

Supporting Information

Copper-Catalyzed Ring Expansion of Cyclopropyl Ketones/Formation of N-acyliminium/ Hetero-[4+2]-Cycloaddition: A Route to Substituted Pentacyclic Isoindolin-1-one

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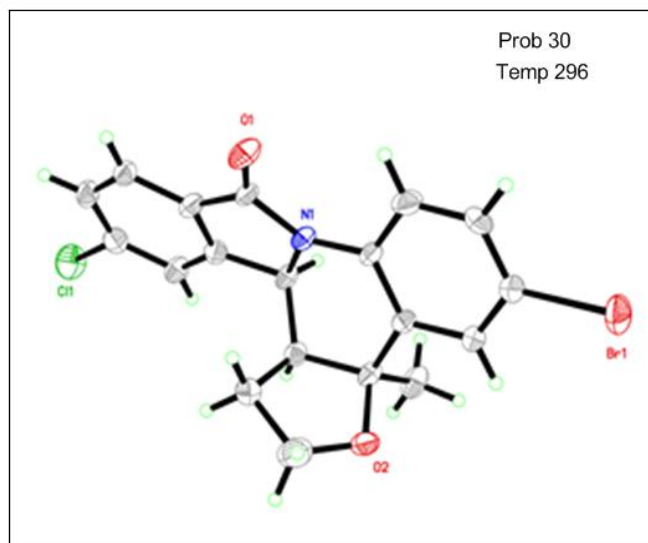


Figure S1. ORTEP drawing (30%) of the crystal structure **4i**

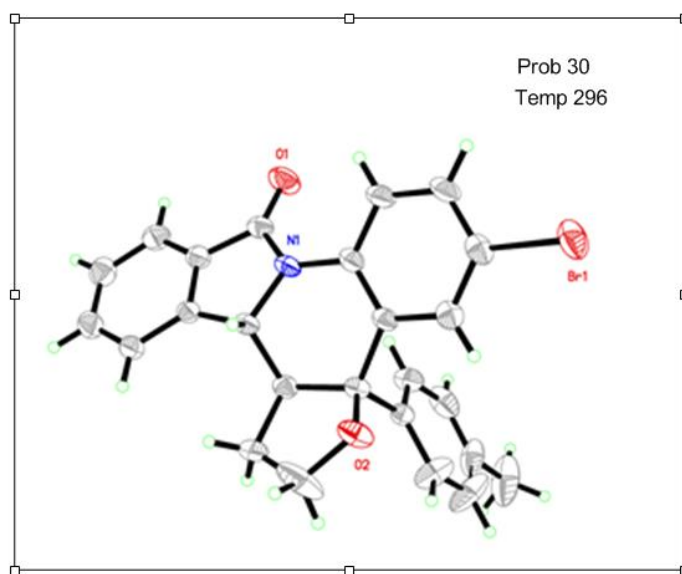


Figure S2. ORTEP drawing (30%) of the crystal structure **4ab**

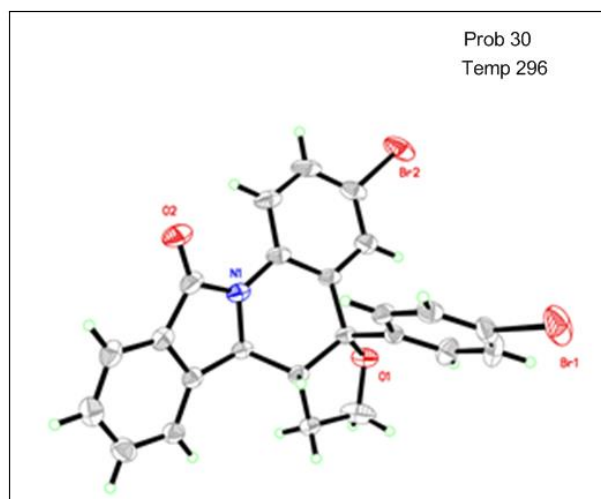
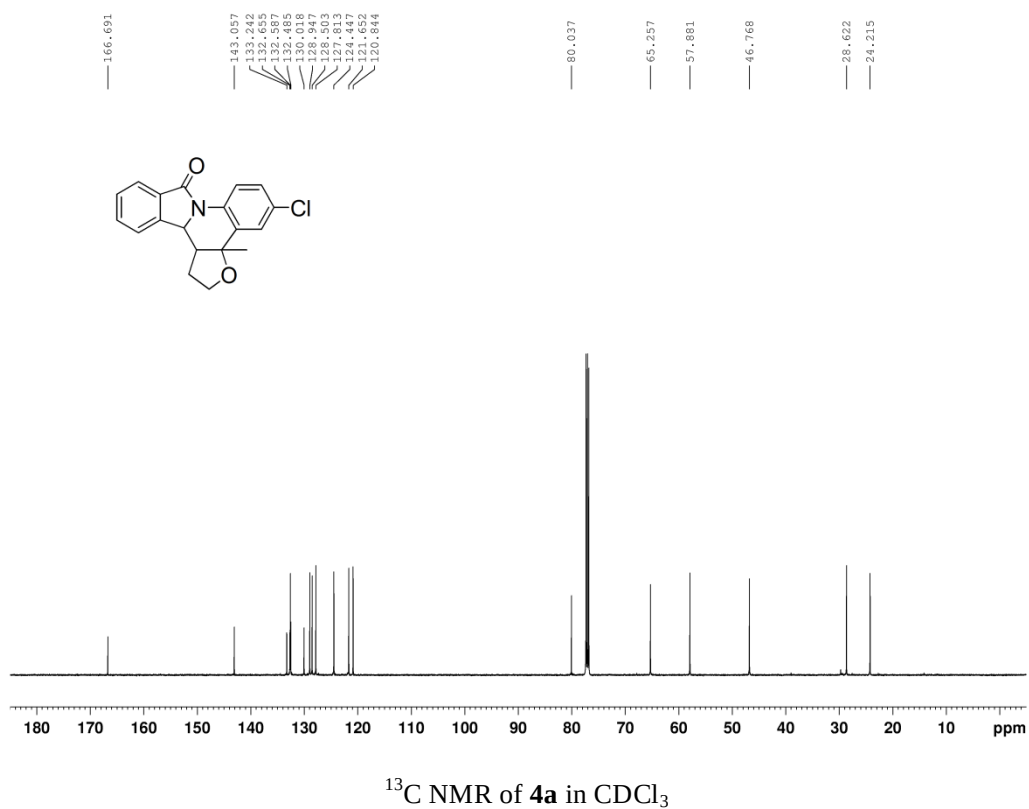
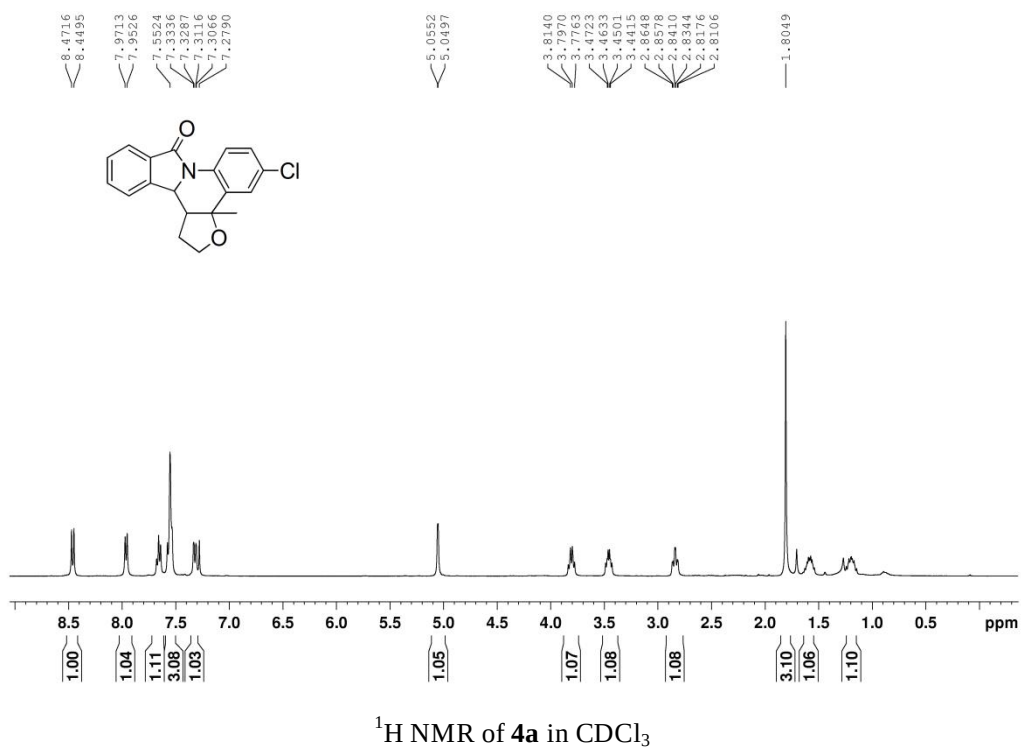
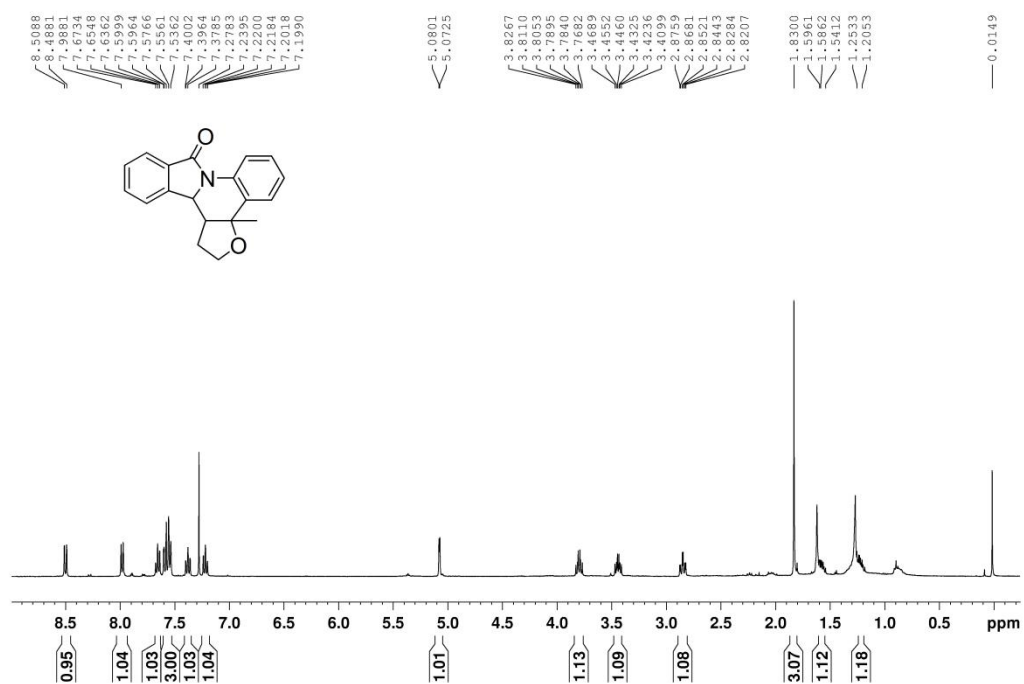


