

Supporting Information

Construction of Chiral Chroman Scaffolds via Catalytic Asymmetric (4+2) Cyclizations of *para*-Quinone Methide Derivatives with 3-Vinylindoles

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Yu-Chen Zhang^{a,*} and Feng Shi^{a,*}

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Medicinal Plants of Jiangsu Province, Jiangsu Normal University, Xuzhou, 221116, China*

^b*Department of Geriatric, the First Affiliated Hospital of Nanjing Medical University, Nanjing,
210029, China.*

E-mail: fshi@jsnu.edu.cn; zhangyc@jsnu.edu.cn; dhxnjmu@126.com

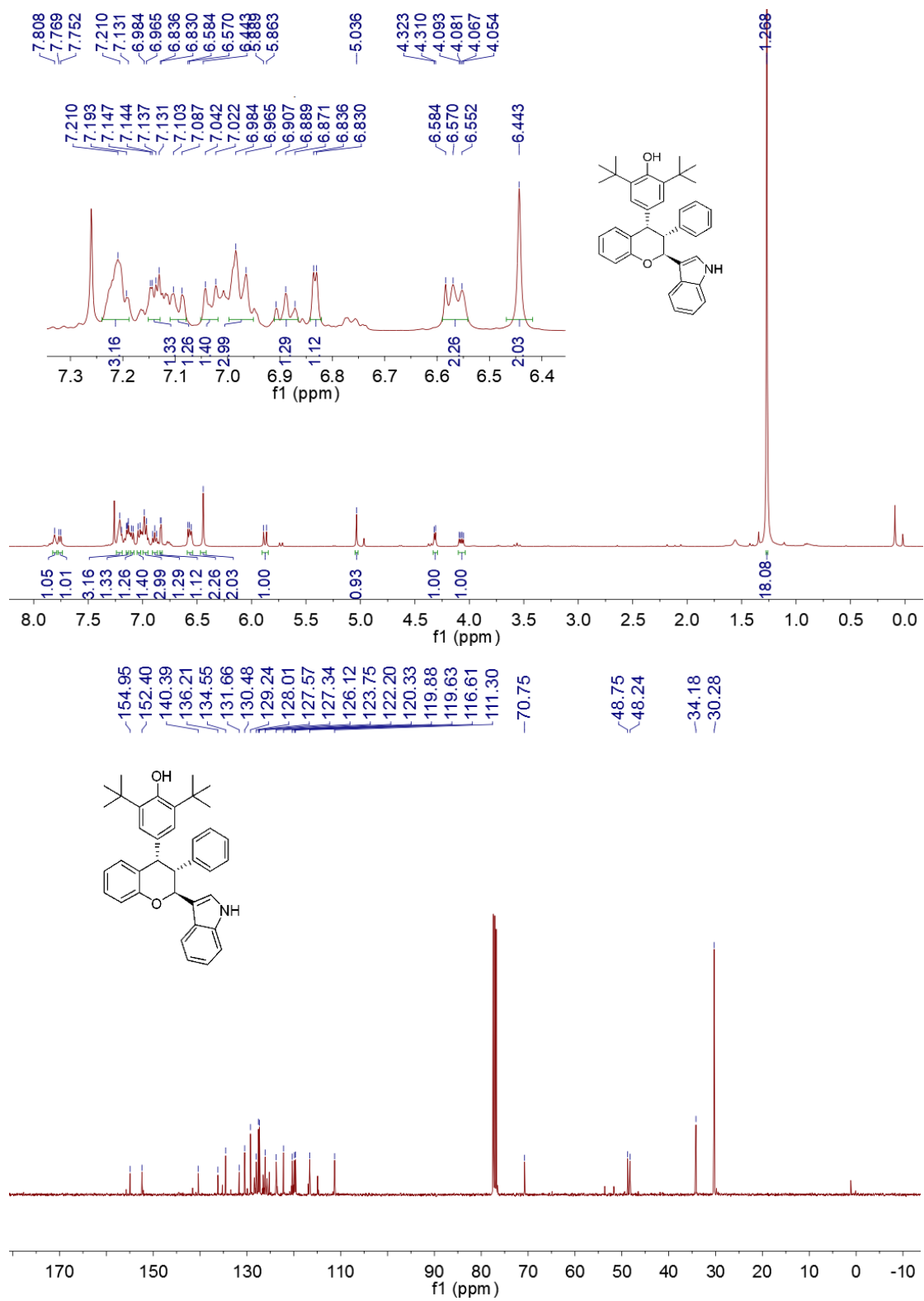
[‡]These authors contributed equally to the work.

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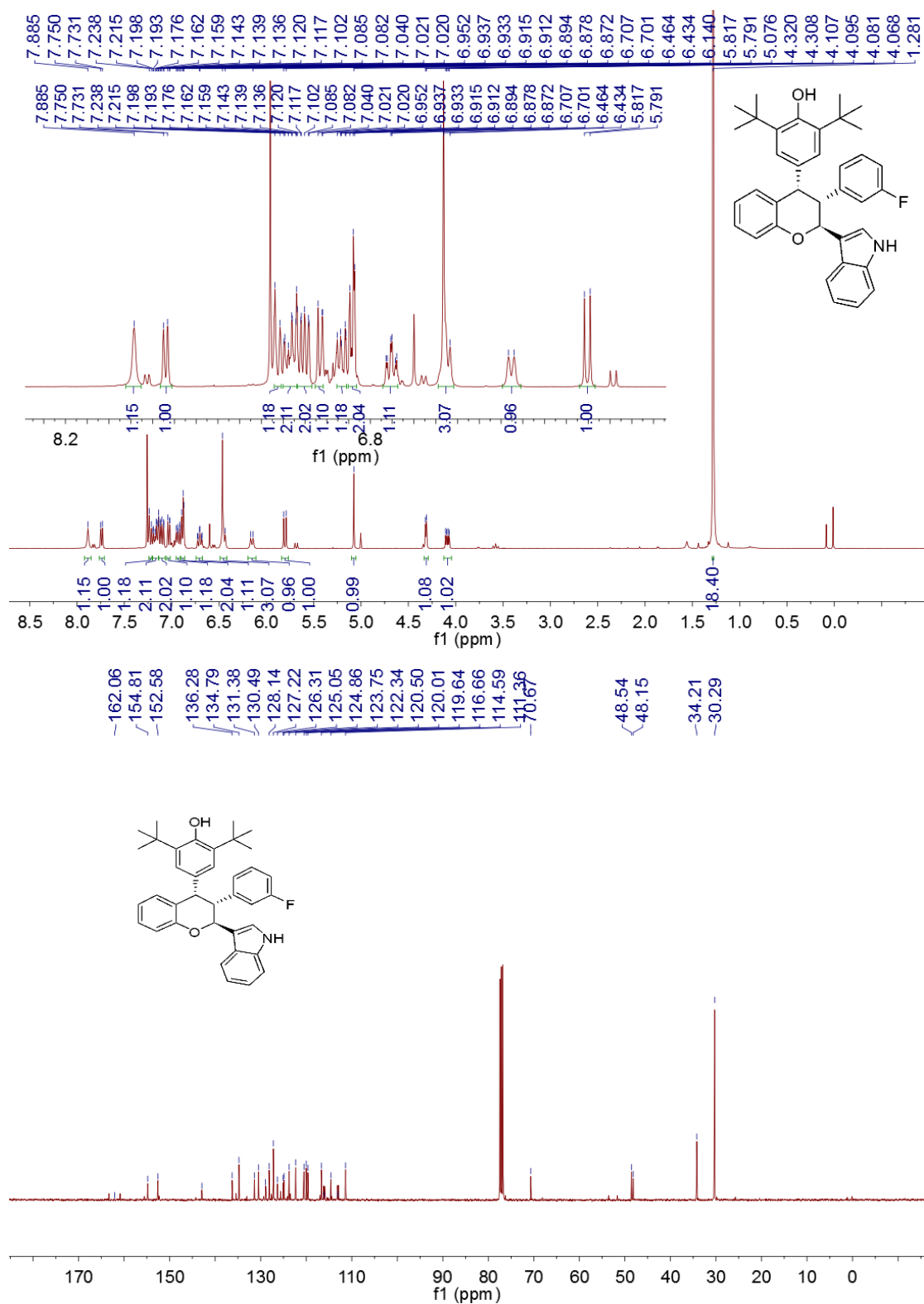
- 1. NMR spectra of products 3 (S2-S26)**
- 2. HPLC copies of products 3 (S27-S53)**
- 3. X-ray single crystal data for compound 3pf (S54-S55)**

1. NMR spectra of products 3

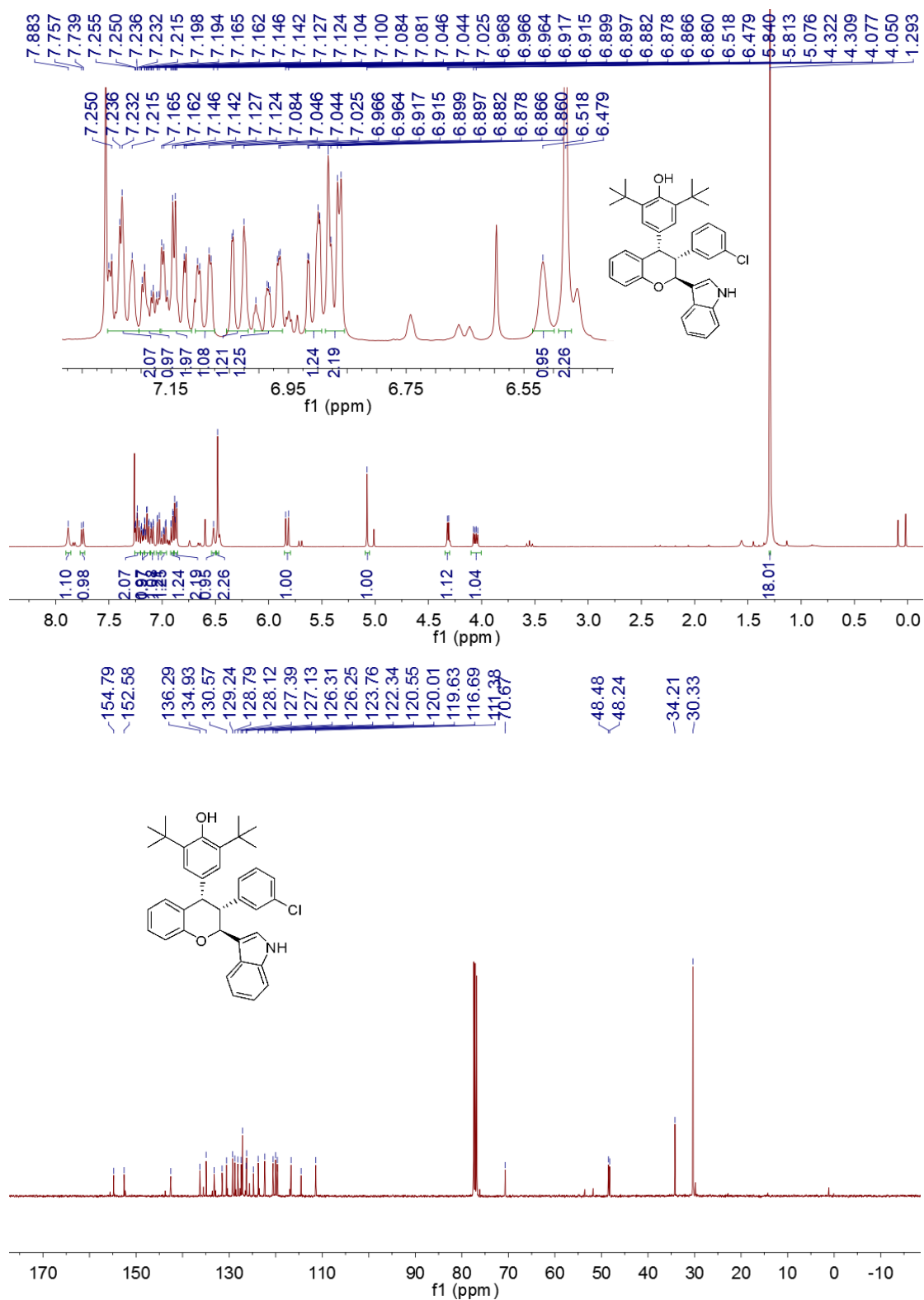
3aa: (inseparable diastereomers, 79:21 dr):



