

Supporting Information

DABCO and Tributyl Phosphine Catalyzed [4+2] and [3+2] Cycloadditions of 3-Acyl-2H-chromen-ones and Ethyl 2,3-Butadienoate

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X-ray diffraction data for **2b** and **3j**

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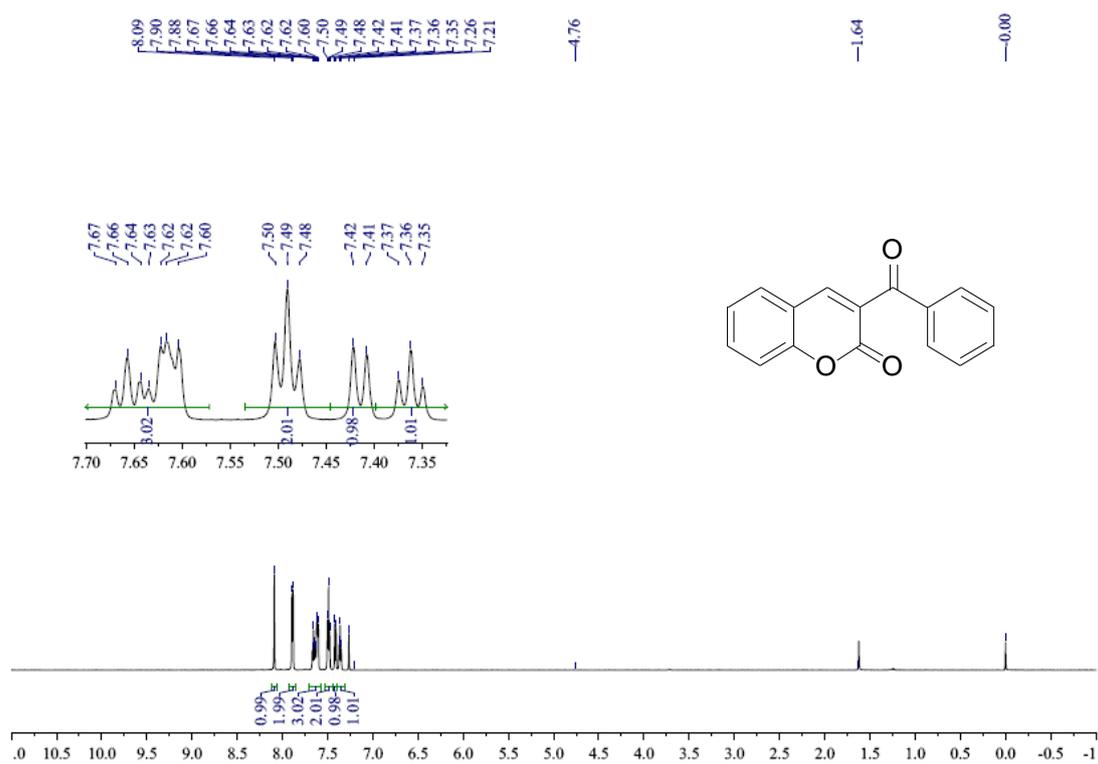


Figure S1. ^1H NMR spectrum (600 MHz, CDCl_3) of 3-benzoyl-chromen-2-one (**1a**)

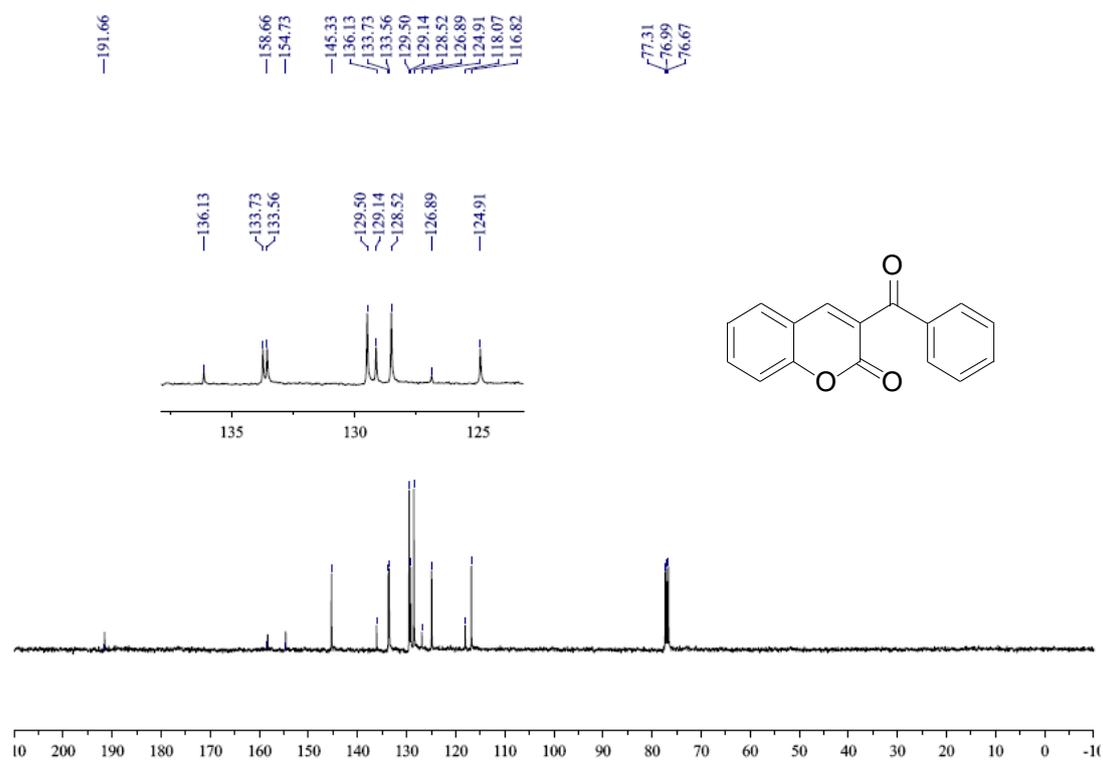


Figure S2. ^{13}C NMR spectrum (150 MHz, CDCl_3) of 3-benzoyl-chromen-2-one (**1a**)

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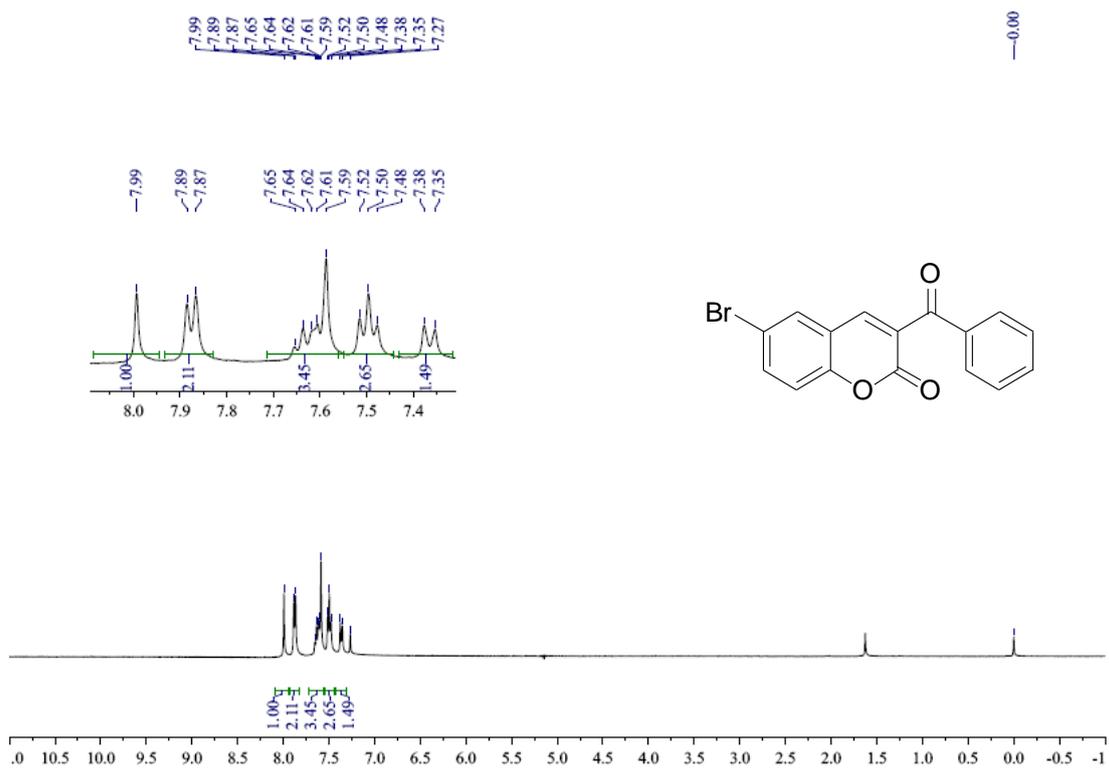


Figure S3. ¹H NMR spectrum (400 MHz, CDCl₃) of 3-benzoyl-6-bromo-chromen-2-one (**1b**)

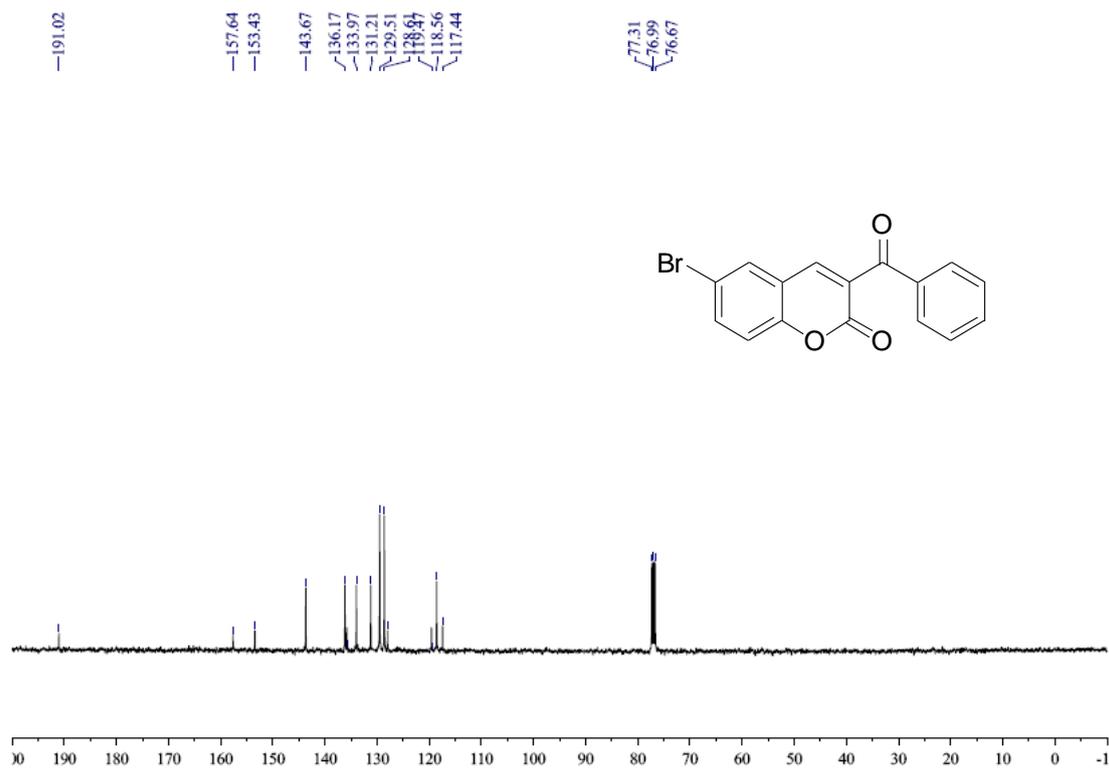


Figure S4. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3-benzoyl-6-bromo-chromen-2-one (**1b**)

Supporting Information

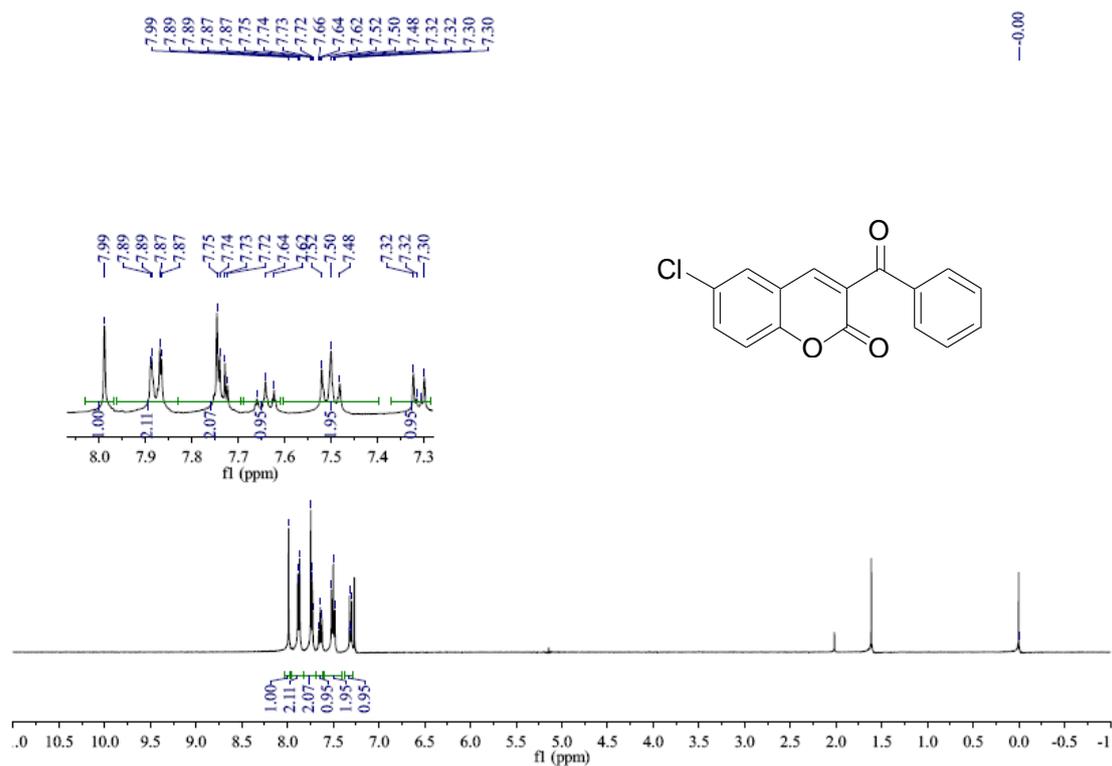


Figure S5. ¹H NMR spectrum (400 MHz, CDCl₃) of 3-benzoyl-6-chloro-chromen-2-one (**1c**)

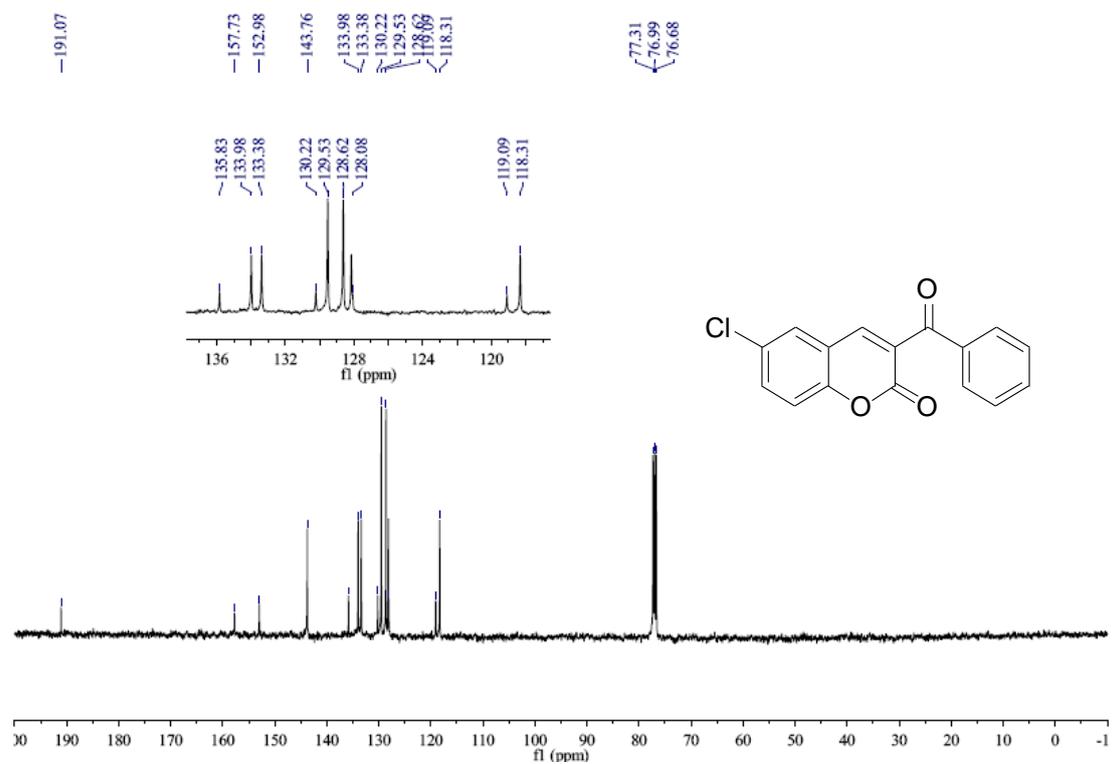


Figure S6. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3-benzoyl-6-chloro-chromen-2-one (**1c**)

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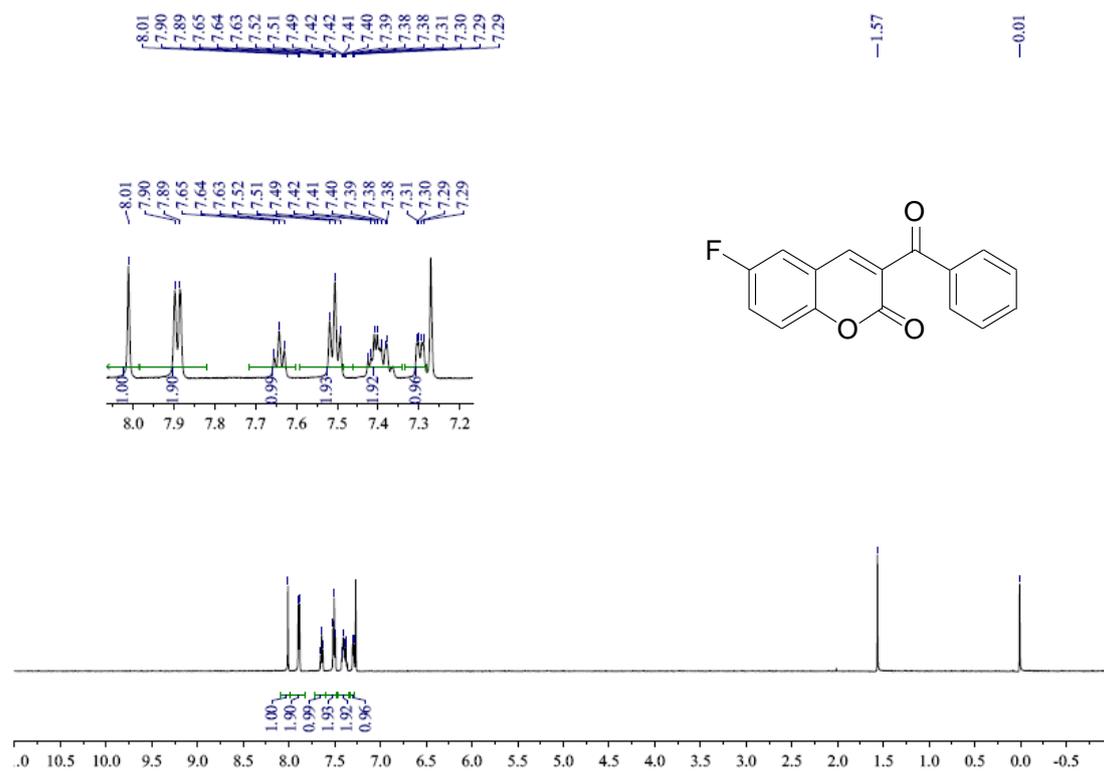


Figure S7. ¹H NMR spectrum (600 MHz, CDCl₃) of 3-benzoyl-6-fluoro-chromen-2-one (**1d**)

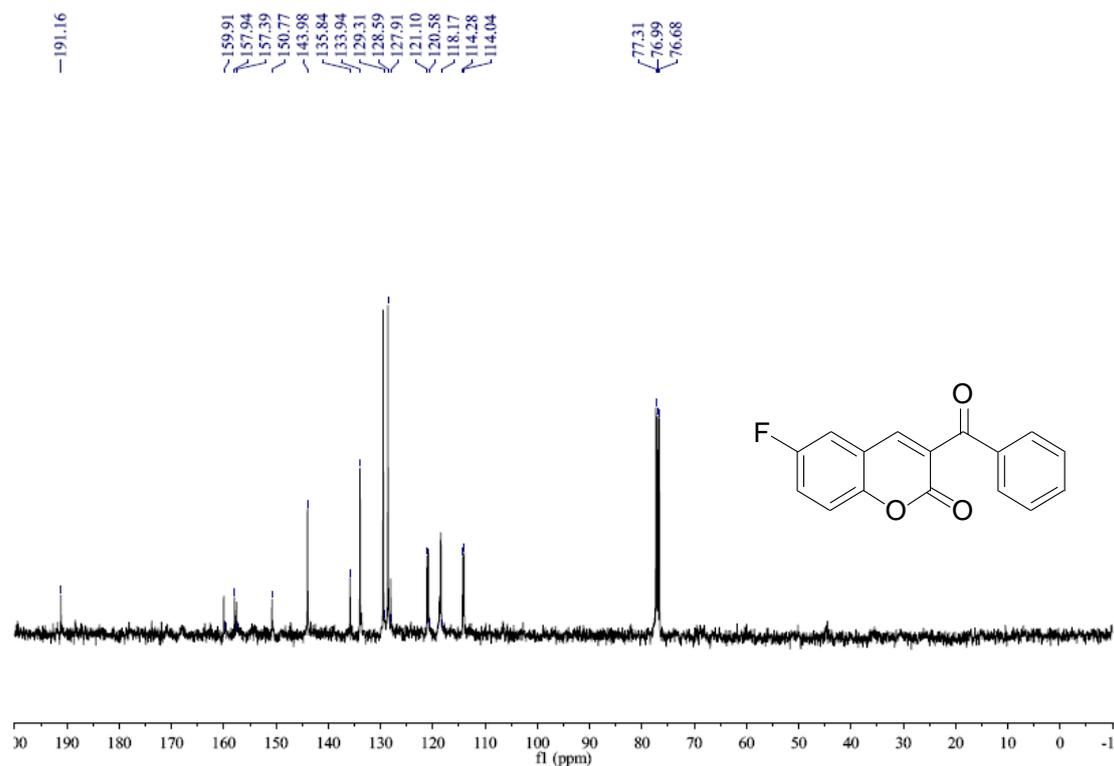


Figure S8. ¹³C NMR spectrum (150 MHz, CDCl₃) of 3-benzoyl-6-fluoro-chromen-2-one (**1d**)

