

Supporting Information

Catalyst-Free [4+2] Cyclization of *para*-Quinone Methide Derivatives with Homophthalic Anhydrides

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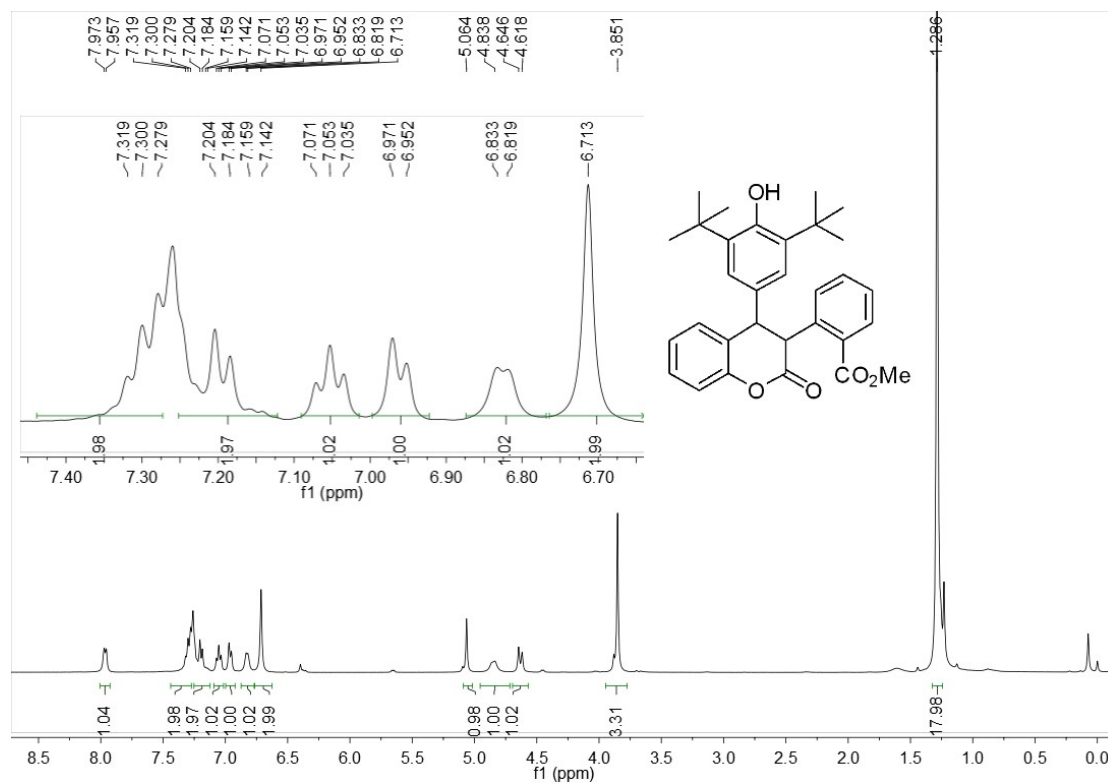
Contents:

1. NMR spectra of products 3 and 4 (S1-S18)

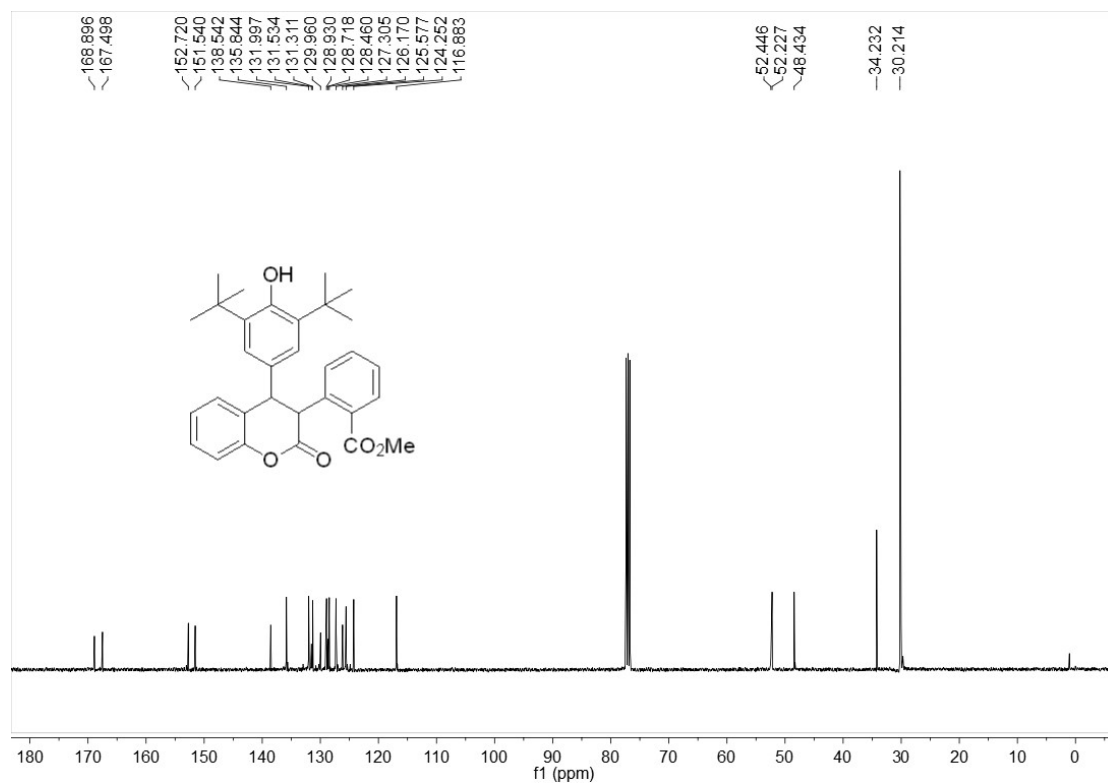
2. X-ray single crystal data for compound 3da (S19-S20)

1. NMR spectra of products 3

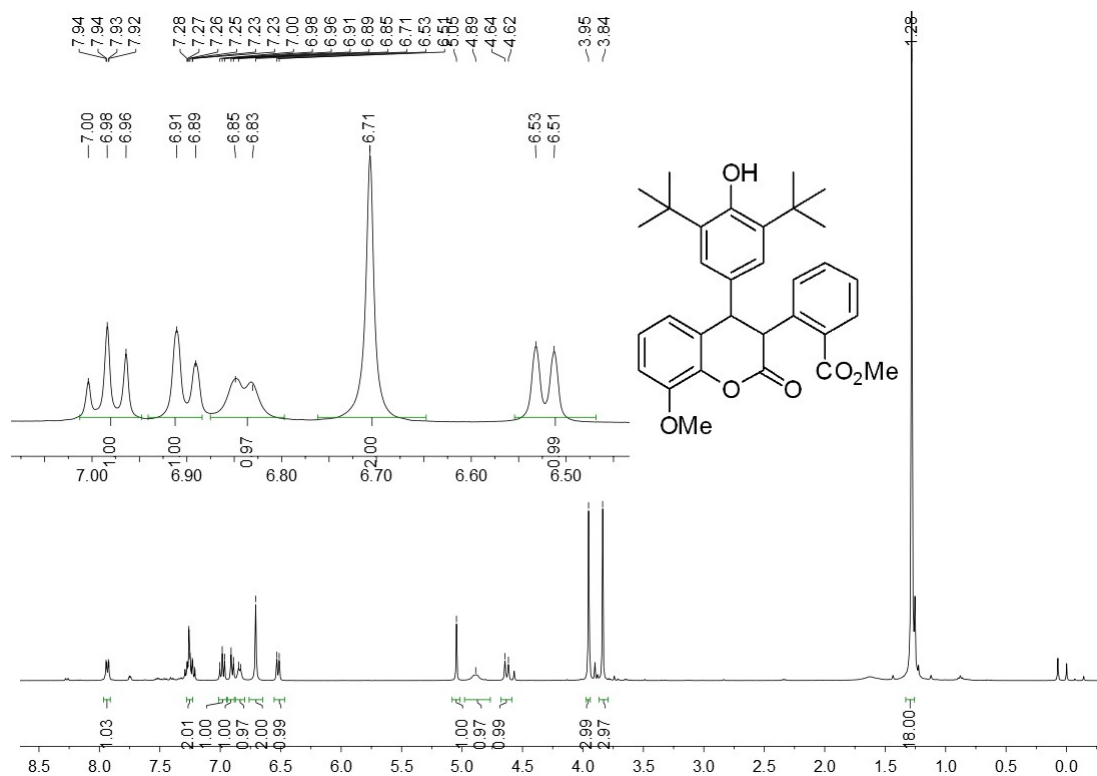
^1H NMR of compound **3aa** (inseparable diastereomers with 91:9 dr)



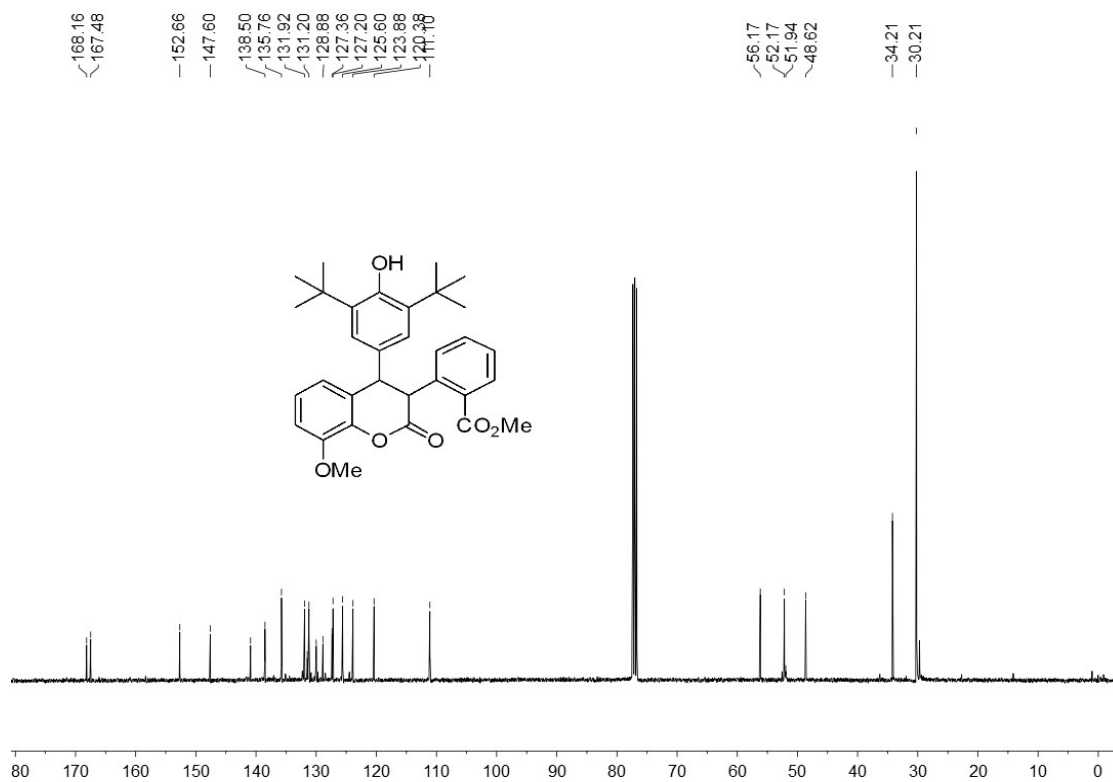
^{13}C NMR of compound **3aa** (inseparable diastereomers with 91:9 dr)