Figure S3. ORTEP drawing (30%) of the crystal structure **4af**

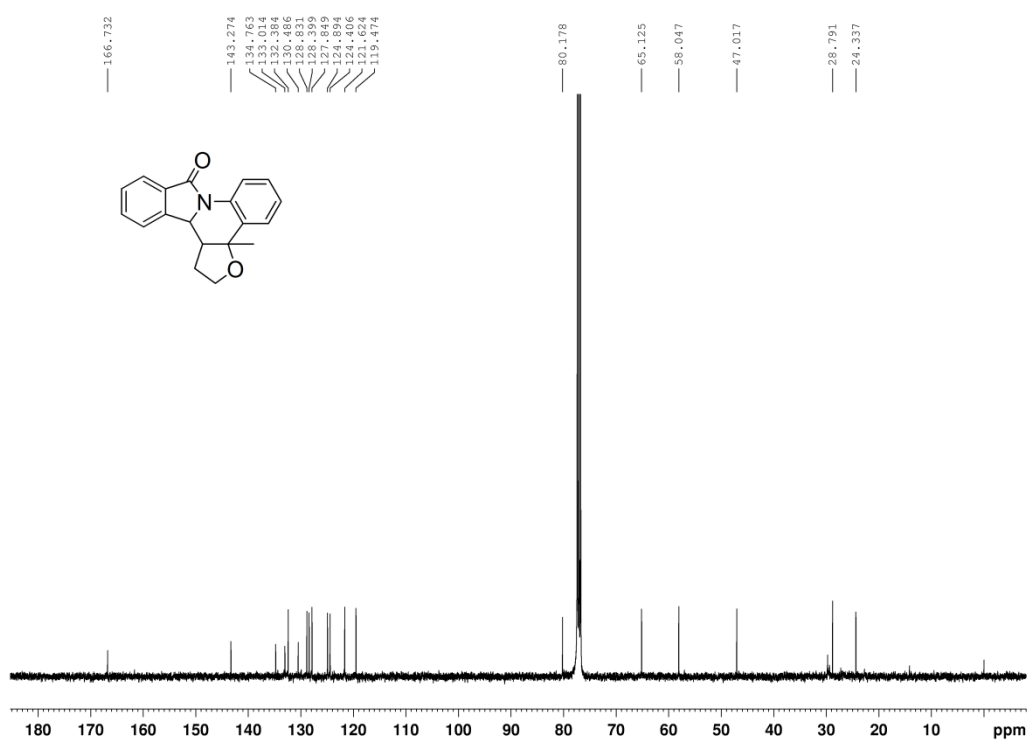
Table S1. Crystal data parameter for compound 4i , 4ab and 4af .			
	4i	4af	4ab
Formula unit	C ₁₉ H ₁₅ BrClNO ₂	C ₂₄ H ₁₇ Br ₂ NO ₂	C ₂₅ H ₂₀ BrNO ₂
Formula wt.	404.68	511.20	446.33
Crystal system	Monoclinic	Monoclinic	Monoclinic
T [K]	296	296	296
<i>a</i> [Å]	31.317(11)	13.498(2)	13.333(2)
<i>b</i> [Å]	6.319(2)	15.224(2)	15.334(2)
<i>c</i> [Å]	19.015(6)	10.0932(15)	10.1707(15)
α [°]	90	90	90
β [°]	116.170(8)	105.787(4)	105.845(4)
γ [°]	90	90	90
Volume [Å ³]	3377(2)	1996.0(5)	2000.4(5)
Space group	C 2/c	P 2 ₁ /c	P 2 ₁ /c
Z	8	4	4
Reflns. Collected	1940	3656	3323
R1 [I>2σ(I)], wR2	0.0824, 0.1673	0.0888, 0.1709	0.0846, 0.1707

