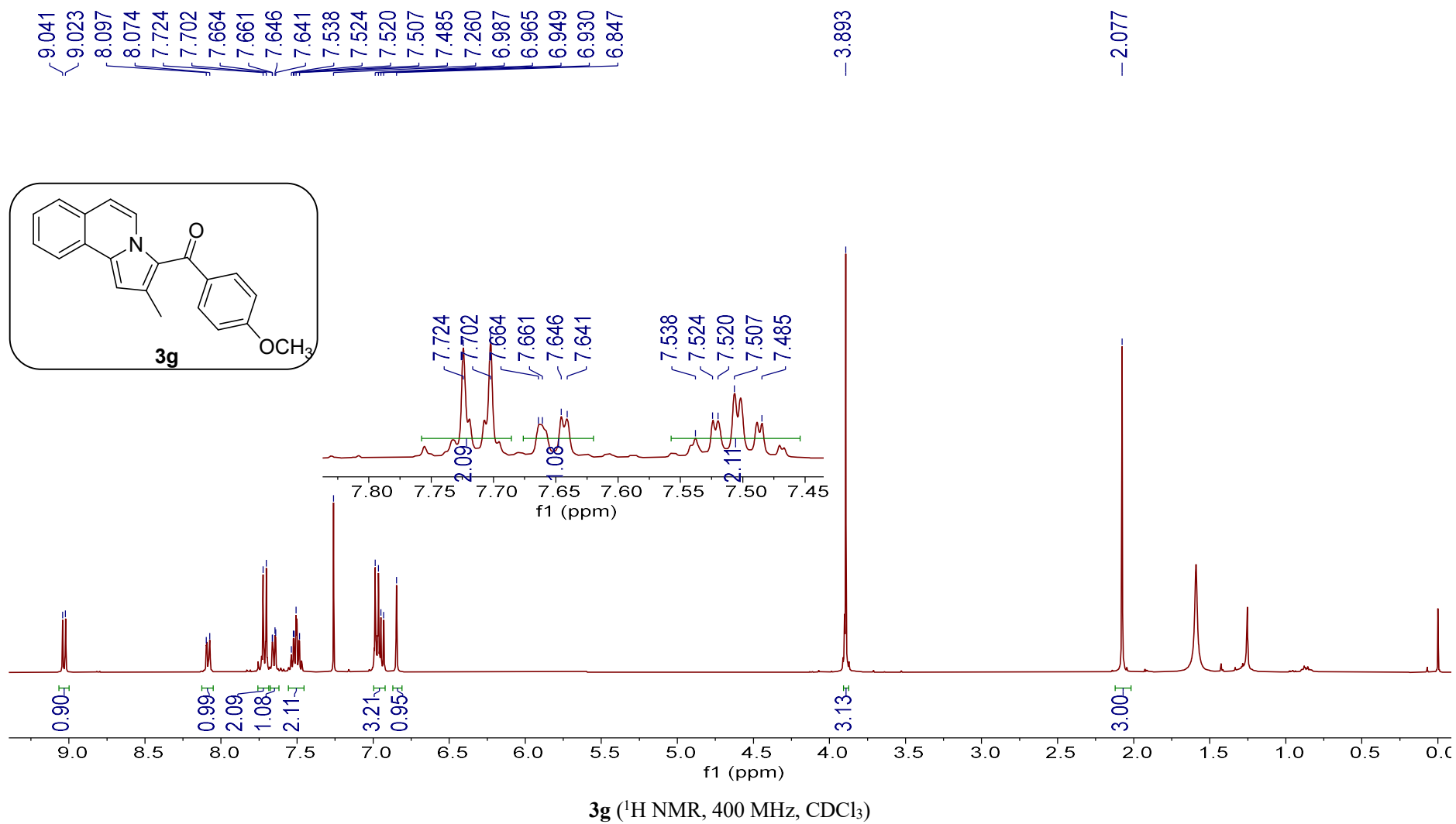


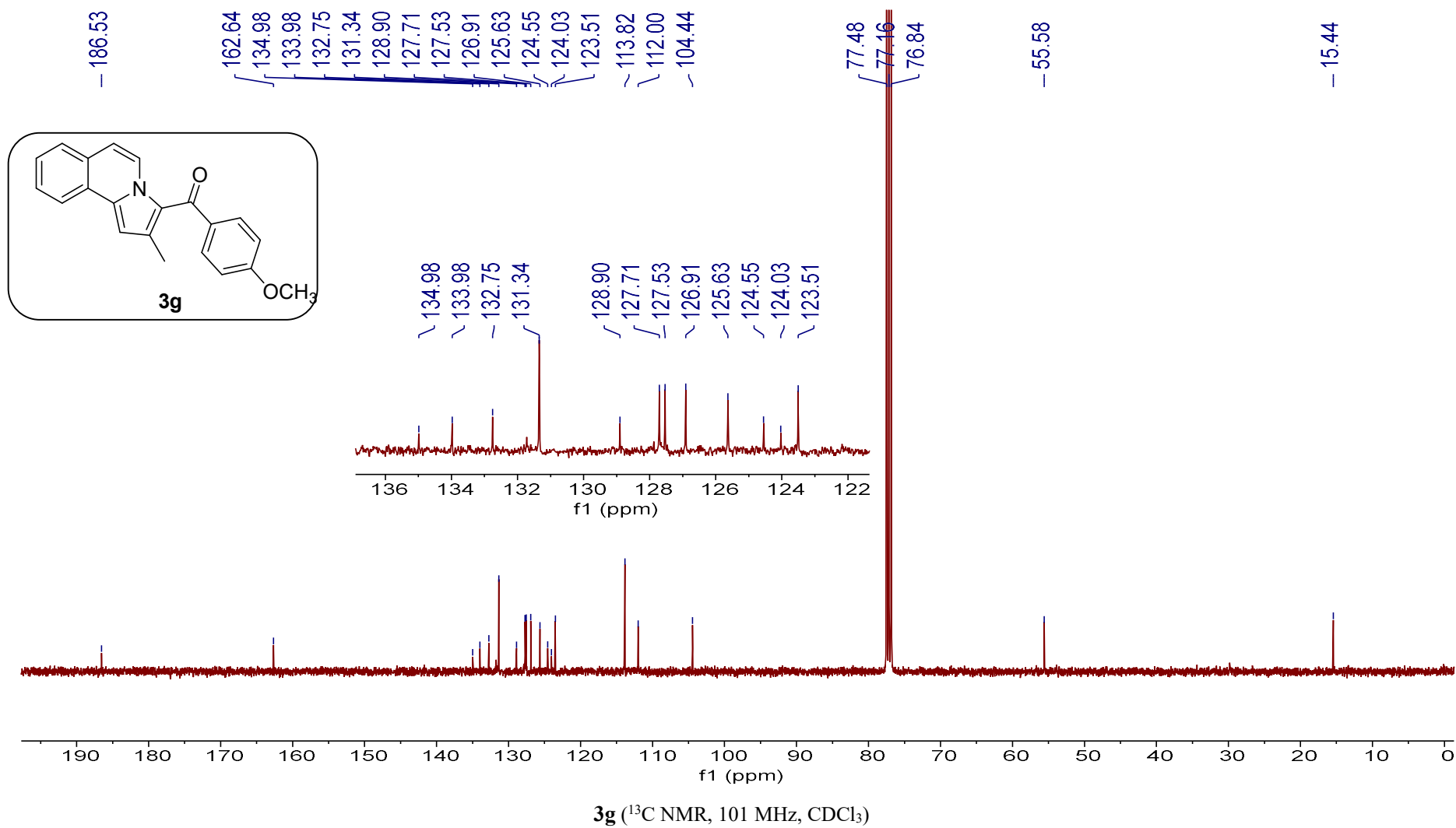


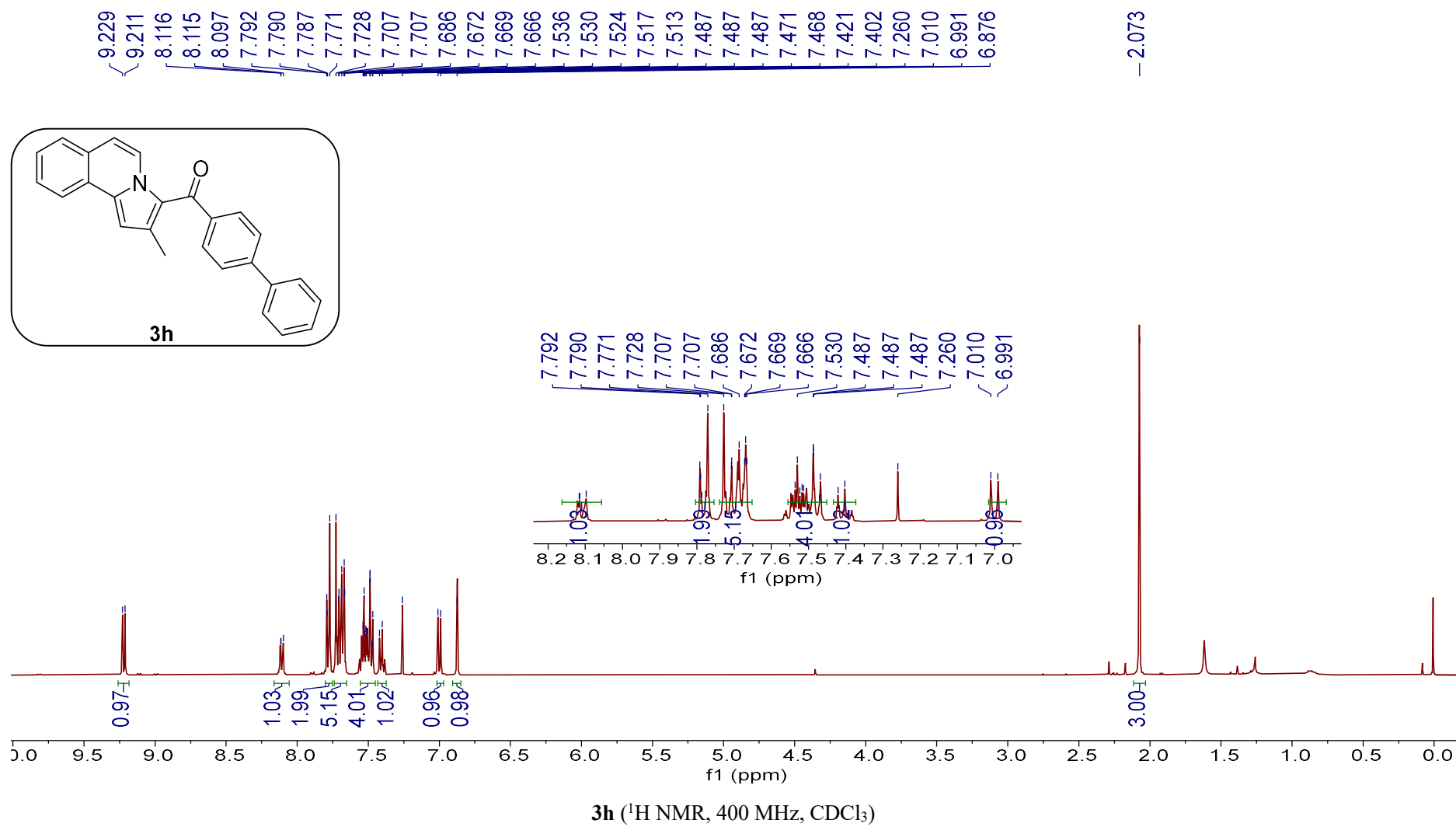
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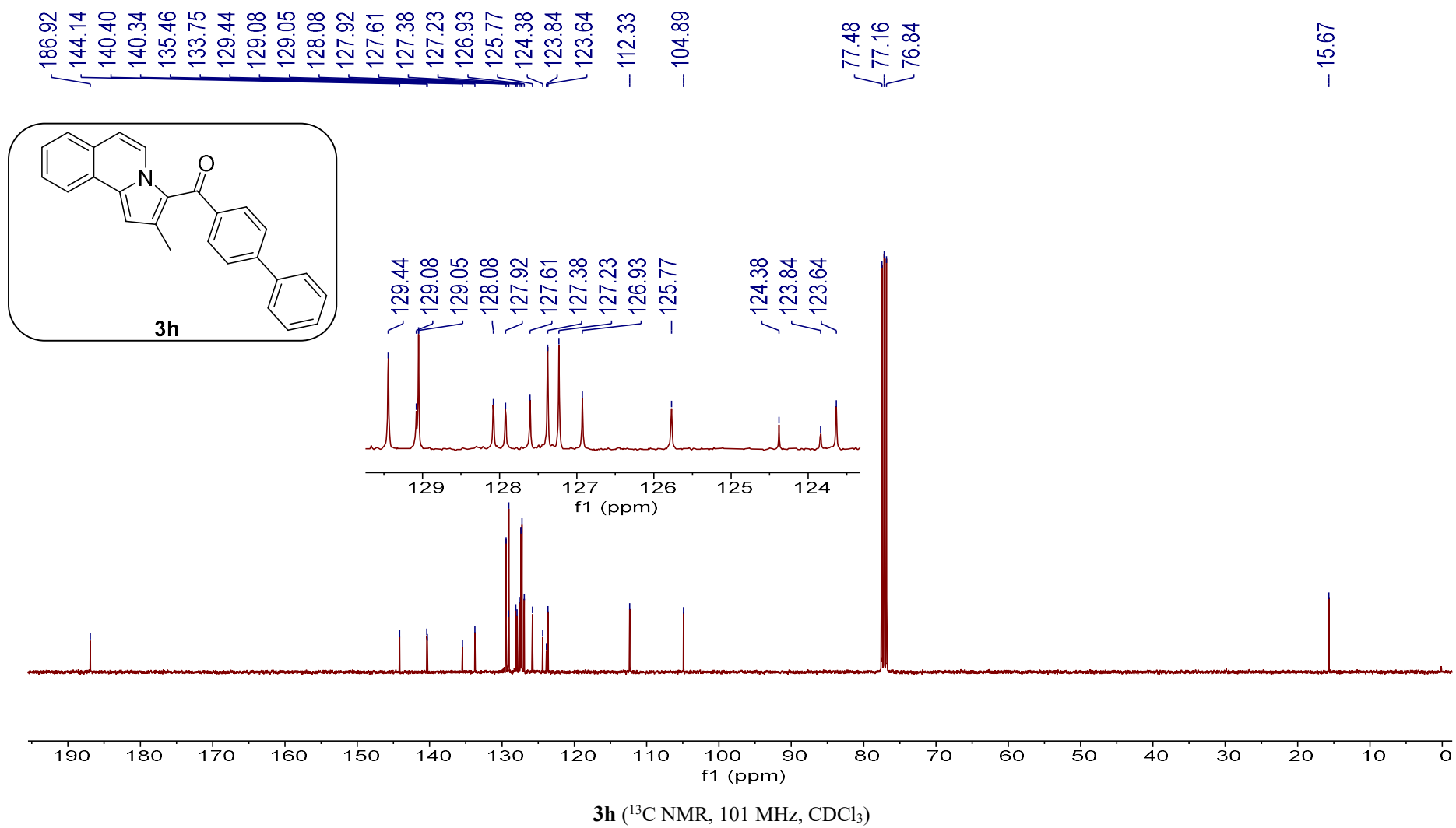


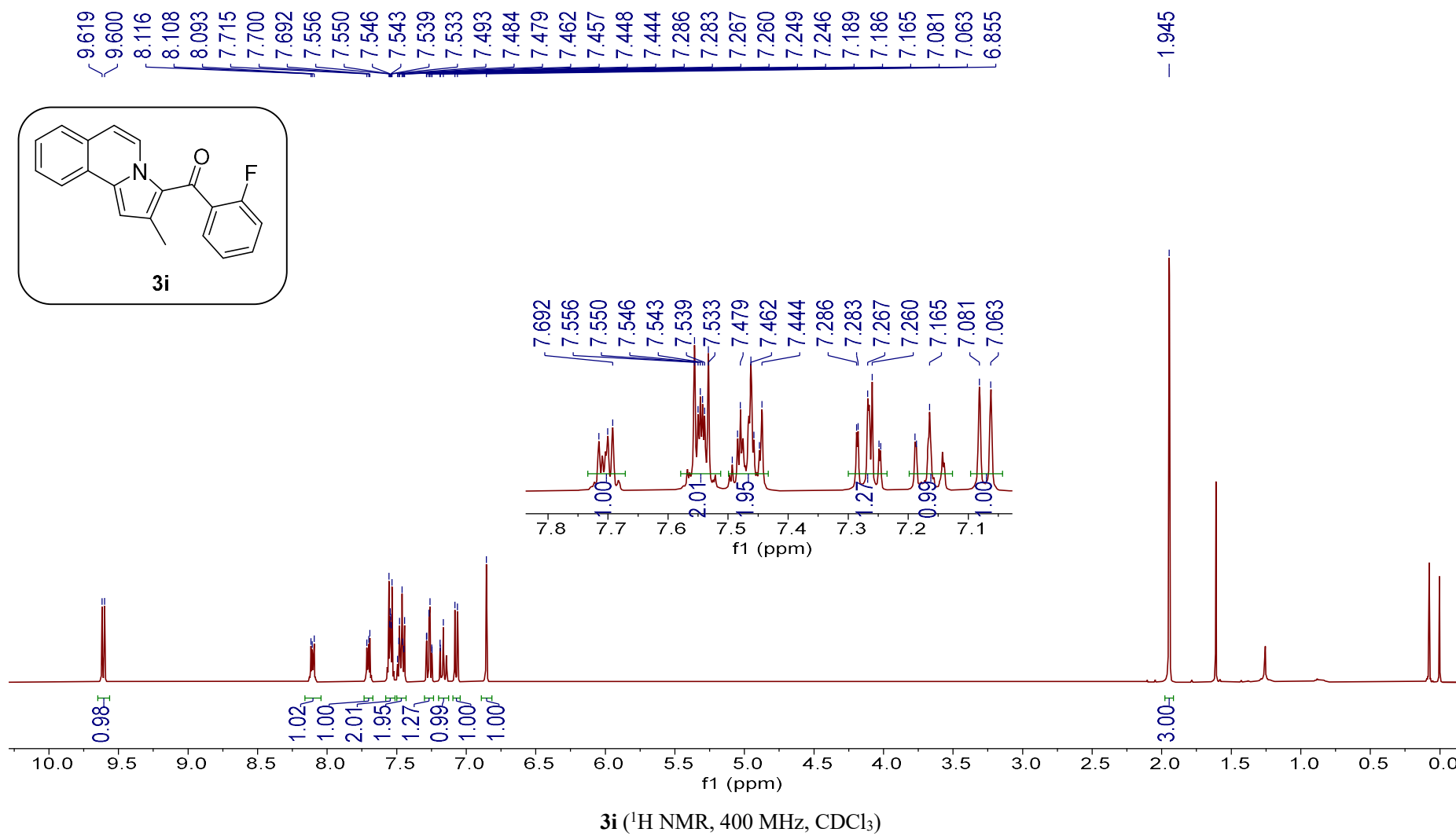


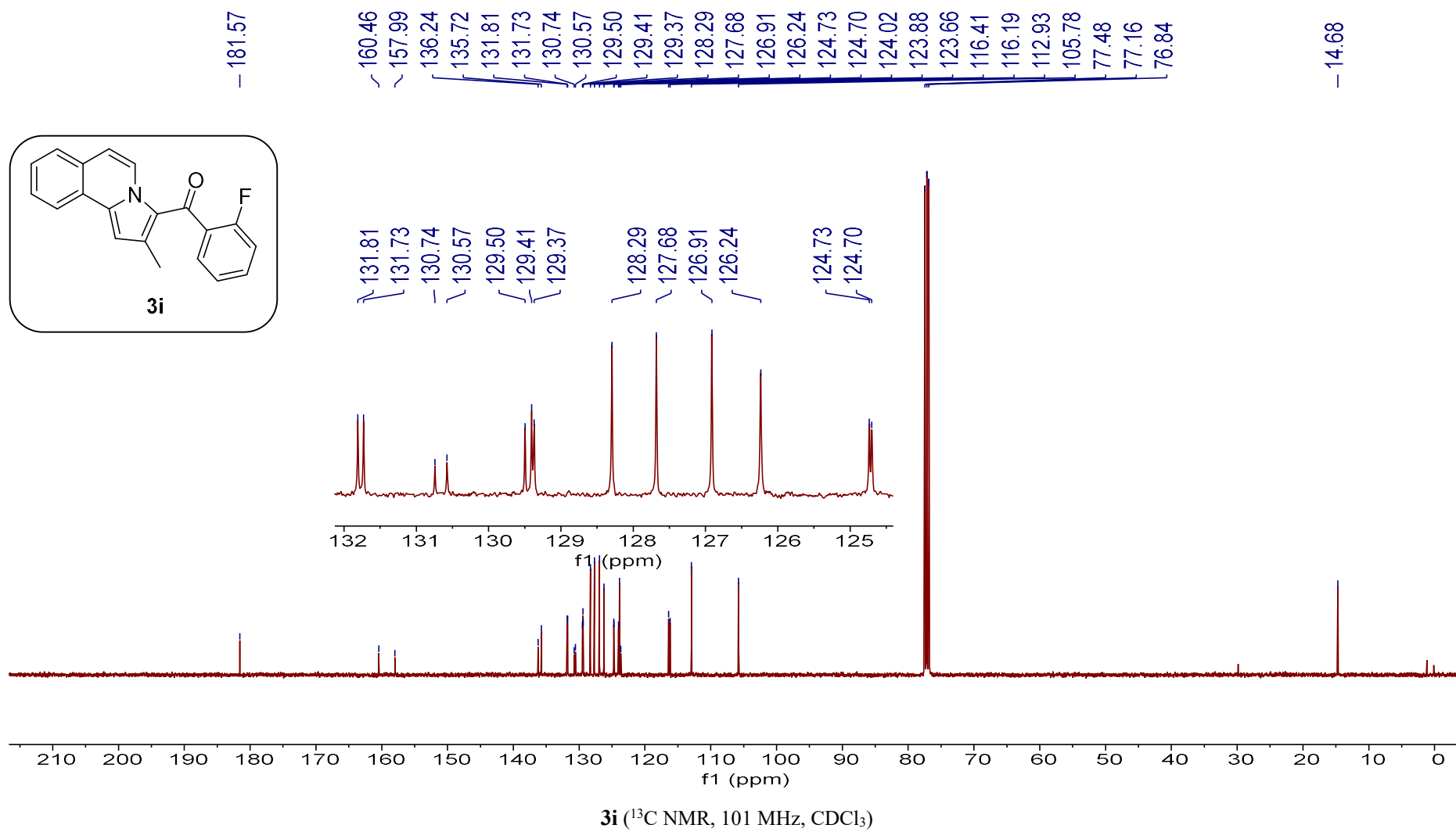
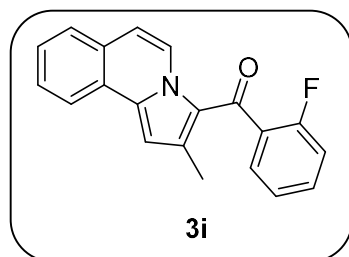


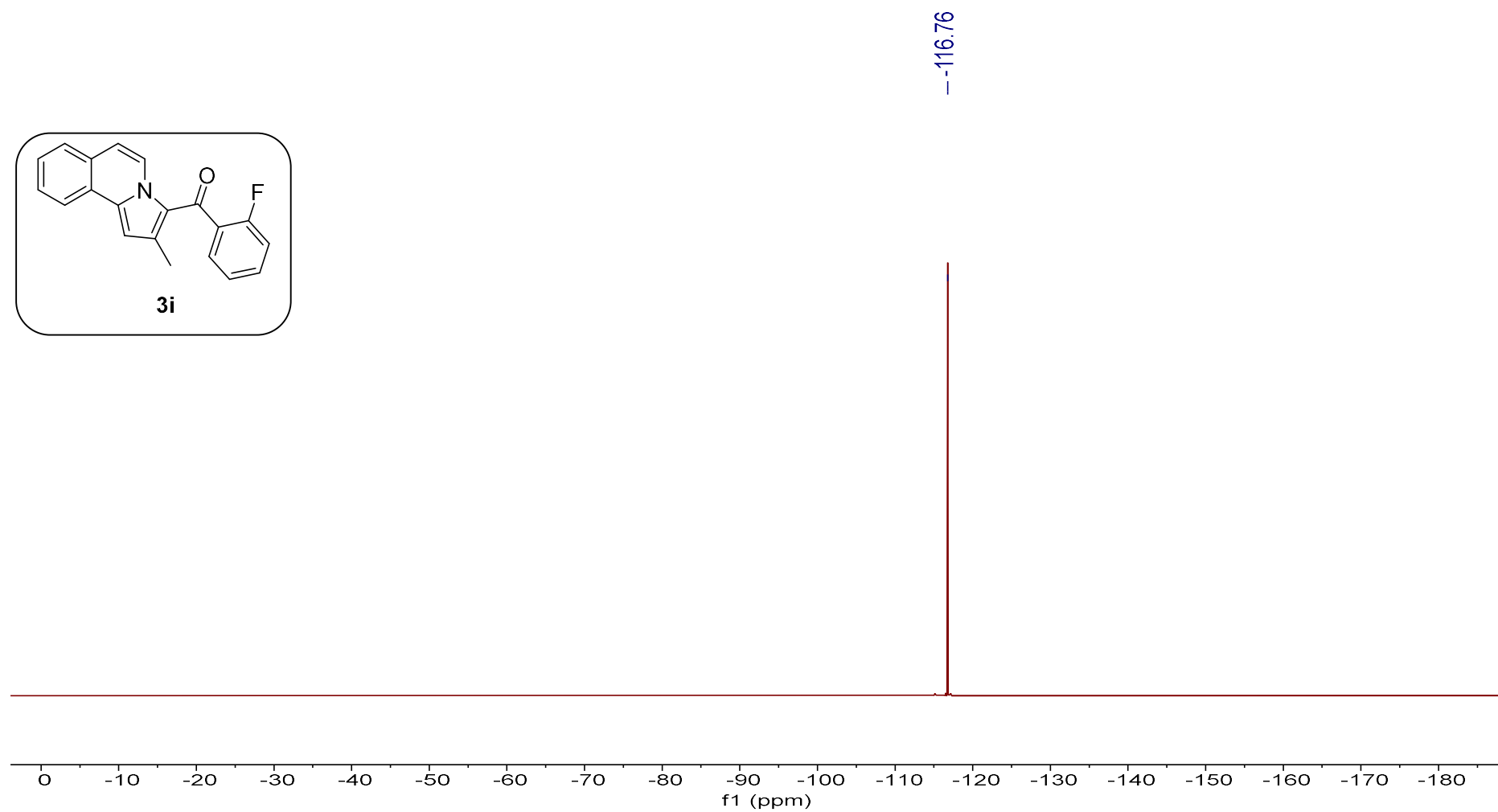
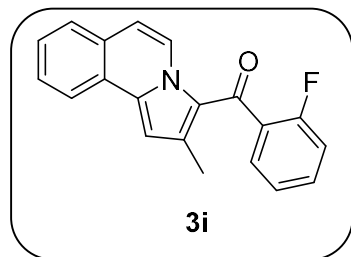