Supporting Information

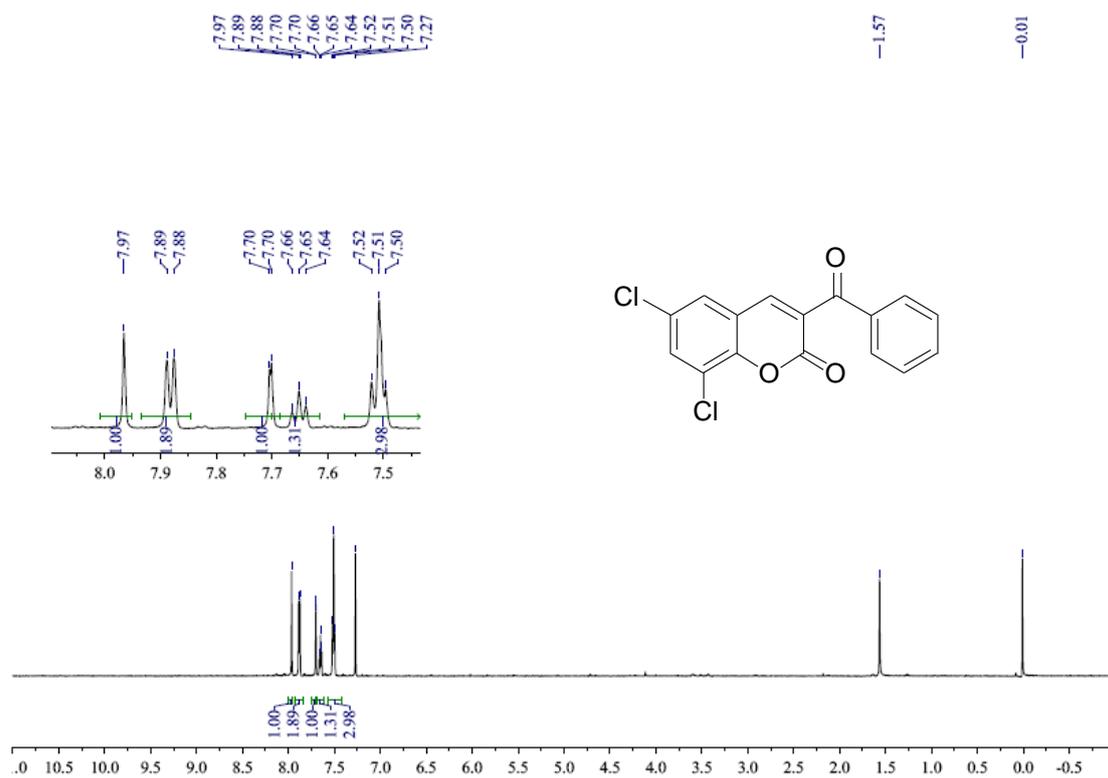


Figure S9. ¹H NMR spectrum (600 MHz, CDCl₃) of 3-benzoyl-6,8-dichloro-chromen-2-one (1e)

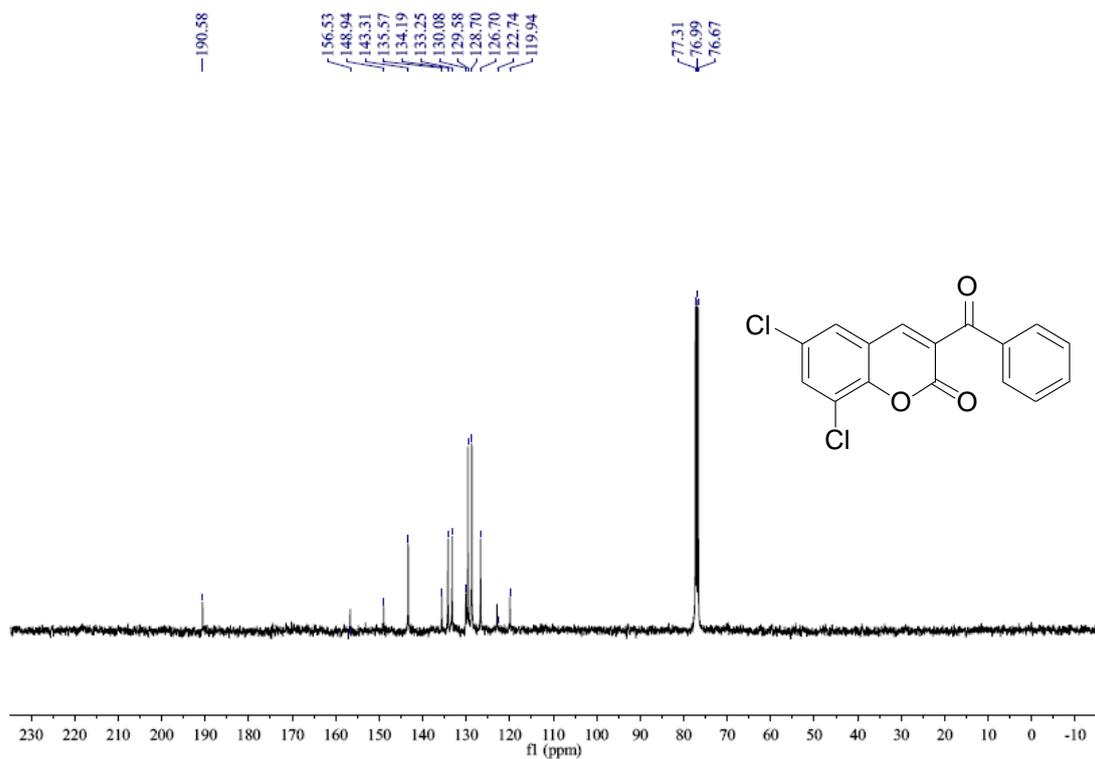


Figure S10. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3-benzoyl-6,8-dichloro-chromen-2-one (1e)

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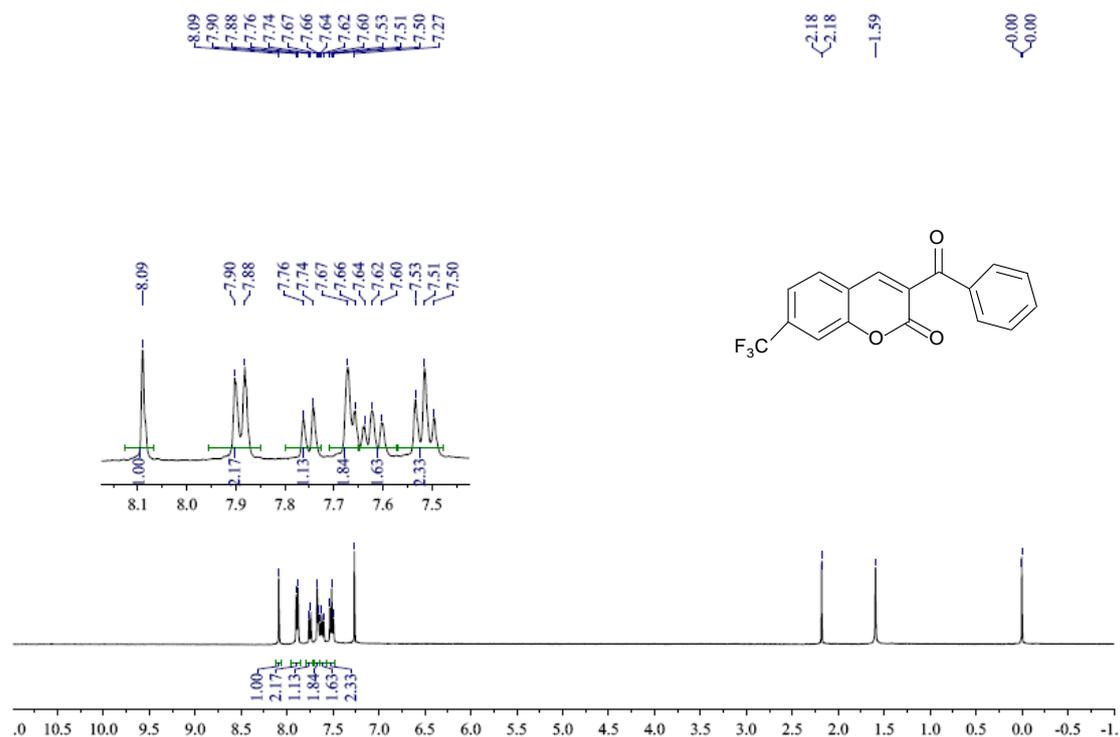


Figure S11. ¹H NMR spectrum (400 MHz, CDCl₃) of 3-benzoyl-7-(trifluoromethyl)-chromen-2-one (**1f**)

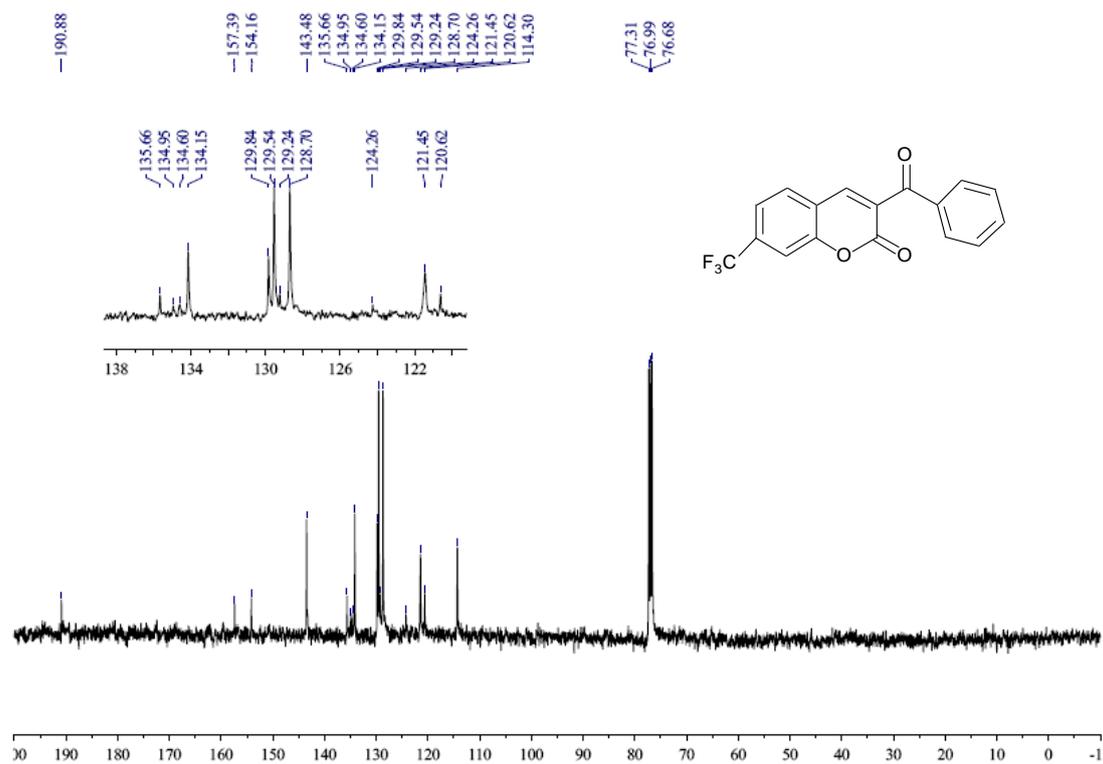


Figure S12. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3-benzoyl-7-(trifluoromethyl)-chromen-2-one (**1f**)

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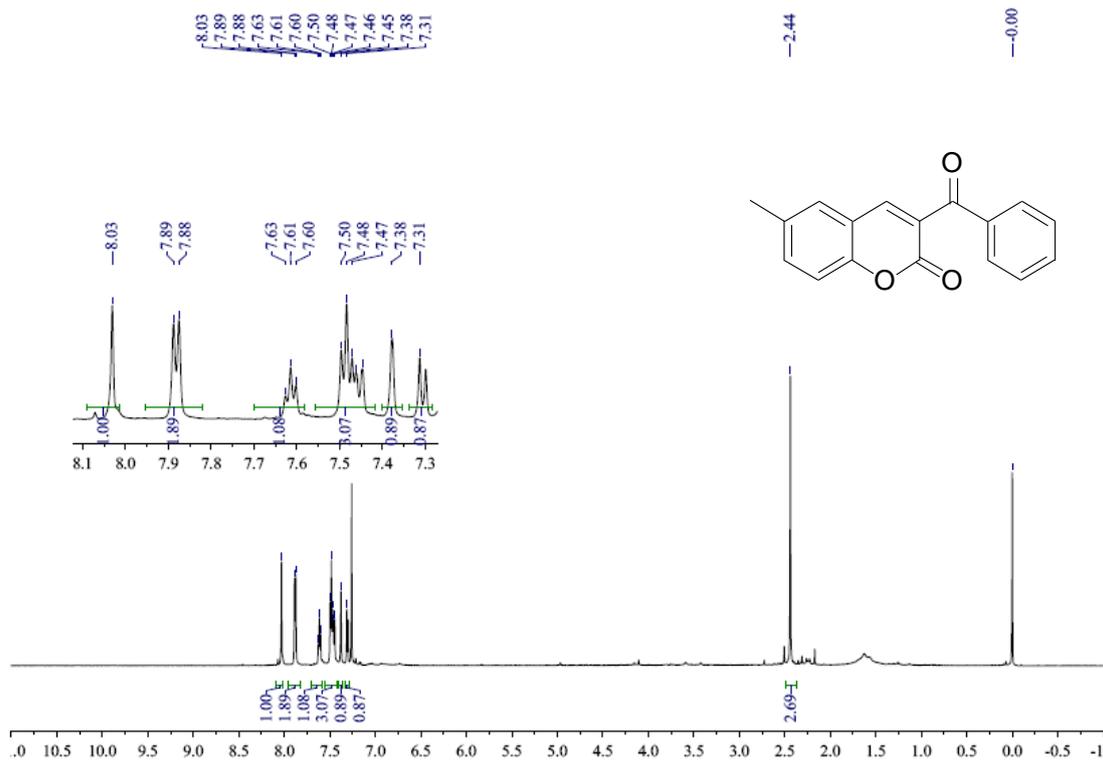


Figure S13. ¹H NMR spectrum (600 MHz, CDCl₃) of 3-benzoyl-6-methyl-chromen-2-one (**1g**)

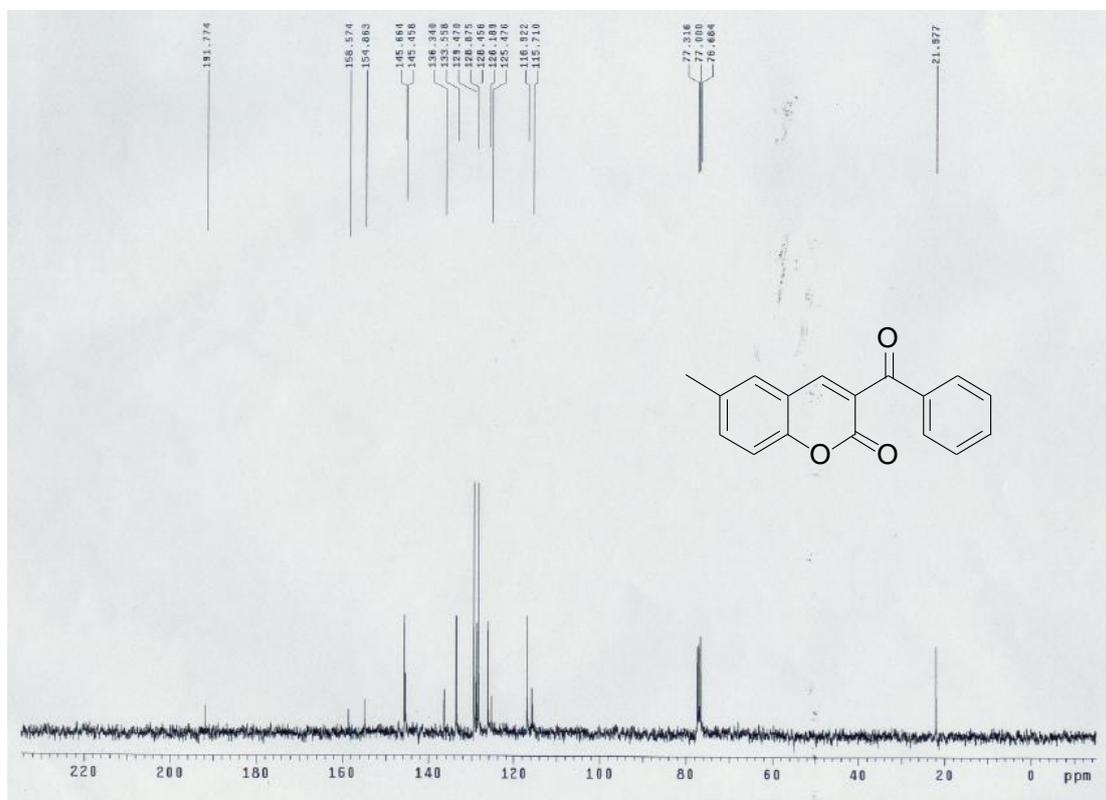


Figure S14. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3-benzoyl-6-methyl-chromen-2-one (**1g**)

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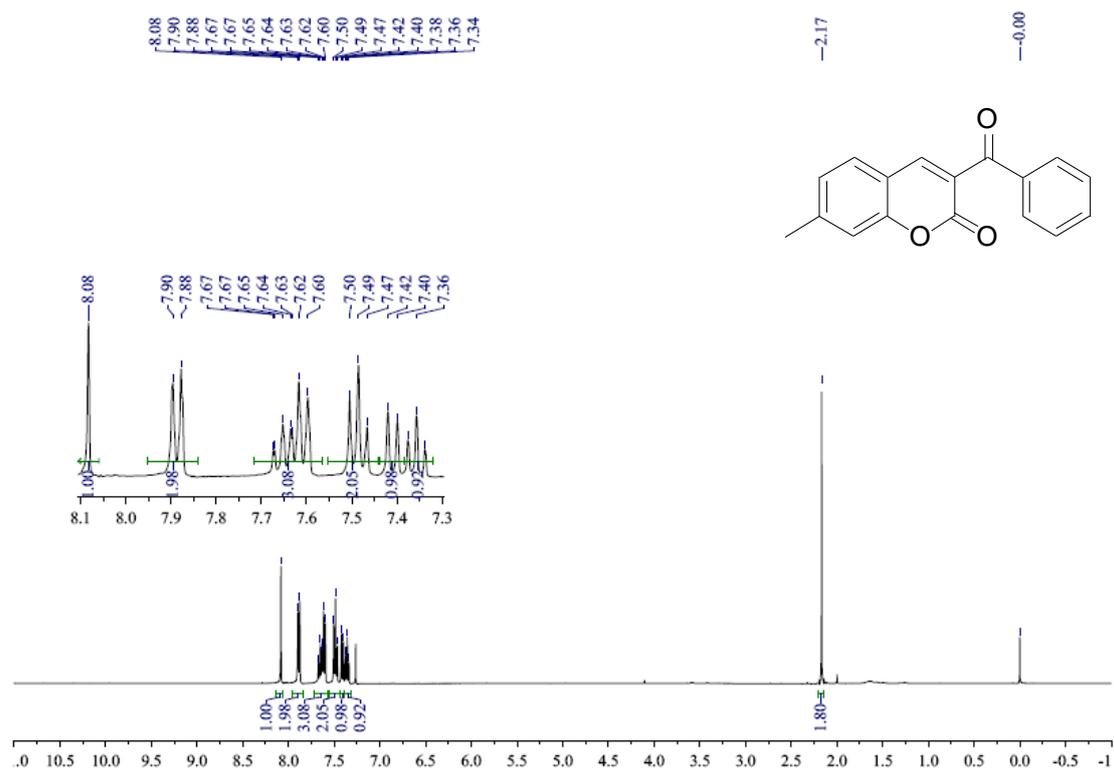


Figure S15. ¹H NMR spectrum (400 MHz, CDCl₃) of 3-benzoyl-7-methyl-chromen-2-one (**1h**)

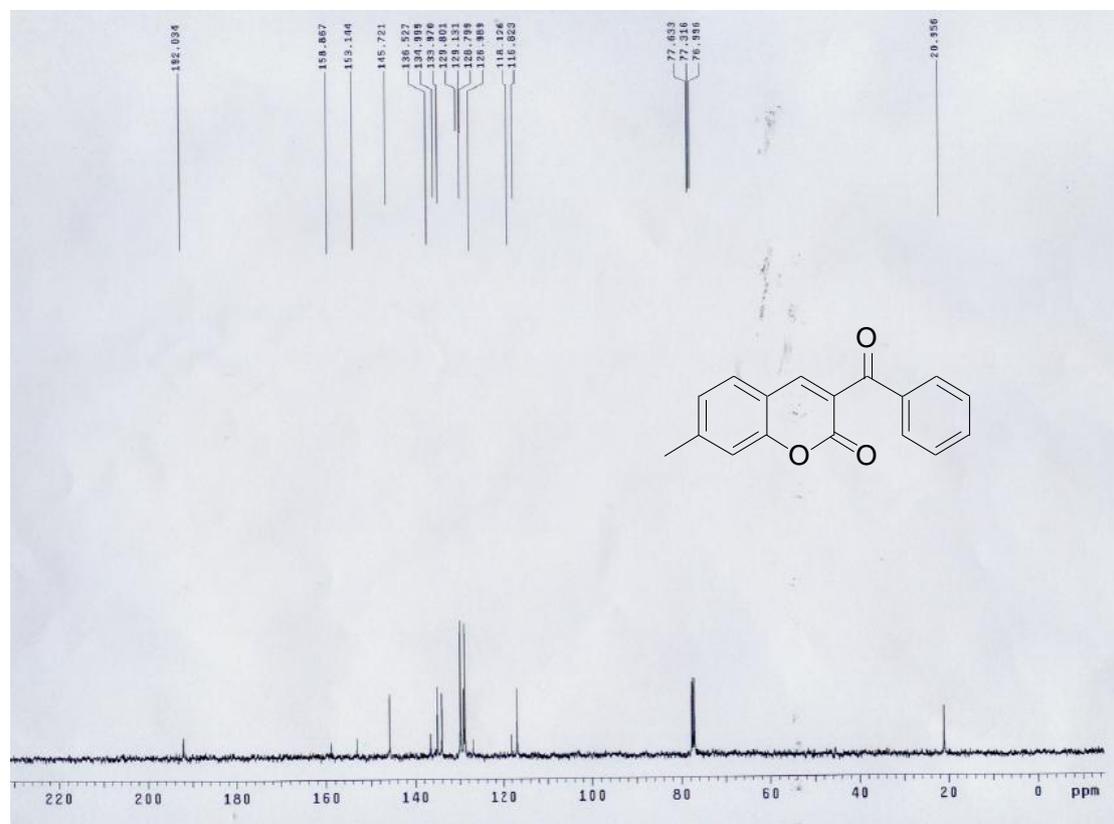


Figure S16. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3-benzoyl-7-methyl-chromen-2-one (**1h**)

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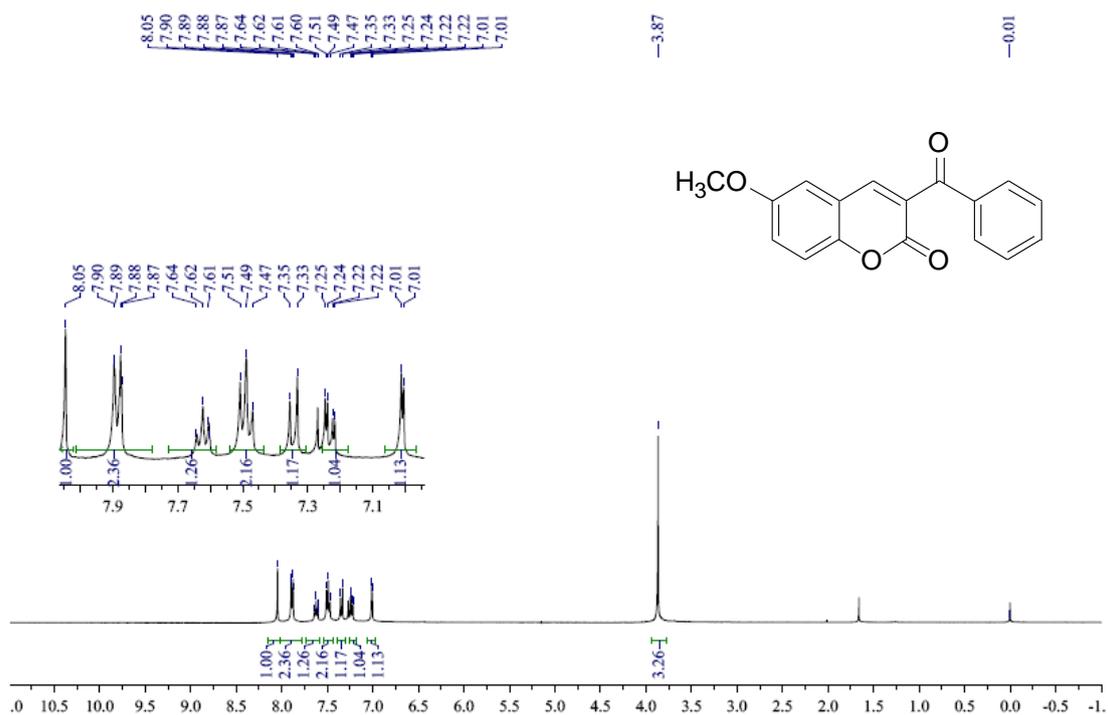


Figure S17. ¹H NMR spectrum (400 MHz, CDCl₃) of 3-benzoyl-6-methoxy-chromen-2-one (**1i**)