GOF	1.014	1.025	1.076
CCDC Reference NO.	1834908	1834907	1834909

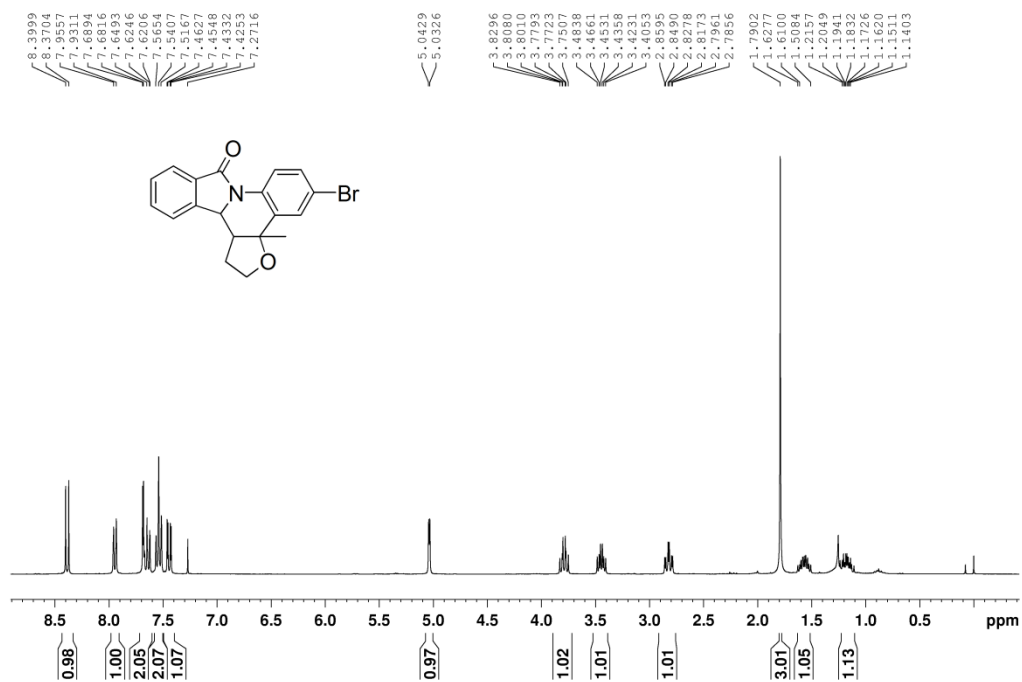




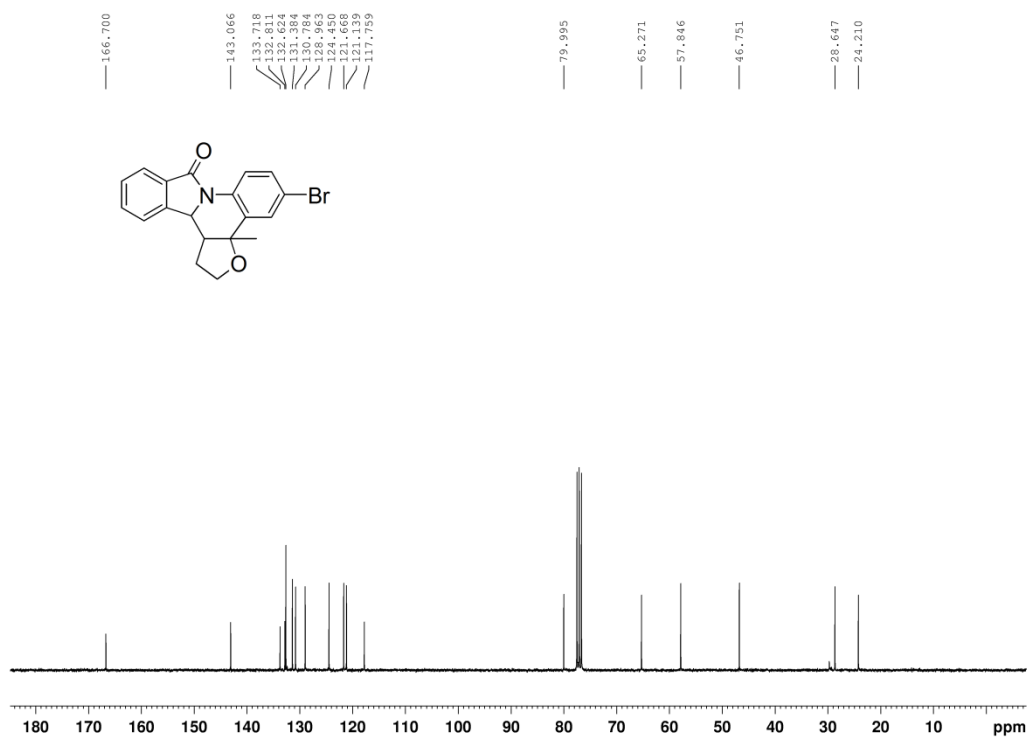
¹H NMR of **4b** in CDCl₃



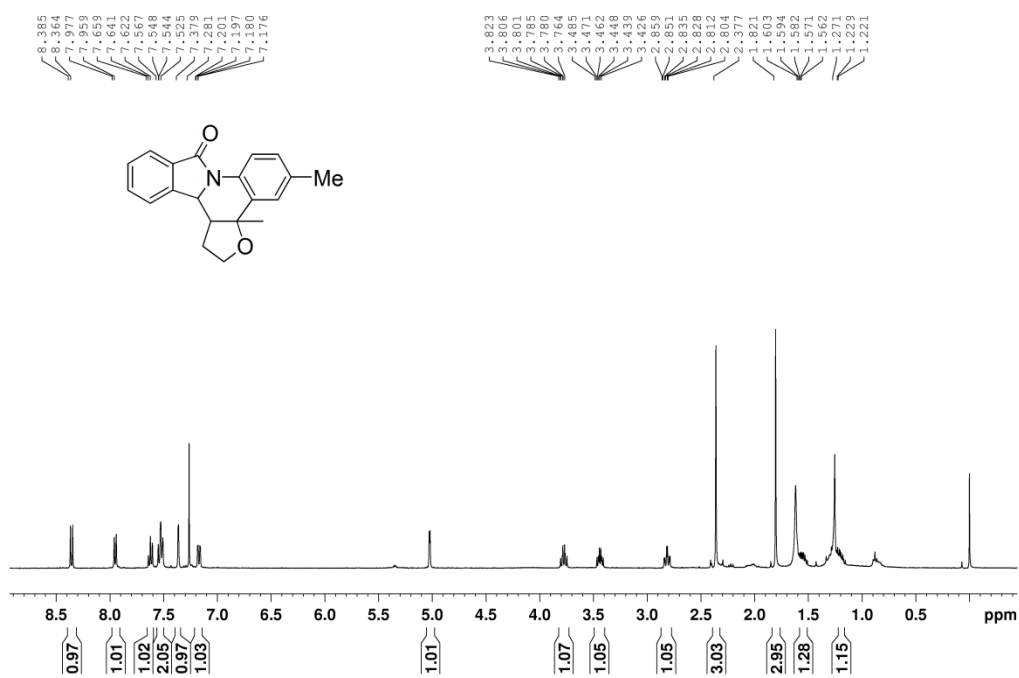
¹³C NMR of **4b** in CDCl₃



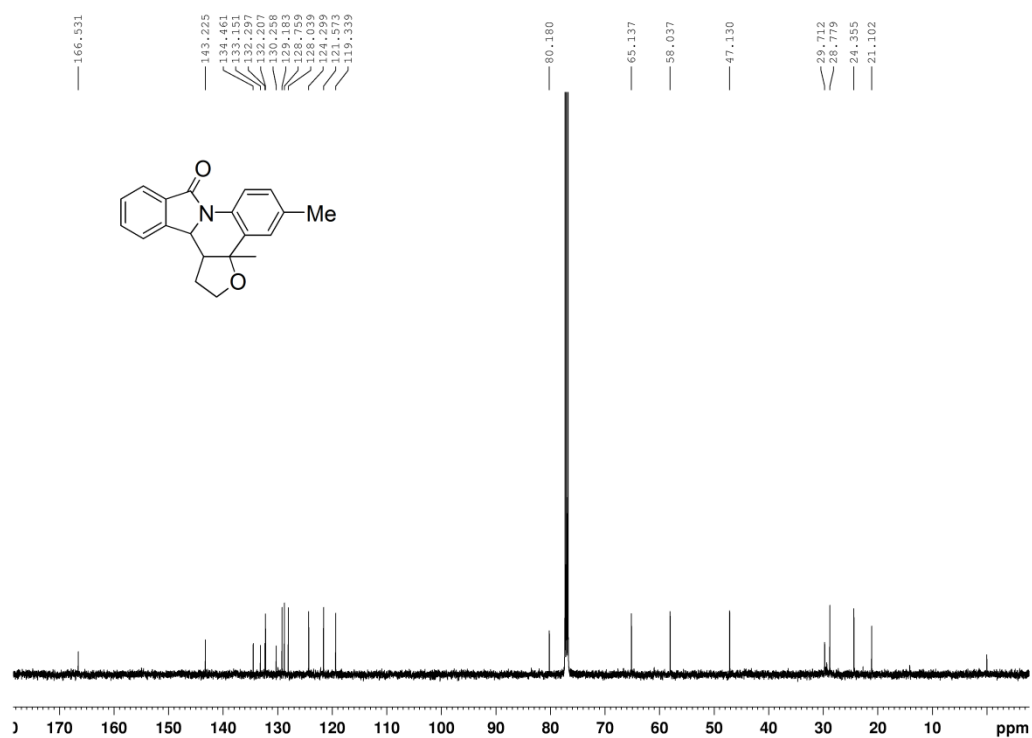
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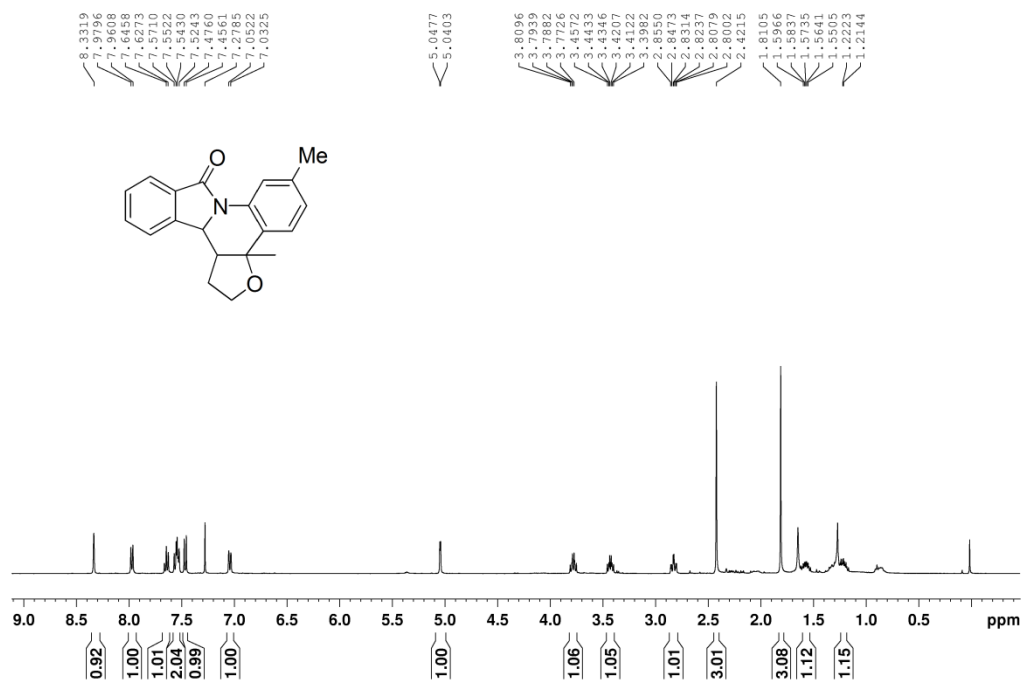
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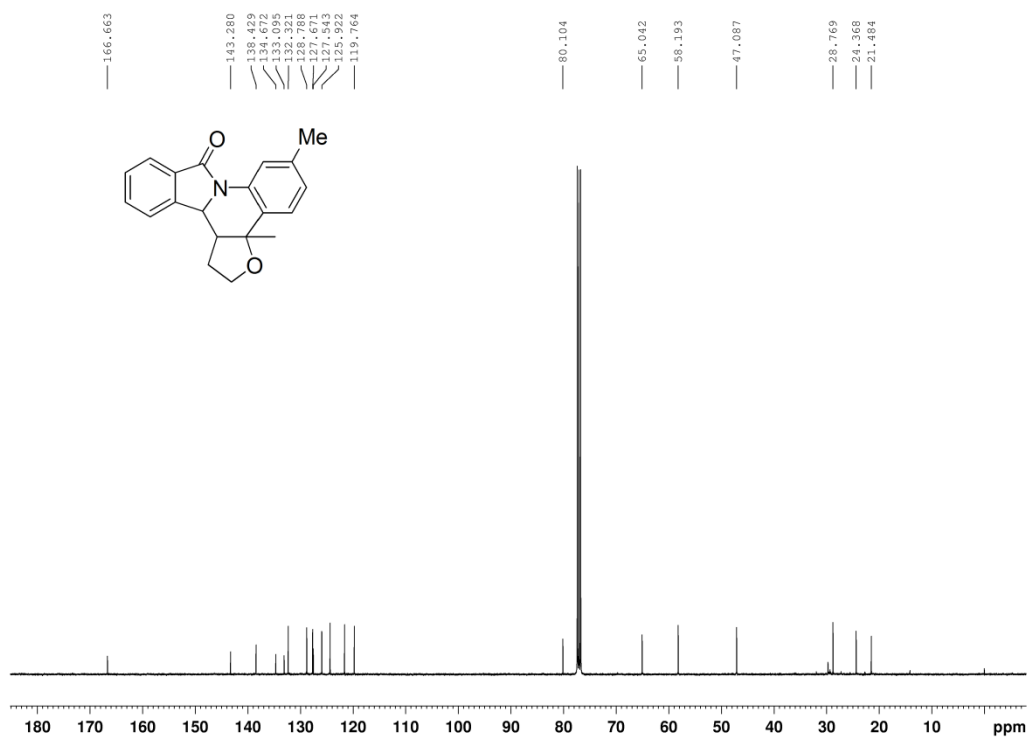
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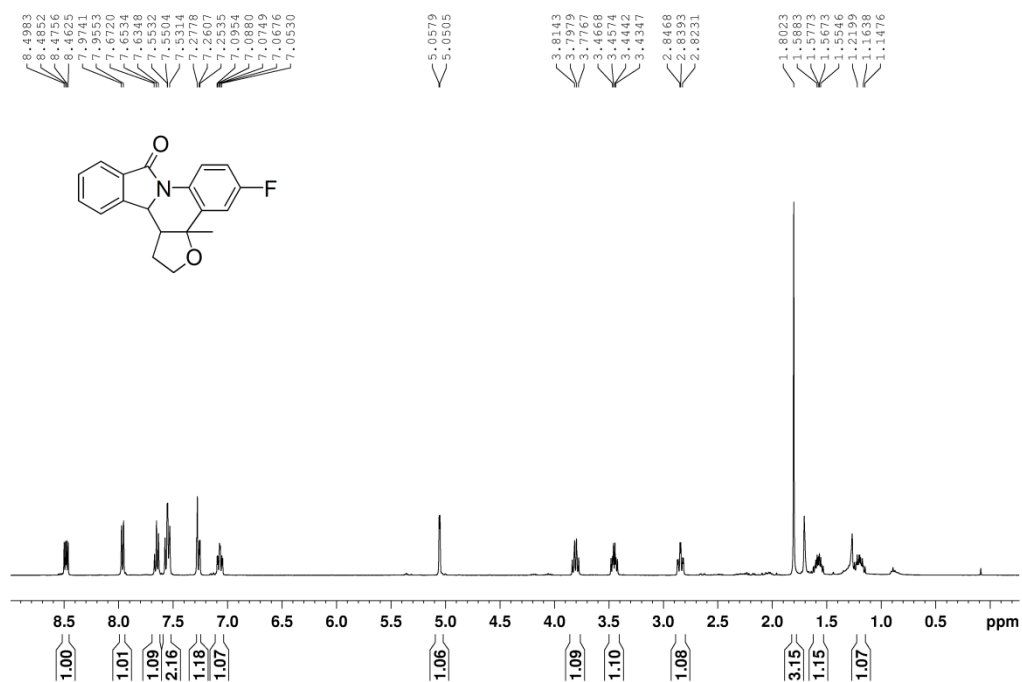
