

## Supplementary Information

### Diastereoselective Synthesis of *trans*-2,3-Dihydroindoles via Formal [4+1] Annulation Reactions of Sulfonium Ylide

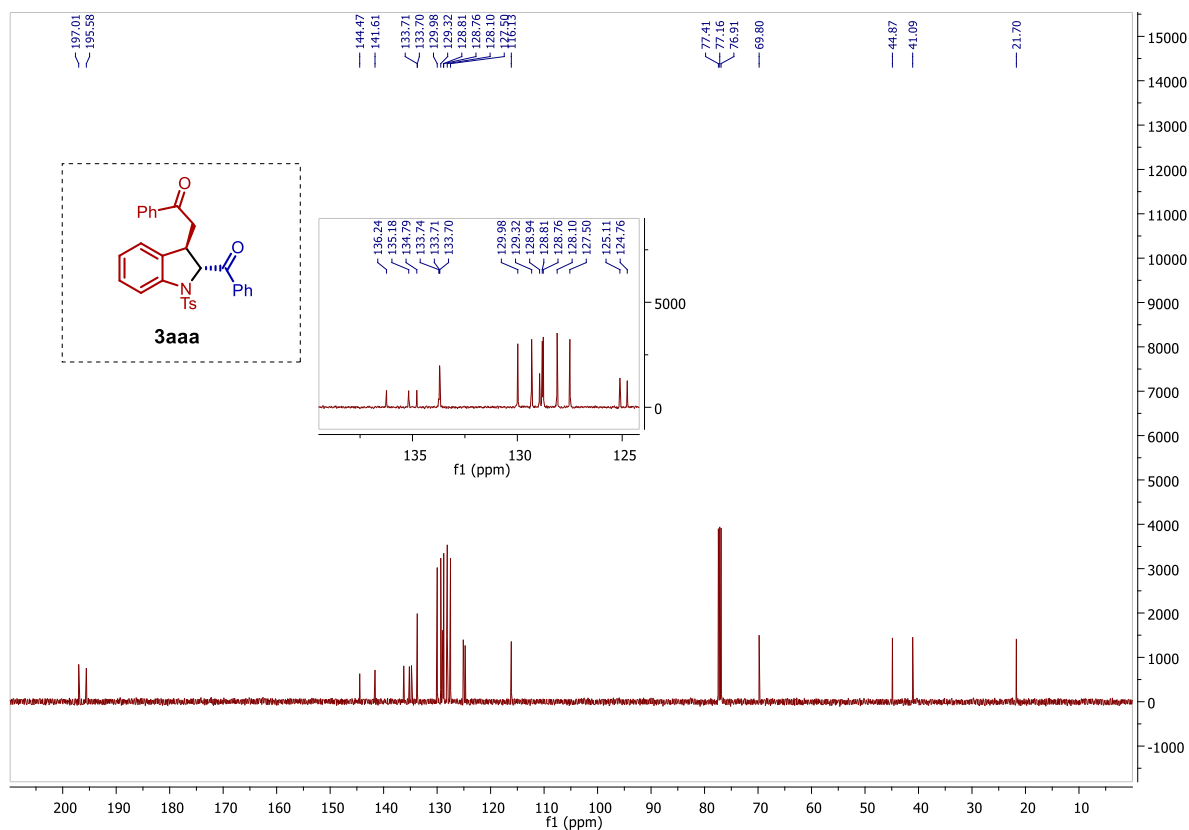
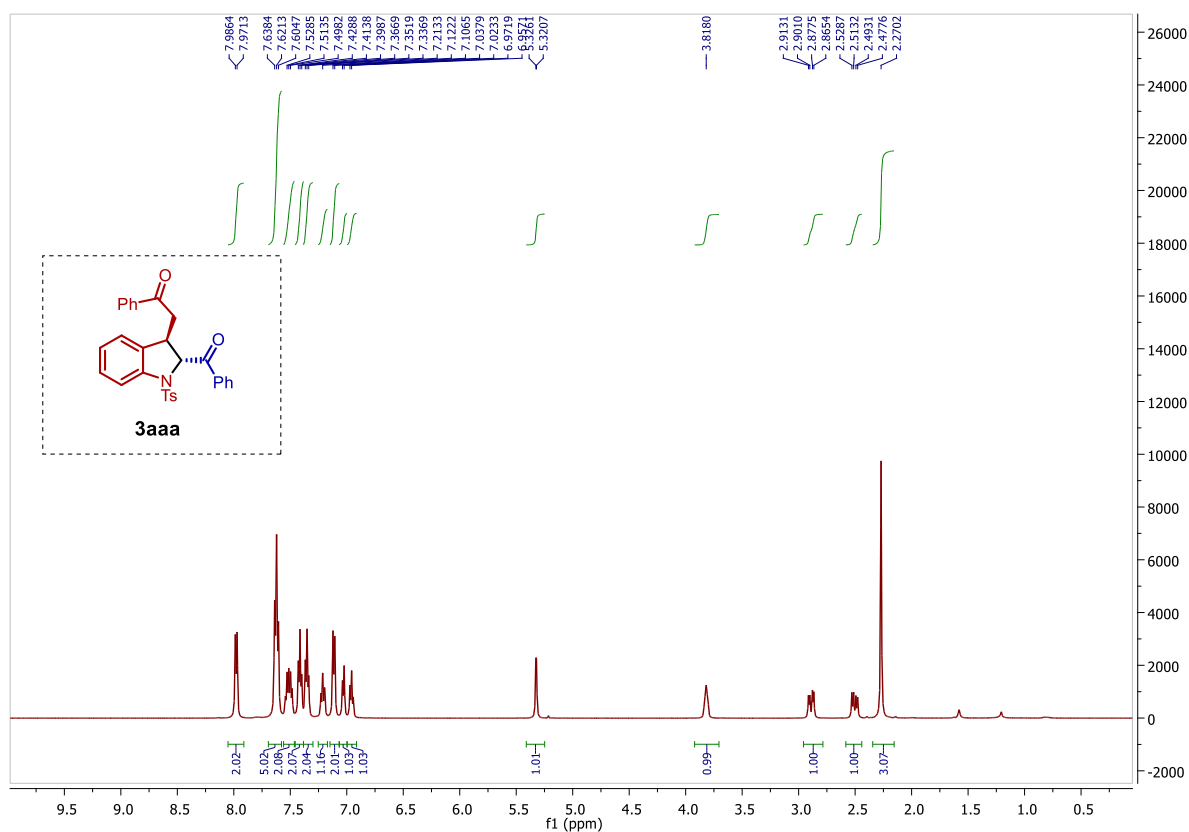