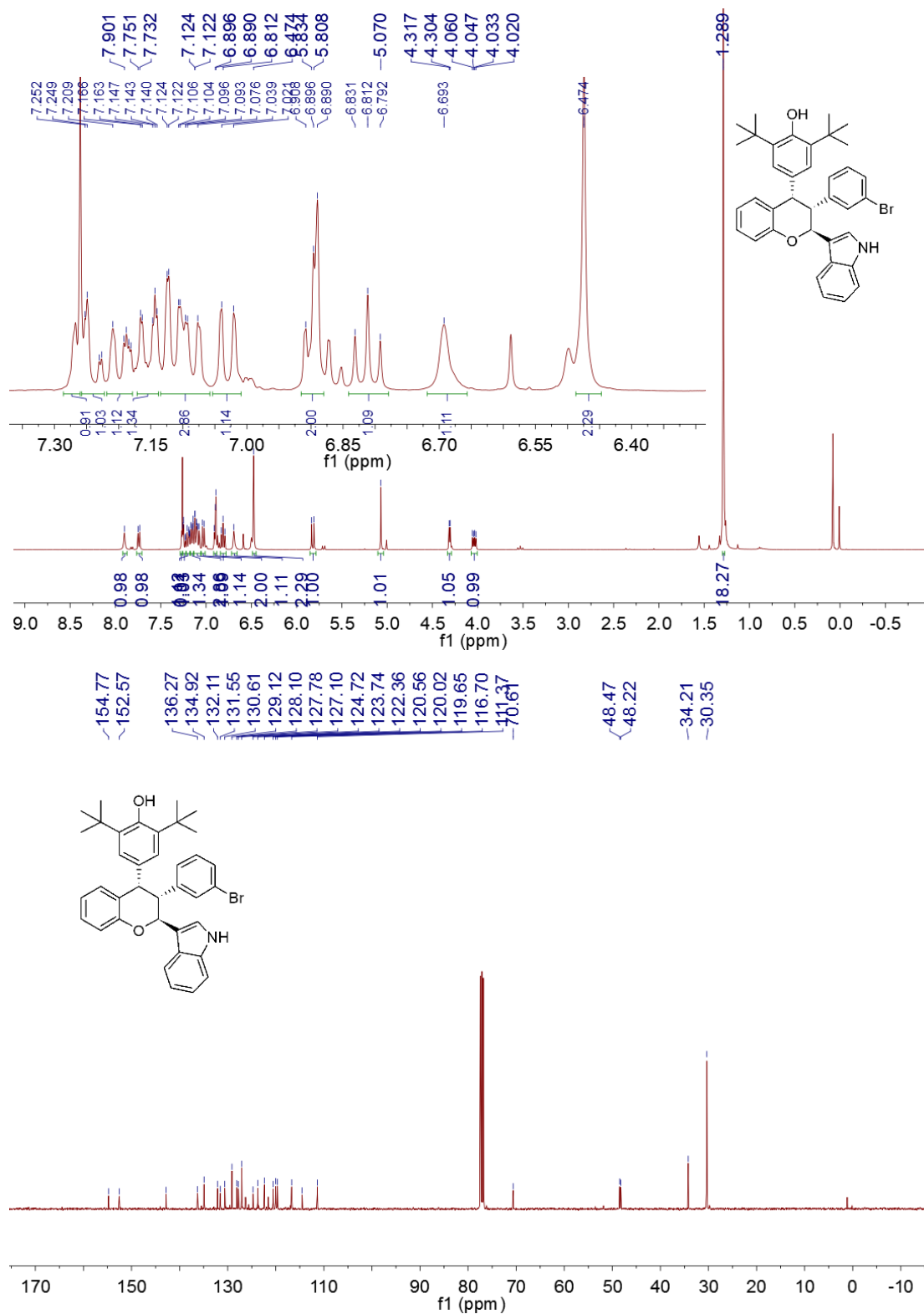
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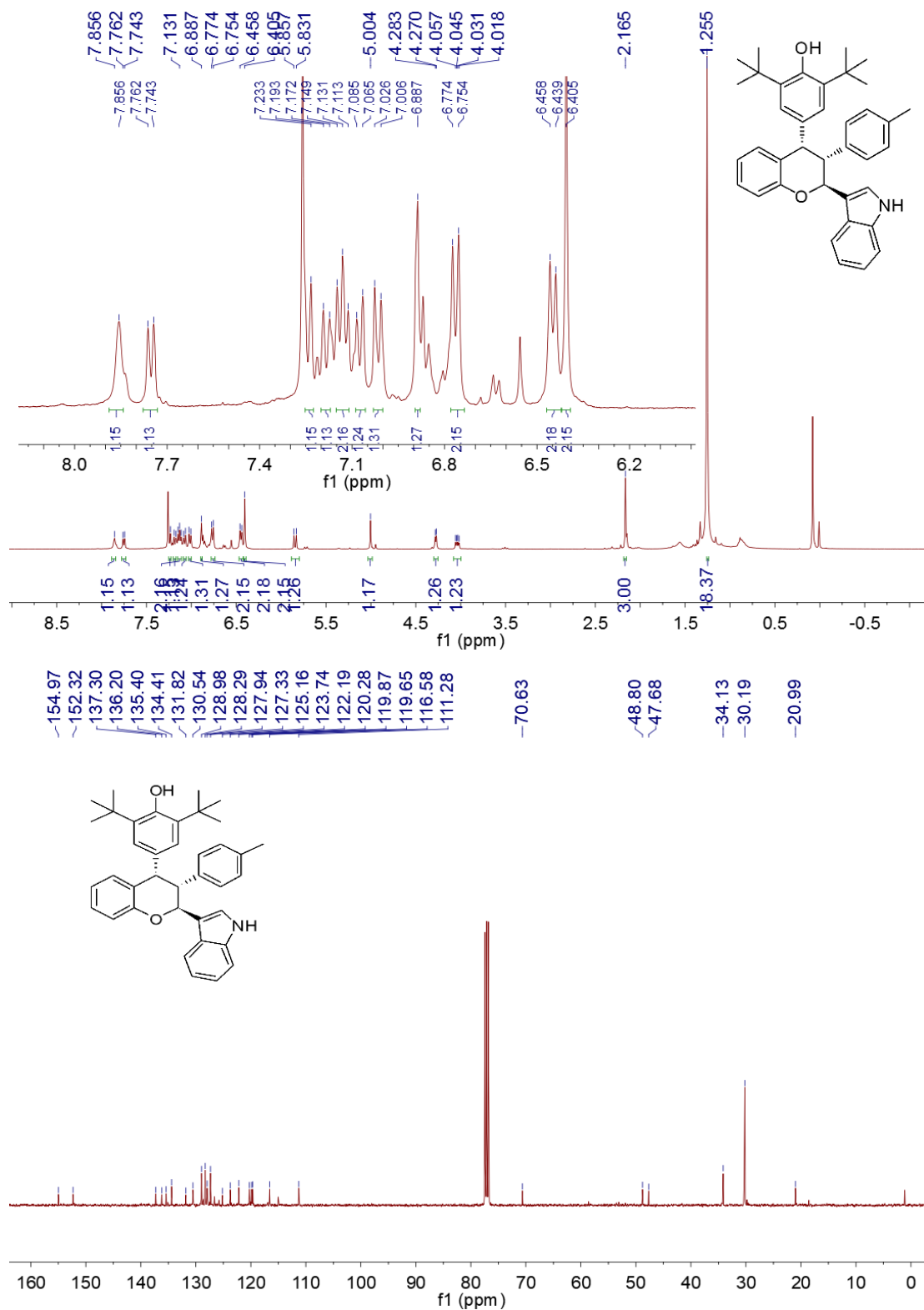
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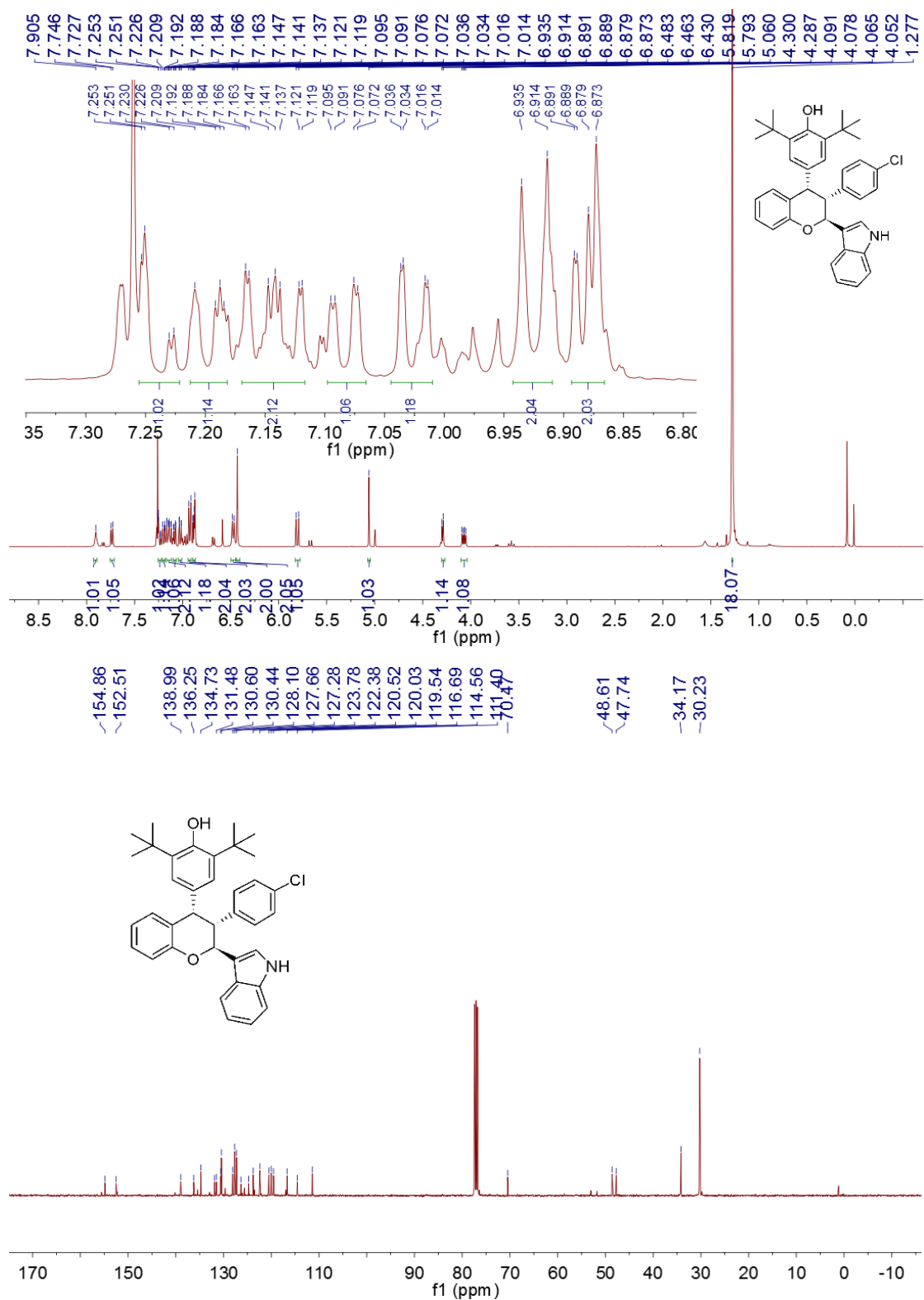
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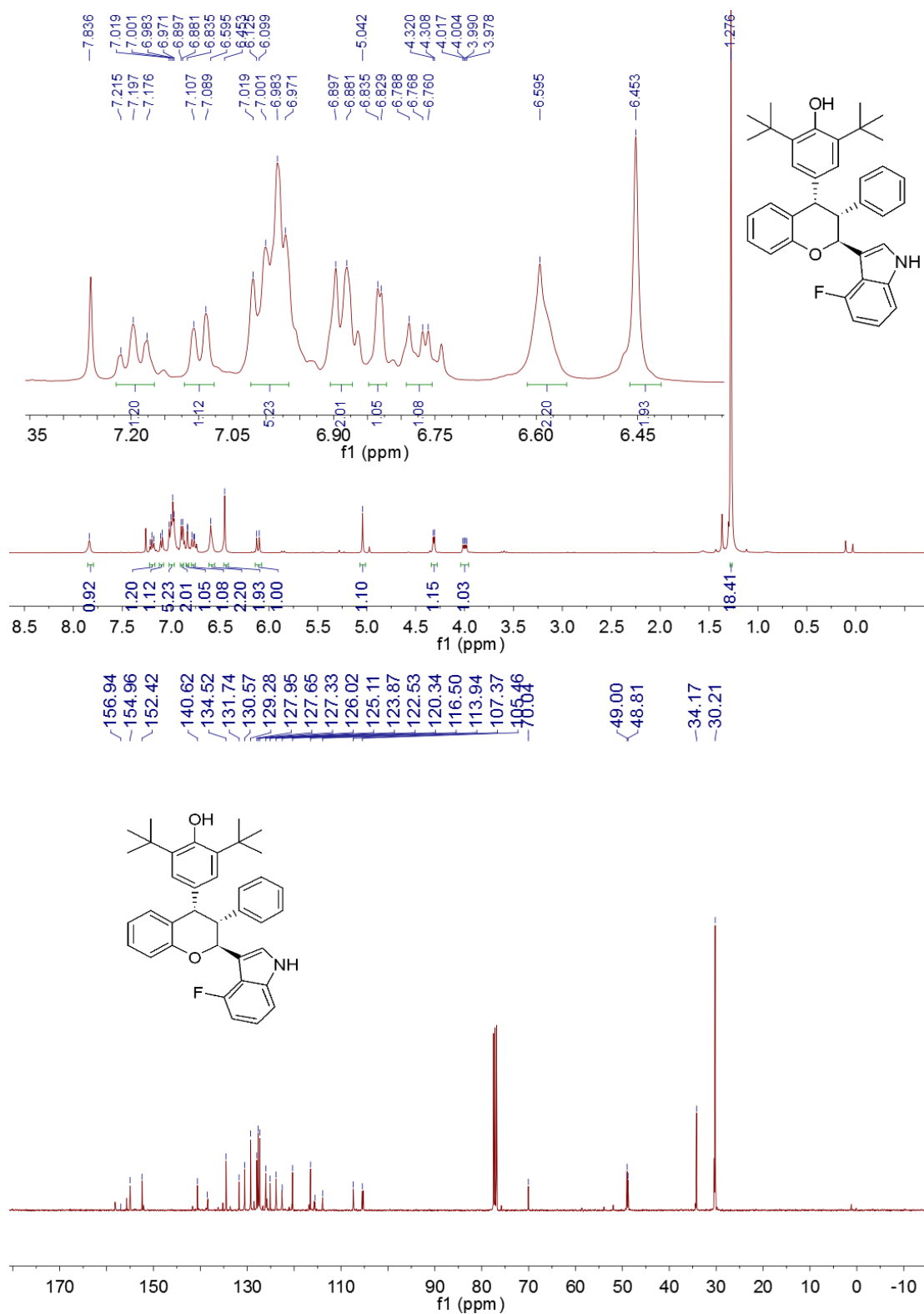
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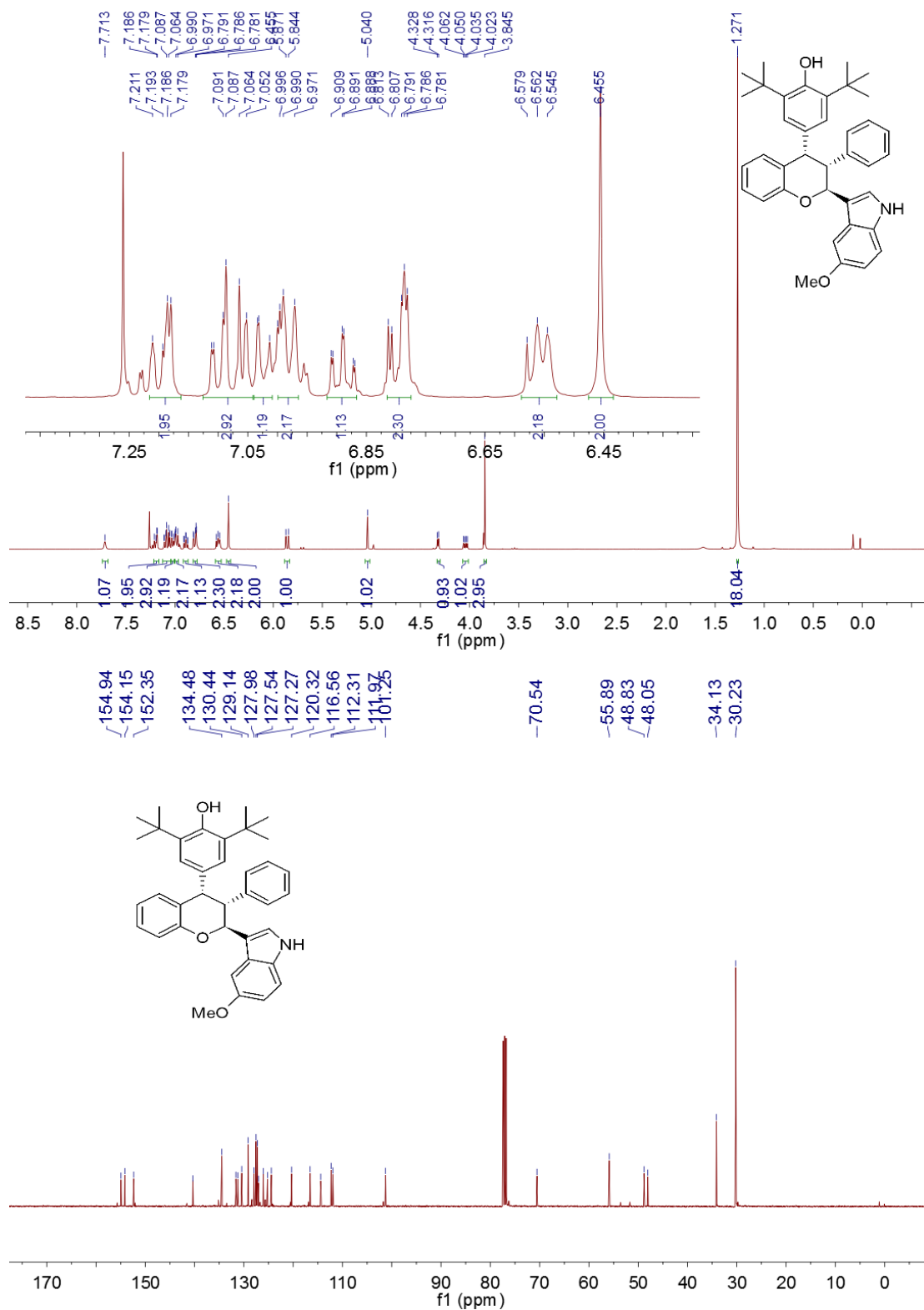
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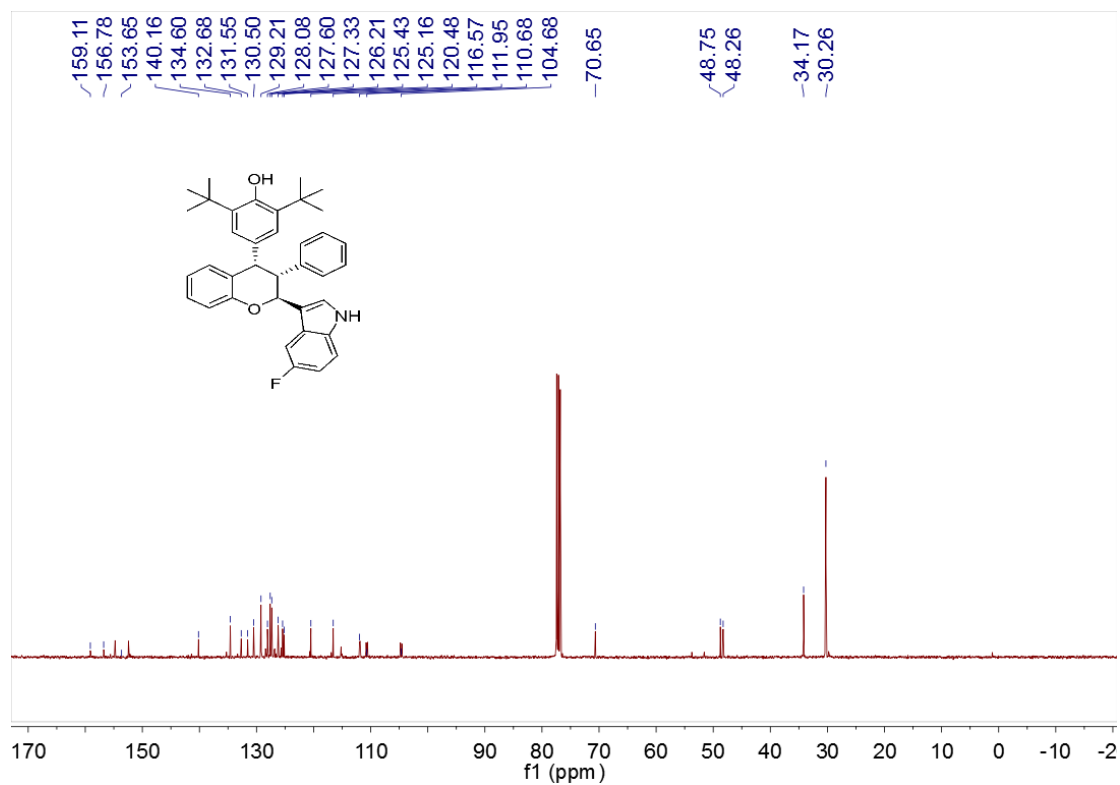
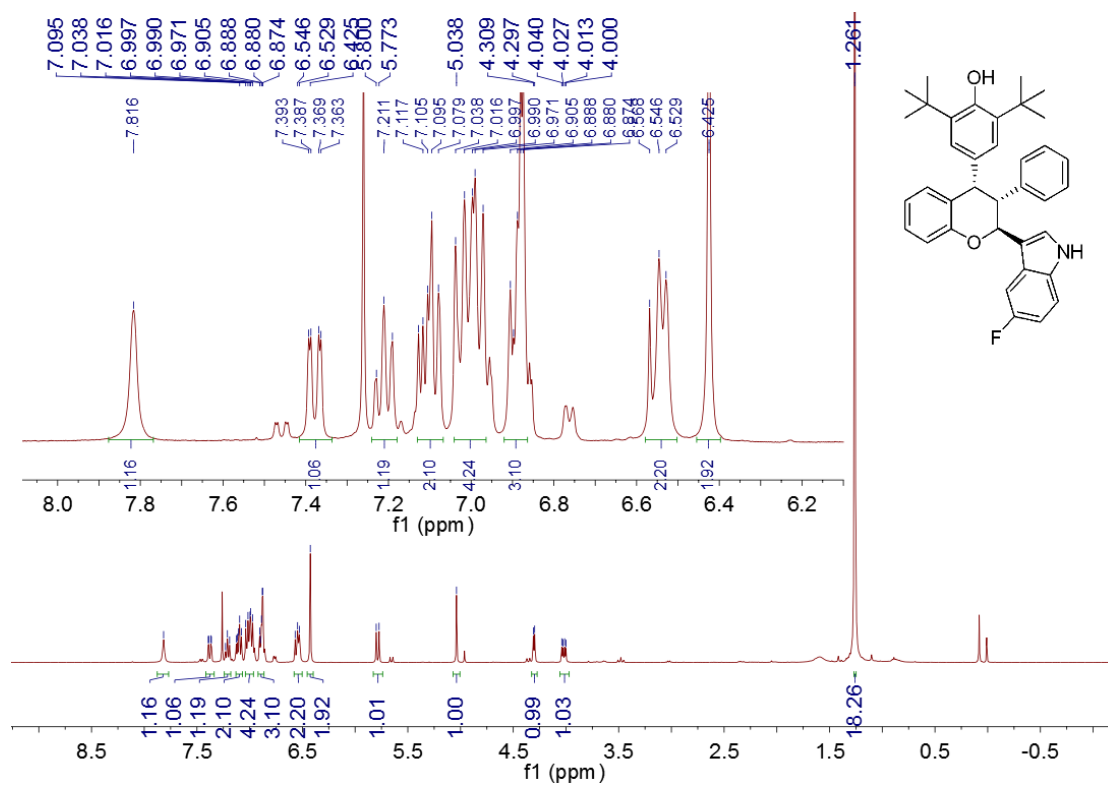
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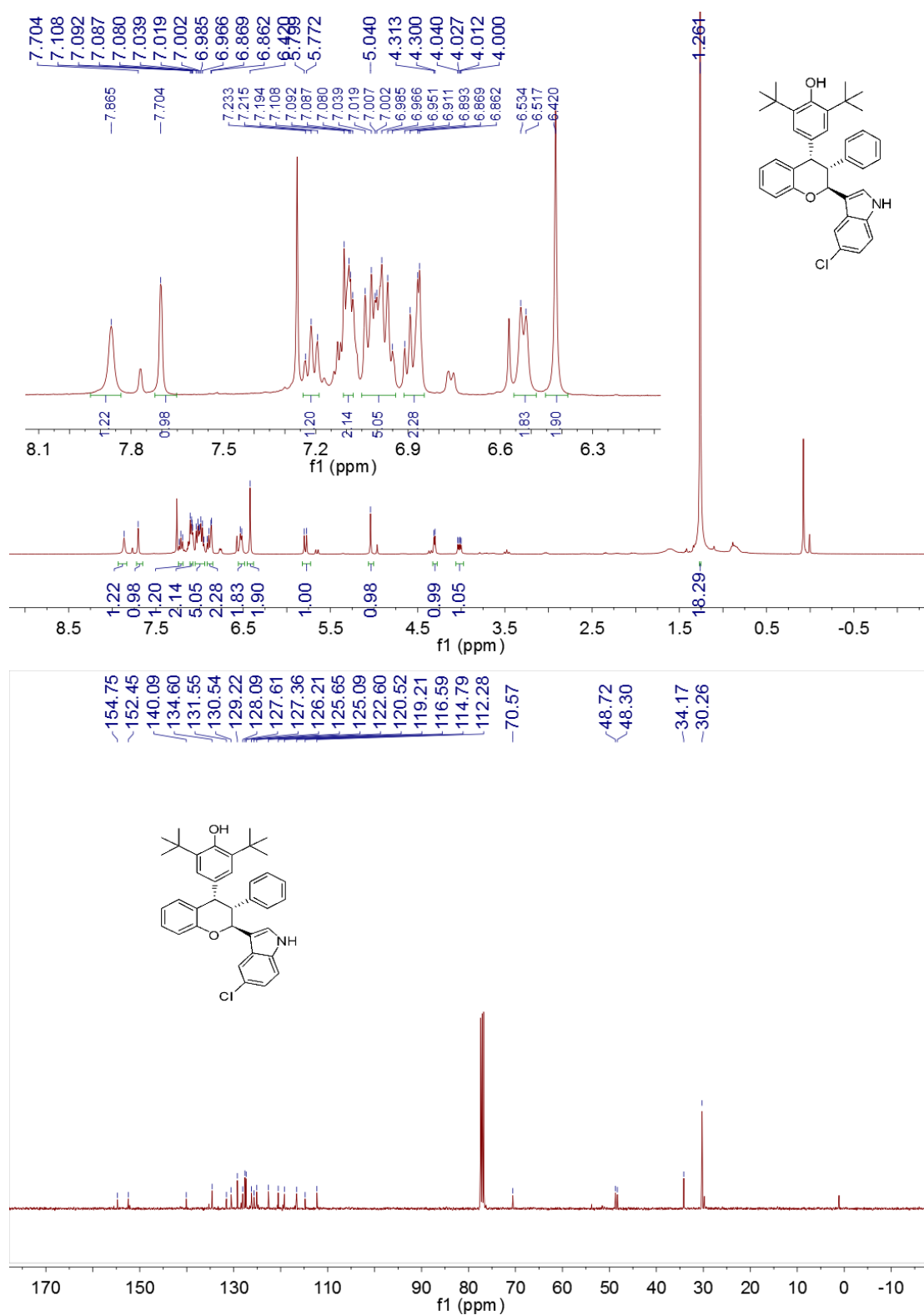
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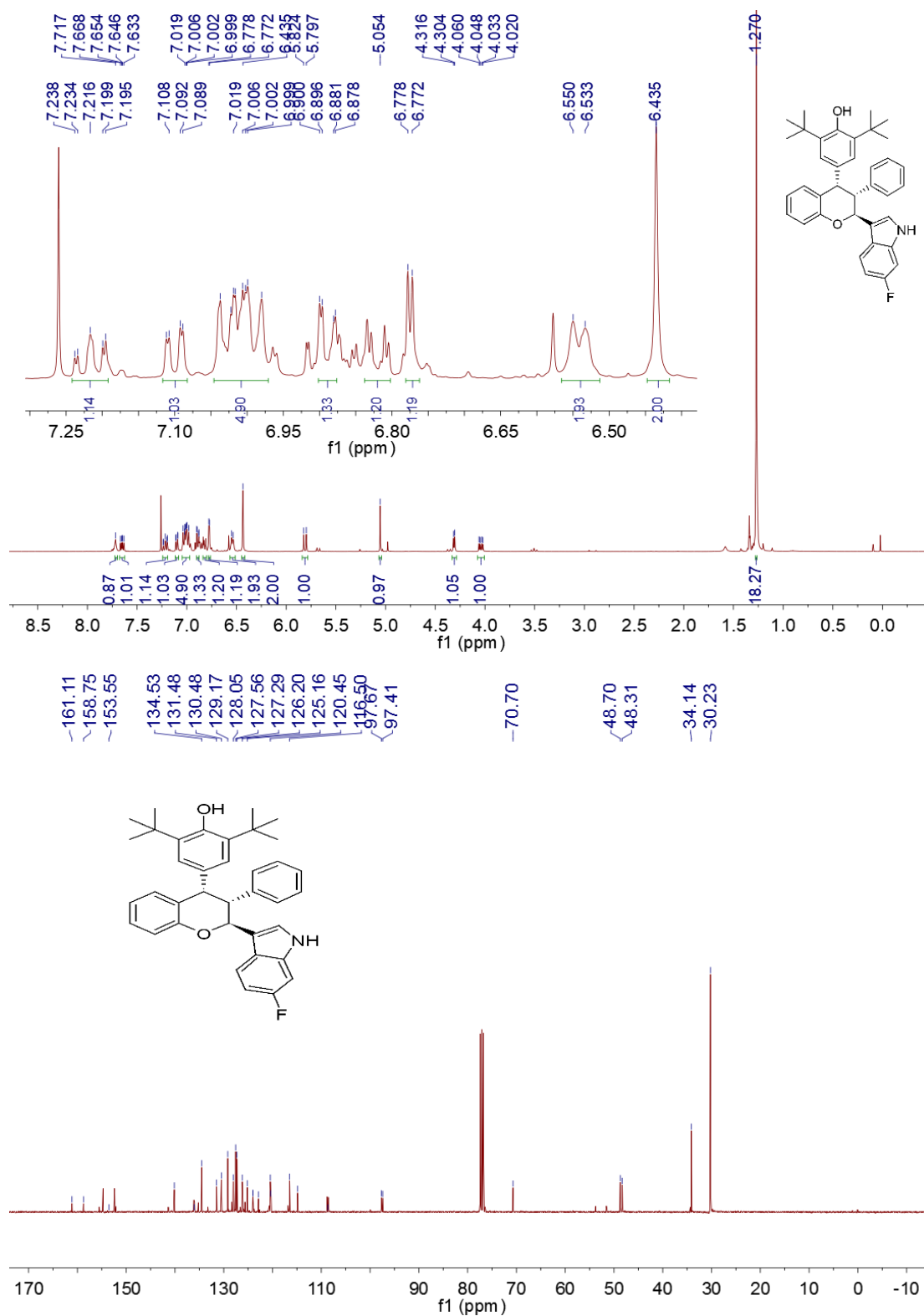
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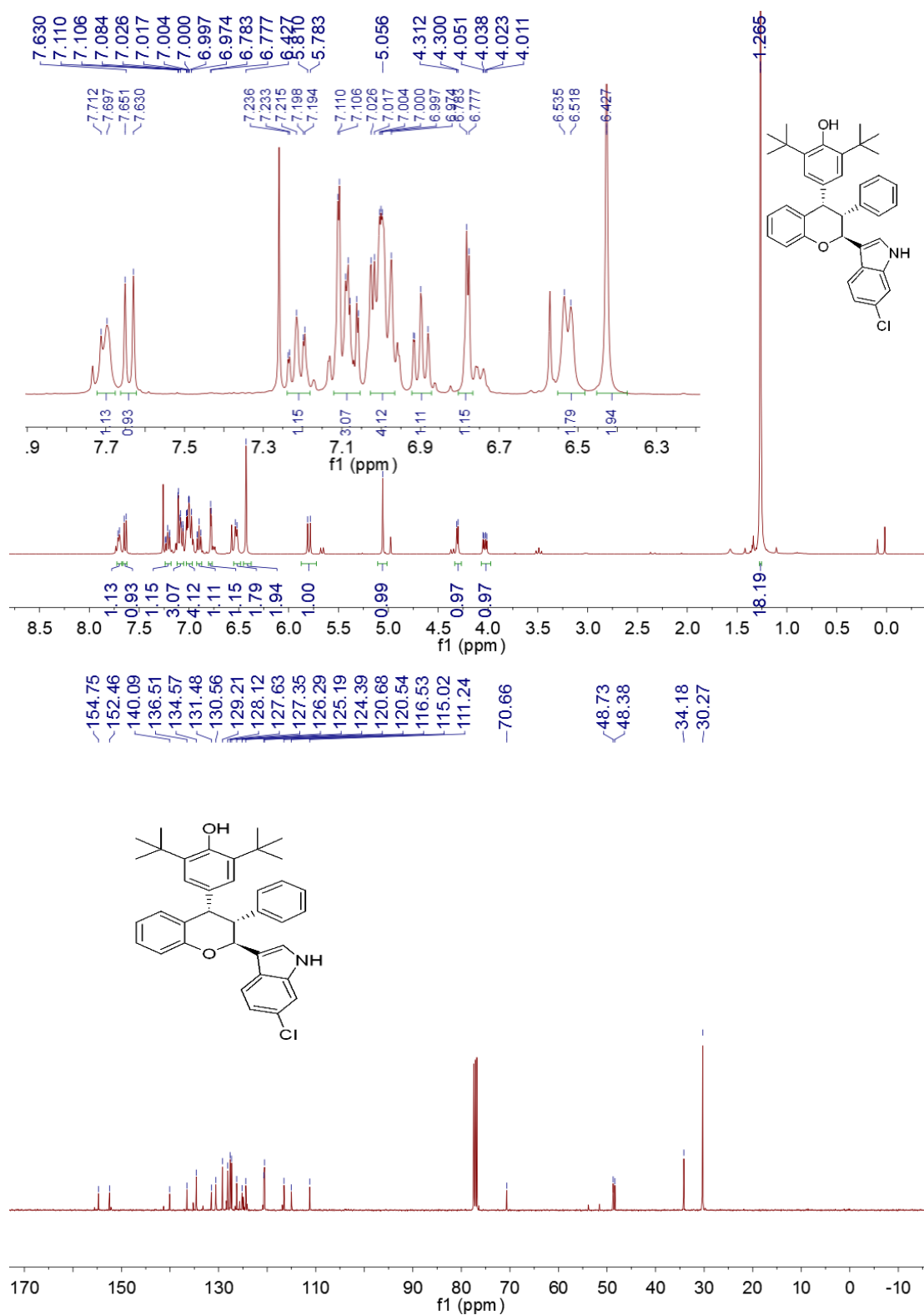
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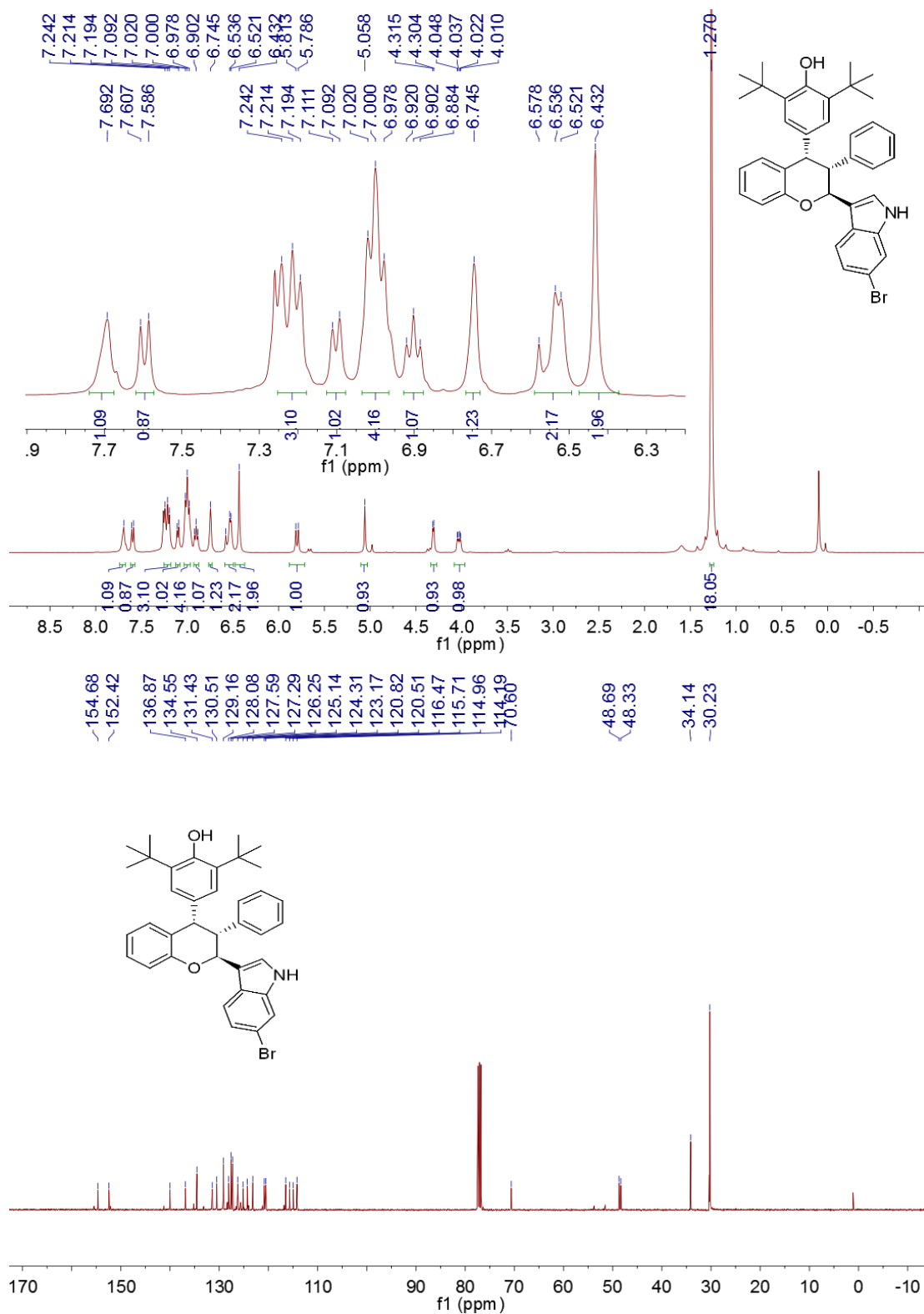
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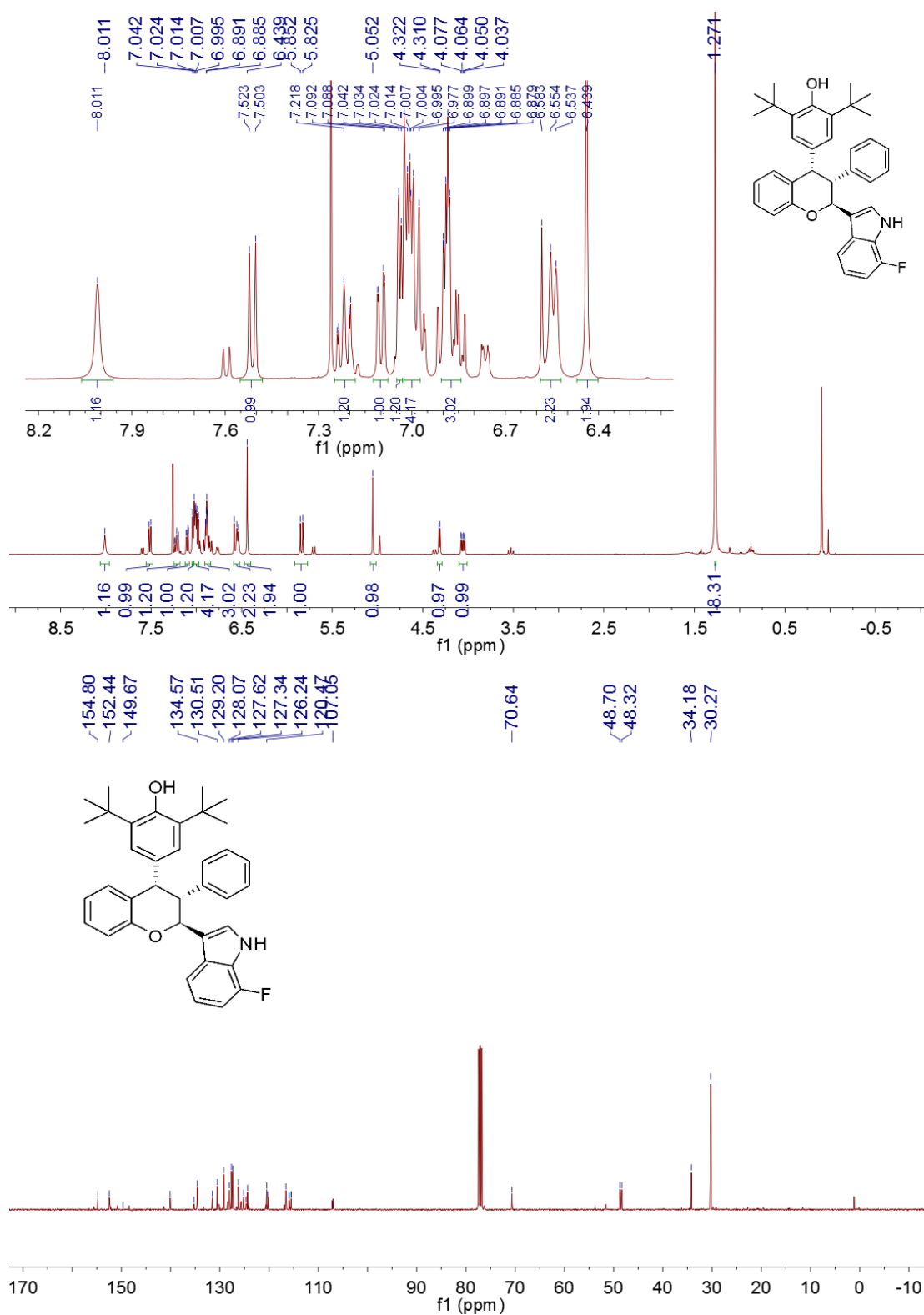
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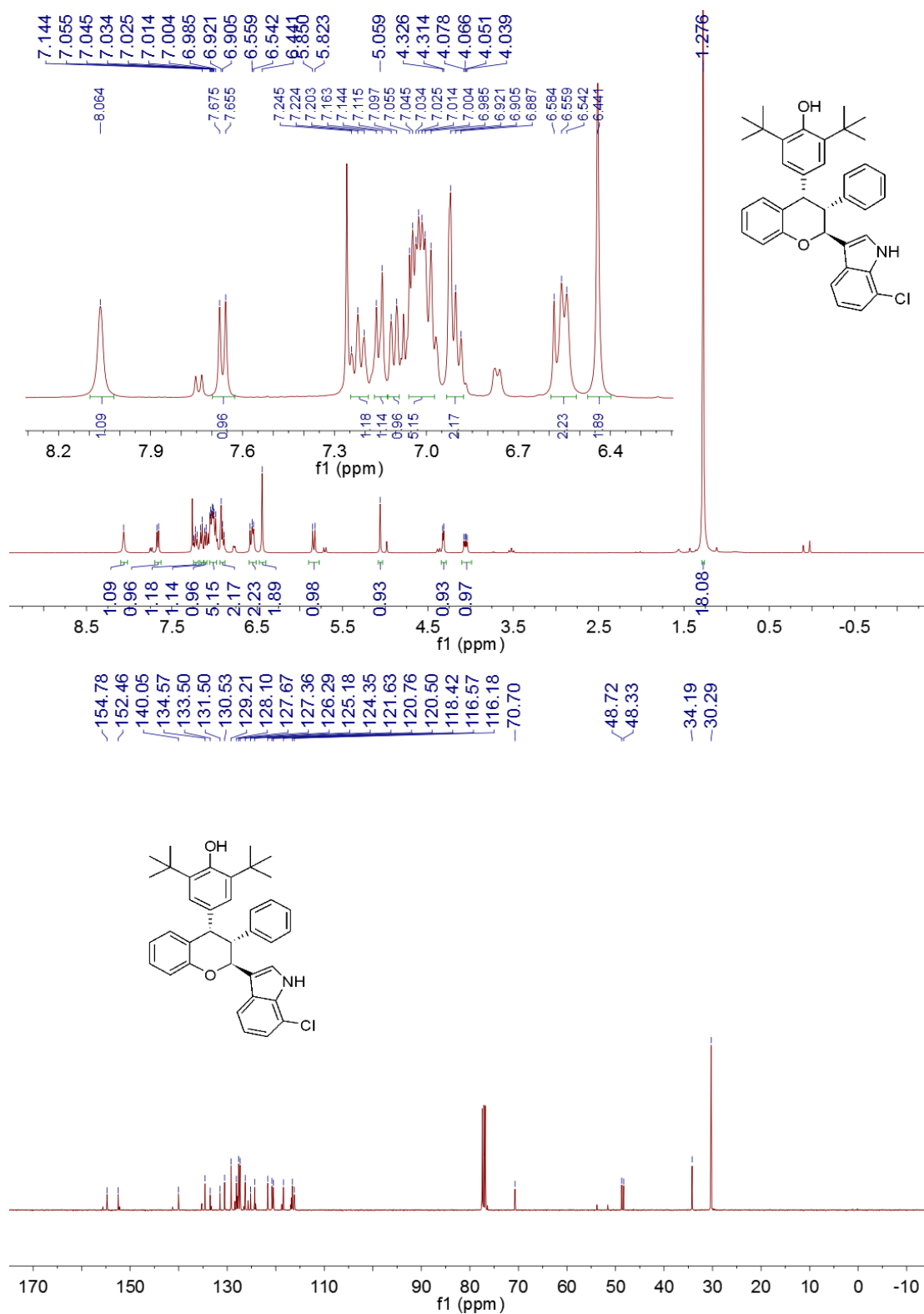
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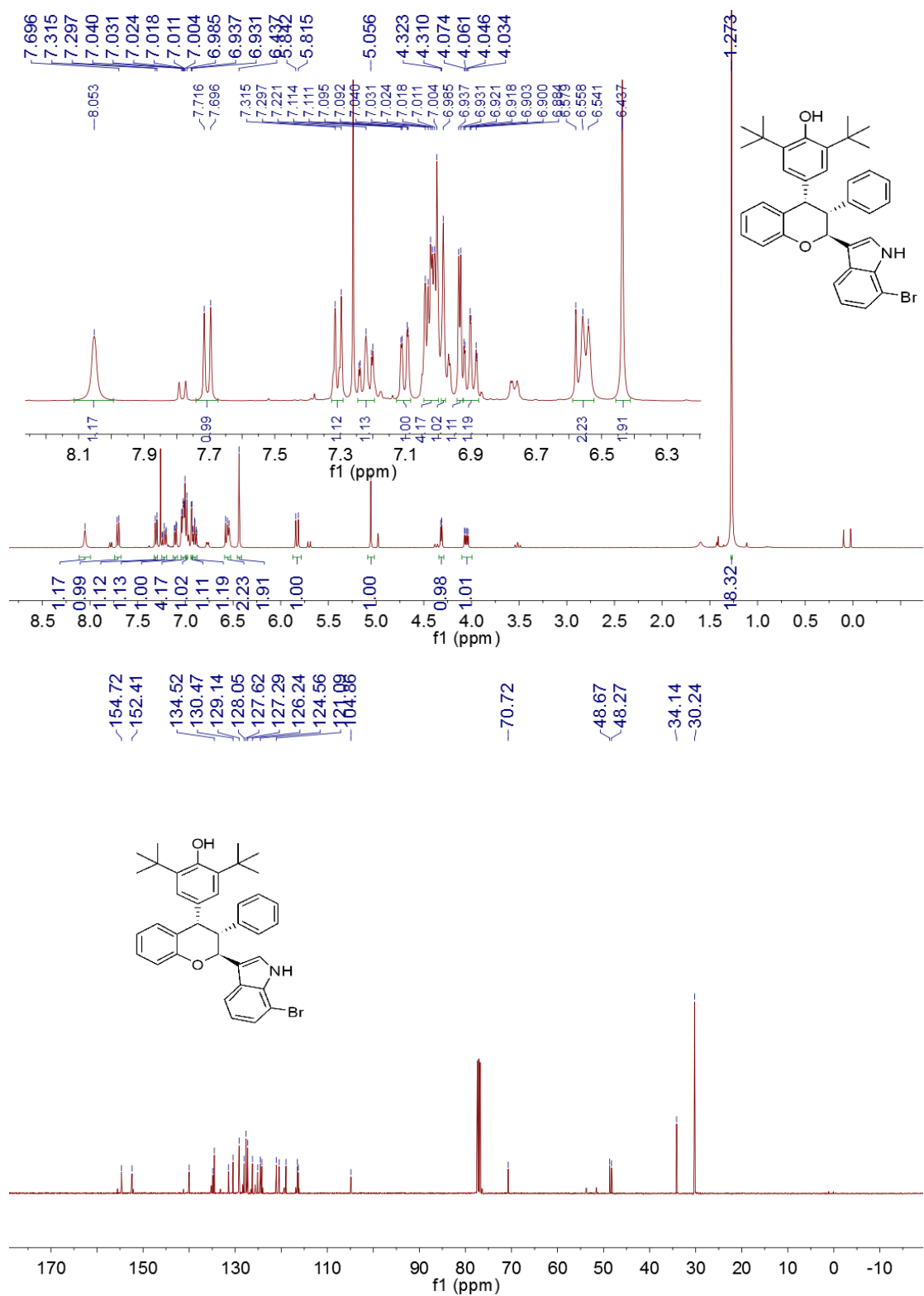
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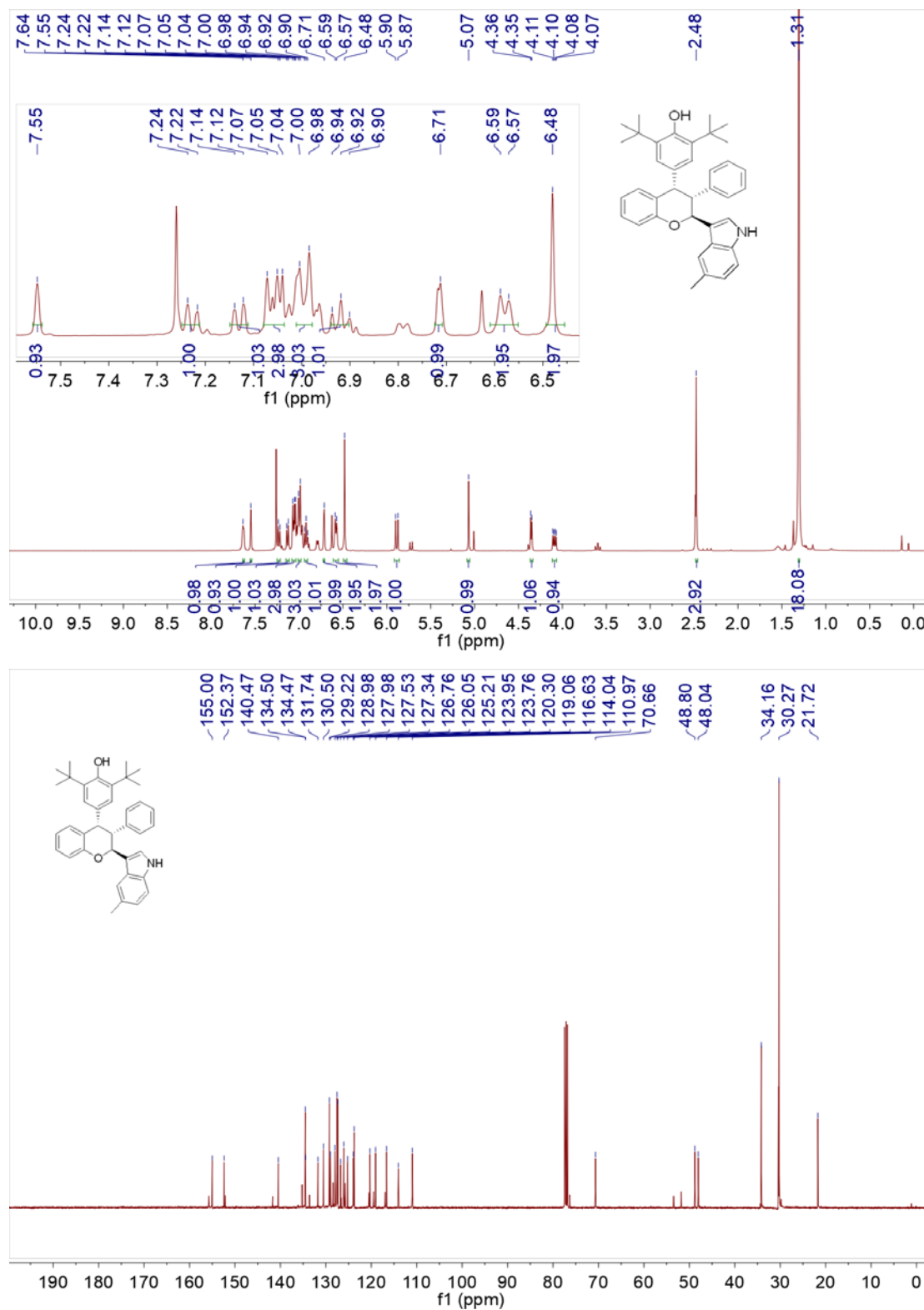
30a: (inseparable diastereomers, 84:16 dr):