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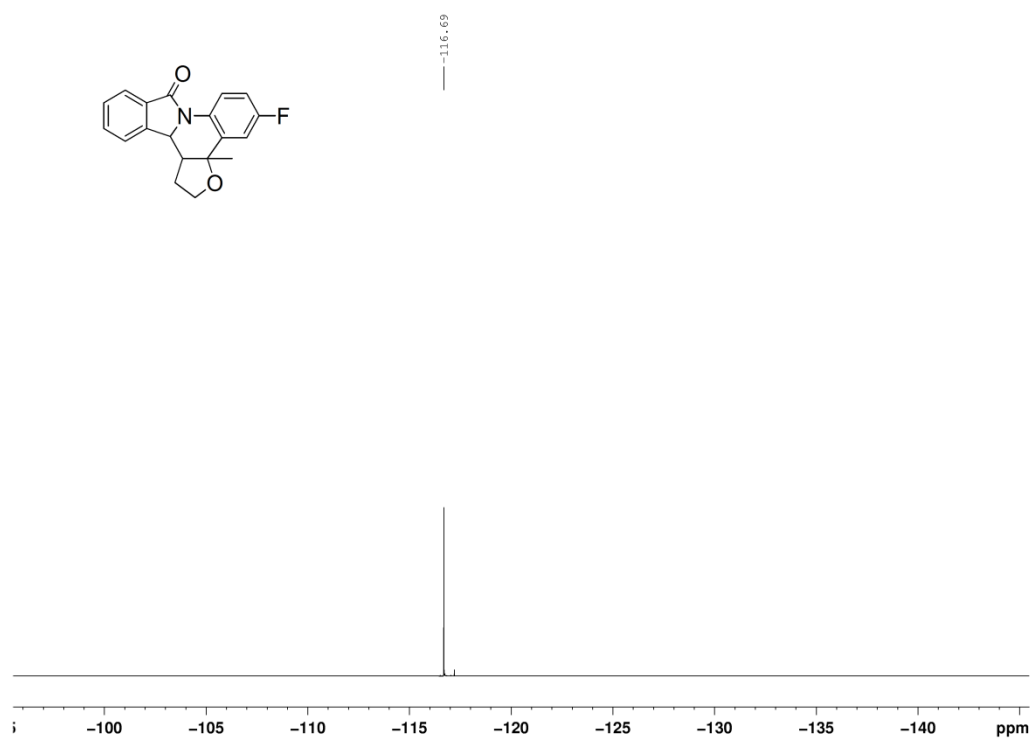
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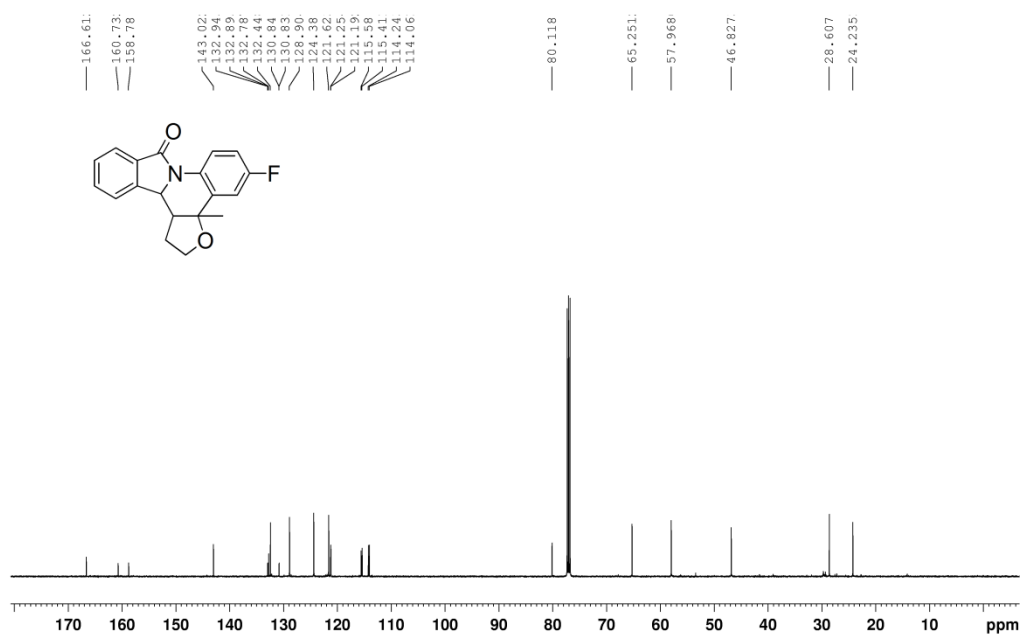
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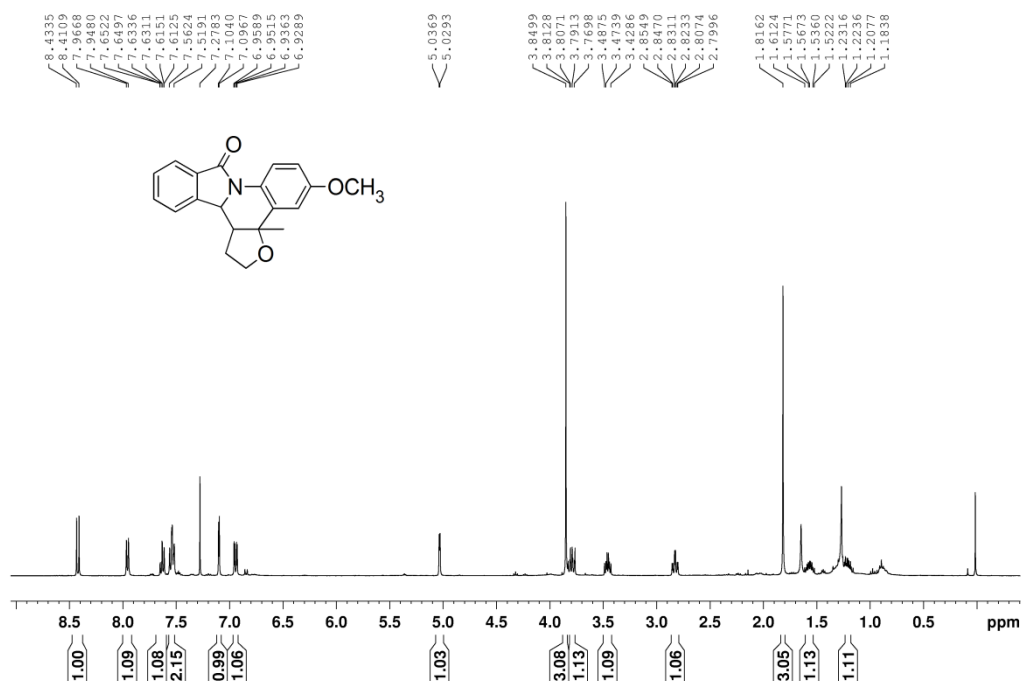
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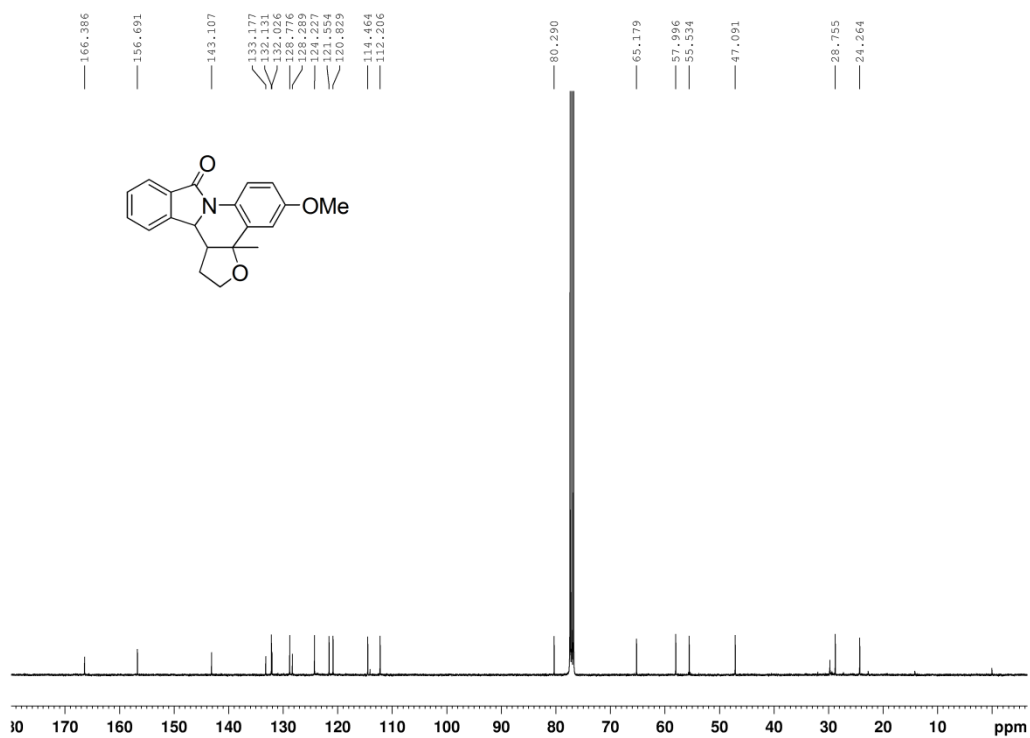
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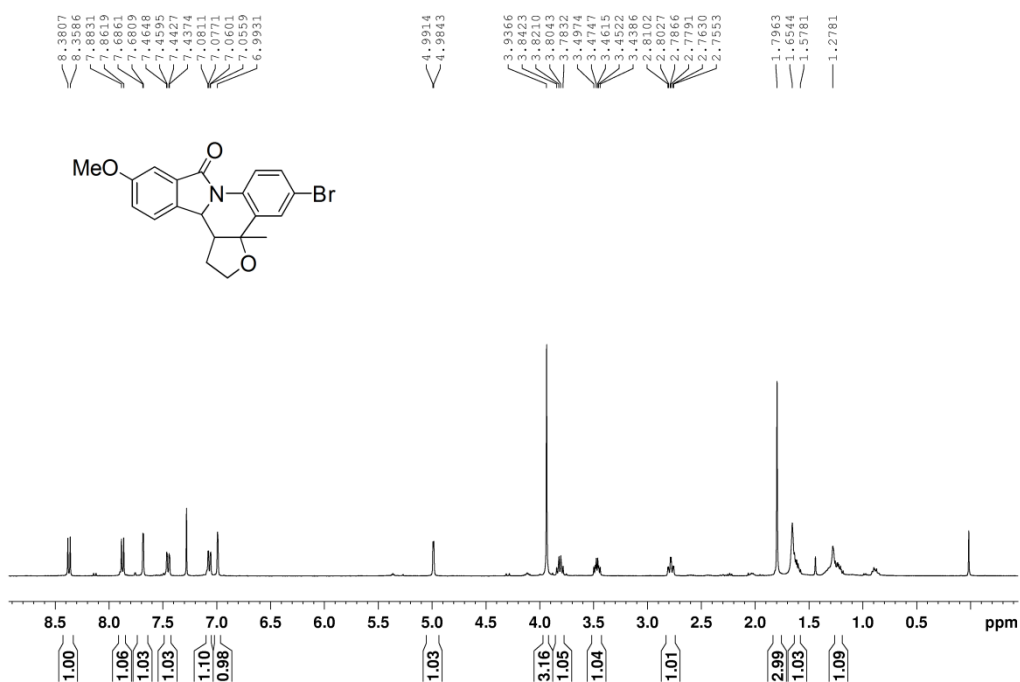
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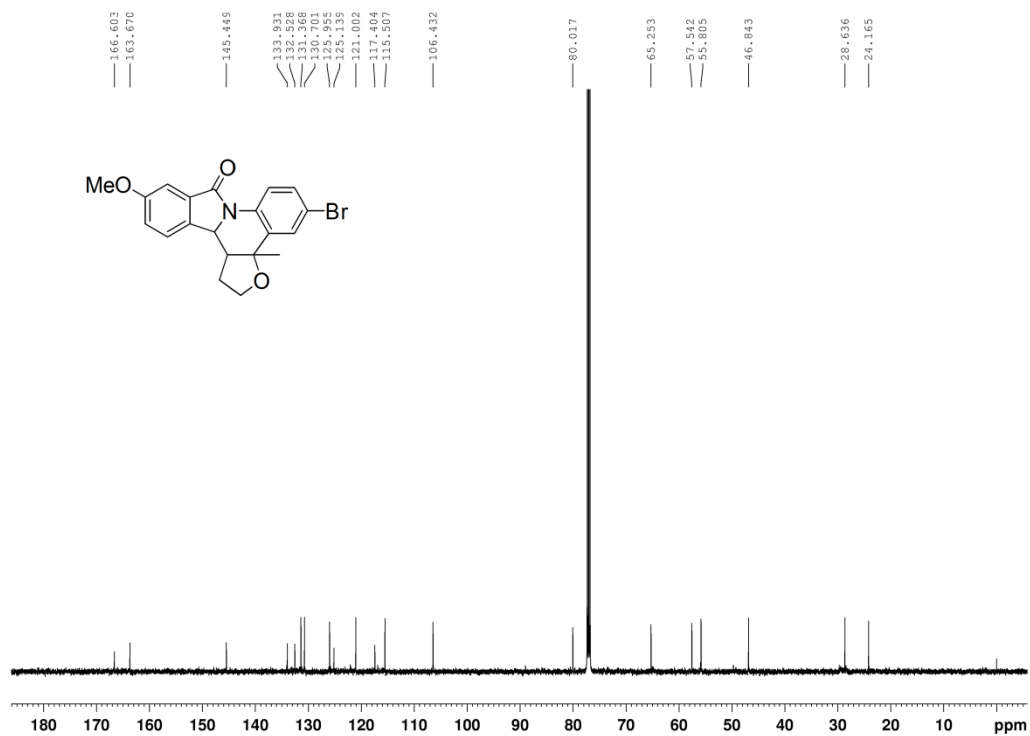
^1H NMR of **4g** in CDCl_3