Anshul Jain,<sup>a</sup> Akanksha Kumari,<sup>a</sup> Ramesh K. Metre,<sup>a</sup> Nirmal K. Rana<sup>a\*</sup>

<sup>a</sup>Department of Chemistry, Indian Institute of Technology Jodhpur, Jodhpur-342030, India

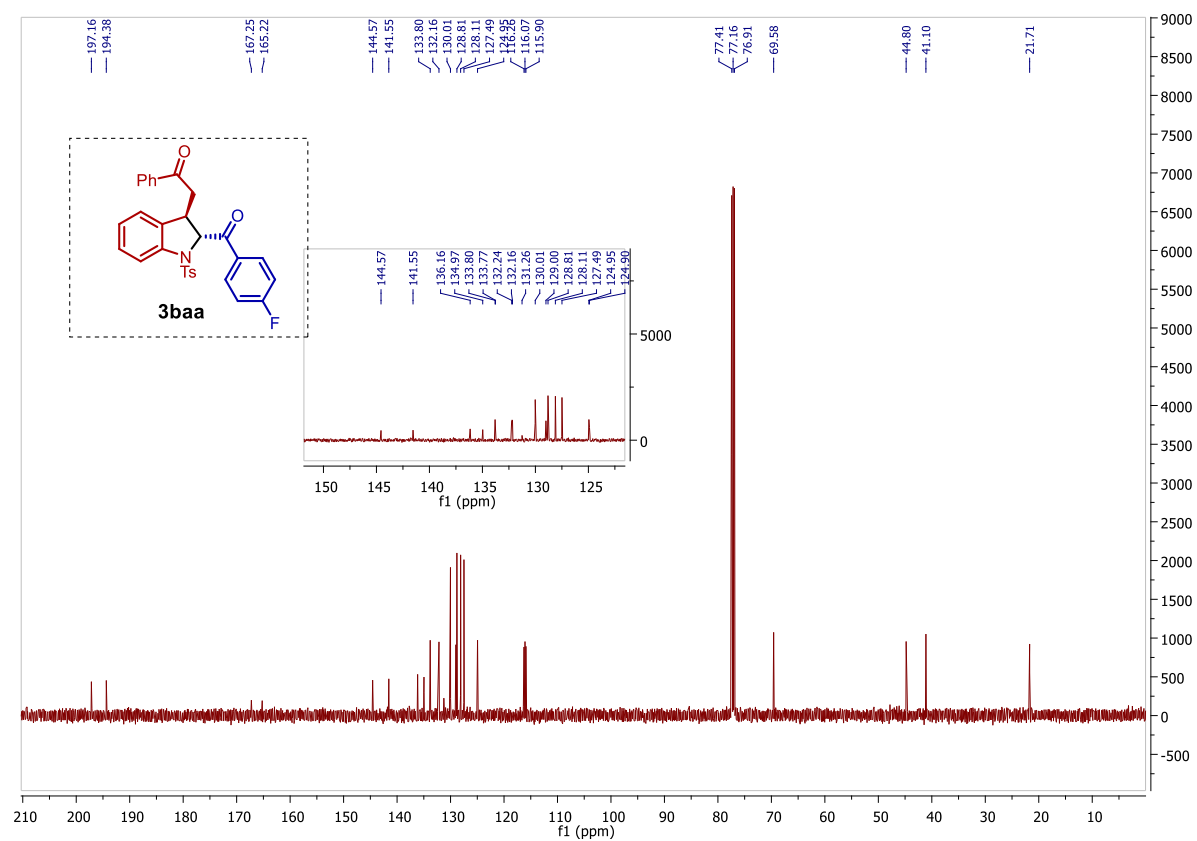
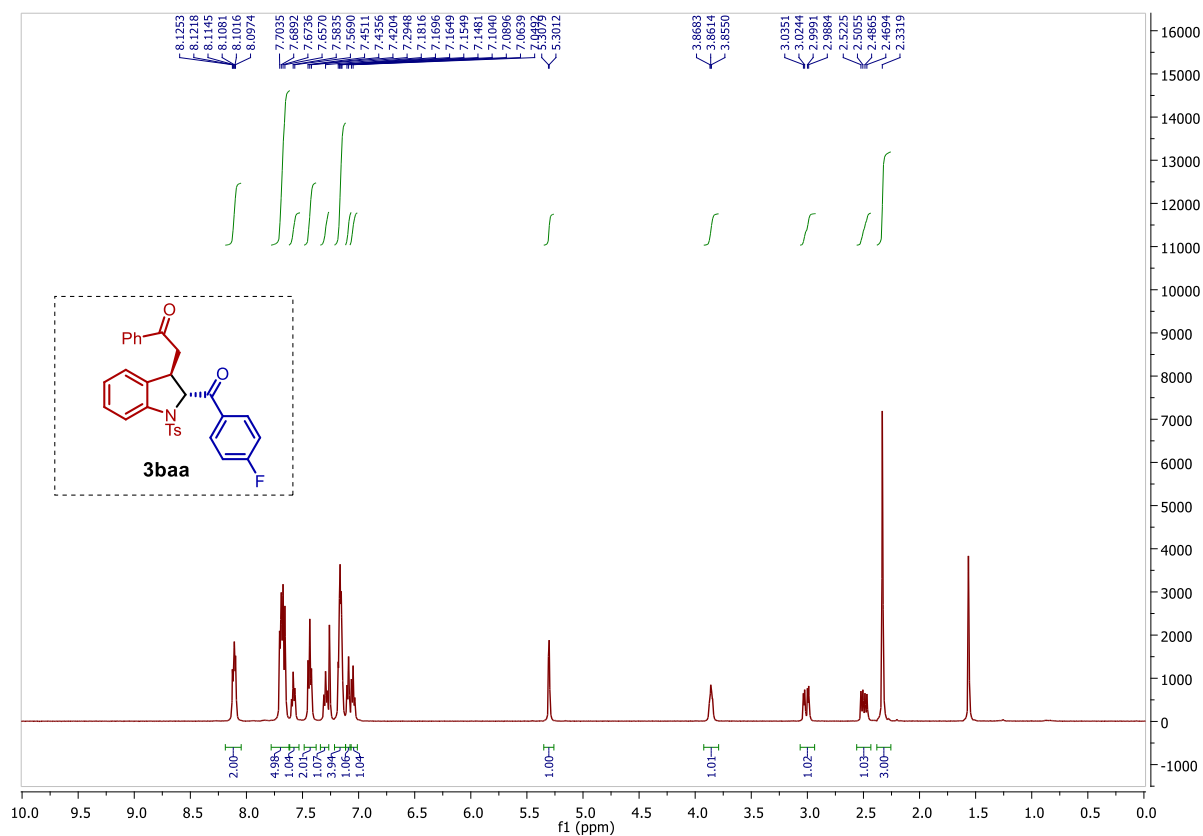
Email: nirmalrana@iitj.ac.in

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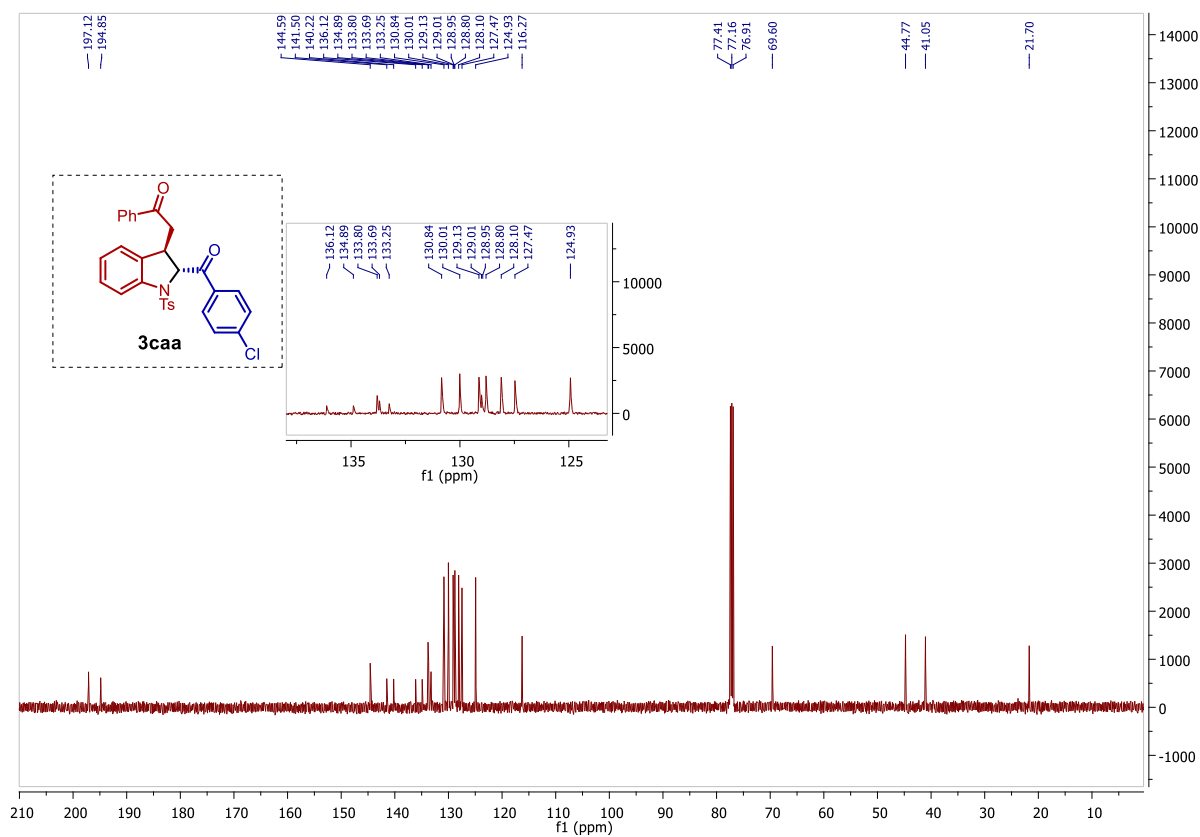
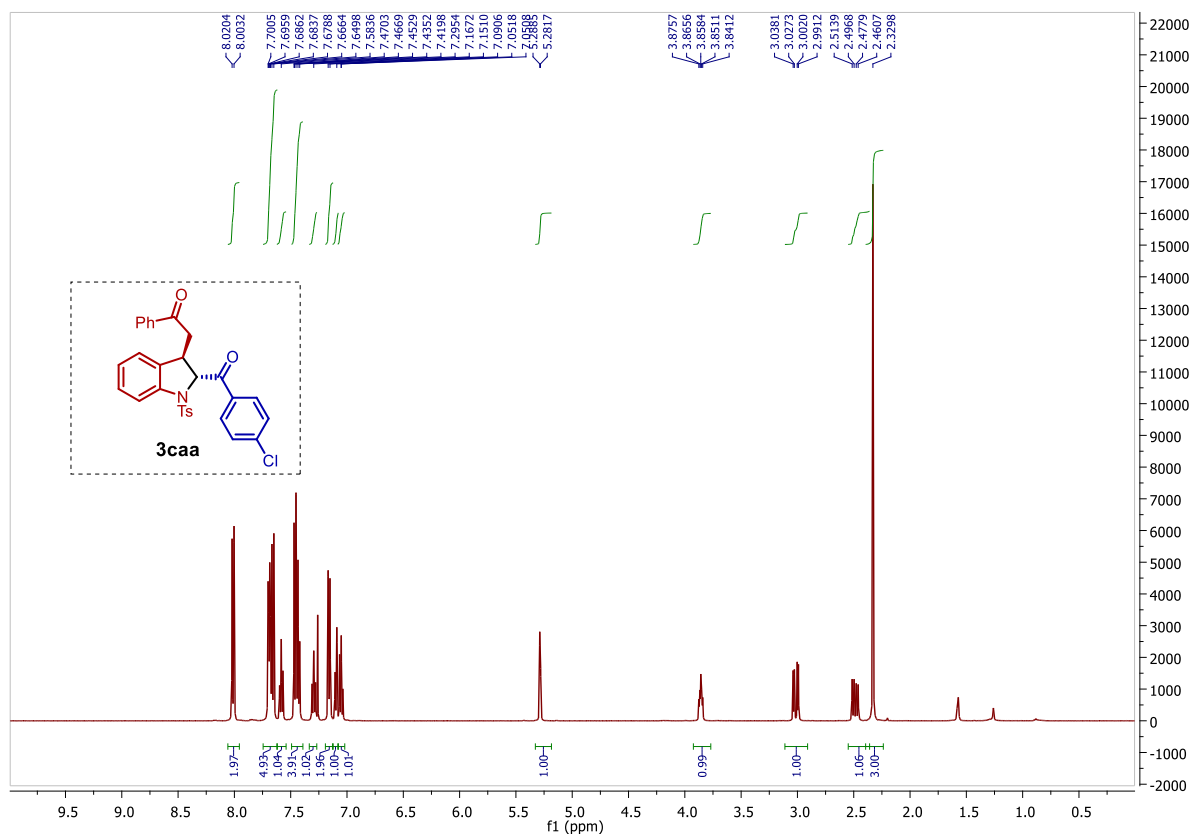