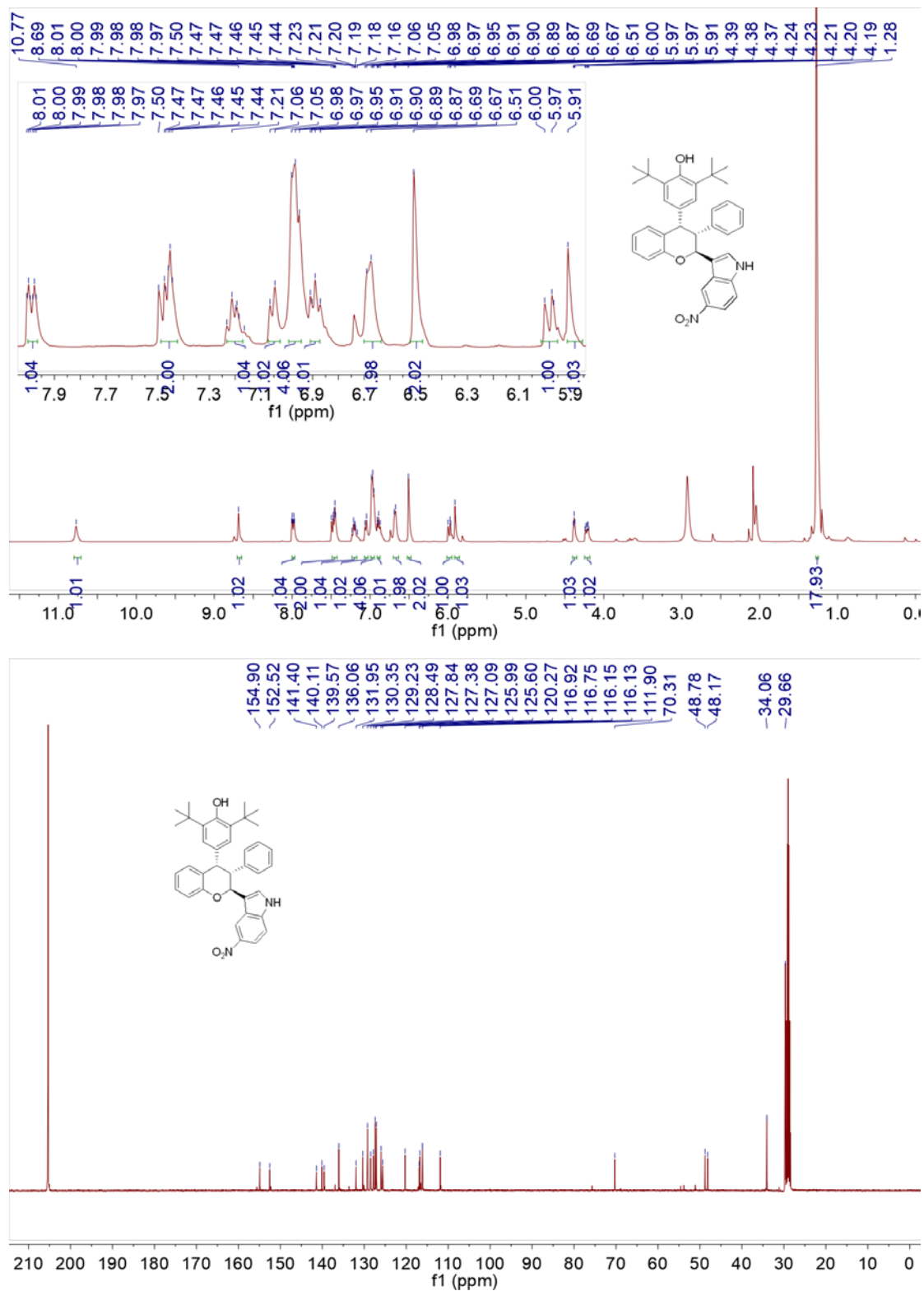
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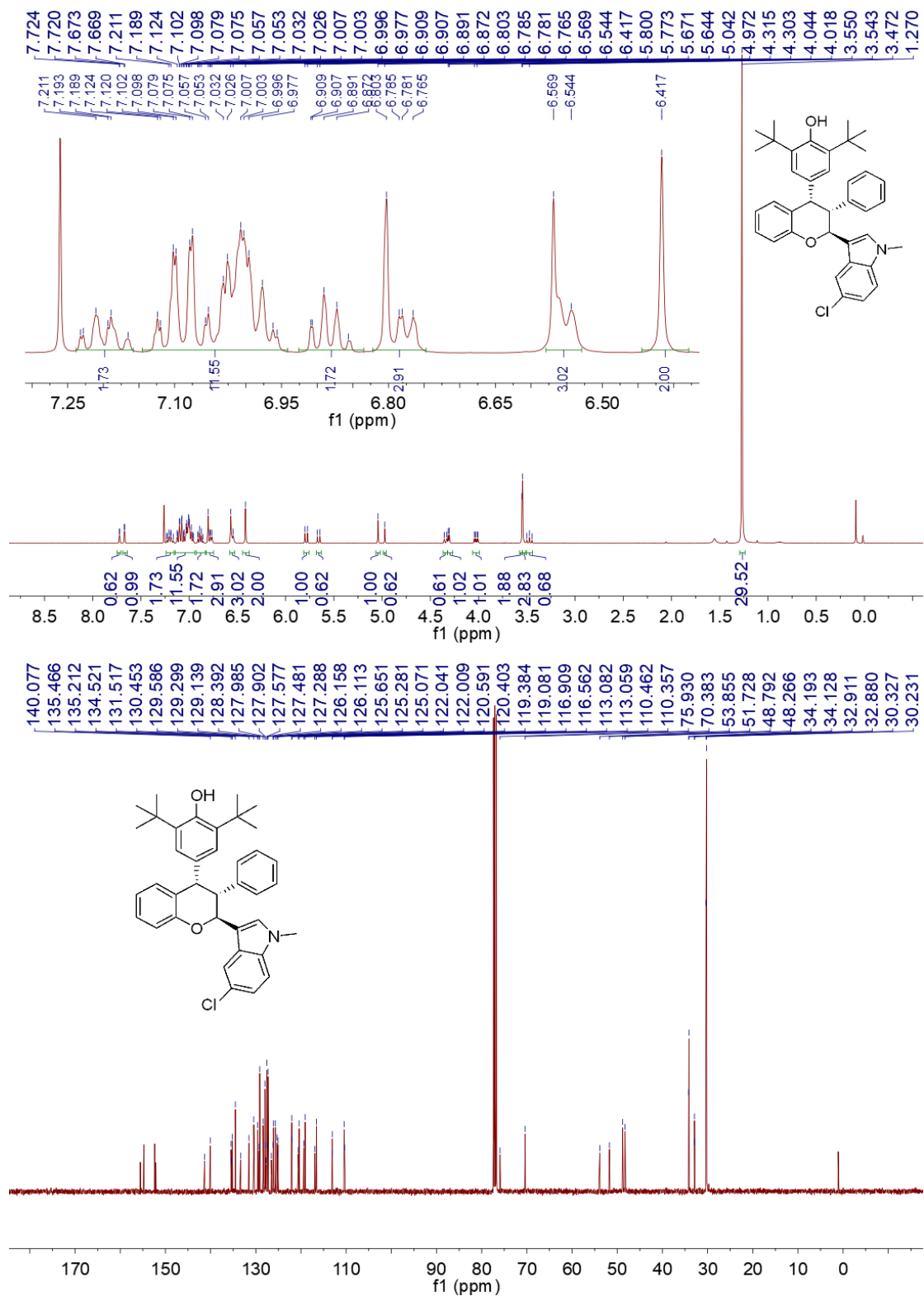
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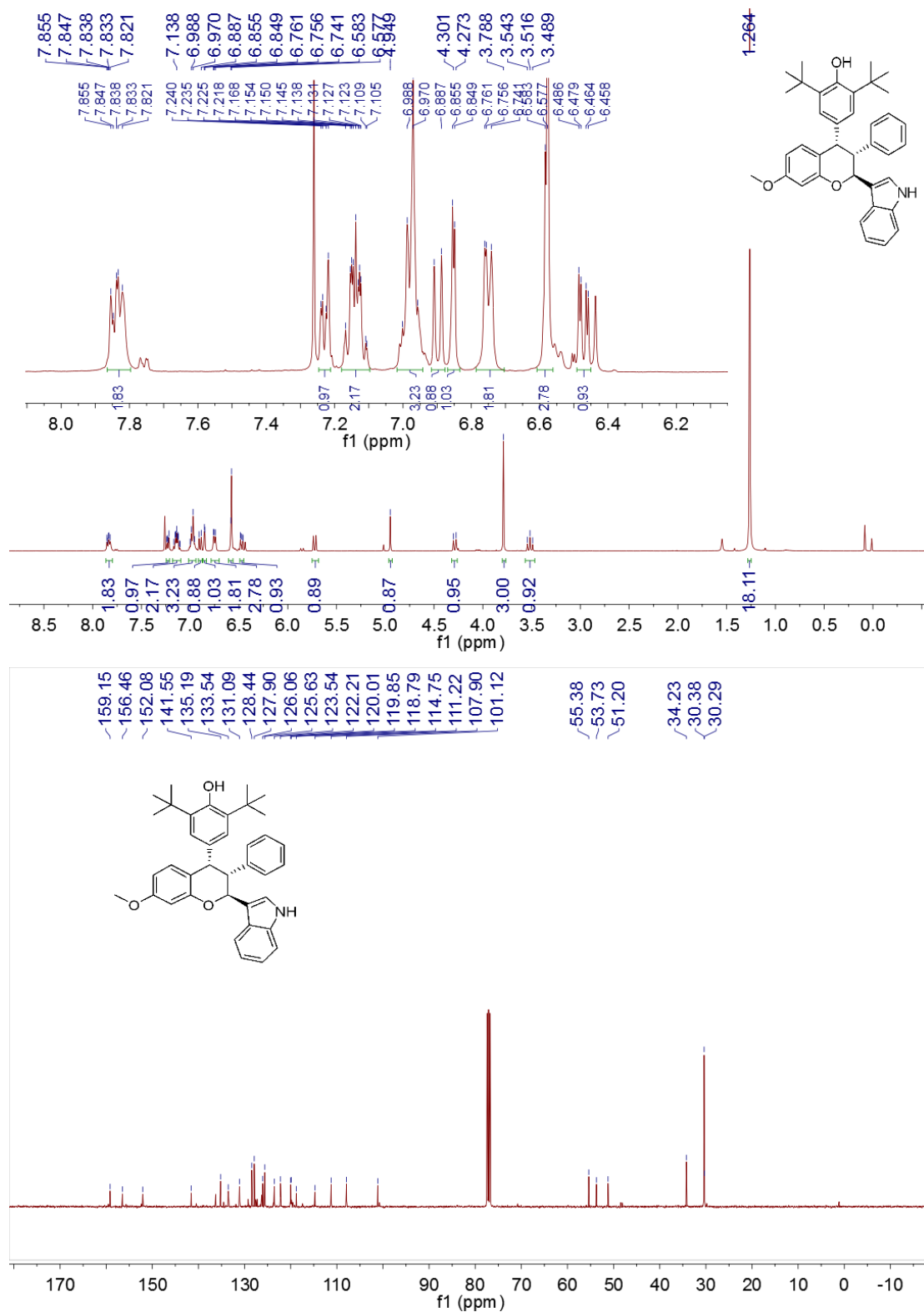
3ra: (inseparable diastereomers, 85:15 dr)



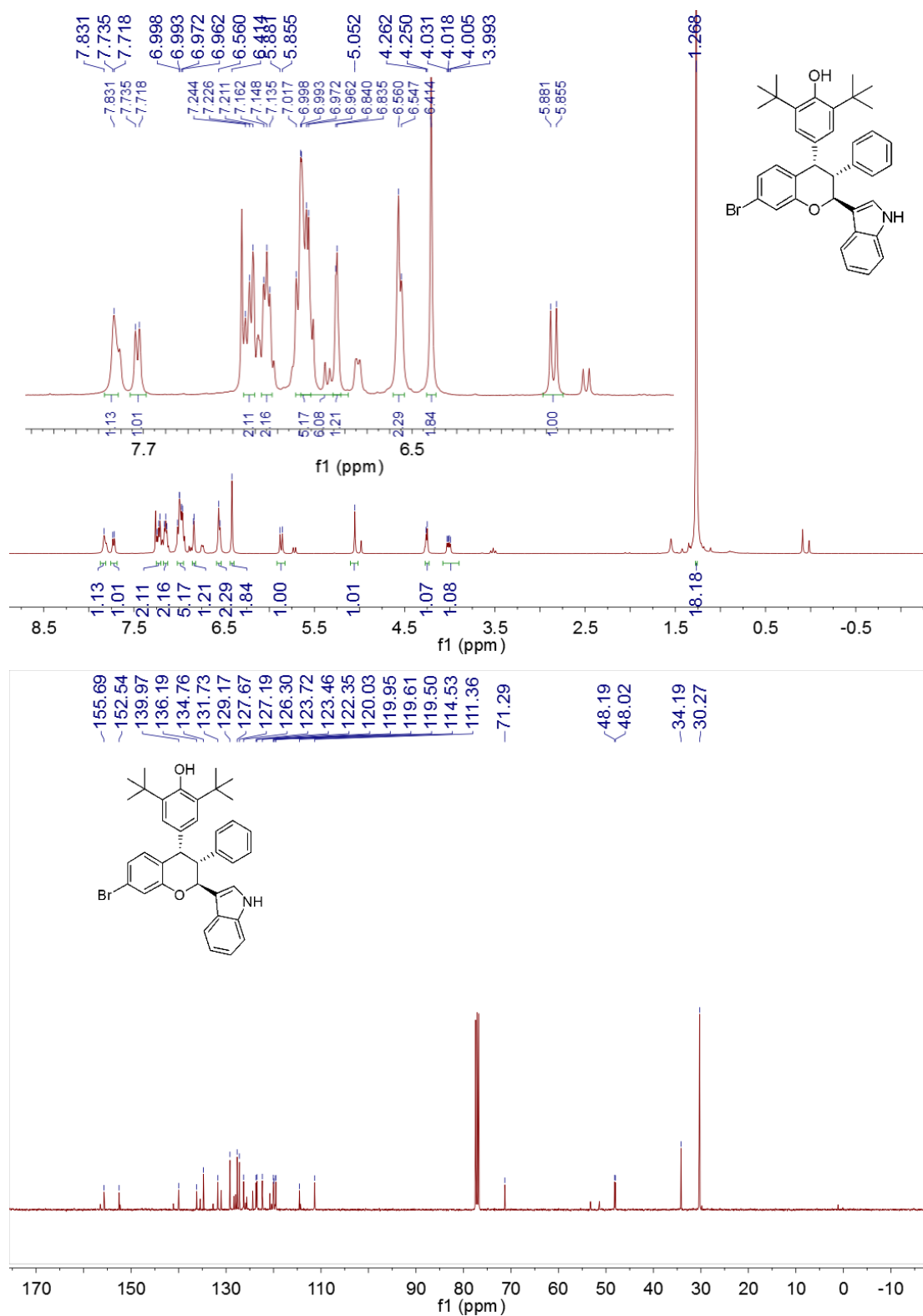
3sa: (inseparable diastereomers, 61:39 dr):



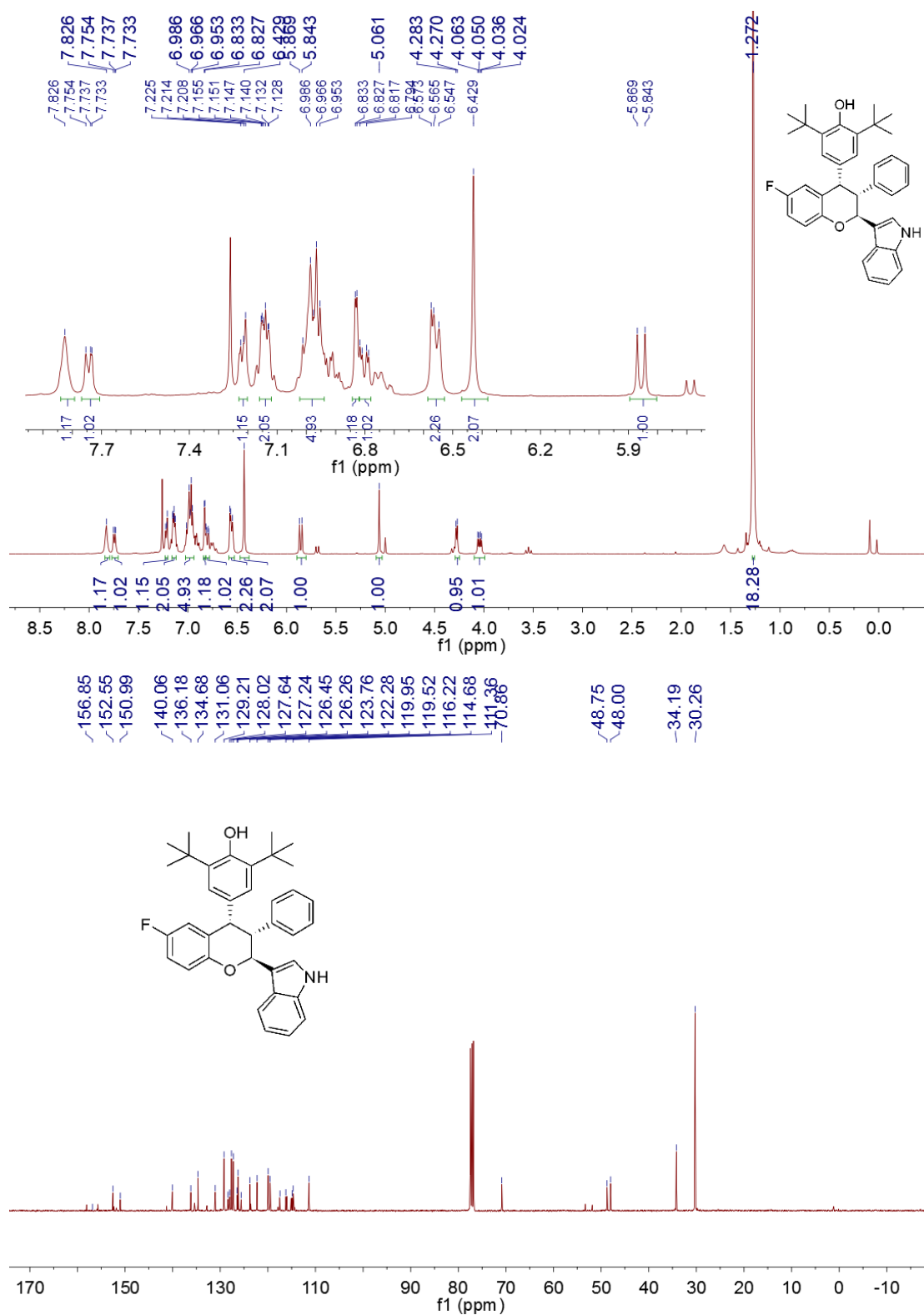
3ab: (inseparable diastereomers, 95:5 dr)