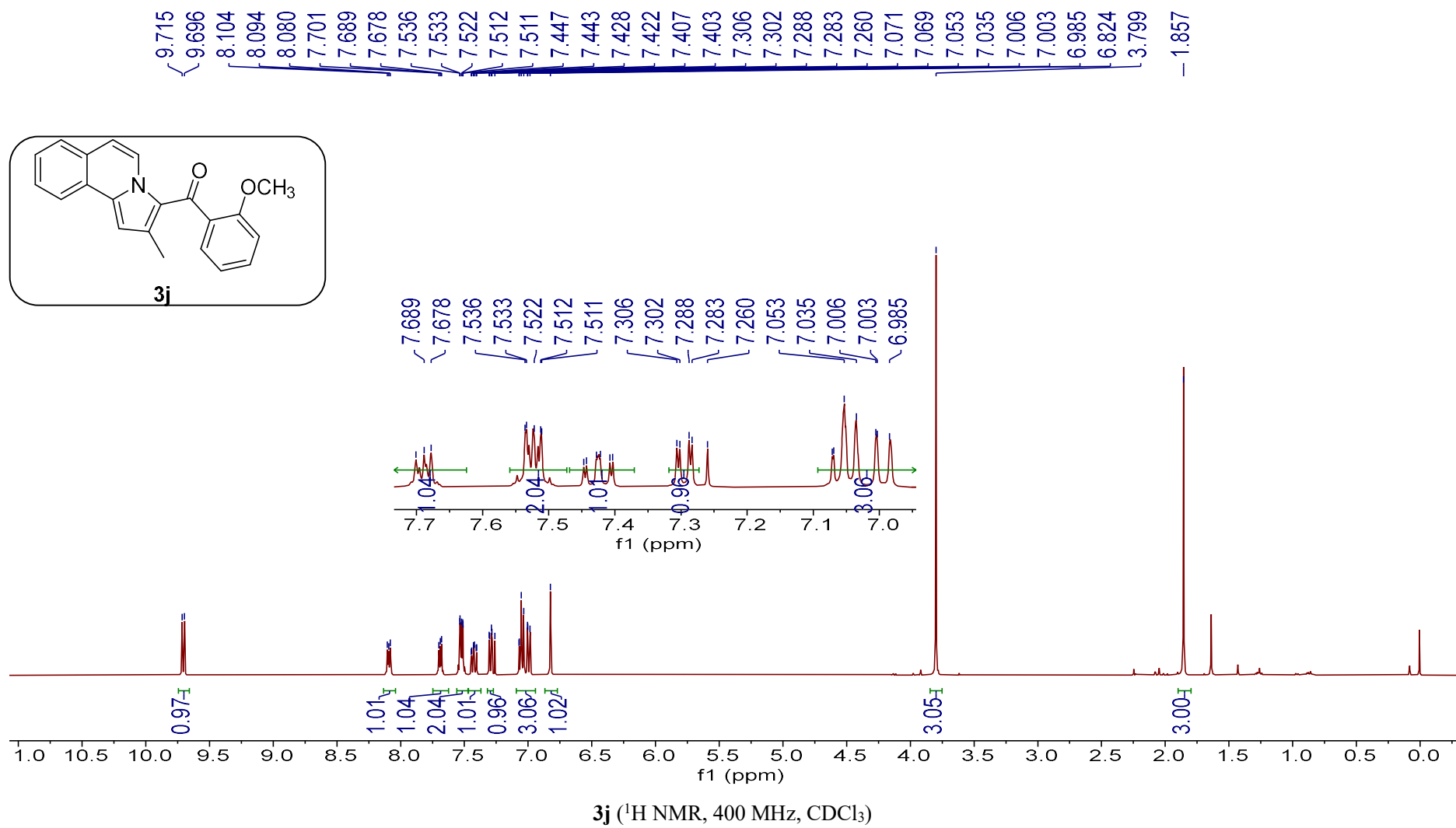


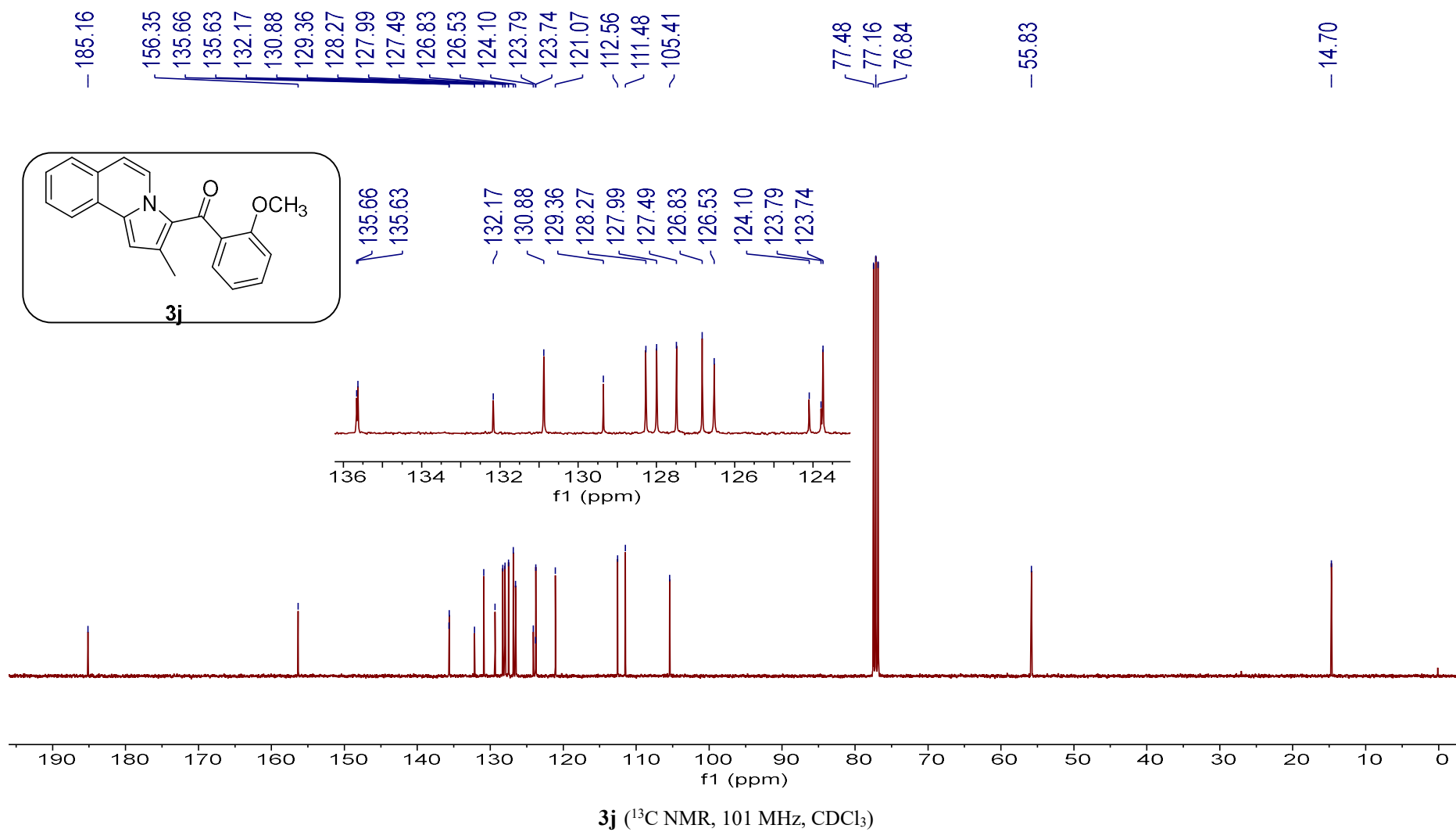


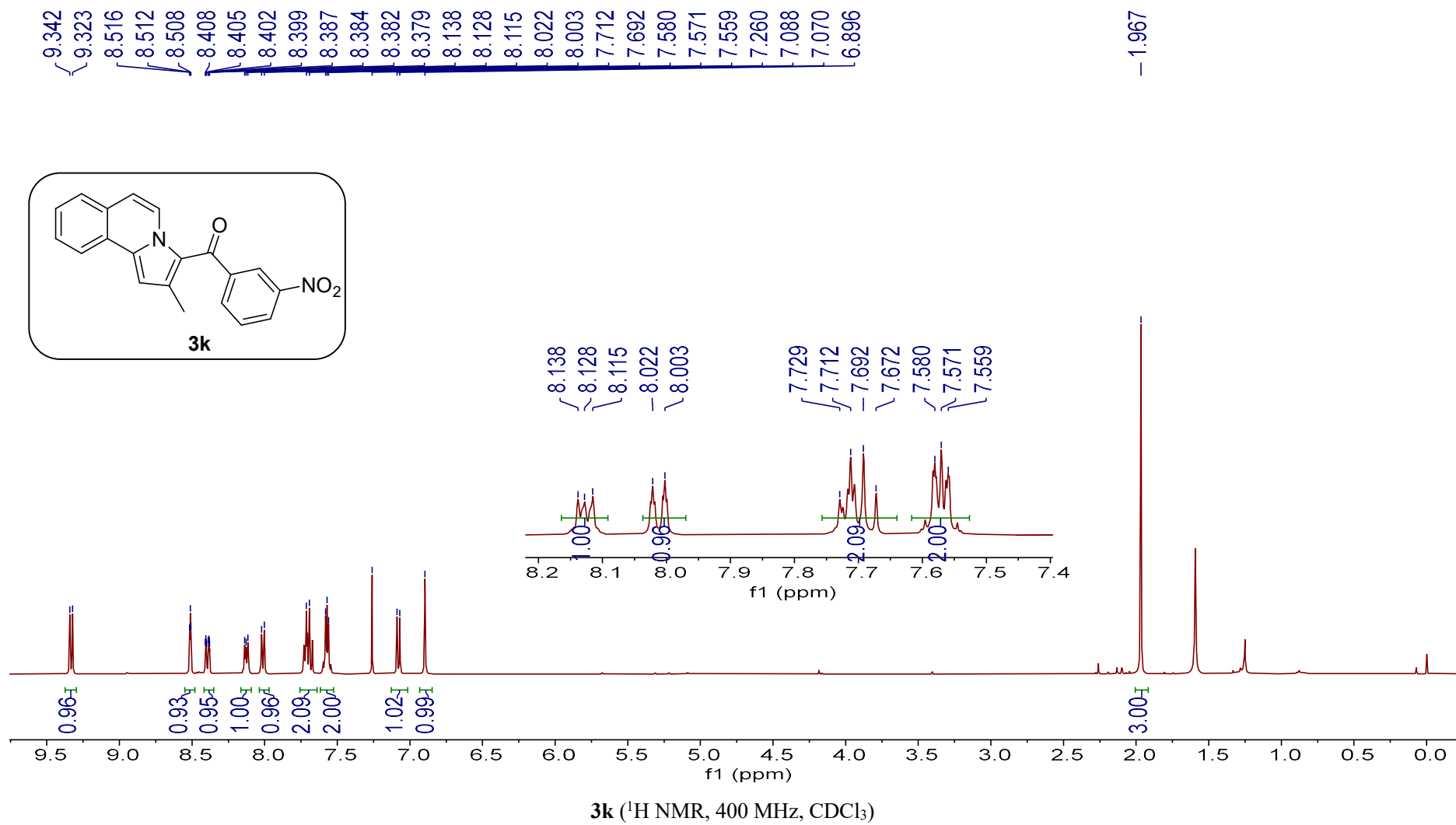


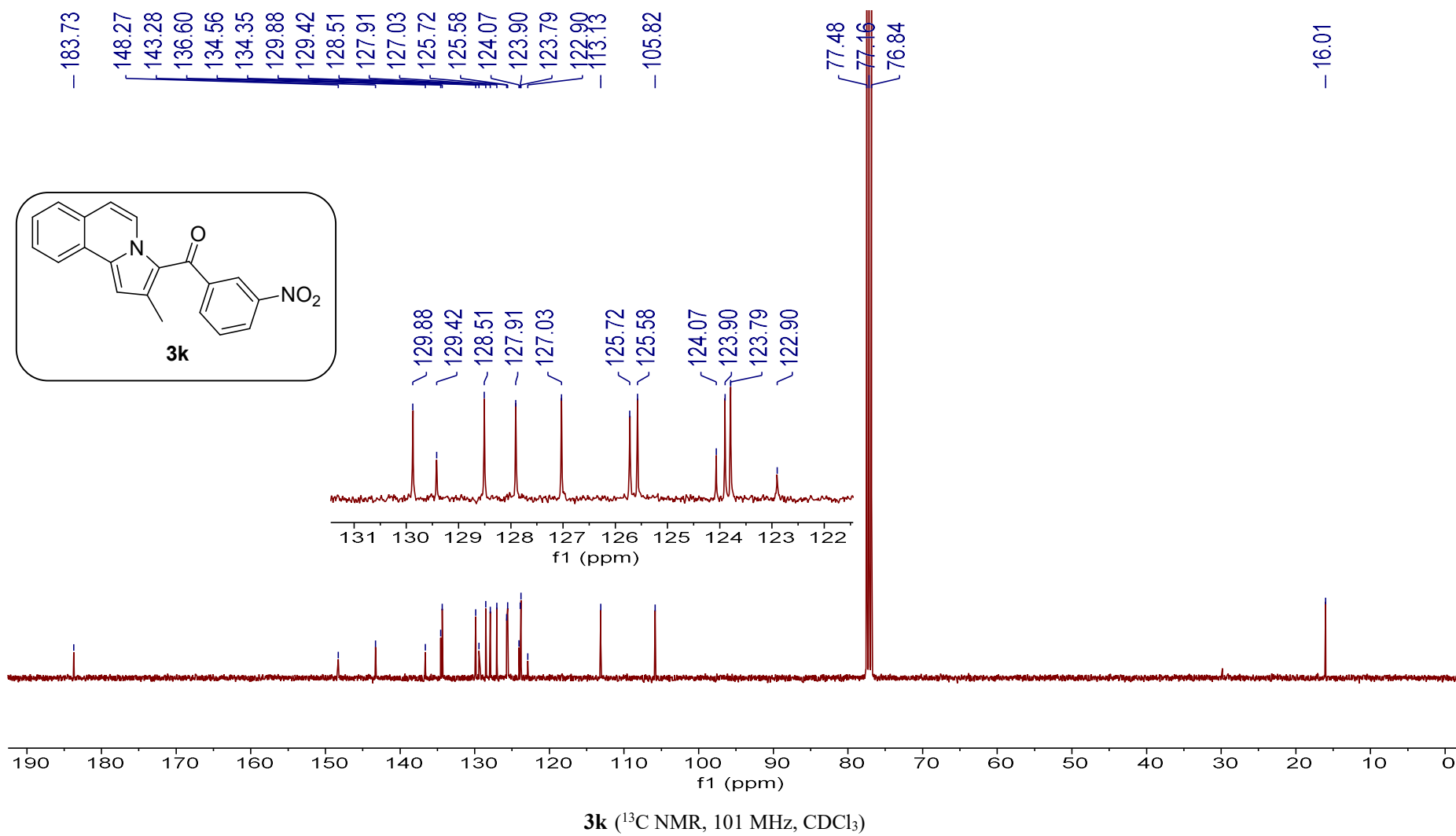


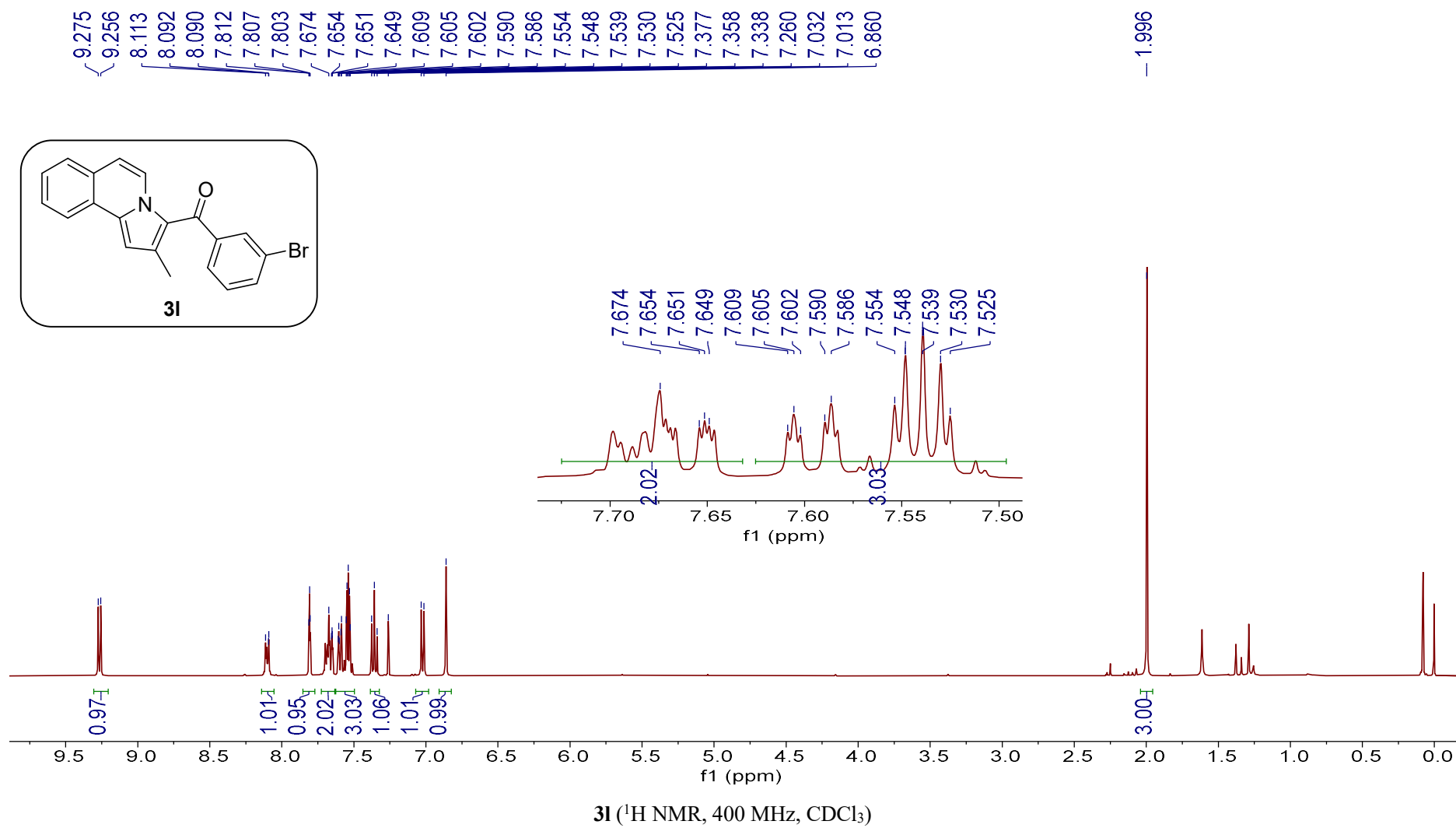
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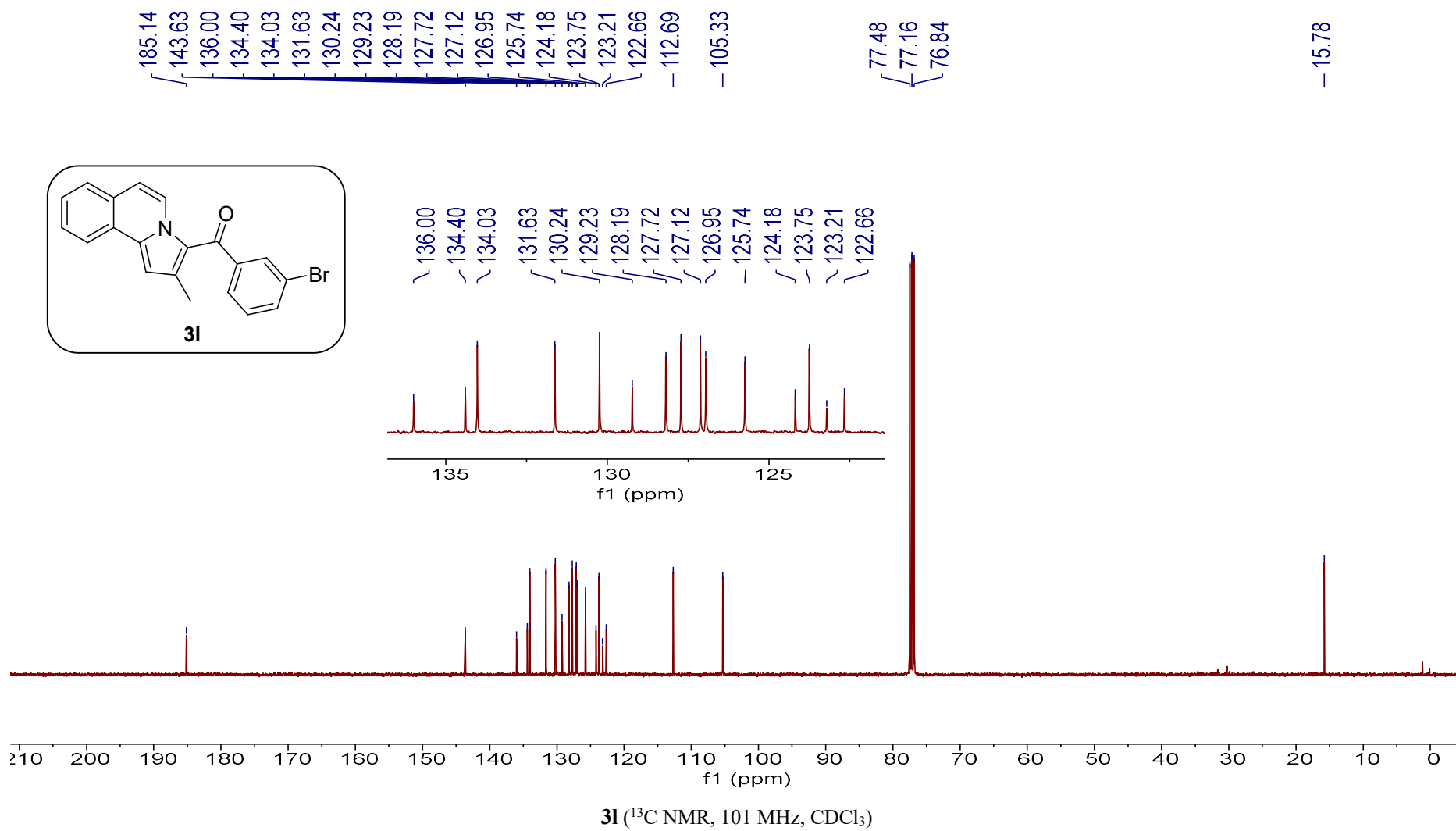