# 1. $^1\text{H}$ and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra



$\text{CDCl}_3$ , 500 MHz  $^1\text{H}$  NMR and 125 MHz  $^{13}\text{C}\{^1\text{H}\}$  NMR Spectra of **3aaa**

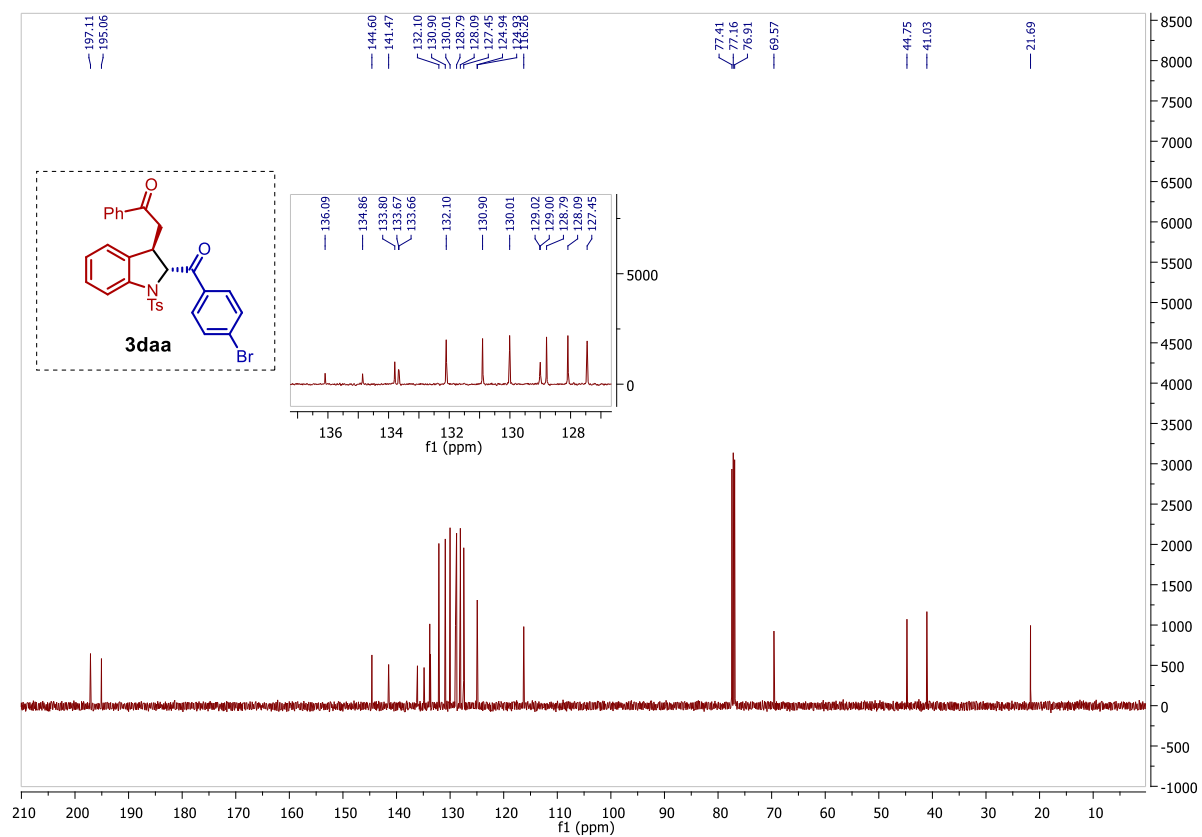