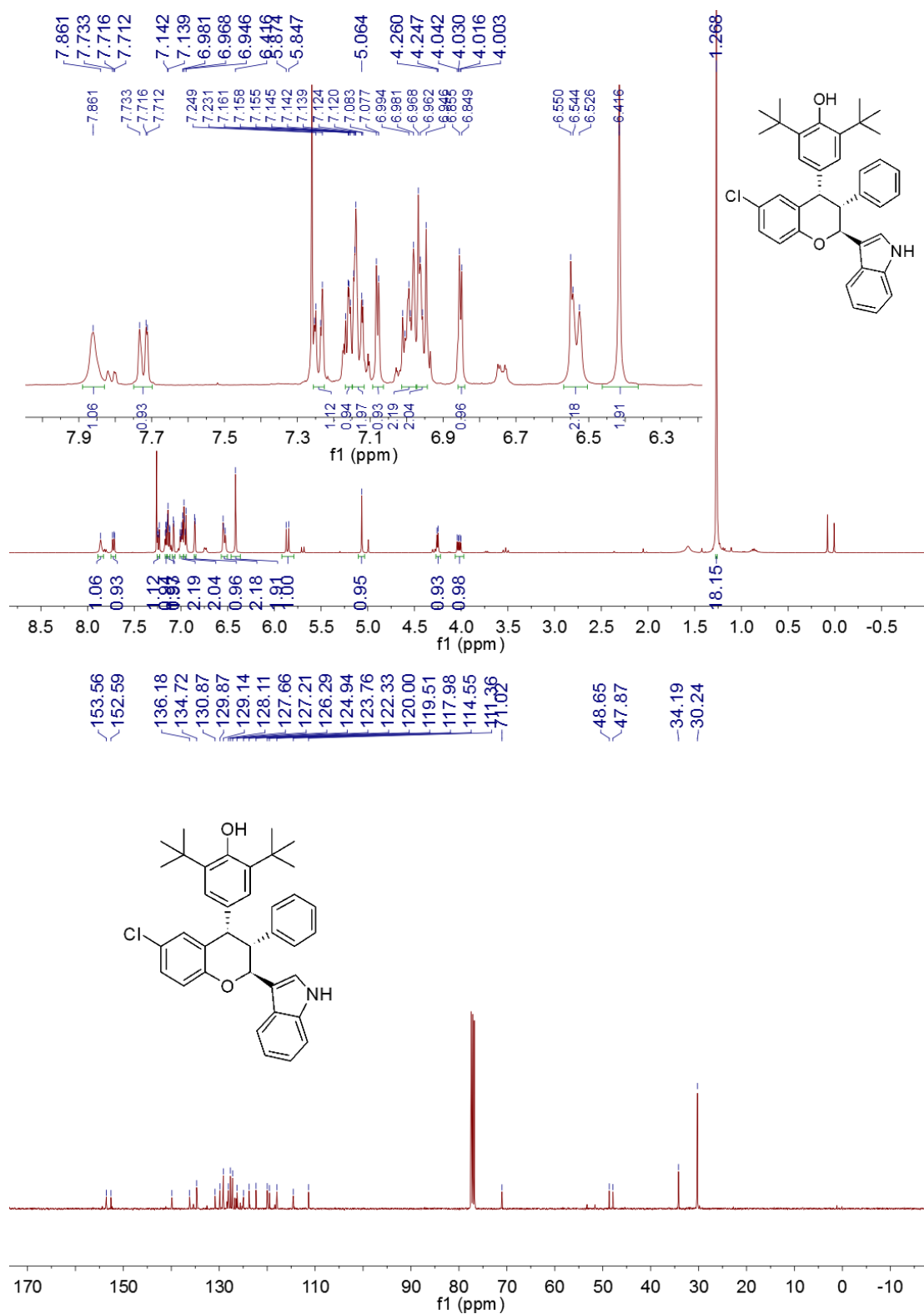
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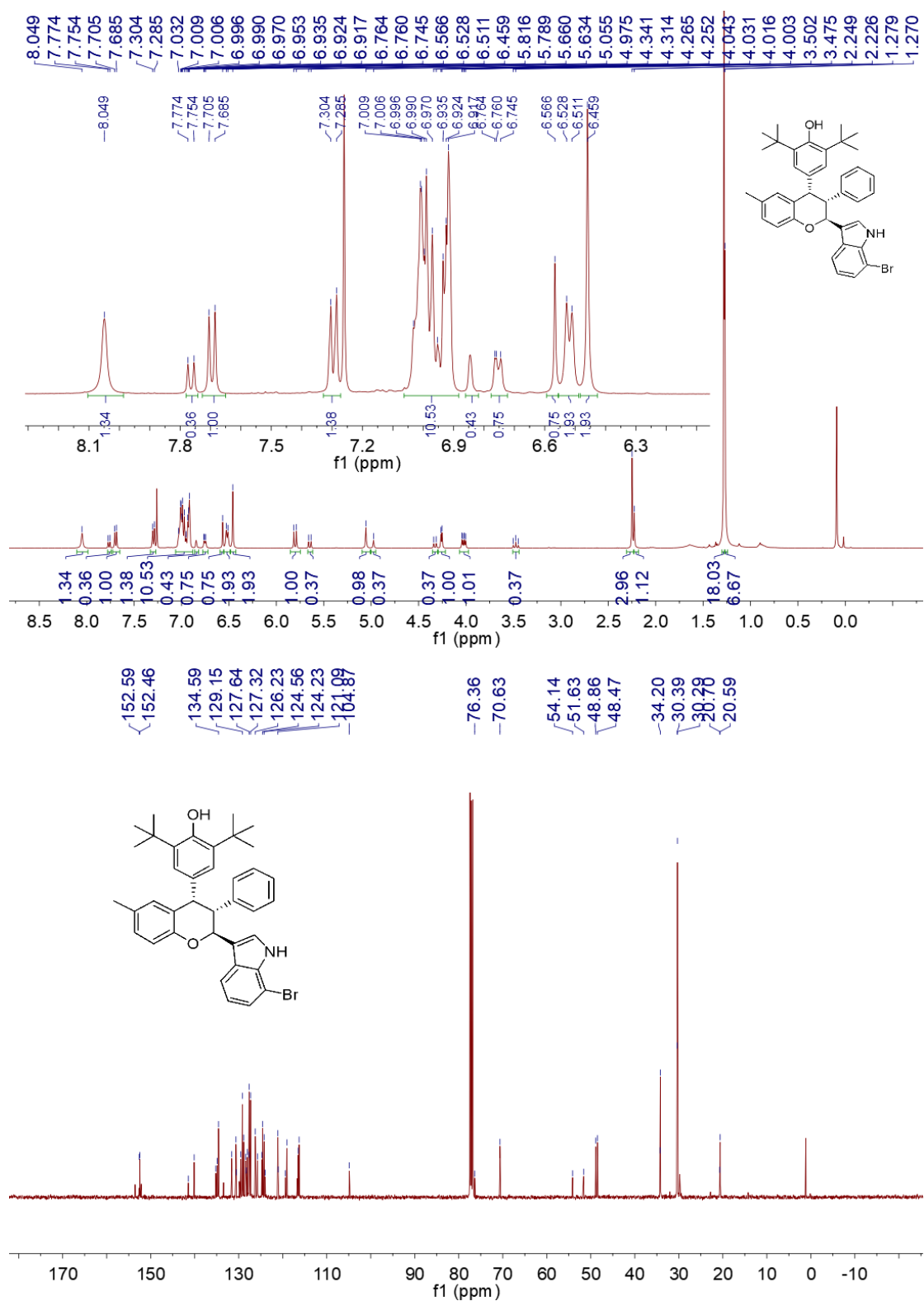
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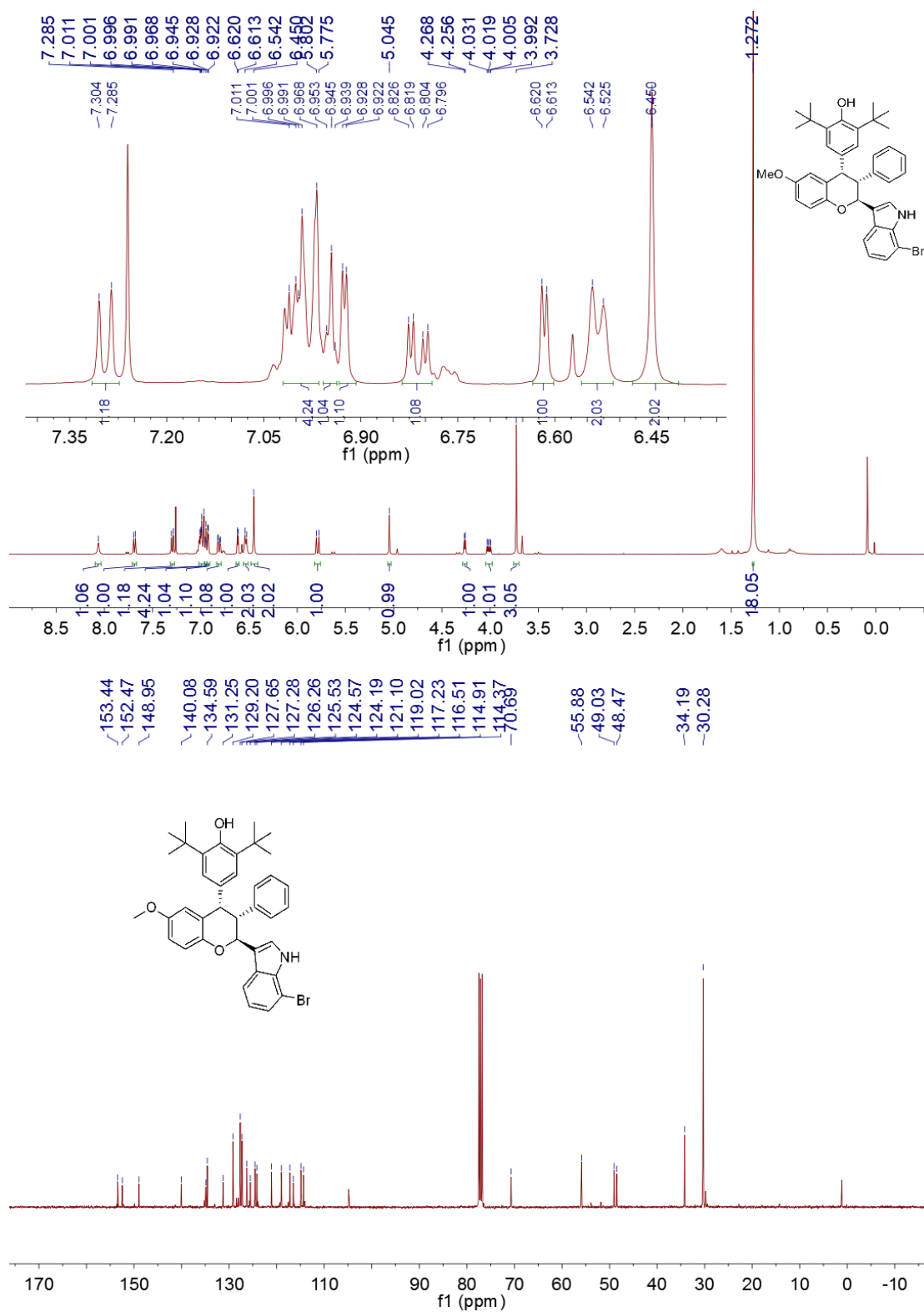
3ae: (inseparable diastereomers, 82:18 dr):



3pf: (inseparable diastereomers, 73:27 dr):

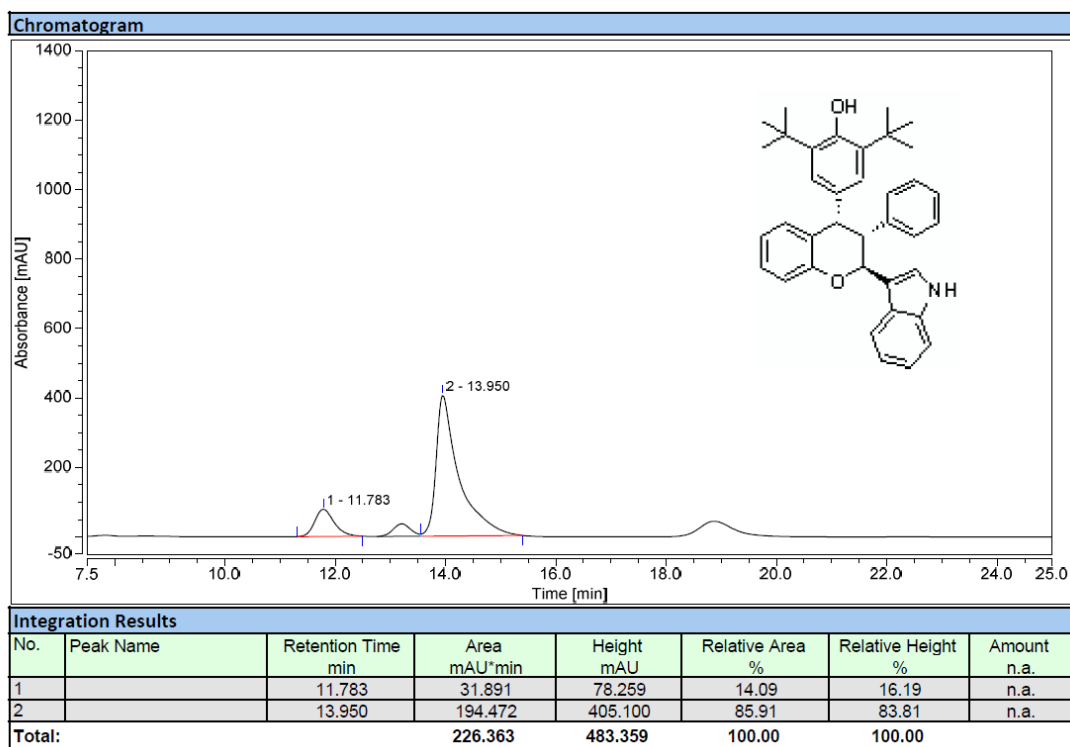
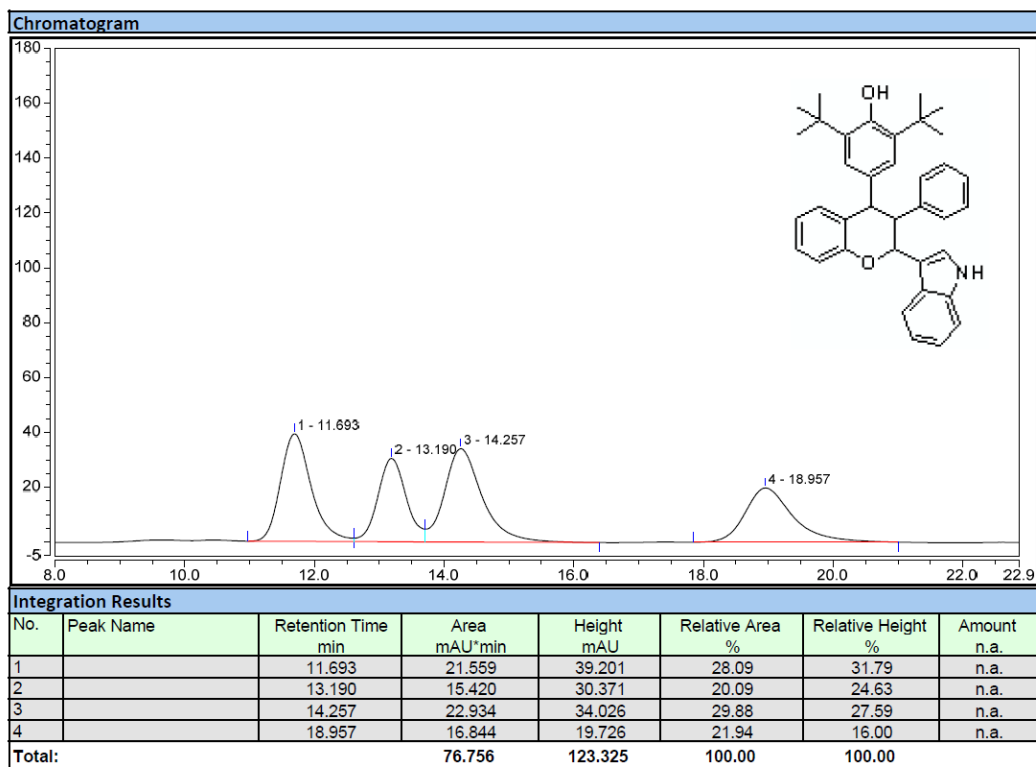


3pg: (inseparable diastereomers, 87:13 dr):

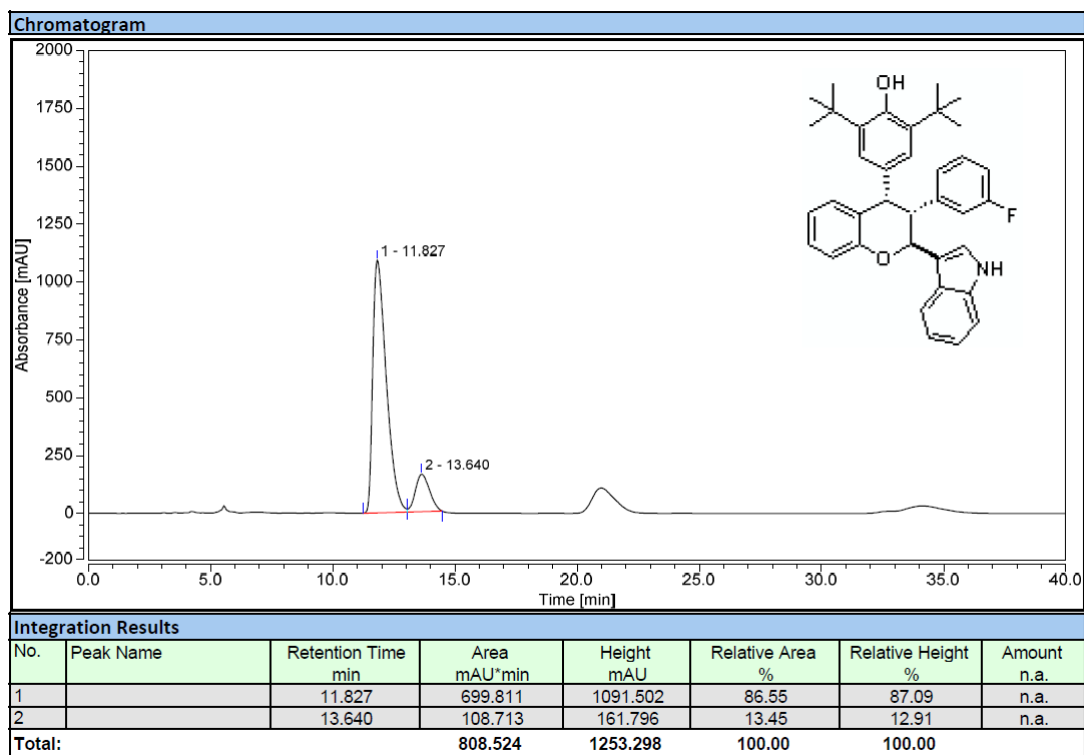
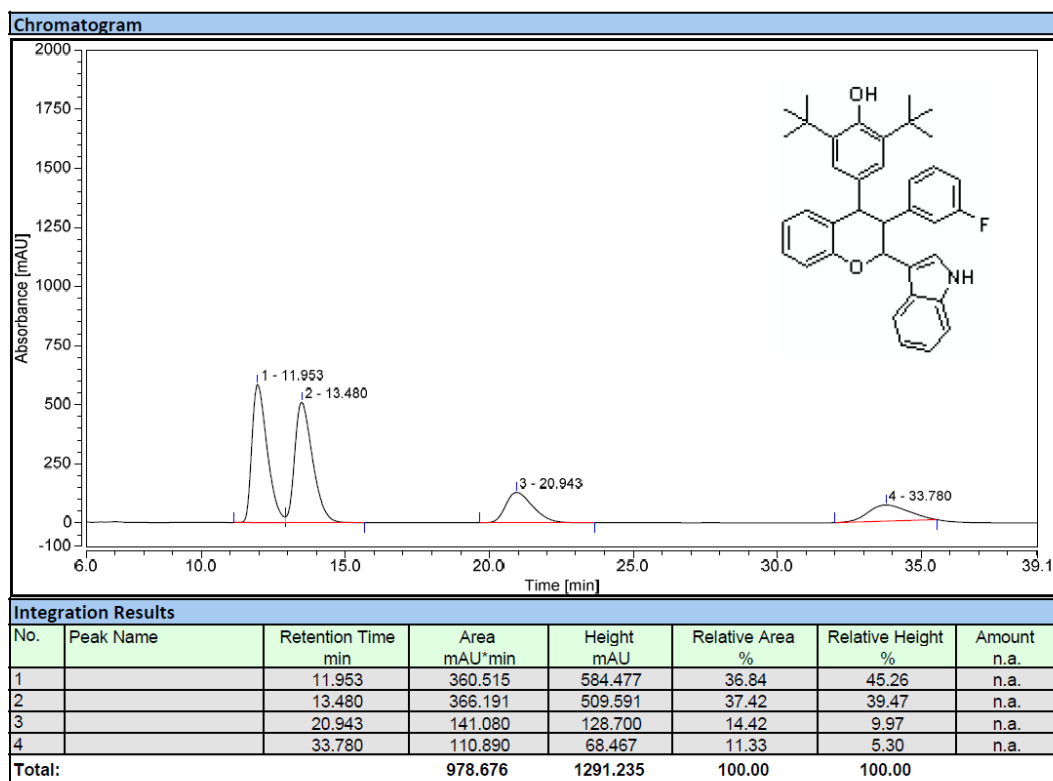


2. HPLC copies of products 3

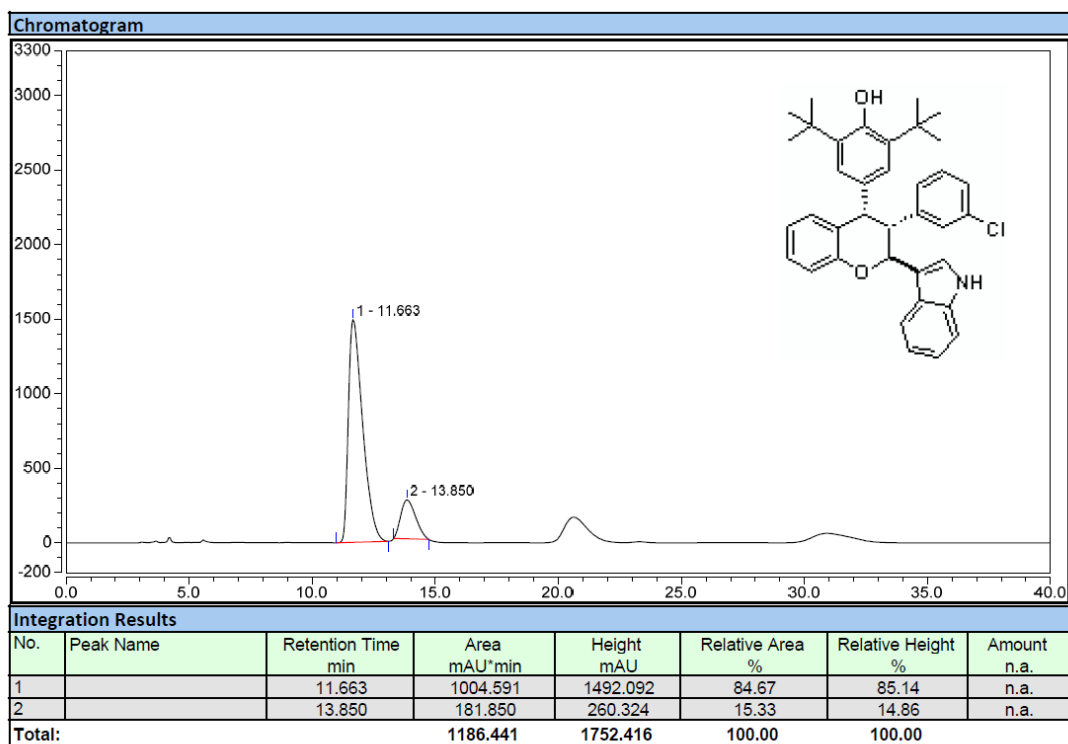
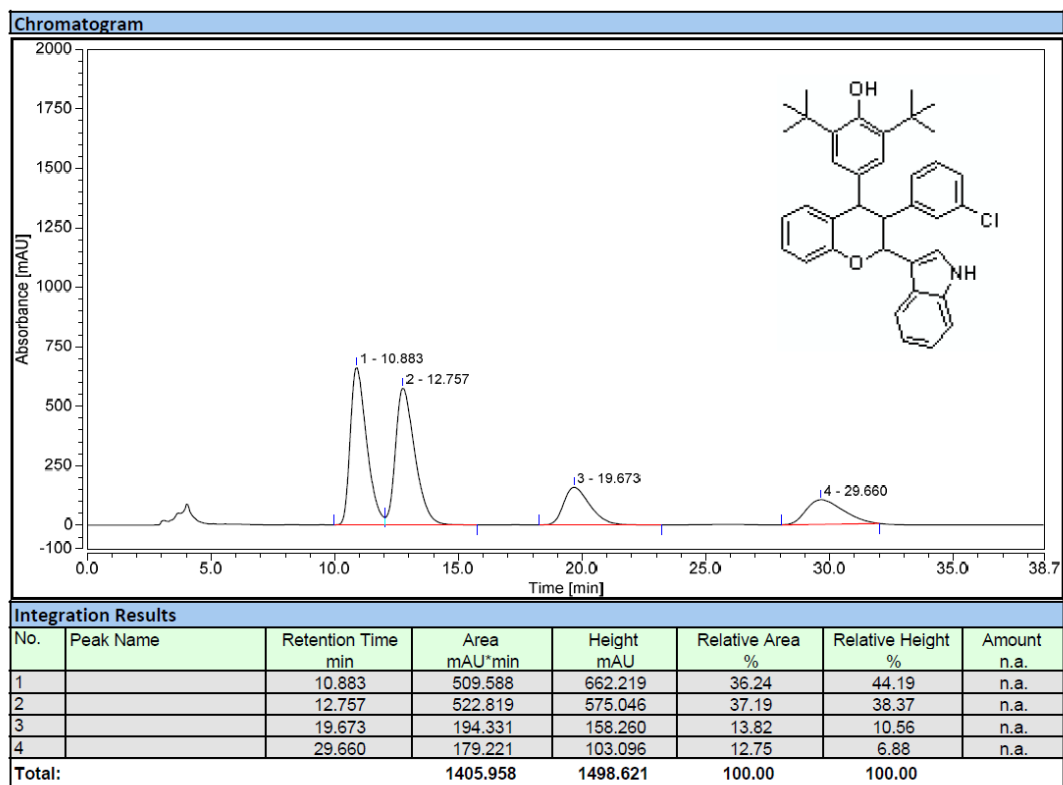
3aa: (inseparable diastereomers, 79:21 dr)