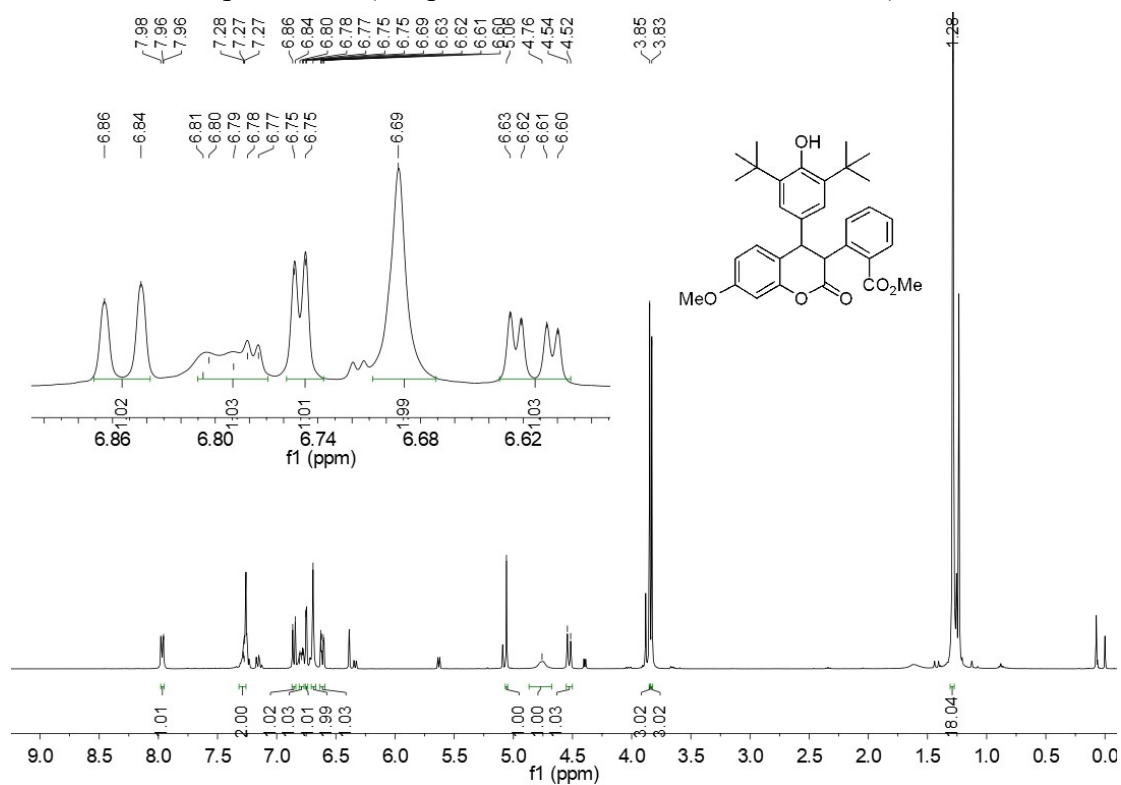
^1H NMR of compound **3ba** (inseparable diastereomers with 85:15 dr)



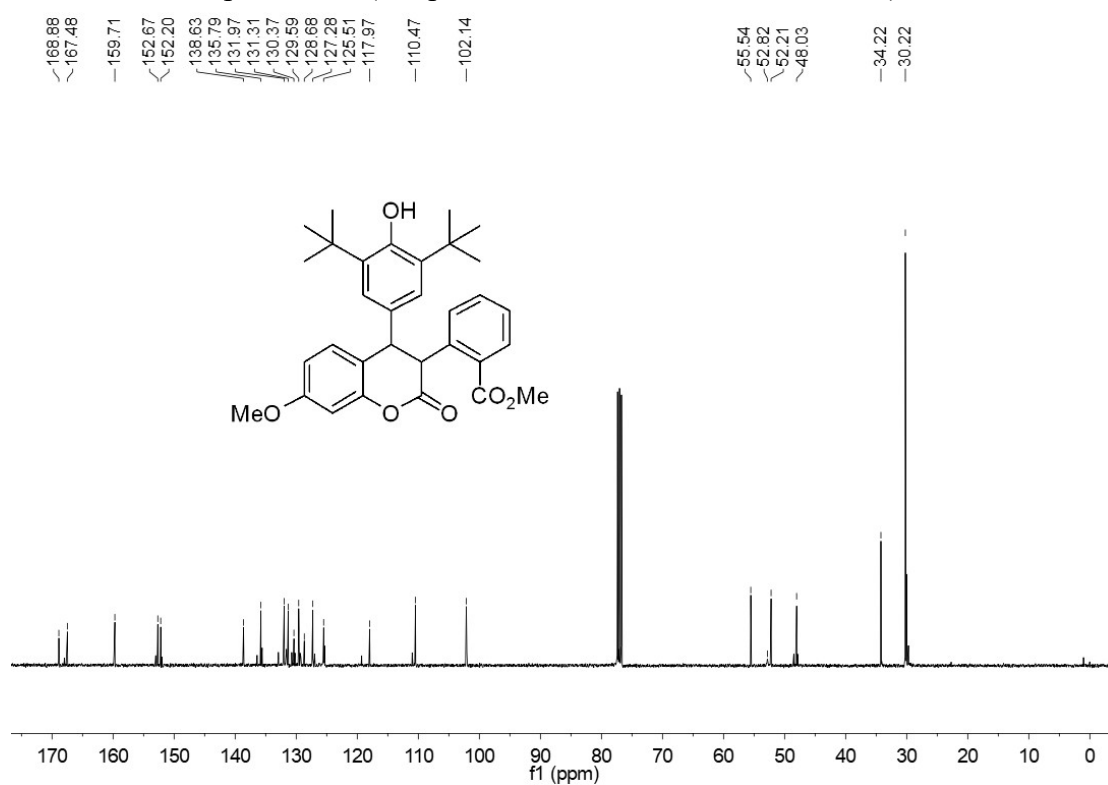
^{13}C NMR of compound **3ba** (inseparable diastereomers with 85:15 dr)



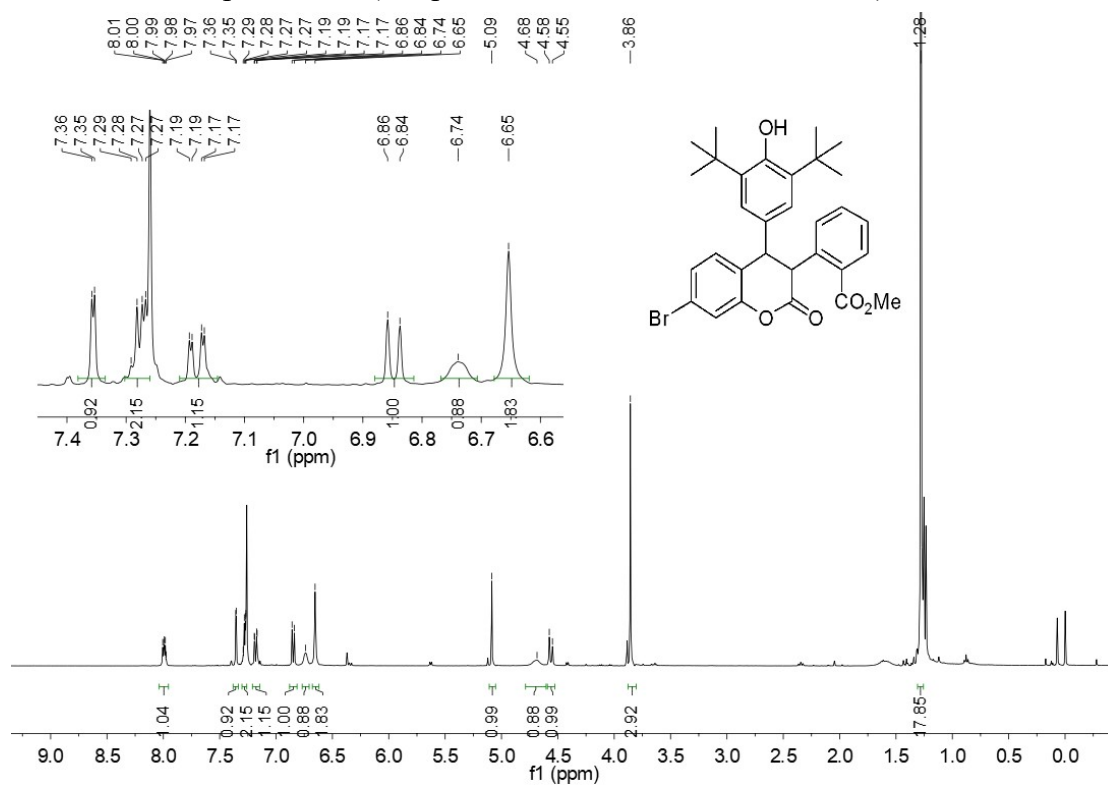
^1H NMR of compound **3ca** (inseparable diastereomers with 80:20 dr)



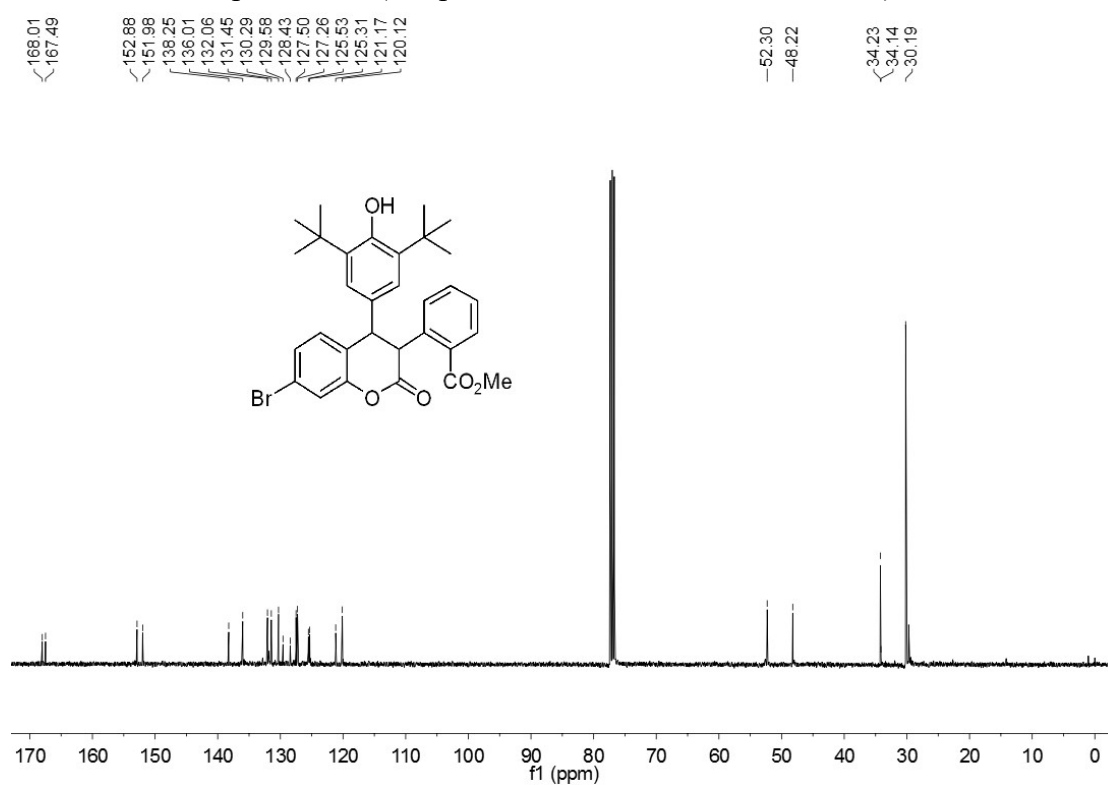
^{13}C NMR of compound **3ca** (inseparable diastereomers with 80:20 dr)



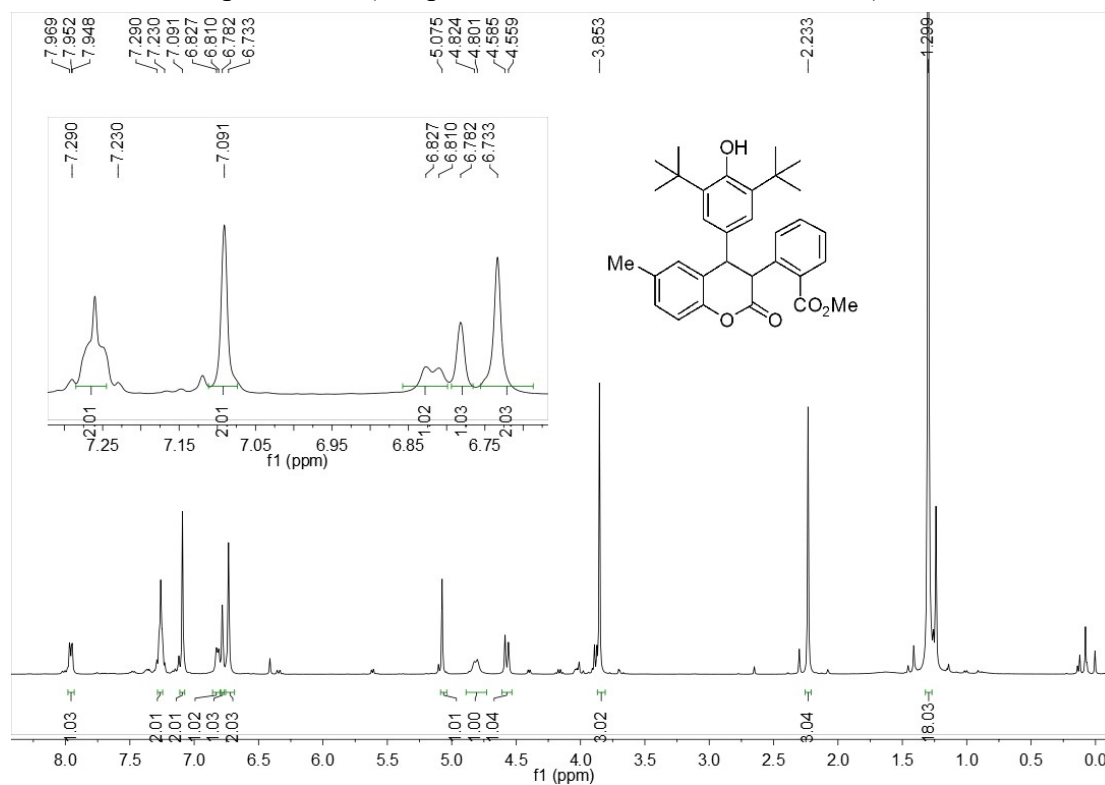
^1H NMR of compound **3da** (inseparable diastereomers with 91:9 dr)