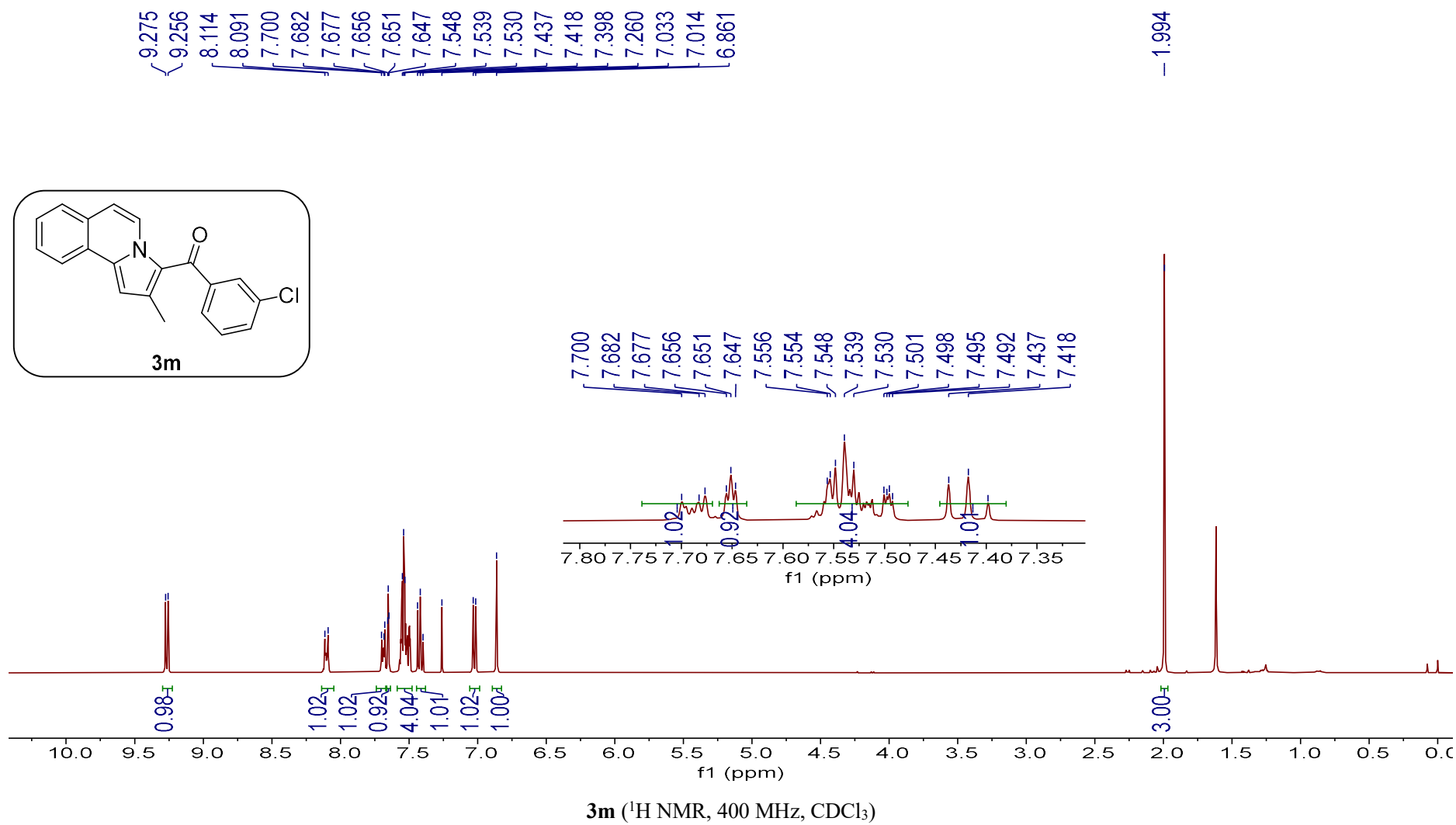


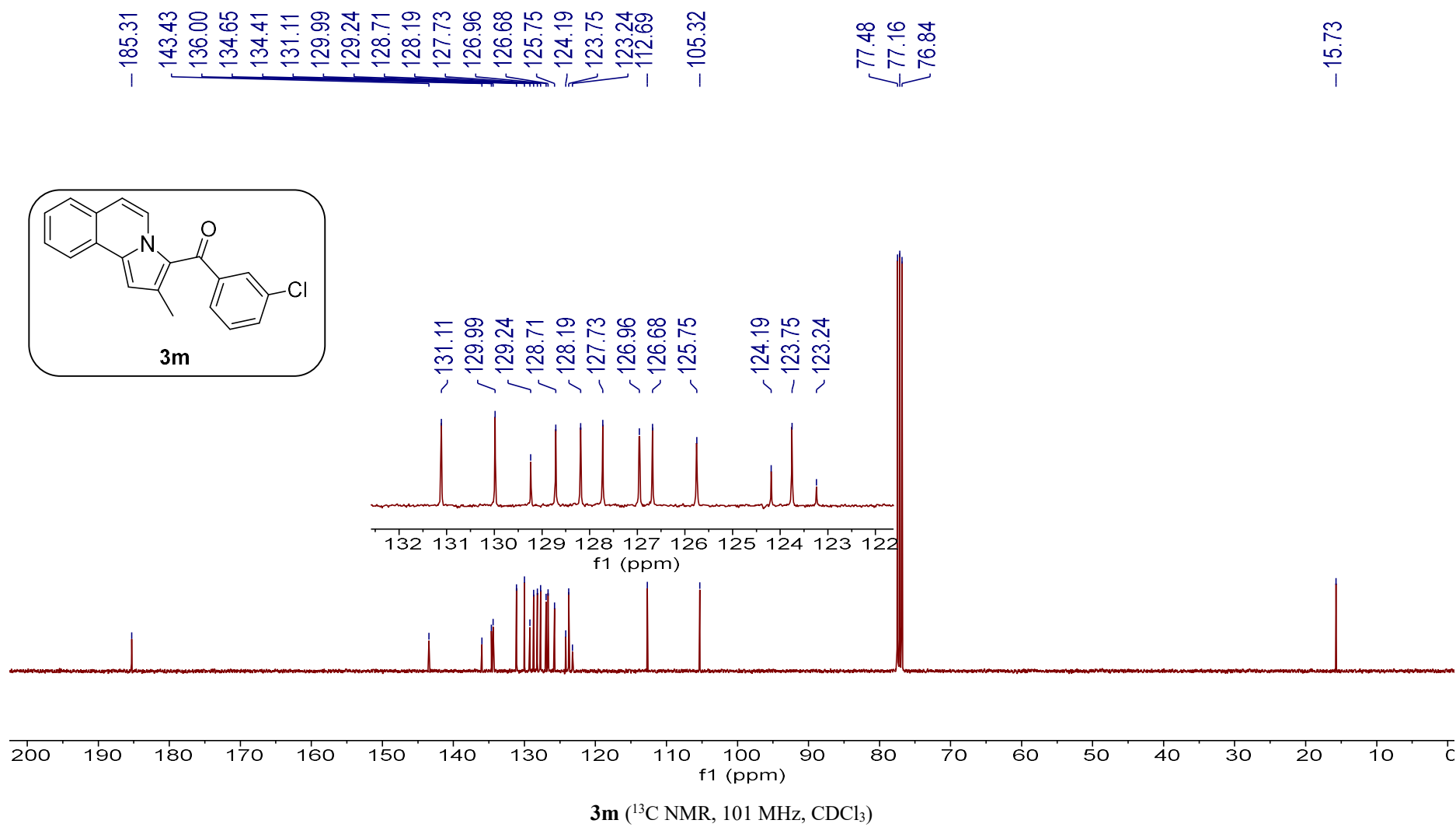


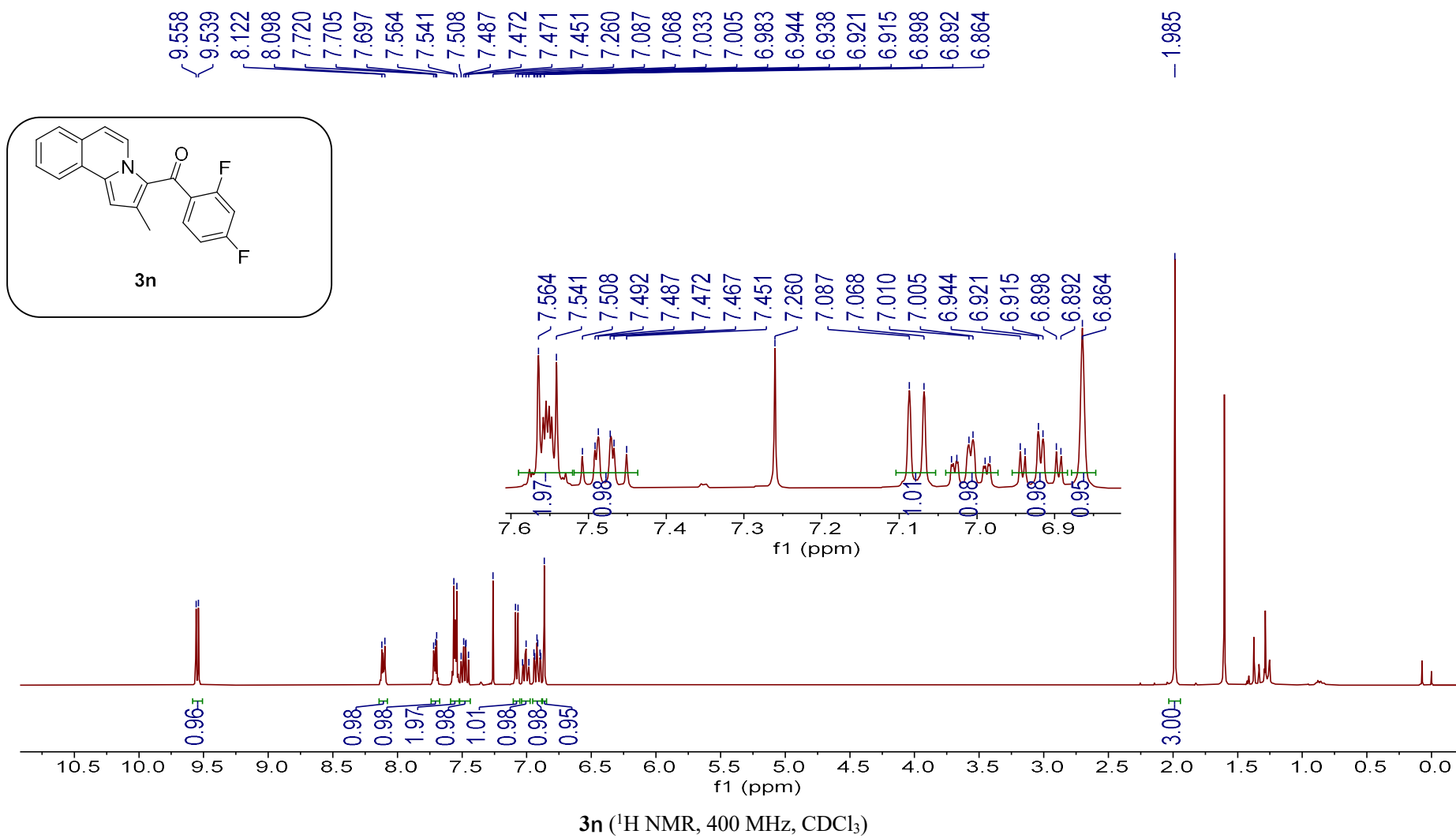


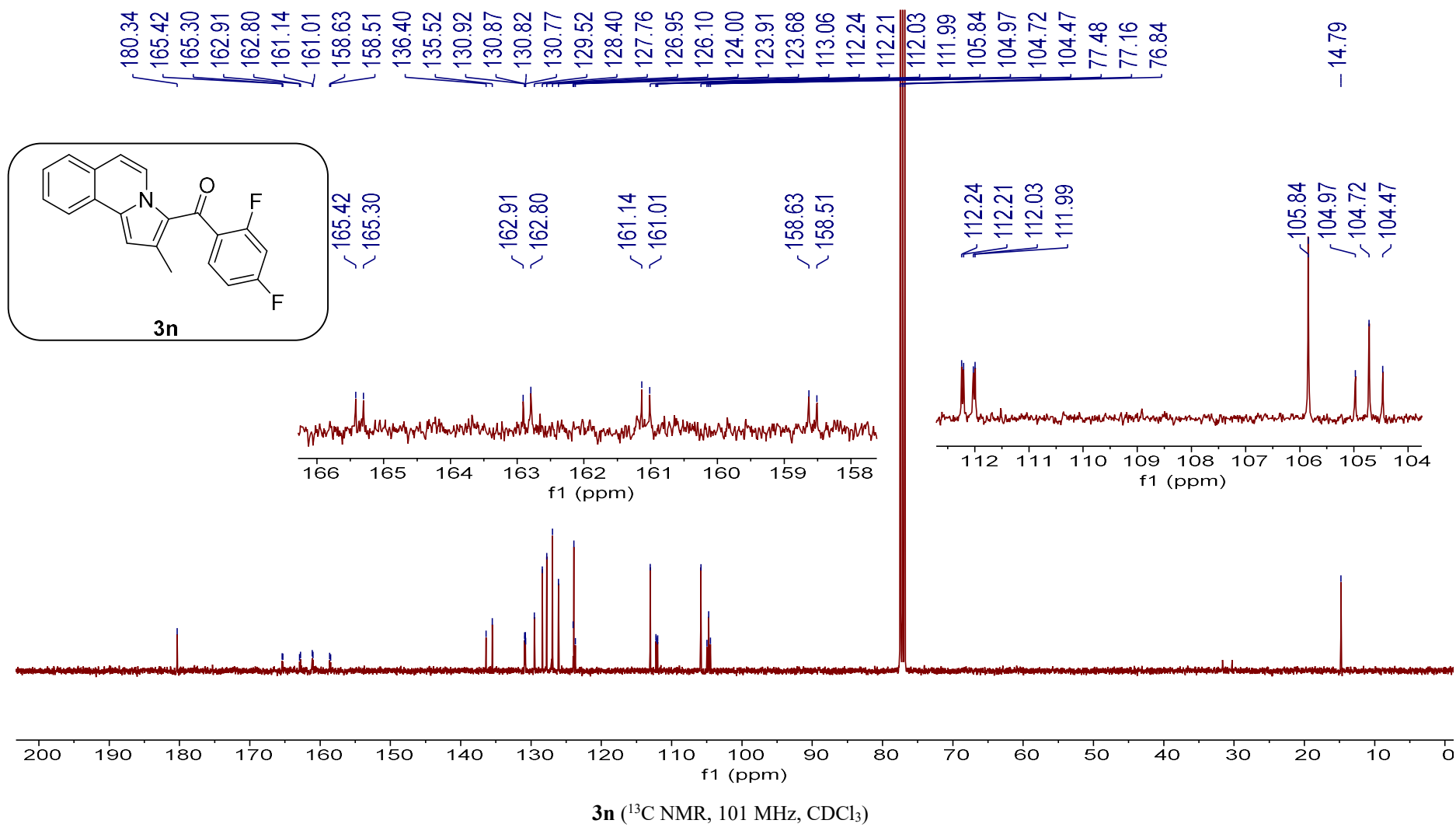


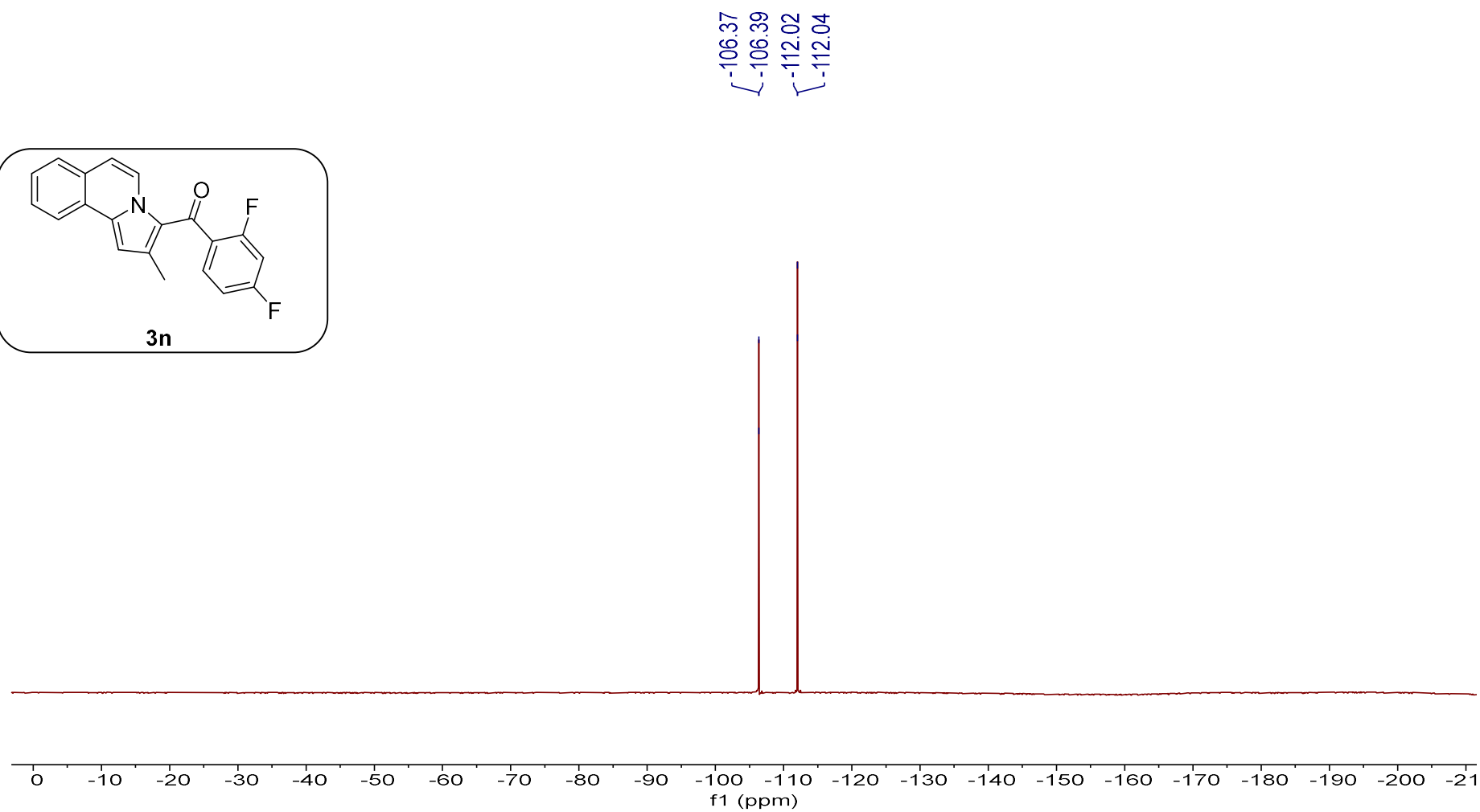
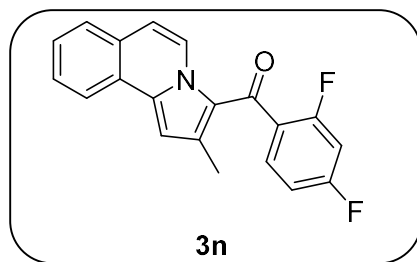