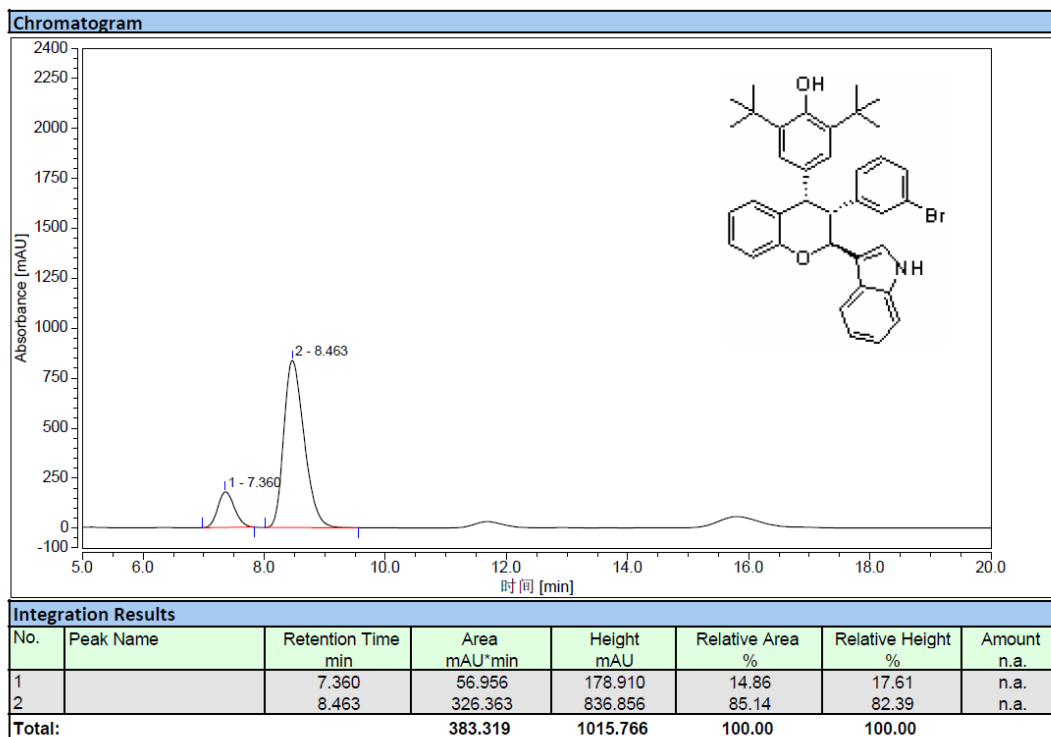
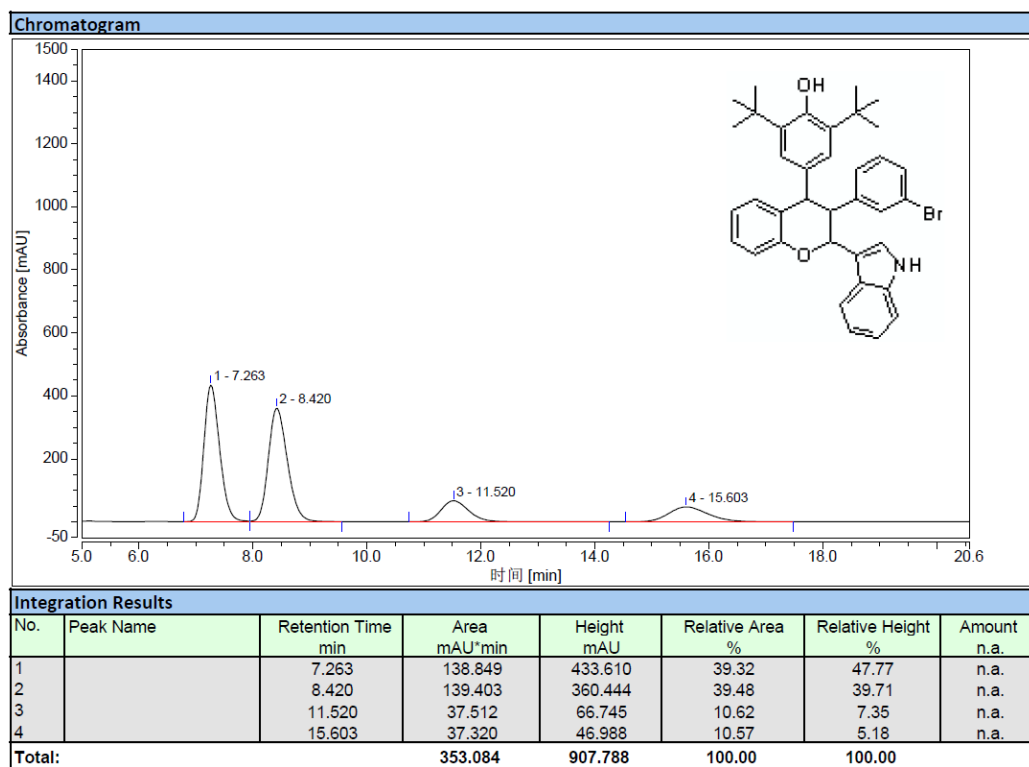
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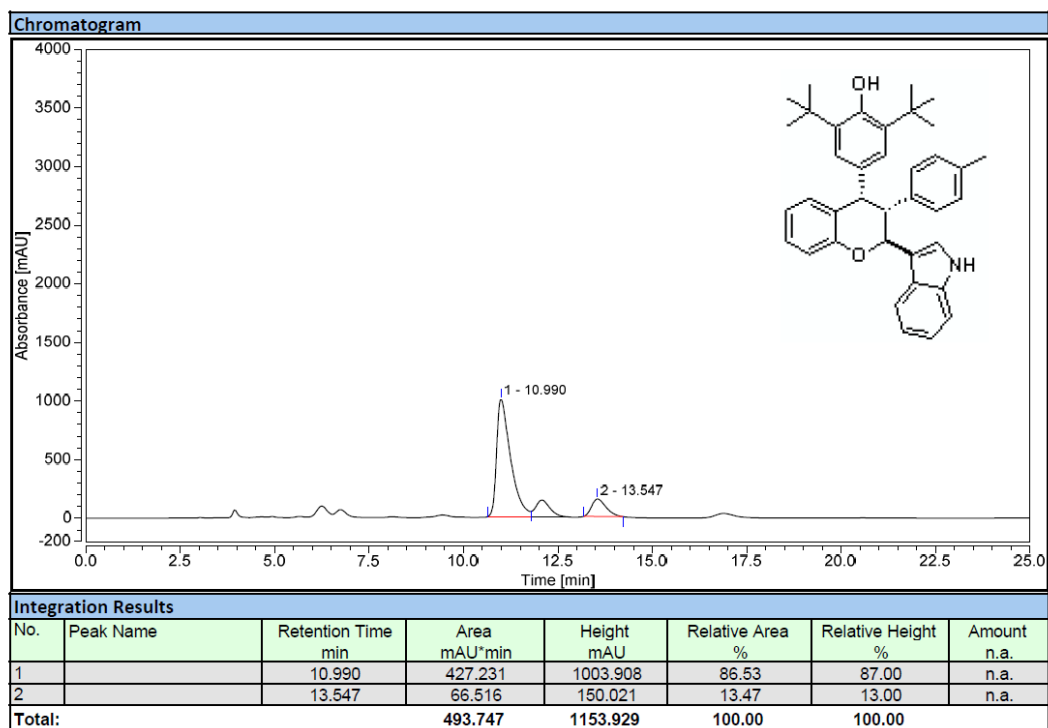
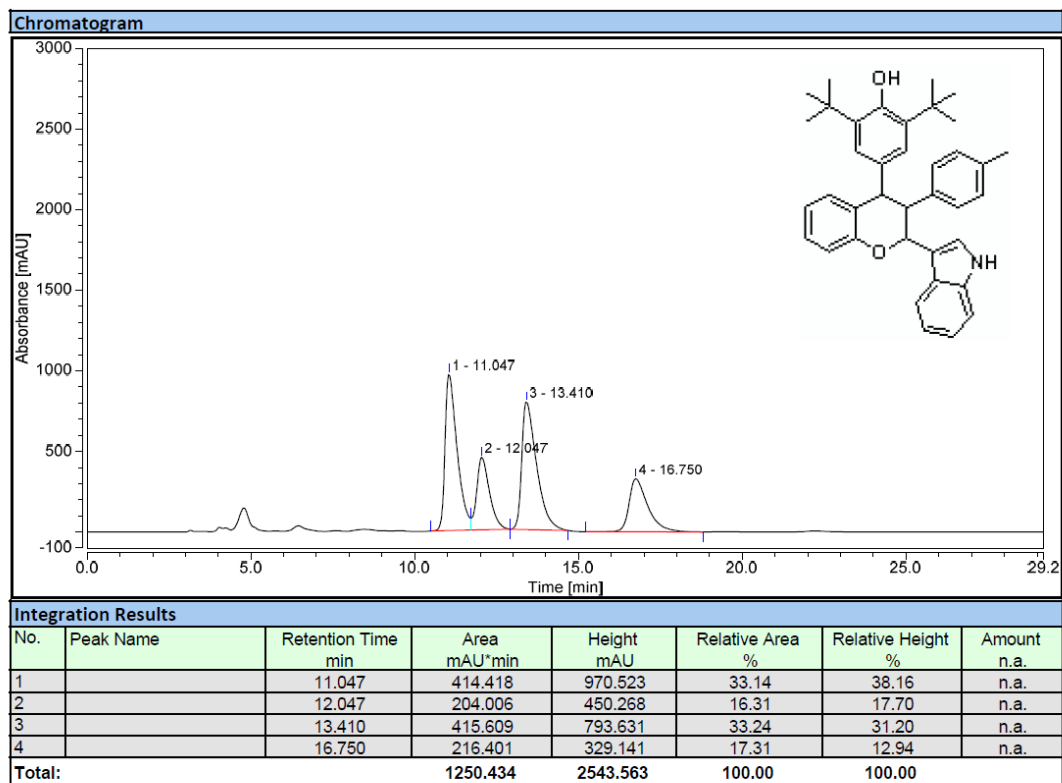
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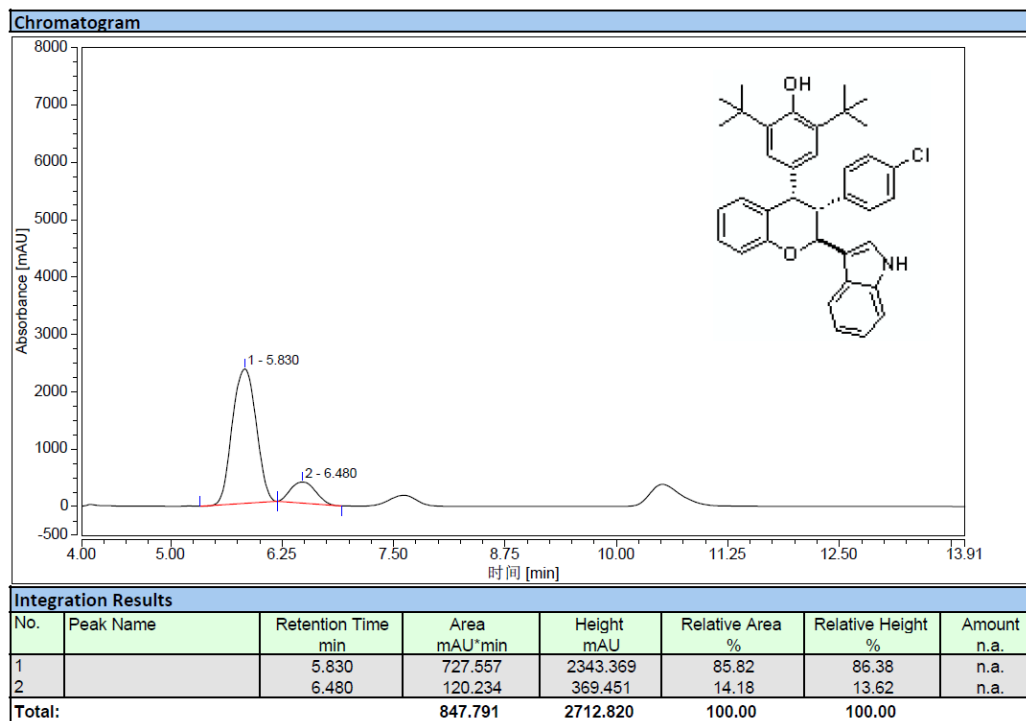
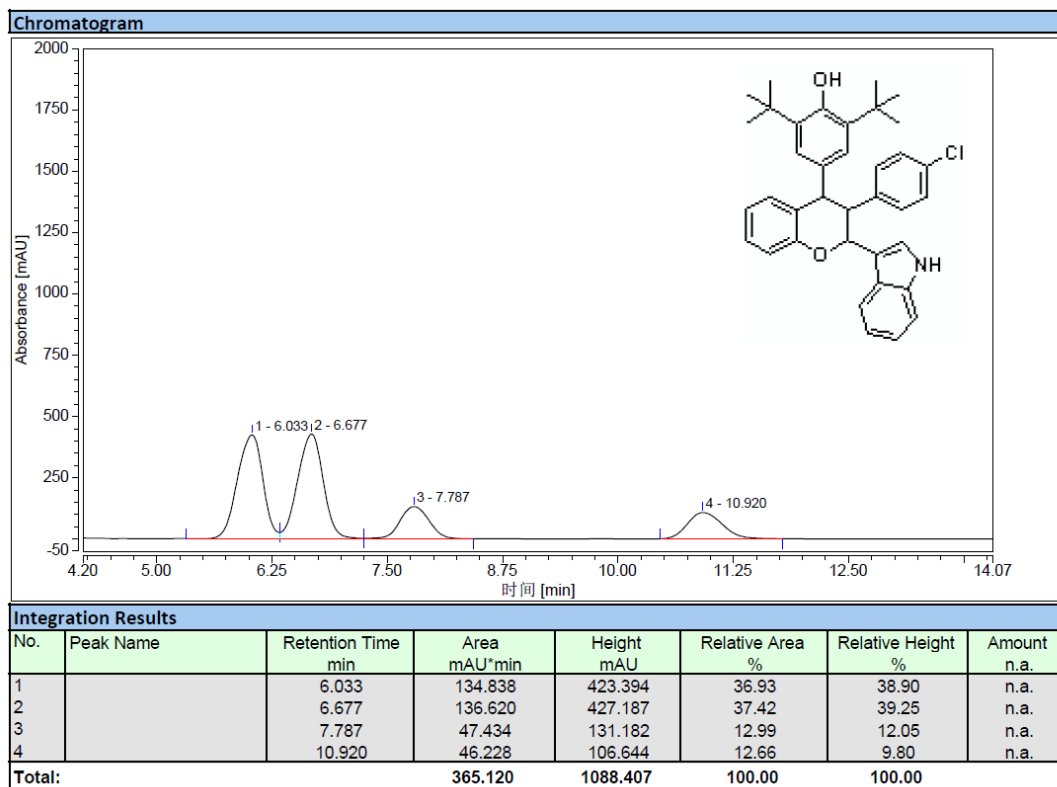
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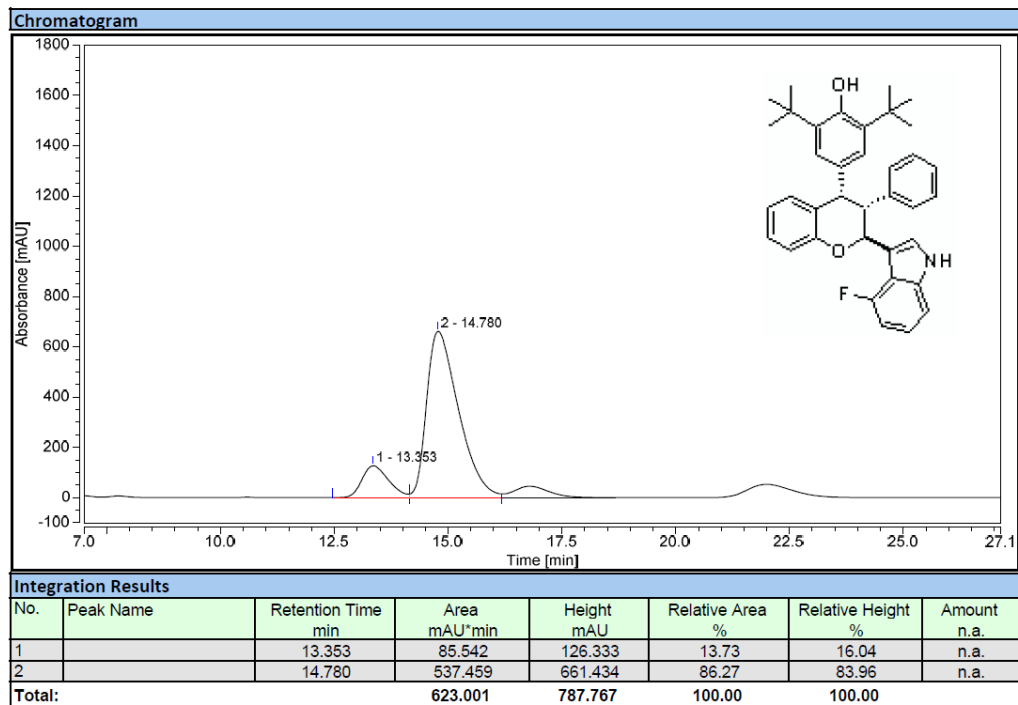
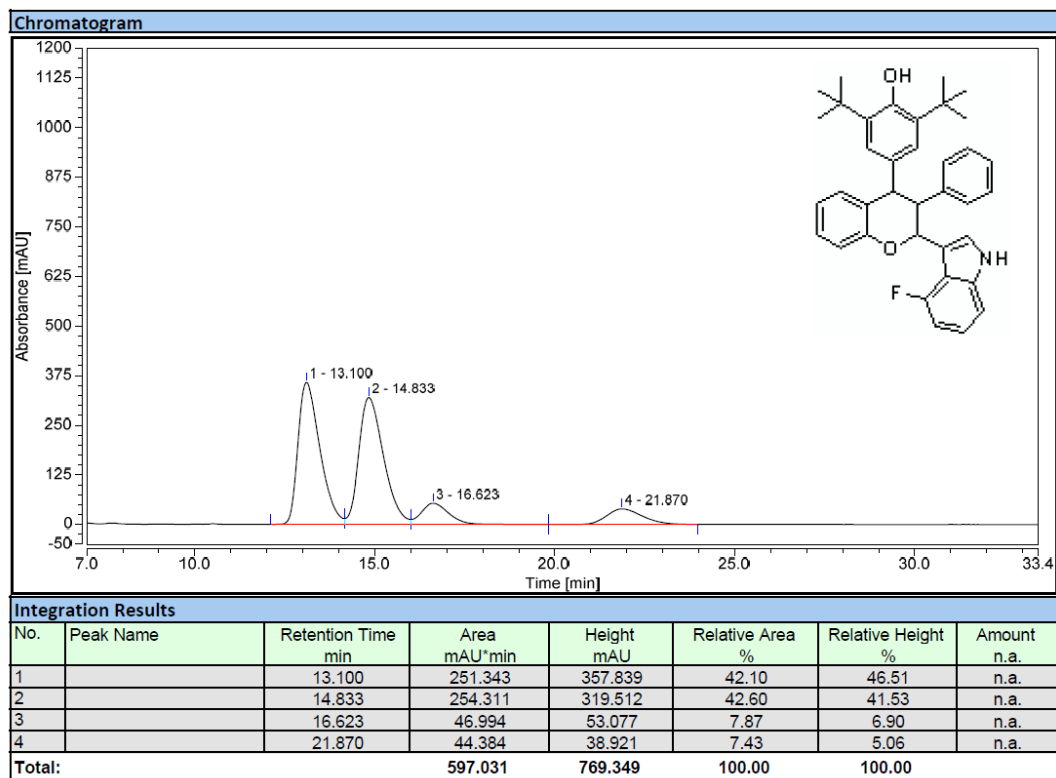
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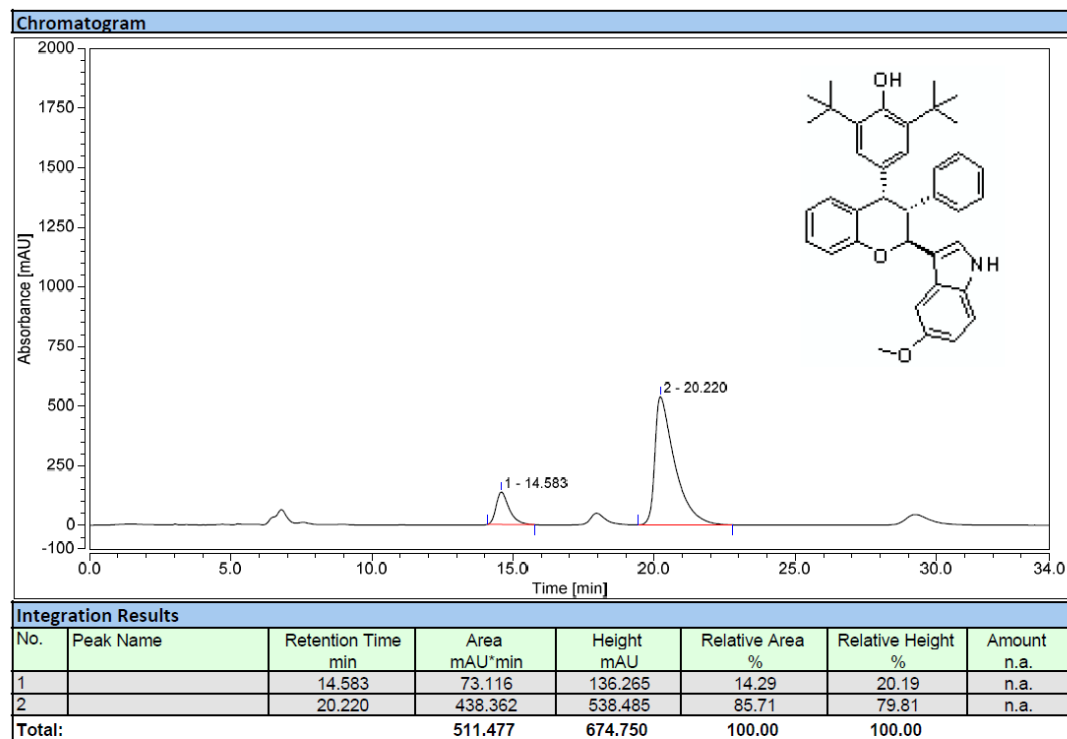
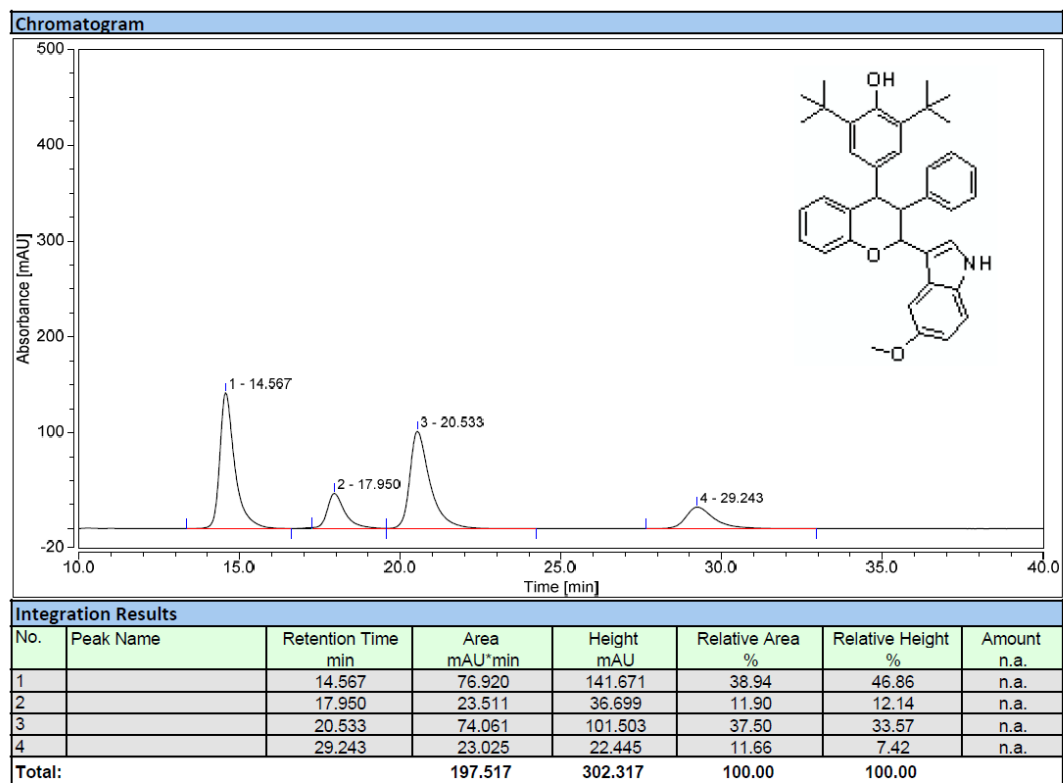
3fa: (inseparable diastereomers, 78:22 dr):