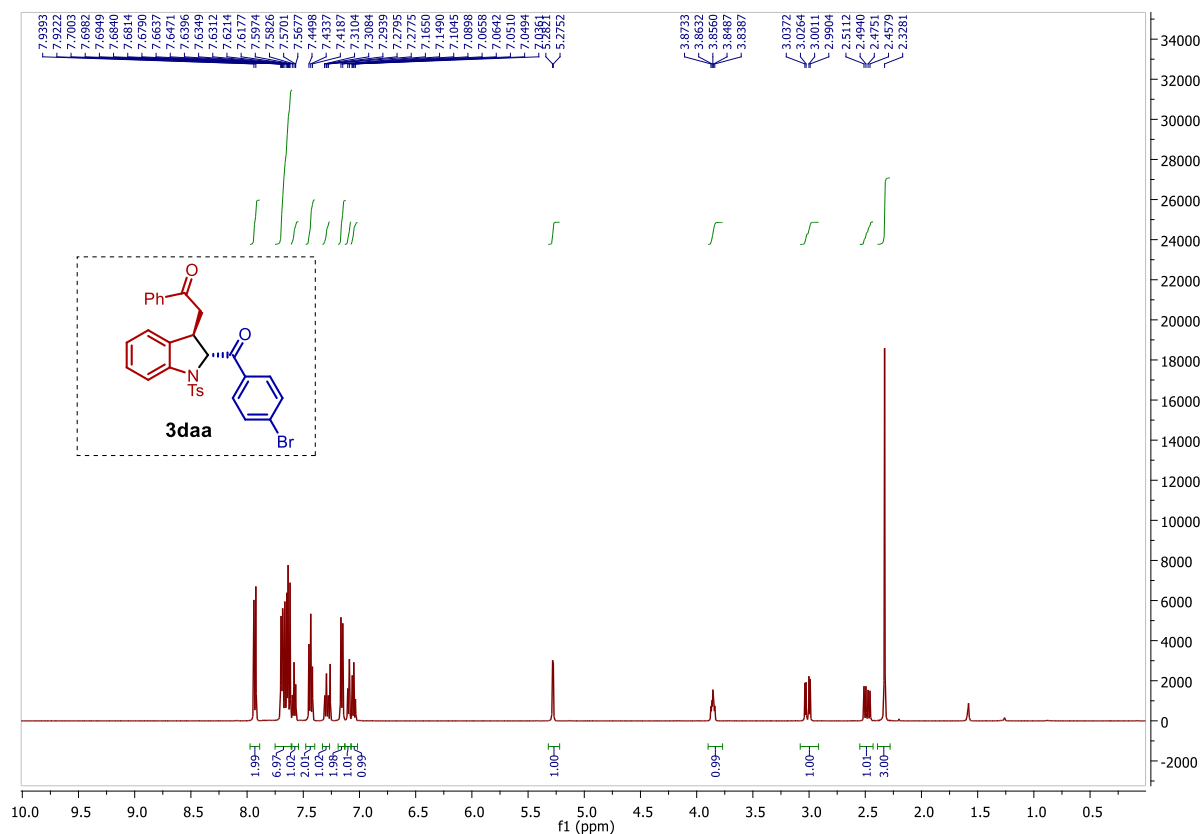


CDCl<sub>3</sub>, 500 MHz <sup>1</sup>H NMR and 125 MHz <sup>13</sup>C{<sup>1</sup>H} NMR Spectra of **3baa**

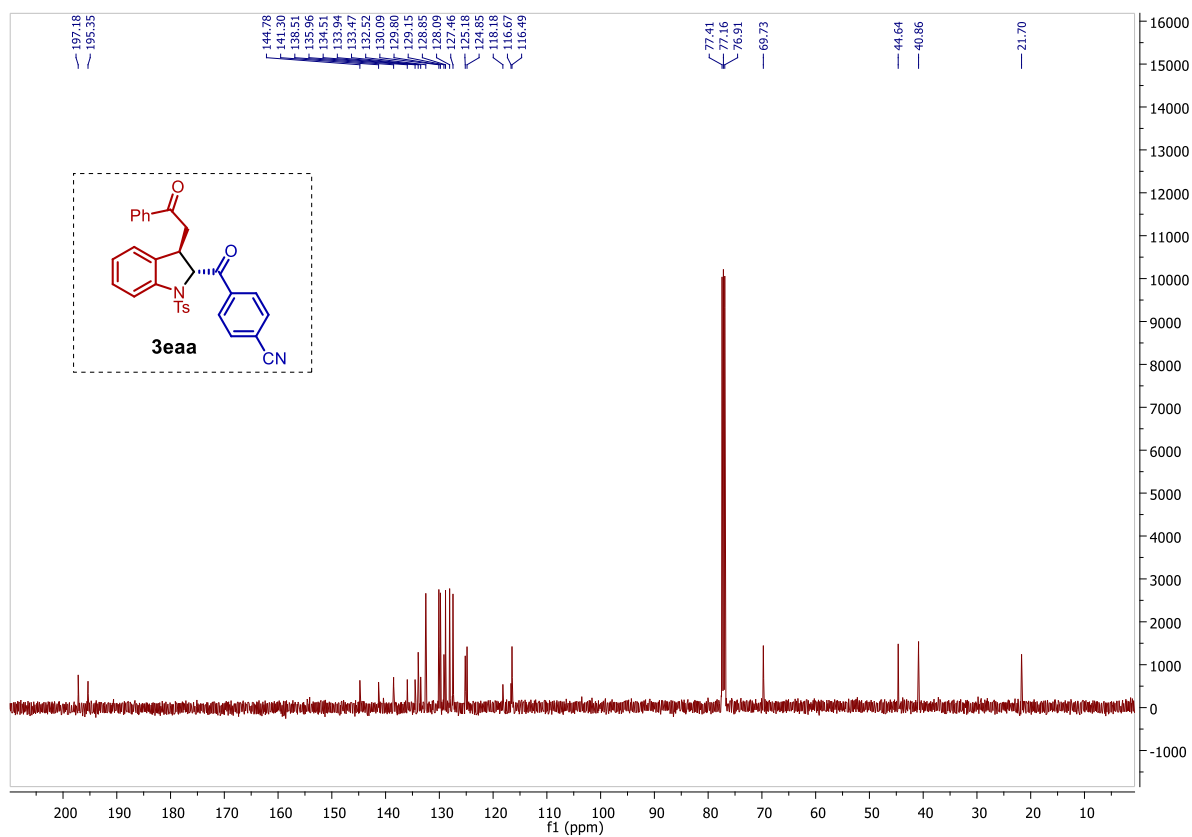
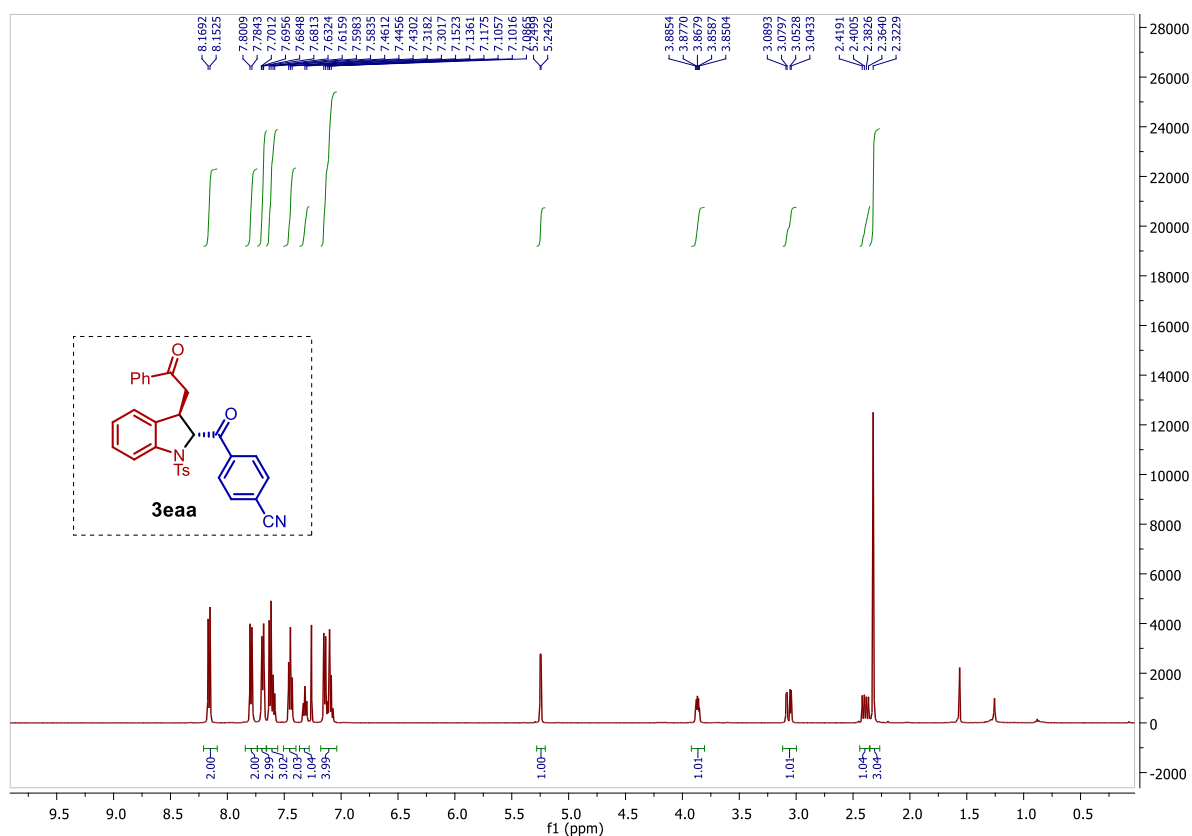