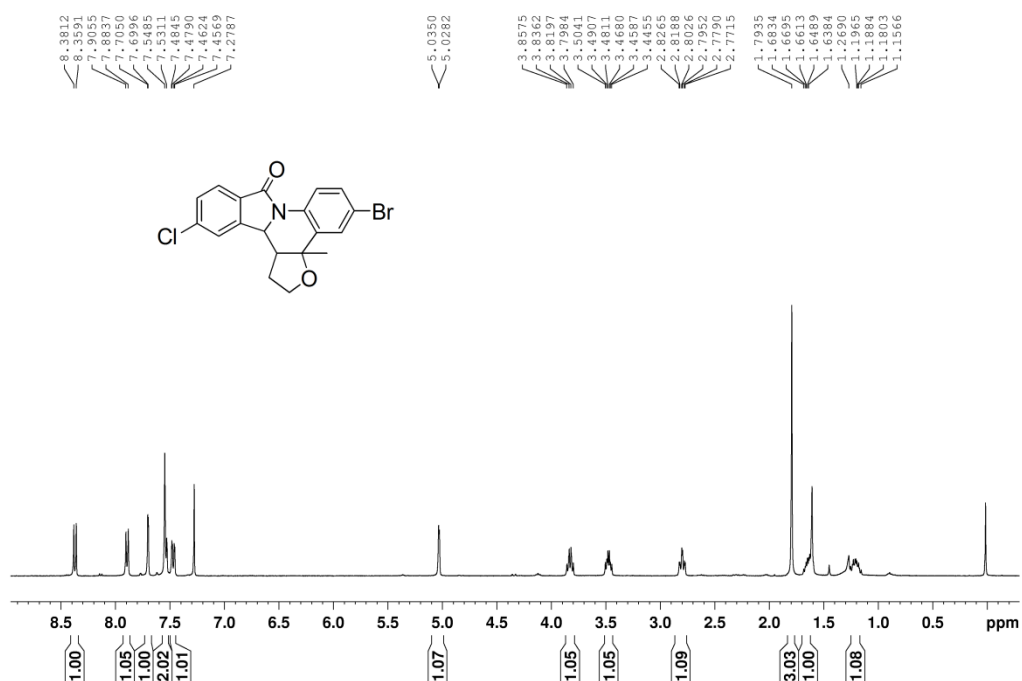
^{13}C NMR of **4g** in CDCl_3



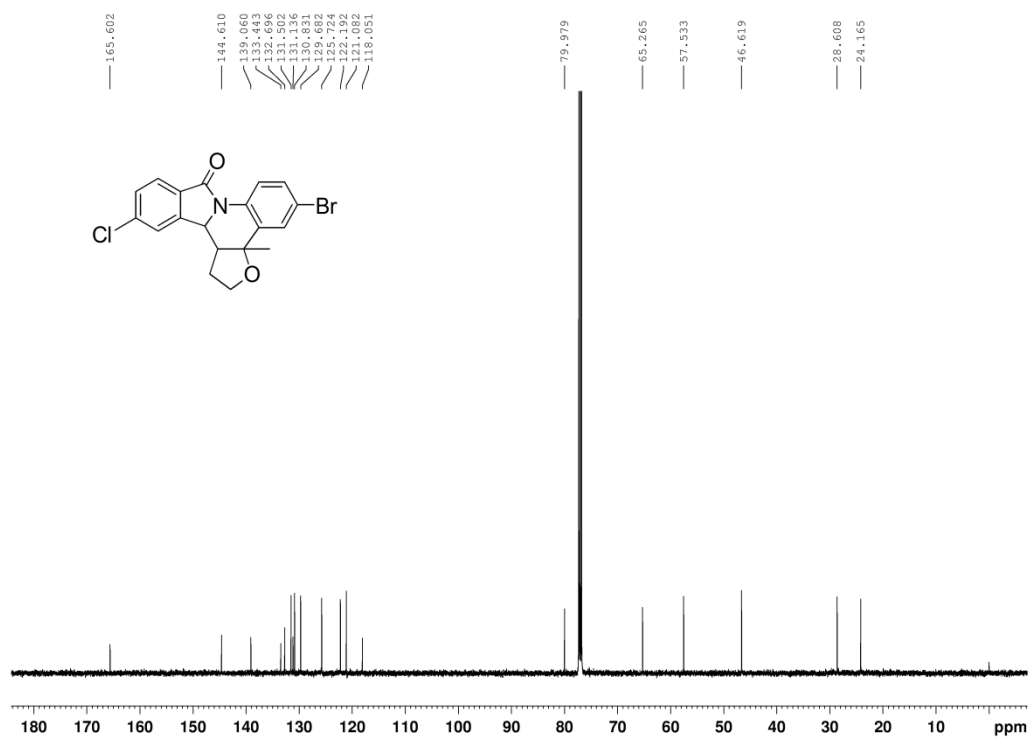
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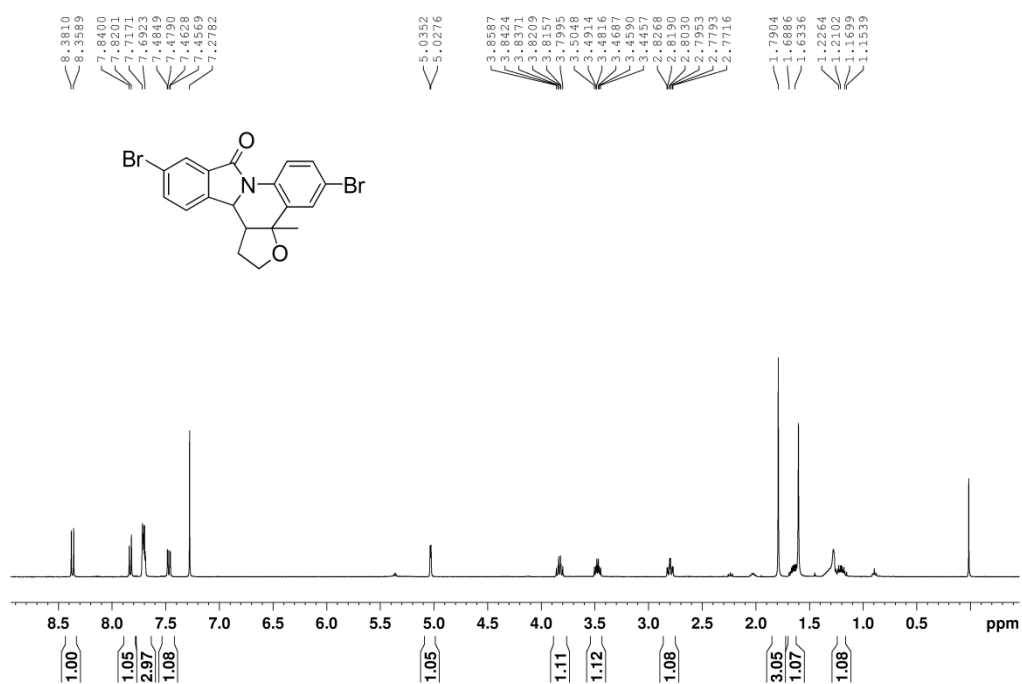
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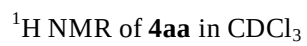
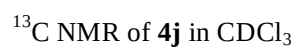
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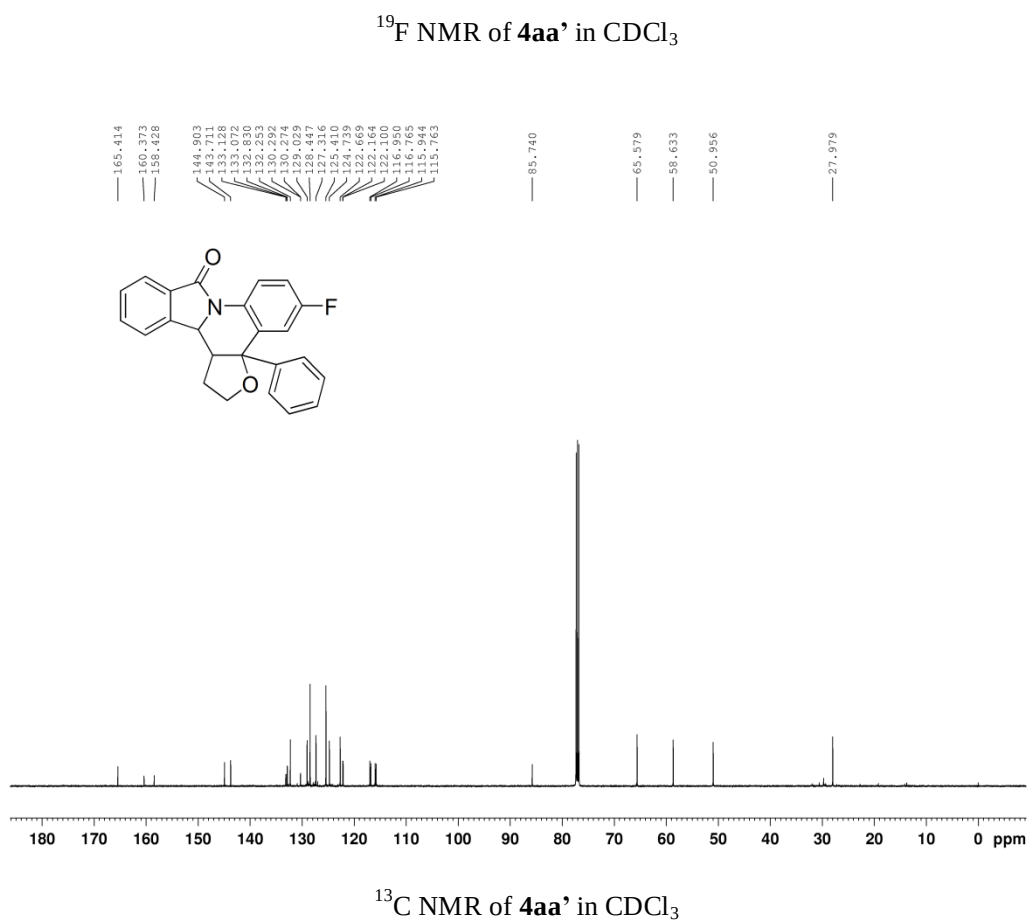
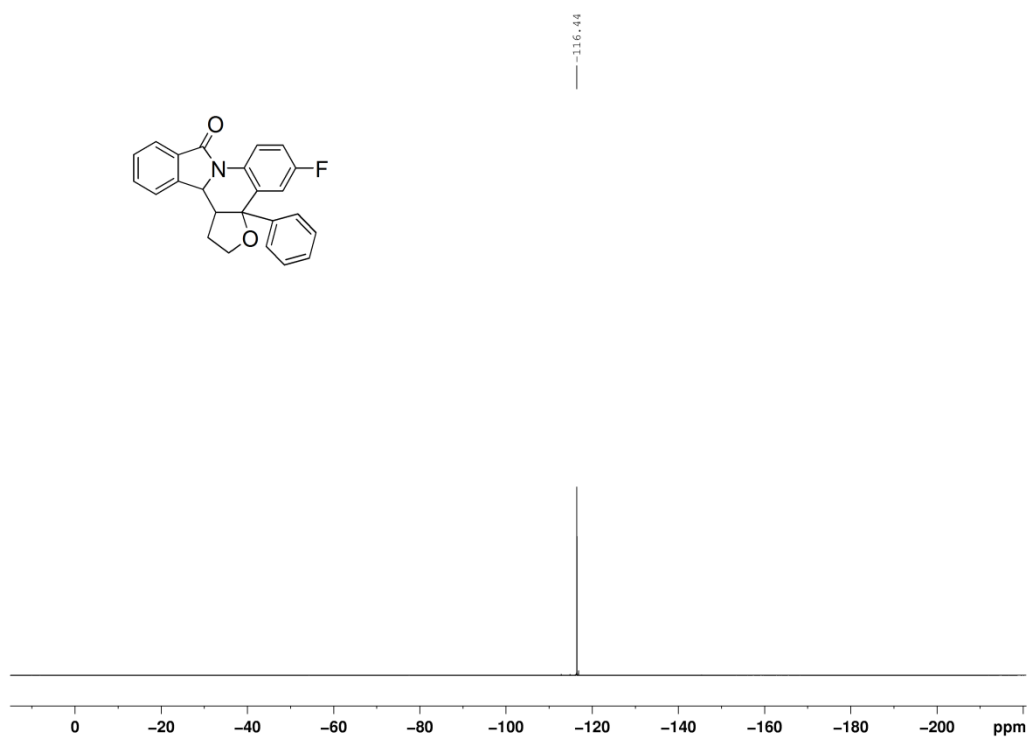


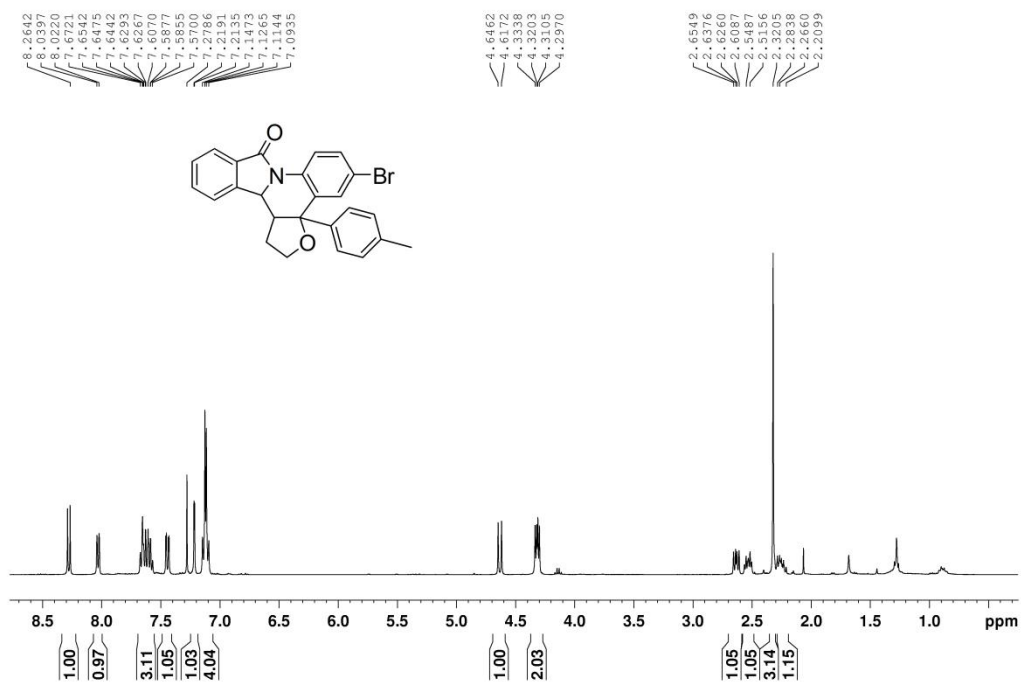
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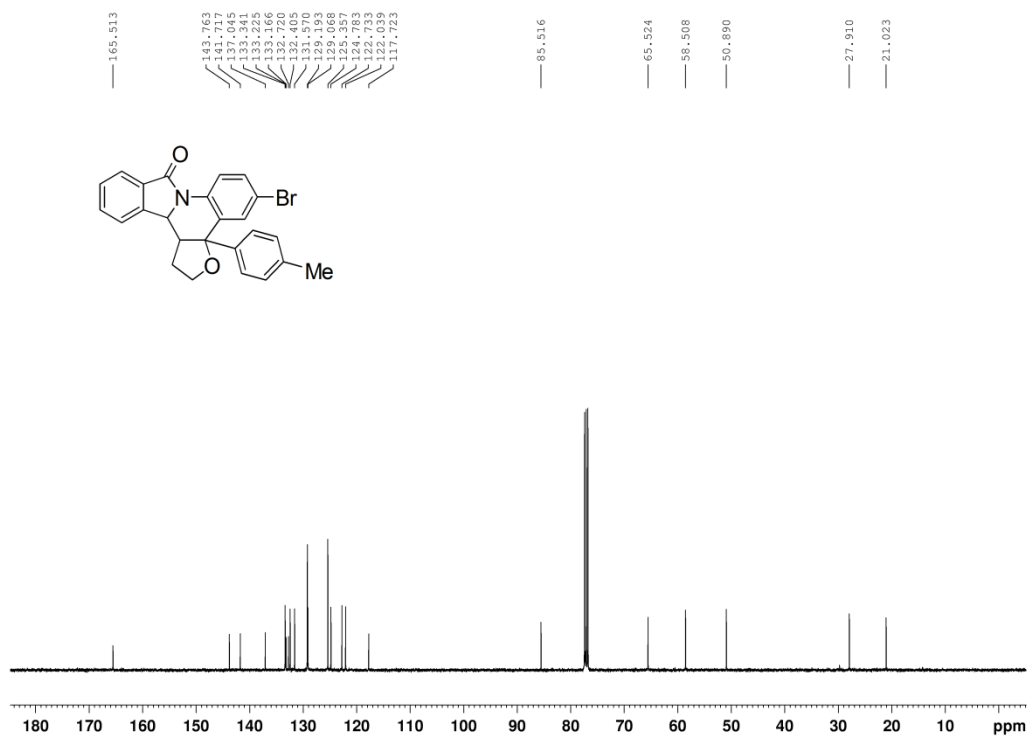
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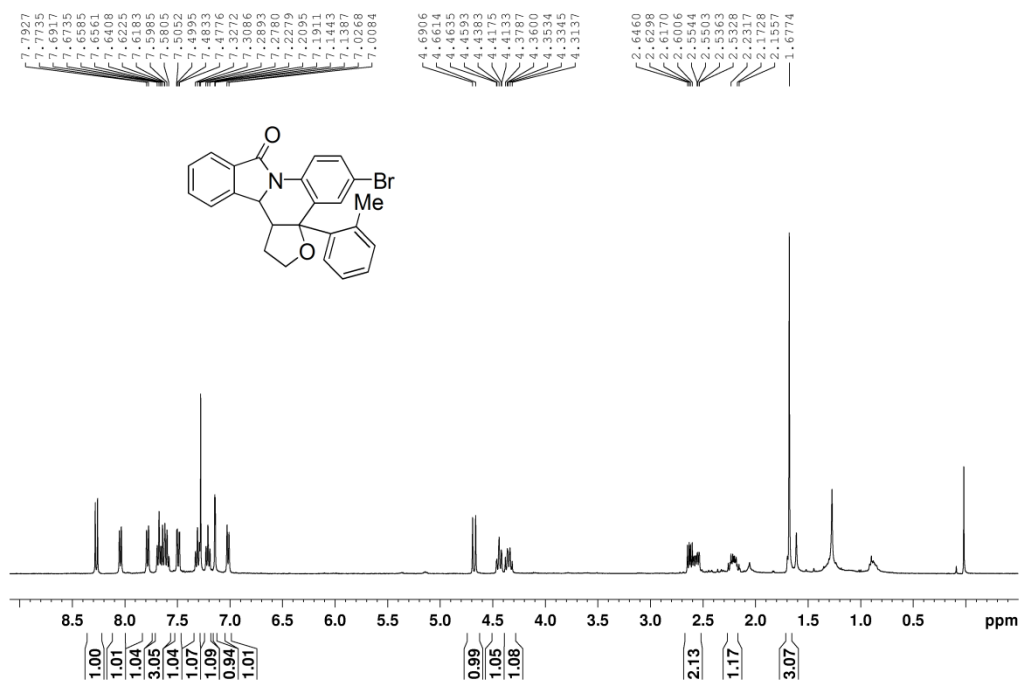