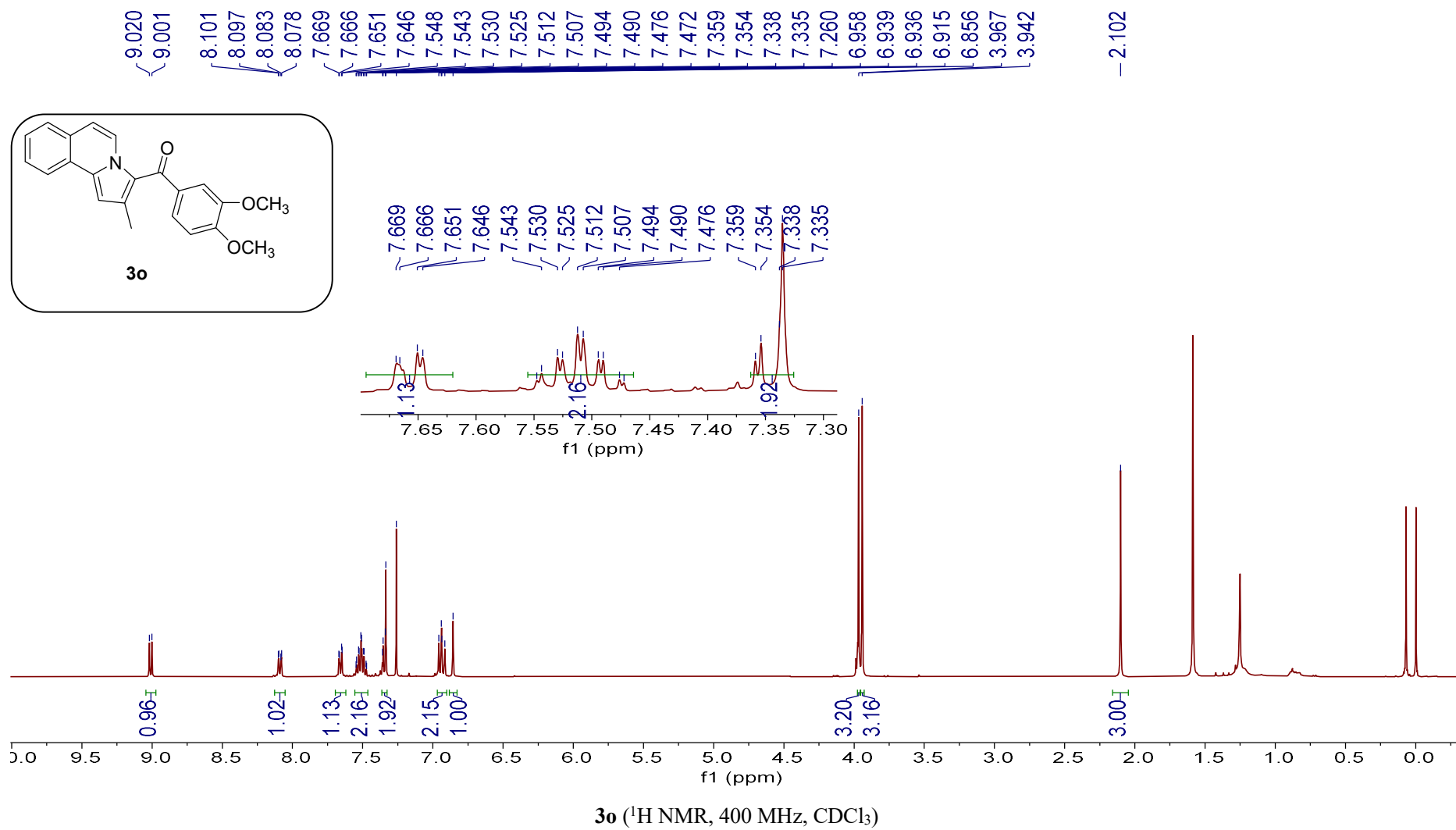


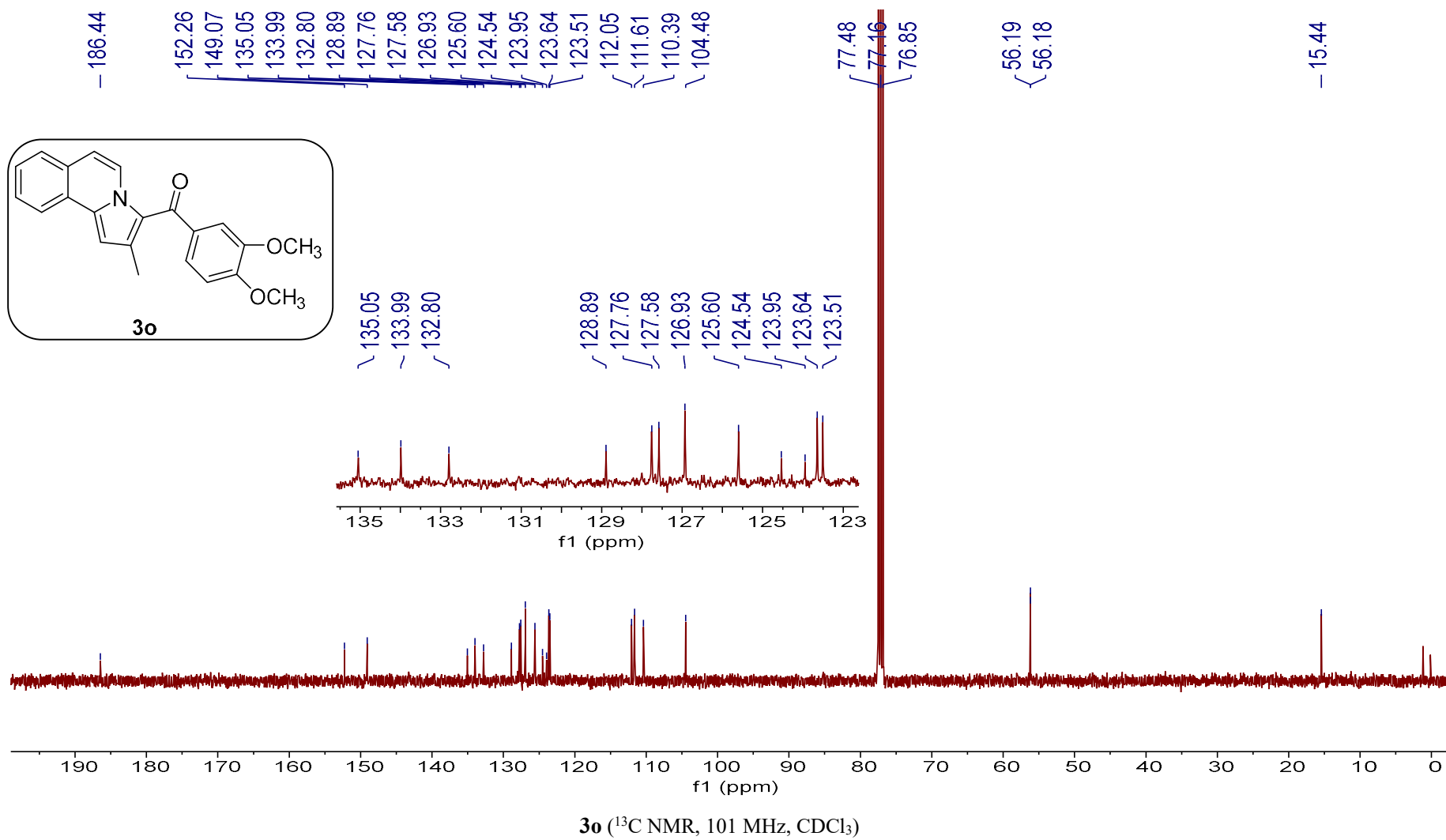


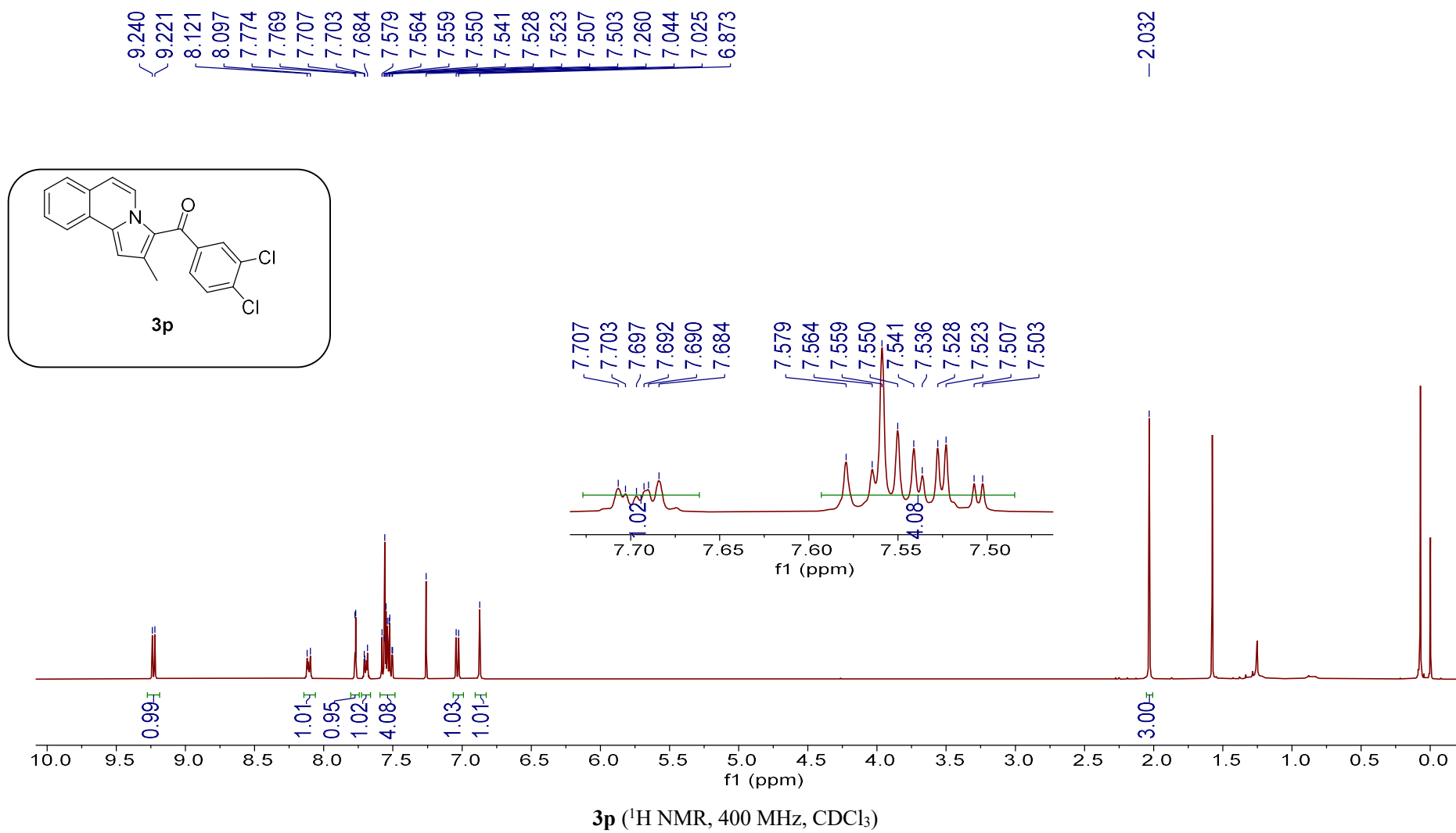


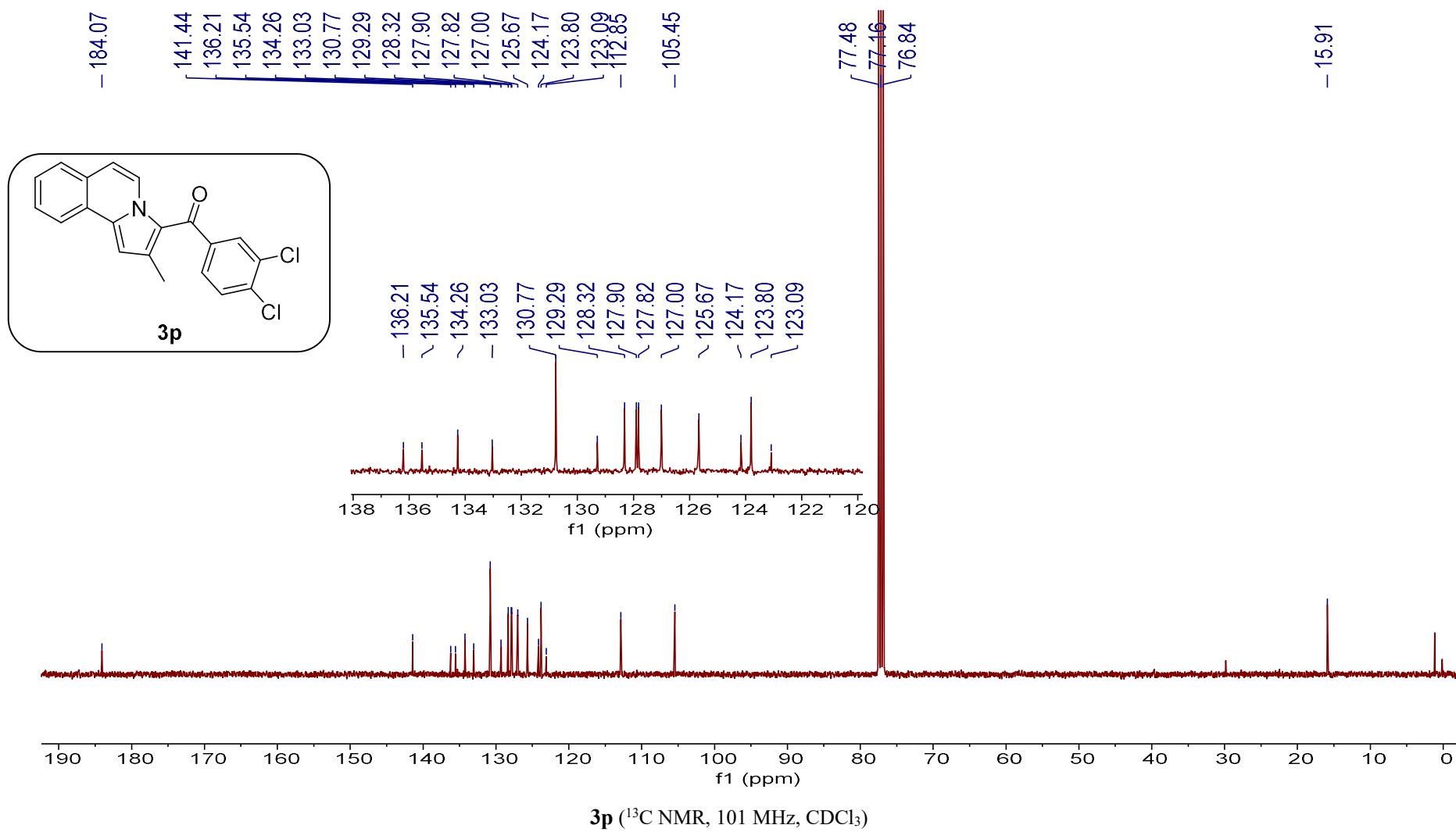


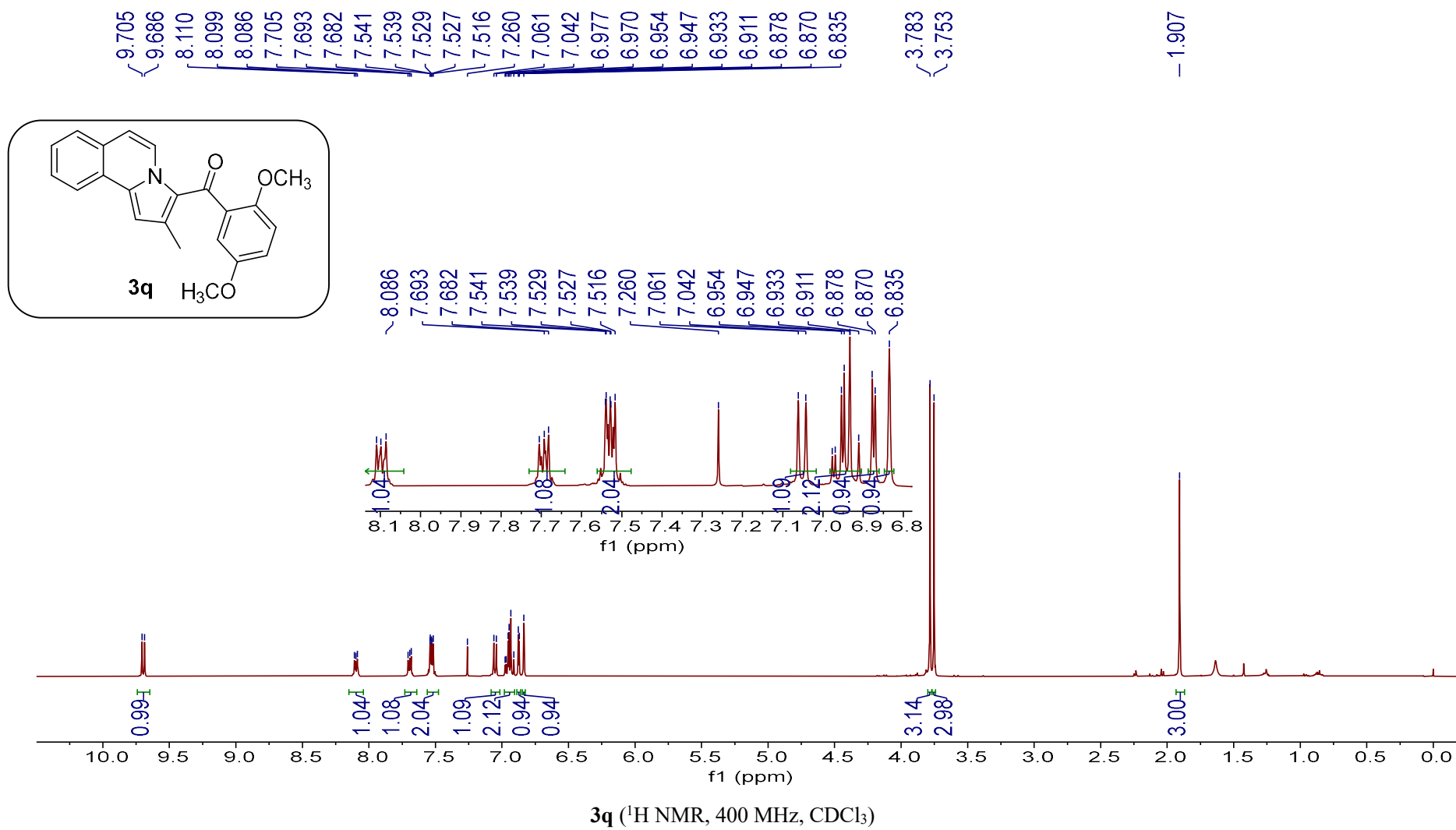
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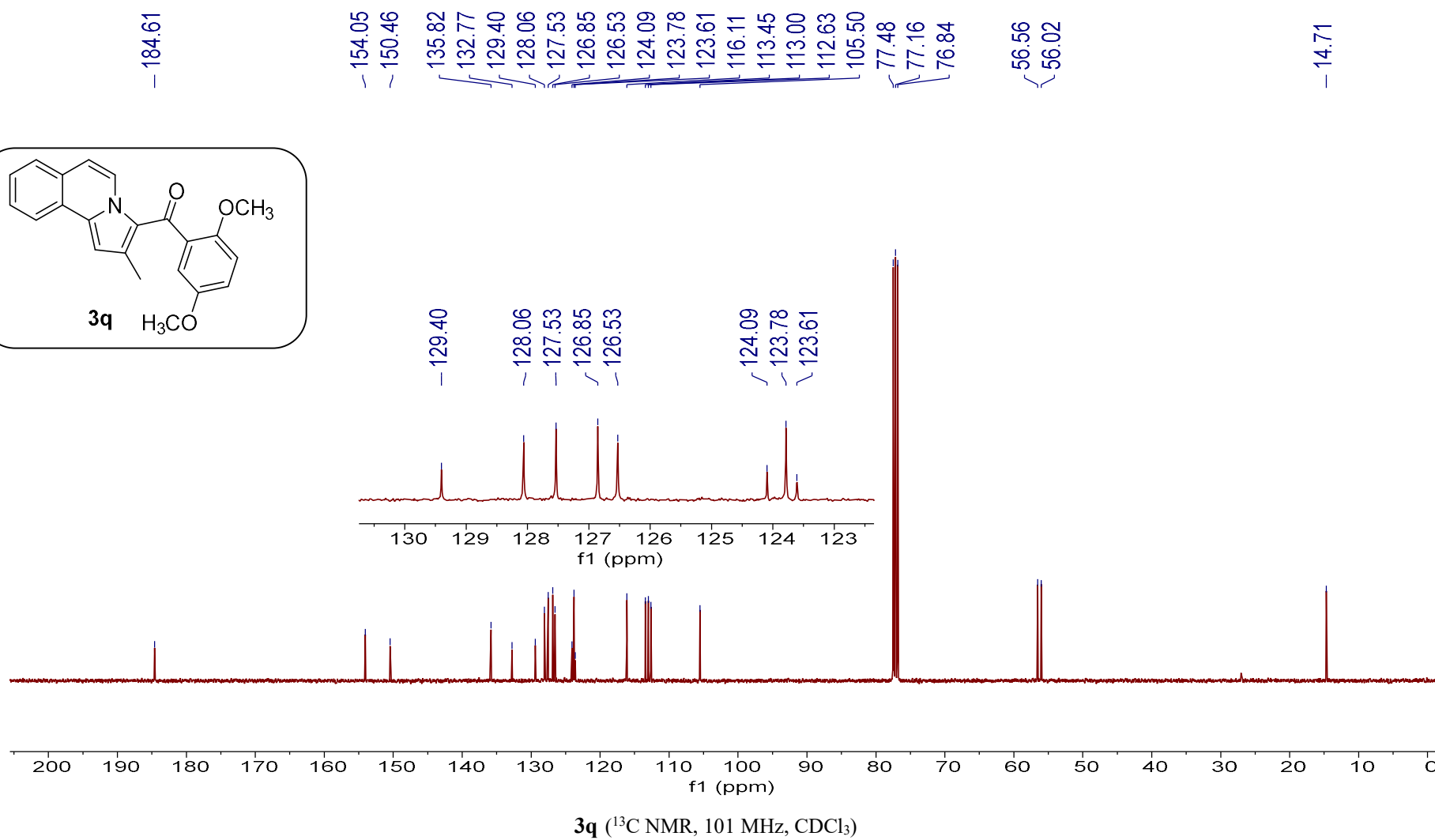
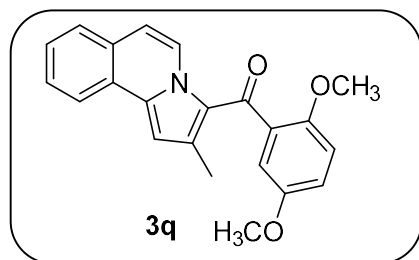