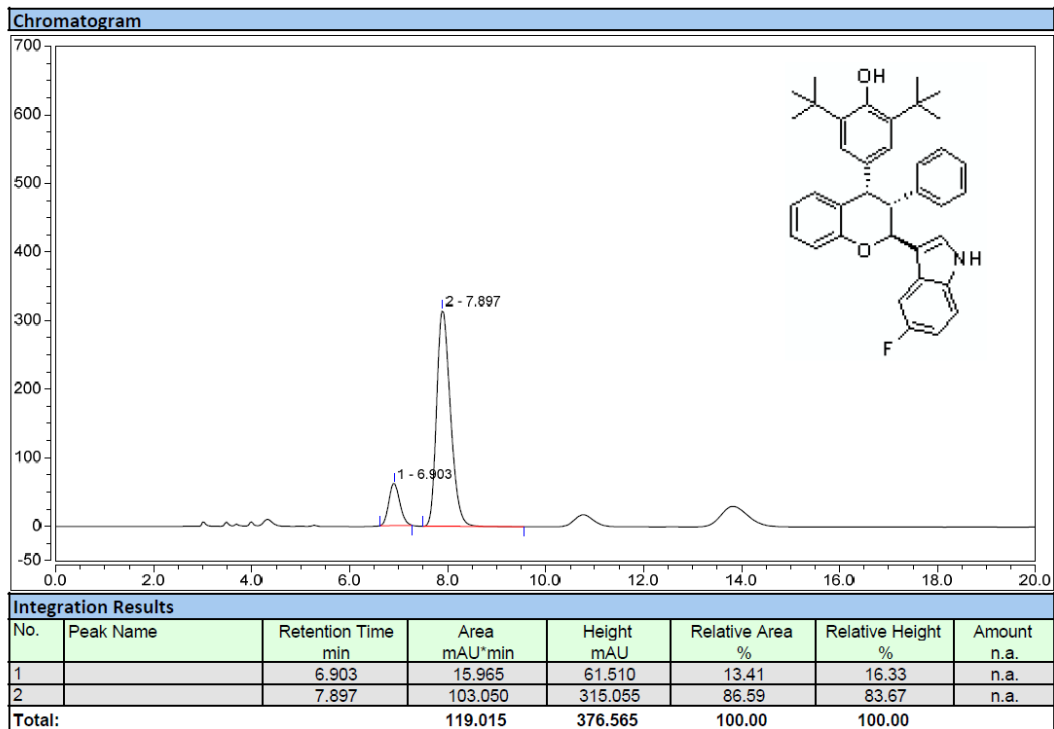
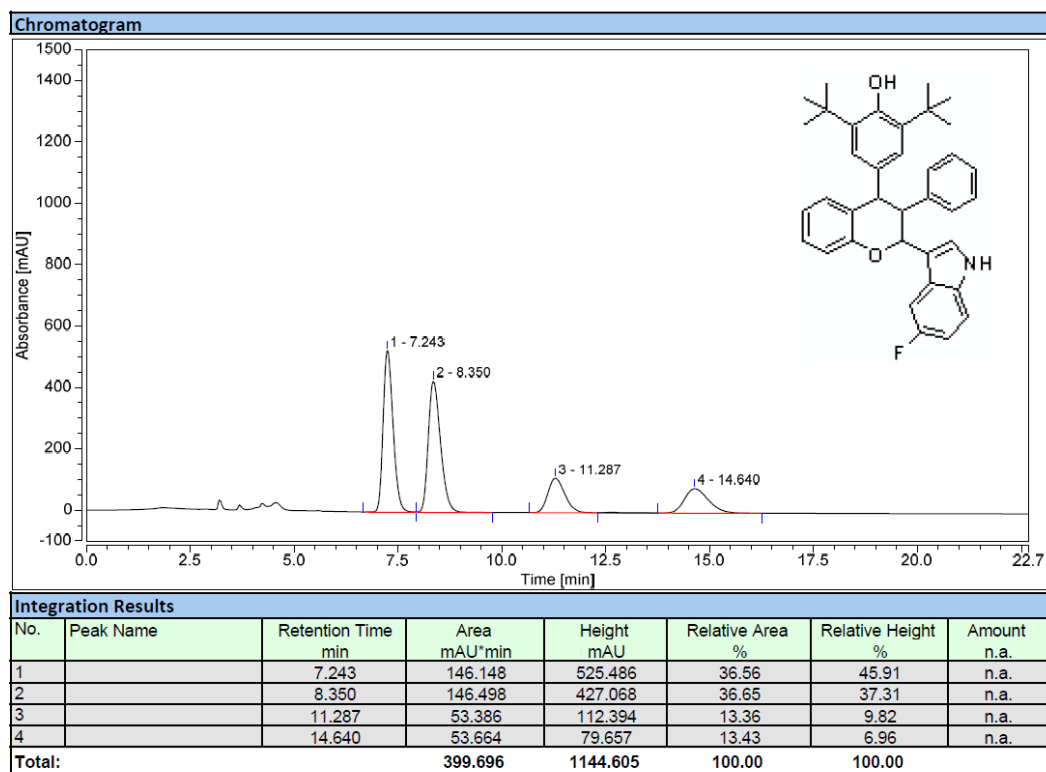
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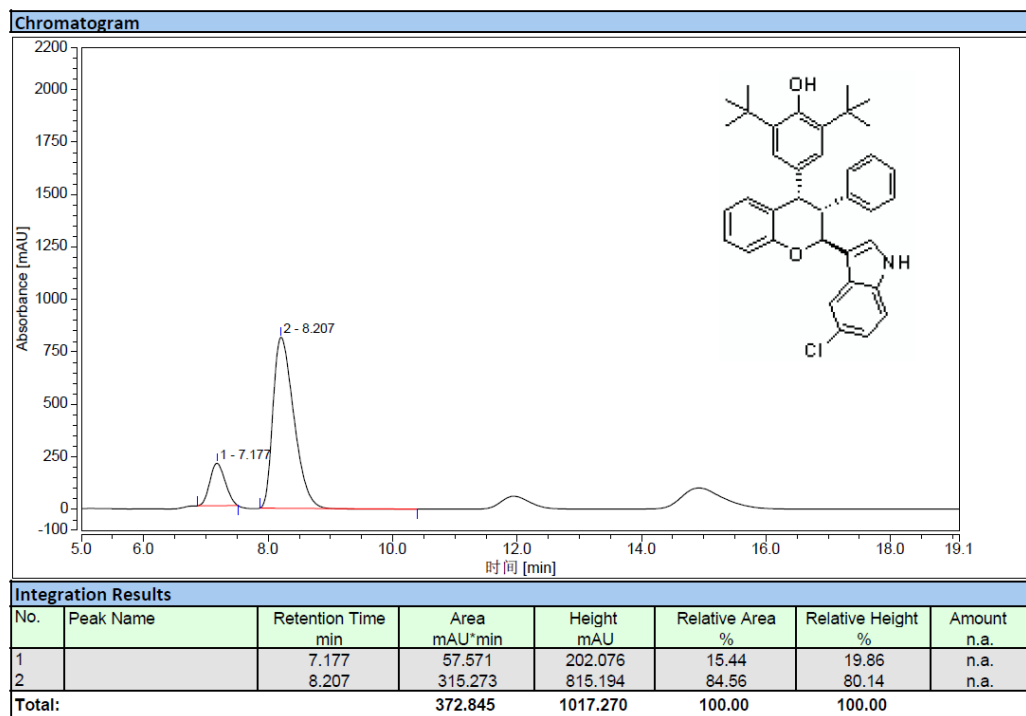
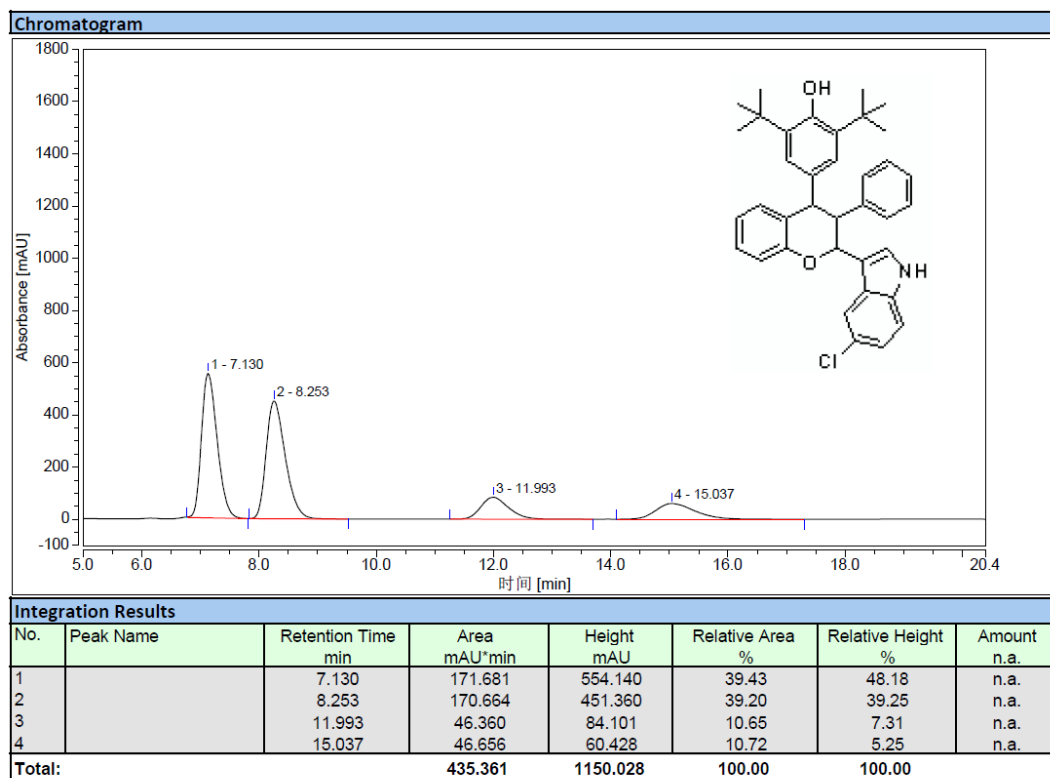
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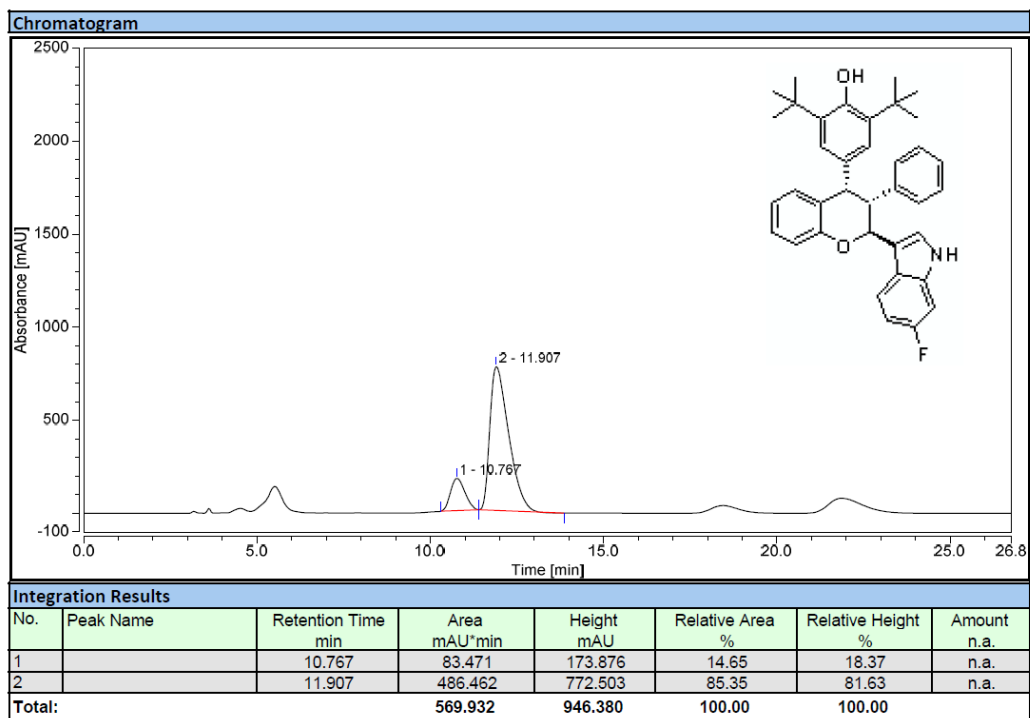
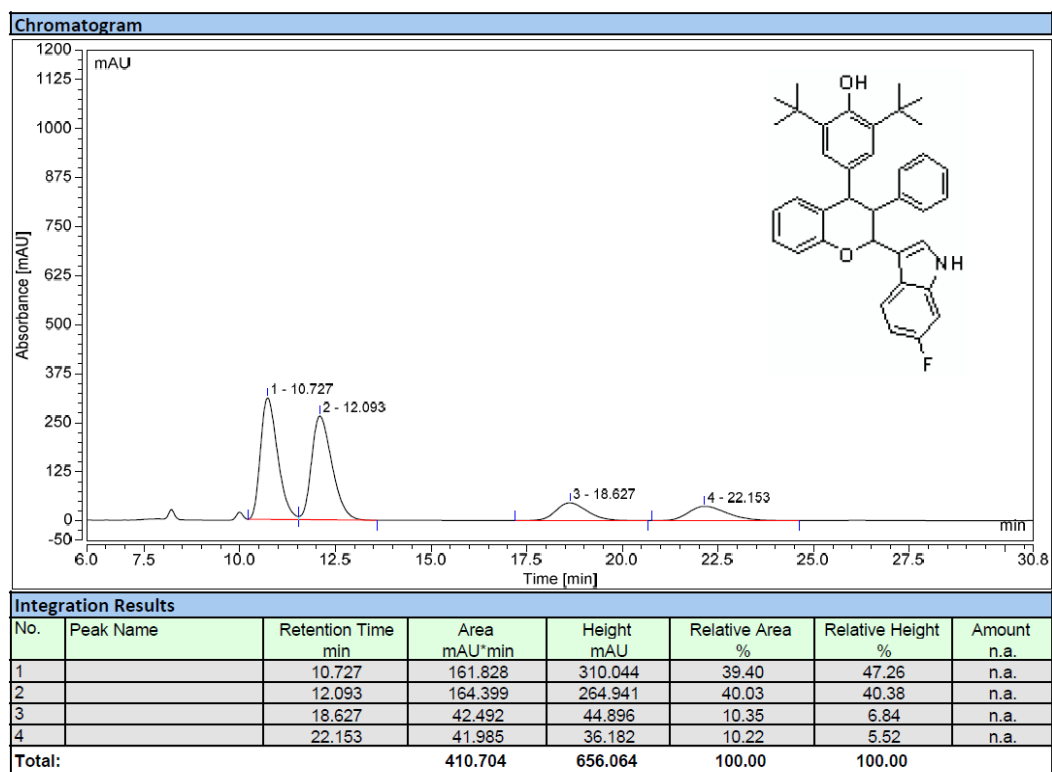
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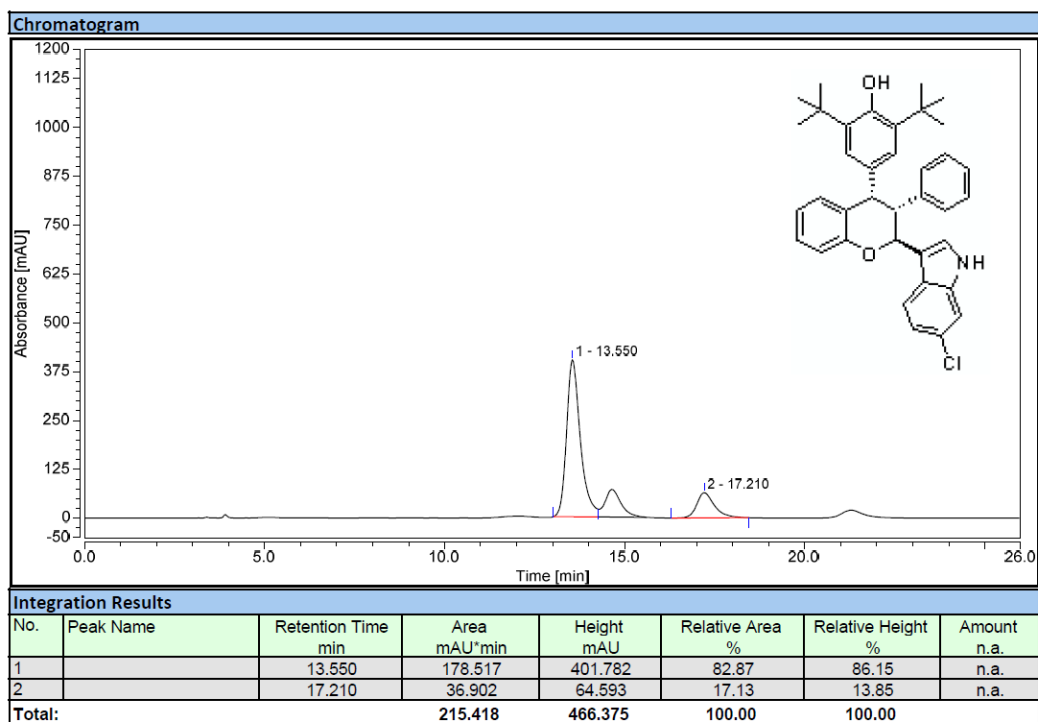
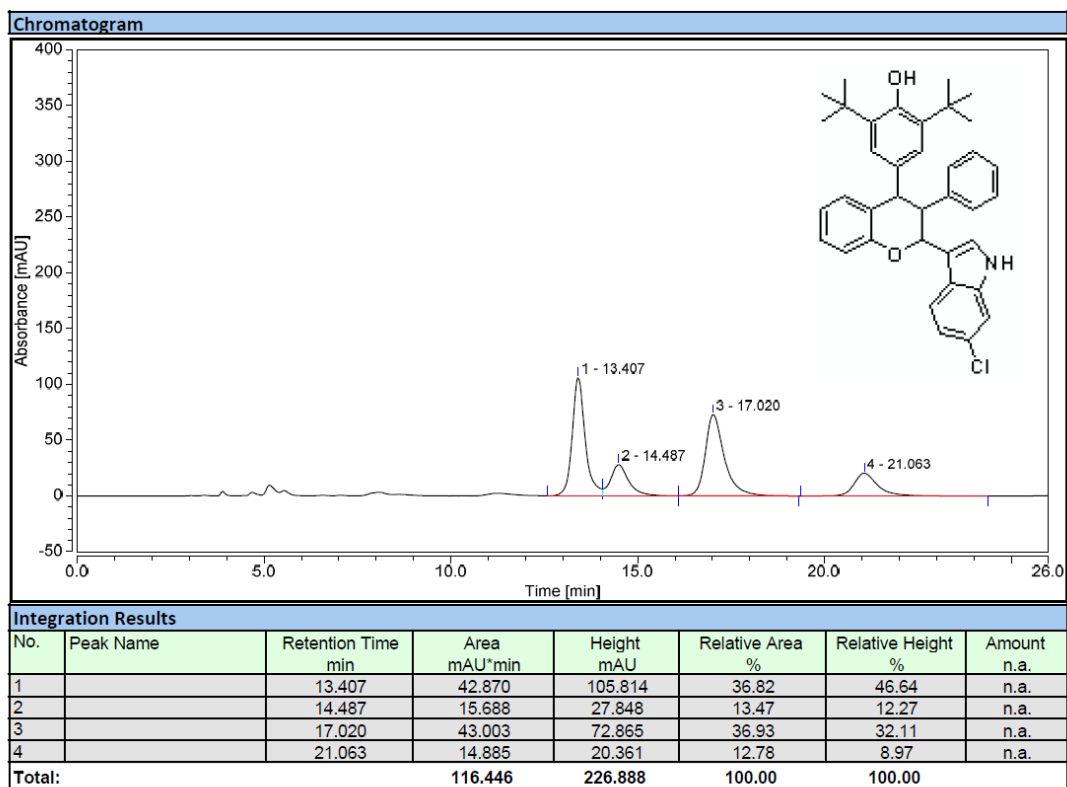
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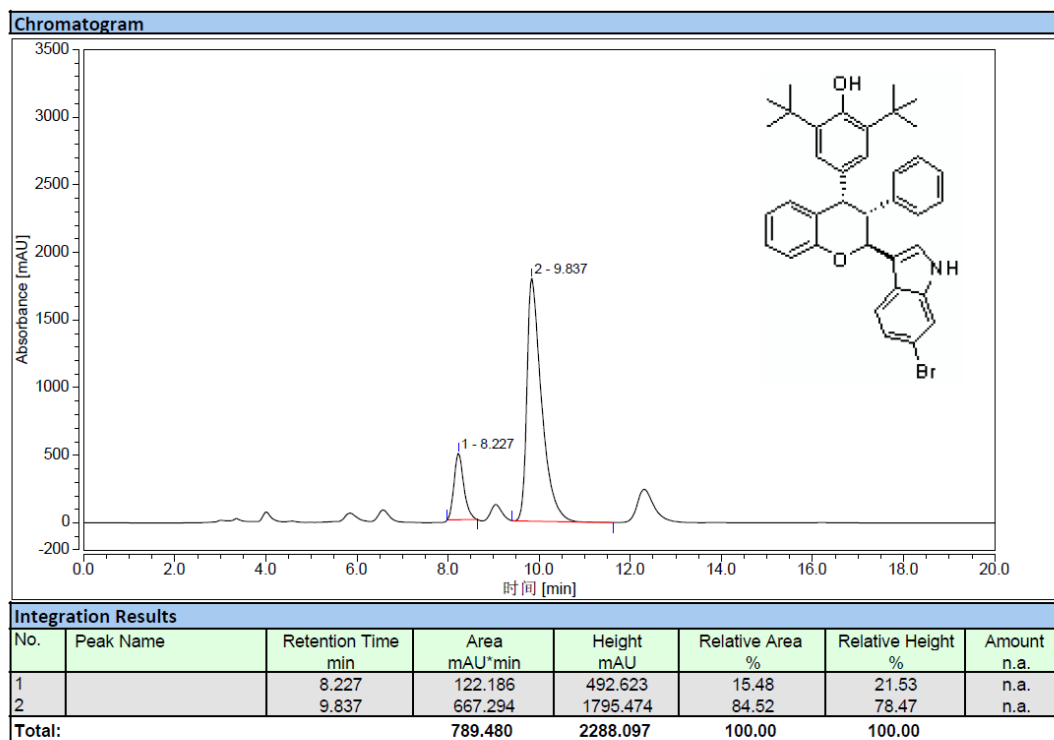
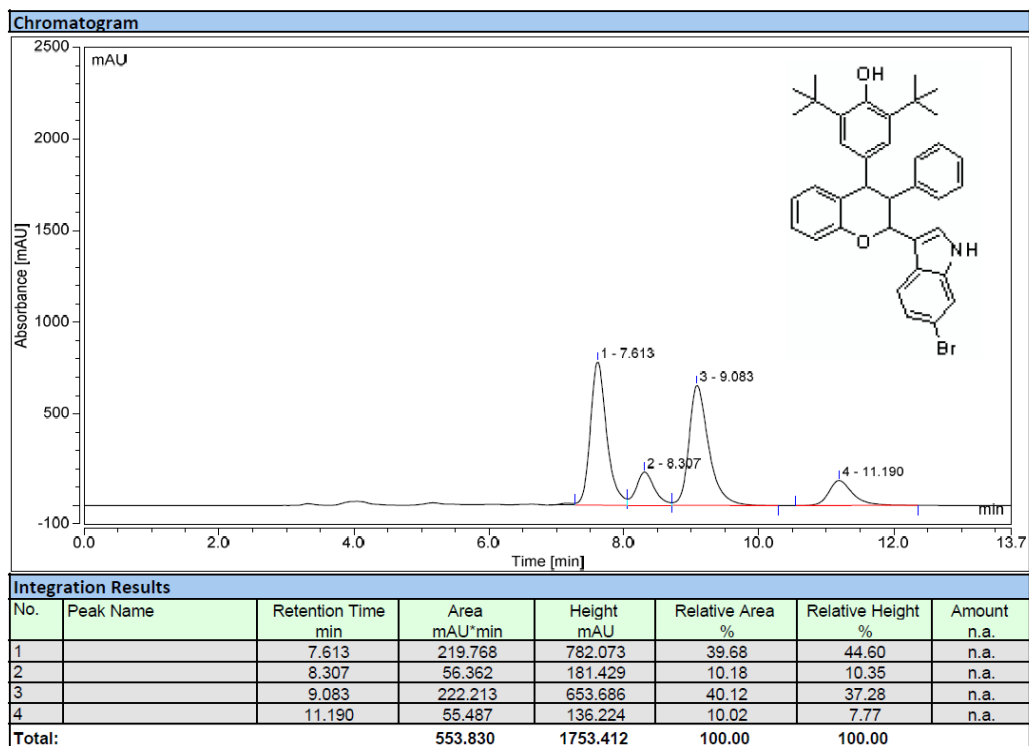
3ka: (inseparable diastereomers, 85:15 dr):



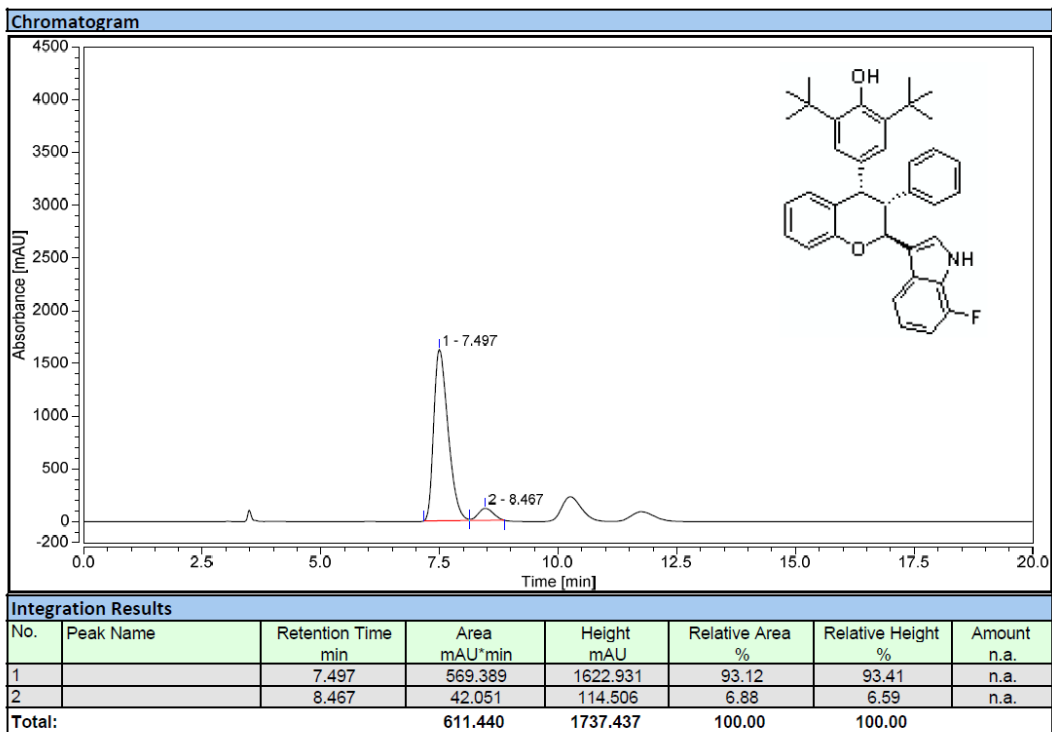
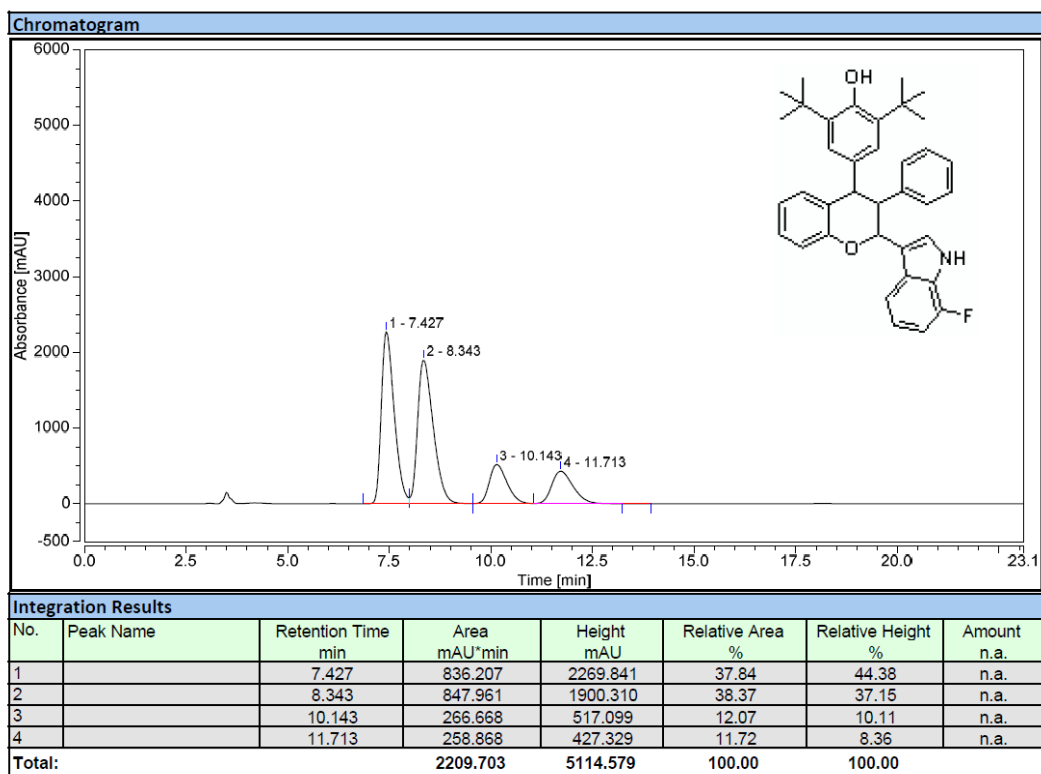
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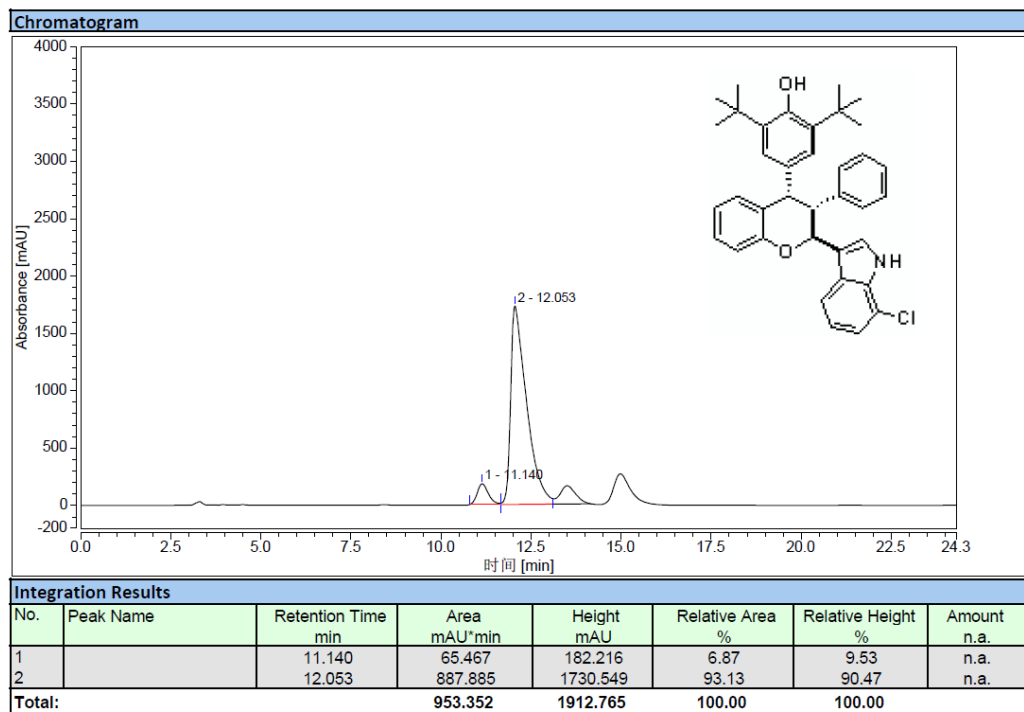
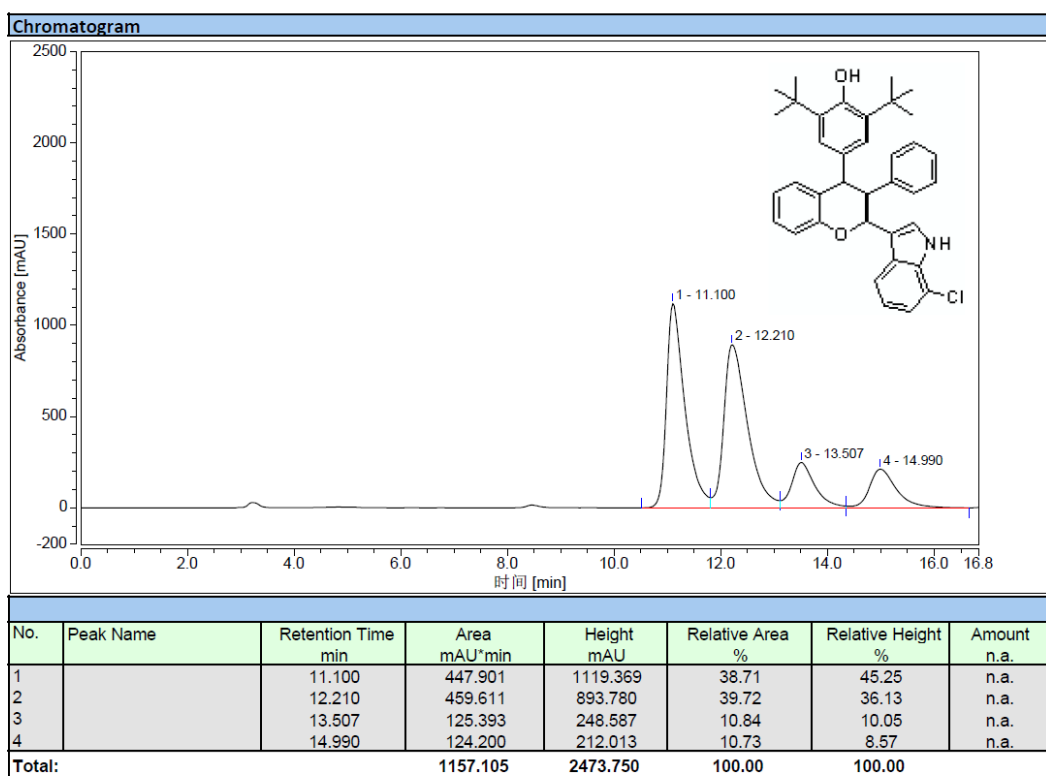
3ma: (inseparable diastereomers, 86:14 dr):



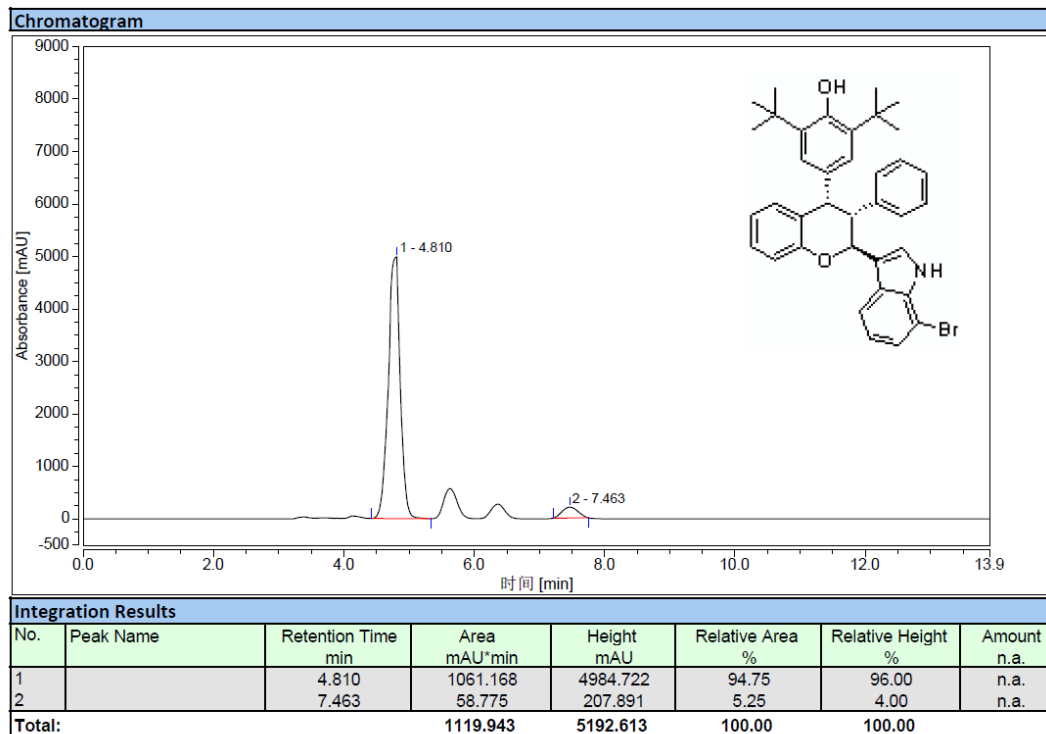
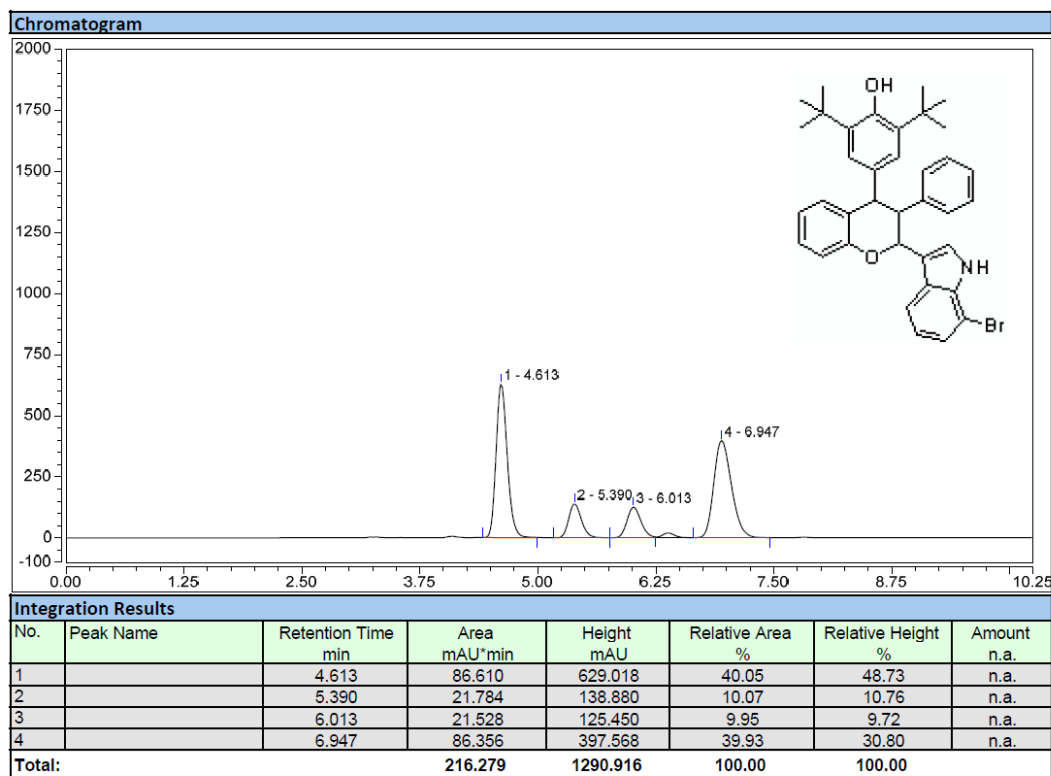
3na: (inseparable diastereomers, 82:18 dr):