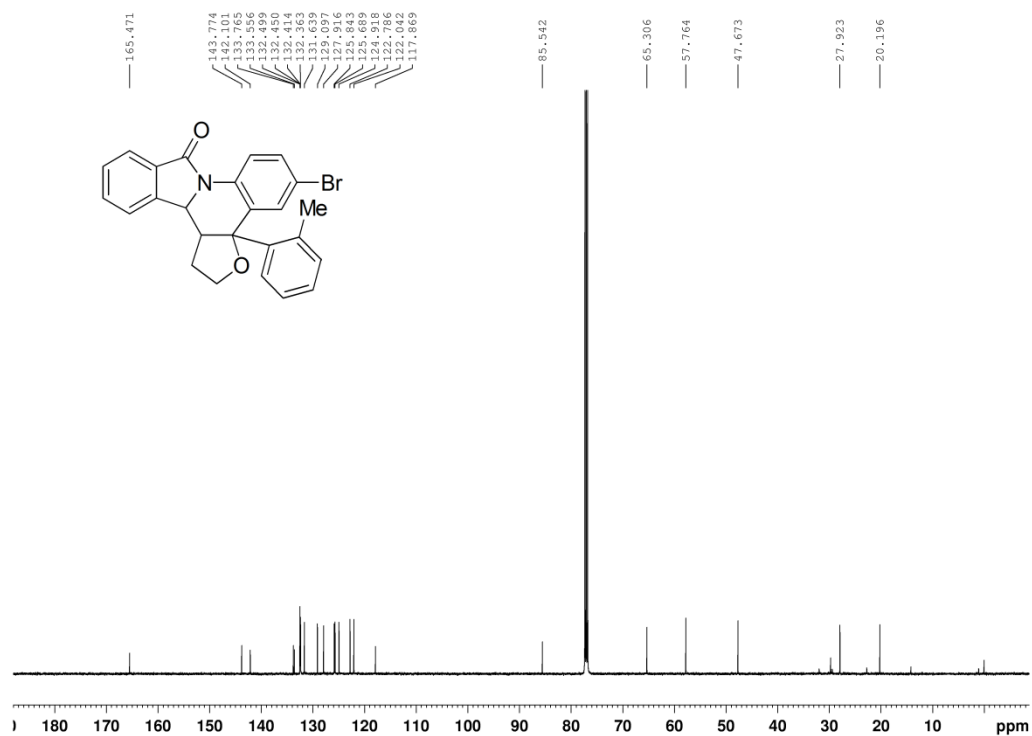
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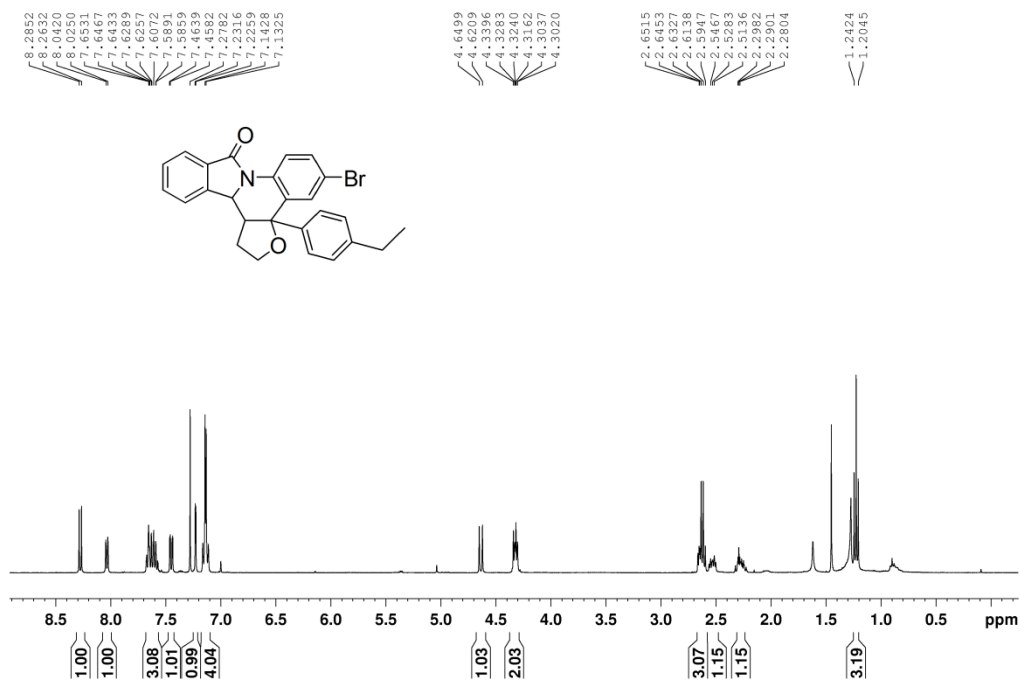
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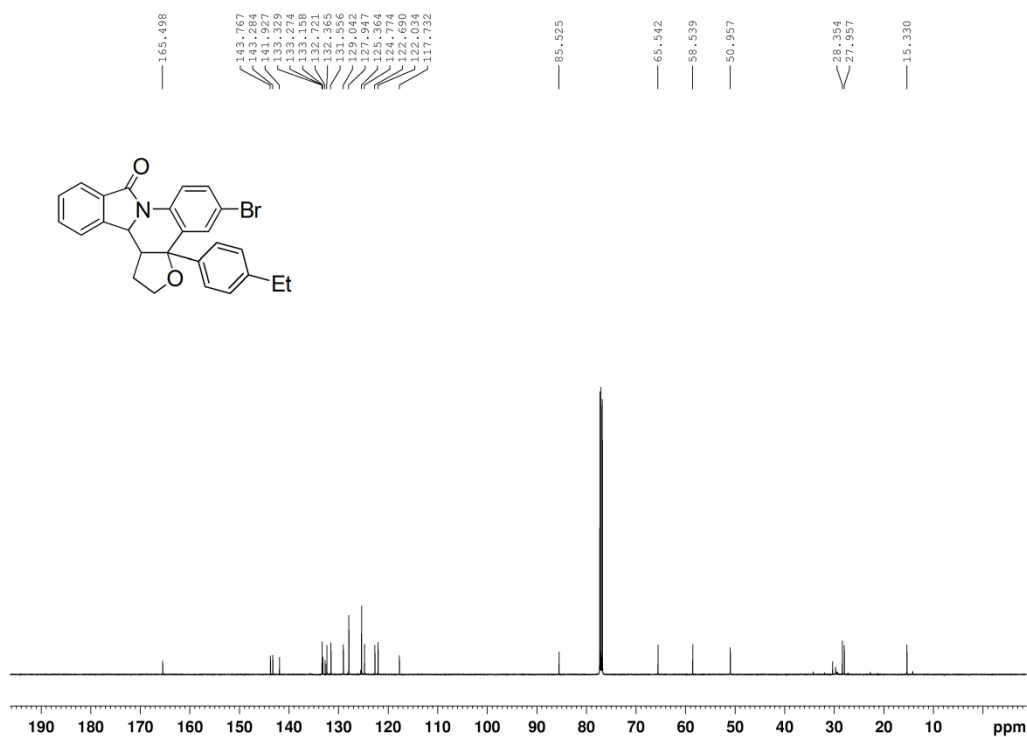
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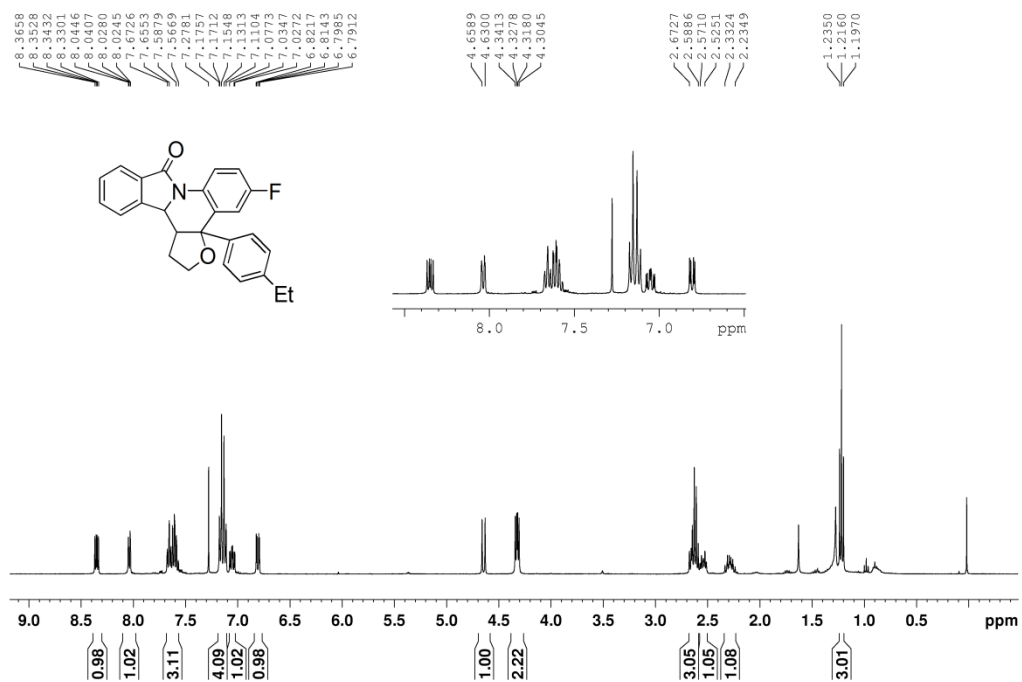
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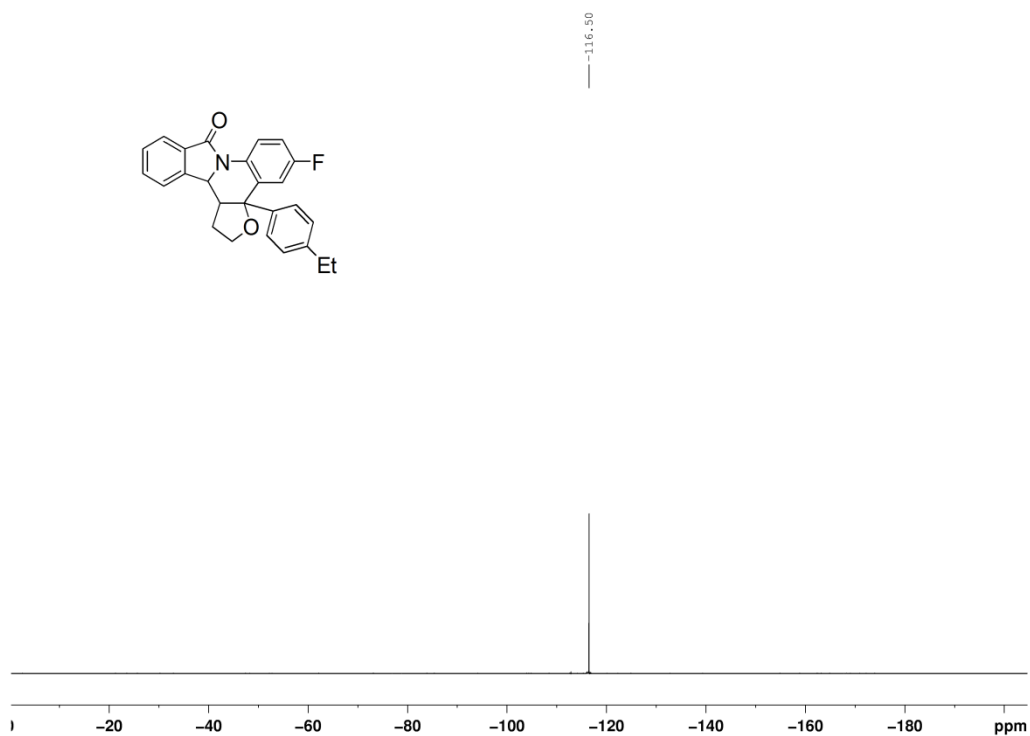
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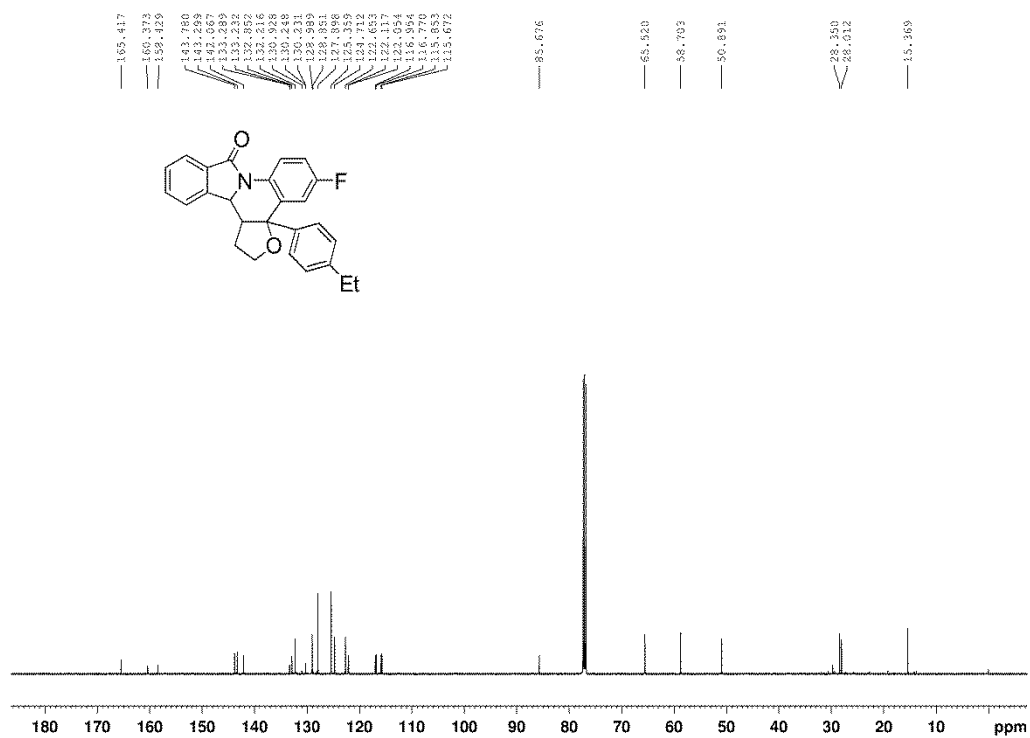