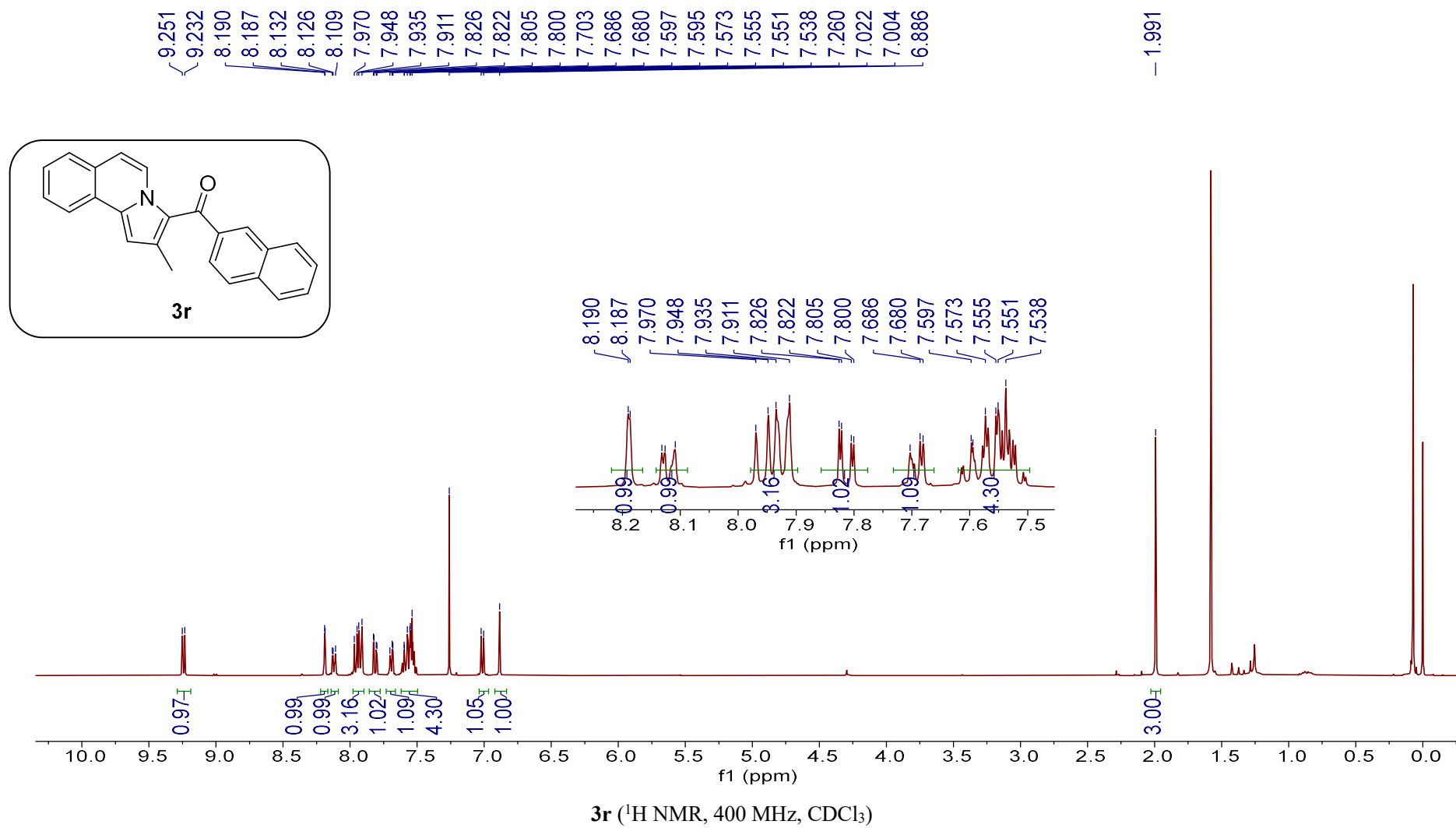


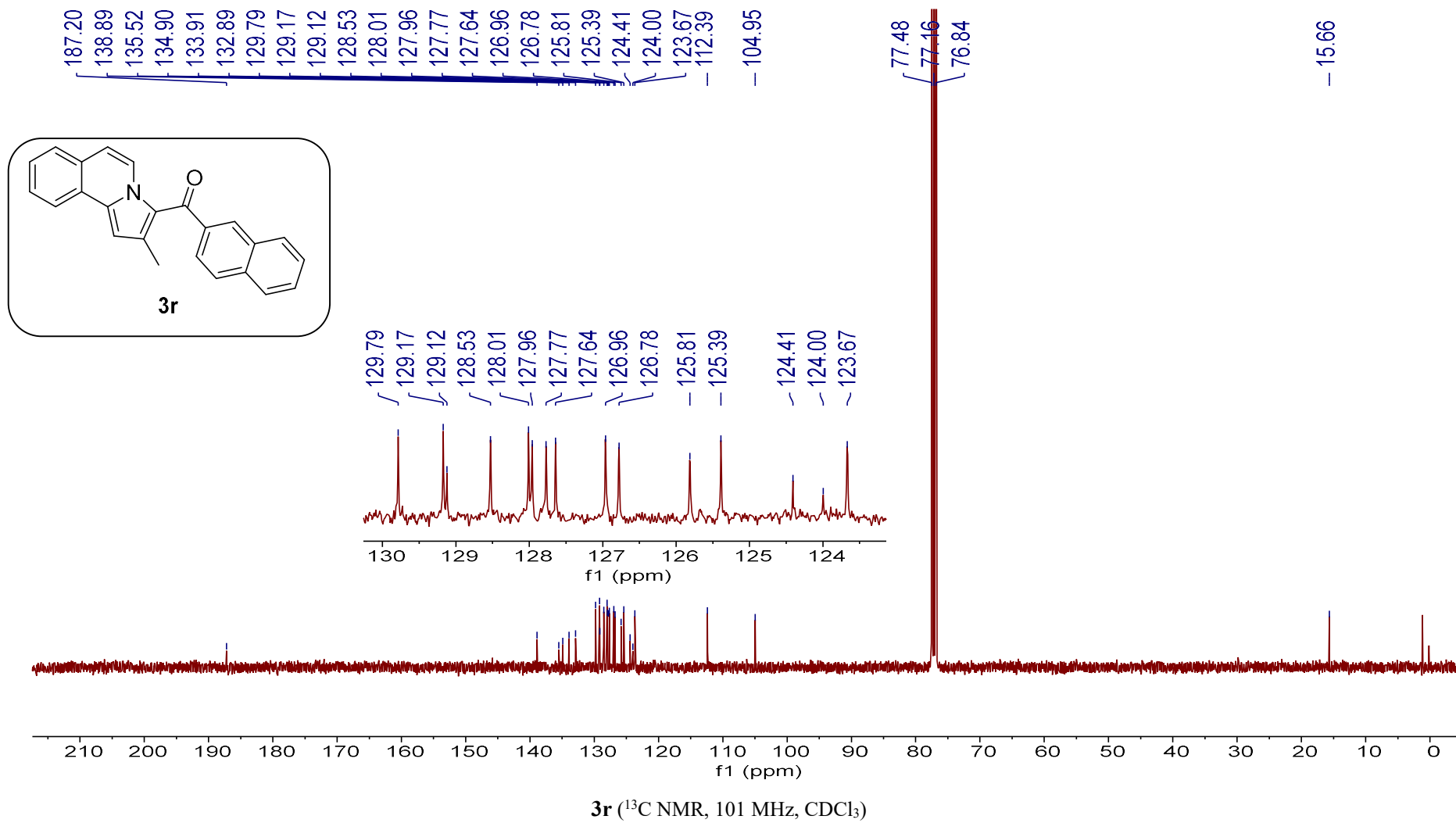


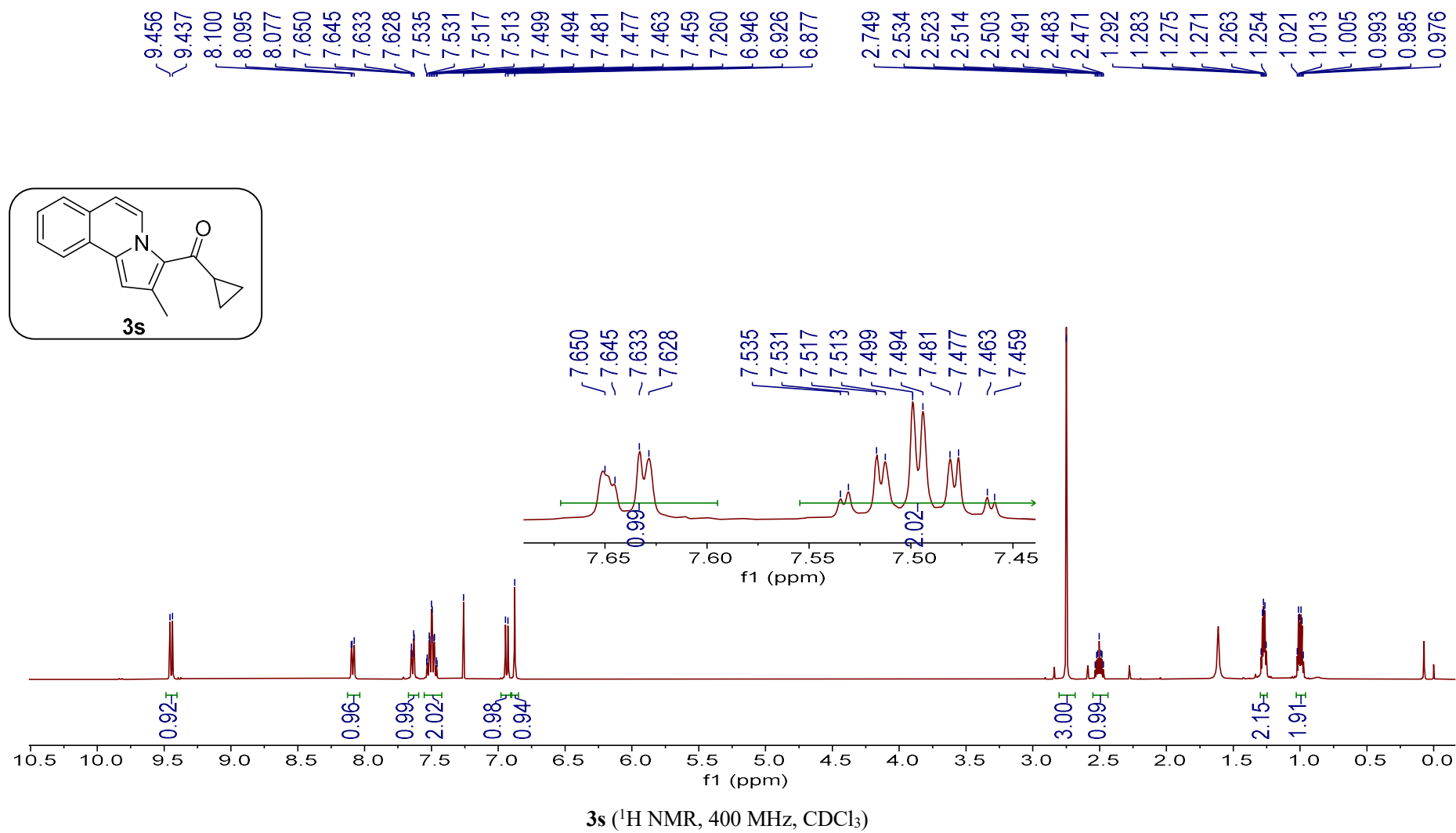


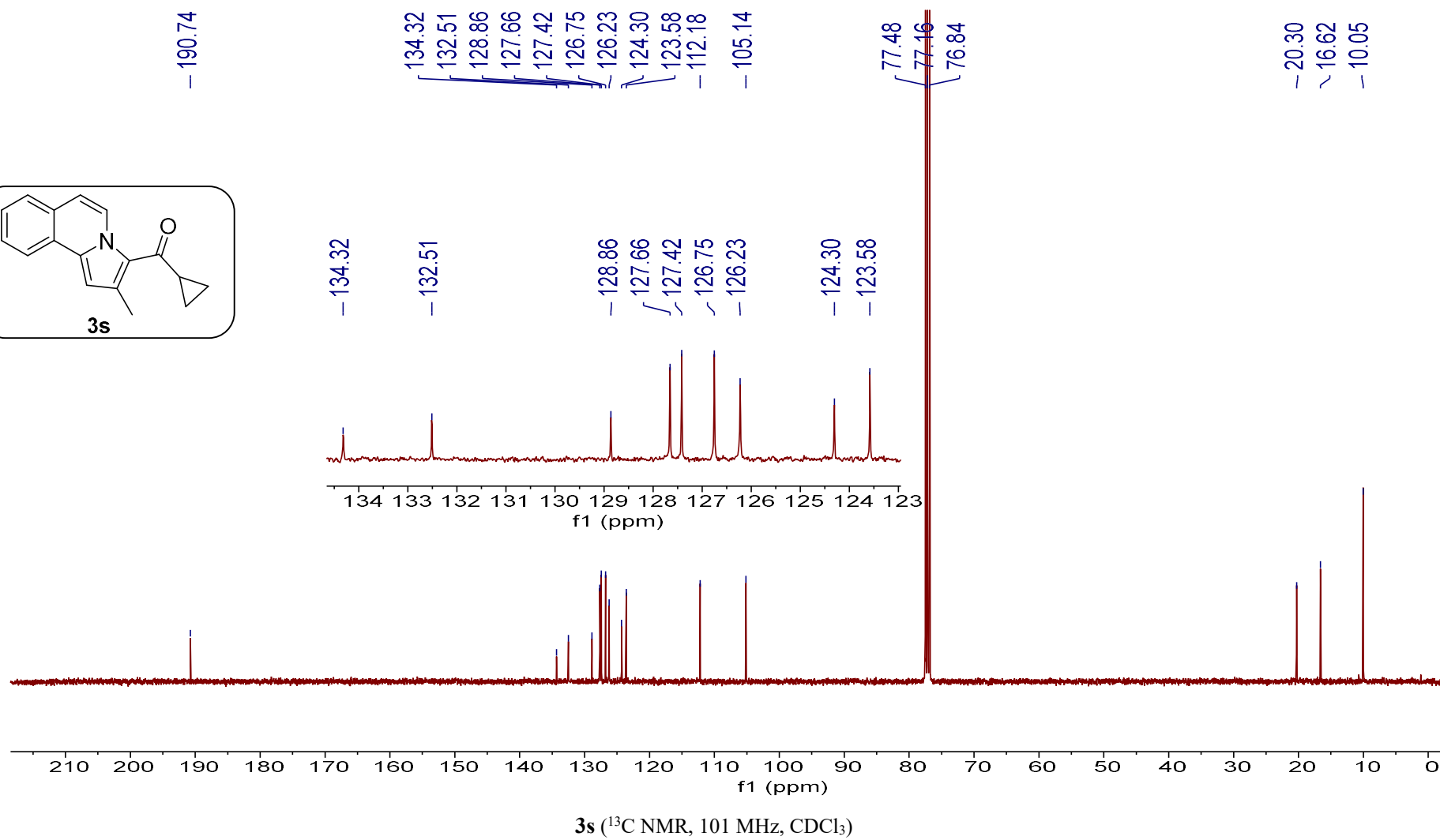
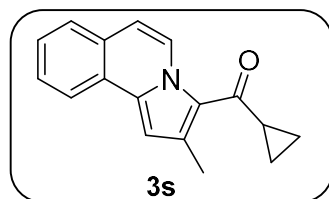