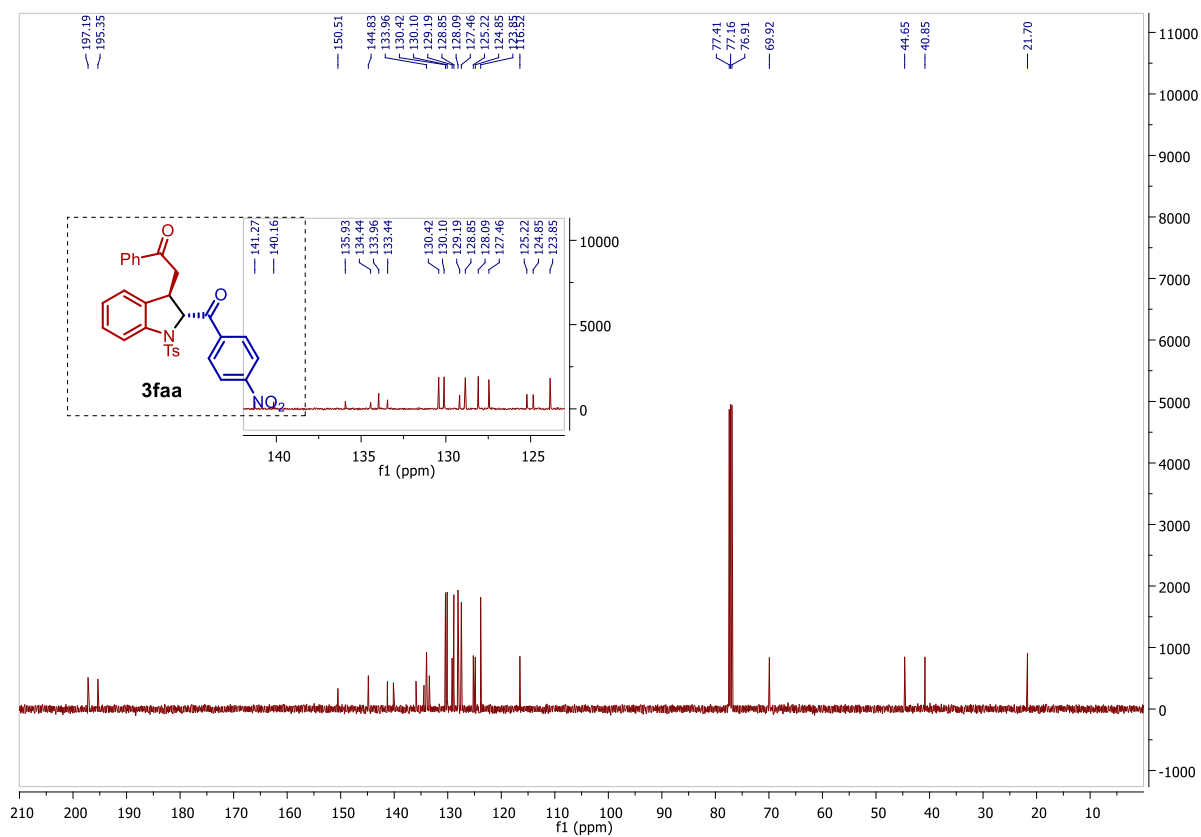
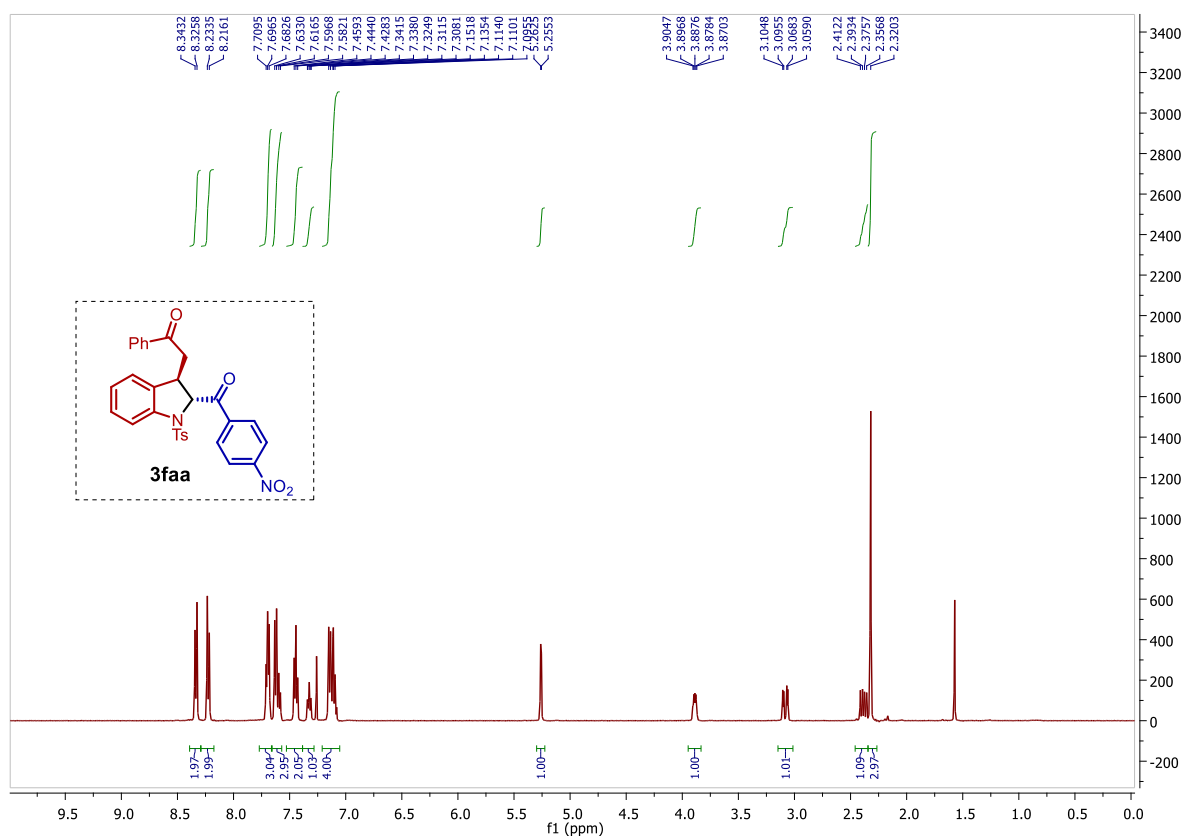
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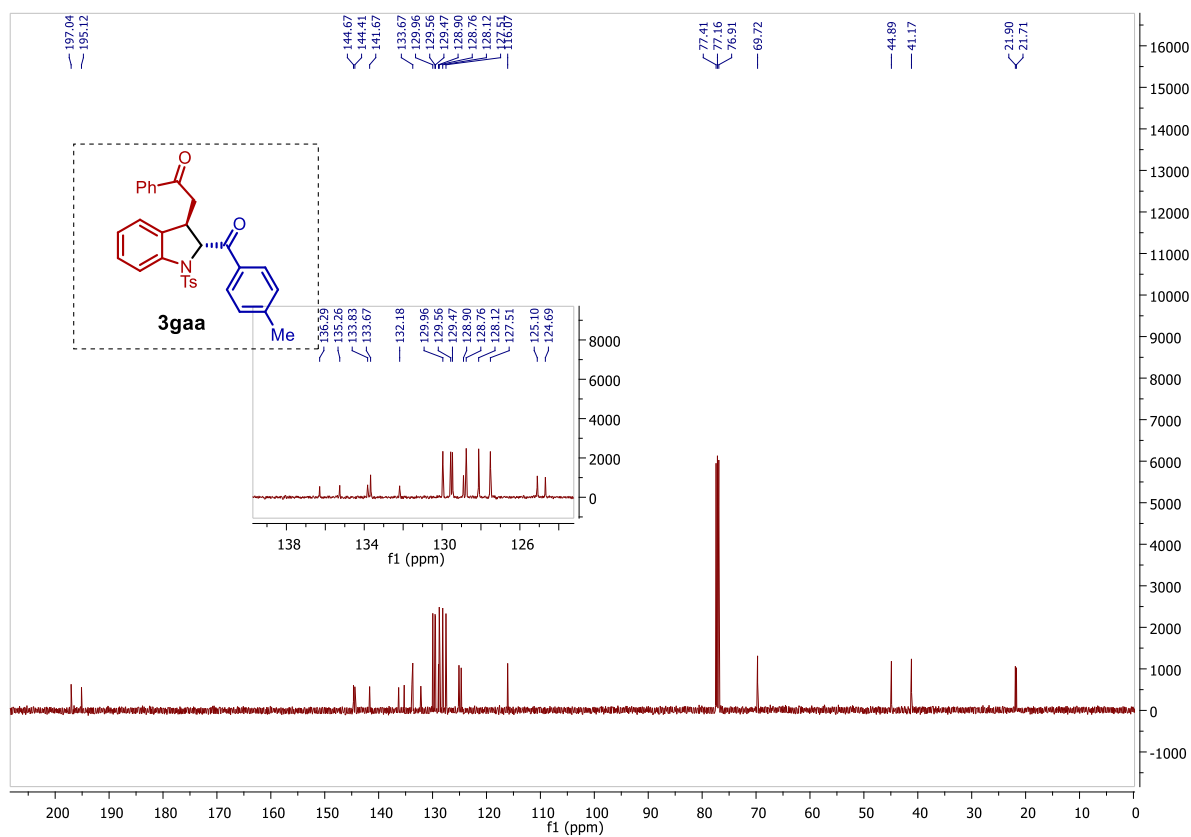
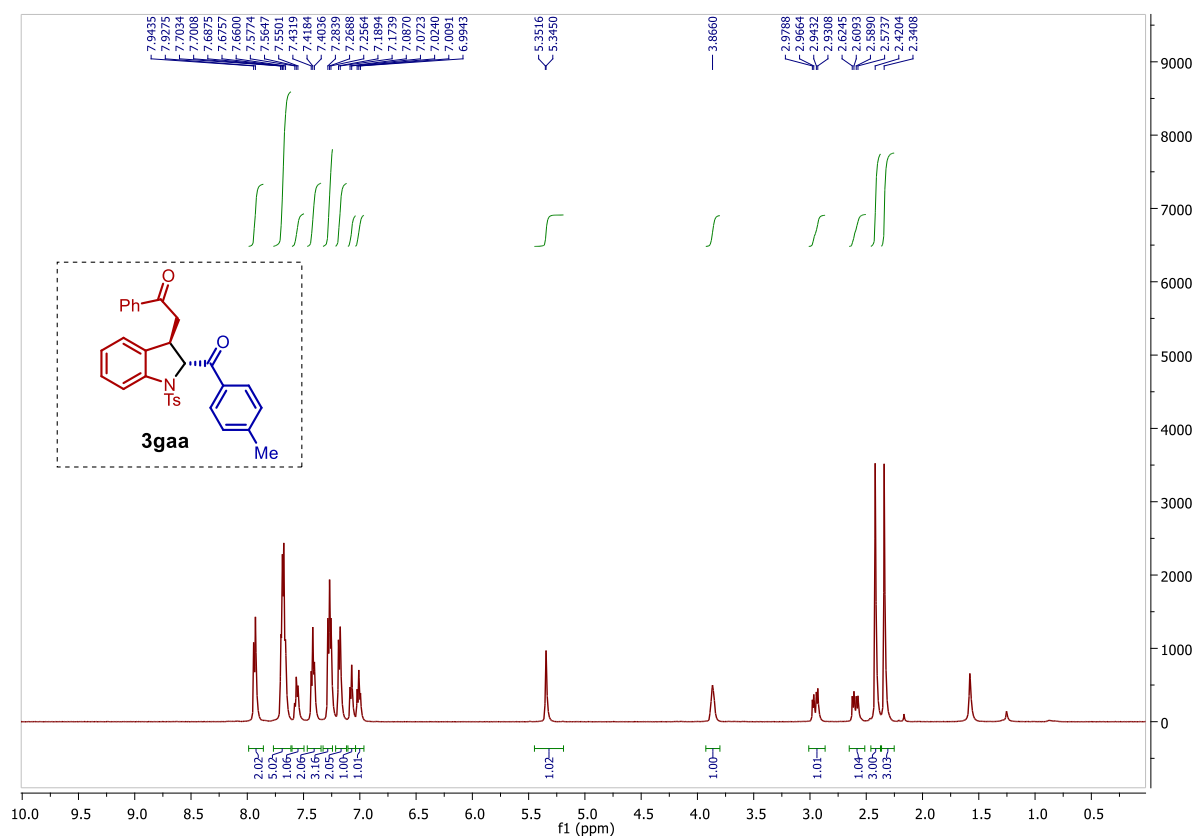