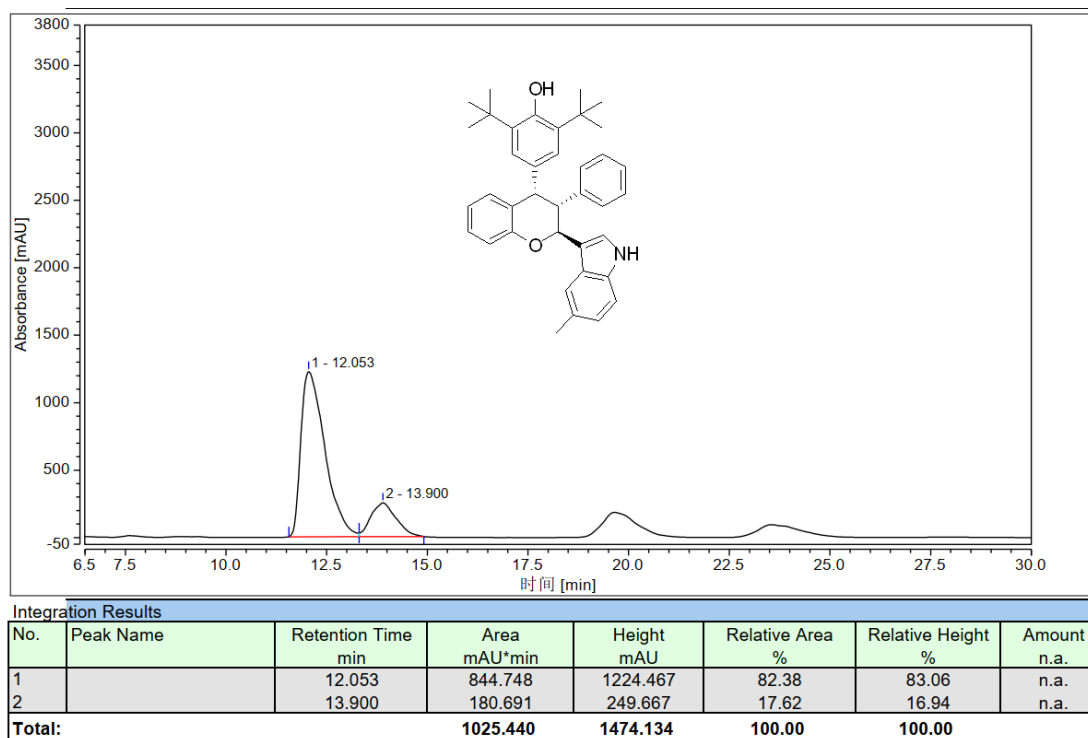
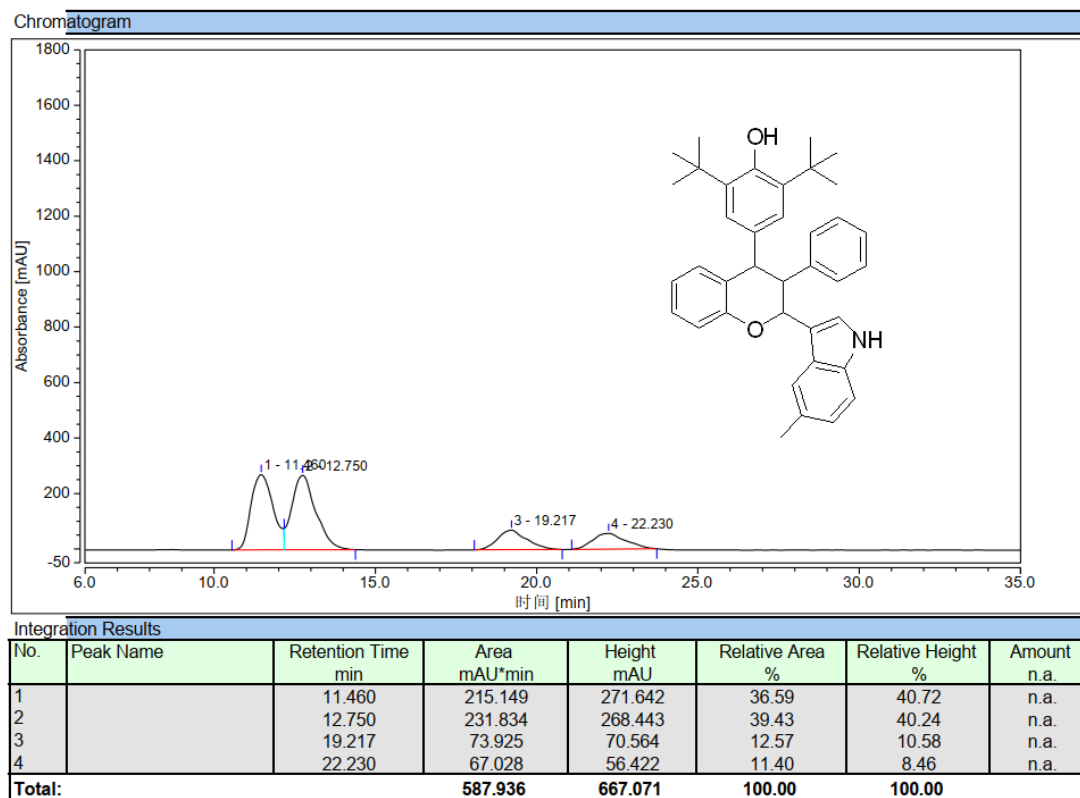
30a: (inseparable diastereomers, 84:16 dr):



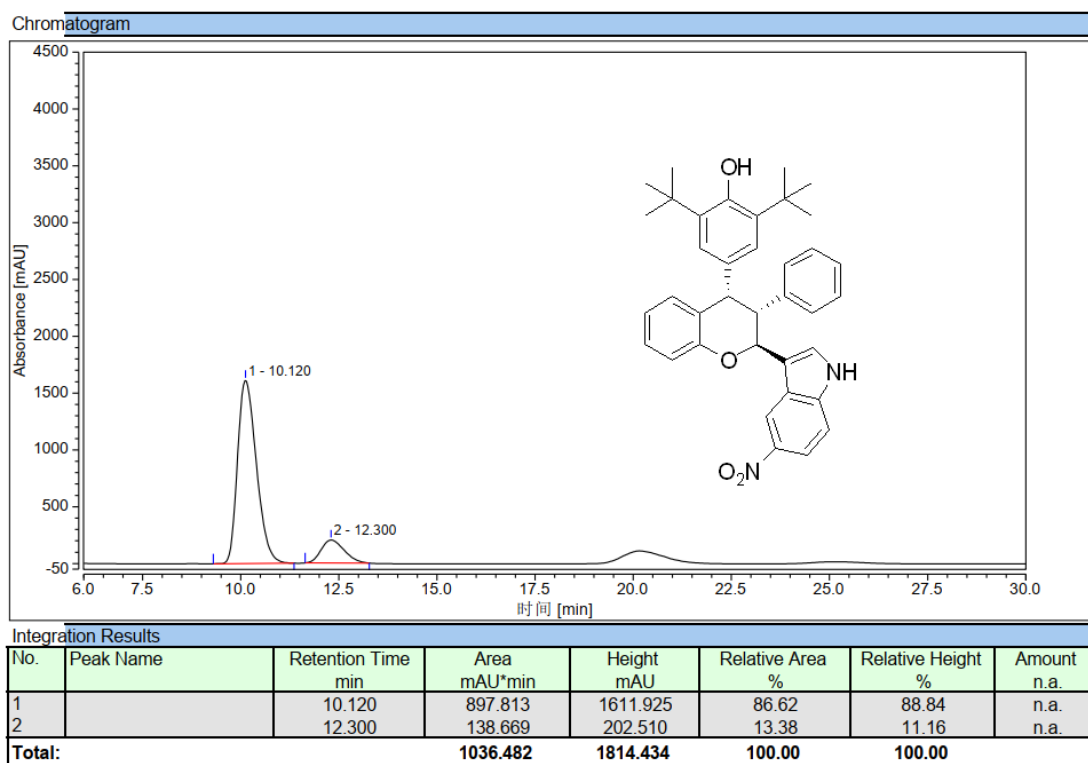
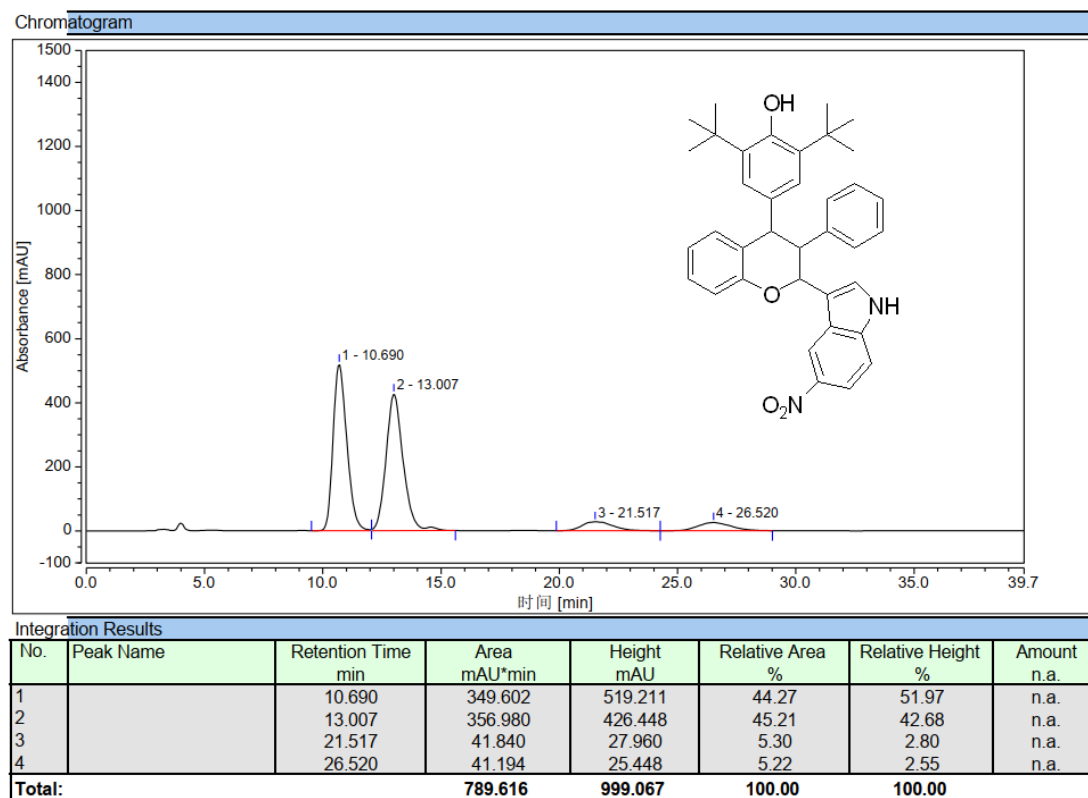
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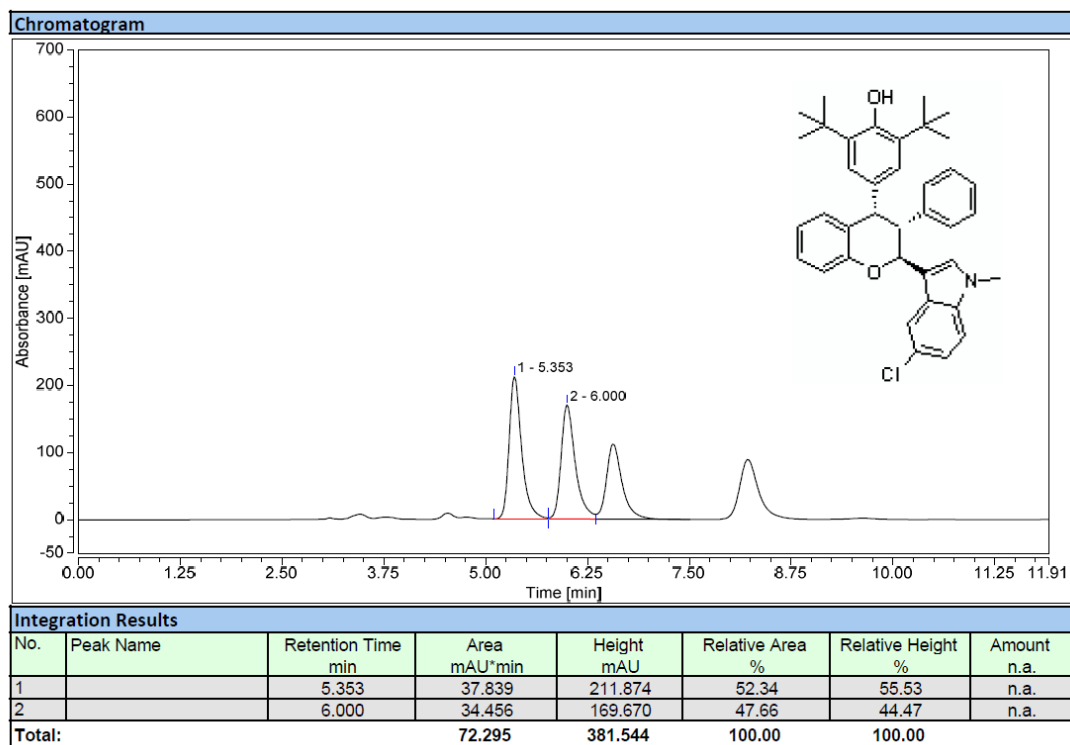
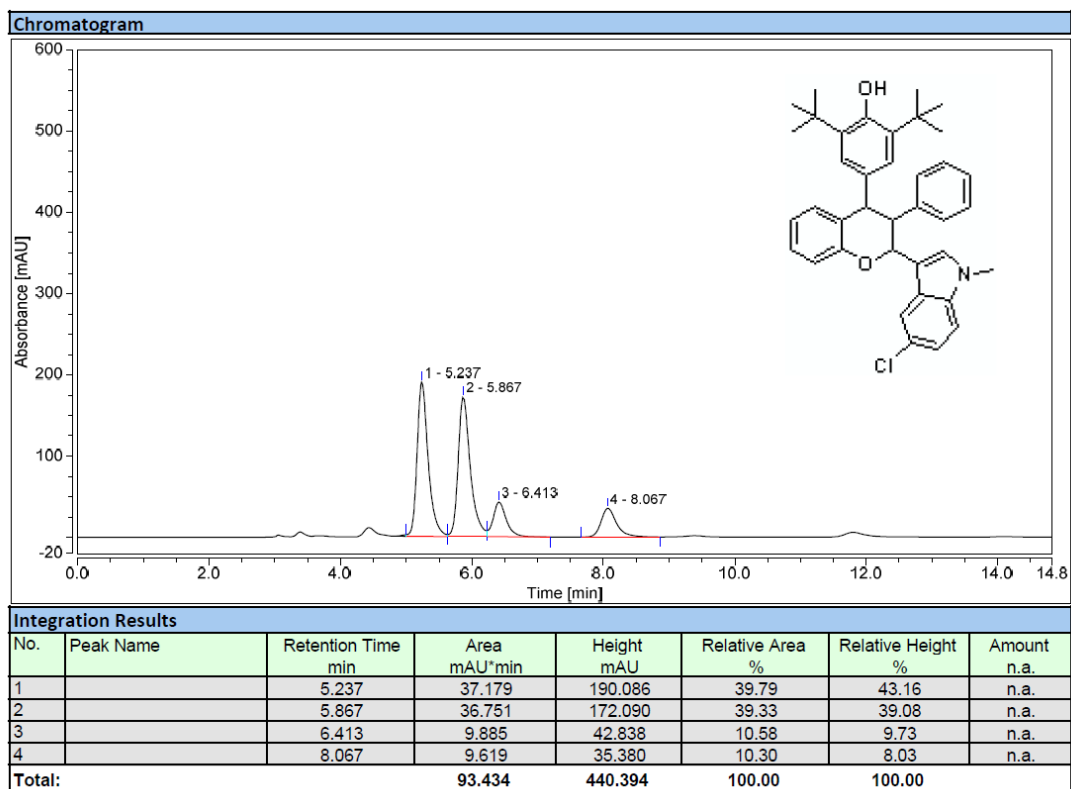
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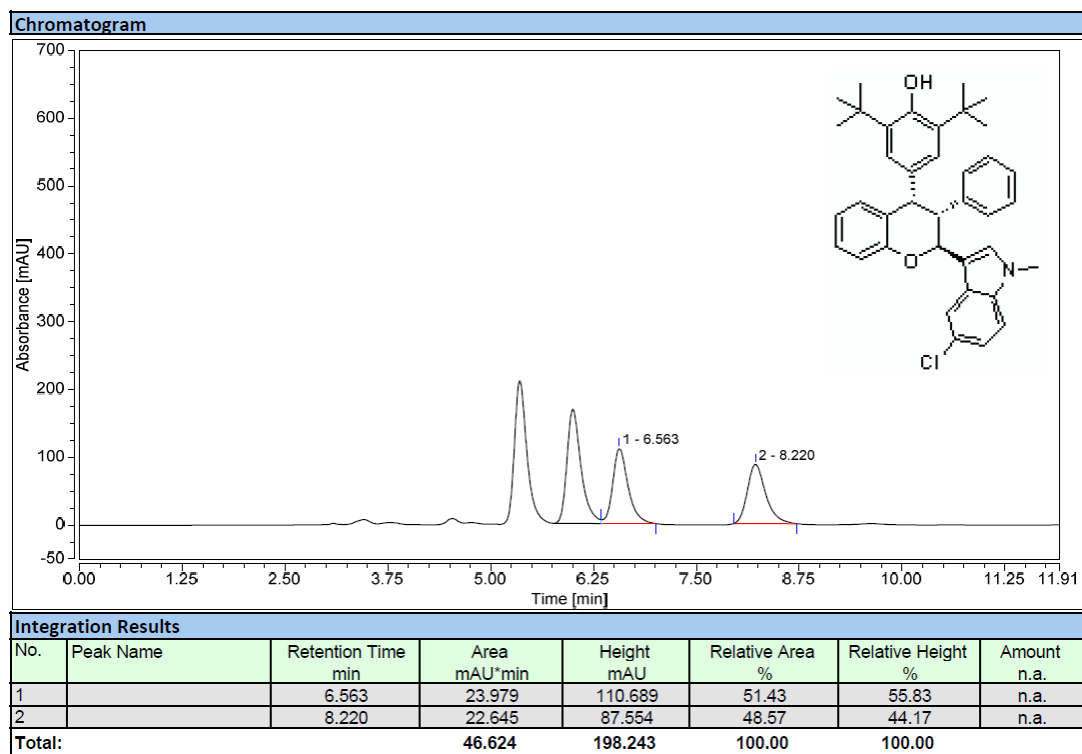


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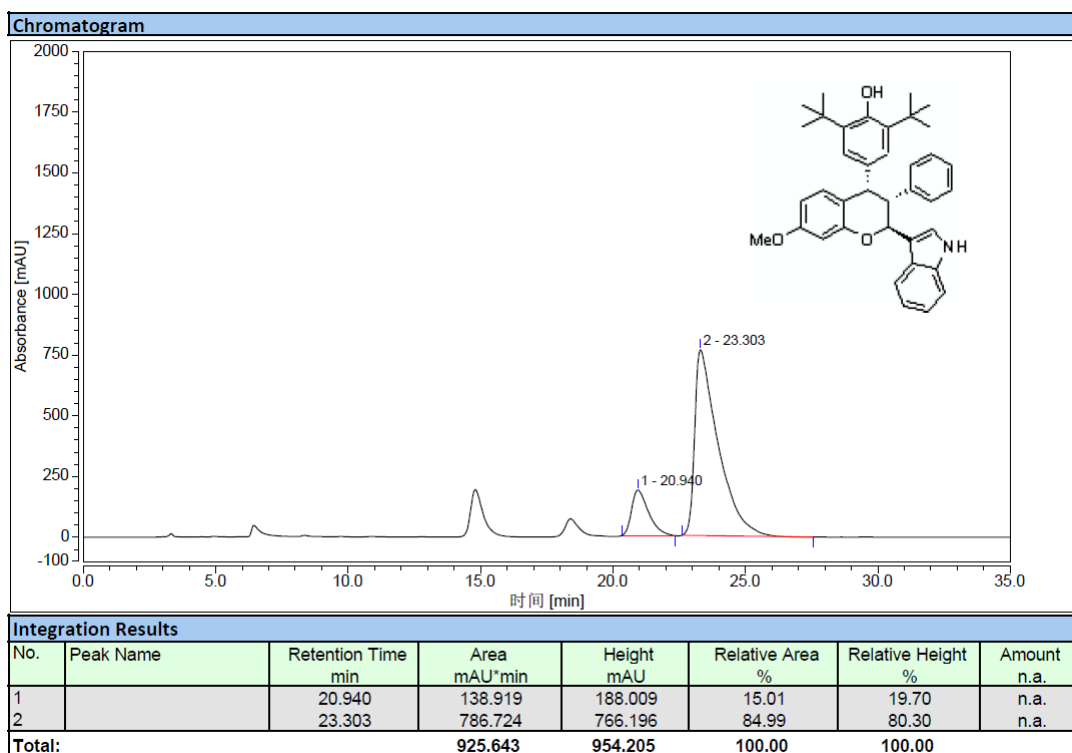
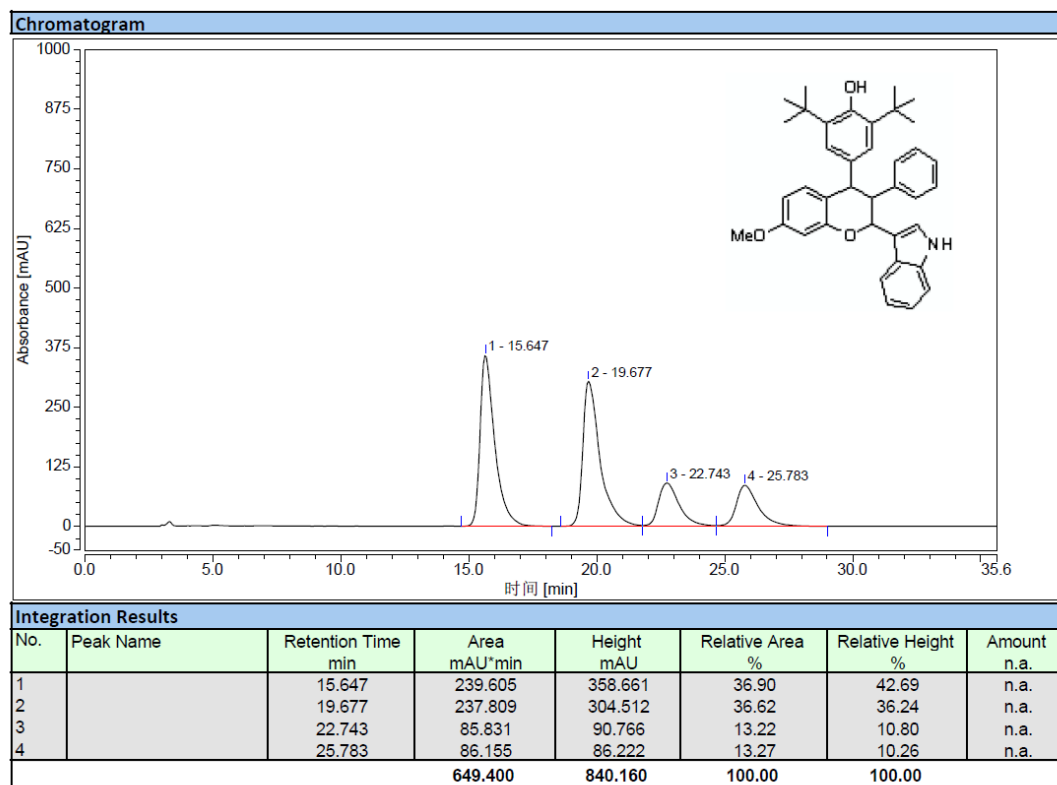


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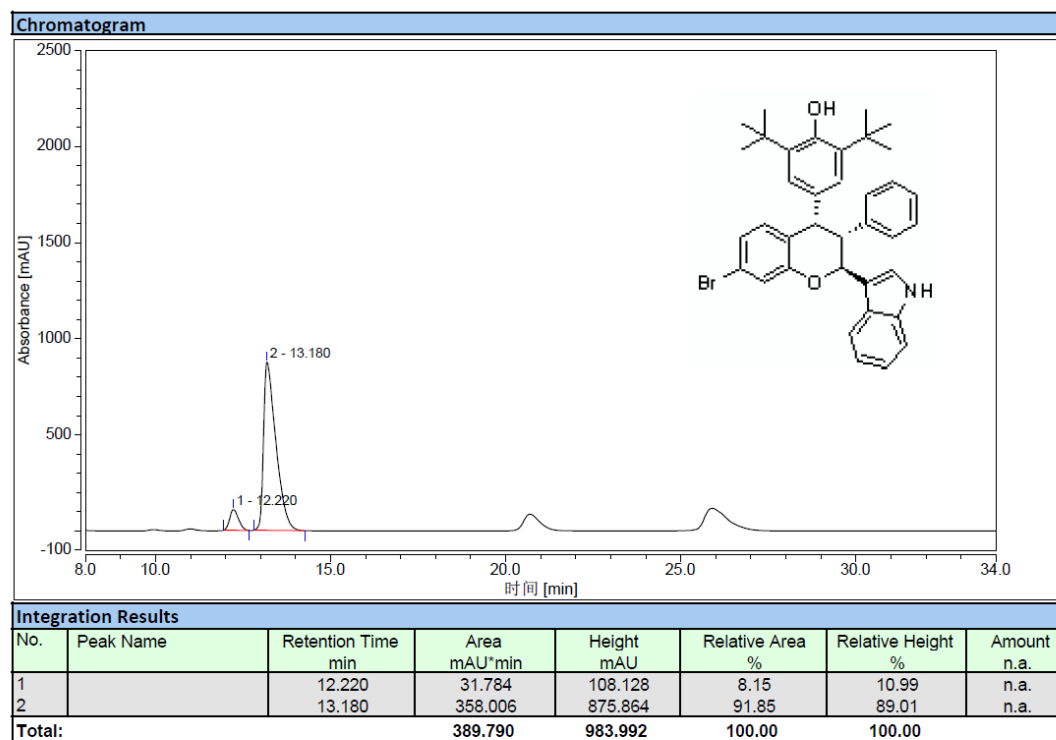
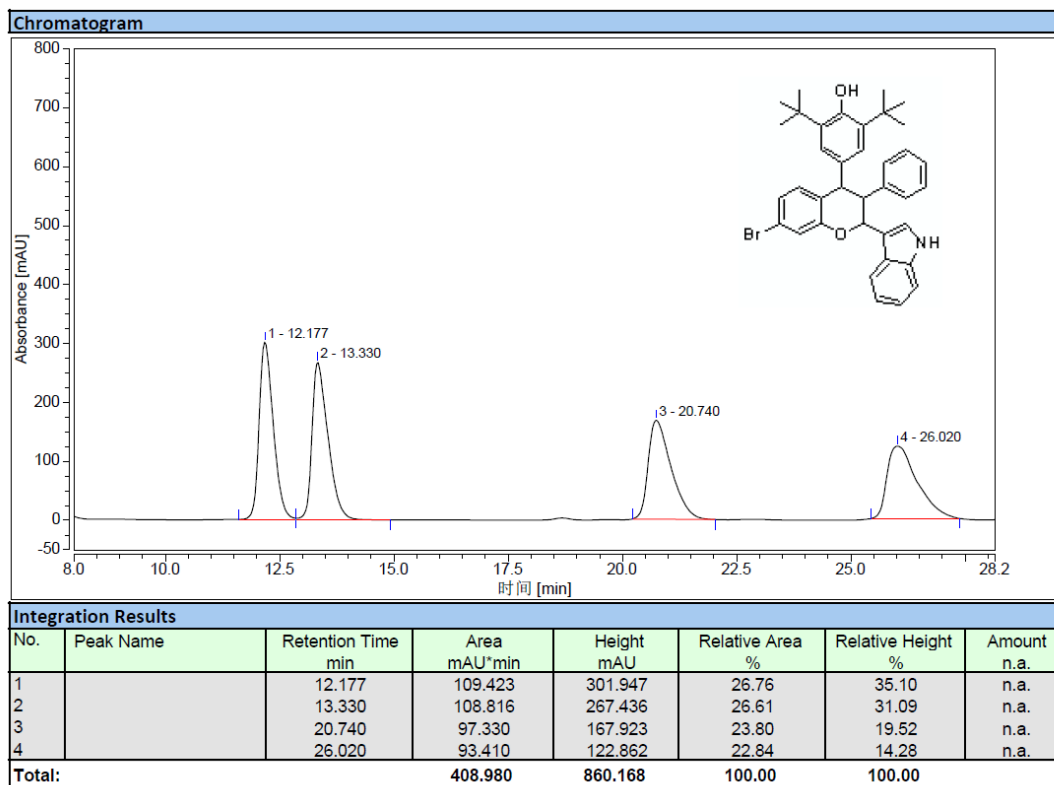