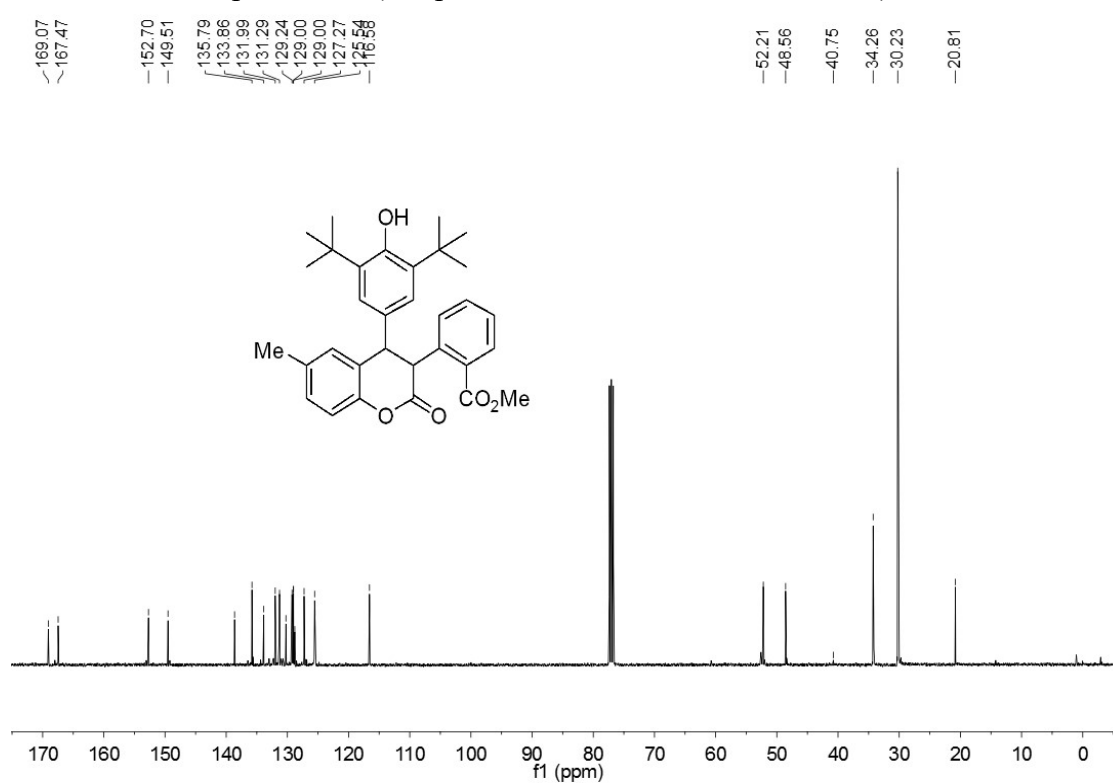
^{13}C NMR of compound **3da** (inseparable diastereomers with 91:9 dr)



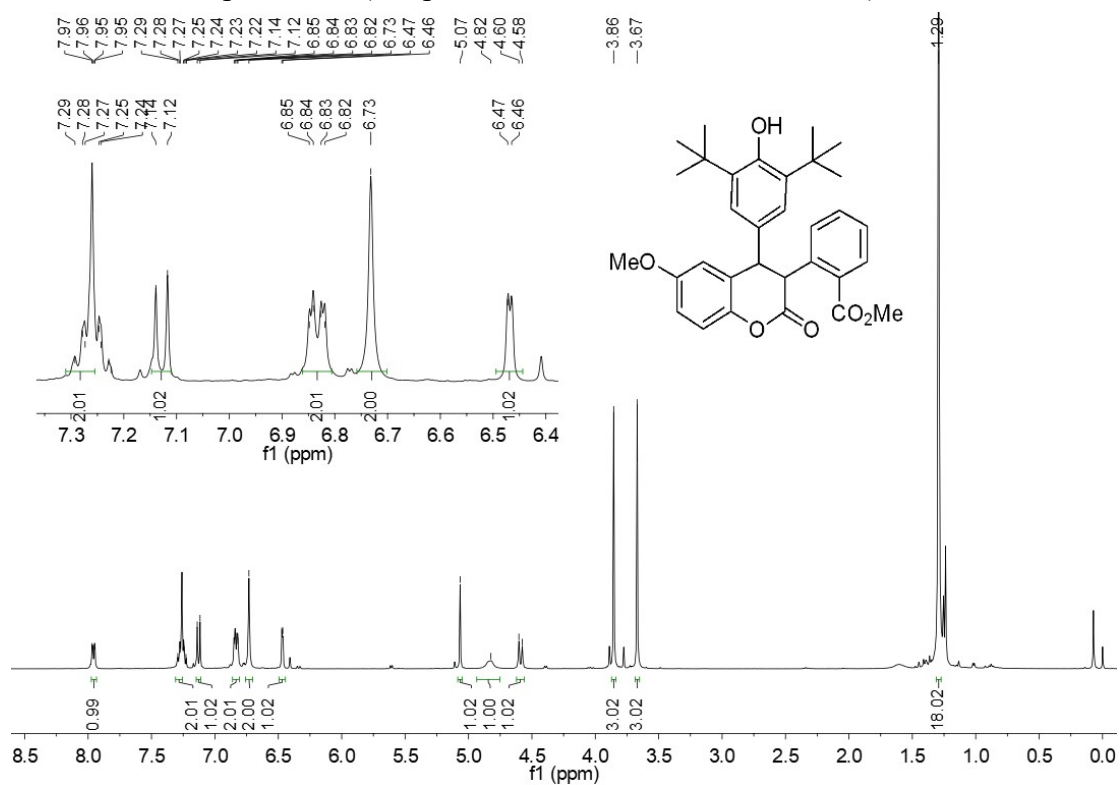
^1H NMR of compound **3ea** (inseparable diastereomers with 91:9 dr)



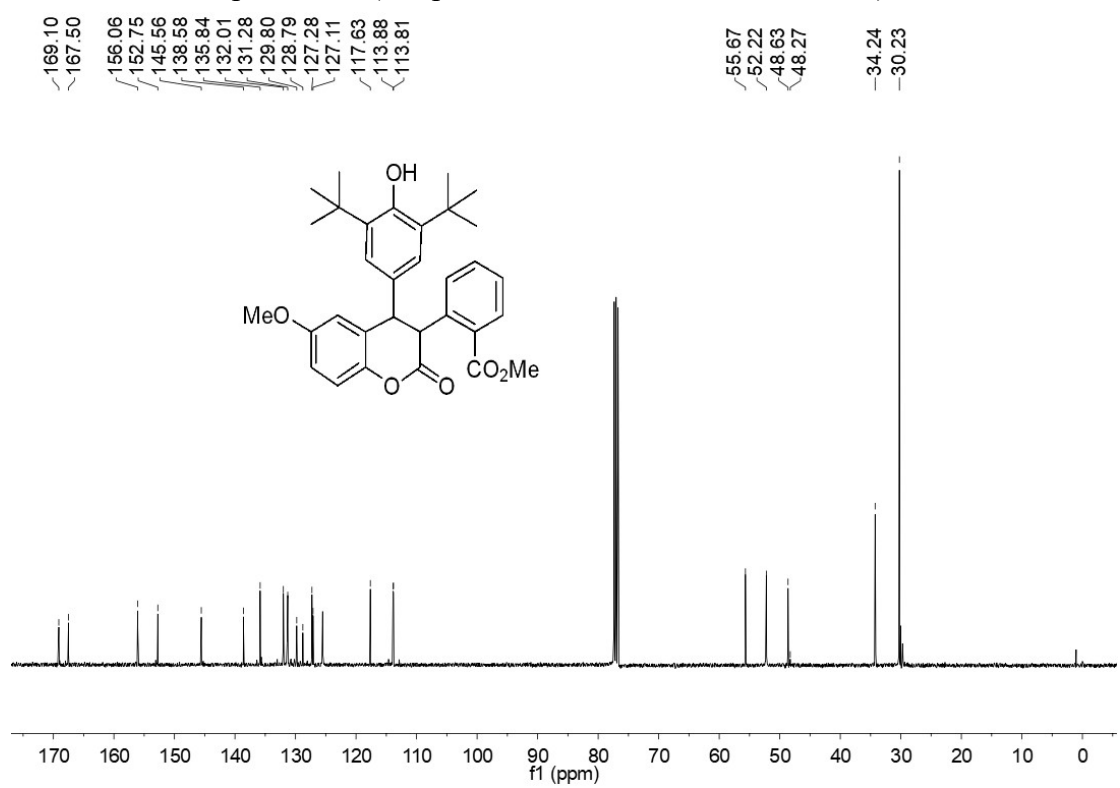
^{13}C NMR of compound **3ea** (inseparable diastereomers with 91:9 dr)



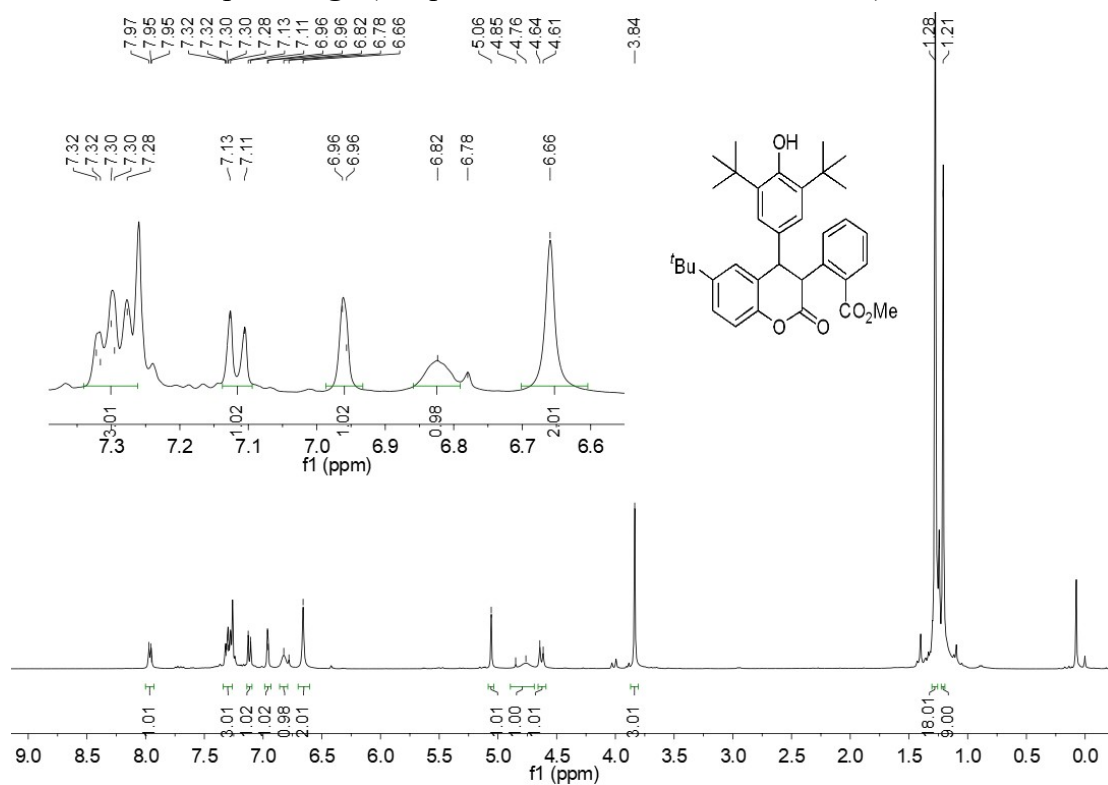
^1H NMR of compound **3fa** (inseparable diastereomers with 91:9 dr)