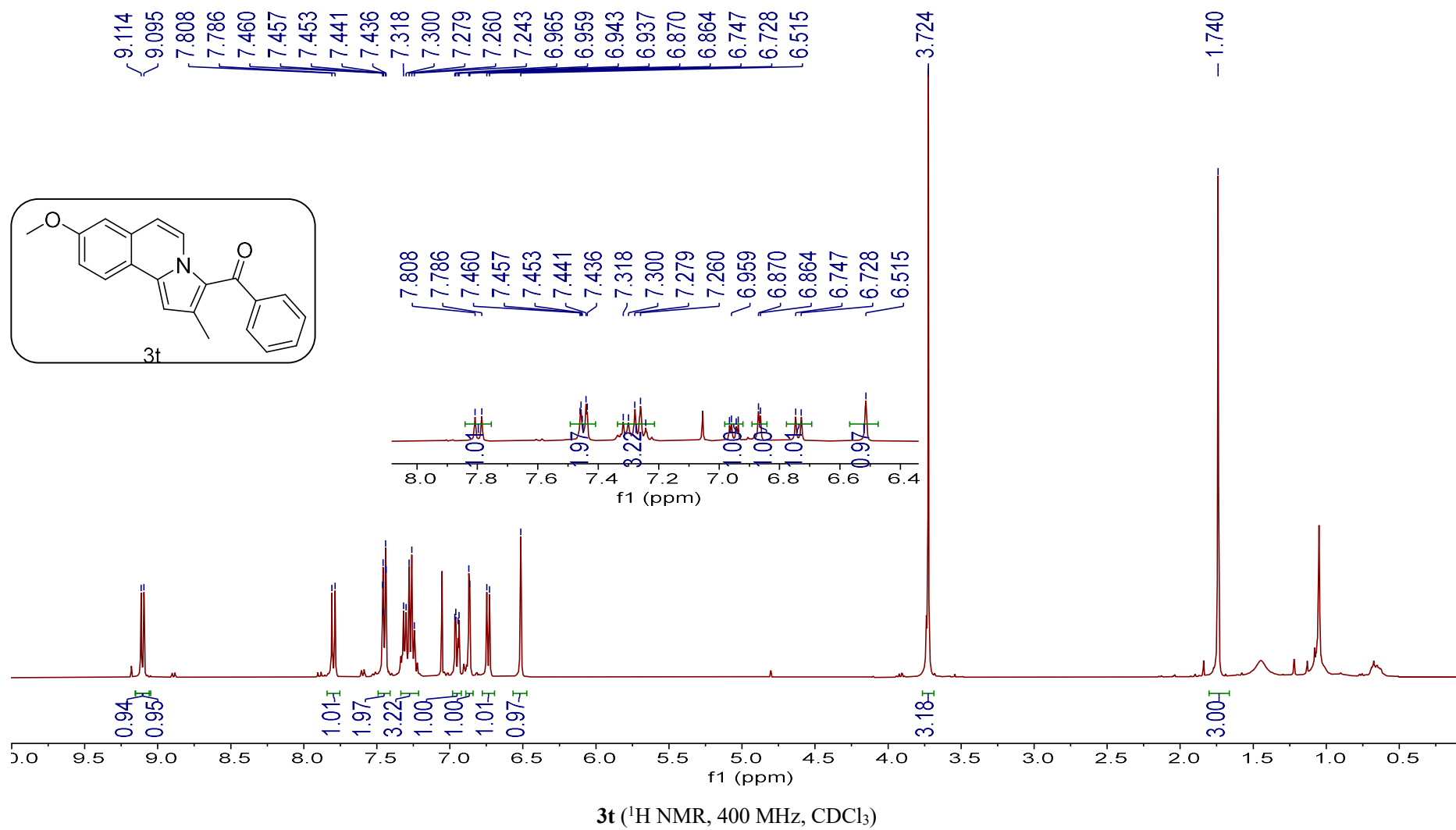


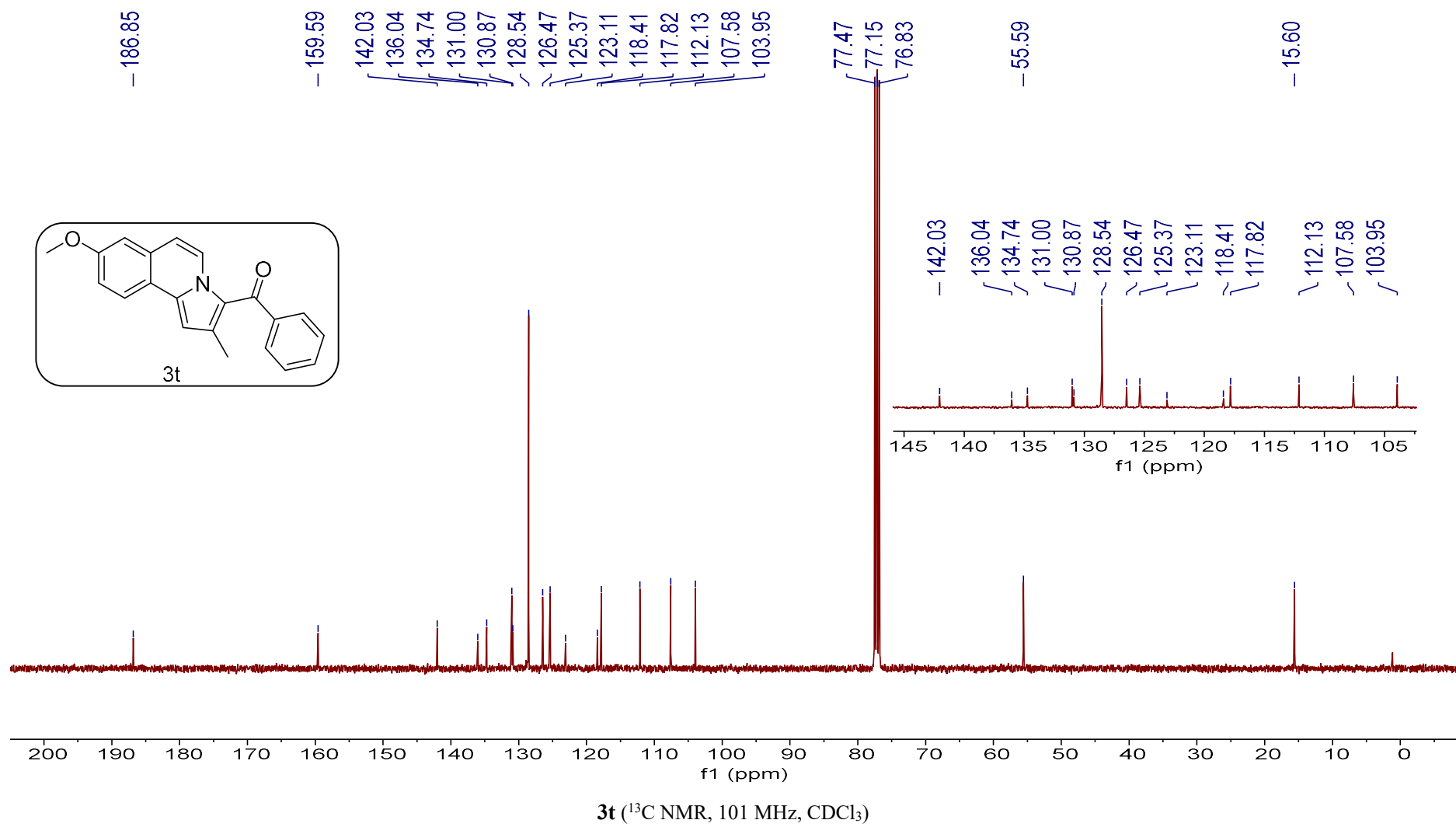


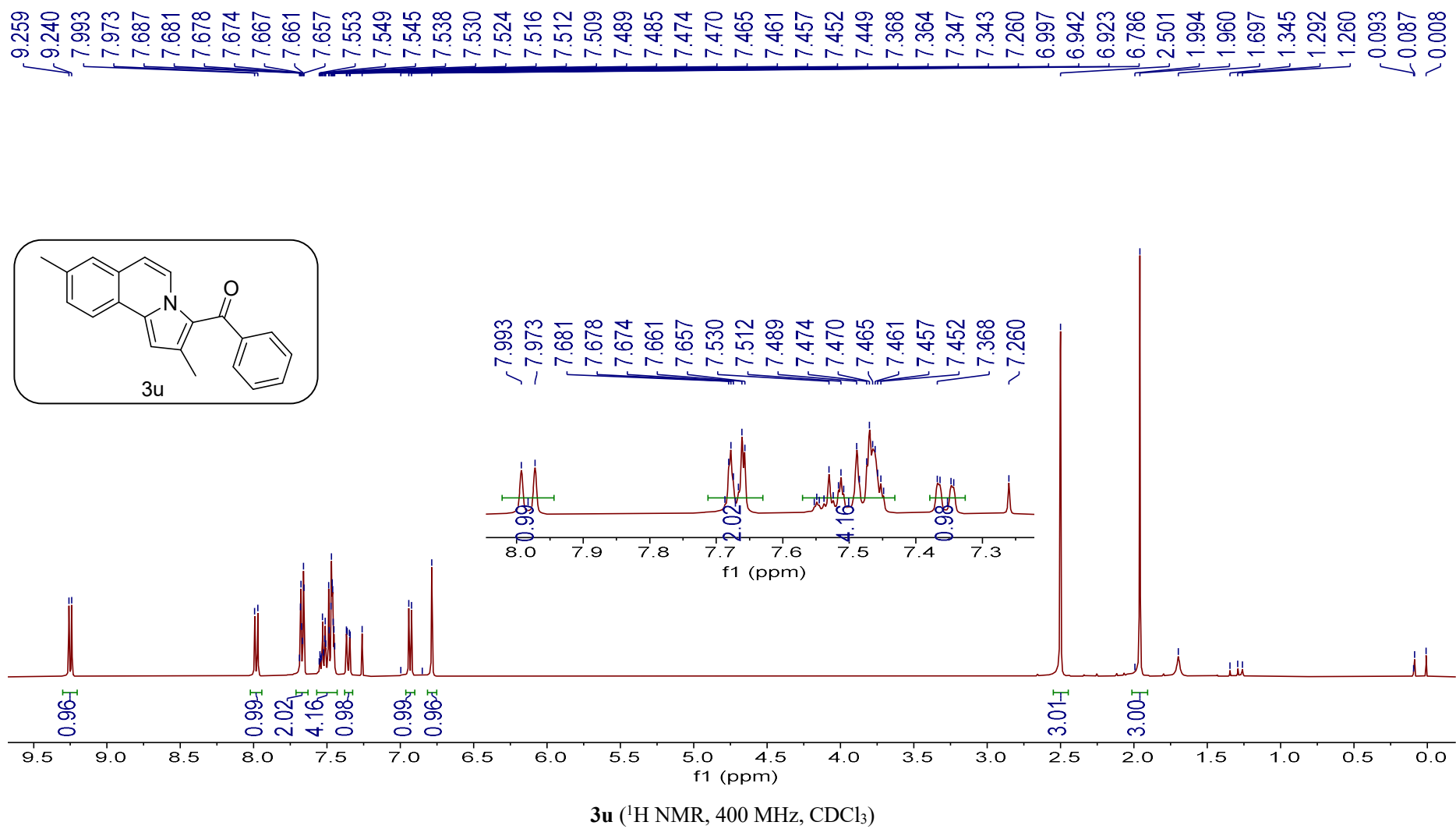


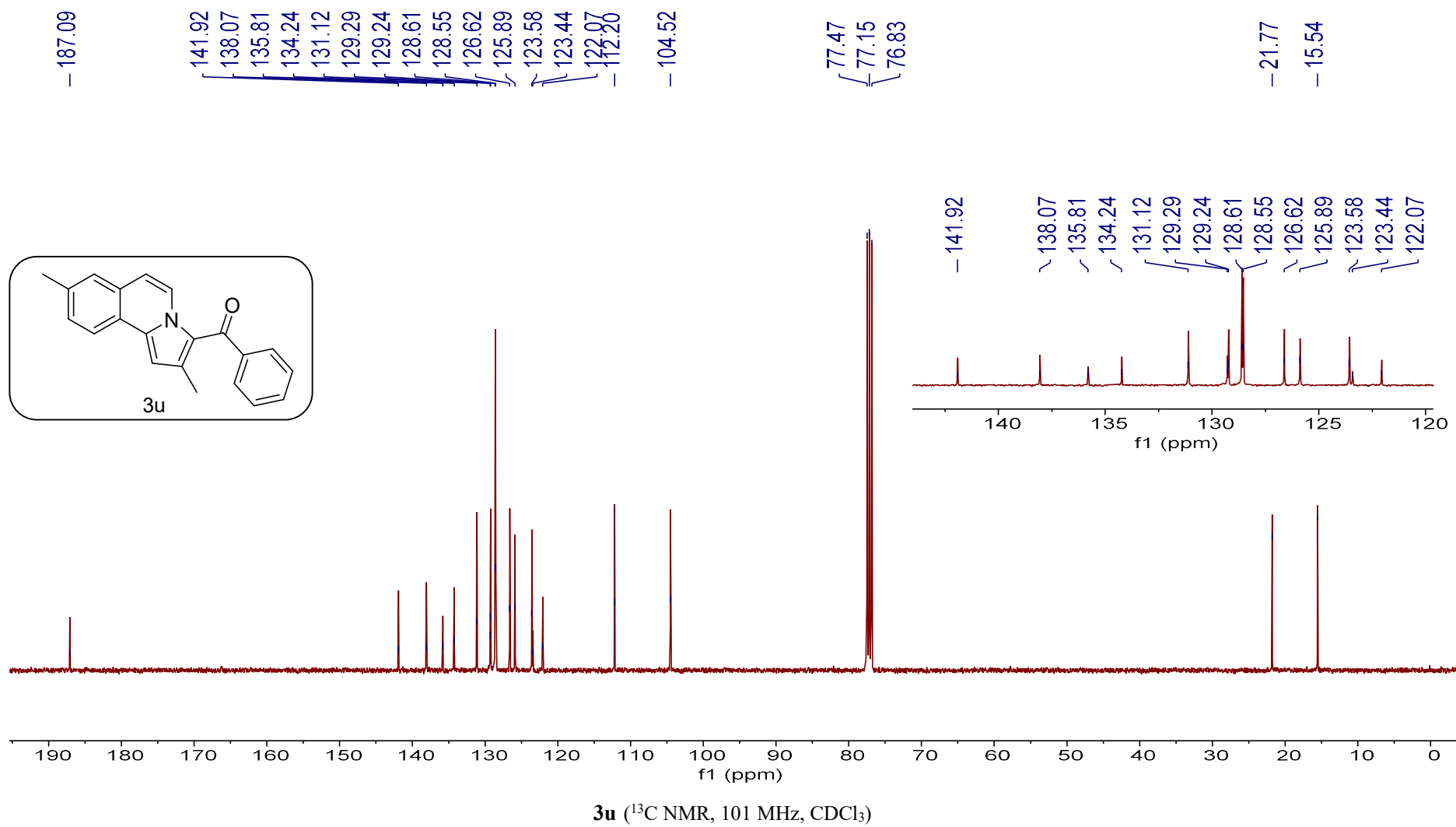


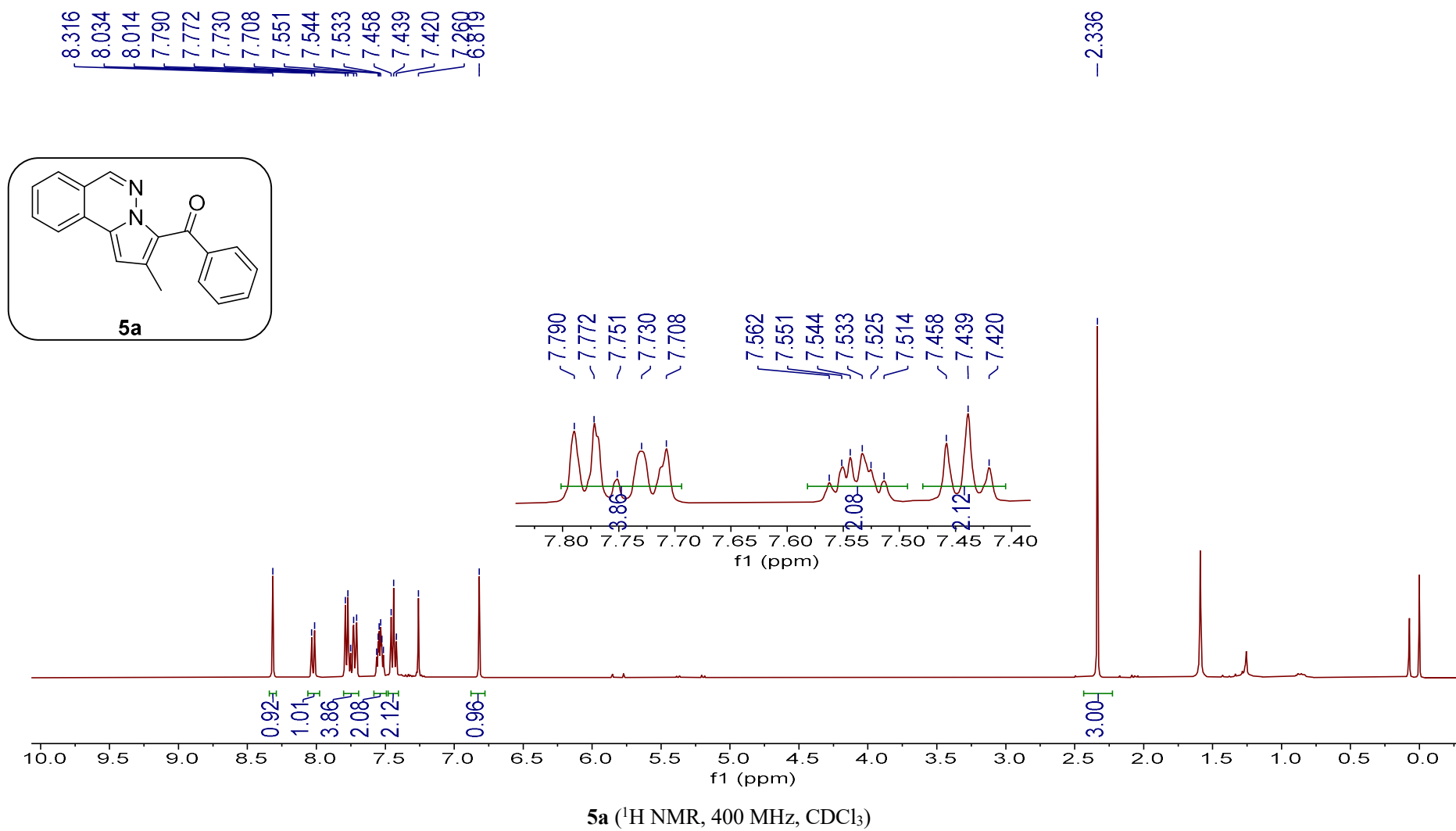


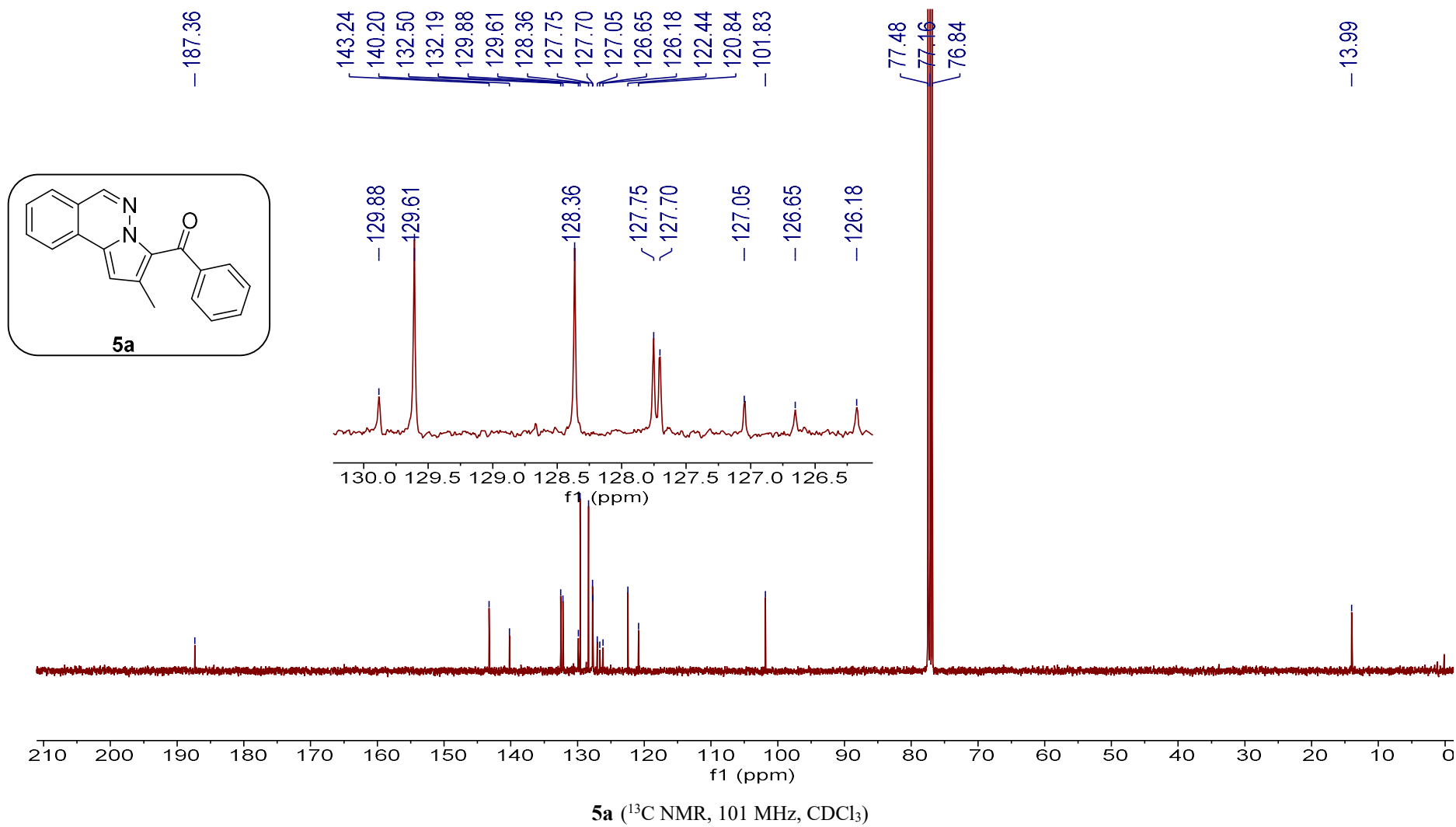


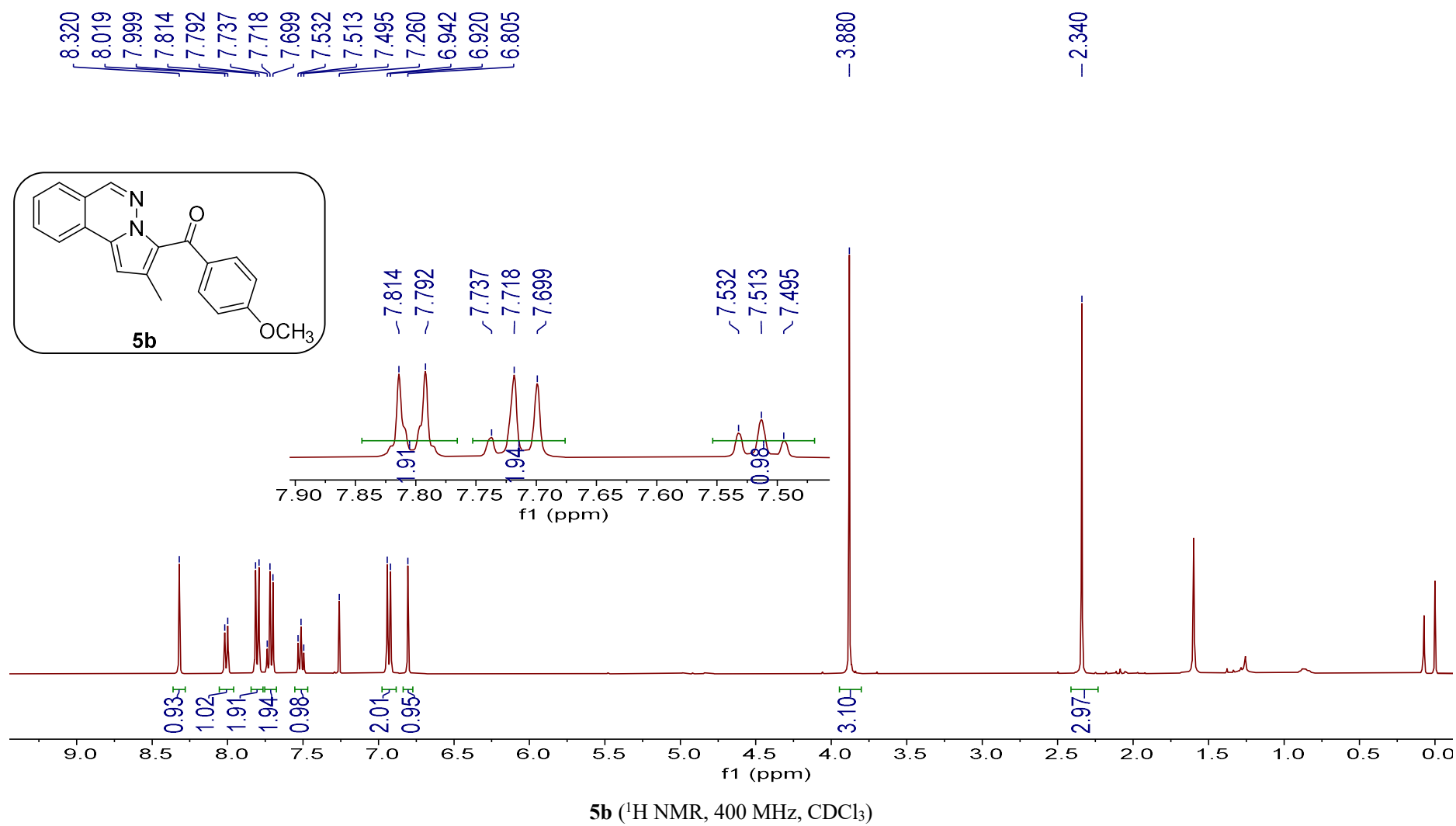


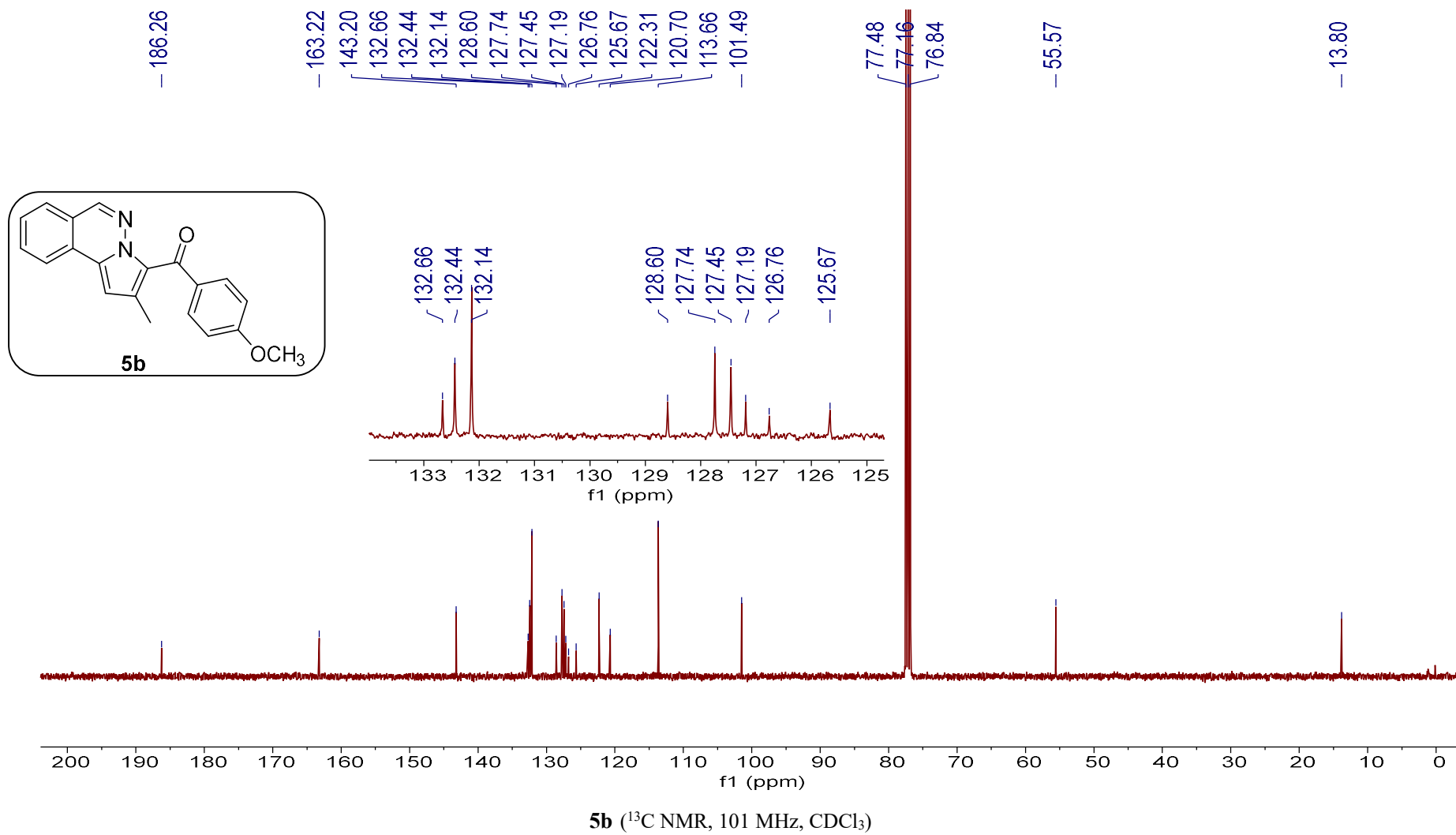


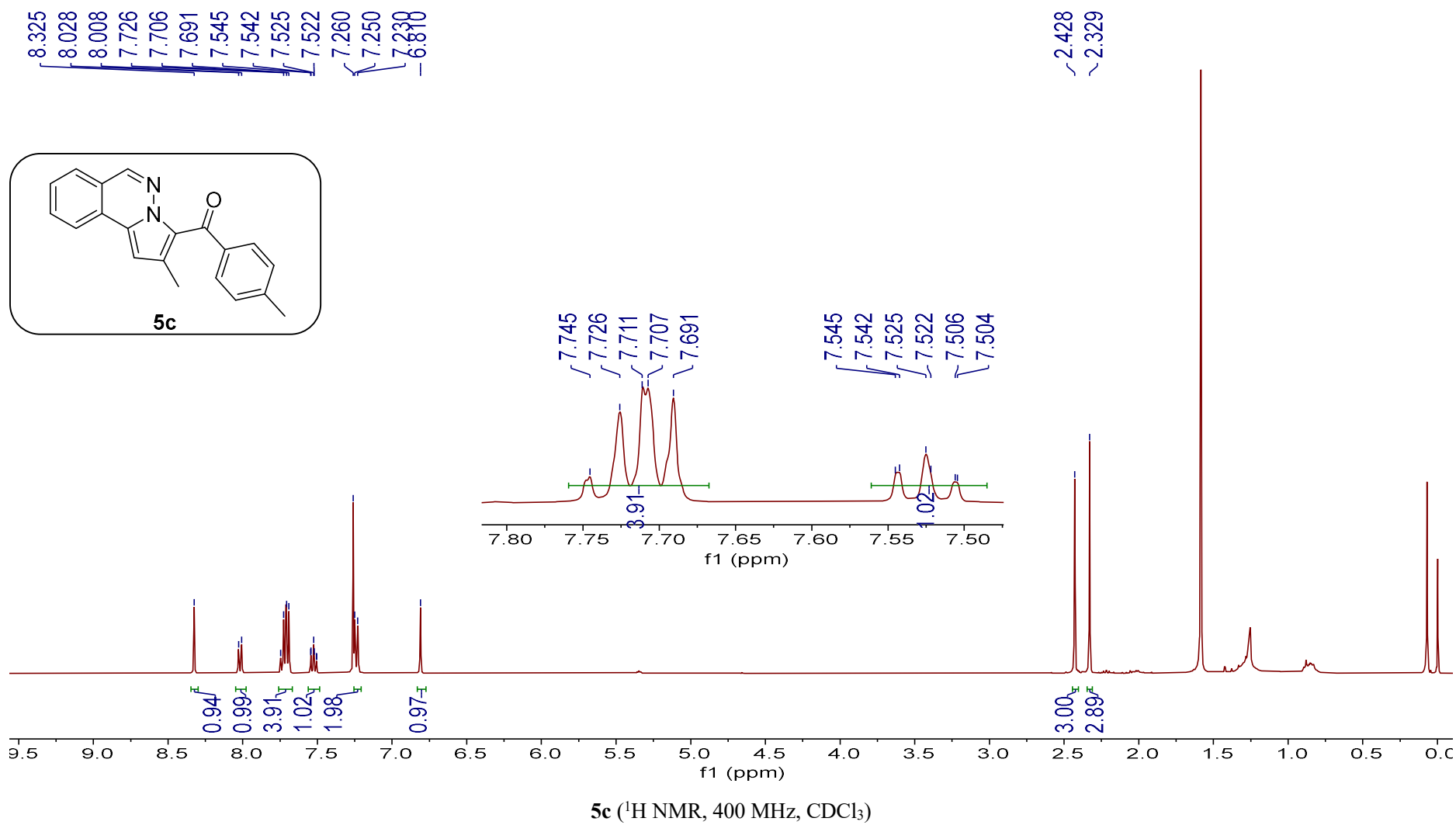


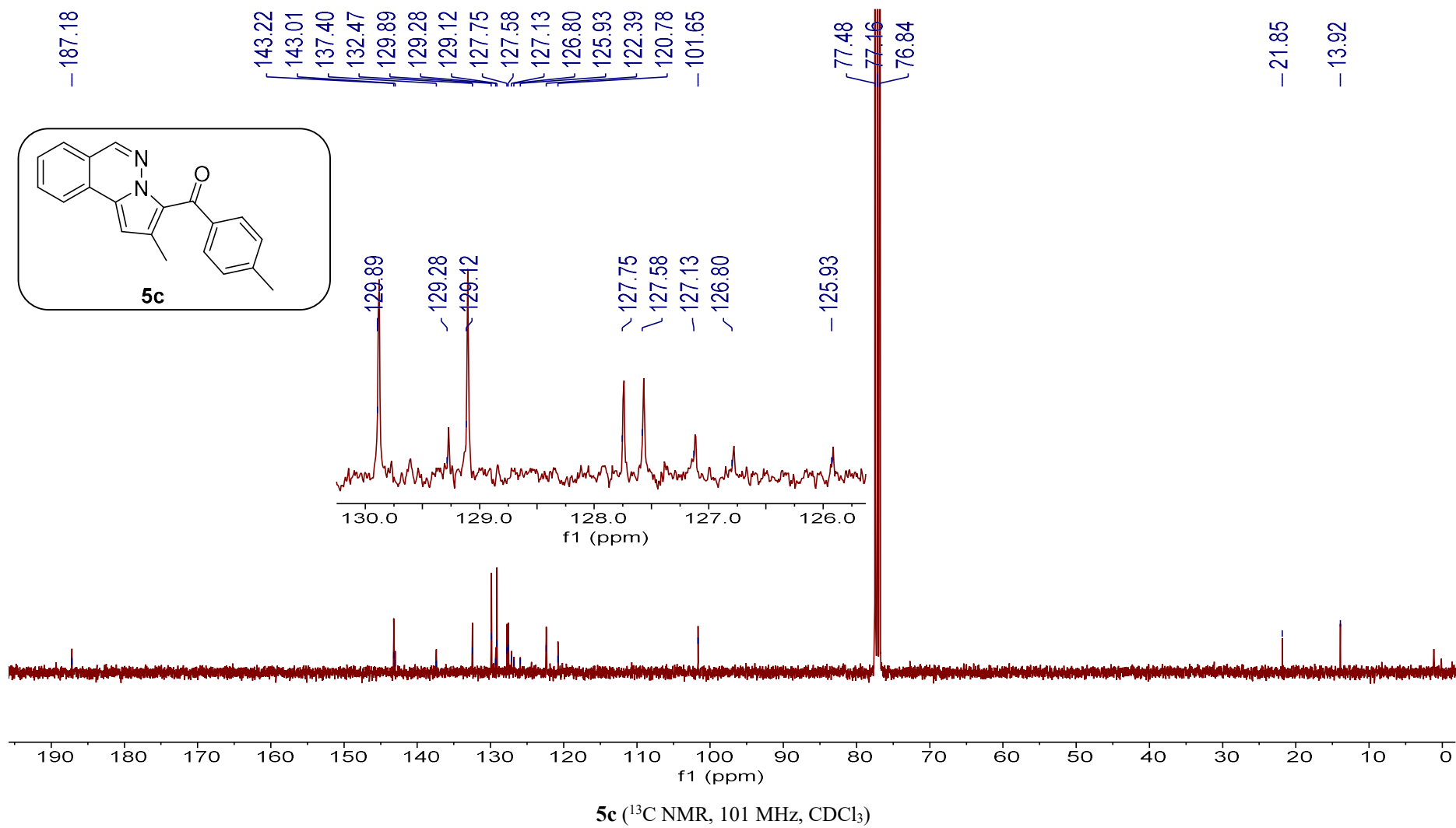