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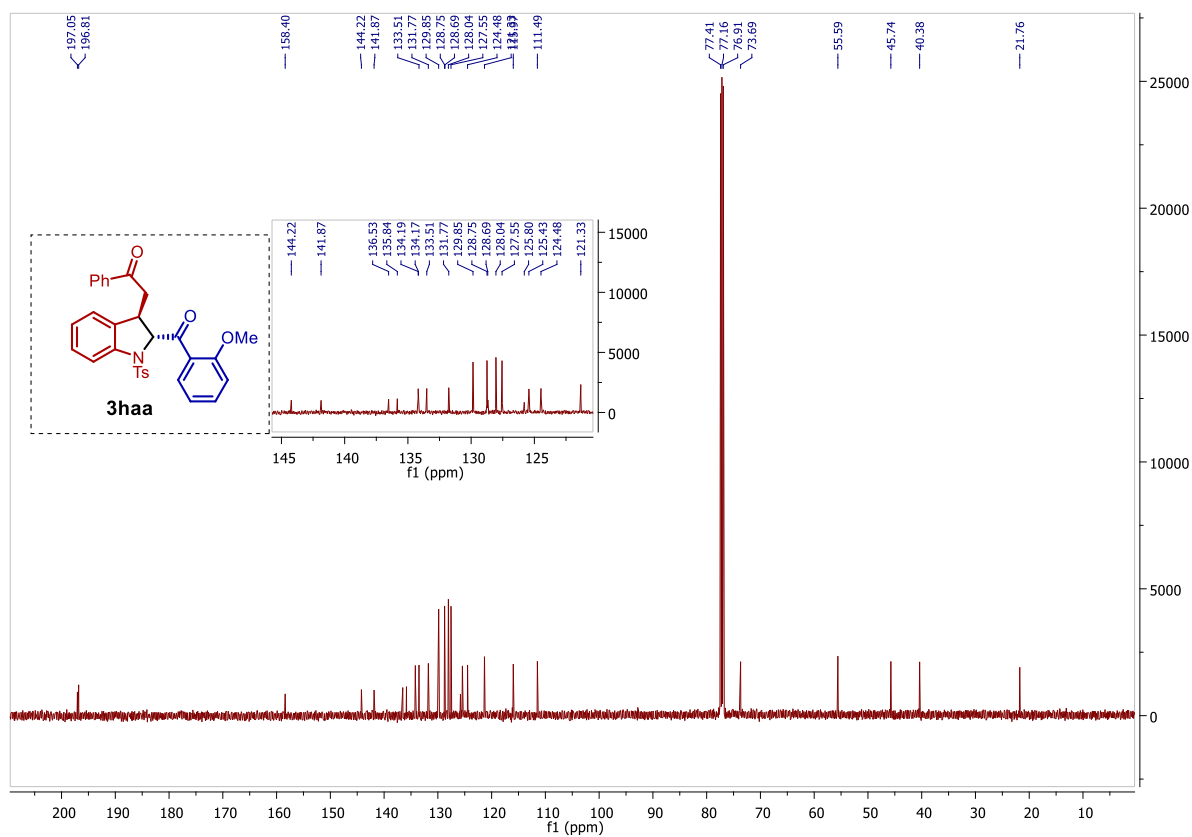
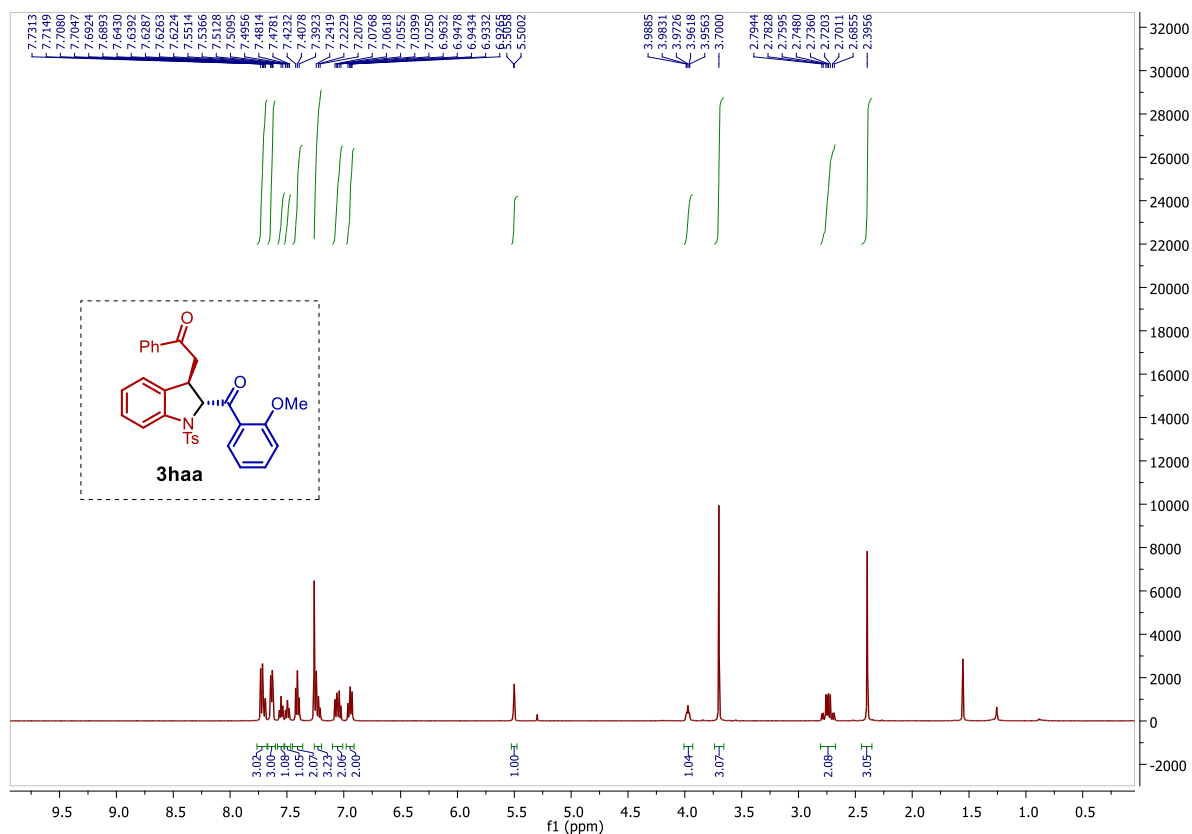
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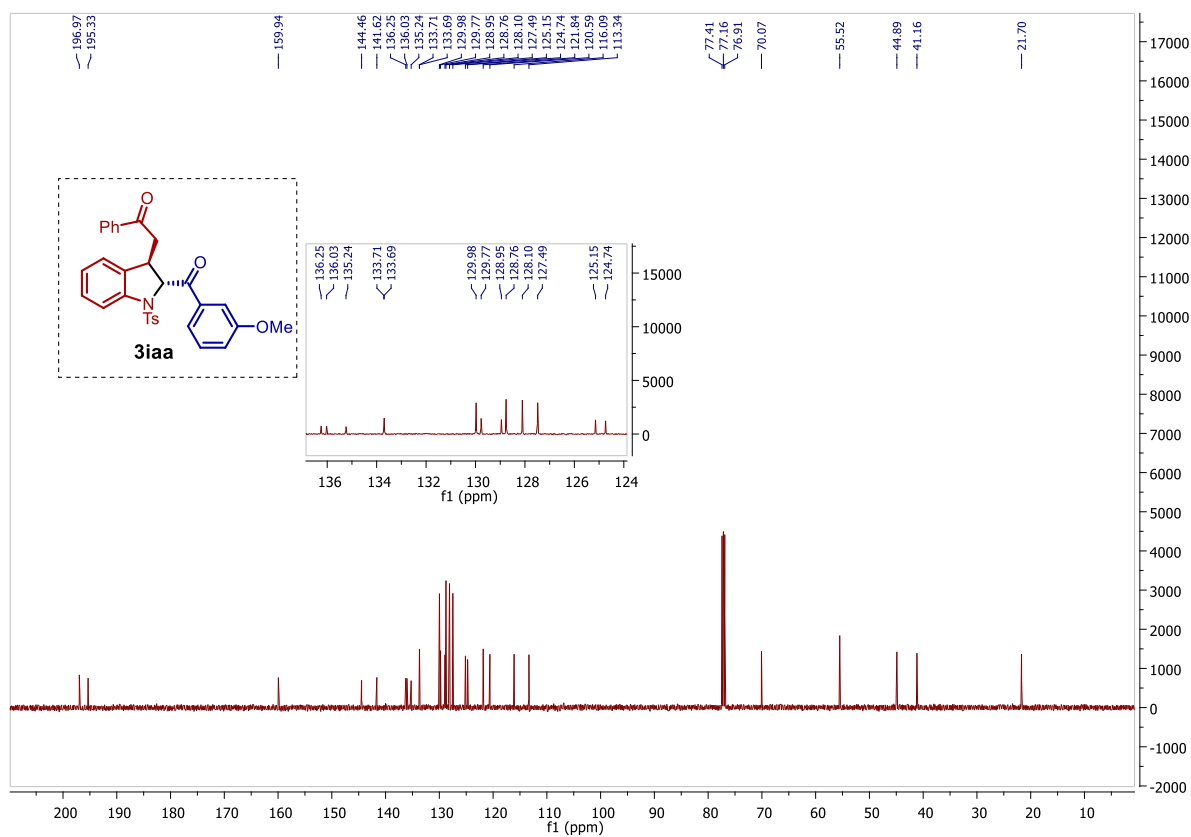