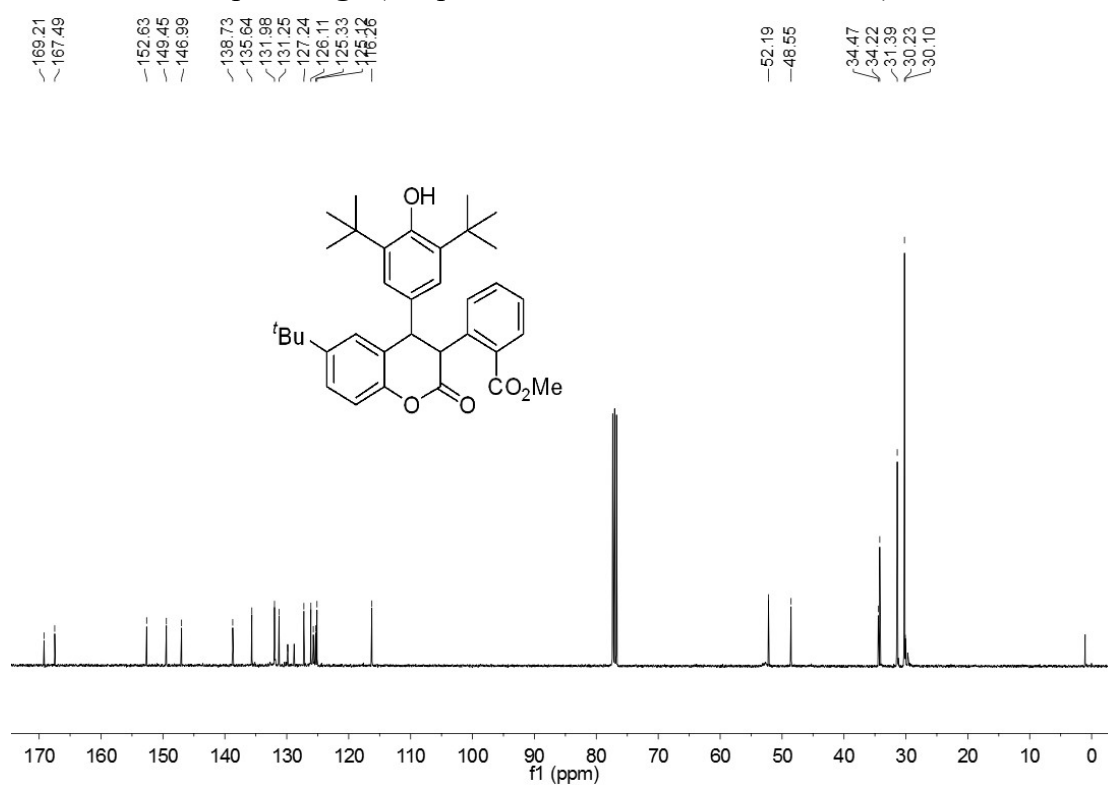
^{13}C NMR spectrum of compound **3fa** (inseparable diastereomers with 91:9 dr)



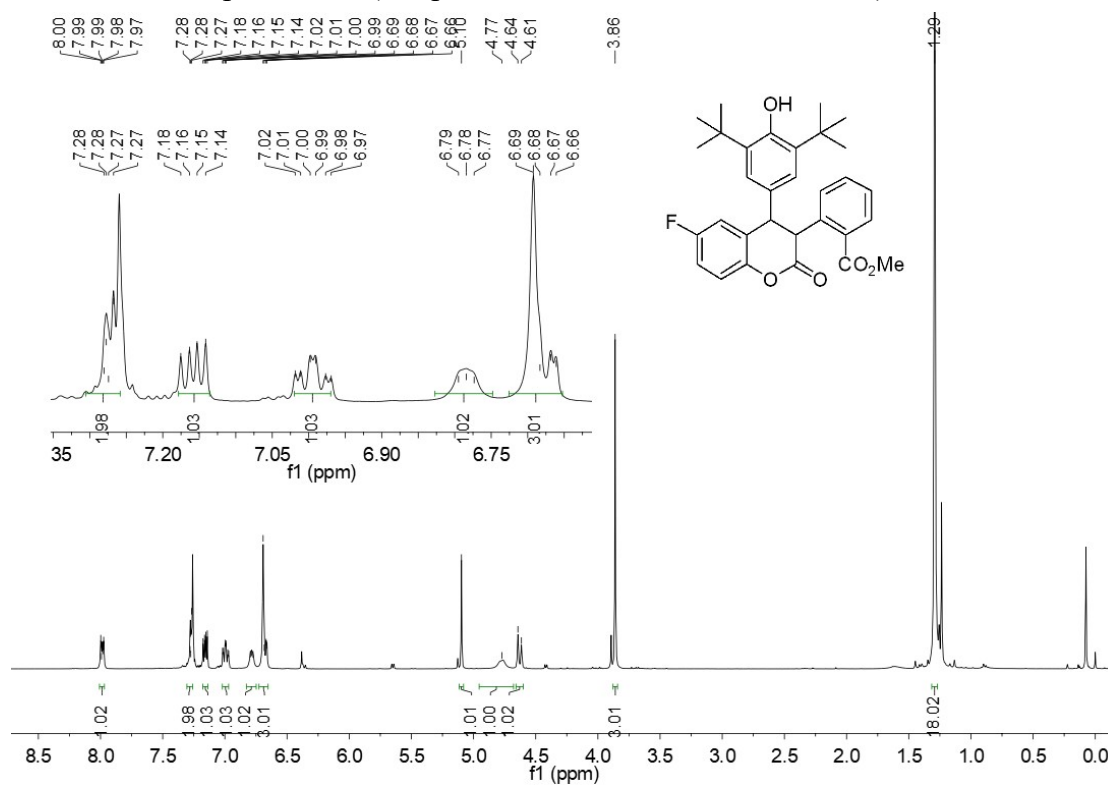
¹H NMR of compound **3ga** (inseparable diastereomers with 91:9 dr)



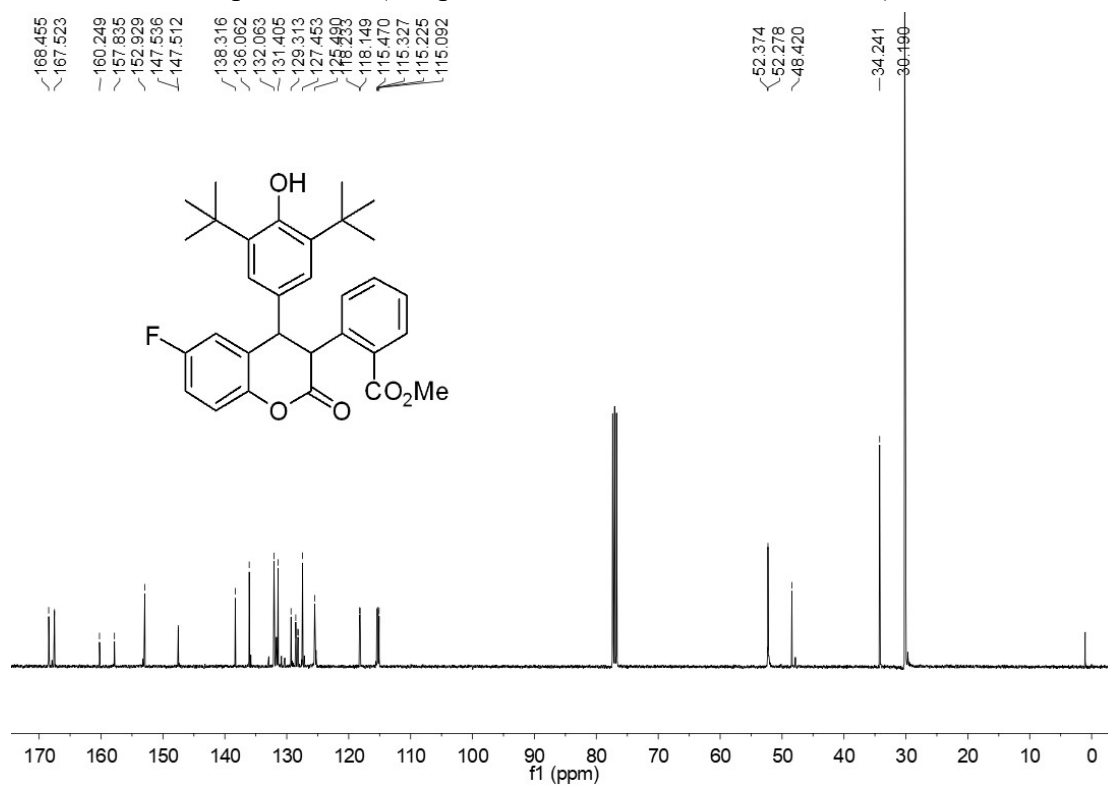
¹³C NMR of compound **3ga** (inseparable diastereomers with 91:9 dr)



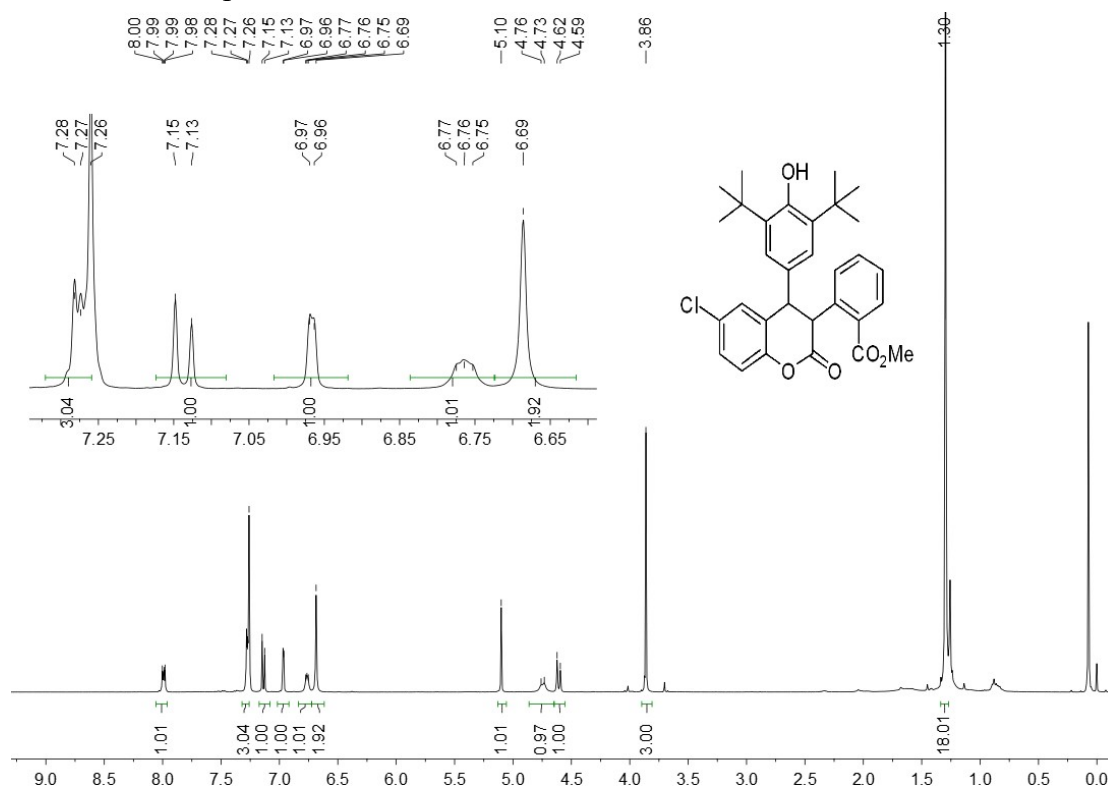
¹H NMR of compound **3ha** (inseparable diastereomers with 91:9 dr)



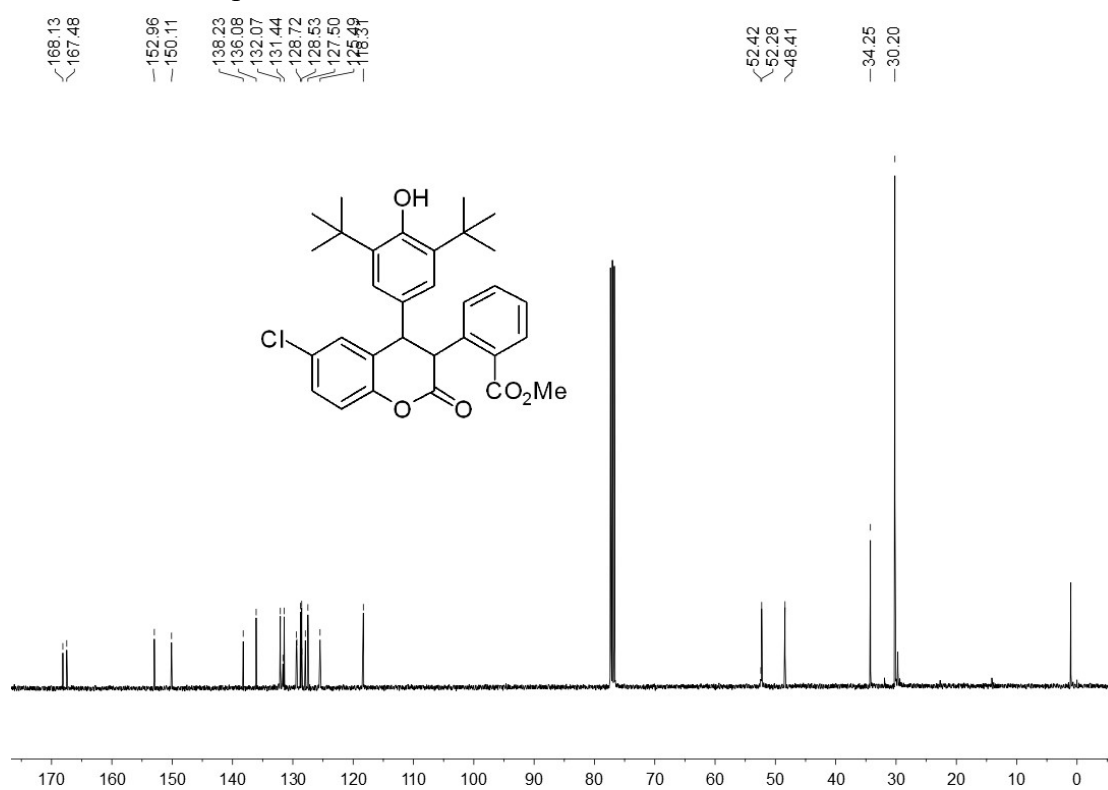
¹³C NMR of compound **3ha** (inseparable diastereomers with 91:9 dr)