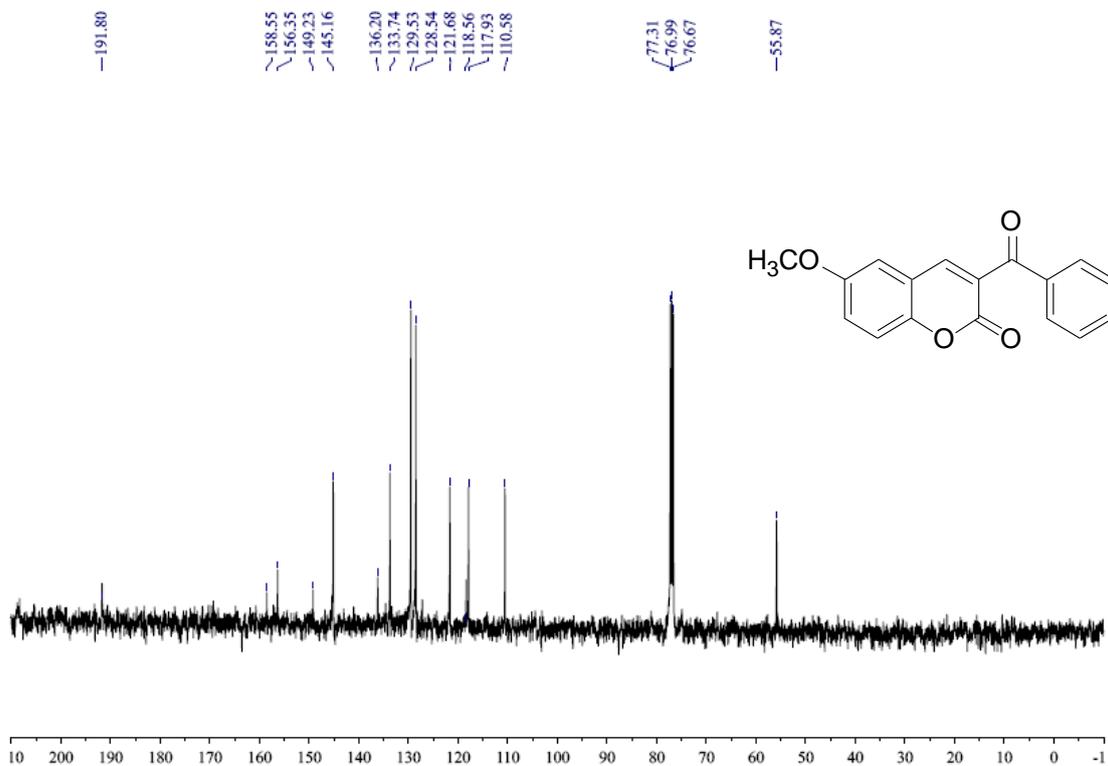


Figure S18. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3-benzoyl-6-methoxy-chromen-2-one (**1i**)

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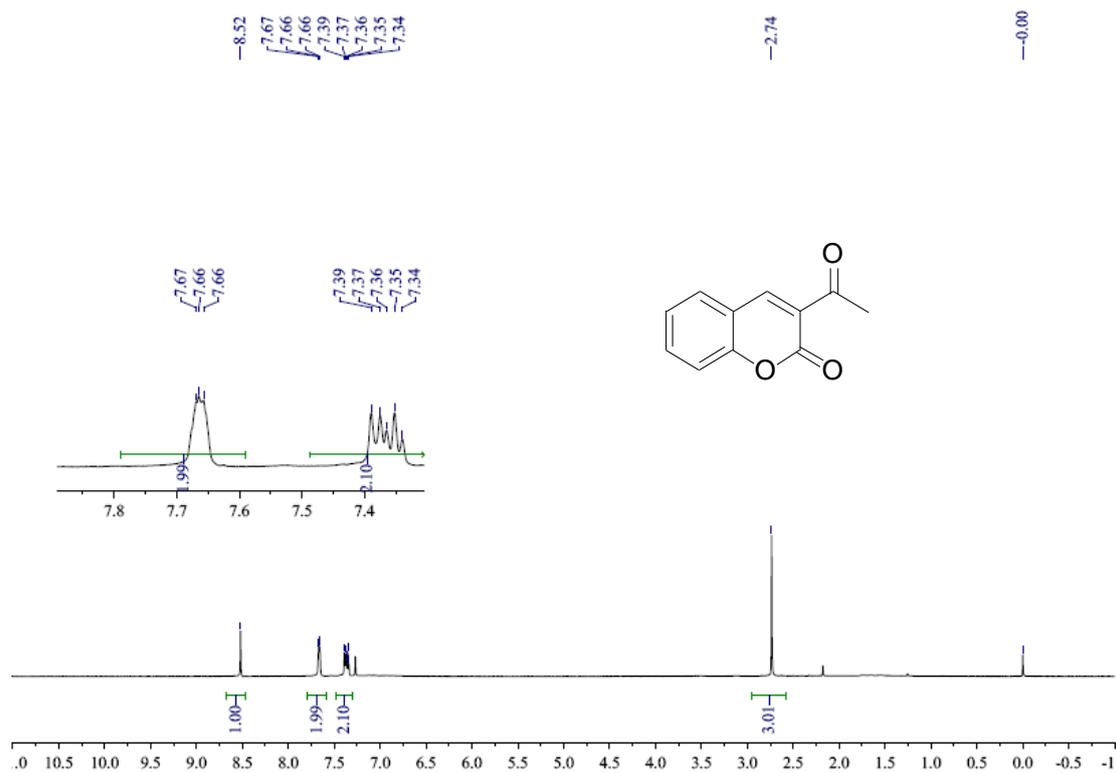


Figure S19. ¹H NMR spectrum (600 MHz, CDCl₃) of 3-acetyl-chromen-2-one (**1j**)

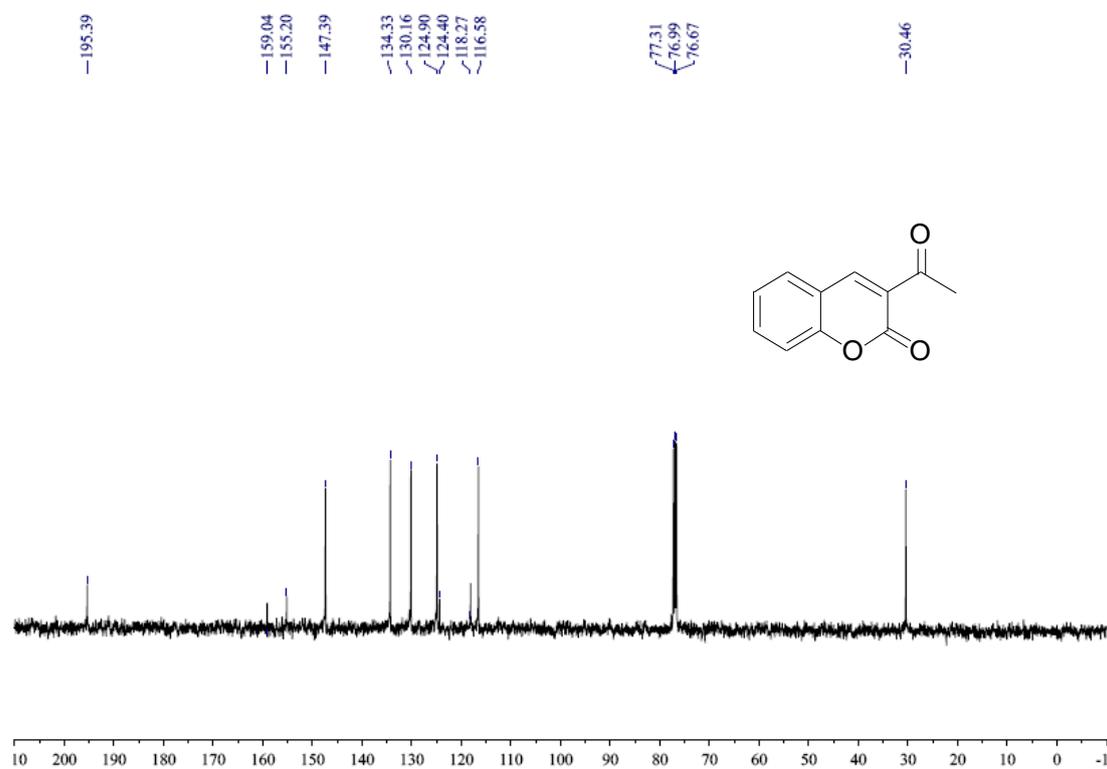


Figure S20. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3-acetyl-chromen-2-one (**1j**)

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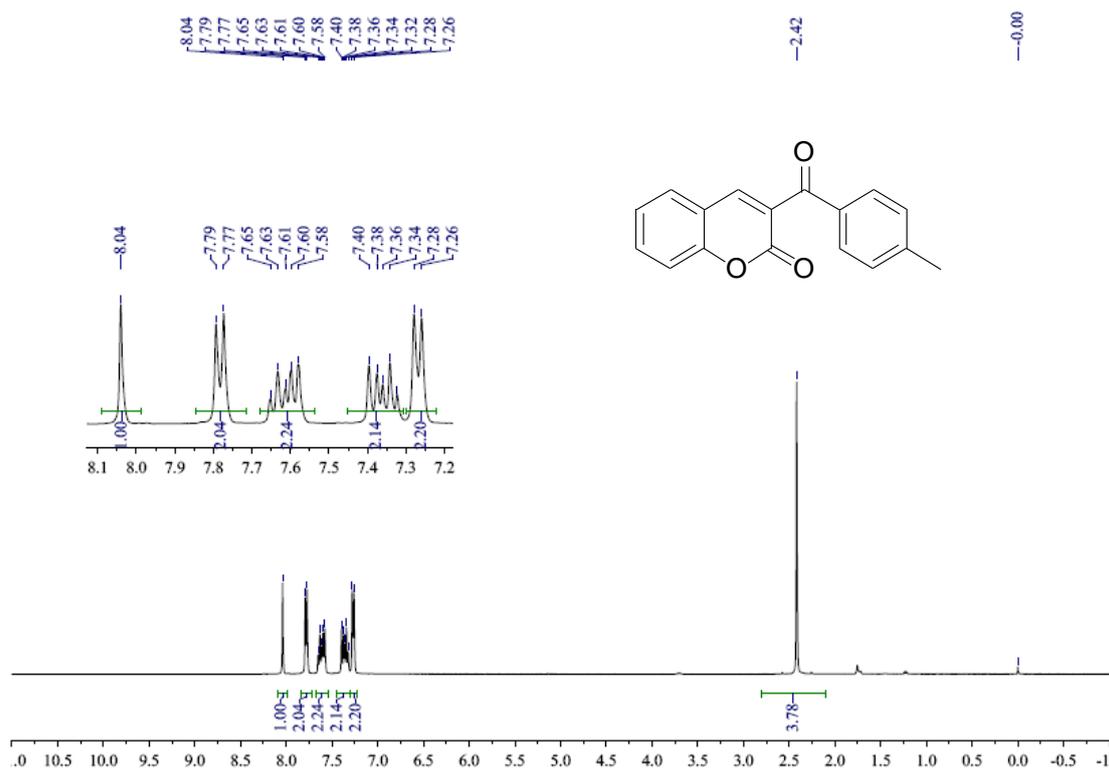


Figure S21. ¹H NMR spectrum (400 MHz, CDCl₃) of 3-(4-methylbenzoyl)-chromen-2-one (**1k**)

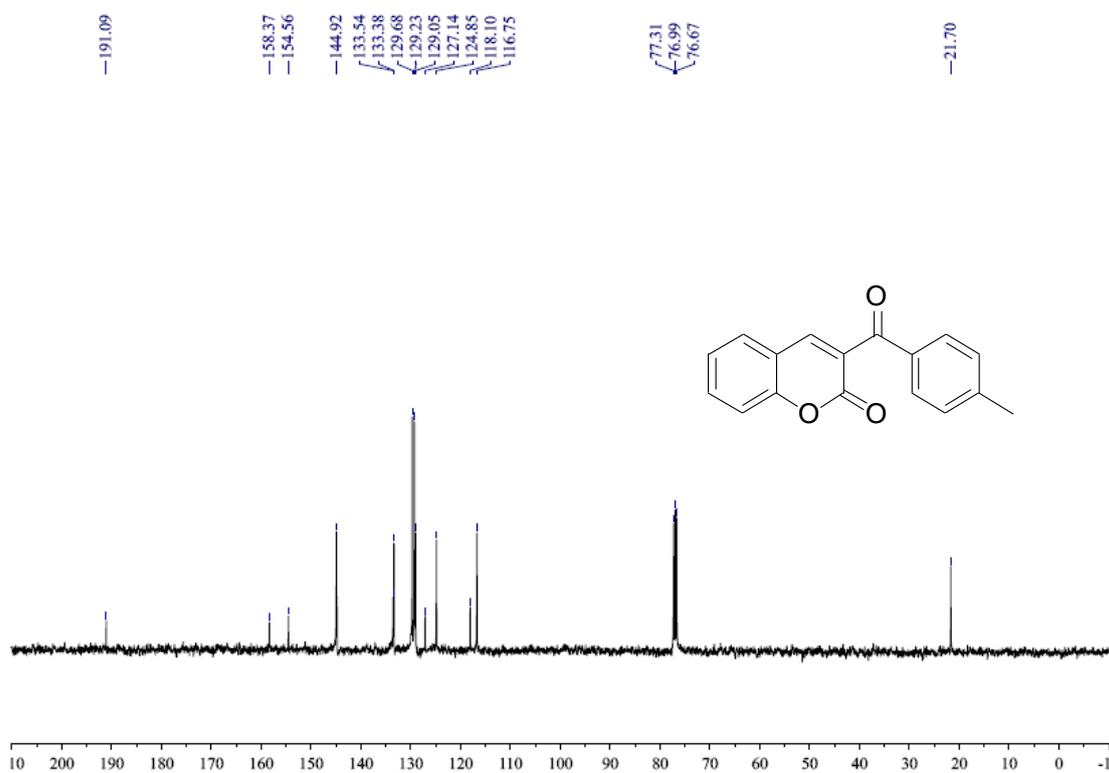


Figure S22. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3-(4-methylbenzoyl)-chromen-2-one (**1k**)

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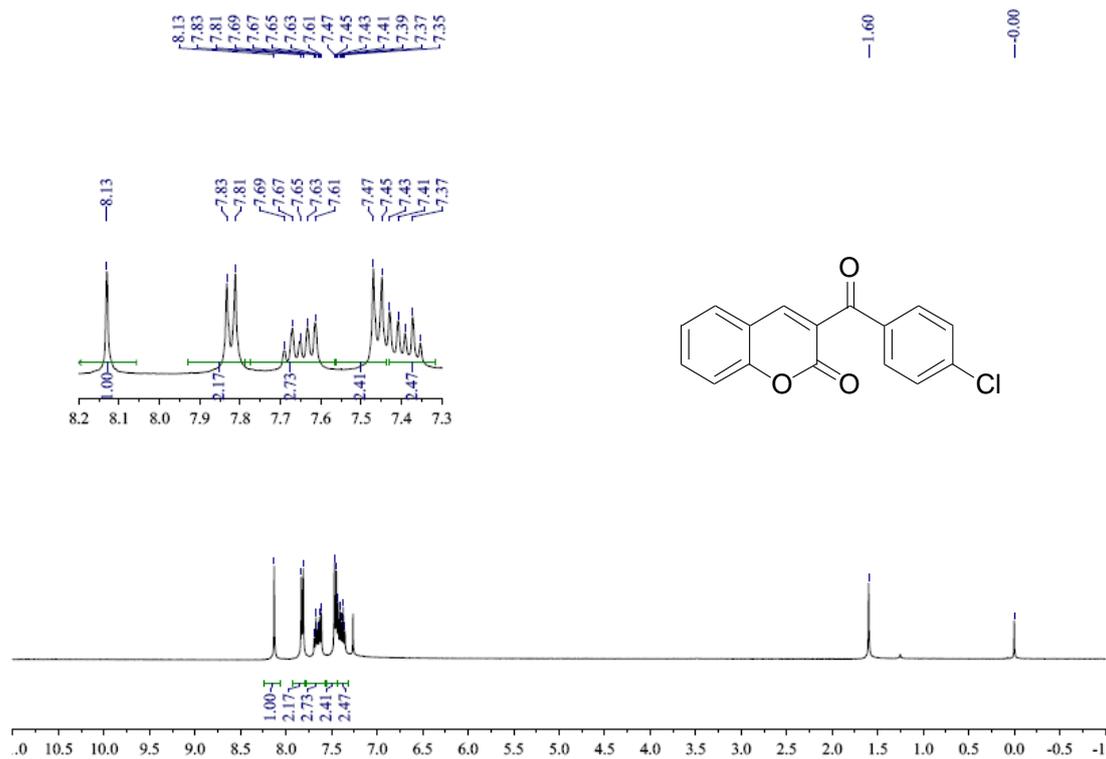


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^1H , ^{13}C NMR-spectra of **2**

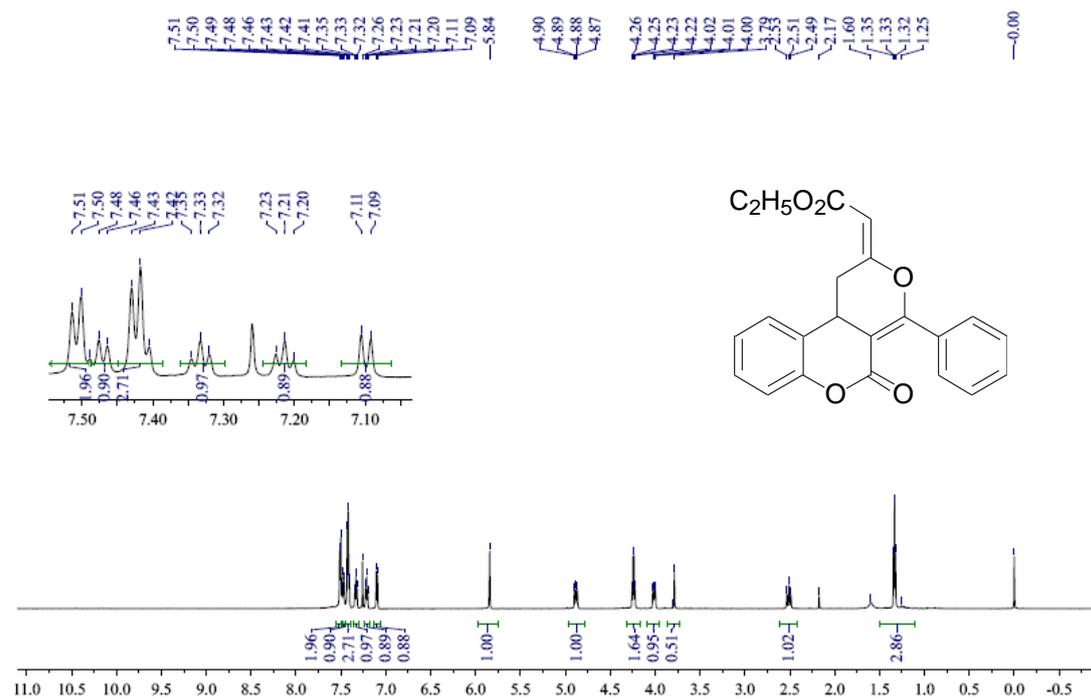


Figure S1. ^1H NMR spectrum (600 MHz, CDCl_3) of **2a**

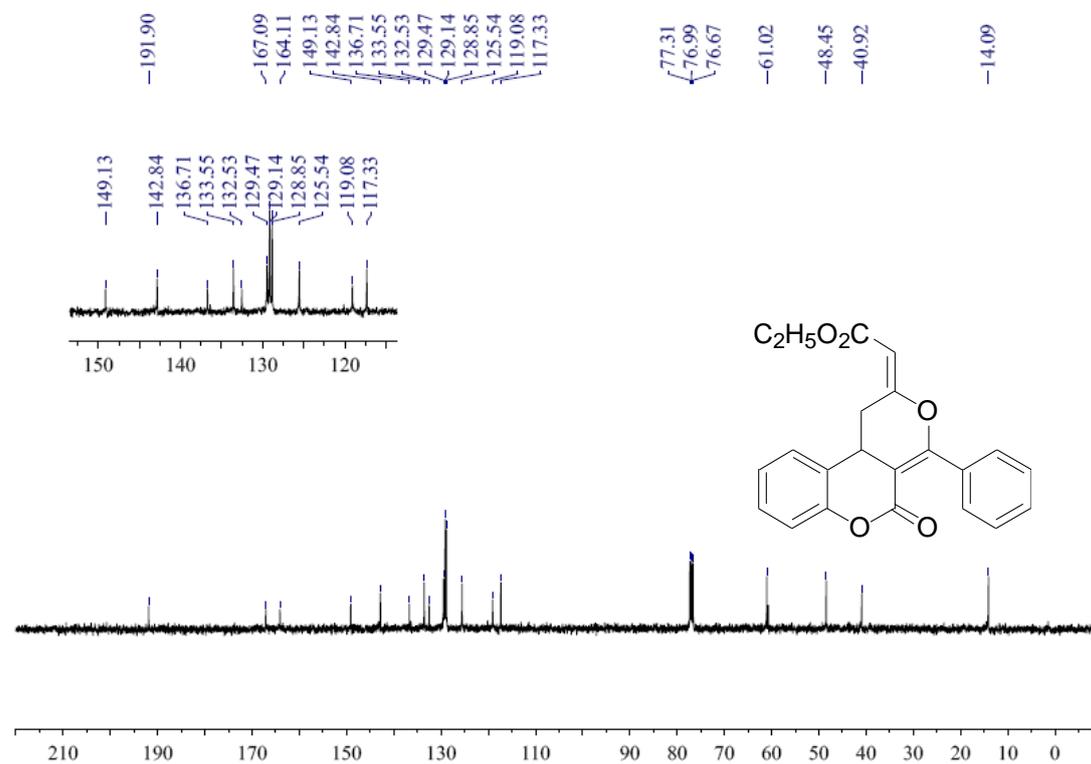


Figure S2. ^{13}C NMR spectrum (100 MHz, CDCl_3) of **2a**

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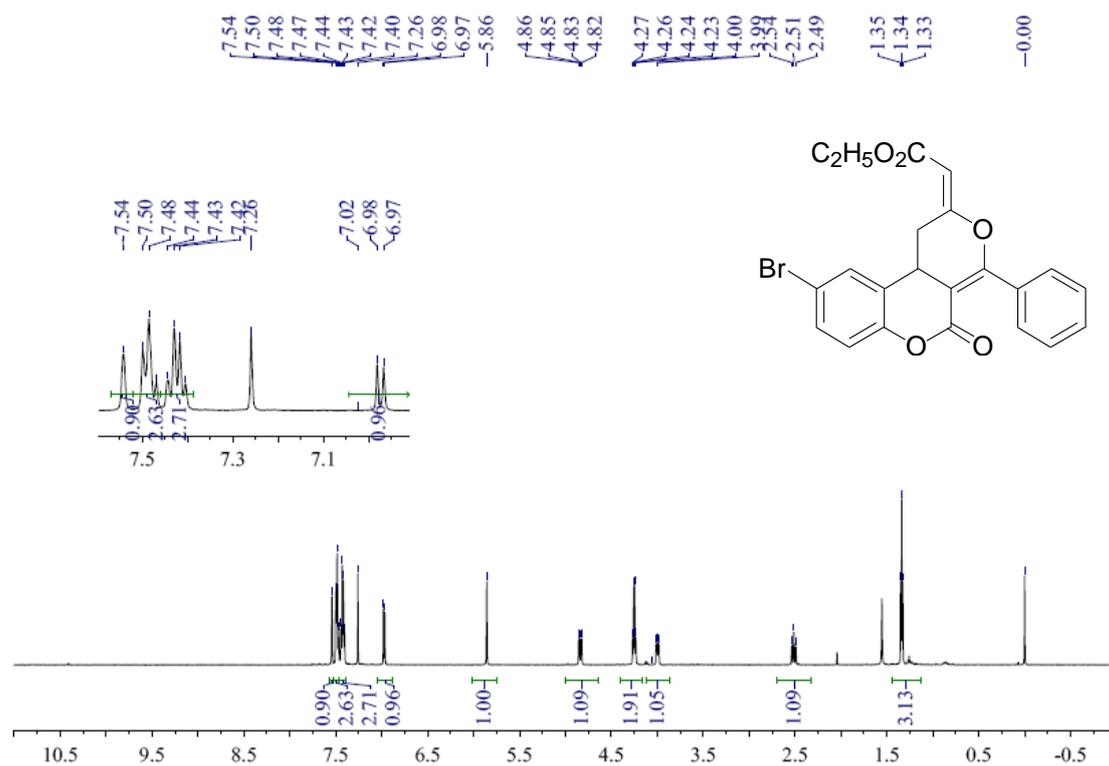