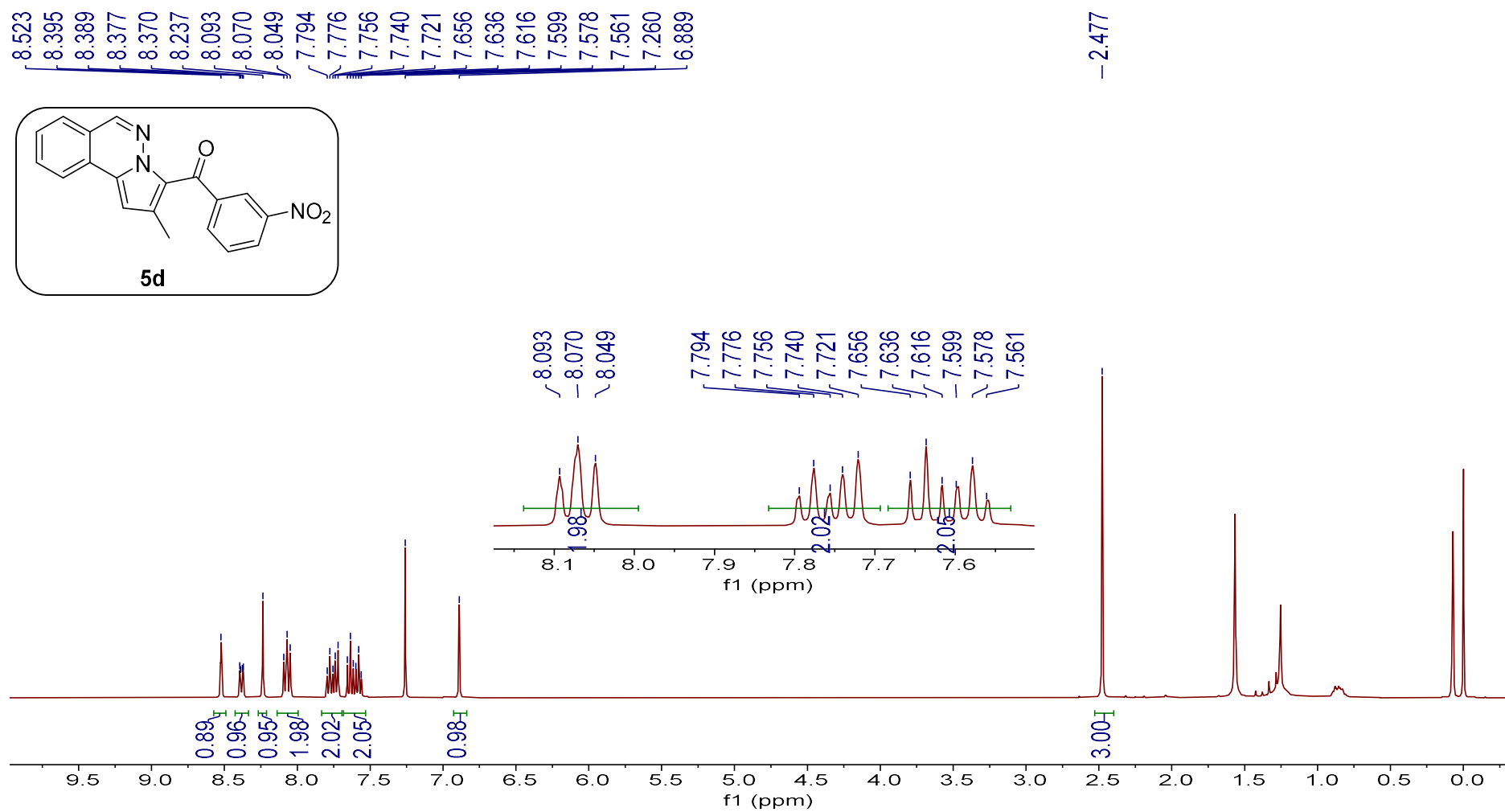




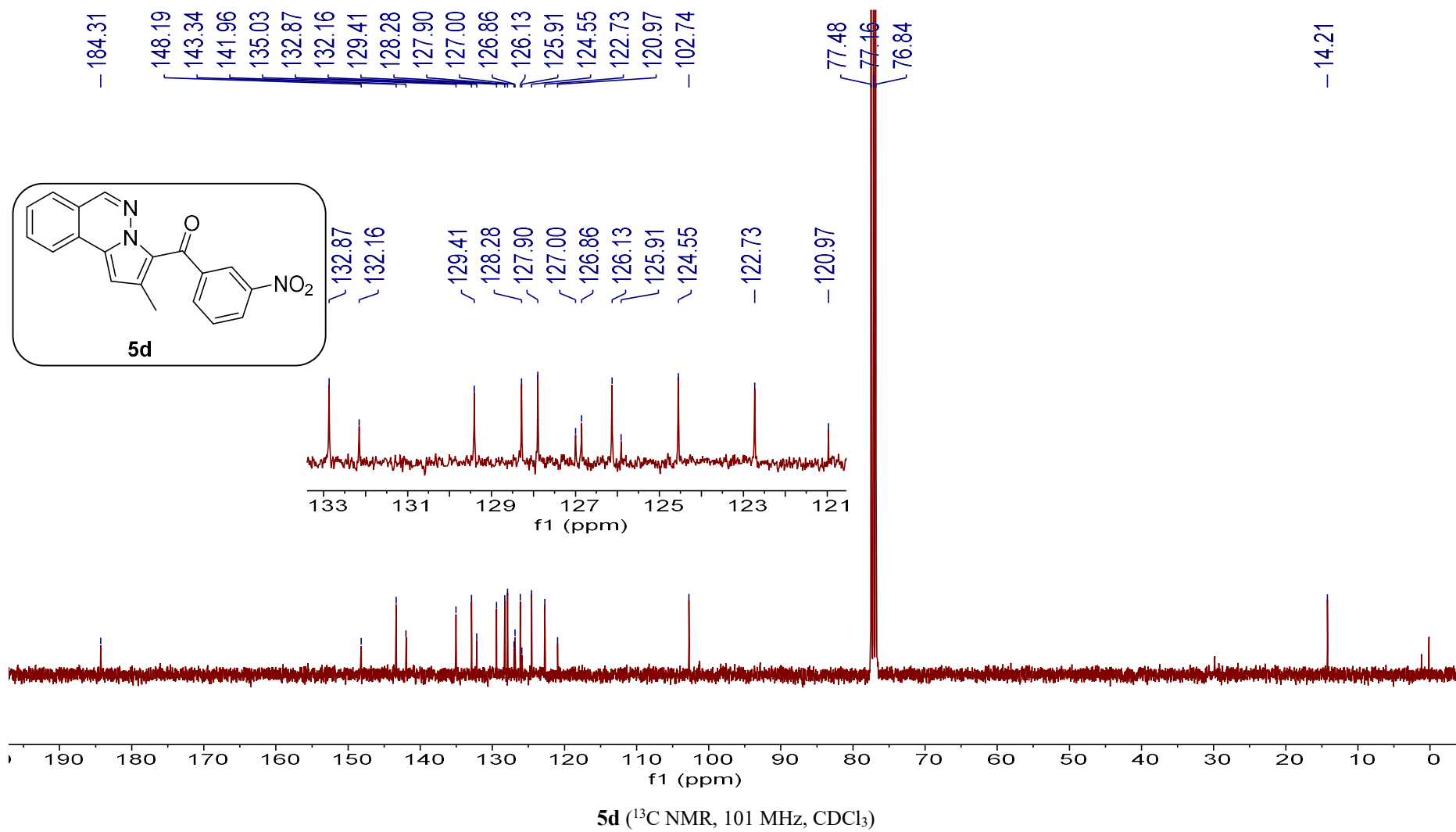


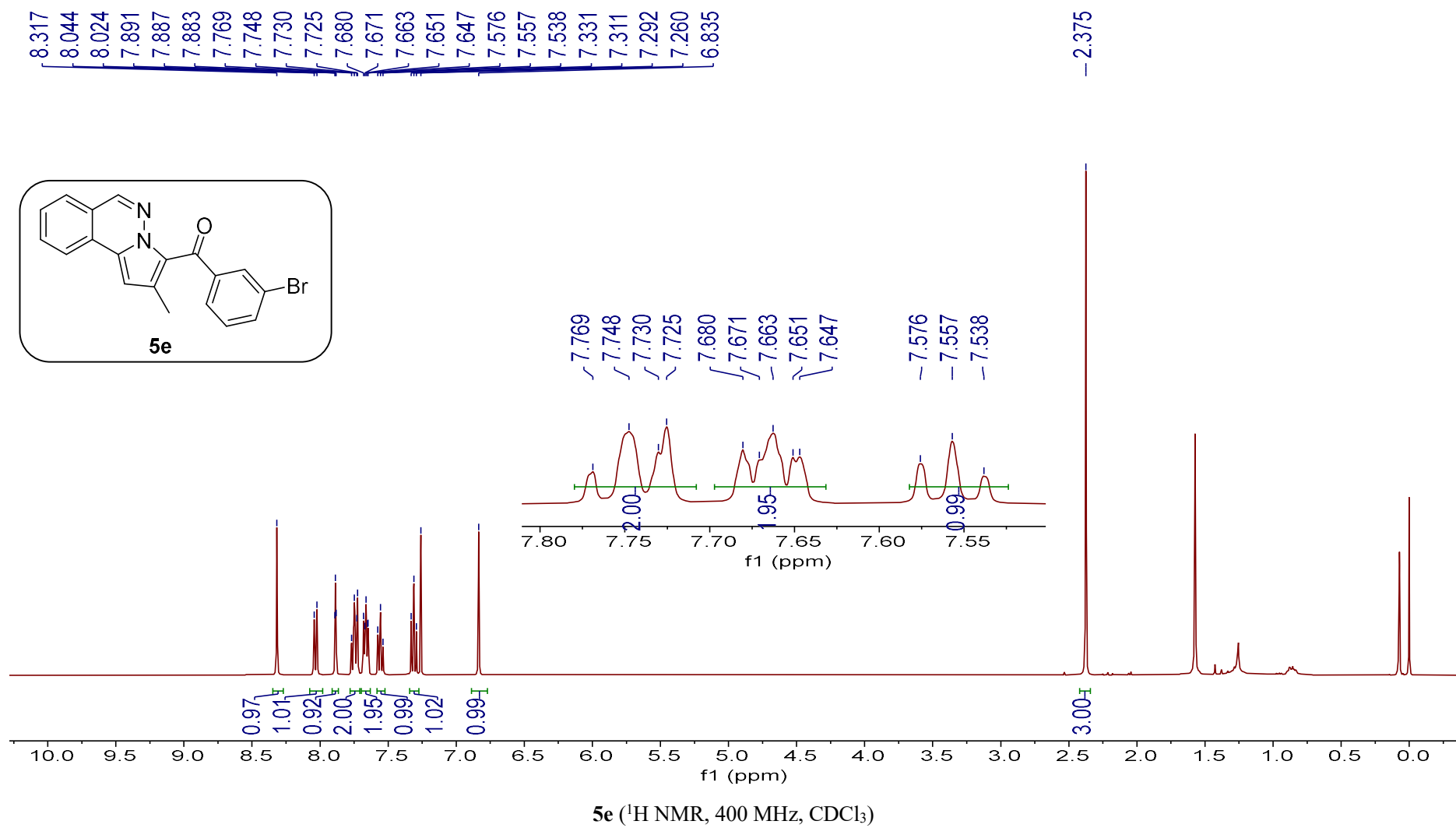


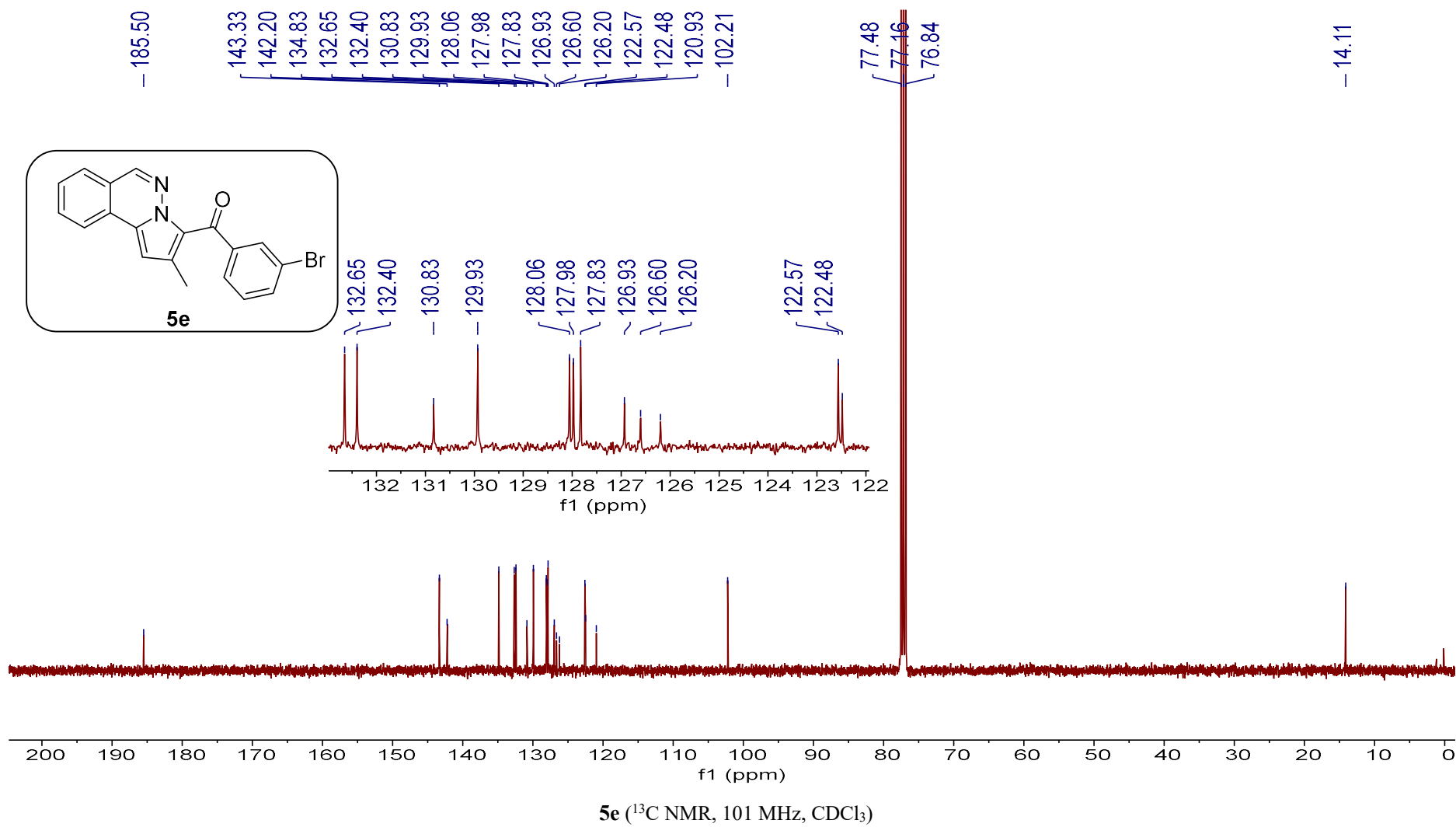


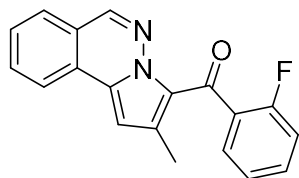


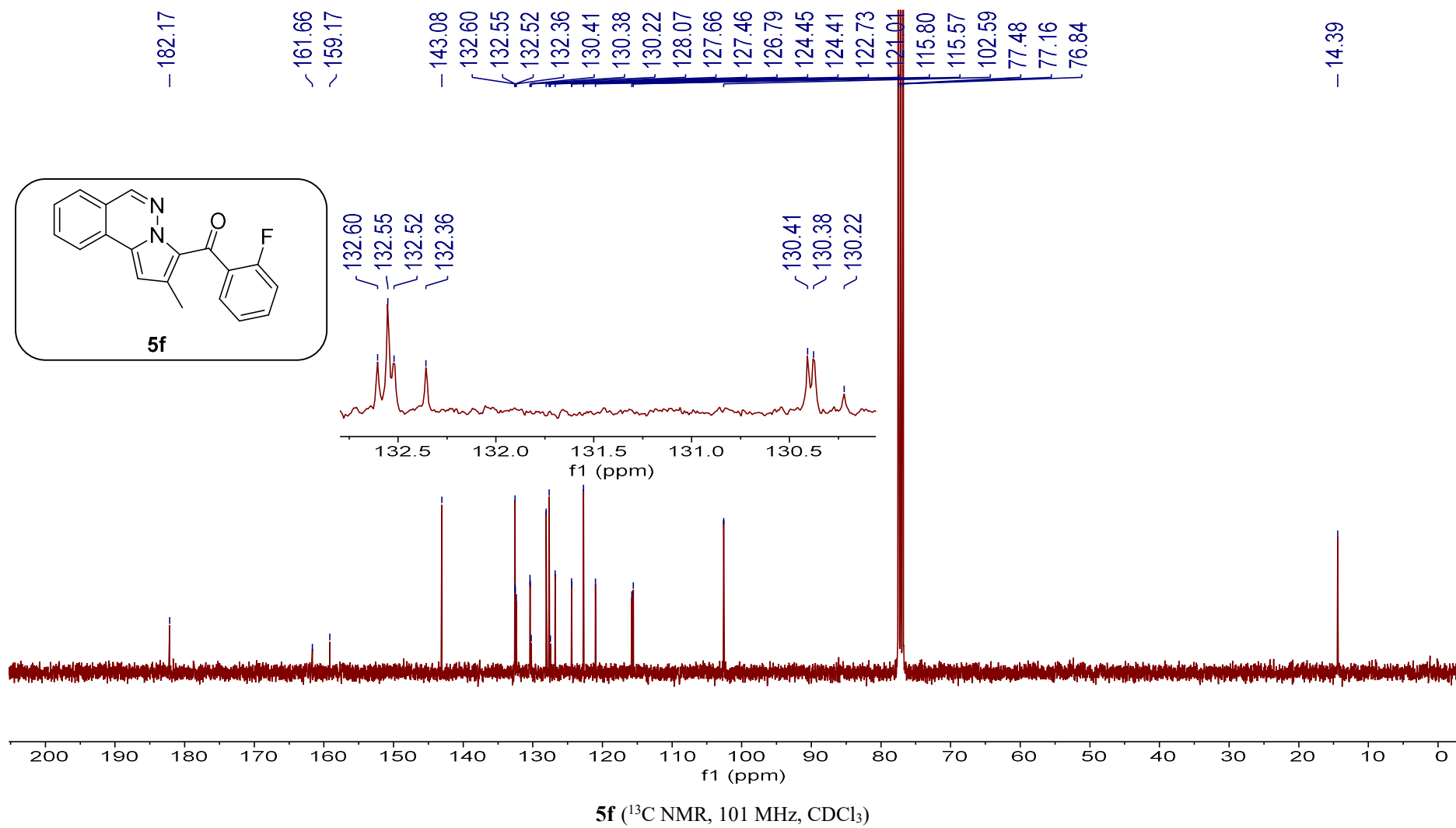
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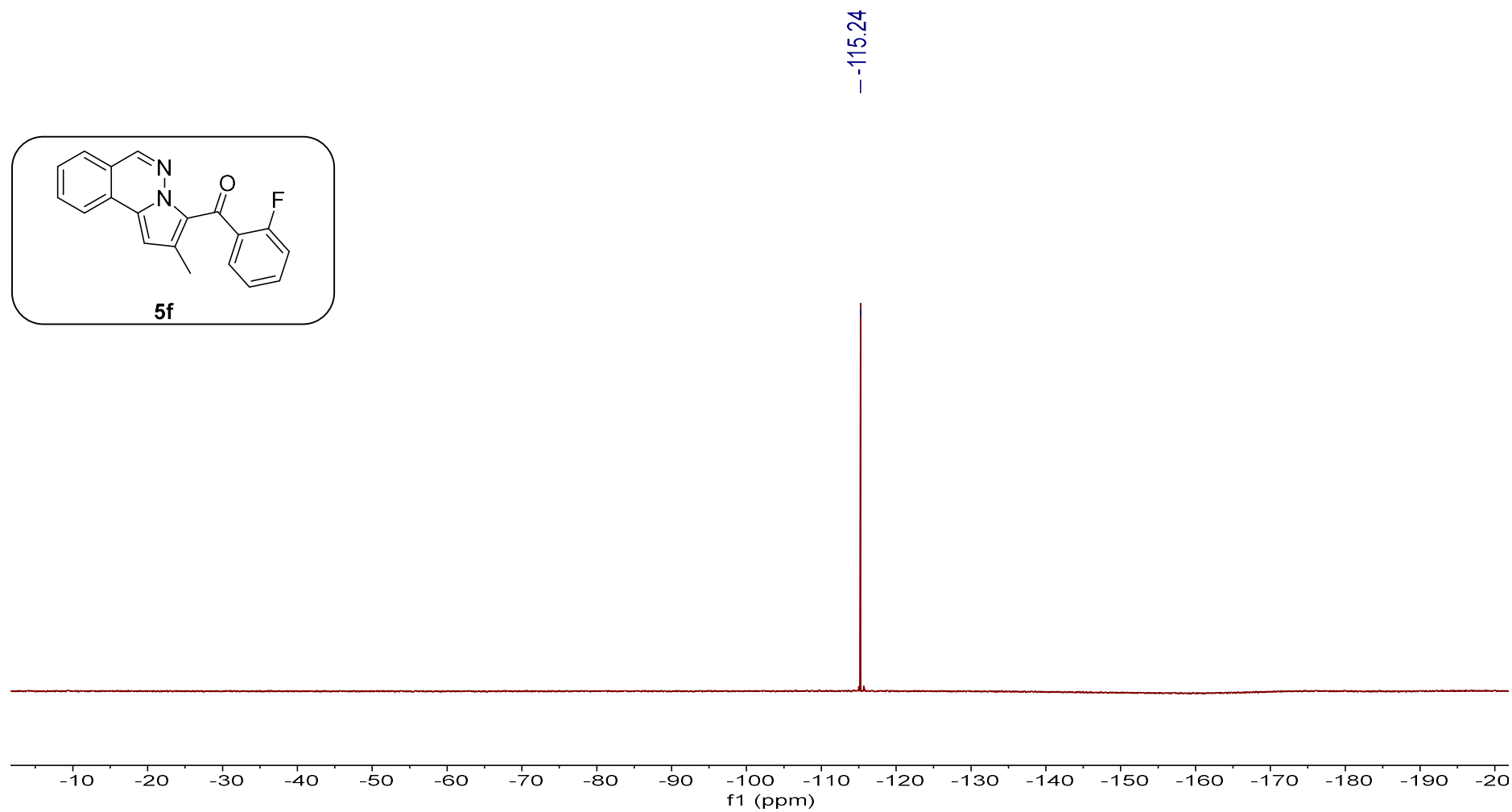
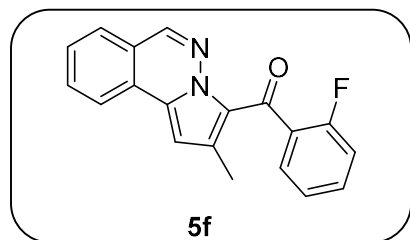