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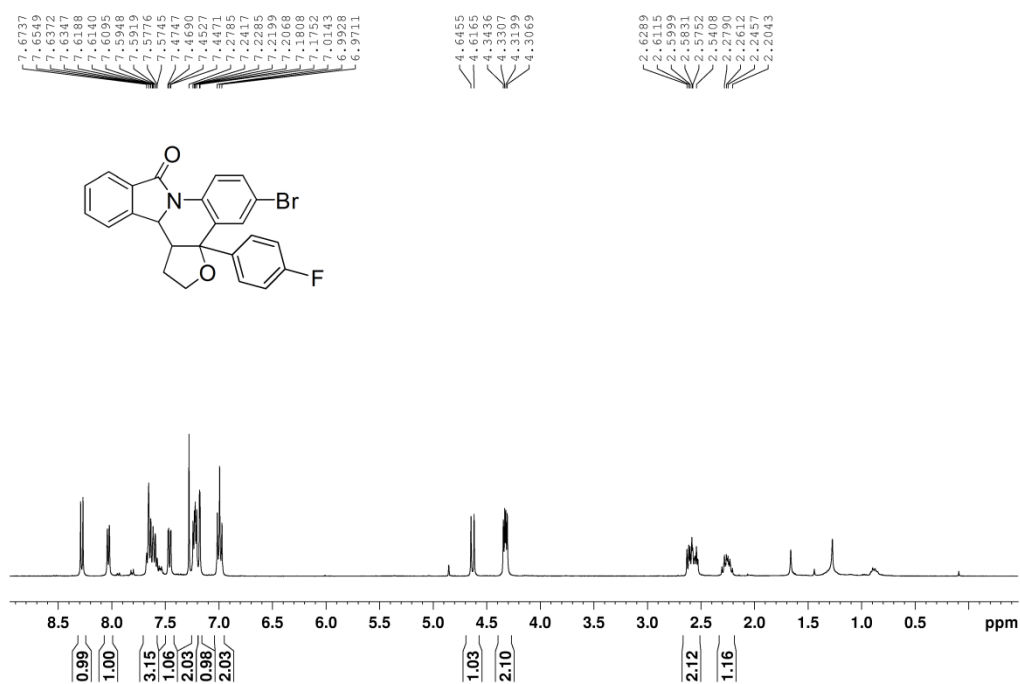
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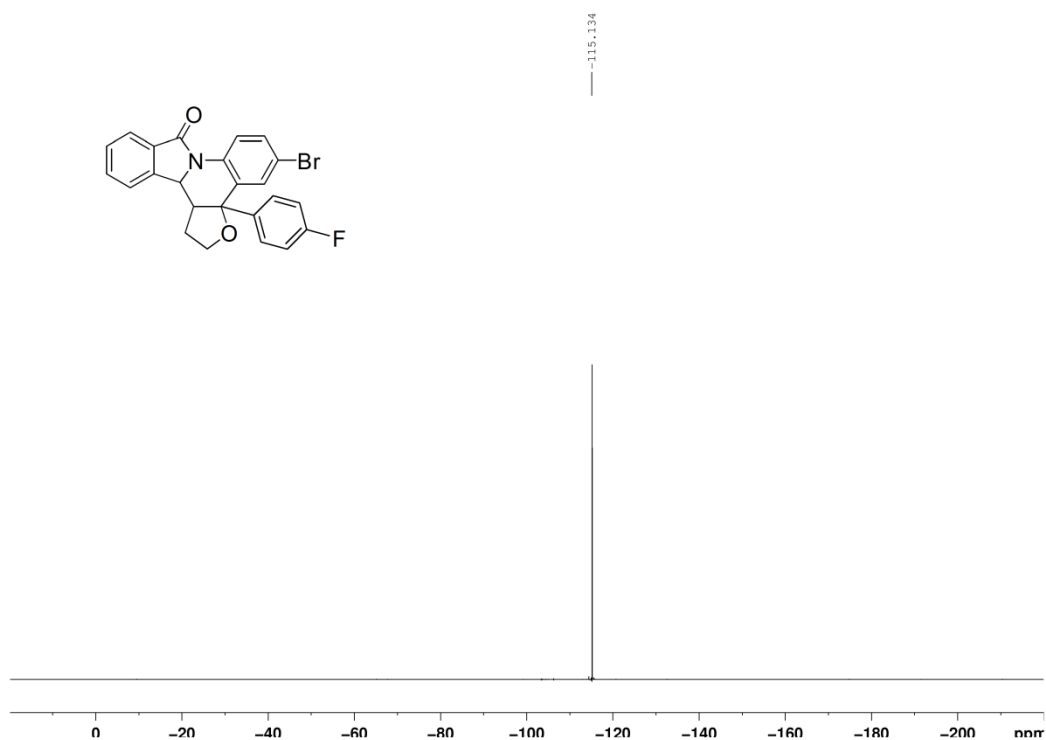
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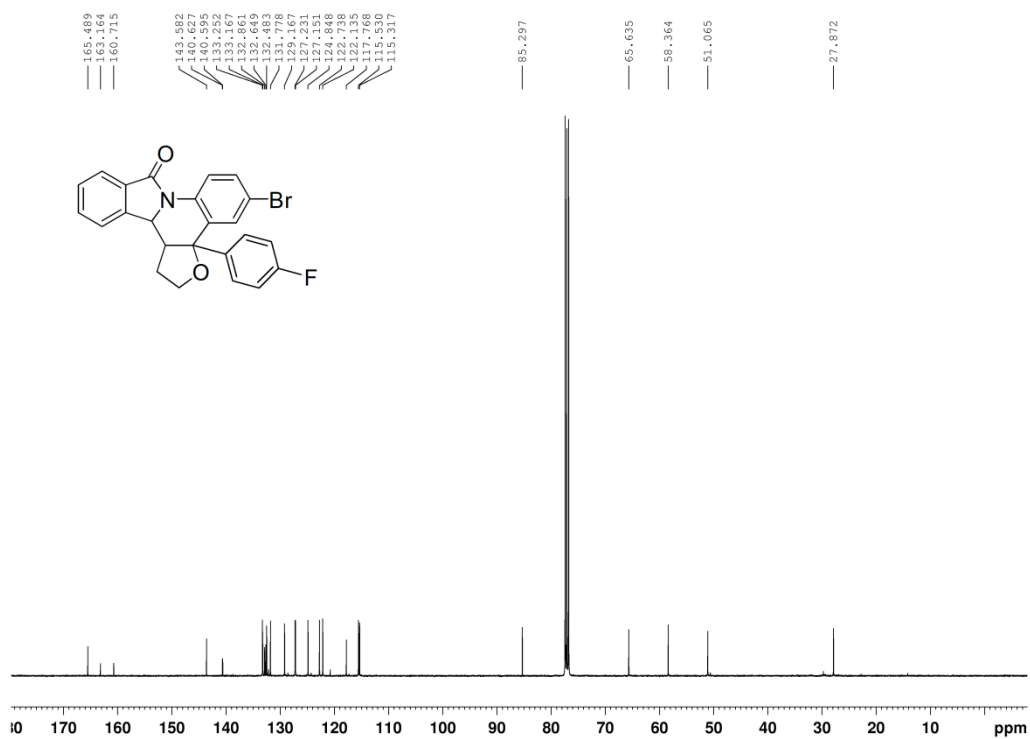
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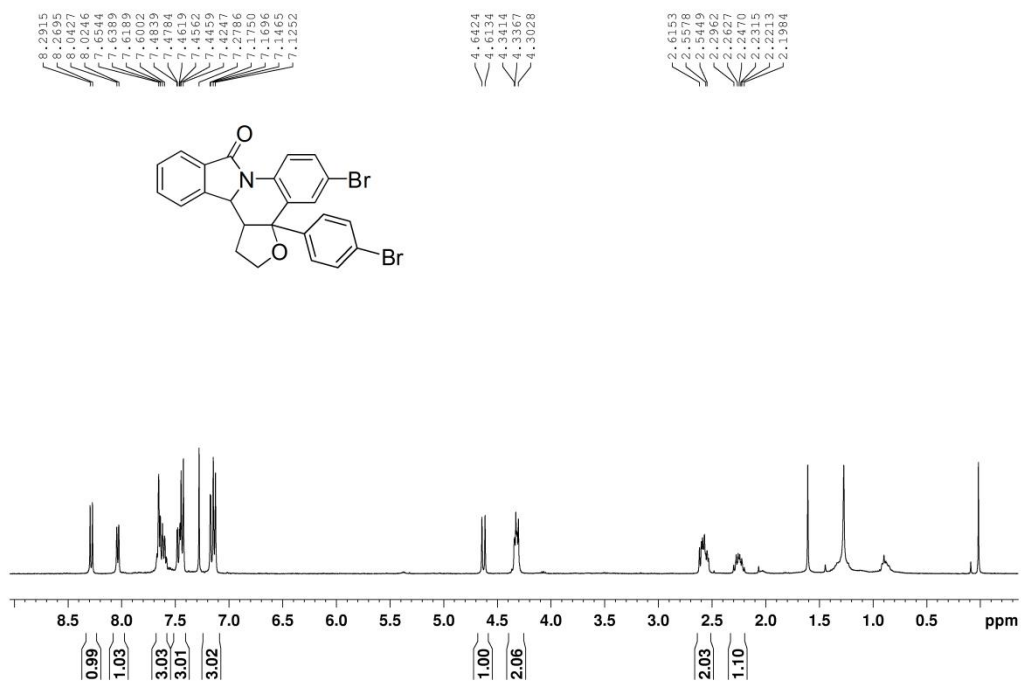
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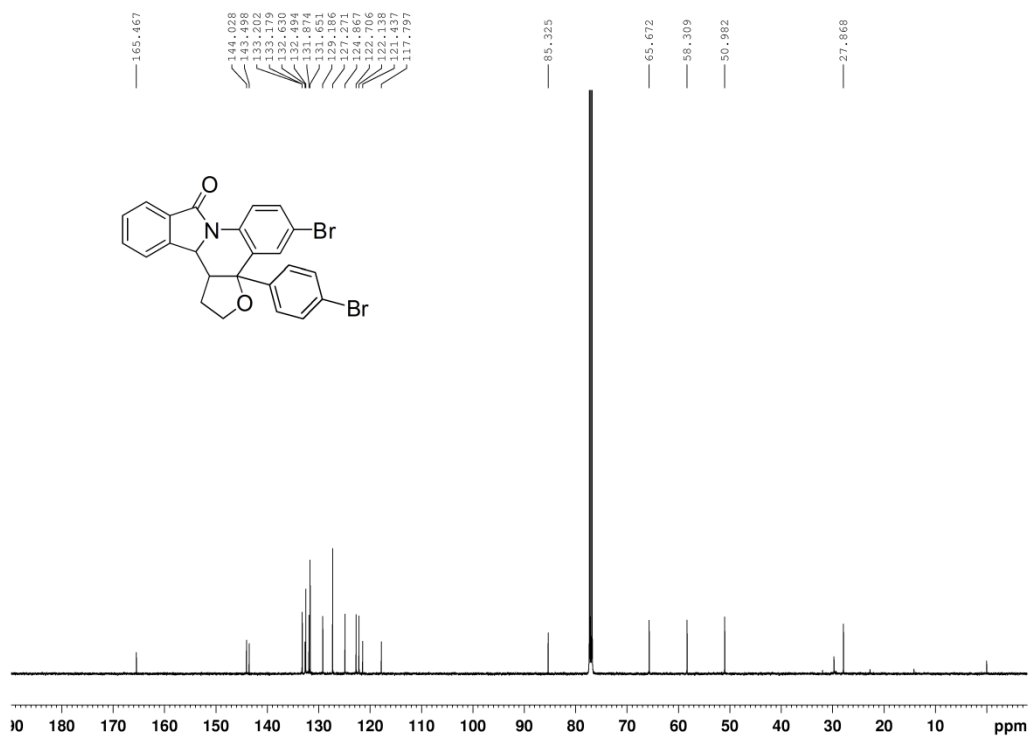
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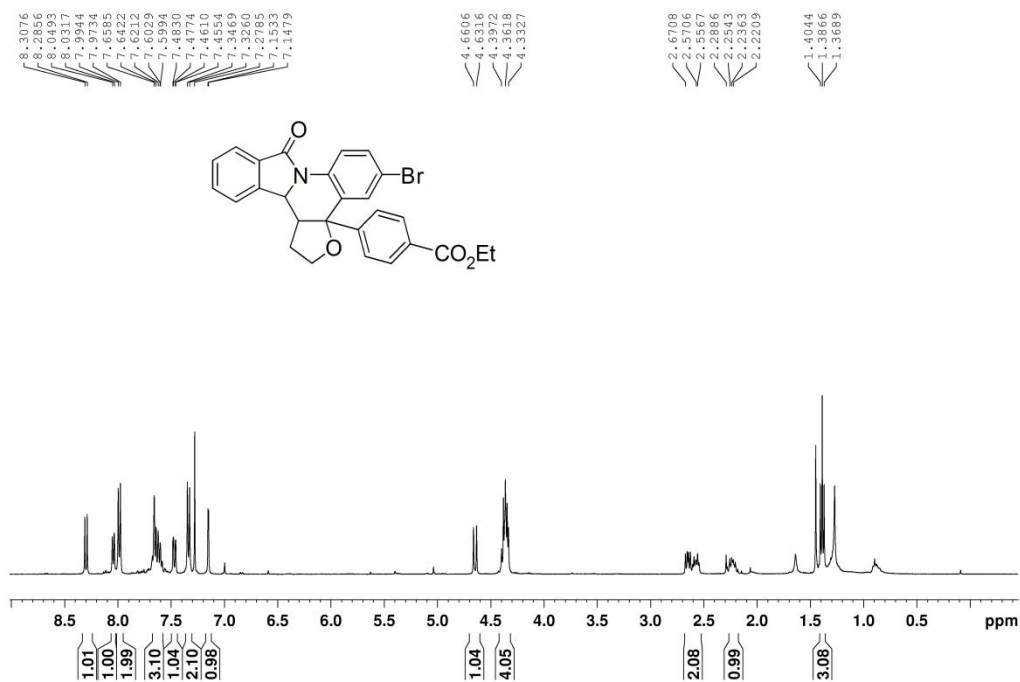