Figure S3. ¹H NMR spectrum (600 MHz, CDCl₃) of **2b**

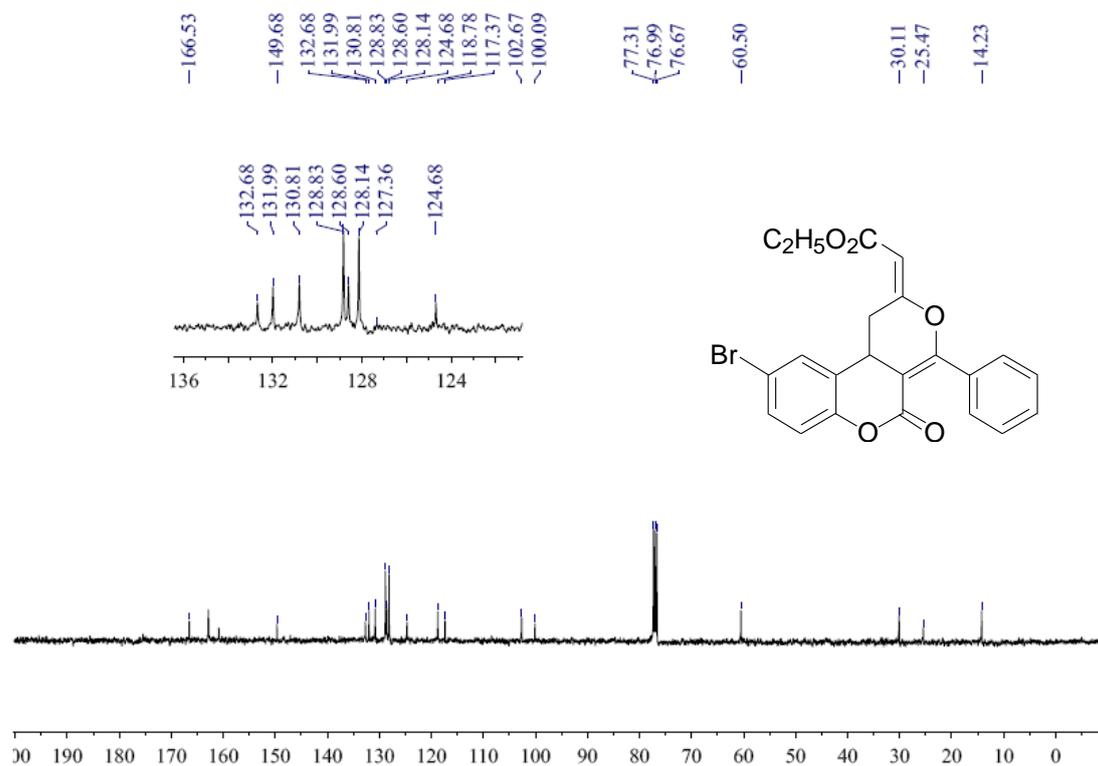


Figure S4. ¹³C NMR spectrum (100 MHz, CDCl₃) of **2b**

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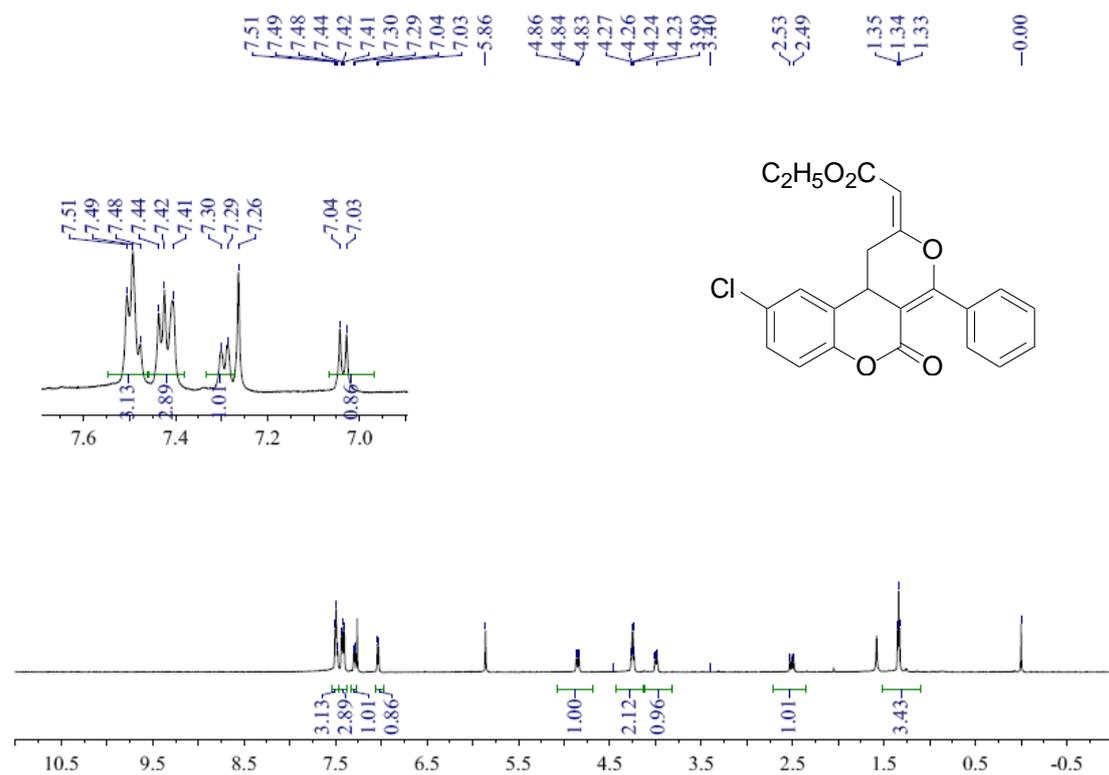


Figure S5. ¹H NMR spectrum (600 MHz, CDCl₃) of **2c**

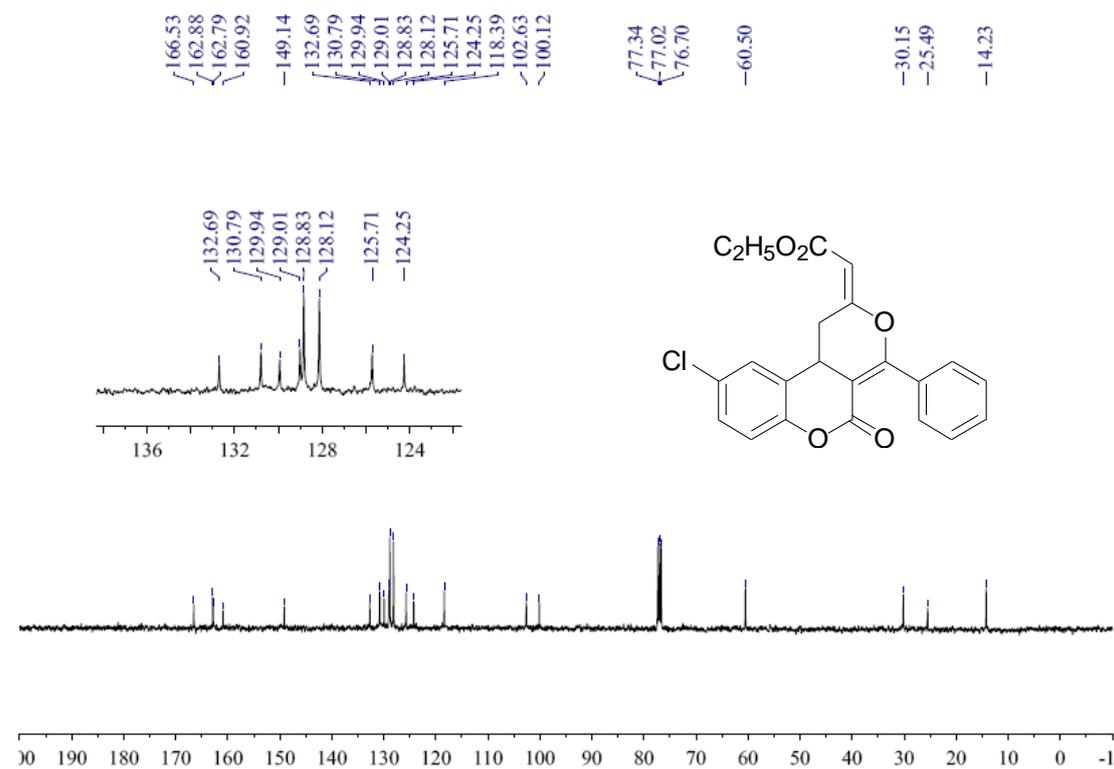


Figure S6. ¹³C NMR spectrum (100 MHz, CDCl₃) of **2c**

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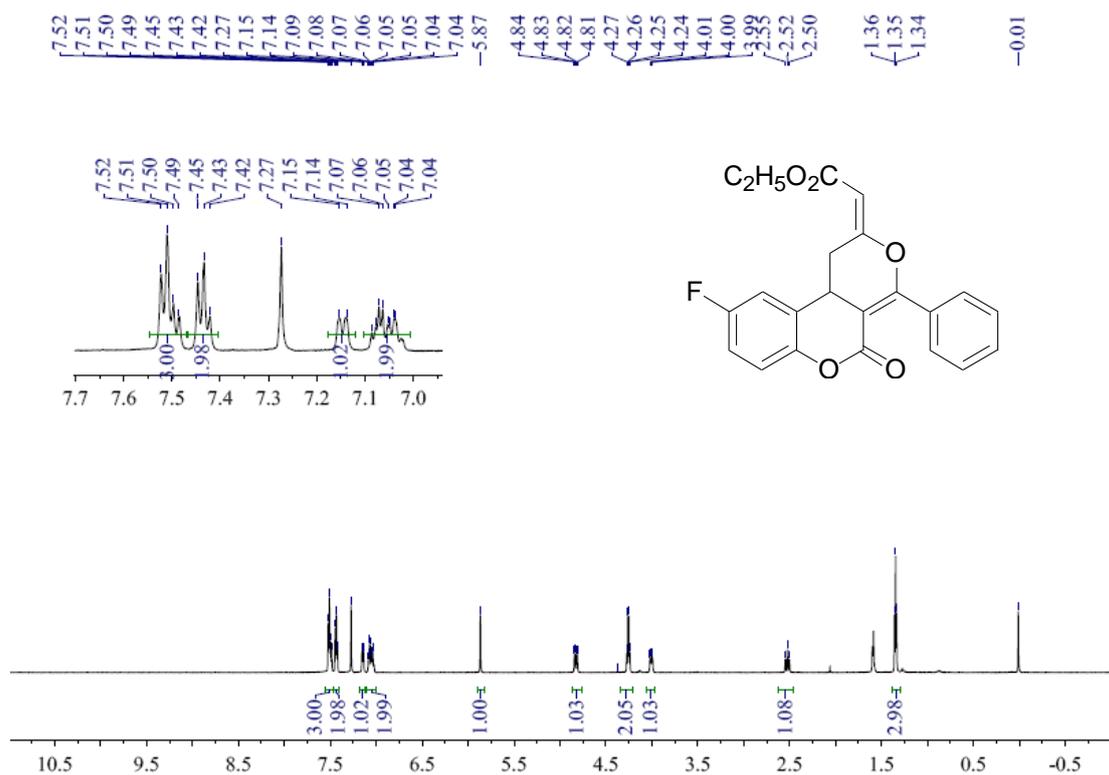


Figure S7. ¹H NMR spectrum (600 MHz, CDCl₃) of **2d**

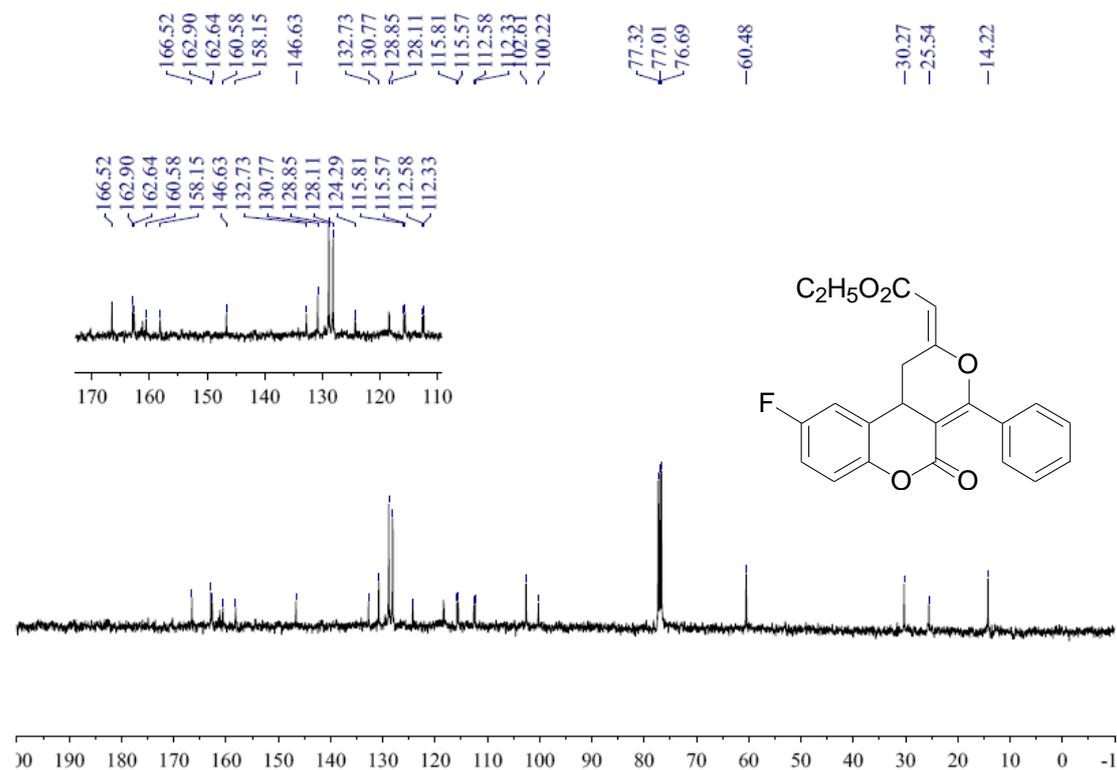


Figure S8. ¹³C NMR spectrum (100 MHz, CDCl₃) of **2d**

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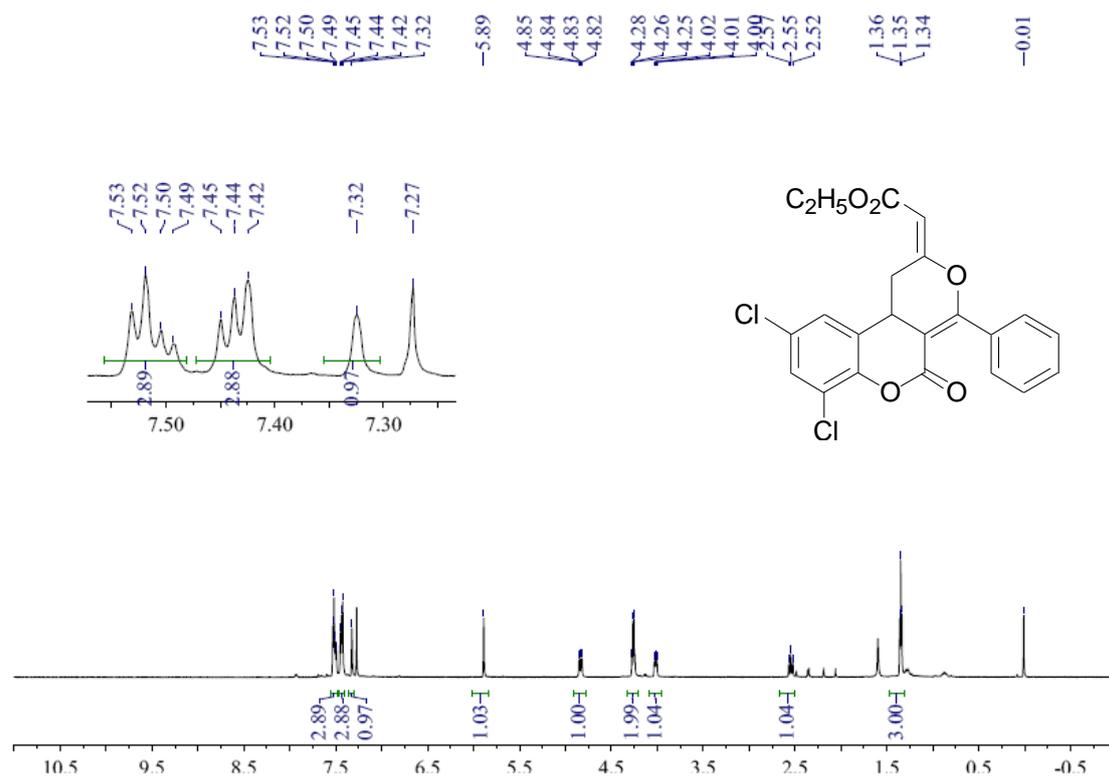


Figure S9. ¹H NMR spectrum (600 MHz, CDCl₃) of **2e**

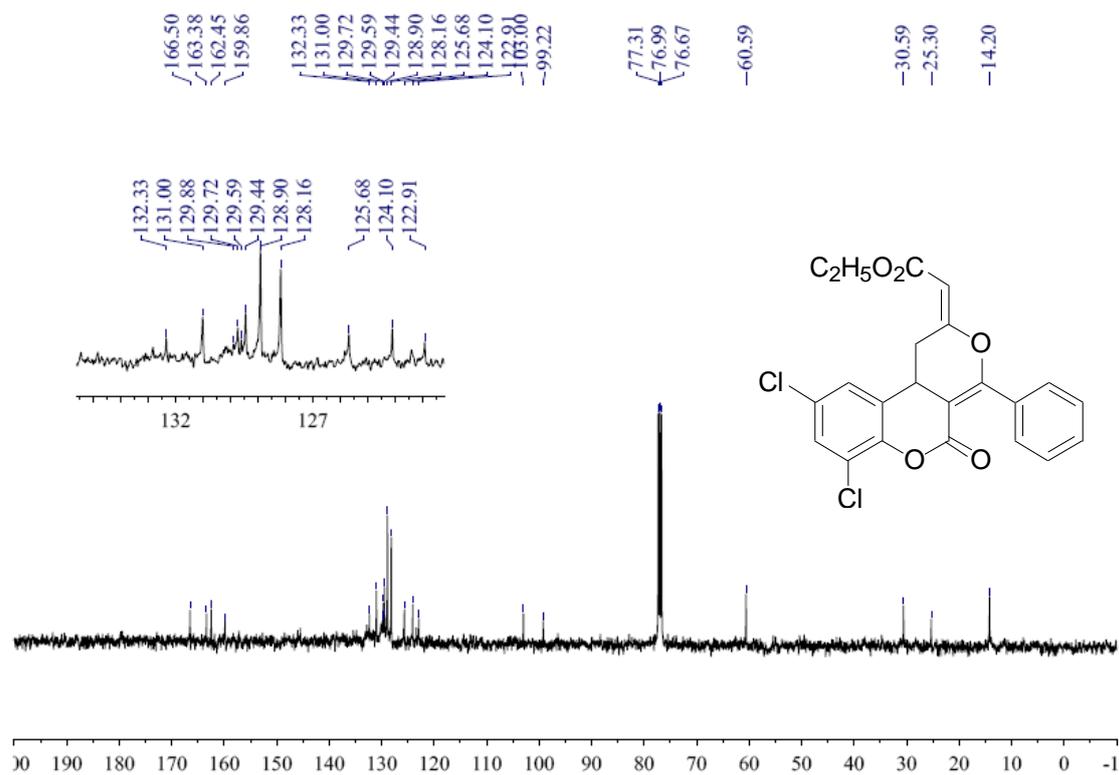


Figure S10. ¹³C NMR spectrum (100 MHz, CDCl₃) of **2e**

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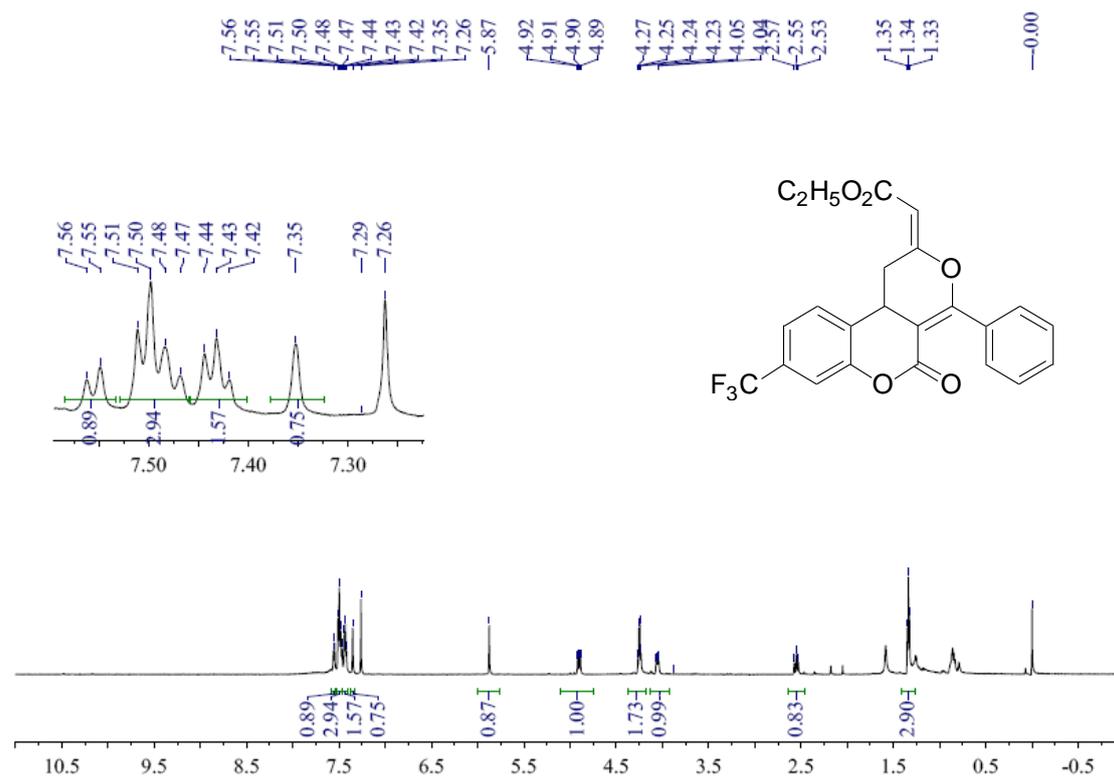