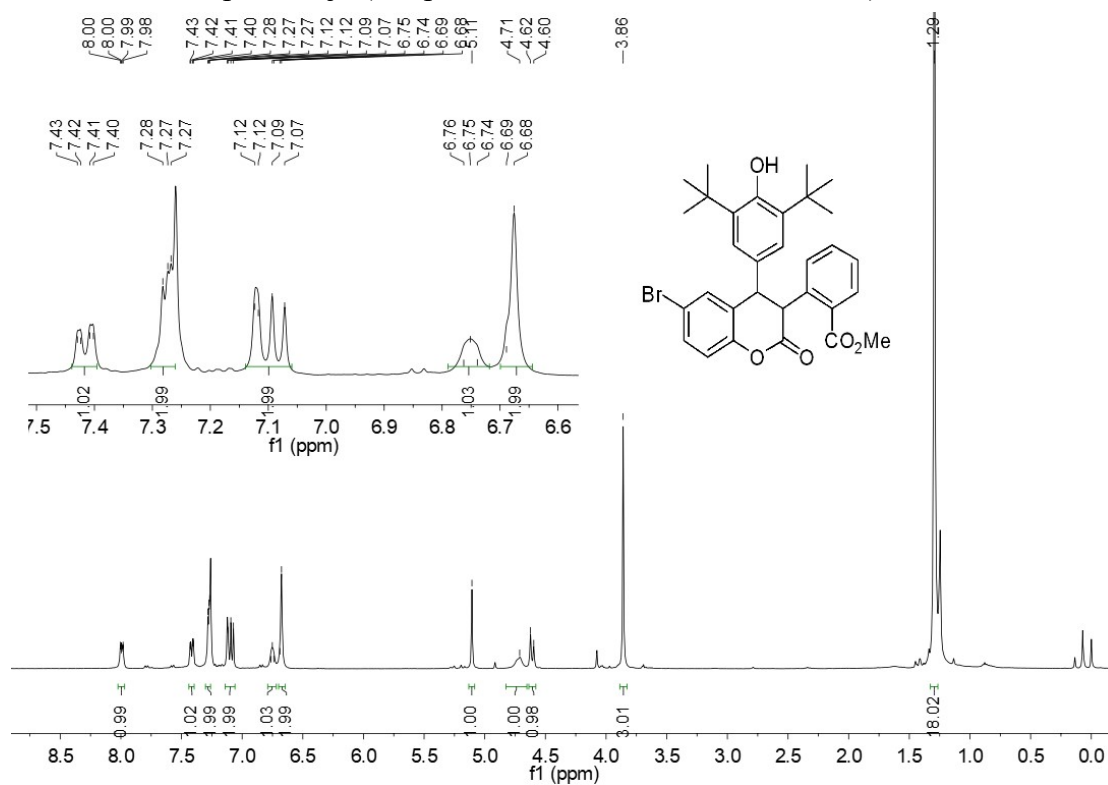
¹H NMR of compound **3ia**



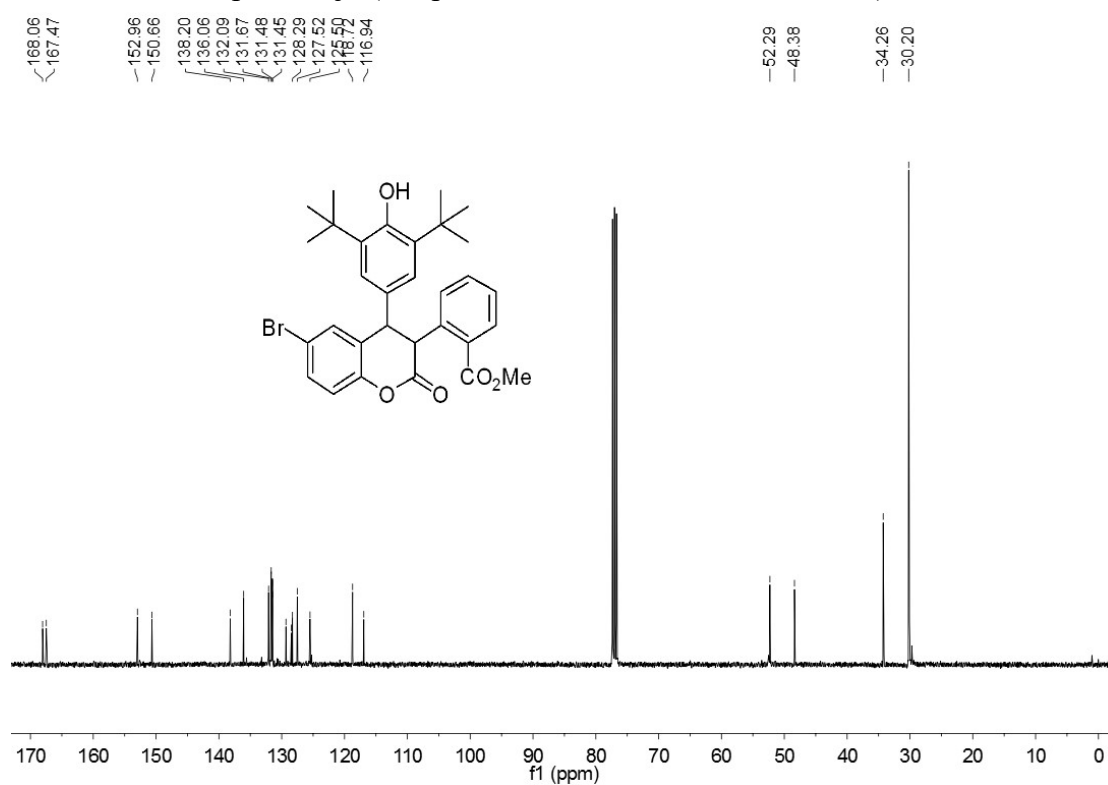
¹³C NMR of compound **3ia**



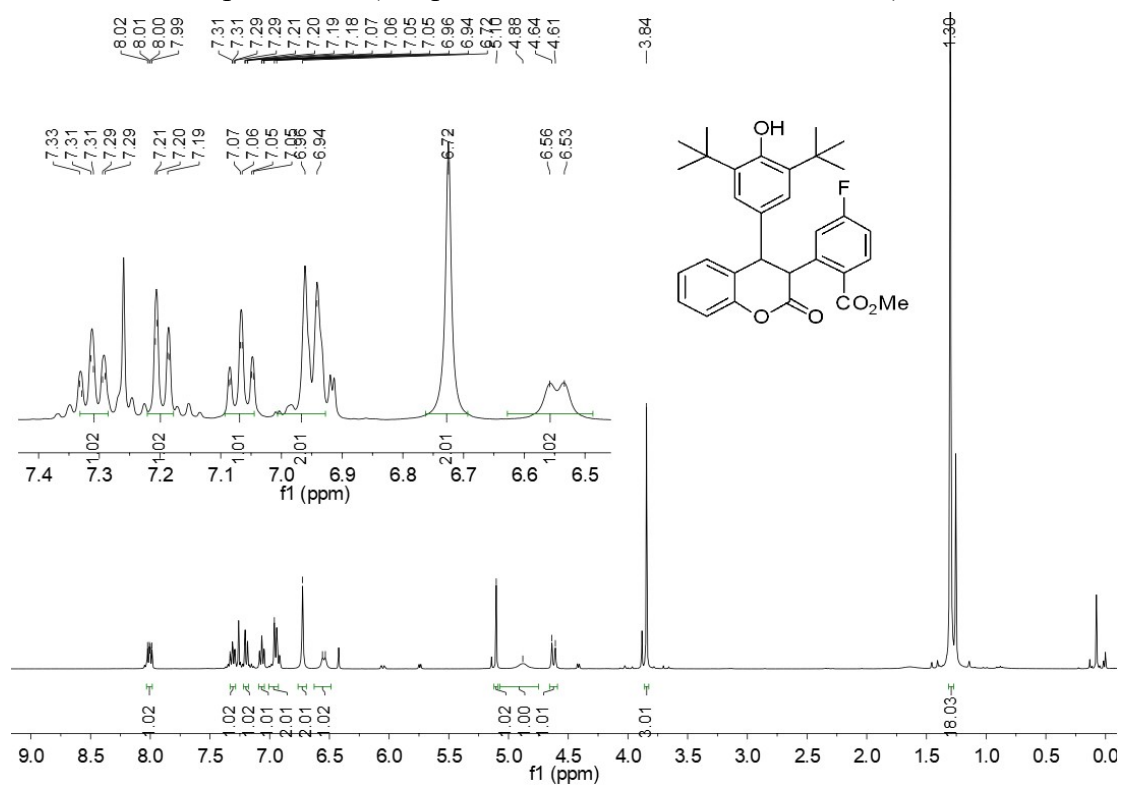
^1H NMR of compound **3ja** (inseparable diastereomers with 91:9 dr)



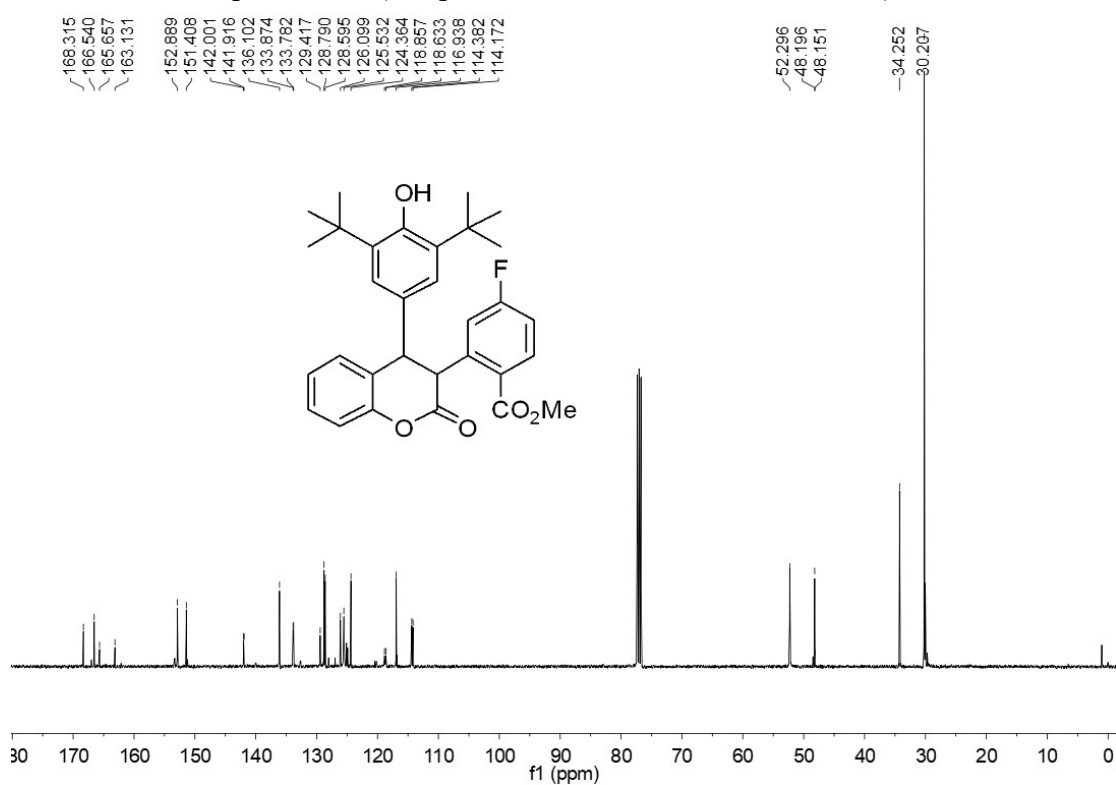
^{13}C NMR of compound **3ja** (inseparable diastereomers with 91:9 dr)