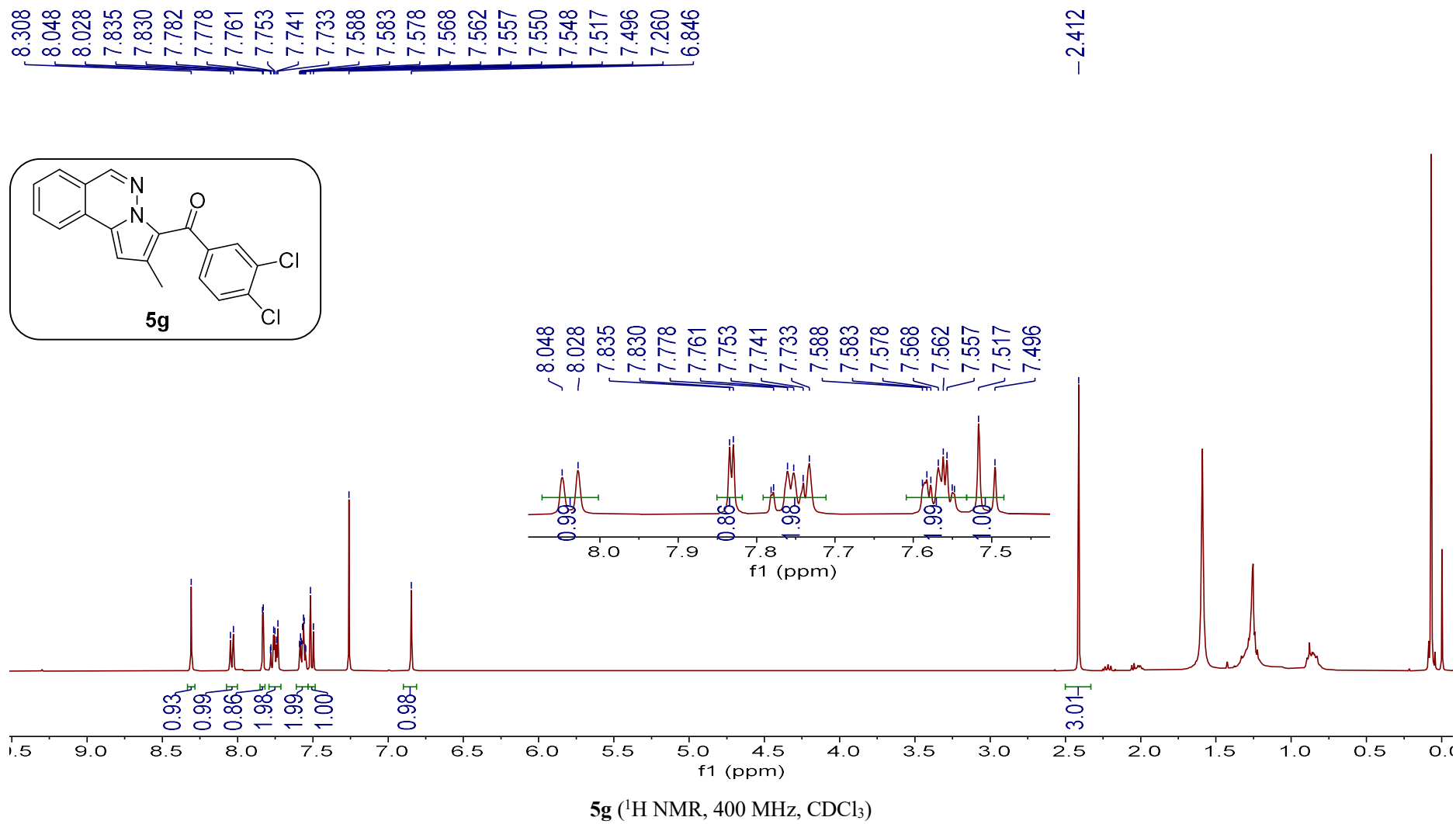


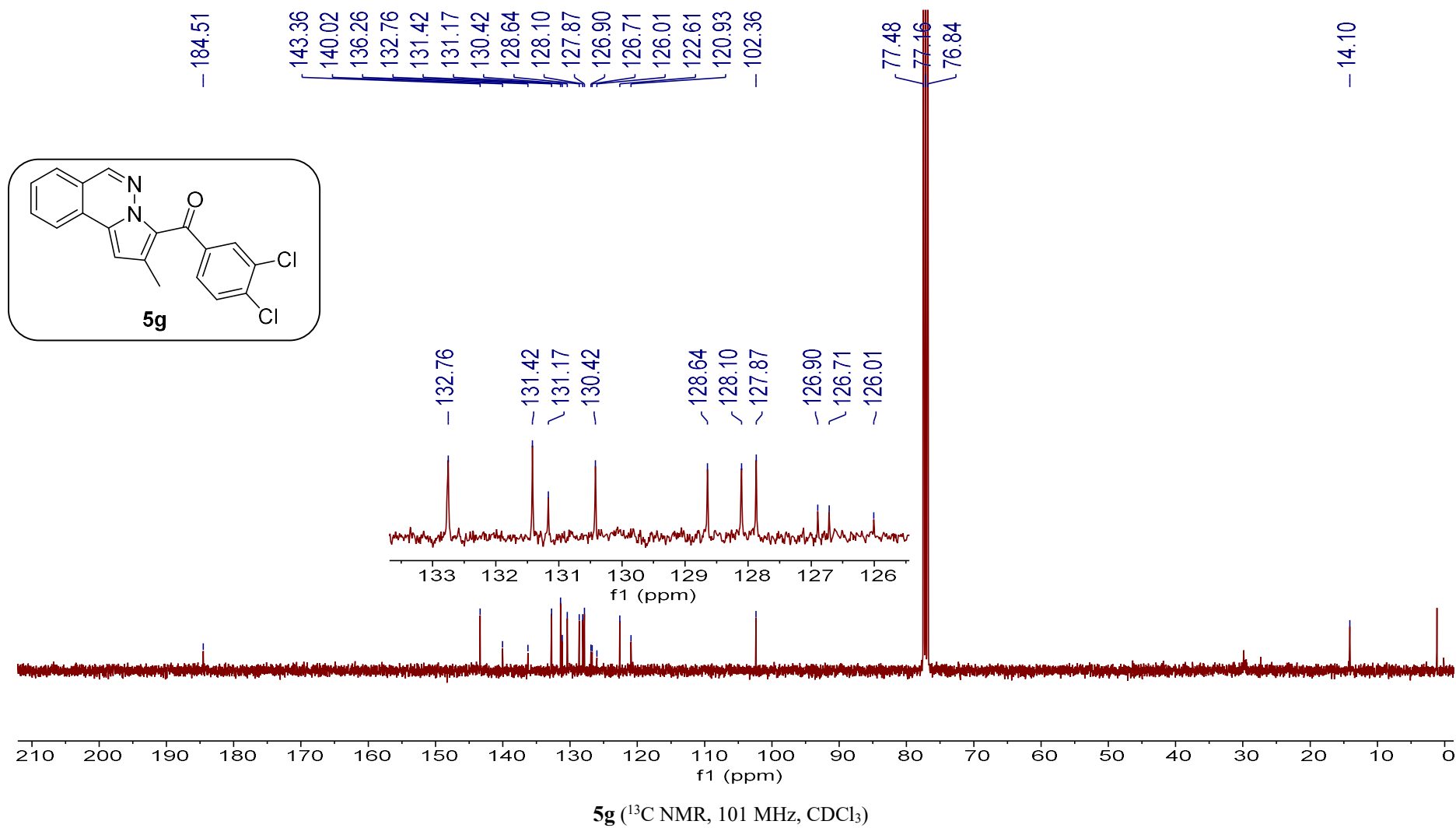


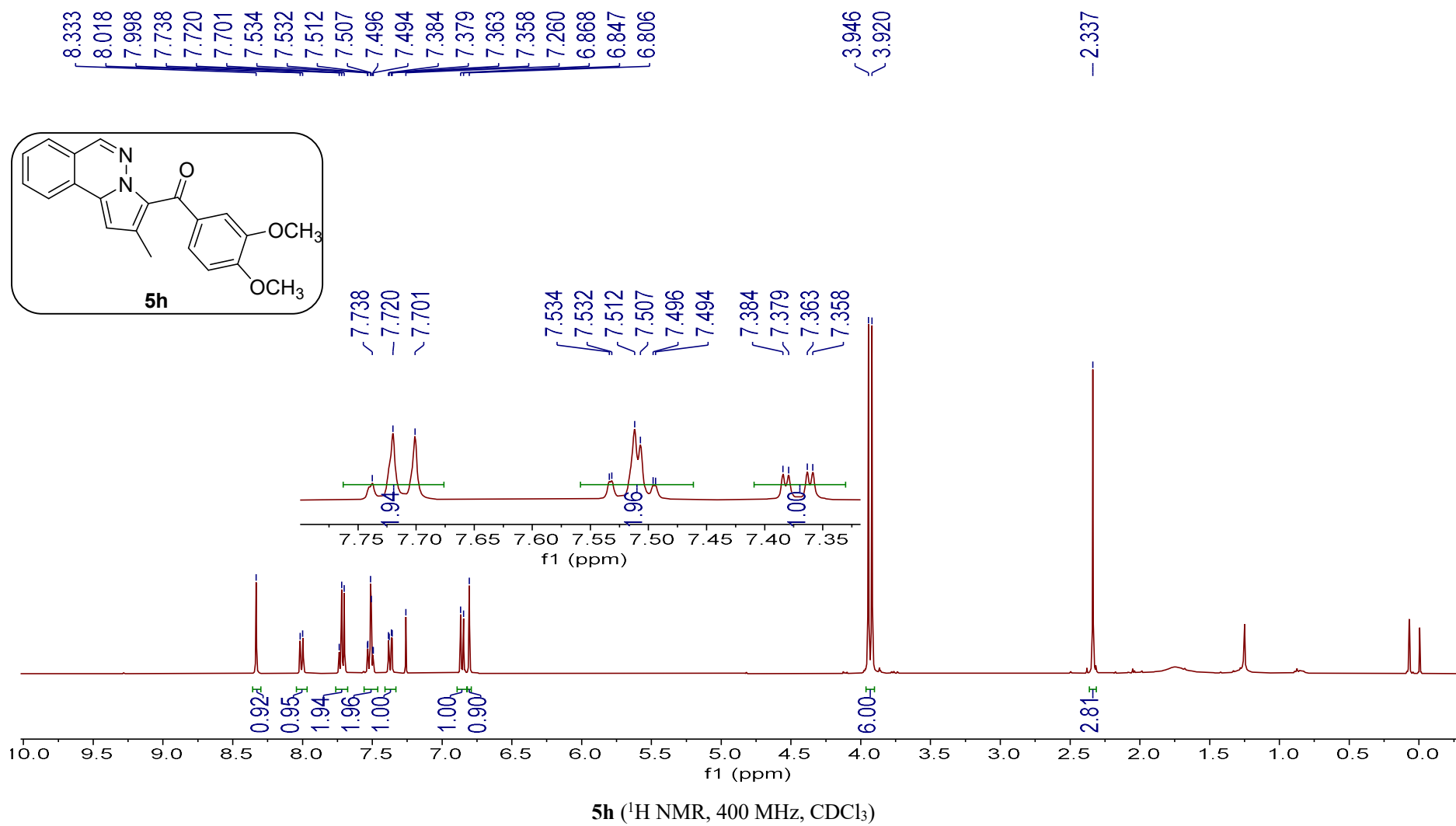


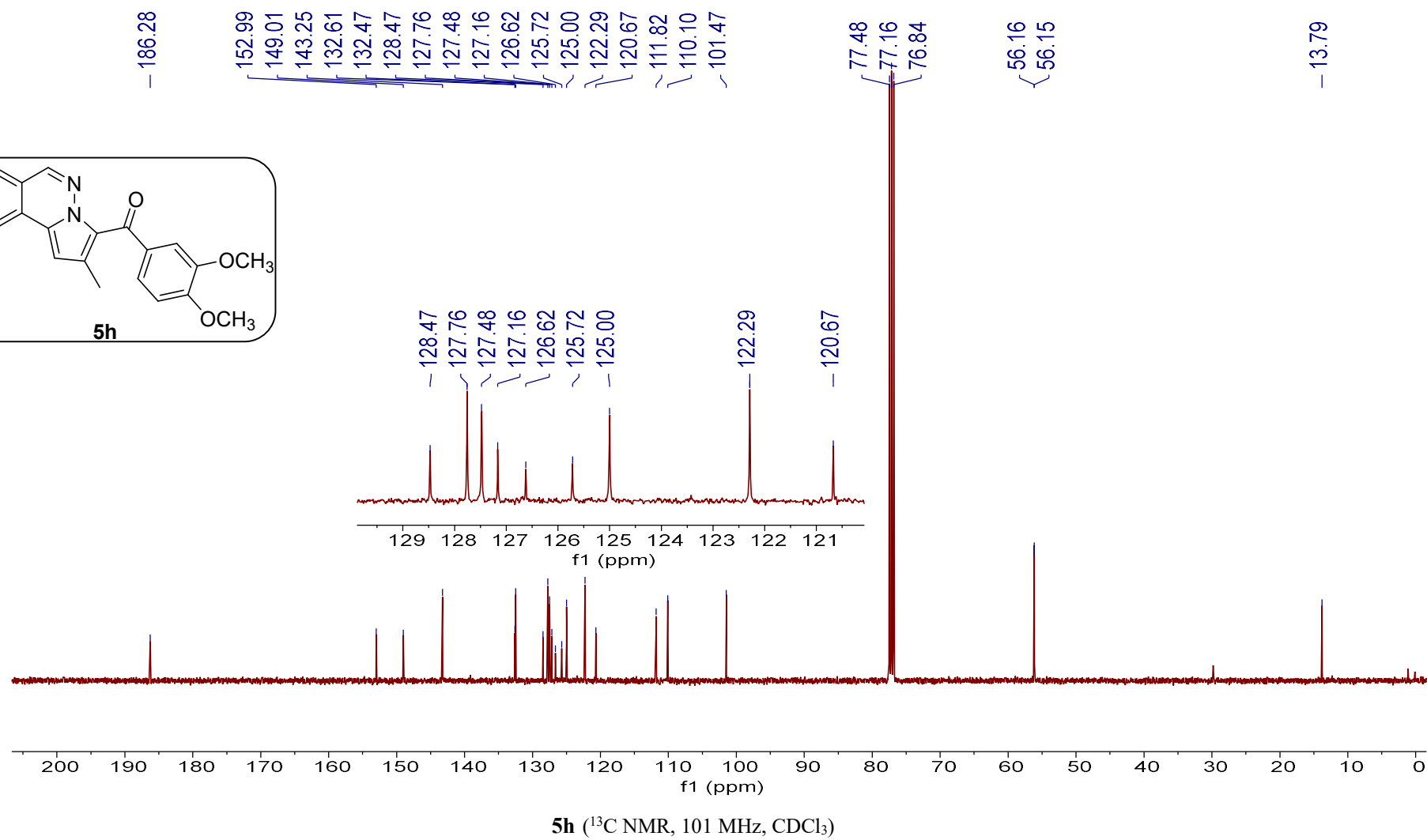
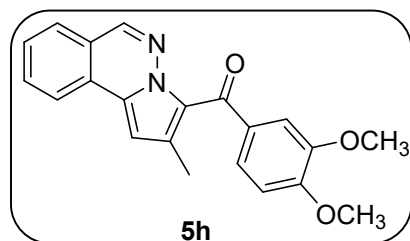


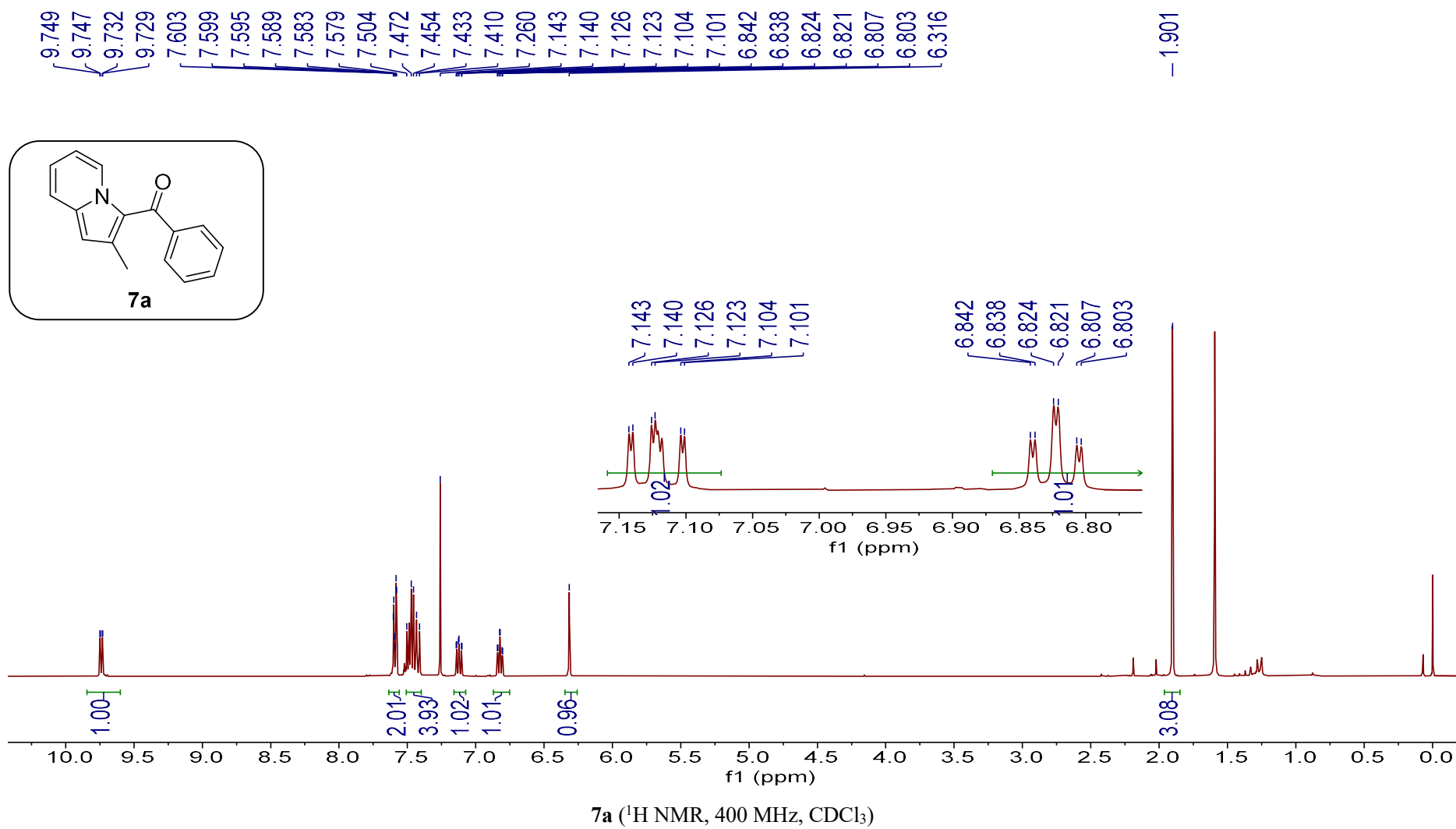
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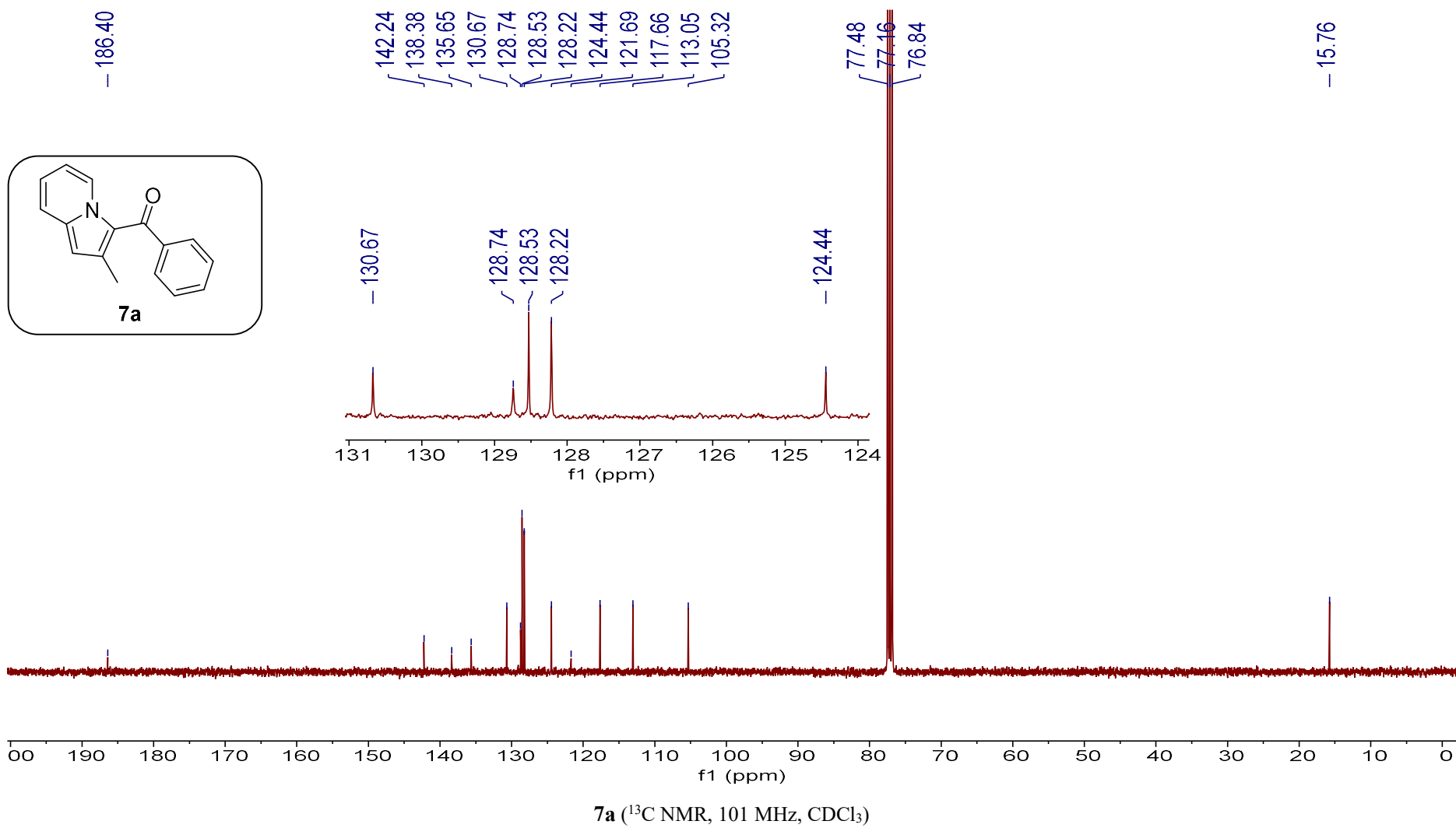


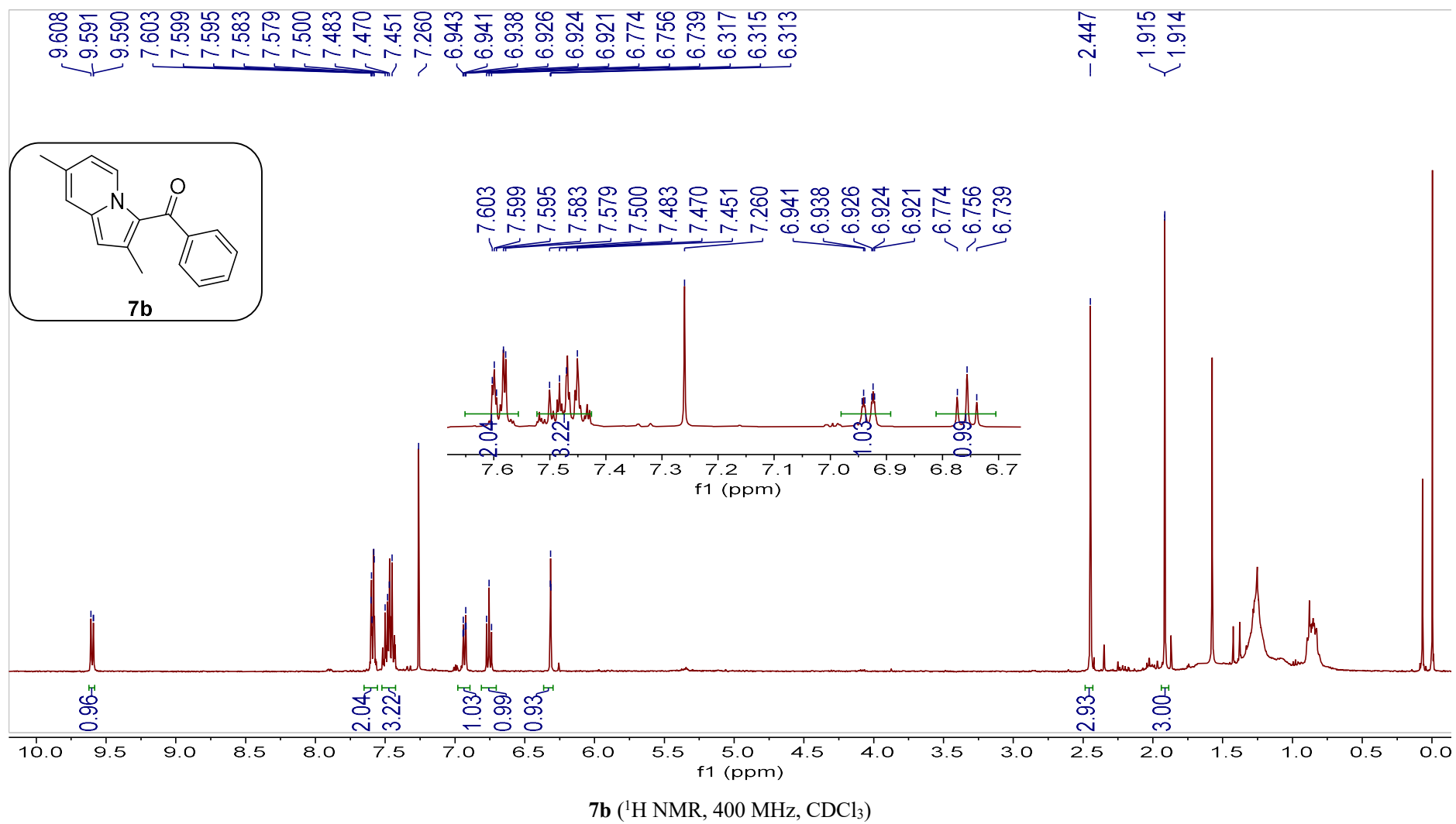


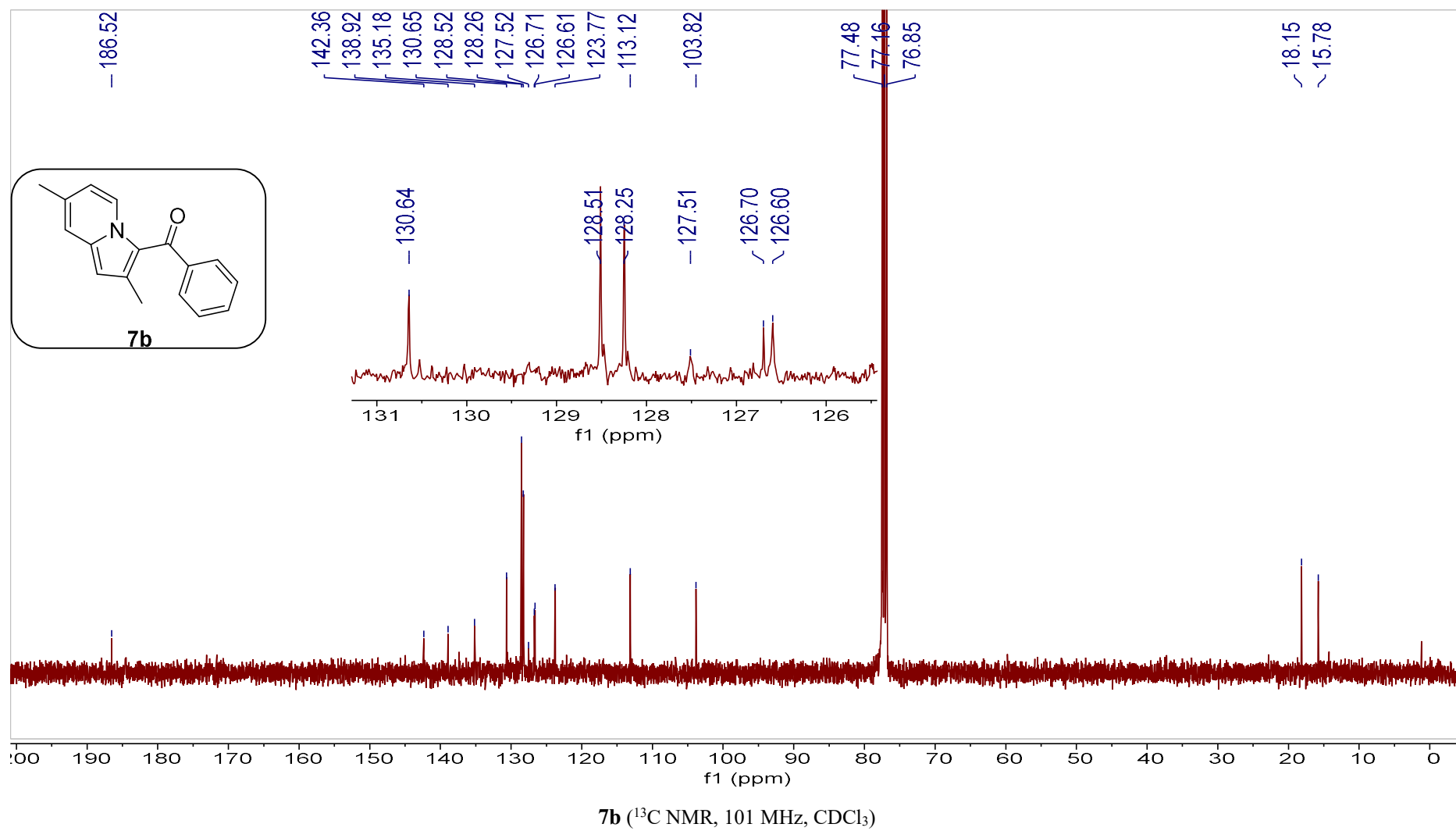




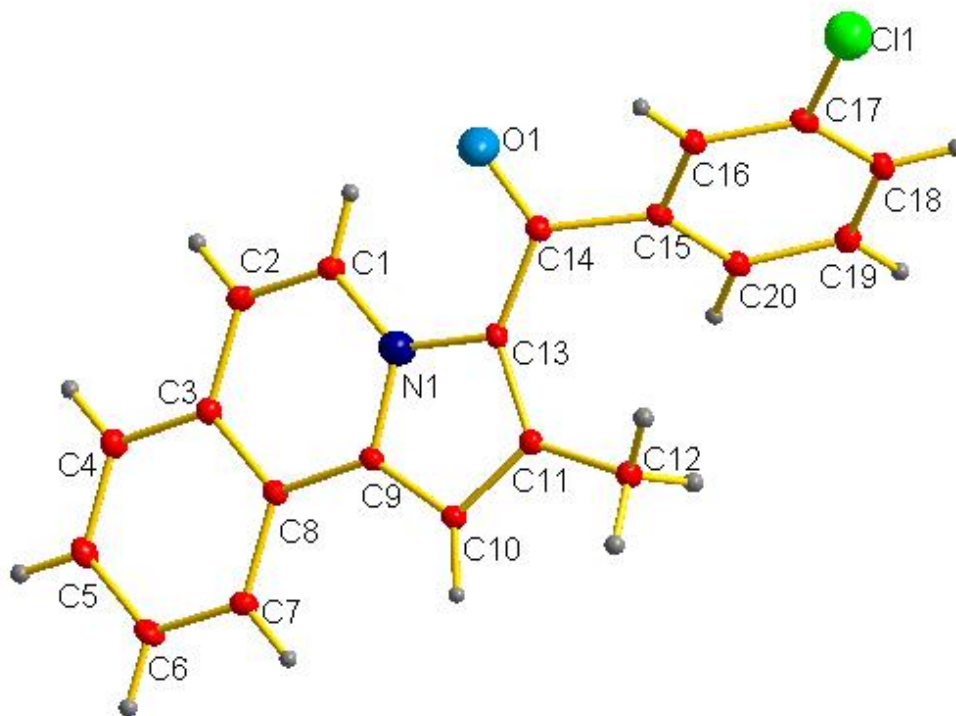








2. X-raycrystal structure of **3m**



Single crystals of **3m** were grown in ethyl acetate and petroleum ether. petroleum ether (2.0 mL) was added to **3m** (15 mg in a 4 mL vial) followed by 3 drops of ethyl acetate. The 4 mL vial was capped and placed at room temperature in the experimental cabinet for 7 days, whereupon crystals formed. A yellow block shaped crystal of **3m** was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 293(2) K, on a Rigaku AFC7R diffractometer. The crystal data of **3m** have been deposited in CCDC with number 2022332 and have been displayed at 50% ellipsoid contour probability level.

Table 1. Crystal data and structure refinement for **3m**.

Identification code	20200702LI_ZNZ5223_2_0m_a	
Empirical formula	C ₂₀ H ₁₄ Cl N O	
Formula weight	319.77	
Temperature	193(2) K	
Wavelength	1.34139 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.0991(3) Å	α = 75.7790(10)°.
	b = 10.0866(3) Å	β = 69.4490(10)°.
	c = 10.5705(3) Å	γ = 67.4610(10)°.
Volume	740.63(4) Å ³	
Z	2	
Density (calculated)	1.434 Mg/m ³	
Absorption coefficient	1.517 mm ⁻¹	
F(000)	332	
Crystal size	0.120 x 0.110 x 0.080 mm ³	
Theta range for data collection	3.918 to 53.902°.	
Index ranges	-9 ≤ h ≤ 9, -12 ≤ k ≤ 12, -12 ≤ l ≤ 12	
Reflections collected	9190	
Independent reflections	2690 [R(int) = 0.0309]	
Completeness to theta = 53.594°	99.4 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2690 / 0 / 209	
Goodness-of-fit on F ²	1.035	
Final R indices [I > 2σ(I)]	R1 = 0.0372, wR2 = 0.0990	
R indices (all data)	R1 = 0.0418, wR2 = 0.1025	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.603 and -0.298 e.Å ⁻³	