Figure S11. ¹H NMR spectrum (600 MHz, CDCl₃) of **2f**

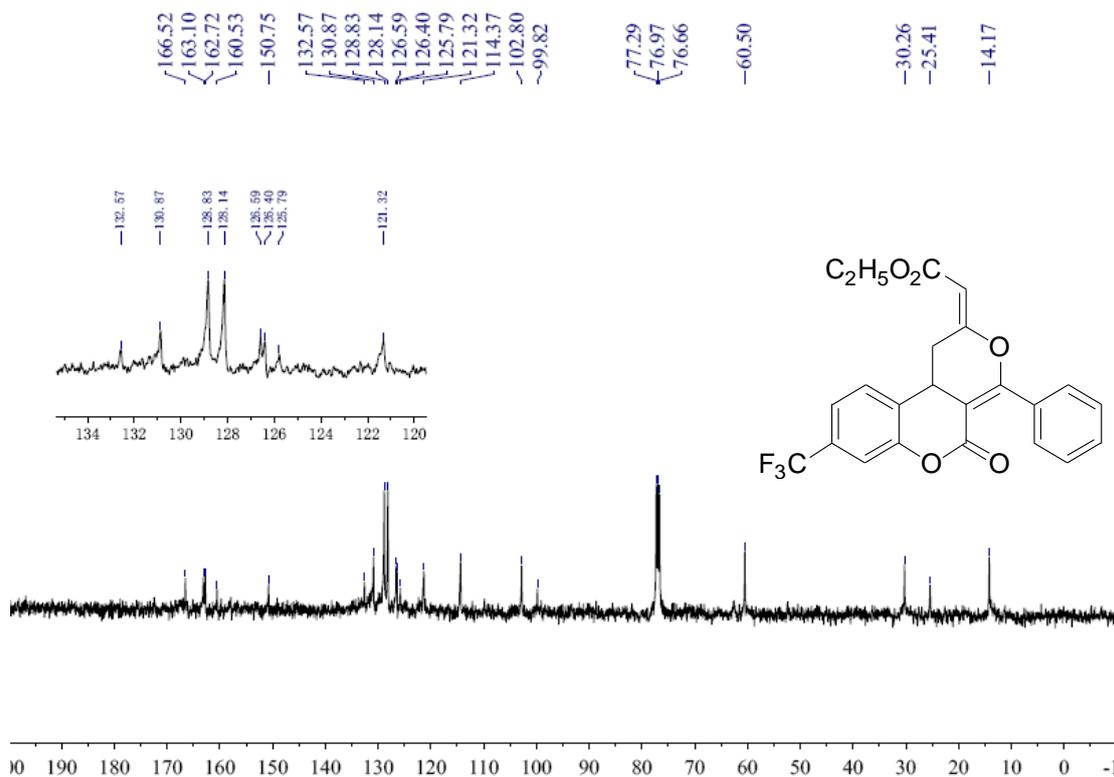


Figure S12. ¹³C NMR spectrum (100 MHz, CDCl₃) of **2f**

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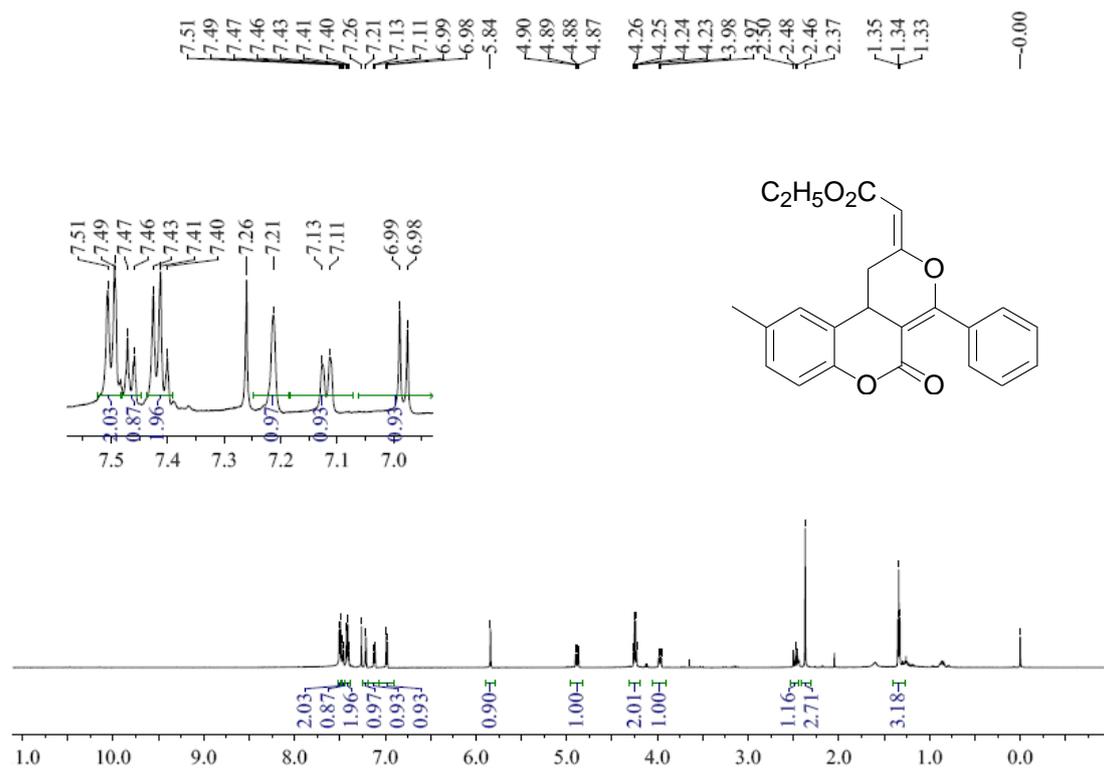


Figure S13. ¹H NMR spectrum (600 MHz, CDCl₃) of **2g**

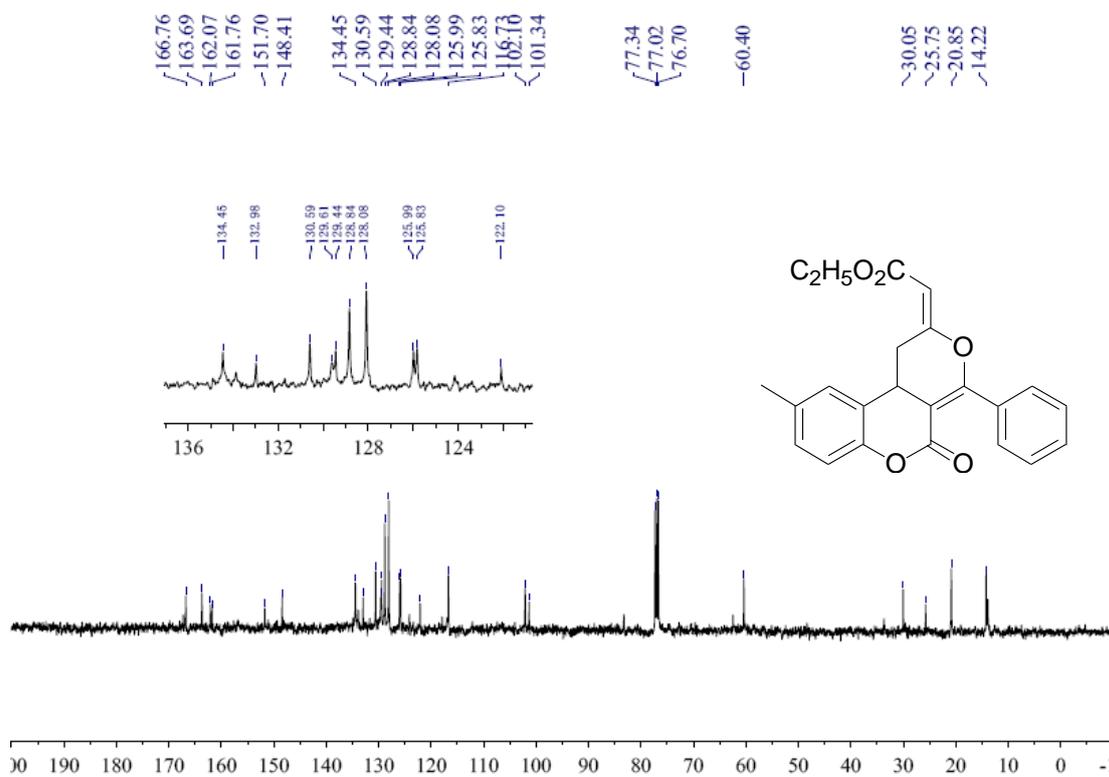


Figure S14. ¹³C NMR spectrum (100 MHz, CDCl₃) of **2g**

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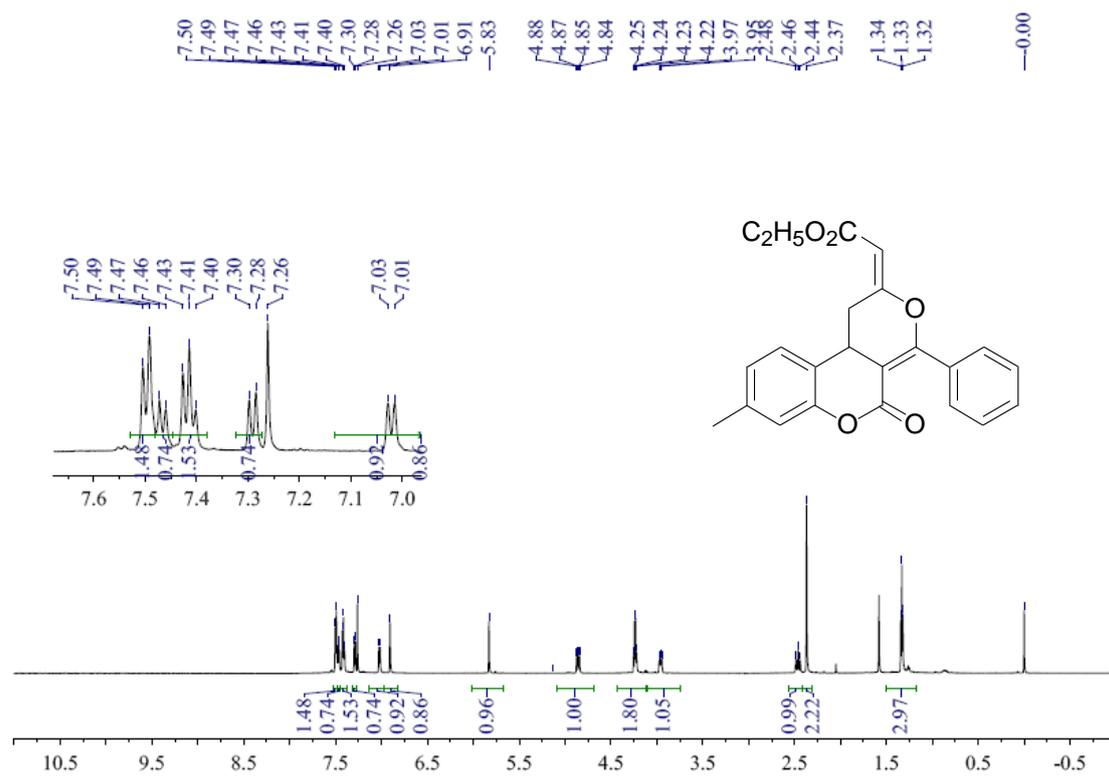


Figure S15. ¹H NMR spectrum (600 MHz, CDCl₃) of **2h**

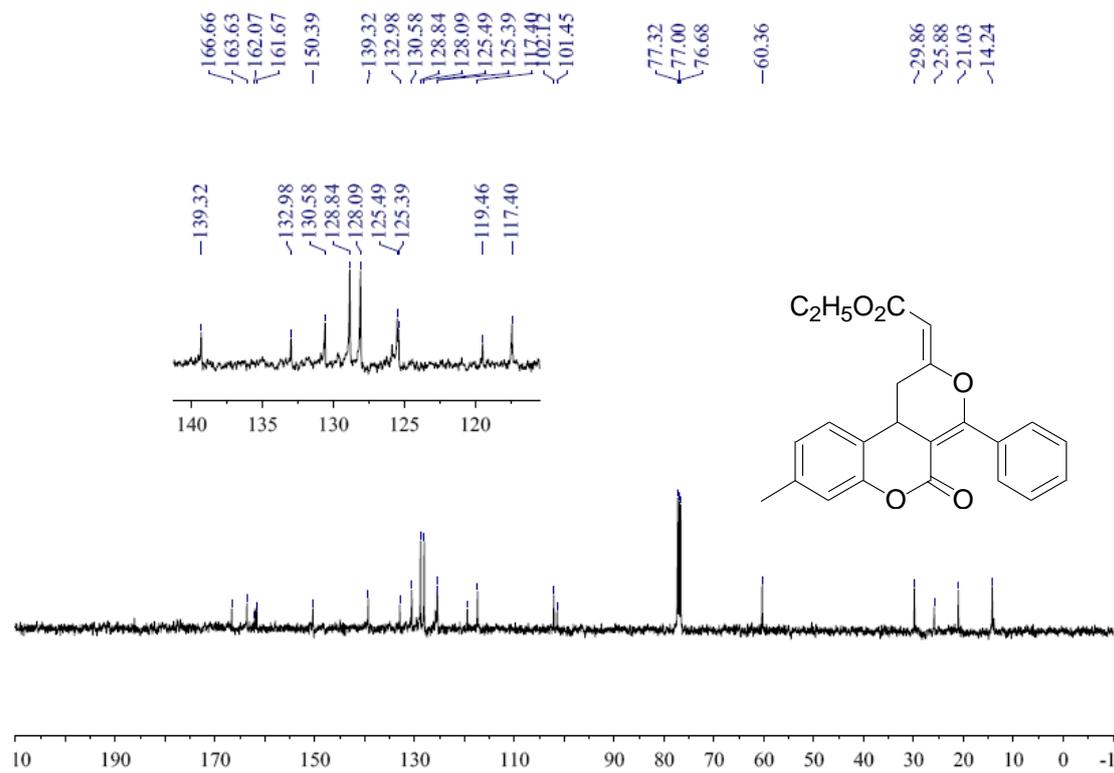


Figure S16. ¹³C NMR spectrum (100 MHz, CDCl₃) of **2h**

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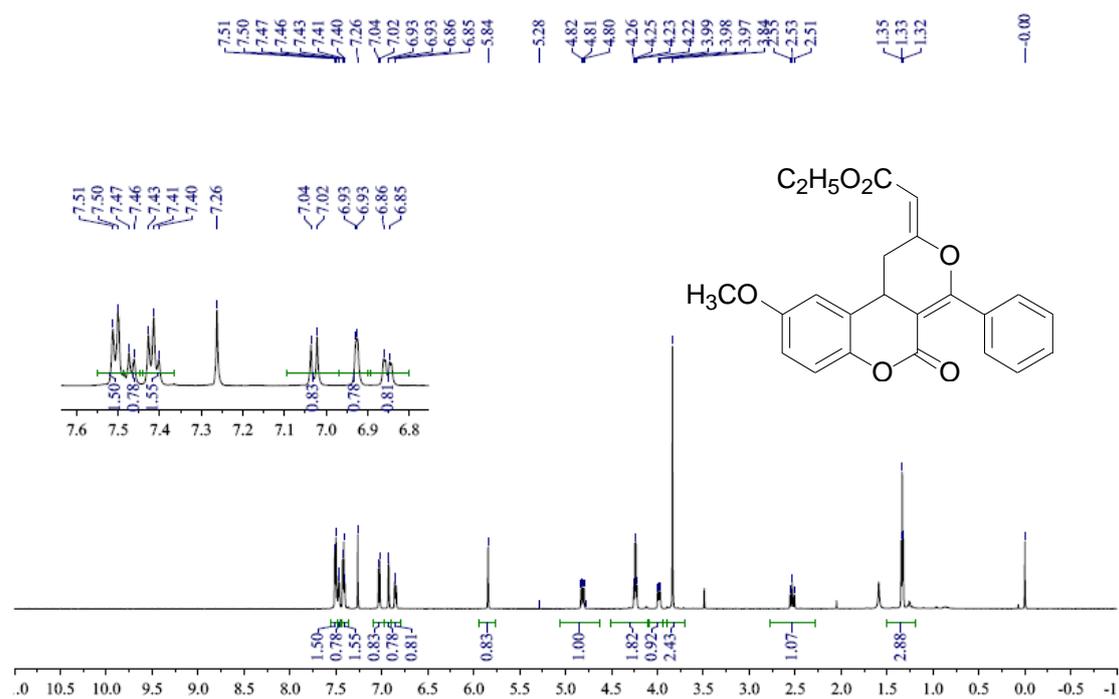


Figure S17. ¹H NMR spectrum (600 MHz, CDCl₃) of **2i**

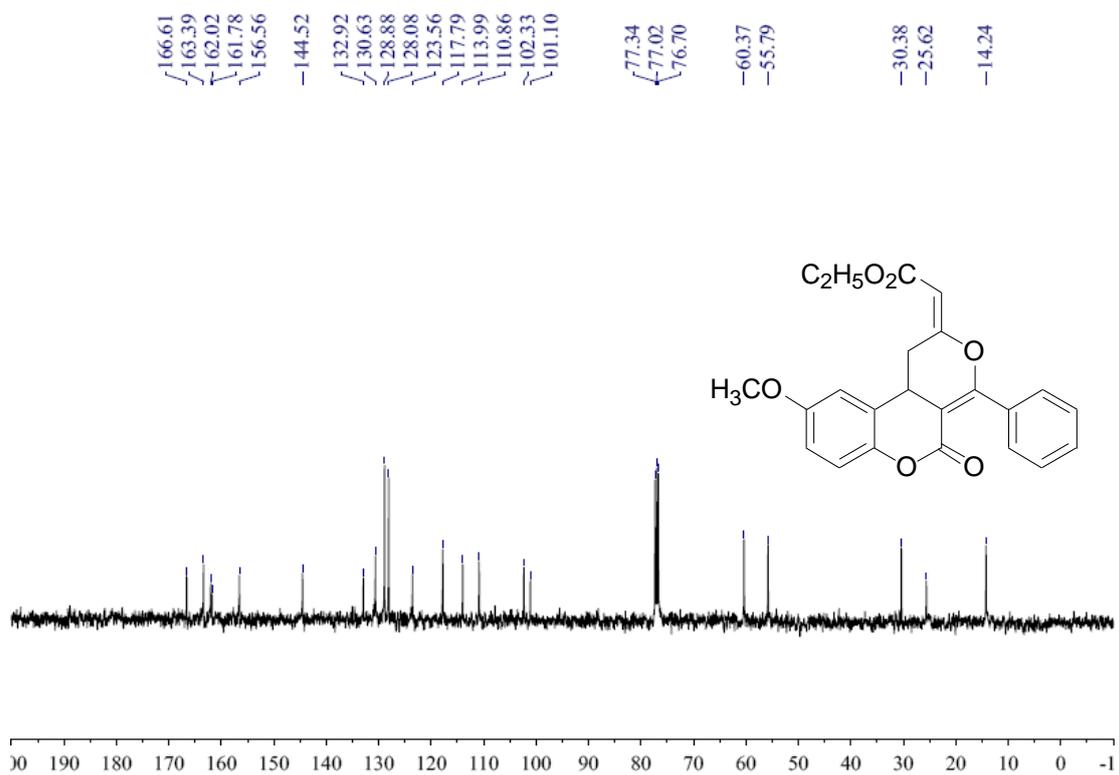


Figure S18. ¹³C NMR spectrum (100 MHz, CDCl₃) of **2i**

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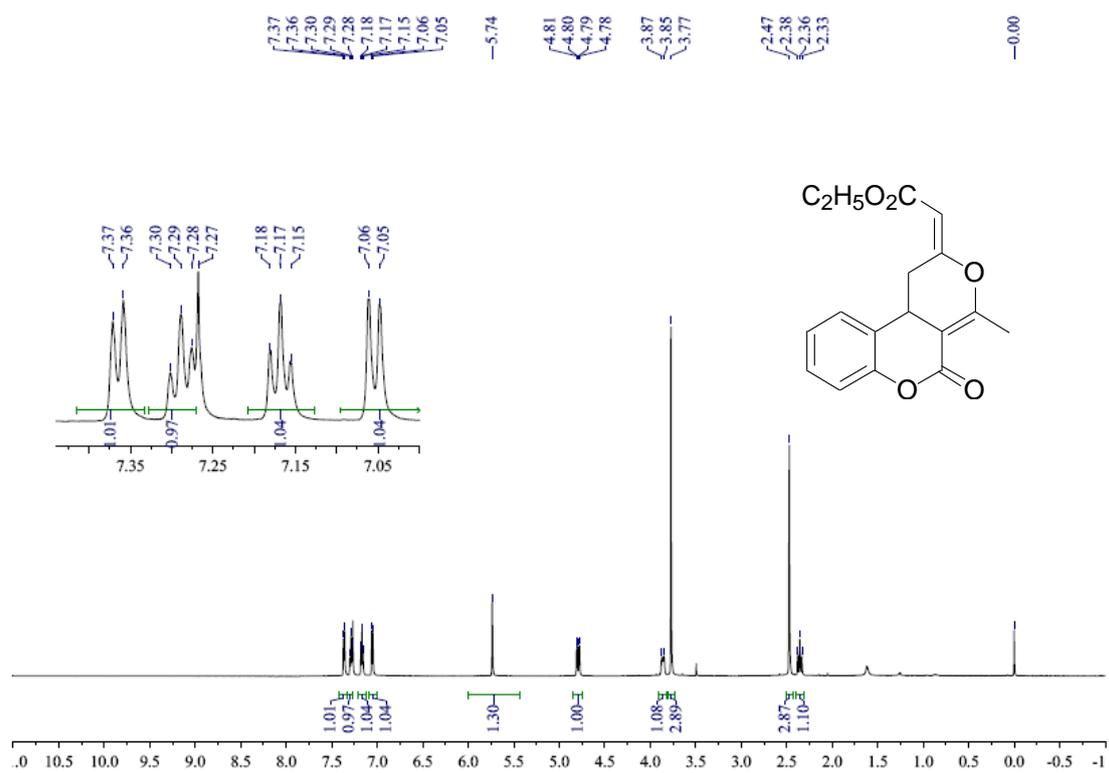


Figure S19. ¹H NMR spectrum (600 MHz, CDCl₃) of **2j**

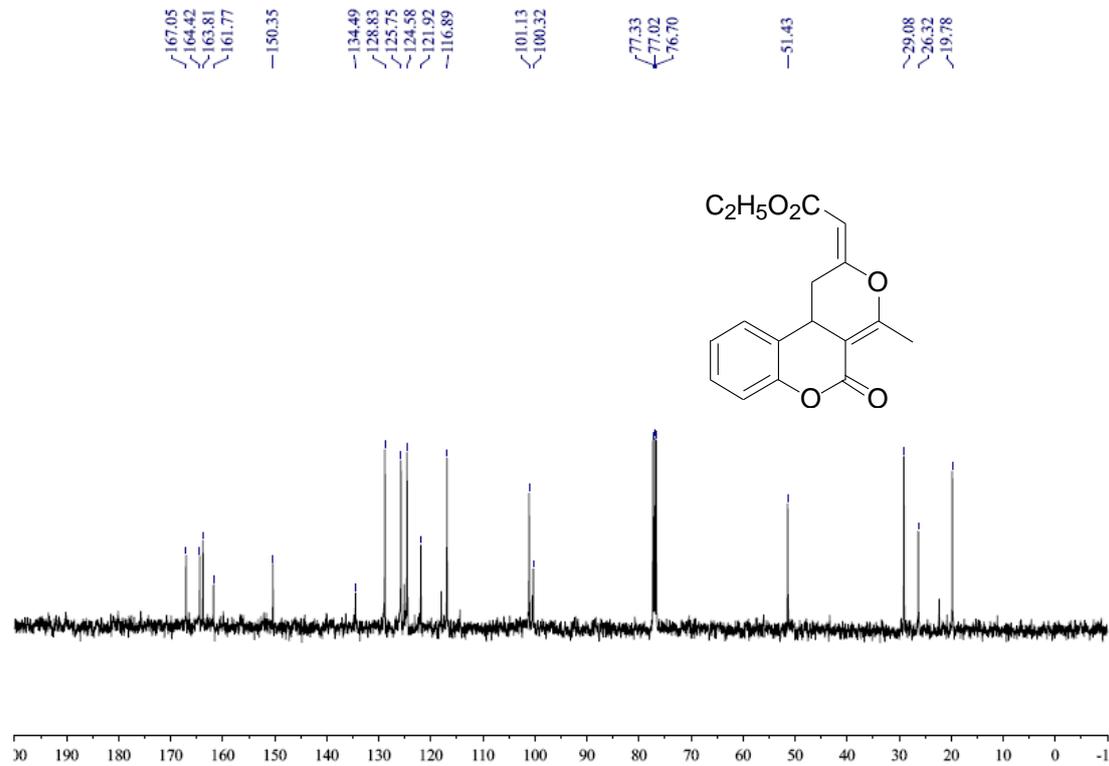


Figure S20. ¹³C NMR spectrum (100 MHz, CDCl₃) of **2j**

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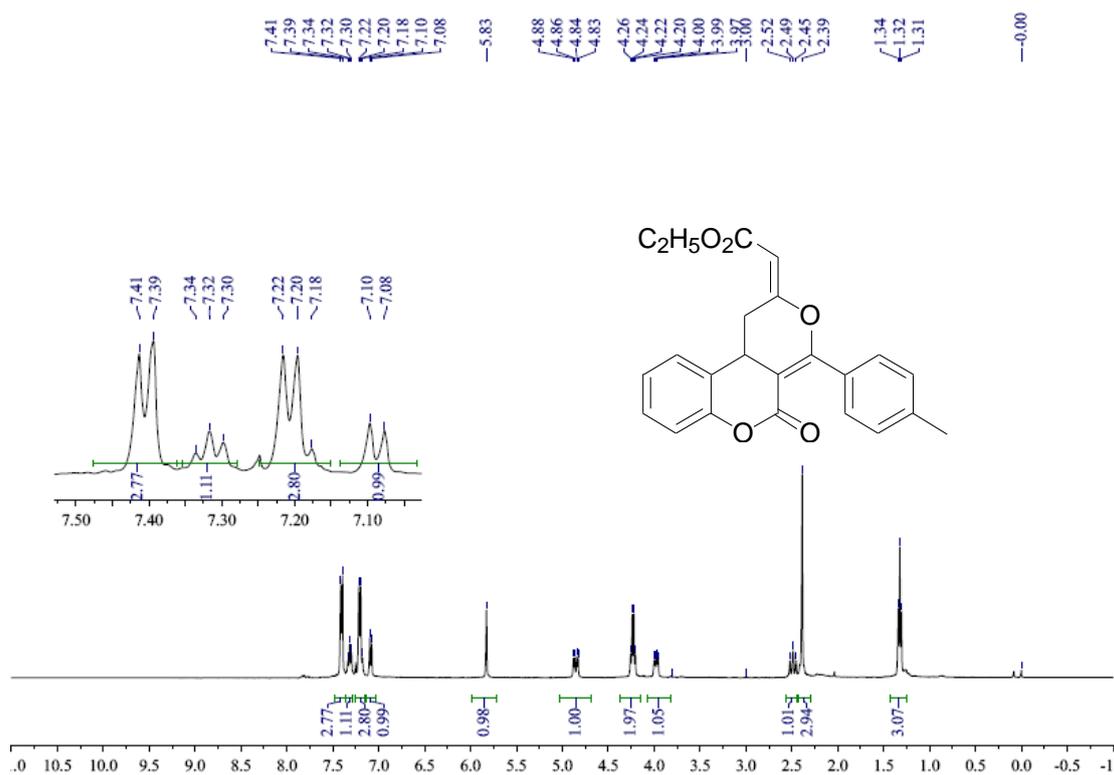