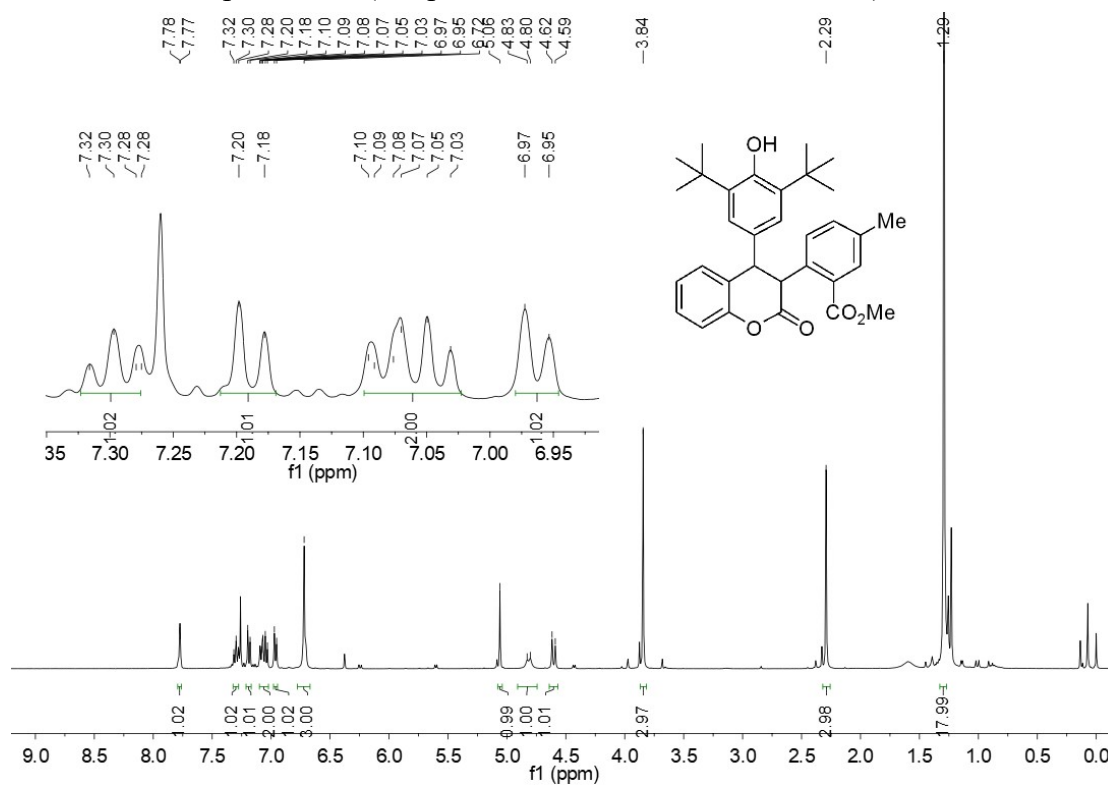
^1H NMR of compound **3ab** (inseparable diastereomers with 88:12 dr)



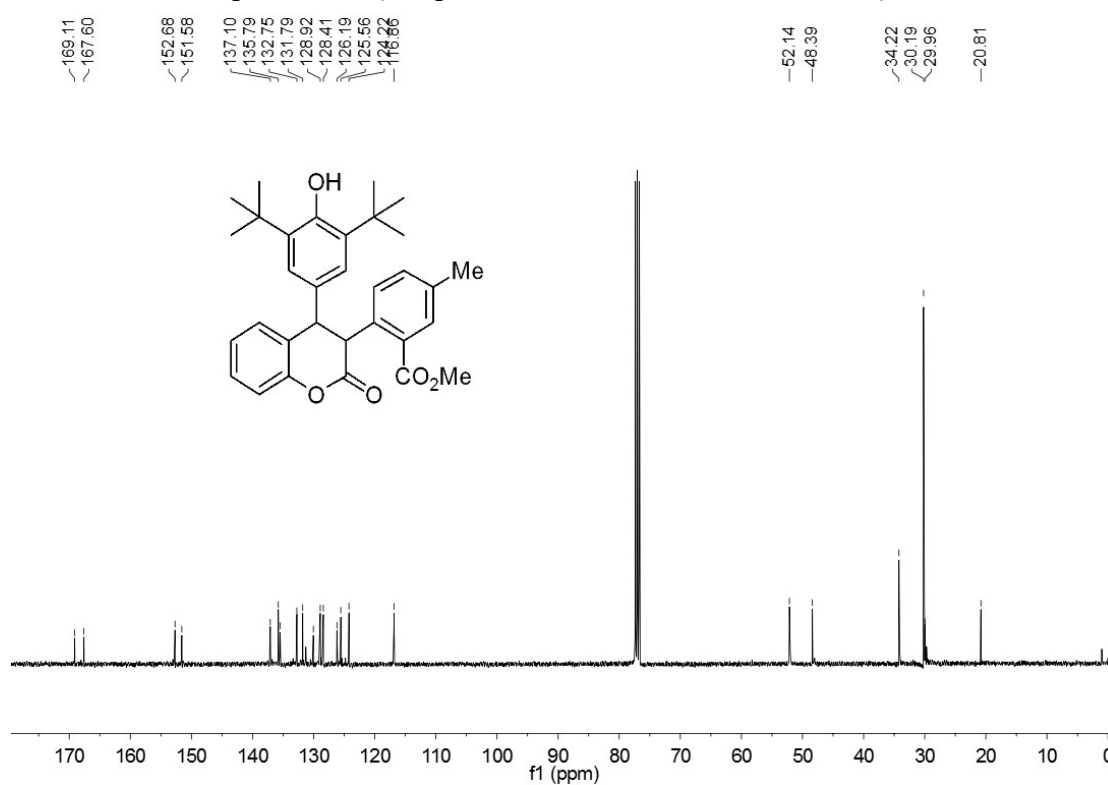
^{13}C NMR of compound **3ab** (inseparable diastereomers with 91:9 dr)



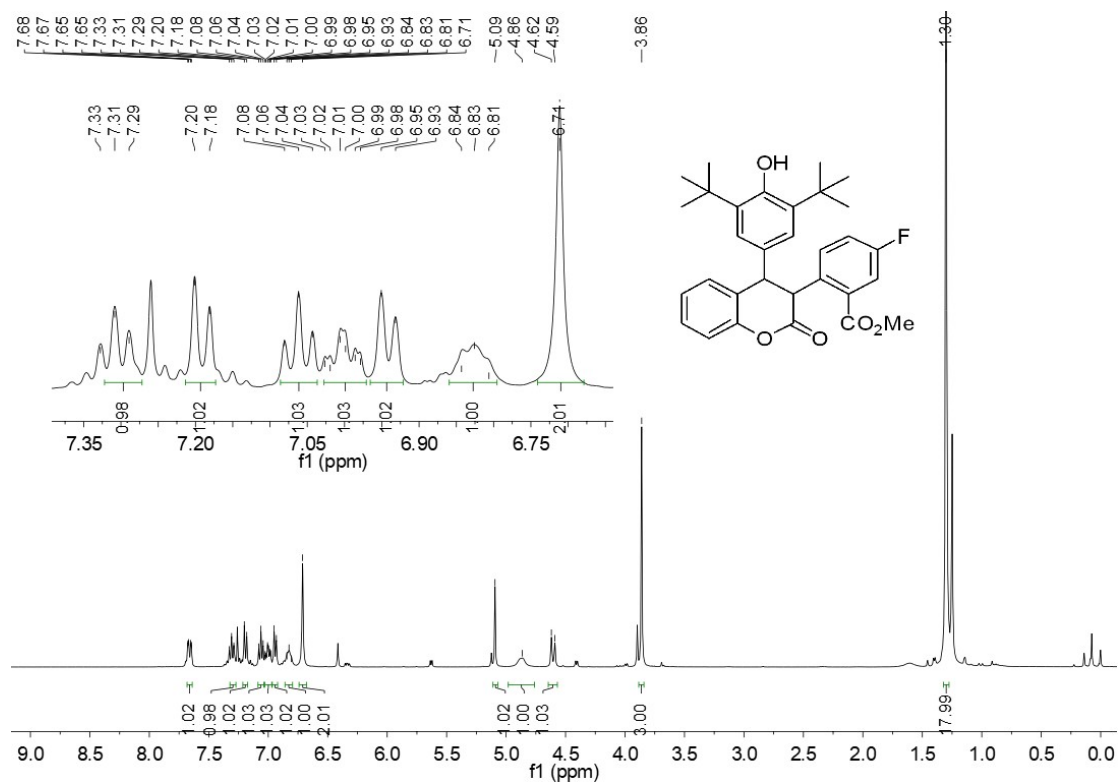
¹H NMR of compound **3ac** (inseparable diastereomers with 91:9 dr)



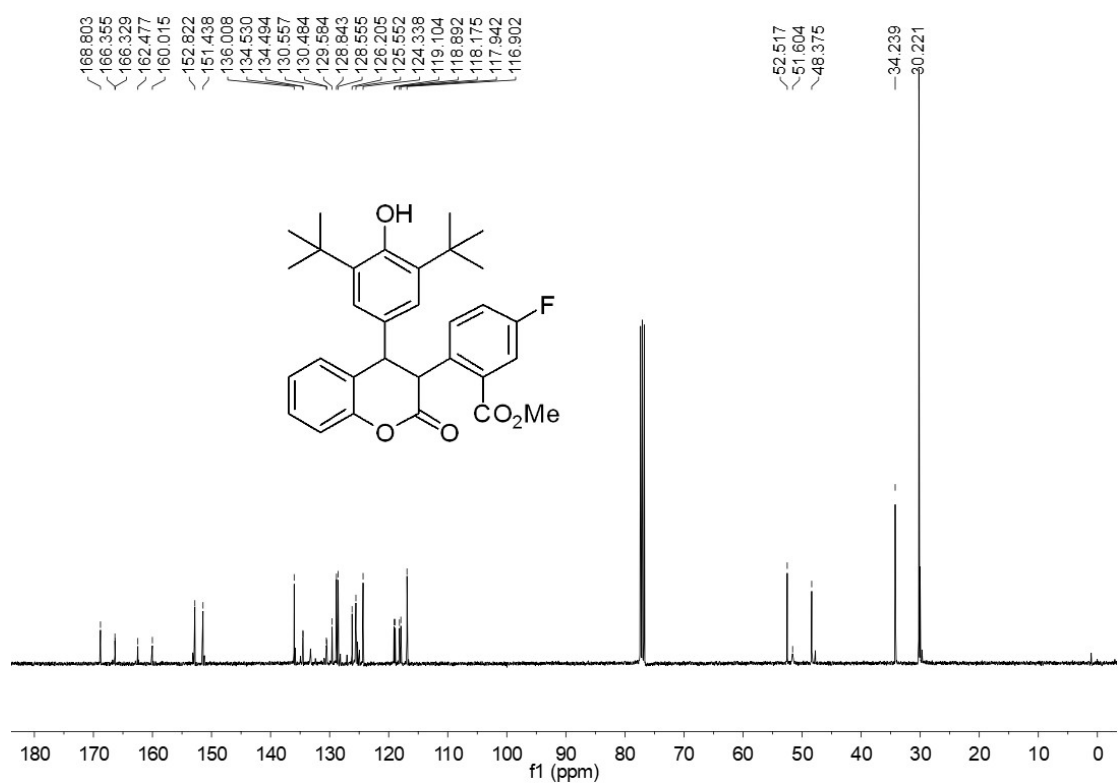
¹³C NMR of compound **3ac** (inseparable diastereomers with 91:9 dr)



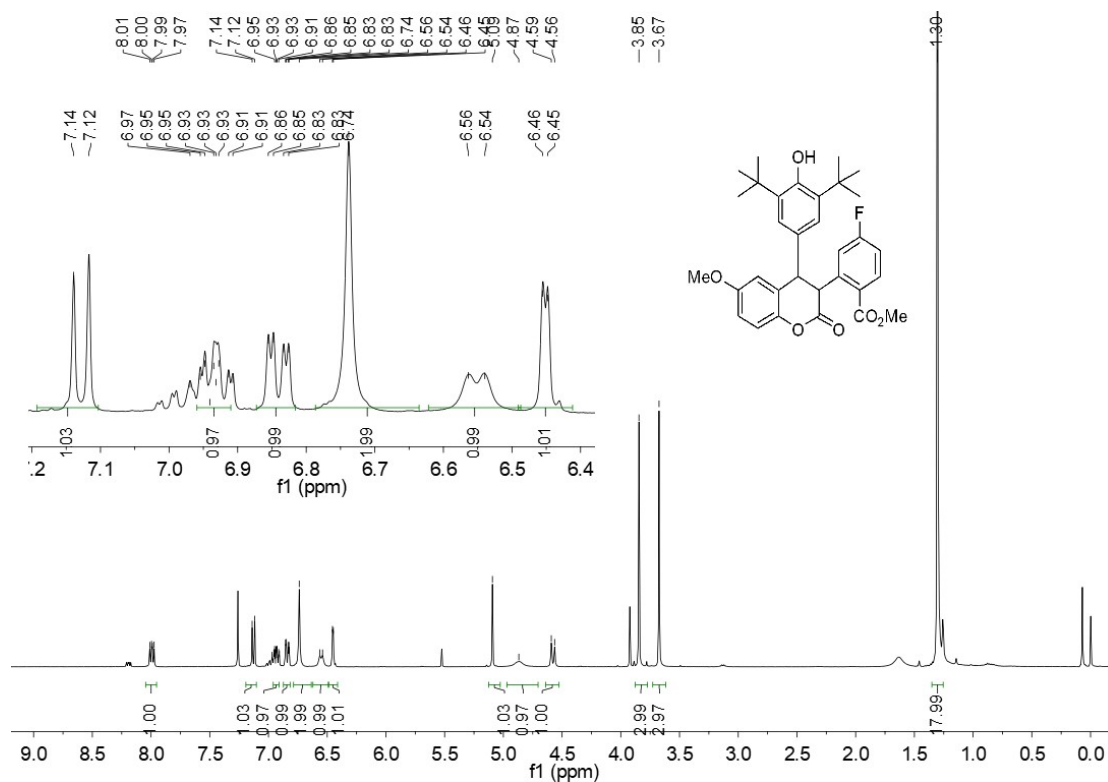
¹H NMR of compound **3ad** (inseparable diastereomers with 85:15 dr)