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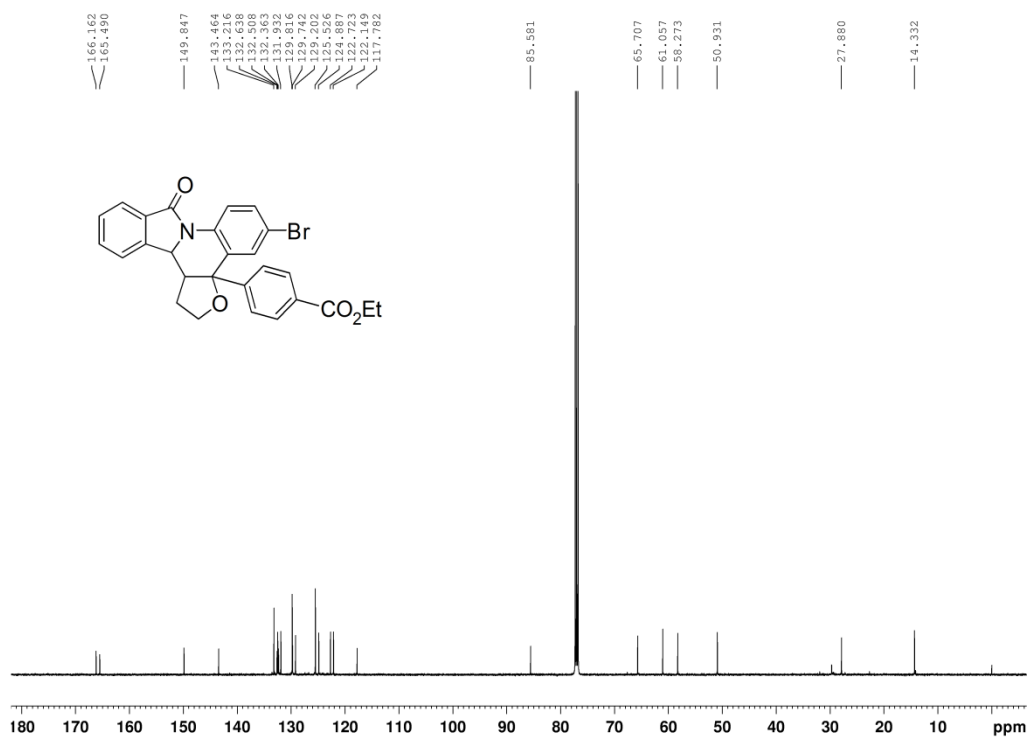
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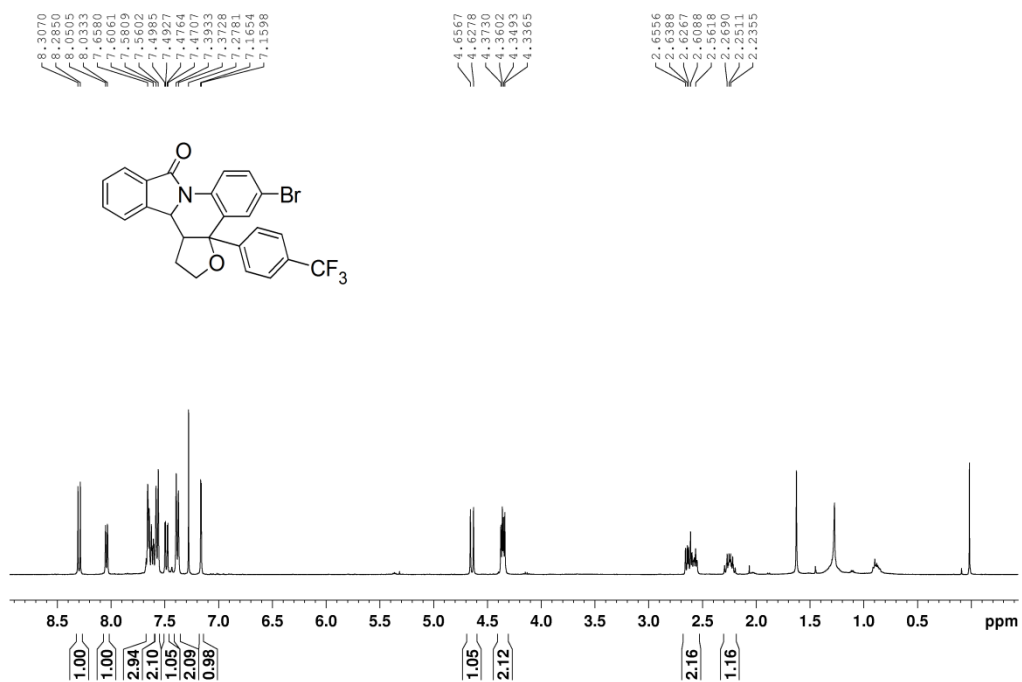
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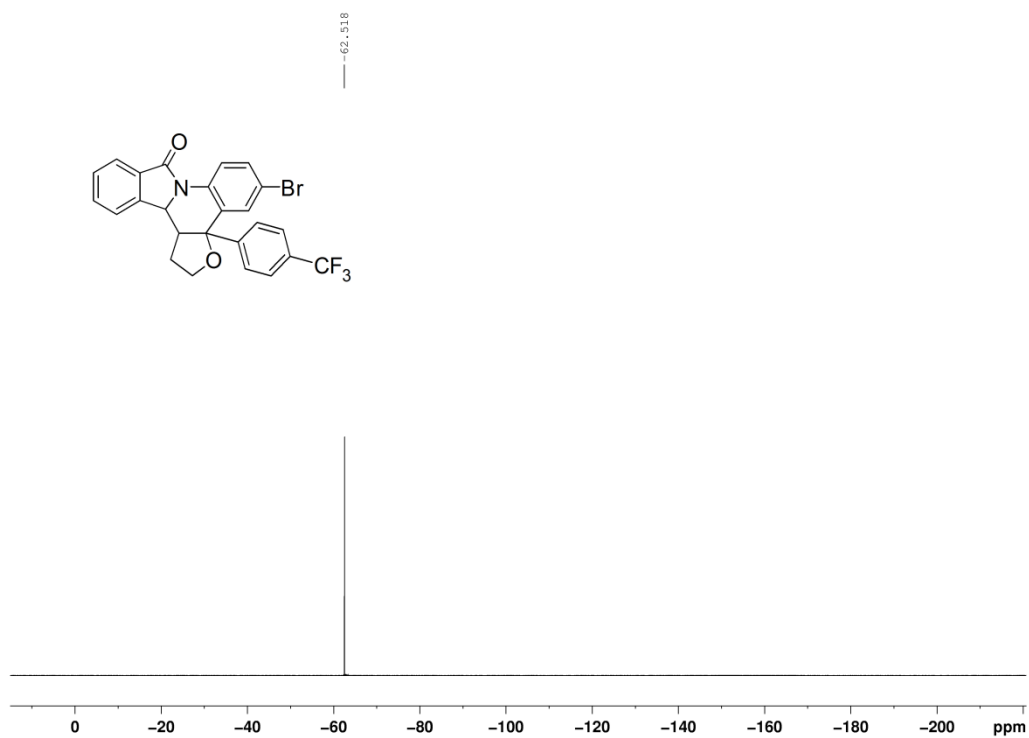
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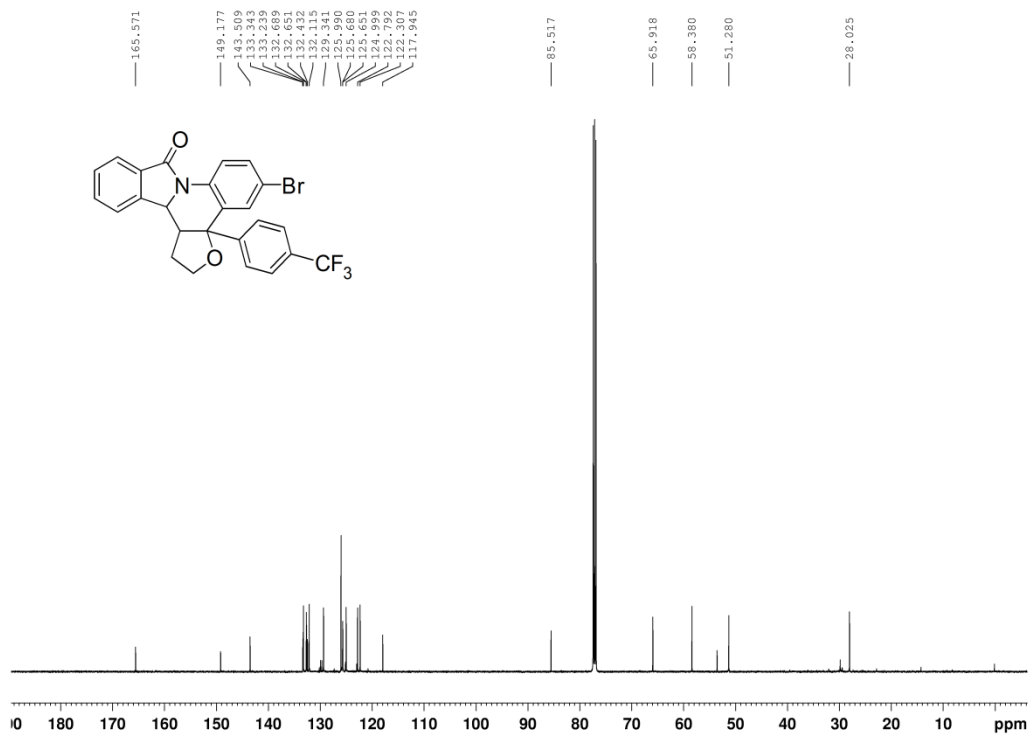
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¹H NMR of **4ah** in CDCl₃



¹⁹F NMR of **4ah** in CDCl₃



^{13}C NMR of **4ah** in CDCl₃