Figure S21. ¹H NMR spectrum (400 MHz, CDCl₃) of **2k**

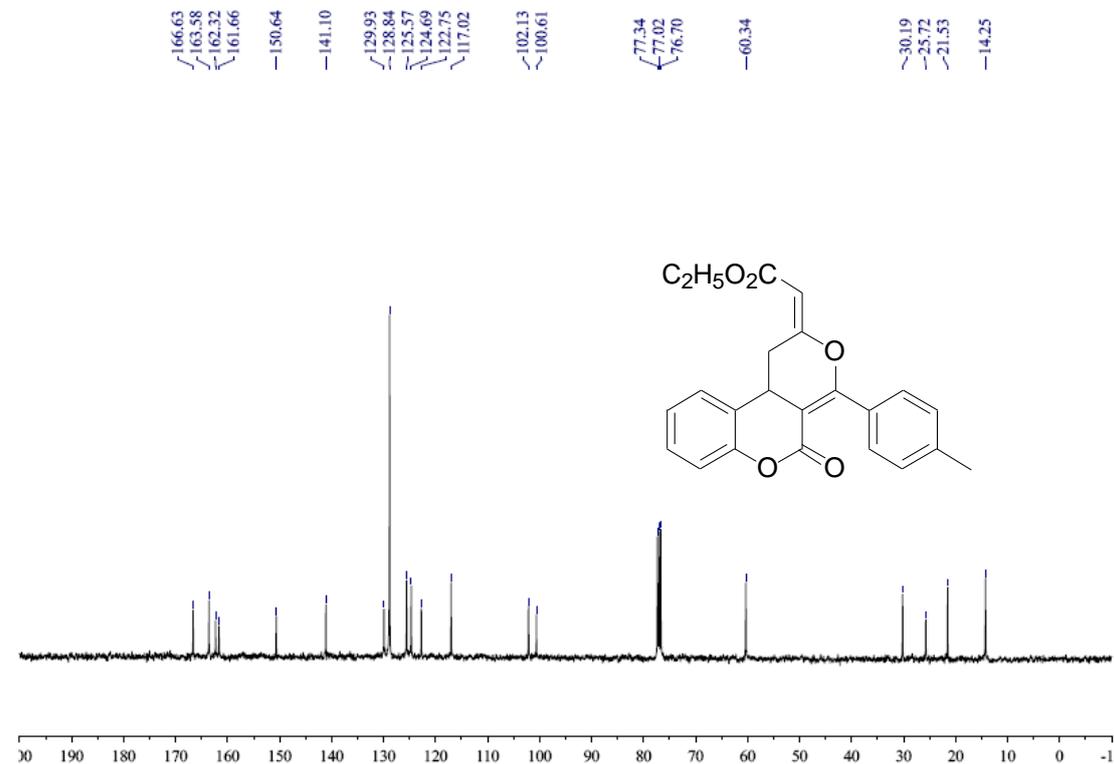


Figure S22. ¹³C NMR spectrum (100 MHz, CDCl₃) of **2k**

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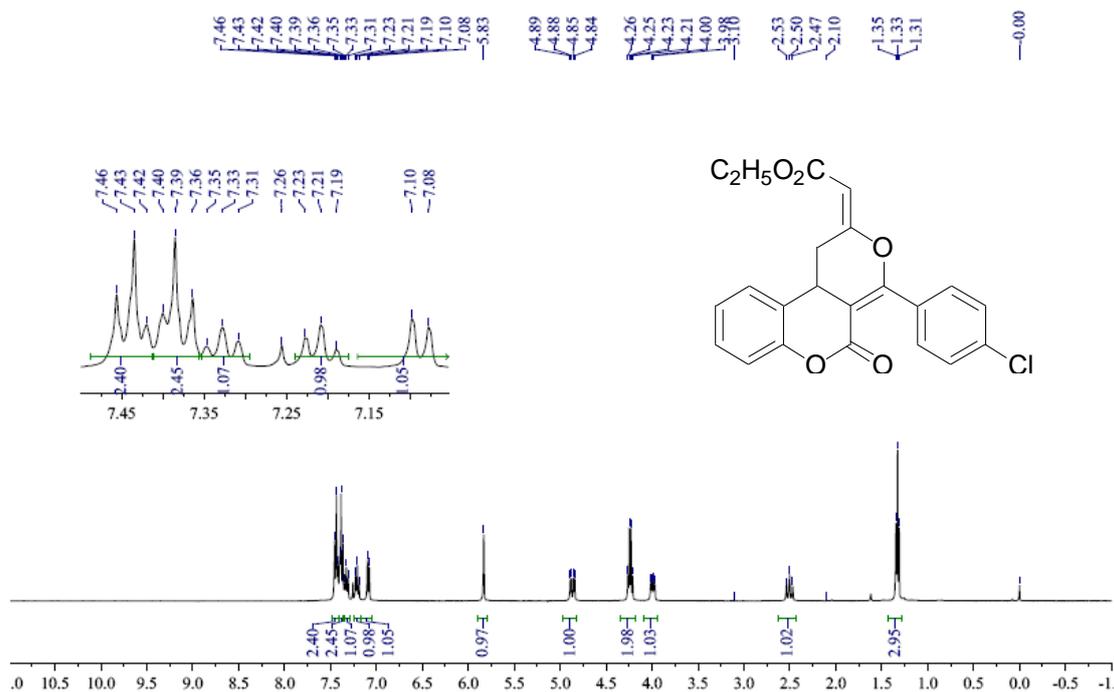


Figure S23. ¹H NMR spectrum (400 MHz, CDCl₃) of **21**

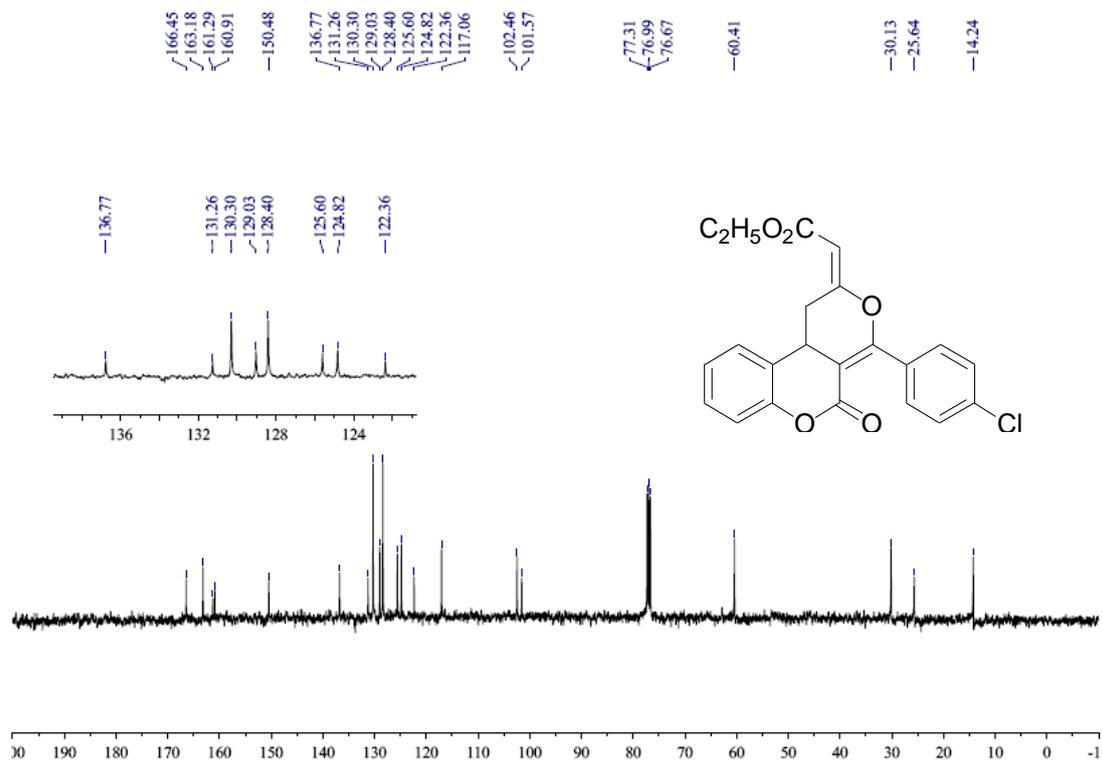


Figure S24. ¹³C NMR spectrum (100 MHz, CDCl₃) of **21**

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^1H , ^{13}C NMR-spectra of **3**

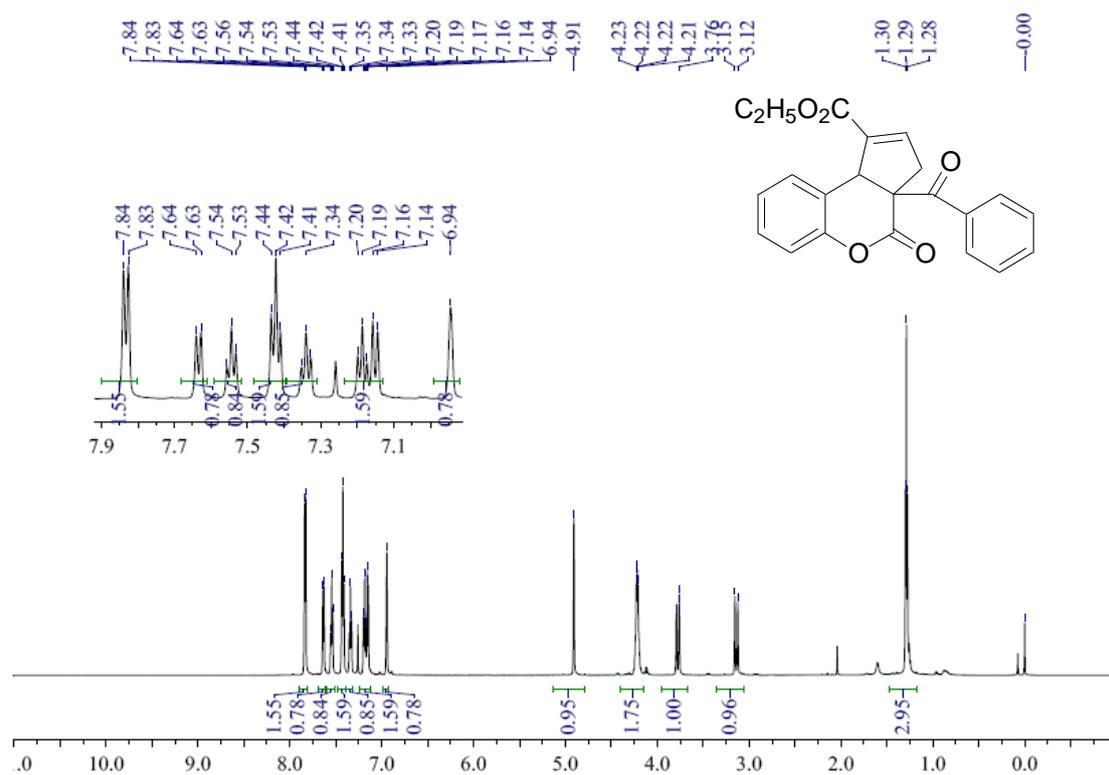


Figure S1. ^1H NMR spectrum (600 MHz, CDCl_3) of **3a**

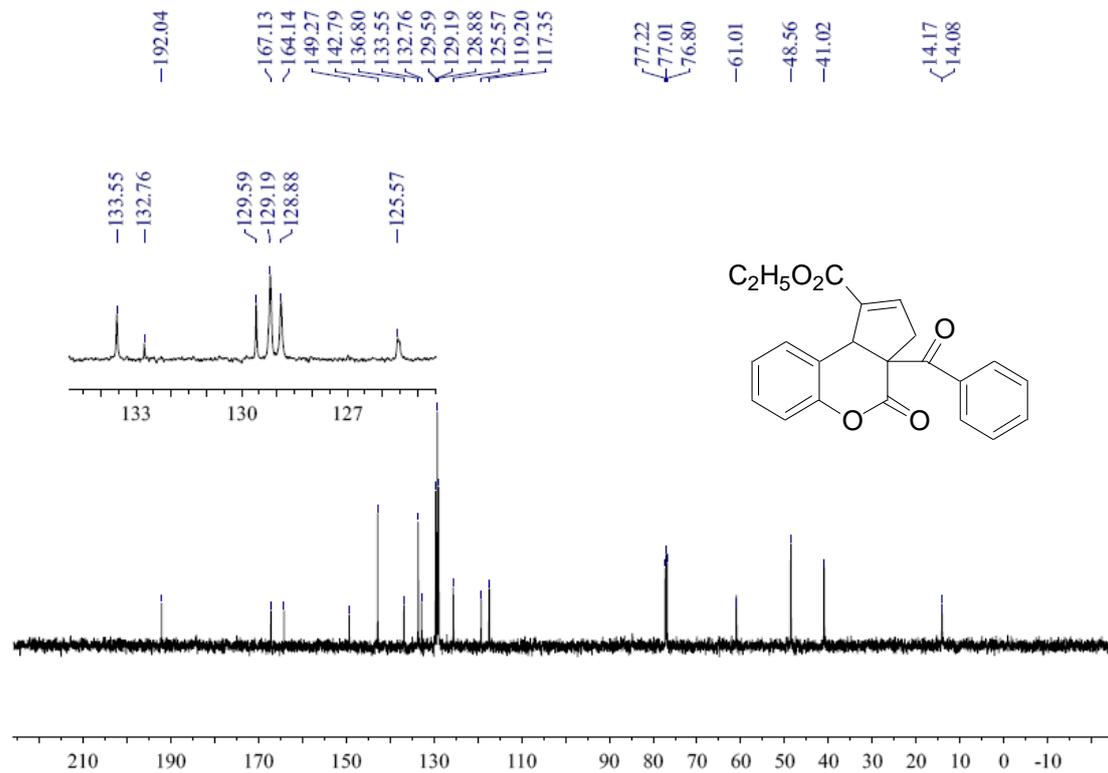


Figure S2. ^{13}C NMR spectrum (100 MHz, CDCl_3) of **3a**

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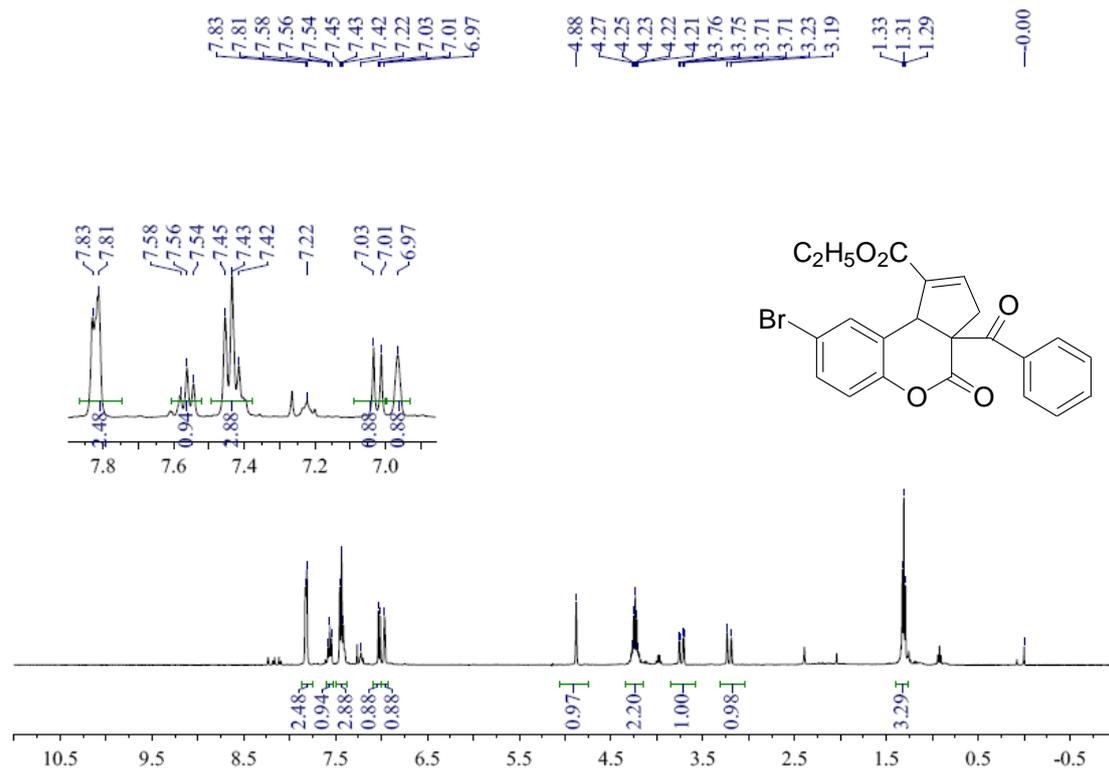


Figure S3. ¹H NMR spectrum (400 MHz, CDCl₃) of **3b**

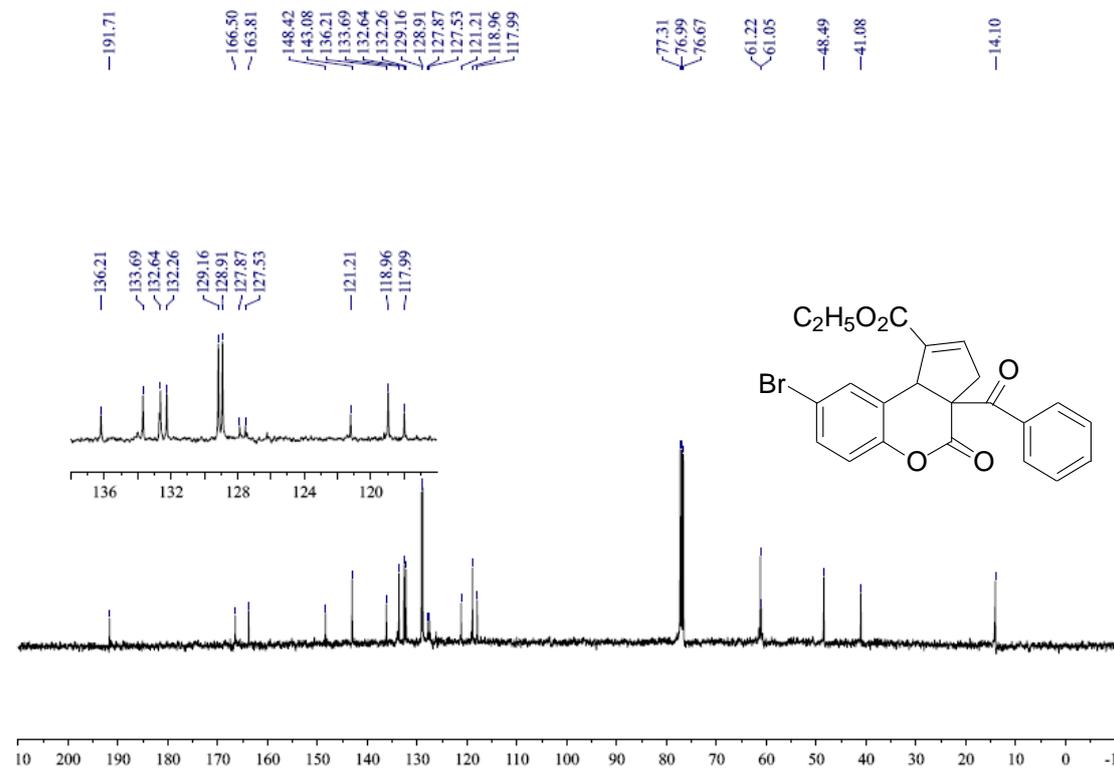


Figure S4. ¹³C NMR spectrum (100 MHz, CDCl₃) of **3b**

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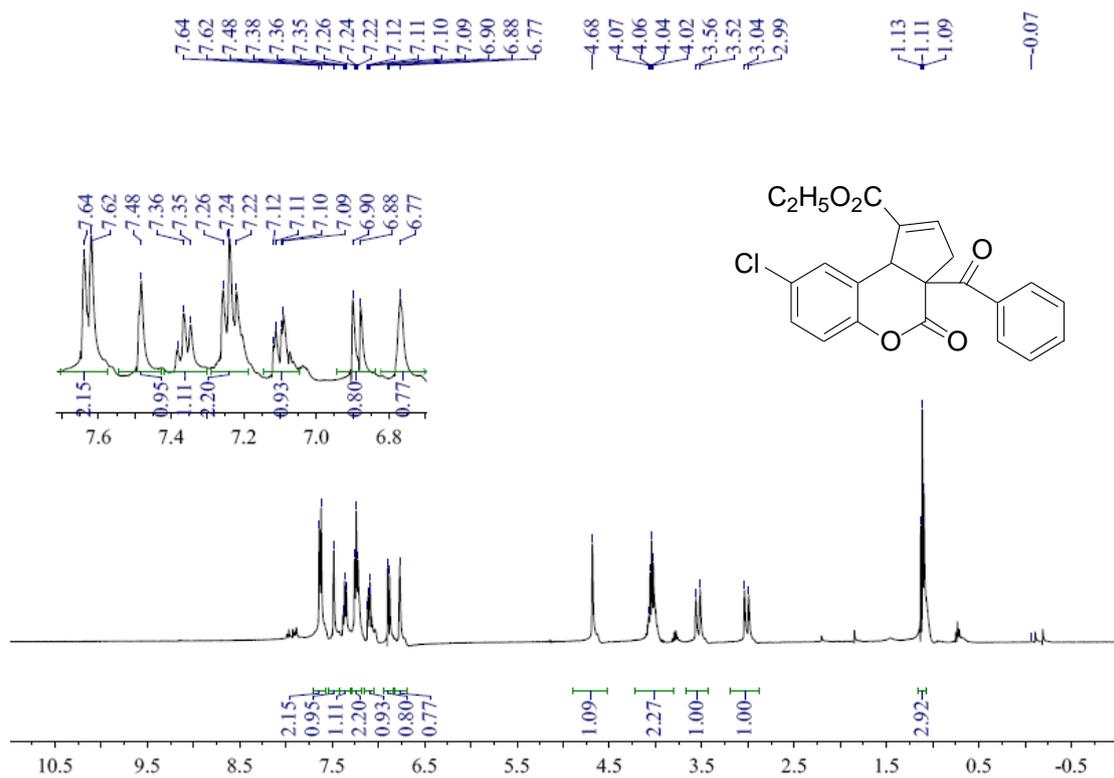