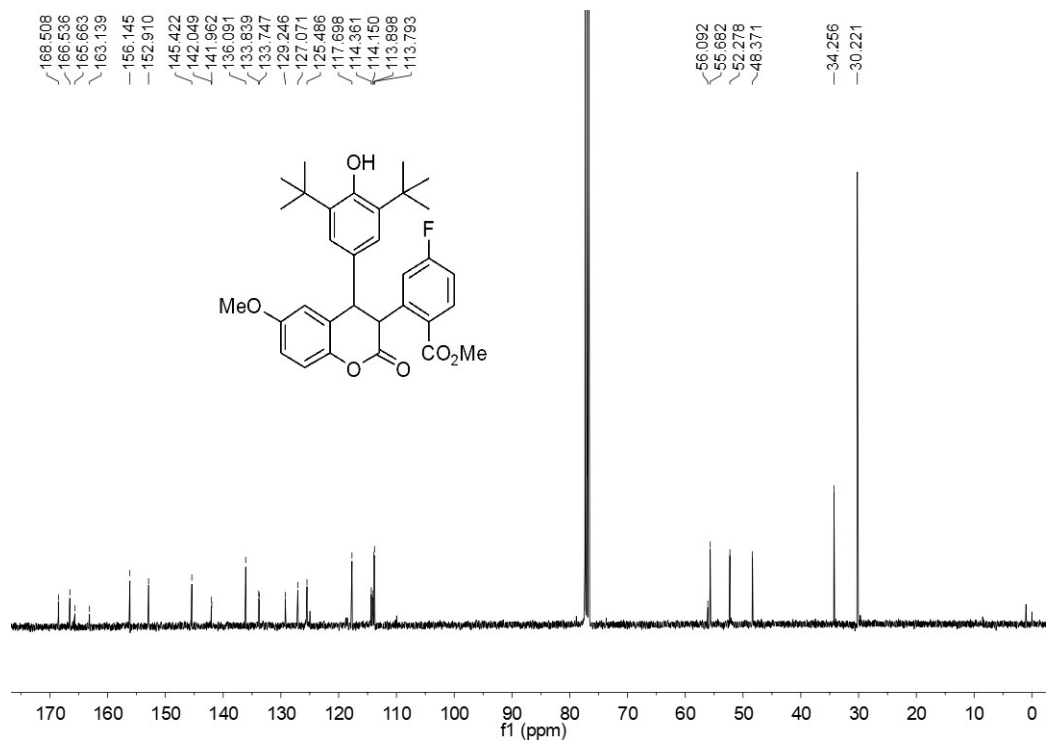
¹³C NMR of compound **3ad** (inseparable diastereomers with 85:15 dr)



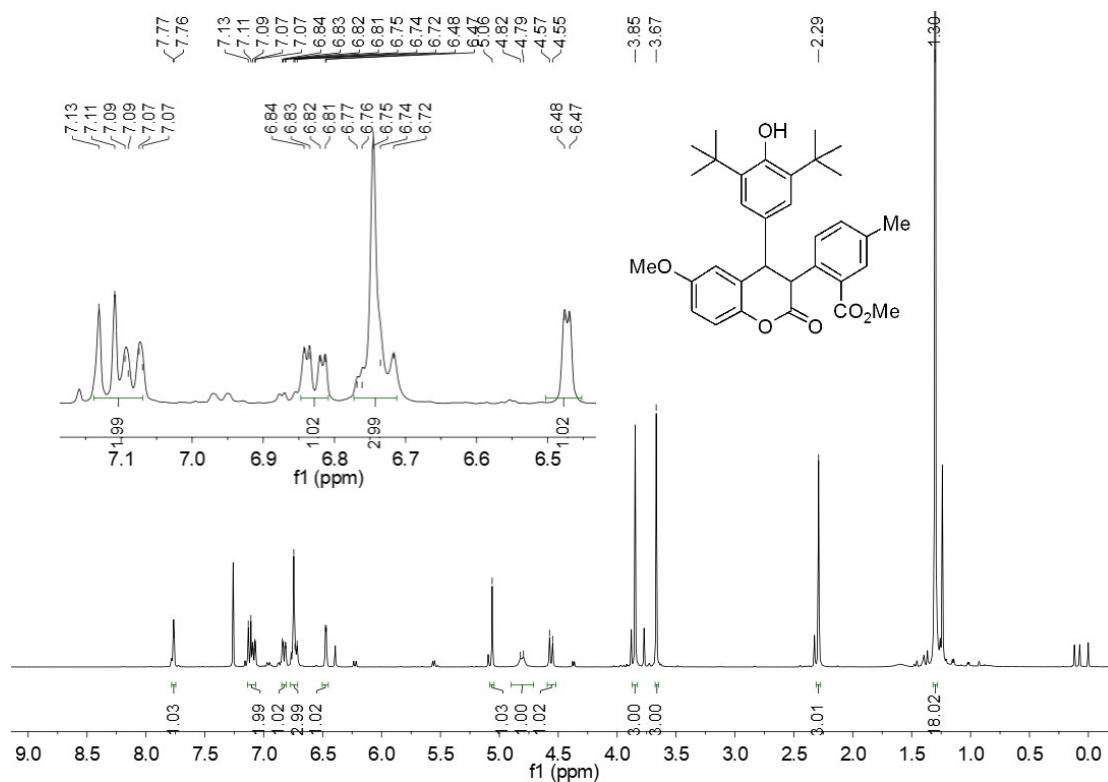
^1H NMR of compound **3fb** (inseparable diastereomers with 83:17 dr)



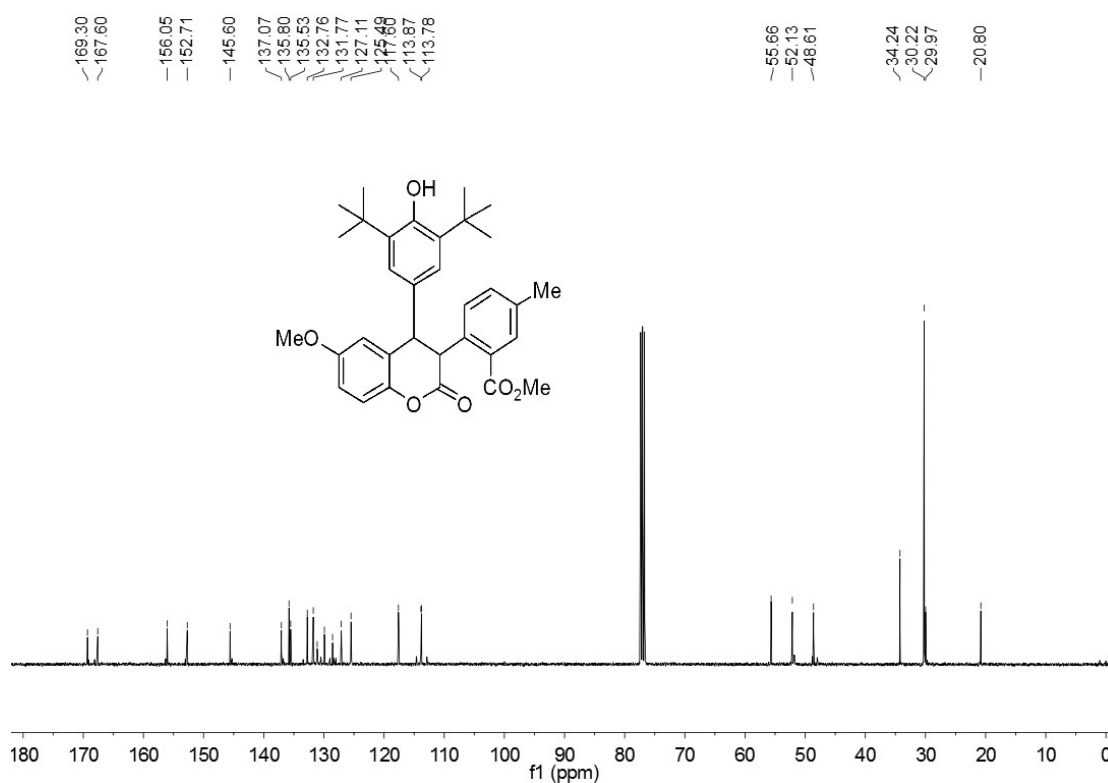
^{13}C NMR of compound **3fb** (inseparable diastereomers with 83:17 dr)



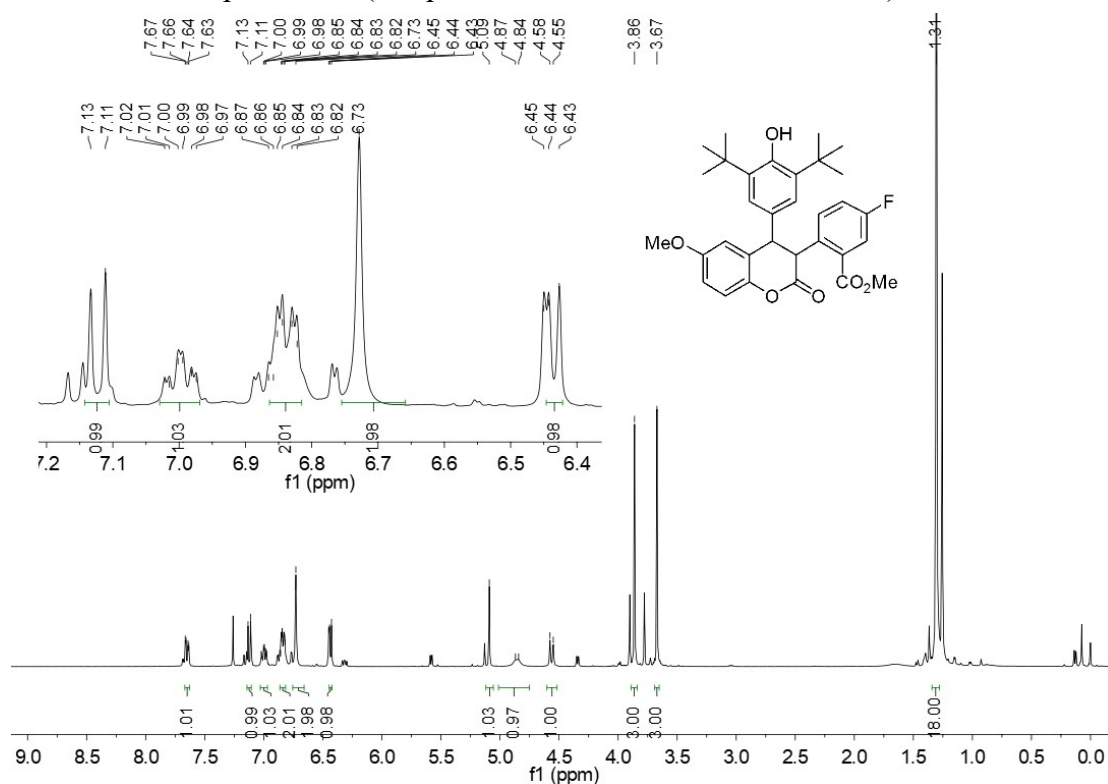
¹H NMR of compound **3fc** (inseparable diastereomers with 87:13 dr)