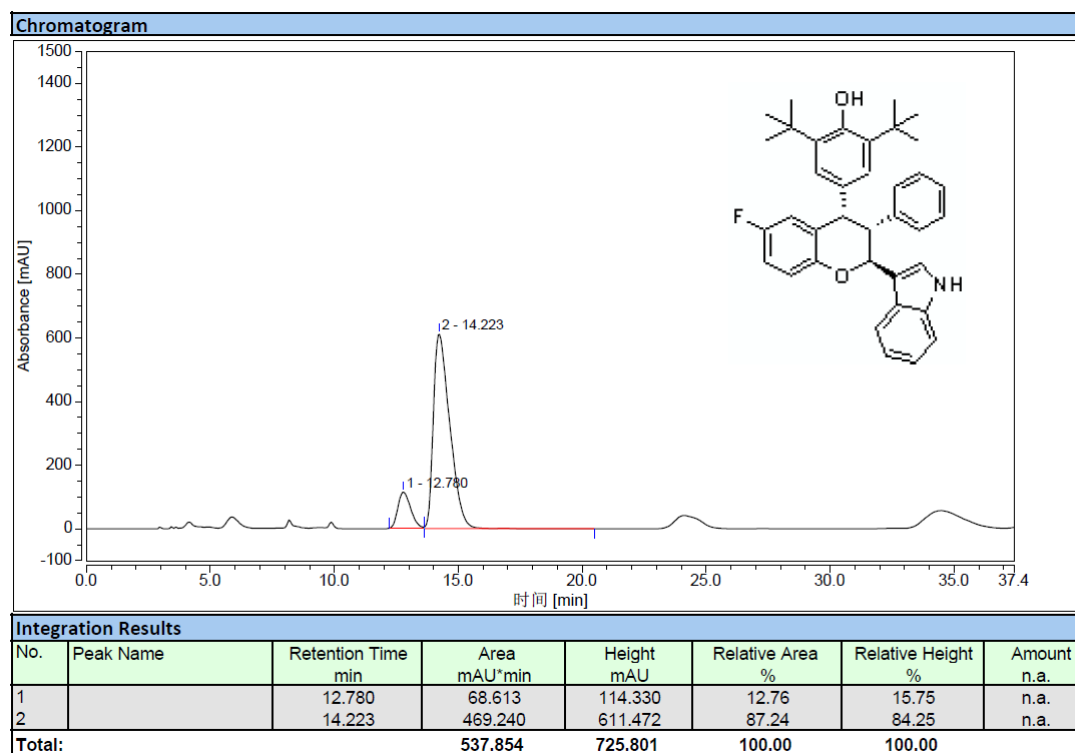
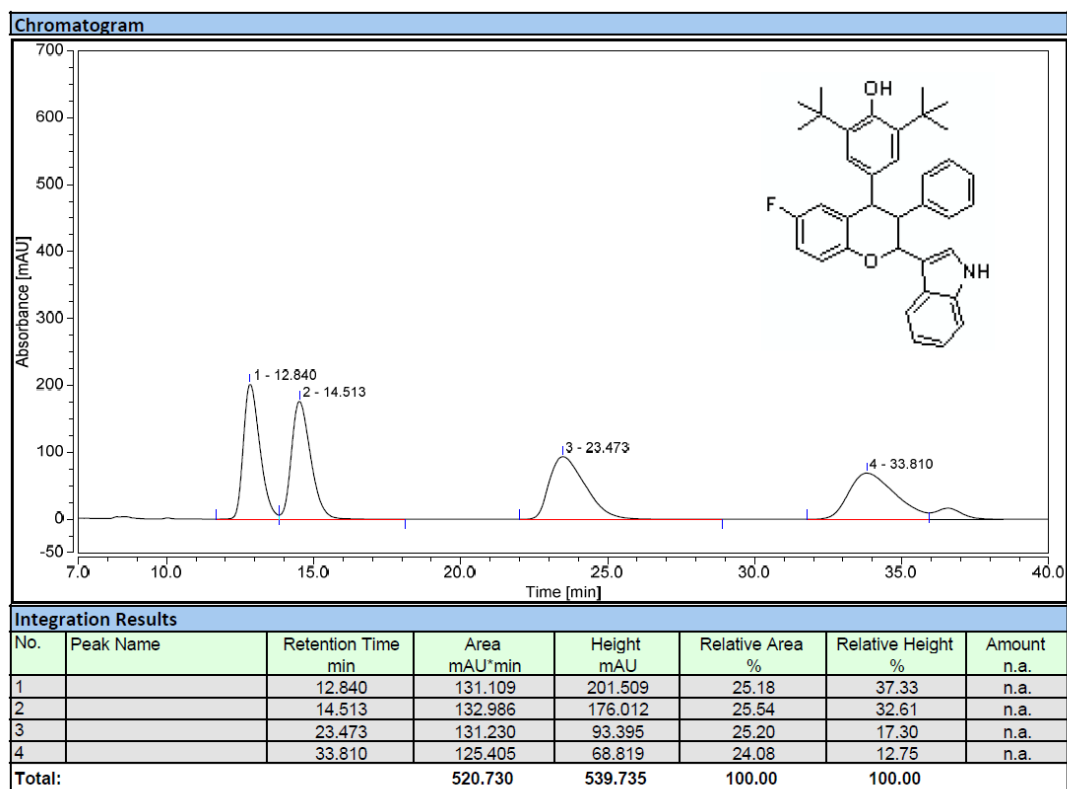
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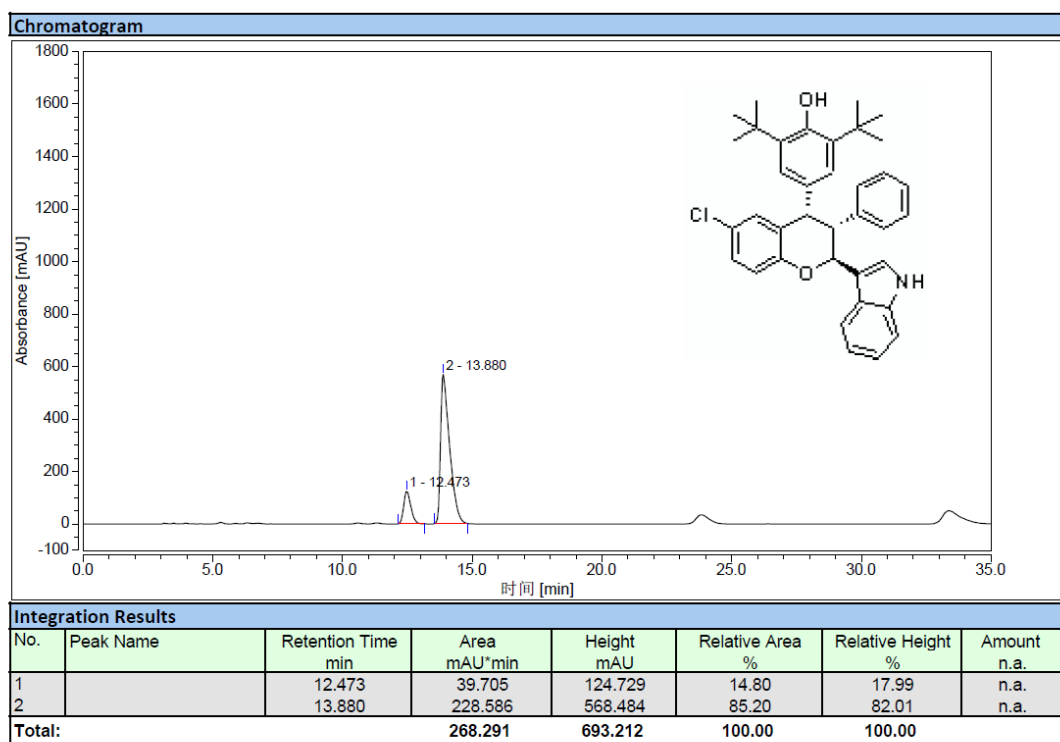
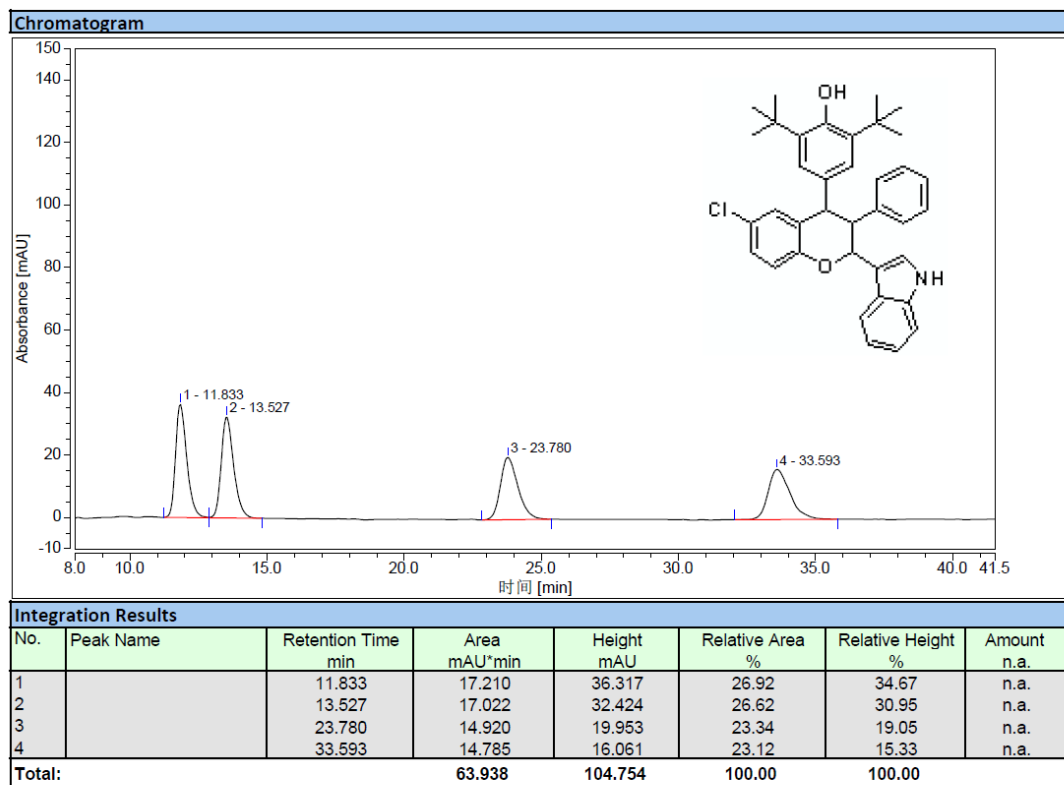
3ac: (inseparable diastereomers, 78:22 dr)



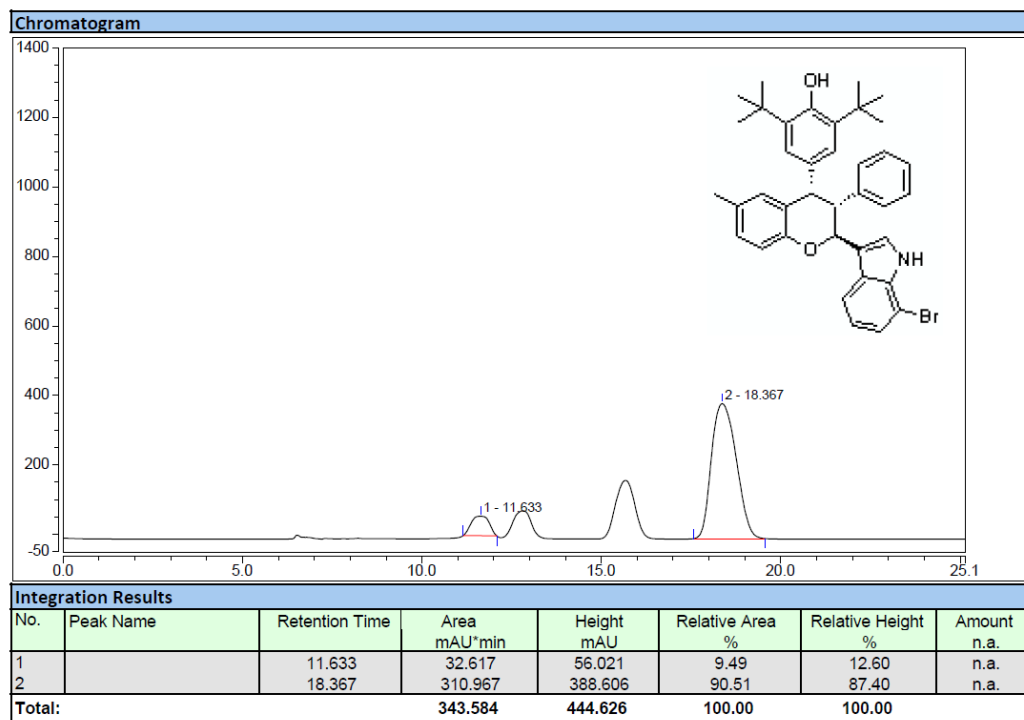
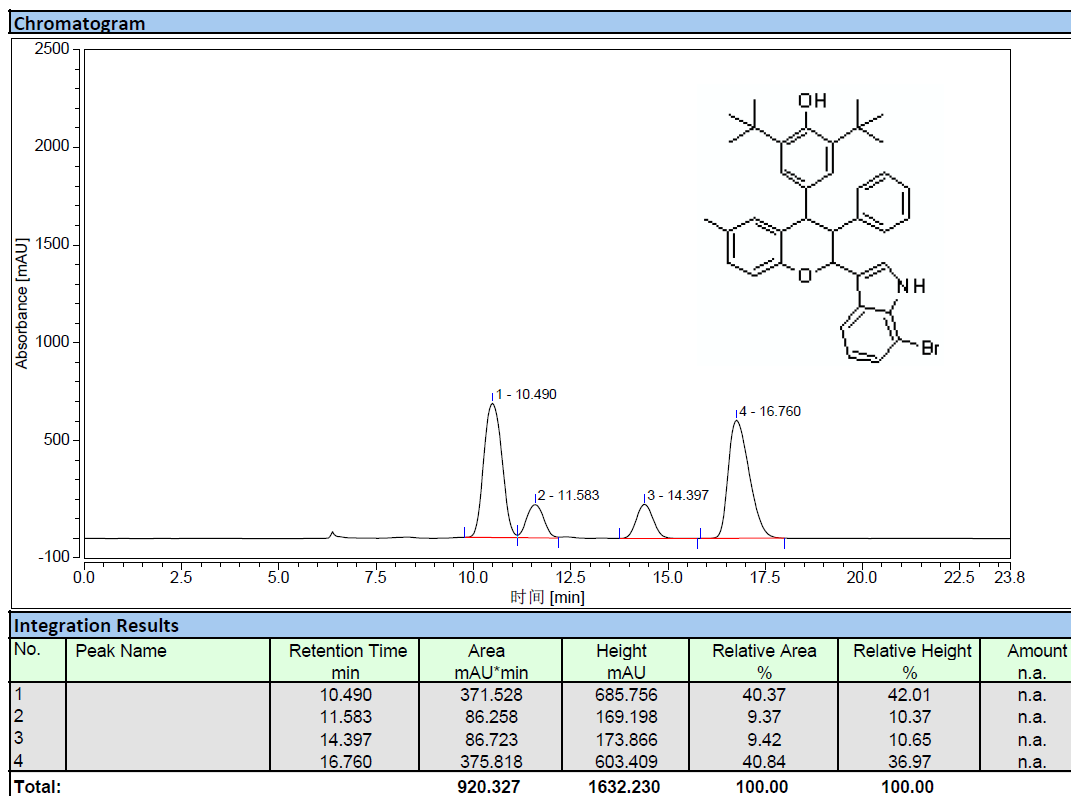
3ad: (inseparable diastereomers, 81:19 dr)

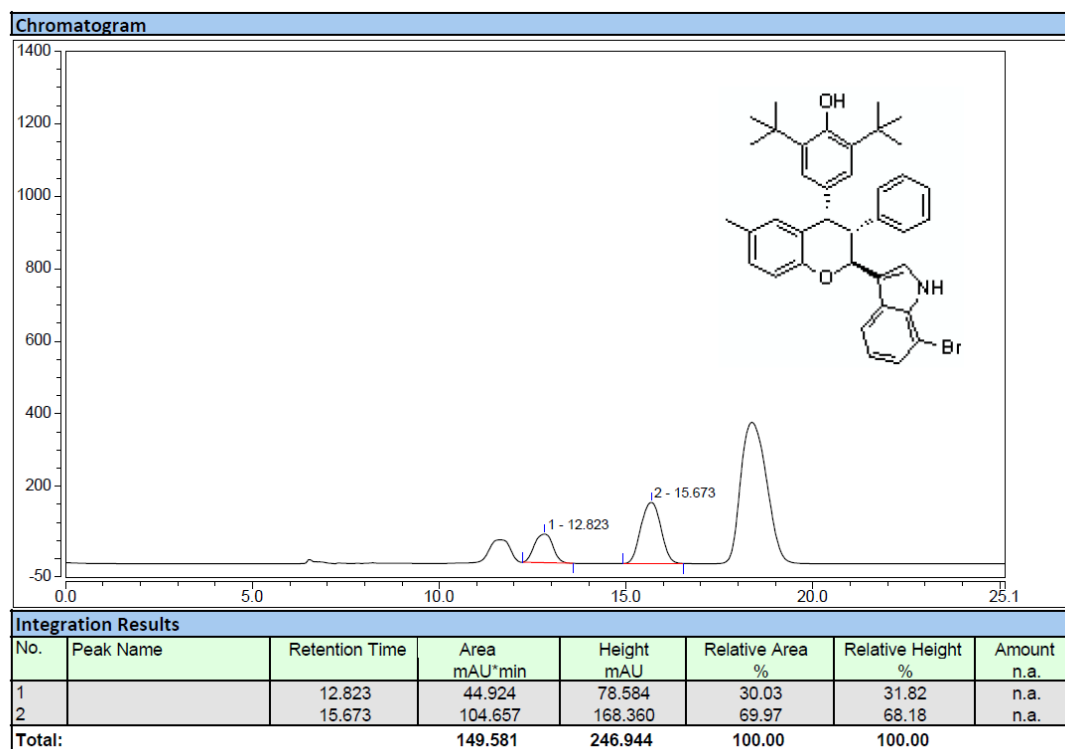


3ae: (inseparable diastereomers, 82:18 dr)

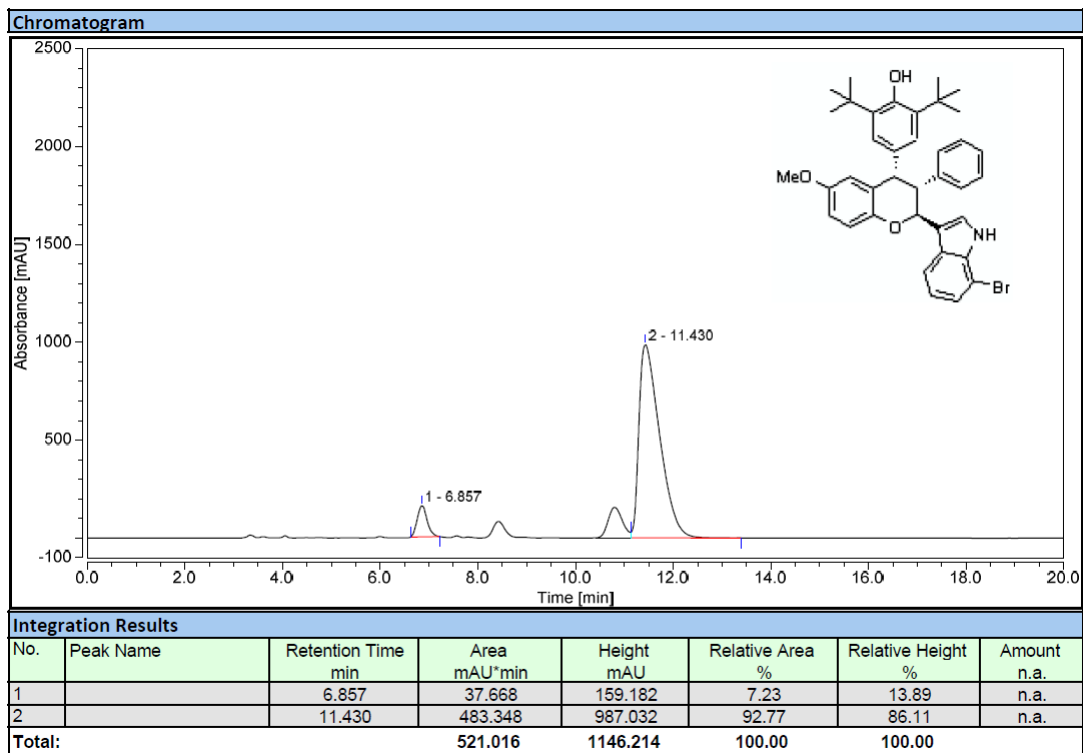
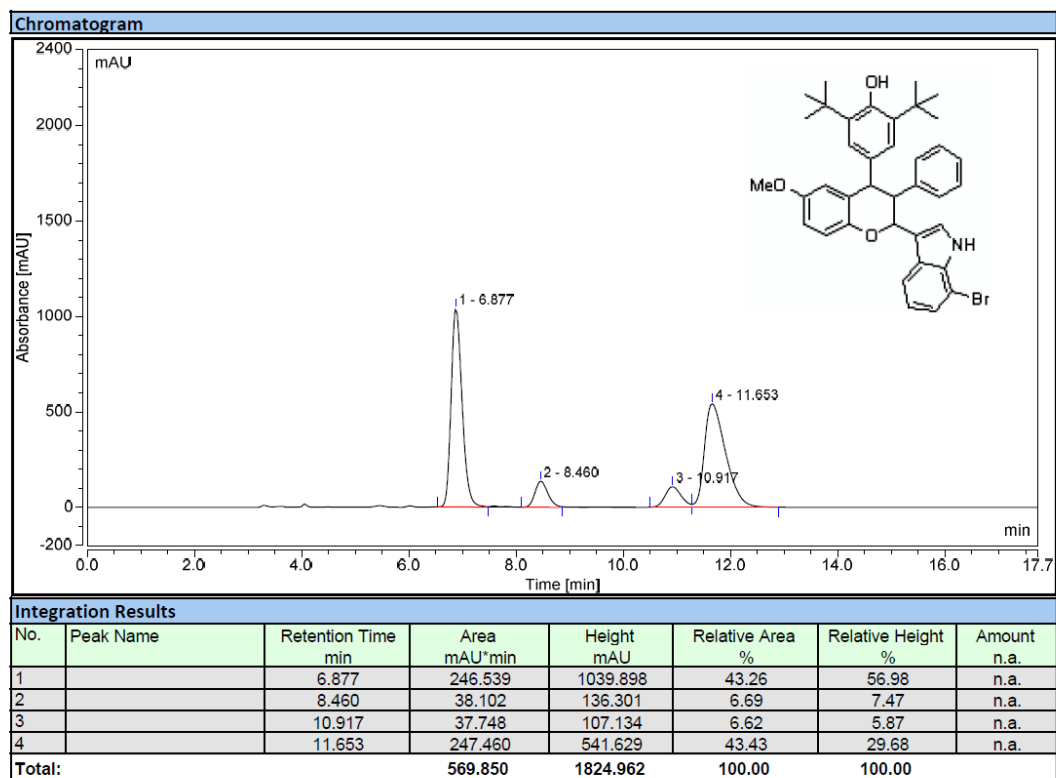


3pf: (inseparable diastereomers, 73:27 dr)

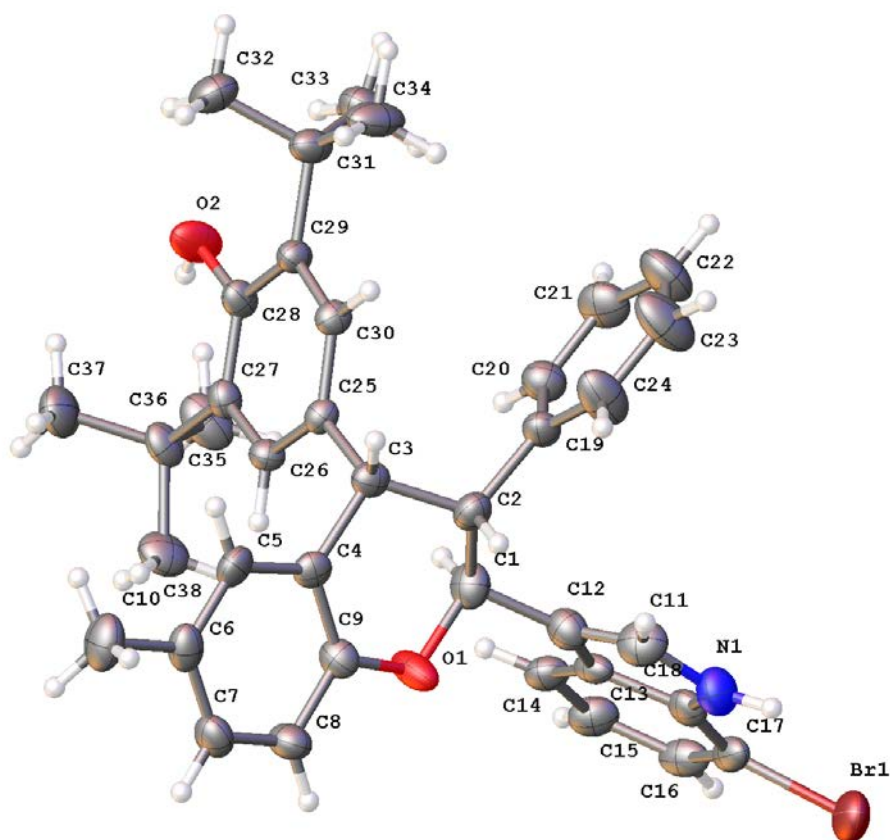
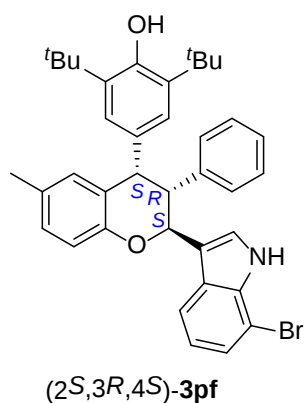




3pg: (inseparable diastereomers, 87:13 dr)



3. X-ray single crystal data for compound 3pf



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

Empirical formula	C ₃₈ H ₄₀ Br N O ₂	
Formula weight	622.62	
Temperature	296.15 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 10.382(3) Å	α = 90°.
	b = 15.766(4) Å	β = 90°.

	c = 20.036(6) Å	$\gamma = 90^\circ$.
Volume	3279.6(16) Å ³	
Z	4	
Density (calculated)	1.261 Mg/m ³	
Absorption coefficient	1.286 mm ⁻¹	
F(000)	1304	
Theta range for data collection	2.777 to 27.501°.	
Index ranges	-13<=h<=11, -20<=k<=20, -26<=l<=21	
Reflections collected	19417	
Independent reflections	7385 [R(int) = 0.0362]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7385 / 3 / 387	
Goodness-of-fit on F ²	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0594, wR2 = 0.1422	
R indices (all data)	R1 = 0.1011, wR2 = 0.1594	
Absolute structure parameter	0.032(6)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.781 and -0.548 e.Å ⁻³	