Figure S5. ¹H NMR spectrum (400 MHz, CDCl₃) of **3c**

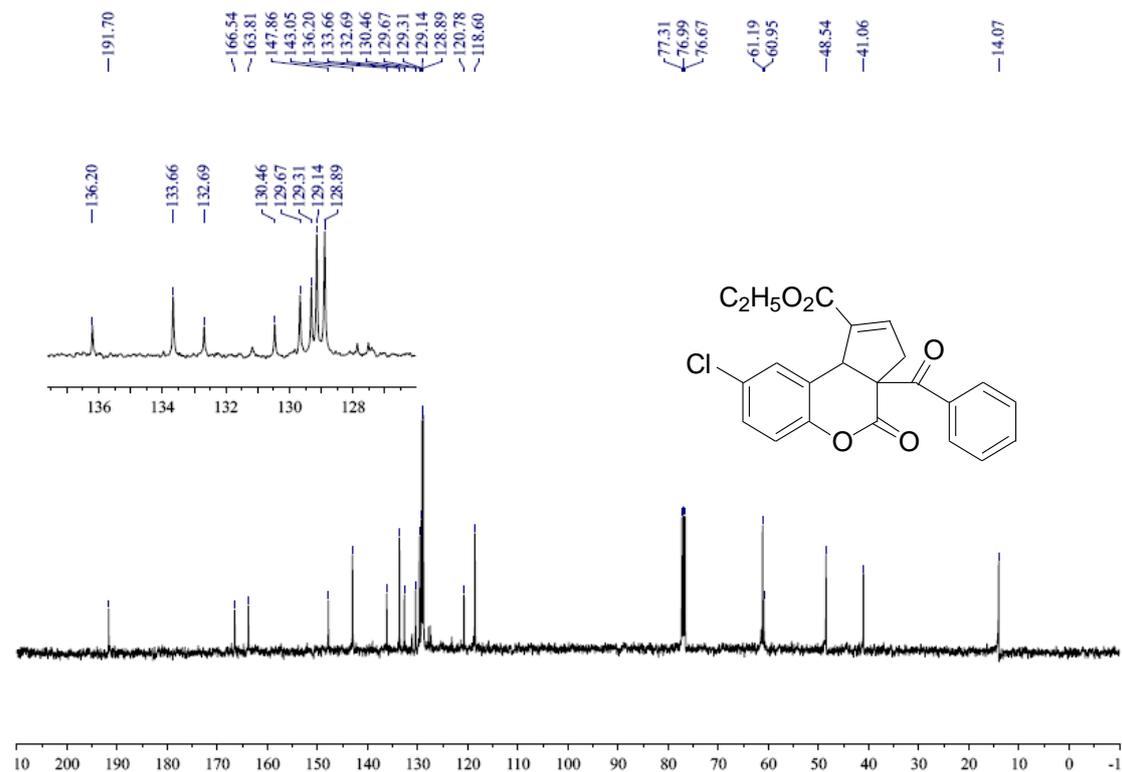


Figure S6. ¹³C NMR spectrum (100 MHz, CDCl₃) of **3c**

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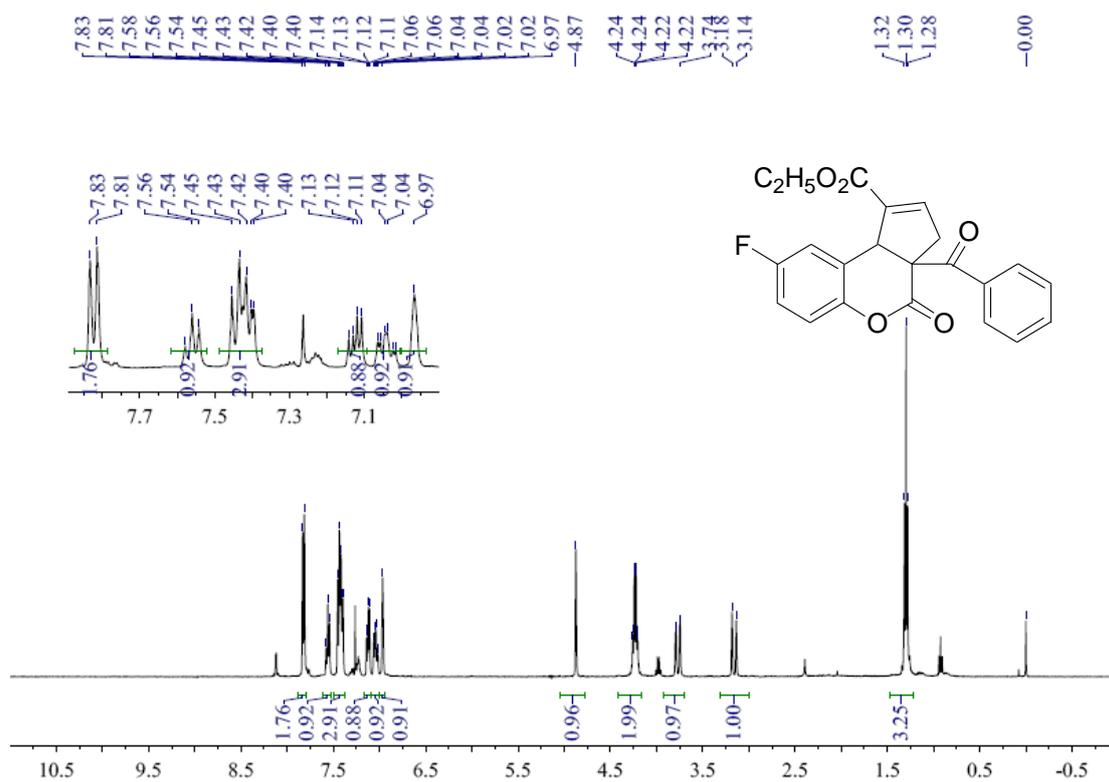


Figure S7. $^1\text{H NMR}$ spectrum (400 MHz, CDCl_3) of **3d**

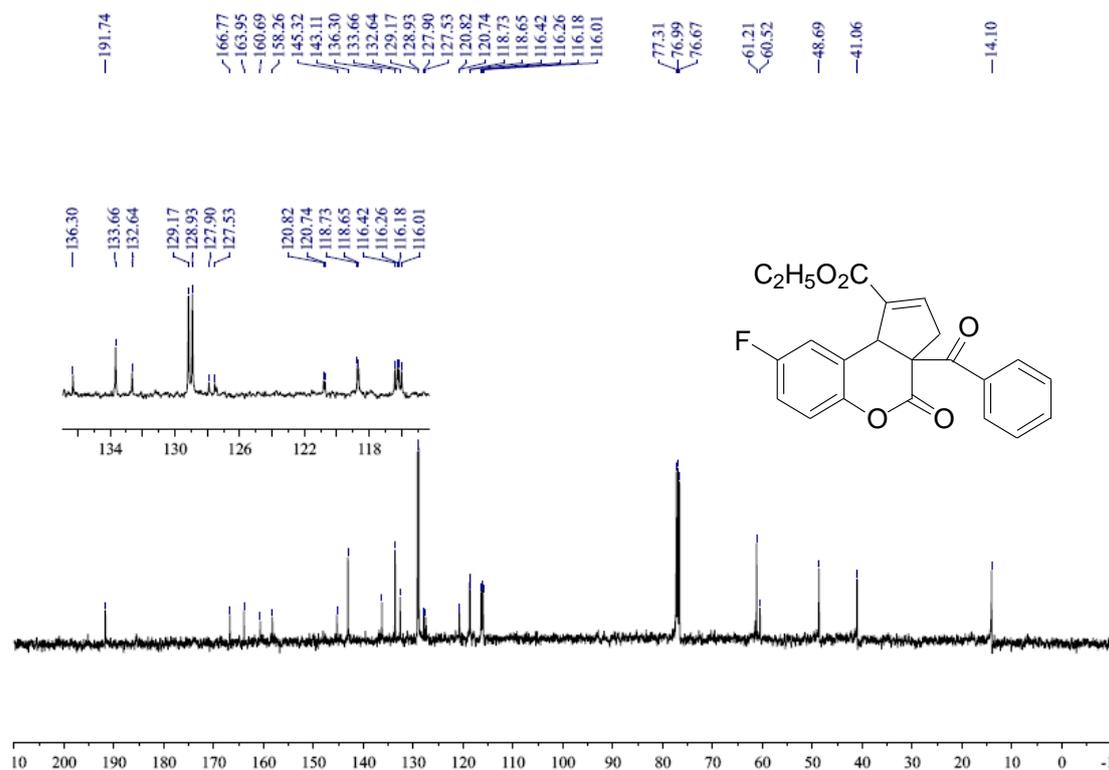


Figure S8. $^{13}\text{C NMR}$ spectrum (100 MHz, CDCl_3) of **3d**

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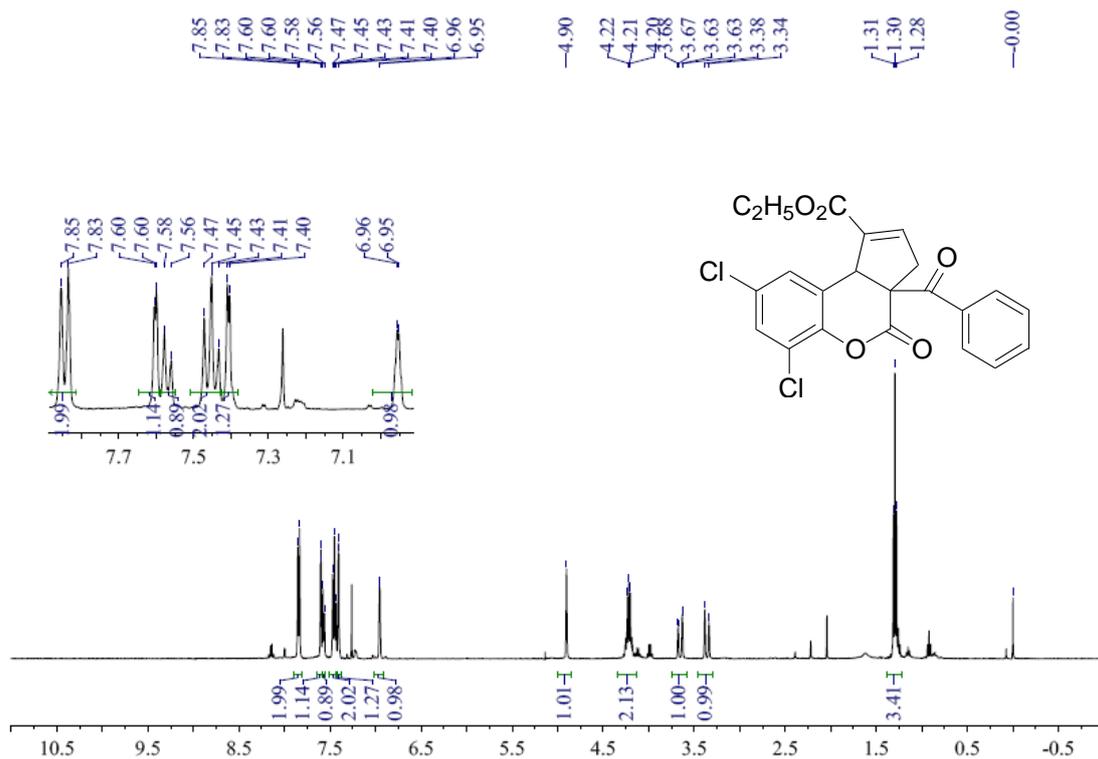


Figure S9. ¹H NMR spectrum (400 MHz, CDCl₃) of 3e

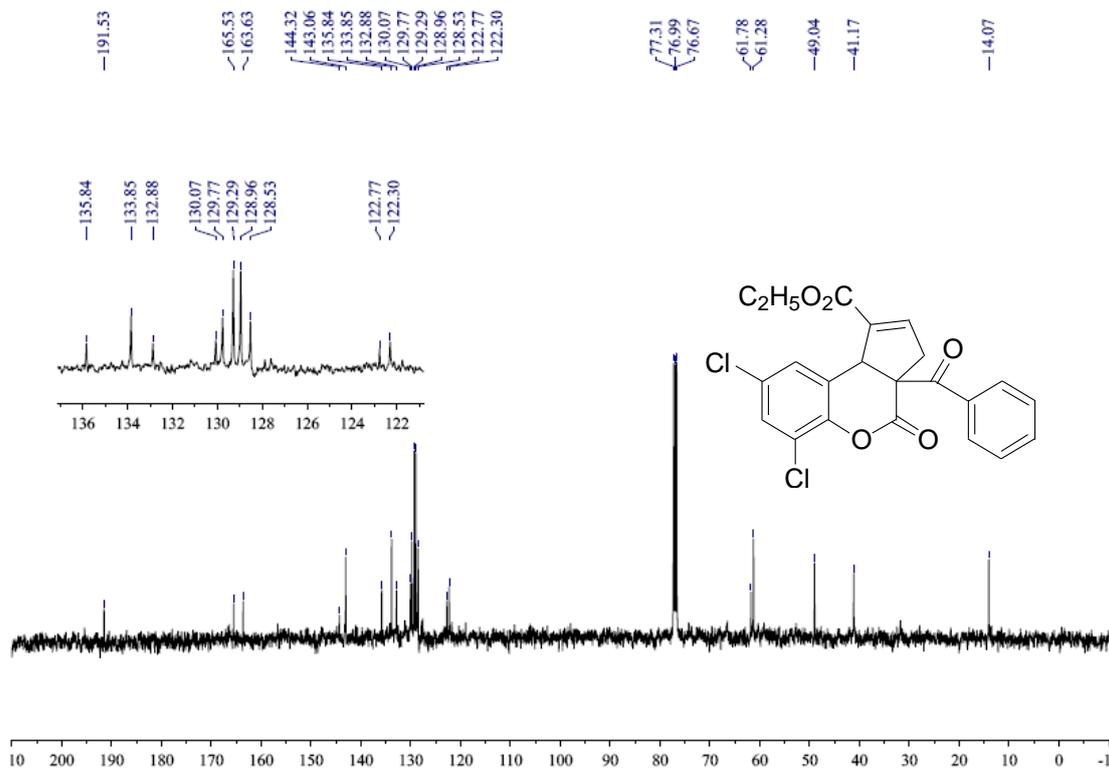


Figure S10. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3e

Supporting Information

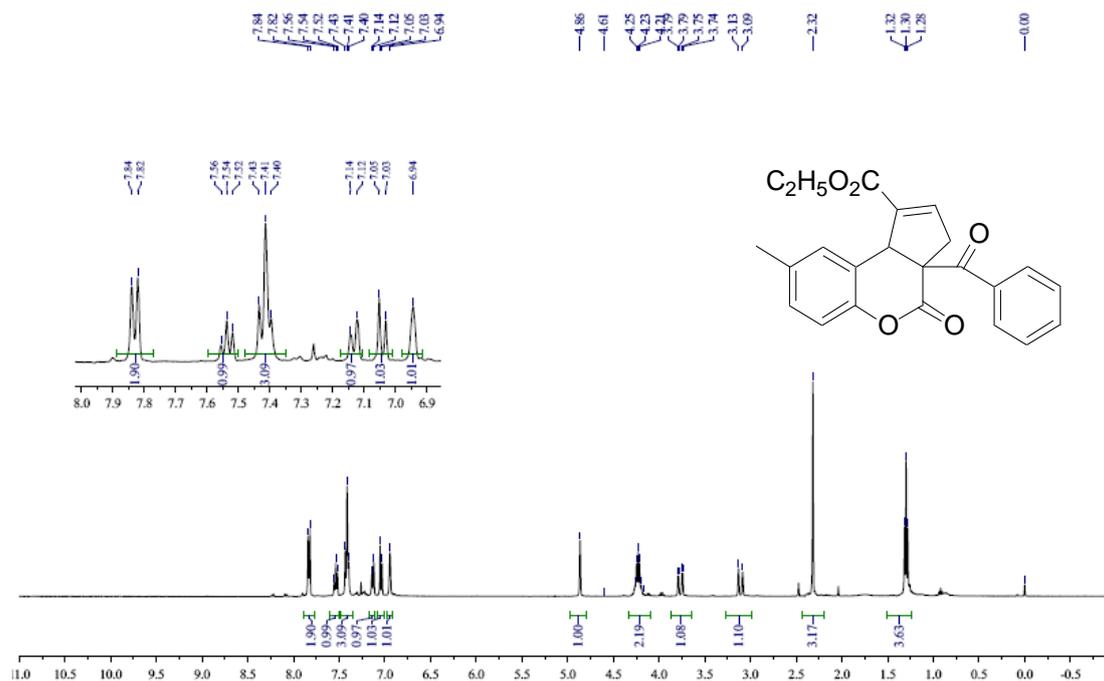


Figure S13. ¹H NMR spectrum (400 MHz, CDCl₃) of 3f

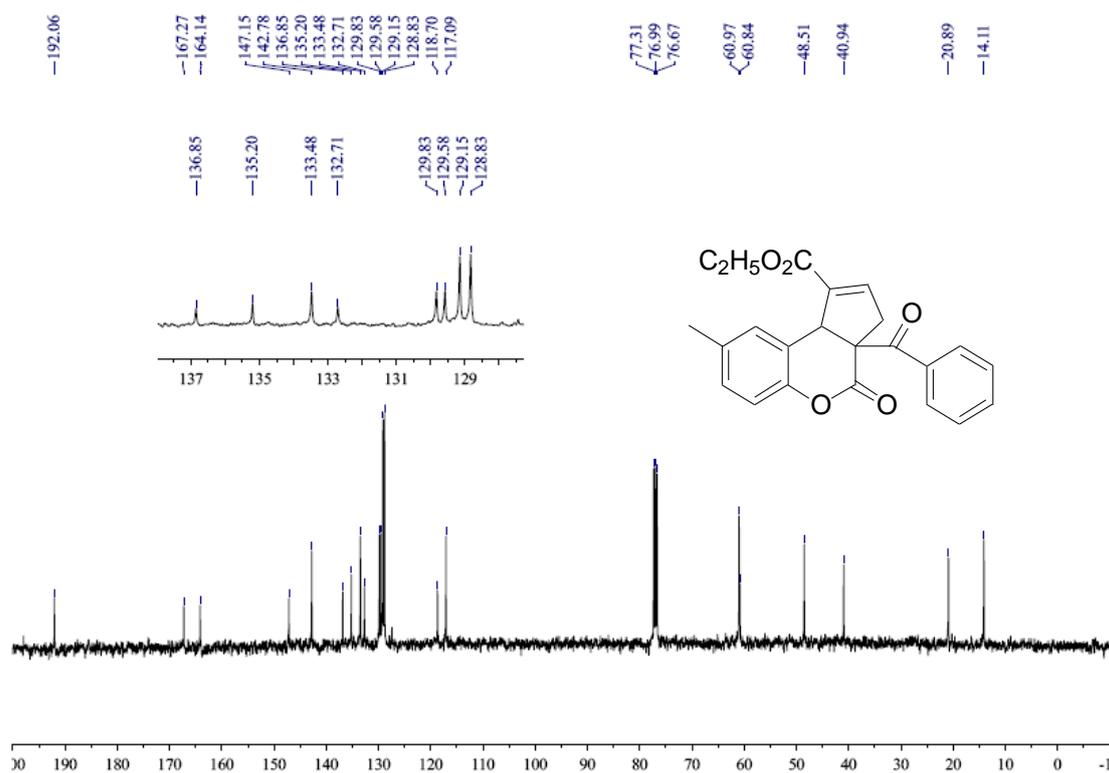


Figure S14. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3f

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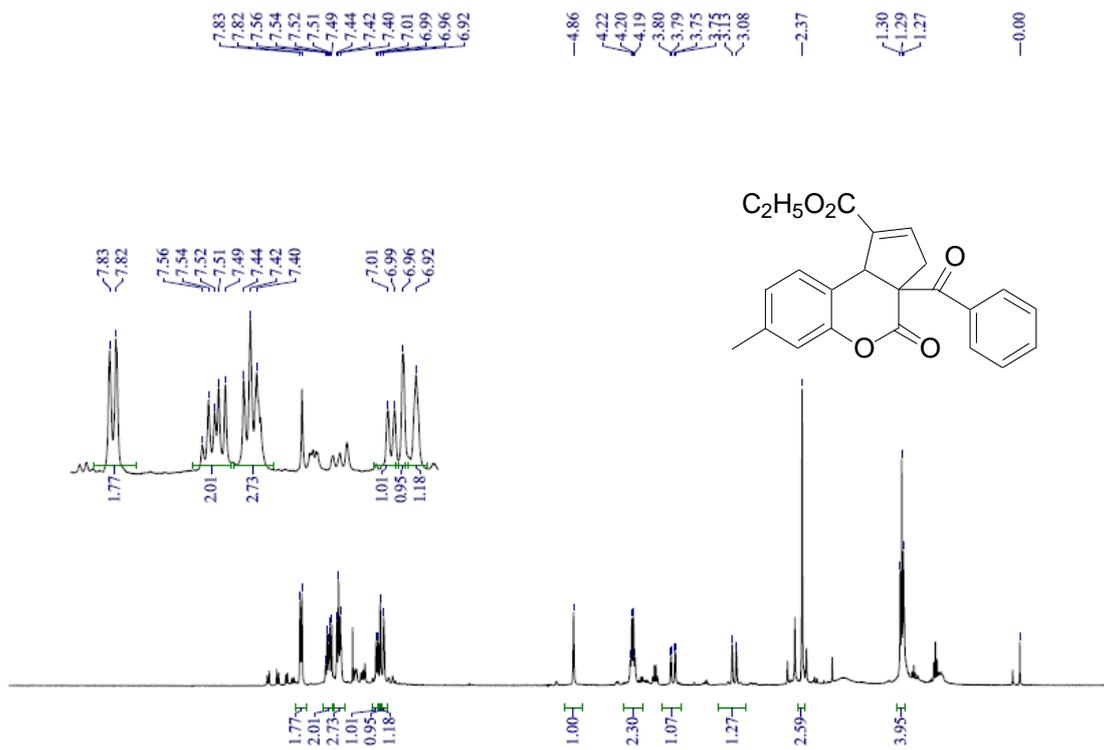