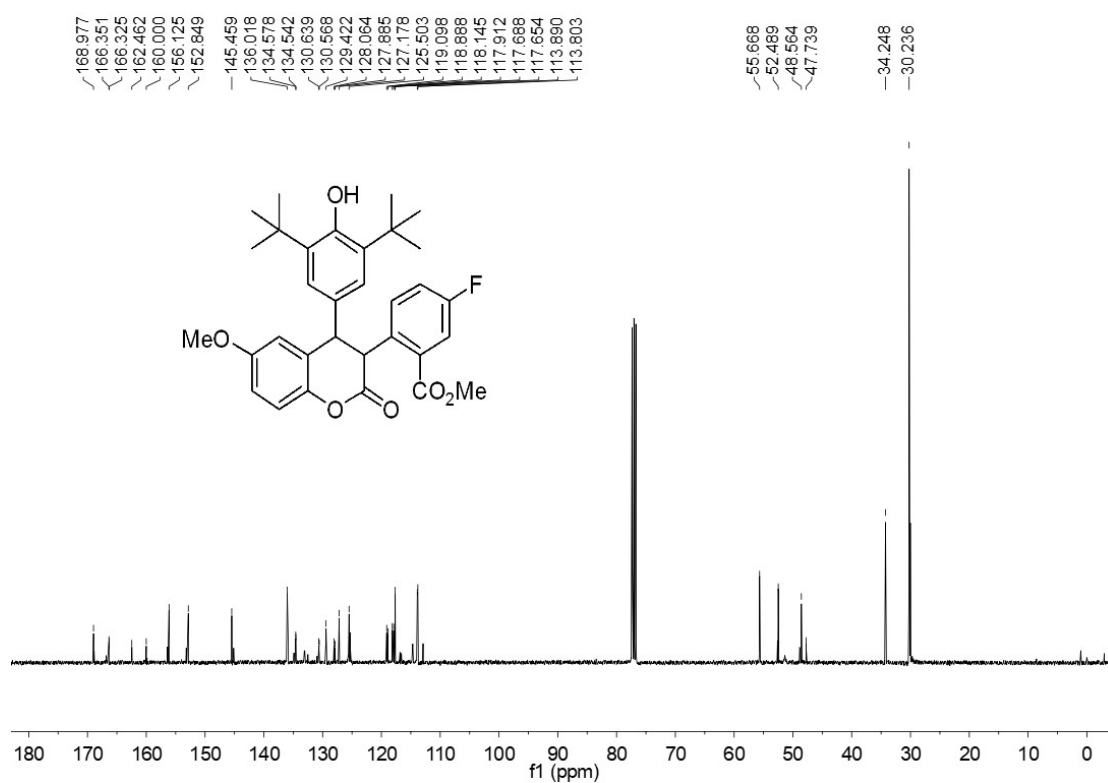
¹³C NMR of compound **3fc** (inseparable diastereomers with 87:13 dr)



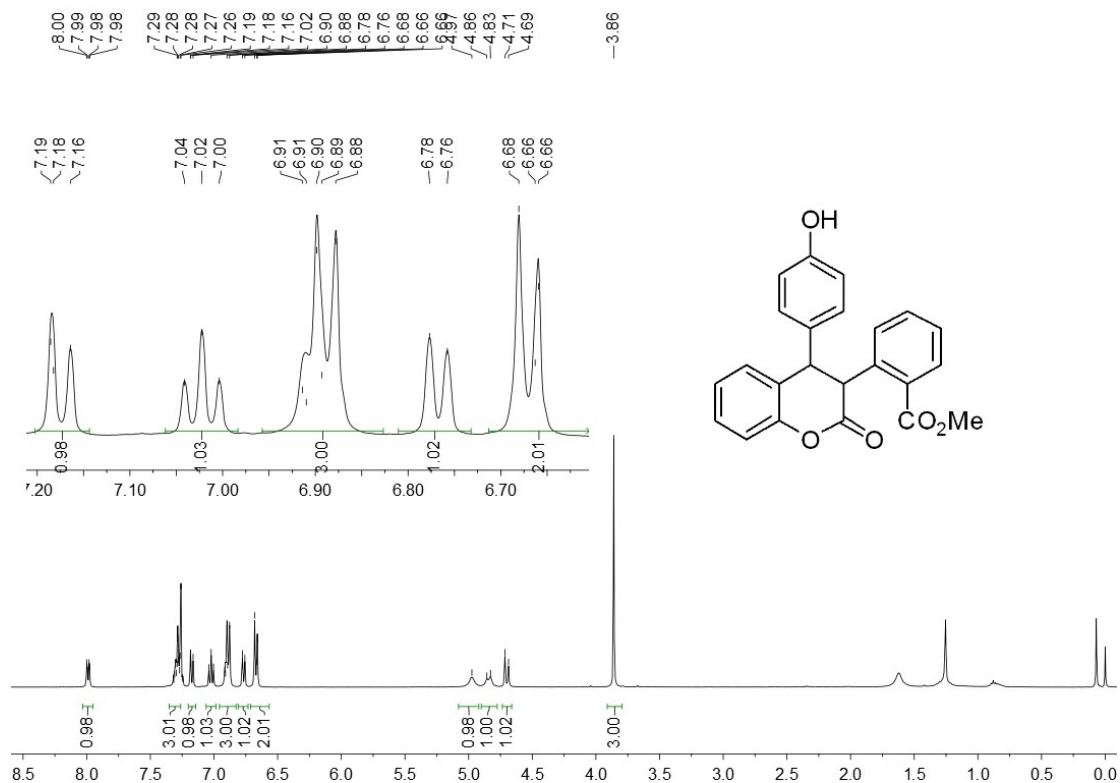
¹H NMR of compound **3fd** (inseparable diastereomers with 77:23 dr)



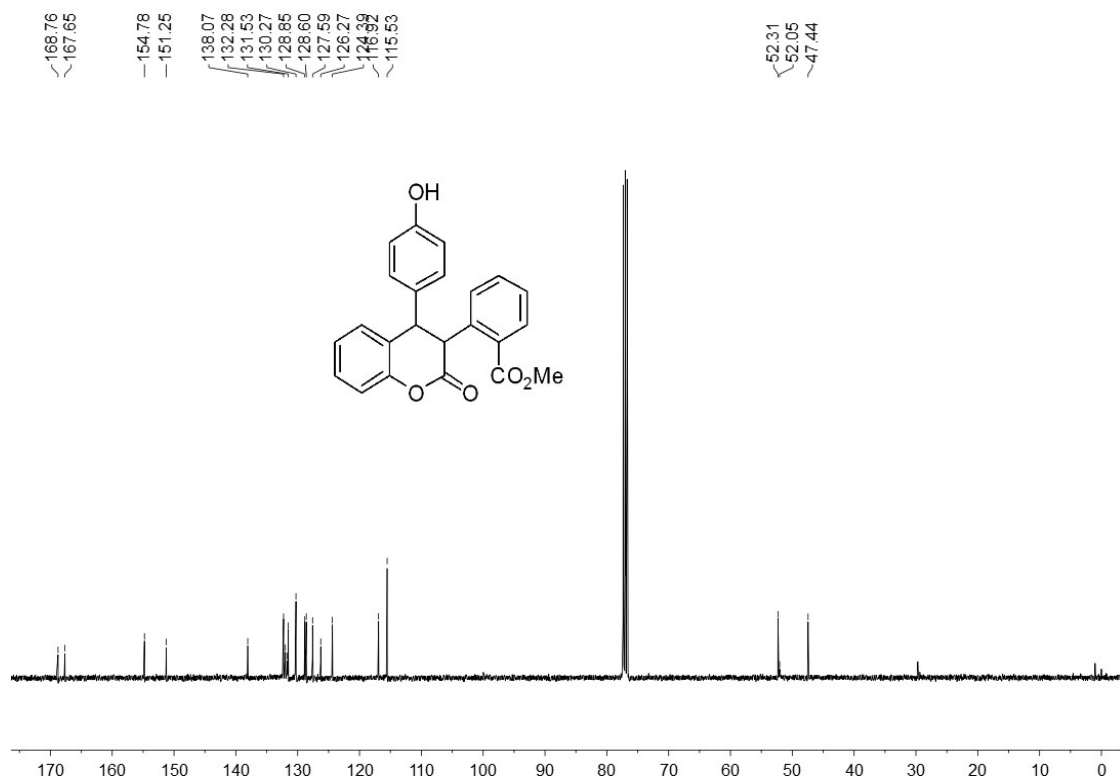
¹³C NMR of compound **3fd** (inseparable diastereomers with 77:23 dr)



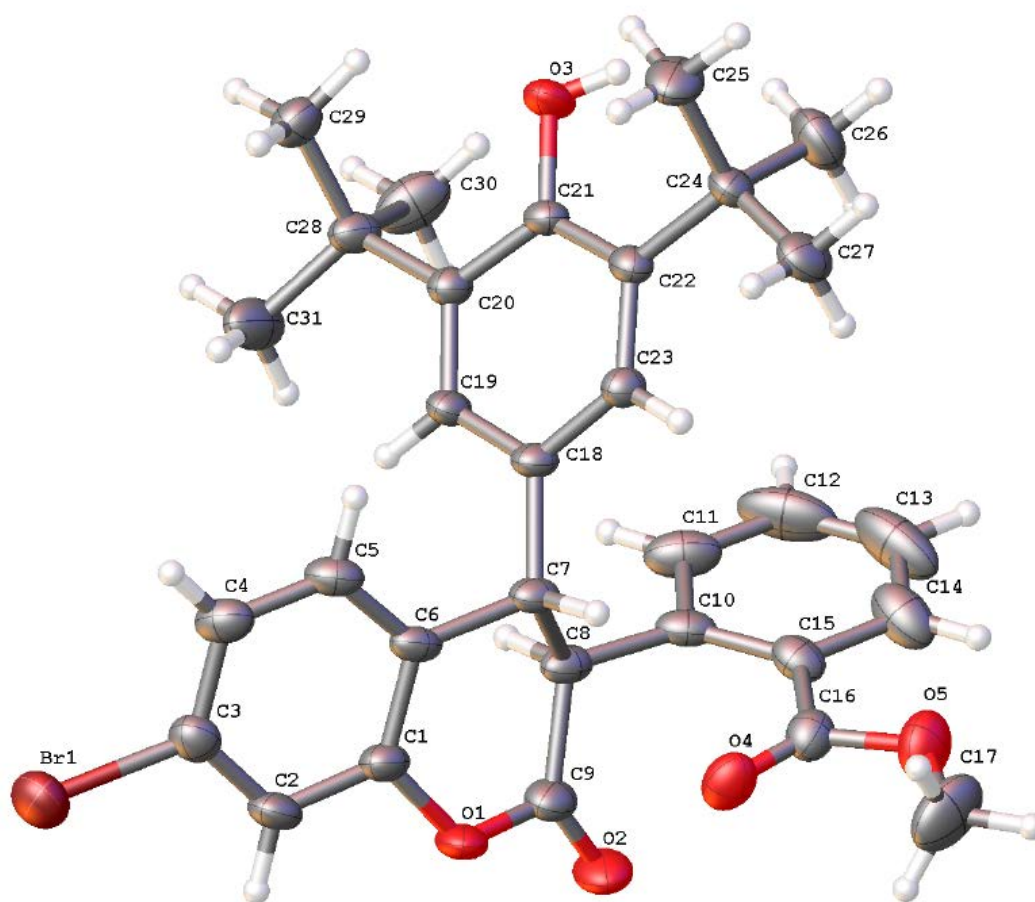
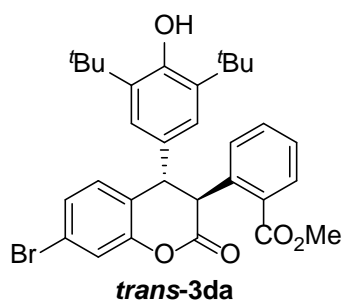
¹H NMR of compound 4



¹³C NMR of compound 4



2. X-ray single crystal data for compound 3da



The thermal ellipsoid was drawn at the 30% probability level.

Empirical formula	C ₃₁ H ₃₃ Br O ₅	
Formula weight	565.48	
Temperature	296.15 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.1745(11) Å	α = 85.634(2)°.
	b = 11.3873(13) Å	β = 82.125(2)°.

	$c = 12.2870(14) \text{ \AA}$	$\gamma = 86.327(2)^\circ$.
Volume	$1404.0(3) \text{ \AA}^3$	
Z	2	
Density (calculated)	1.338 Mg/m^3	
Absorption coefficient	1.501 mm^{-1}	
F(000)	588	
Crystal size	$0.5 \times 0.3 \times 0.3 \text{ mm}^3$	
Theta range for data collection	2.451 to 26.371° .	
Index ranges	$-9 \leq h \leq 12$, $-12 \leq k \leq 14$, $-15 \leq l \leq 13$	
Reflections collected	7863	
Independent reflections	5602 [$R(\text{int}) = 0.0169$]	
Completeness to $\theta = 25.242^\circ$	98.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6451	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5602 / 1 / 341	
Goodness-of-fit on F^2	1.010	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0447$, $wR2 = 0.1012$	
R indices (all data)	$R1 = 0.0892$, $wR2 = 0.1172$	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.385 and $-0.447 \text{ e.\AA}^{-3}$	