Figure S15. ¹H NMR spectrum (400 MHz, CDCl₃) of **3g**

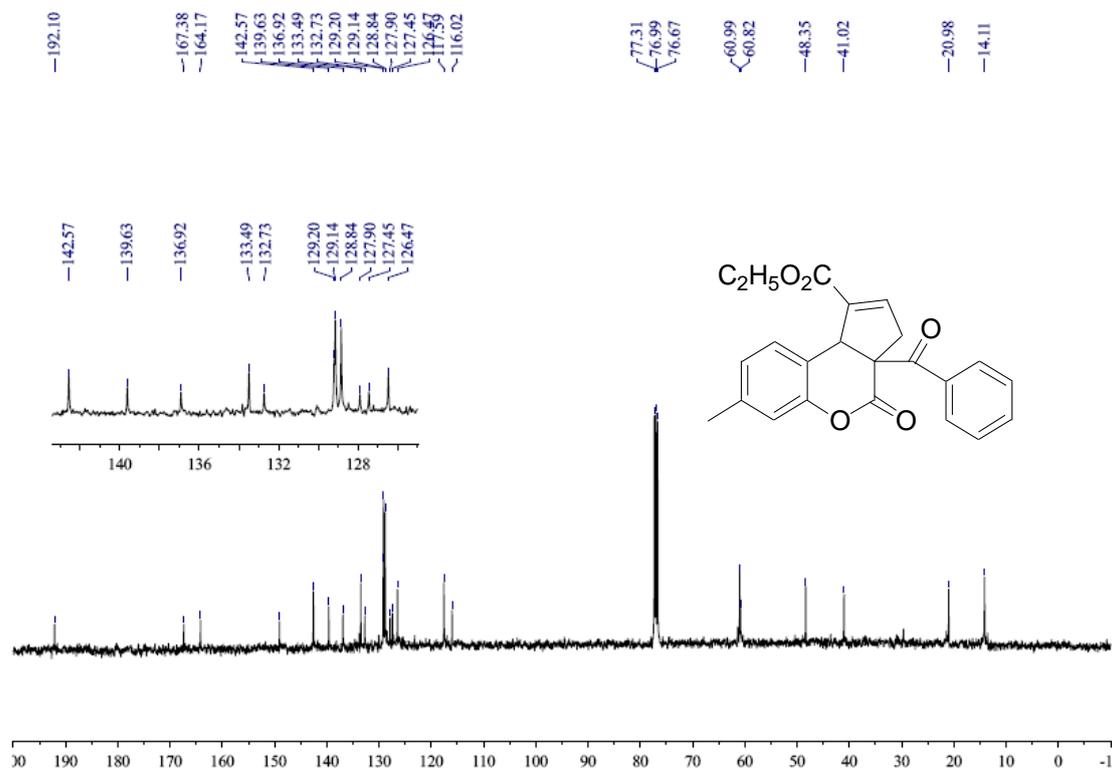


Figure S16. ¹³C NMR spectrum (100 MHz, CDCl₃) of **3g**

Supporting Information

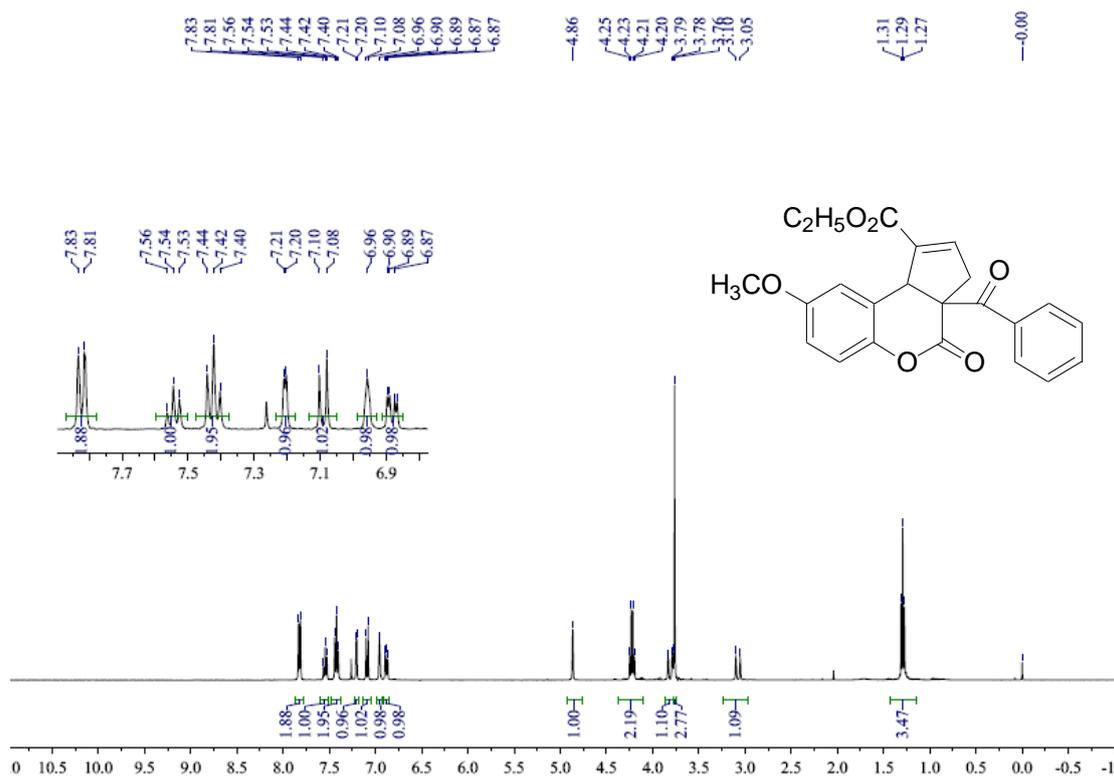


Figure S17. ¹H NMR spectrum (400 MHz, CDCl₃) of **3h**

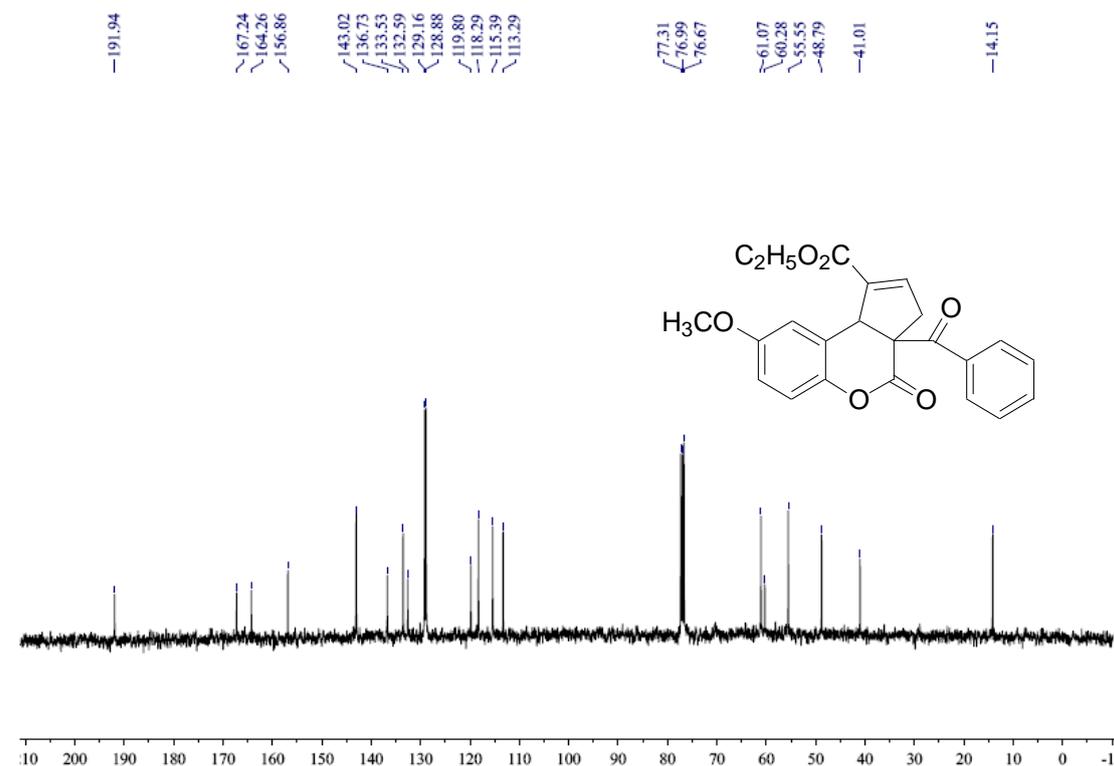


Figure S18. ¹³C NMR spectrum (100 MHz, CDCl₃) of **3h**

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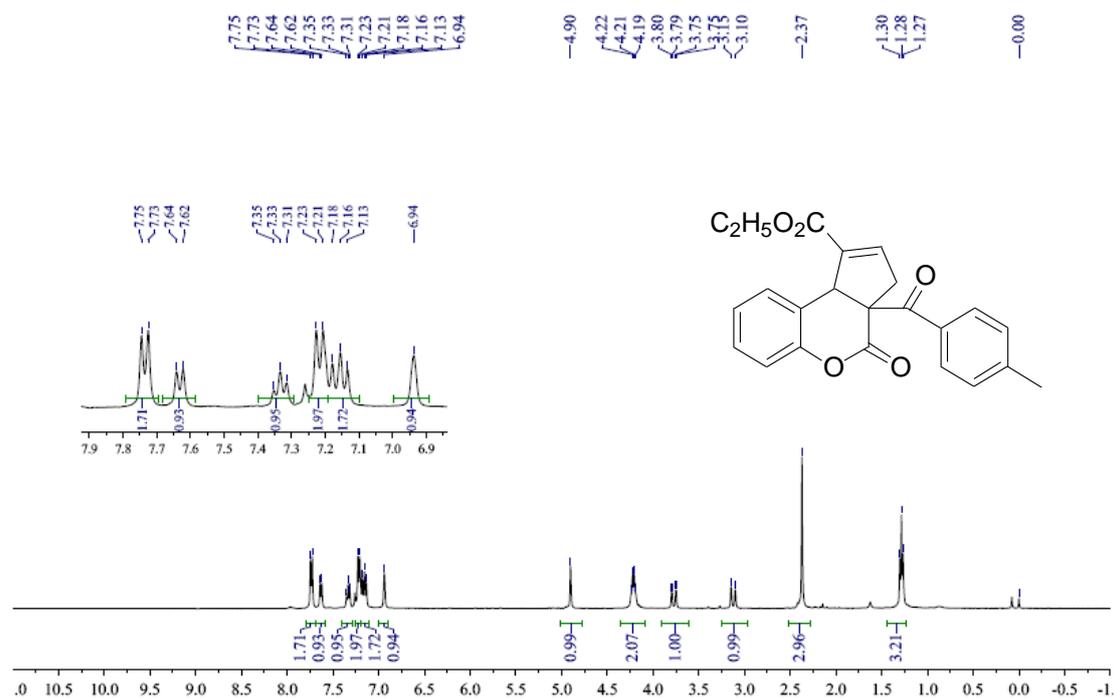


Figure S21. ¹H NMR spectrum (400 MHz, CDCl₃) of **3i**

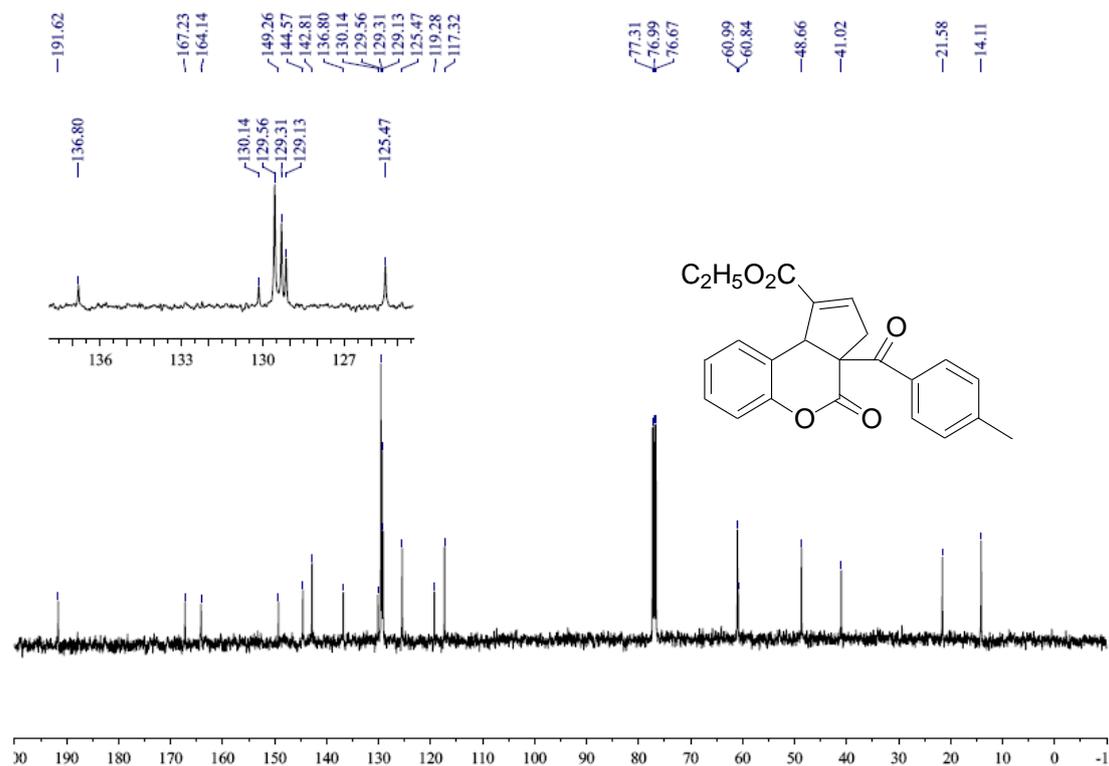


Figure S22. ¹³C NMR spectrum (100 MHz, CDCl₃) of **3i**

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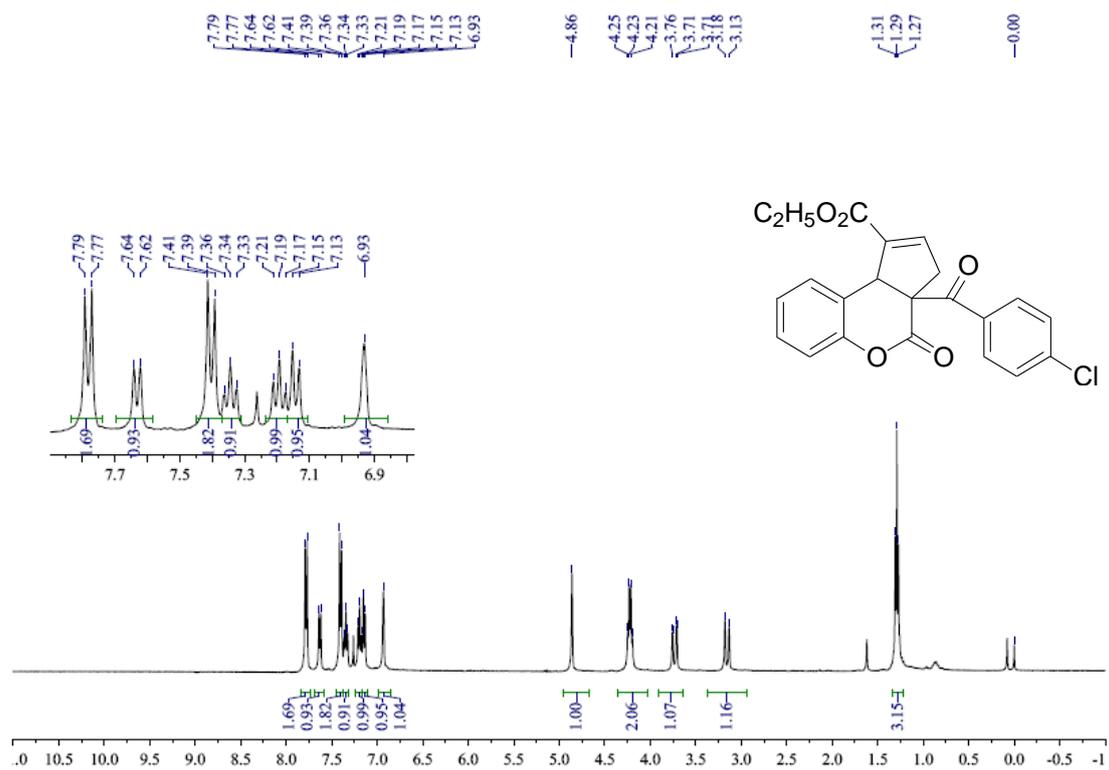


Figure S23. ¹H NMR spectrum (400 MHz, CDCl₃) of **3j**

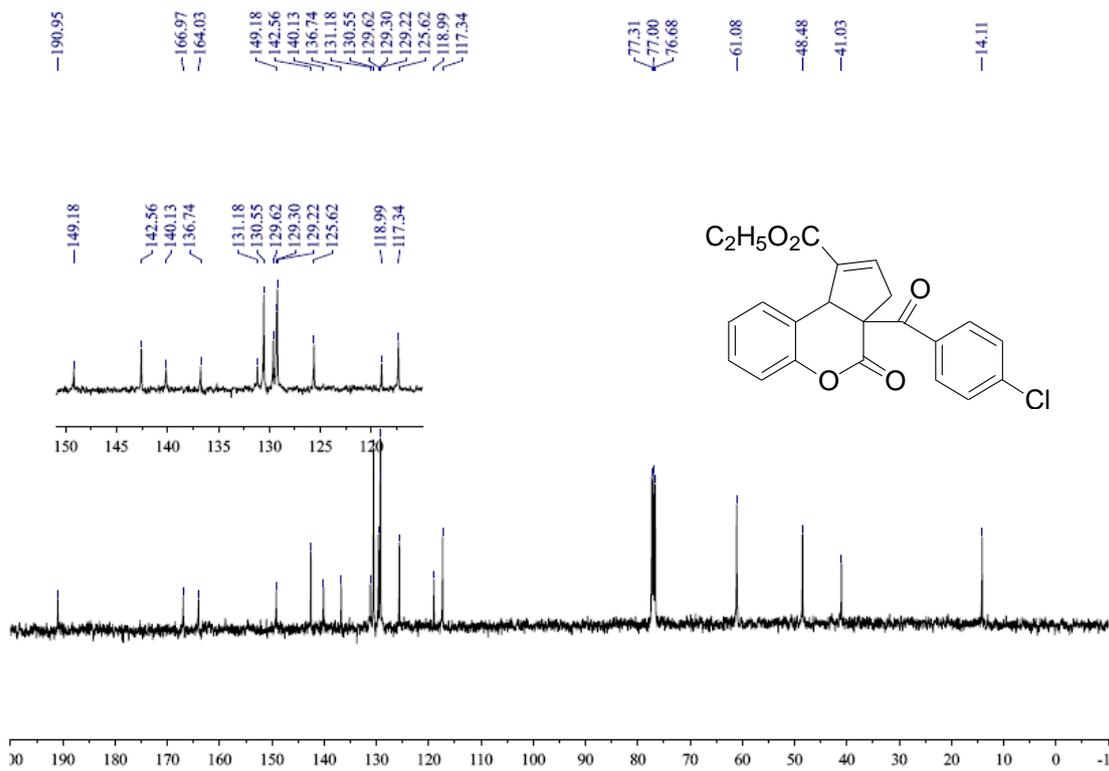


Figure S24. ¹³C NMR spectrum (100 MHz, CDCl₃) of **3j**

X-ray diffraction data for **2b**

The crystal data of **2b** have been deposited in CCDC with number 889494.

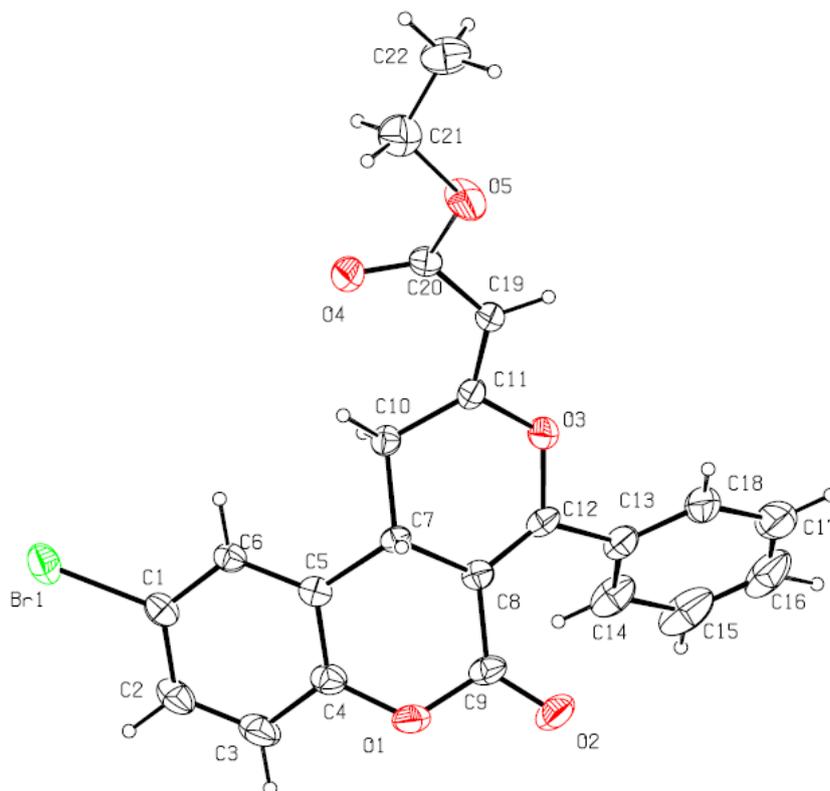


Table 1. Crystal data and structure refinement for mo_120507e.

Identification code	e:20507e	
Empirical formula	C ₂₂ H ₁₇ Br O ₅	
Formula weight	441.27	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna2(1)	
Unit cell dimensions	a = 11.756 Å	α = 90°.
	b = 14.575 Å	β = 90°.
	c = 11.520 Å	γ = 90°.
Volume	1973.9 Å ³	
Z	4	
Density (calculated)	1.485 Mg/m ³	
Absorption coefficient	2.113 mm ⁻¹	
F(000)	896	
Crystal size	0.20 x 0.10 x 0.10 mm ³	

Supporting Information

Theta range for data collection	2.23 to 26.48°.
Index ranges	-14<=h<=14, -17<=k<=18, -14<=l<=14
Reflections collected	14075
Independent reflections	3918 [R(int) = 0.0520]
Completeness to theta = 26.48°	99.6 %
Absorption correction	None
Max. and min. transmission	0.8165 and 0.6773
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3918 / 9 / 271
Goodness-of-fit on F ²	0.986
Final R indices [I>2sigma(I)]	R1 = 0.0394, wR2 = 0.0809
R indices (all data)	R1 = 0.0920, wR2 = 0.0971
Absolute structure parameter	0.009(11)
Largest diff. peak and hole	0.220 and -0.211 e.Å ⁻³

X-ray diffraction data for **3j**

The crystal data of **3j** have been deposited in CCDC with number 889495.

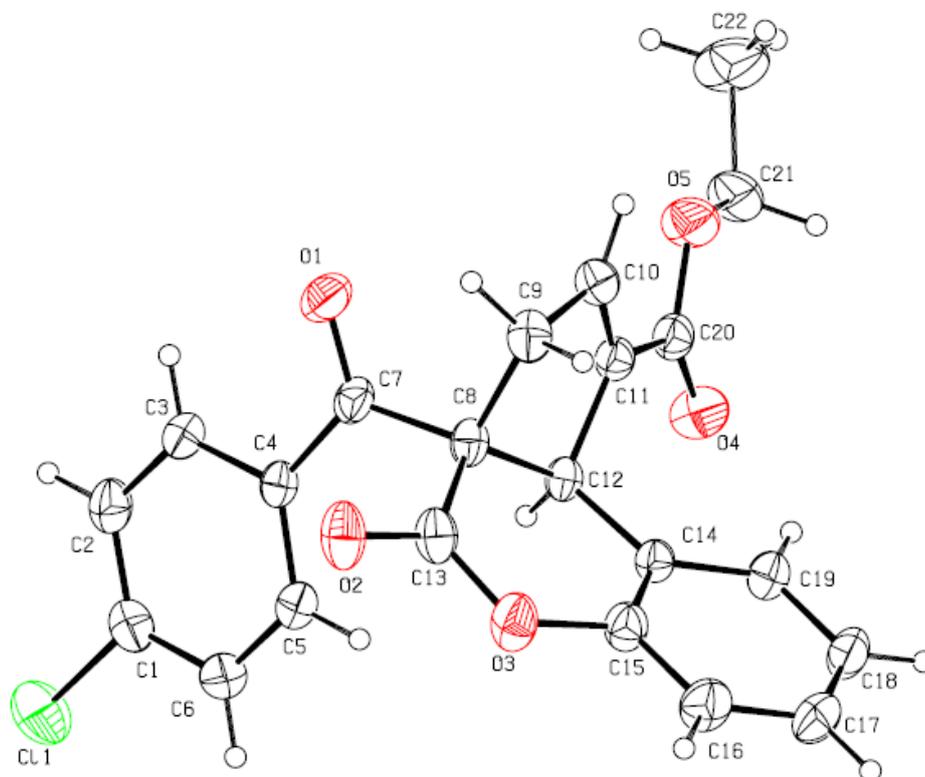


Table 1. Crystal data and structure refinement for mo_120509_0m

Identification code	120509b_0m
Empirical formula	C ₂₂ H ₁₇ Cl O ₅
Formula weight	396.81
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.7129(16) Å \angle = 107.550(2) $^\circ$ b = 10.5113(17) Å \angle = 105.744(2) $^\circ$ c = 10.7041(17) Å \angle = 98.461(2) $^\circ$
Volume	971.2(3) Å ³
Z	2
Density (calculated)	1.357 Mg/m ³
Absorption coefficient	0.227 mm ⁻¹
F(000)	412
Crystal size	? x ? x ? mm ³
Theta range for data collection	2.10 to 25.50 $^\circ$.
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 12, -12 ≤ l ≤ 12

Supporting Information

Reflections collected	7083
Independent reflections	3559 [R(int) = 0.0246]
Completeness to theta = 25.50	98.5 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3559 / 6 / 275
Goodness-of-fit on F ²	1.086
Final R indices [I>2sigma(I)]	R1 = 0.0499, wR2 = 0.1514
R indices (all data)	R1 = 0.0618, wR2 = 0.1632
Extinction coefficient	0.000(4)
Largest diff. peak and hole	0.295 and -0.413 e. ⁻³