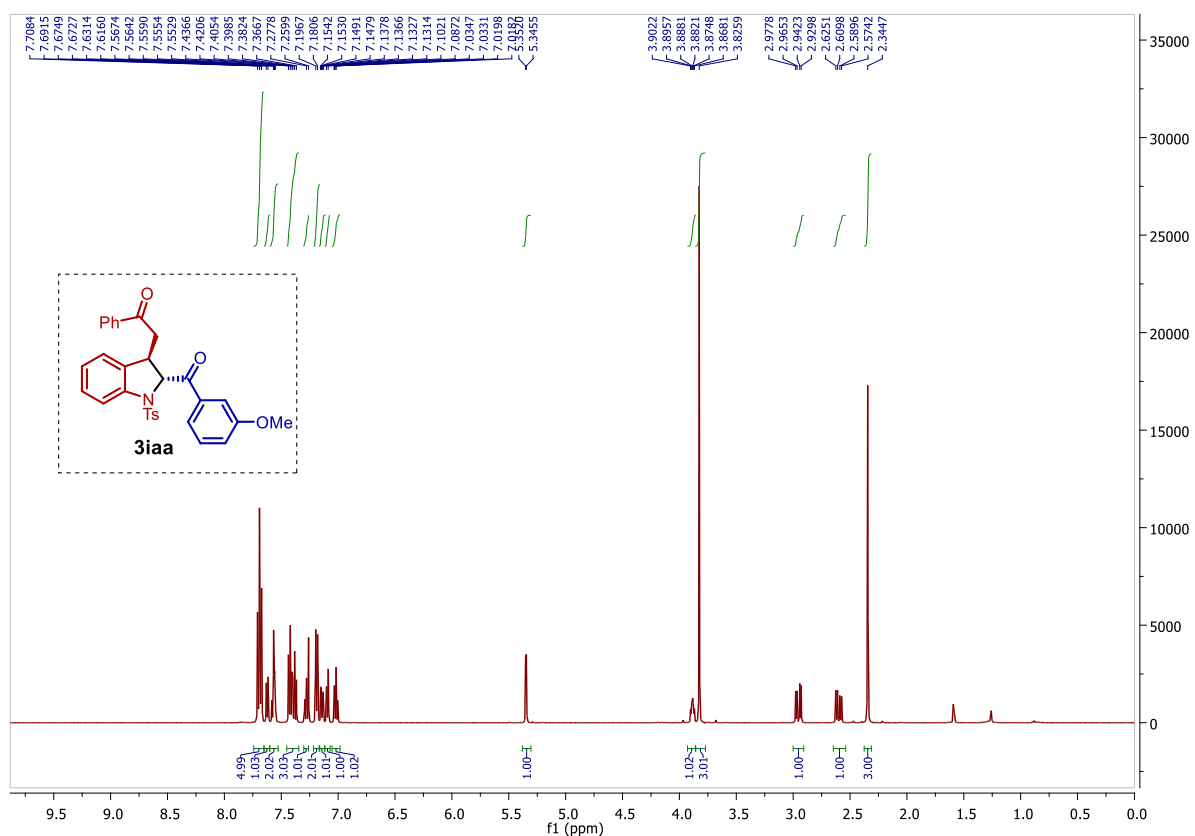
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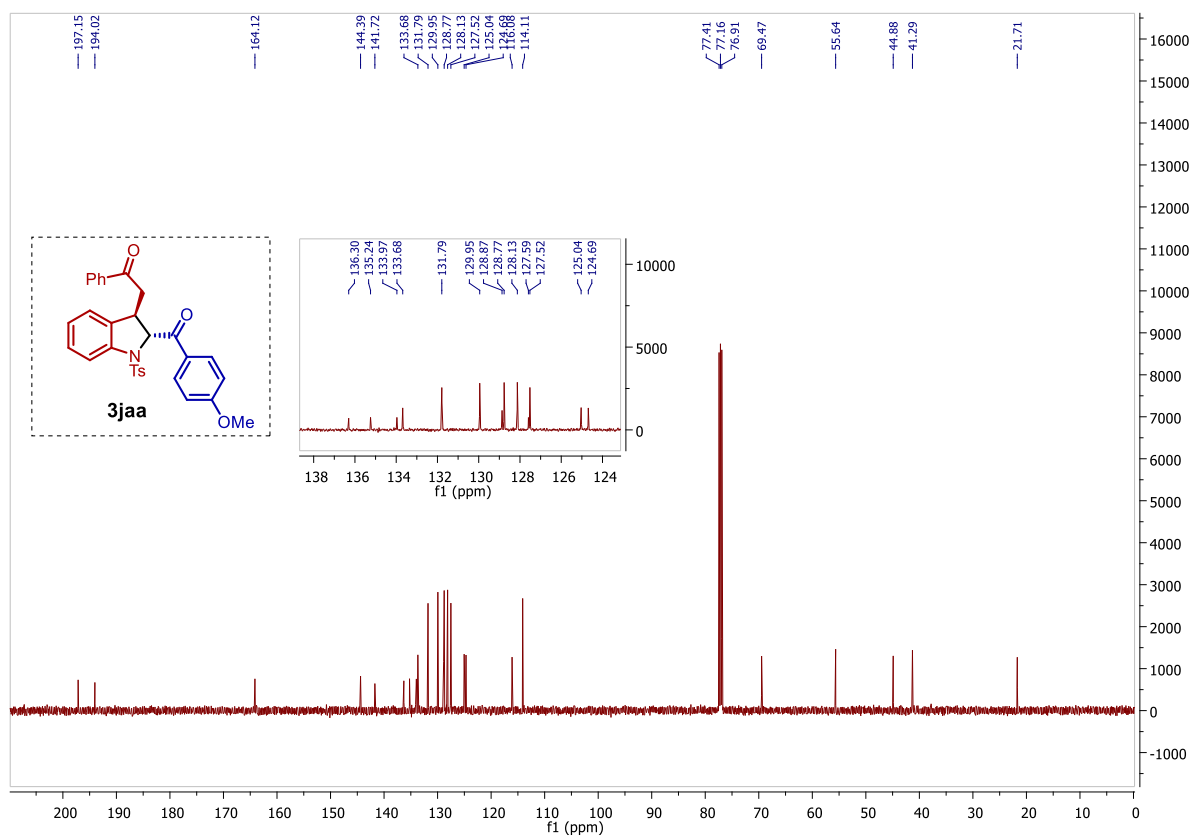
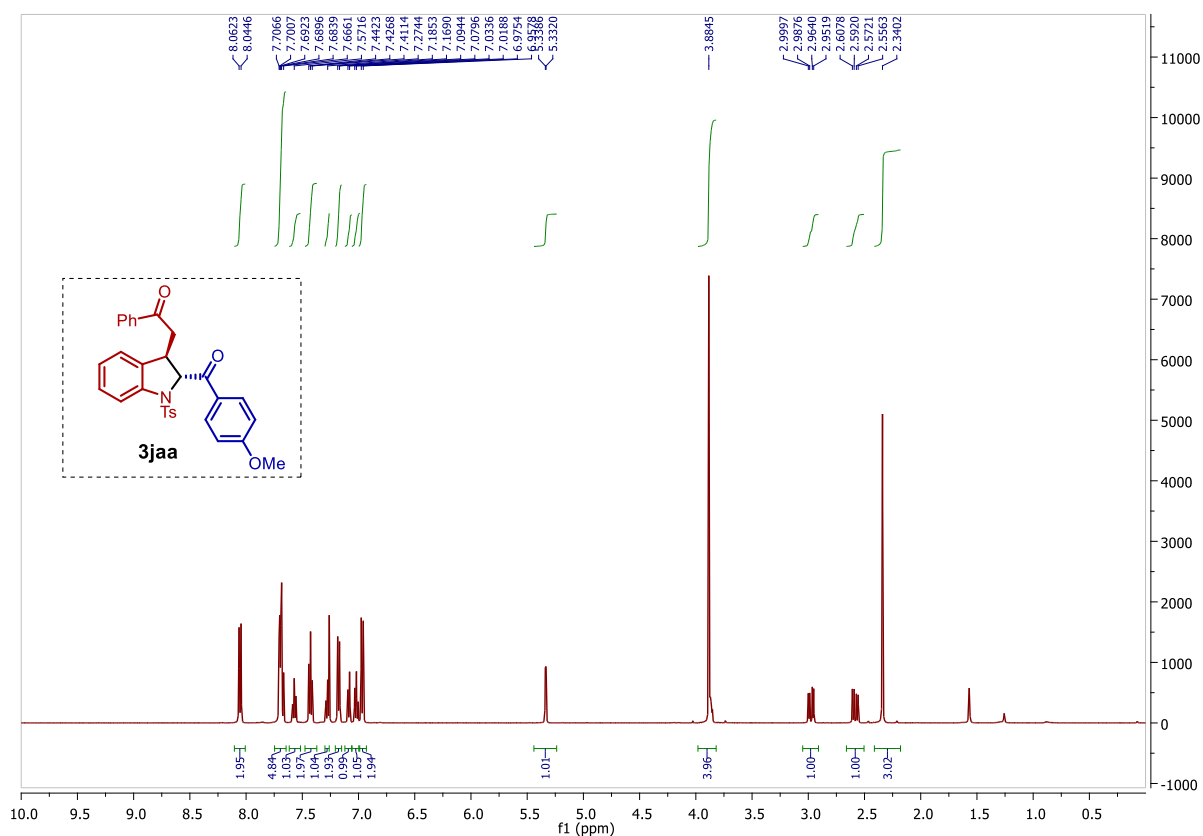
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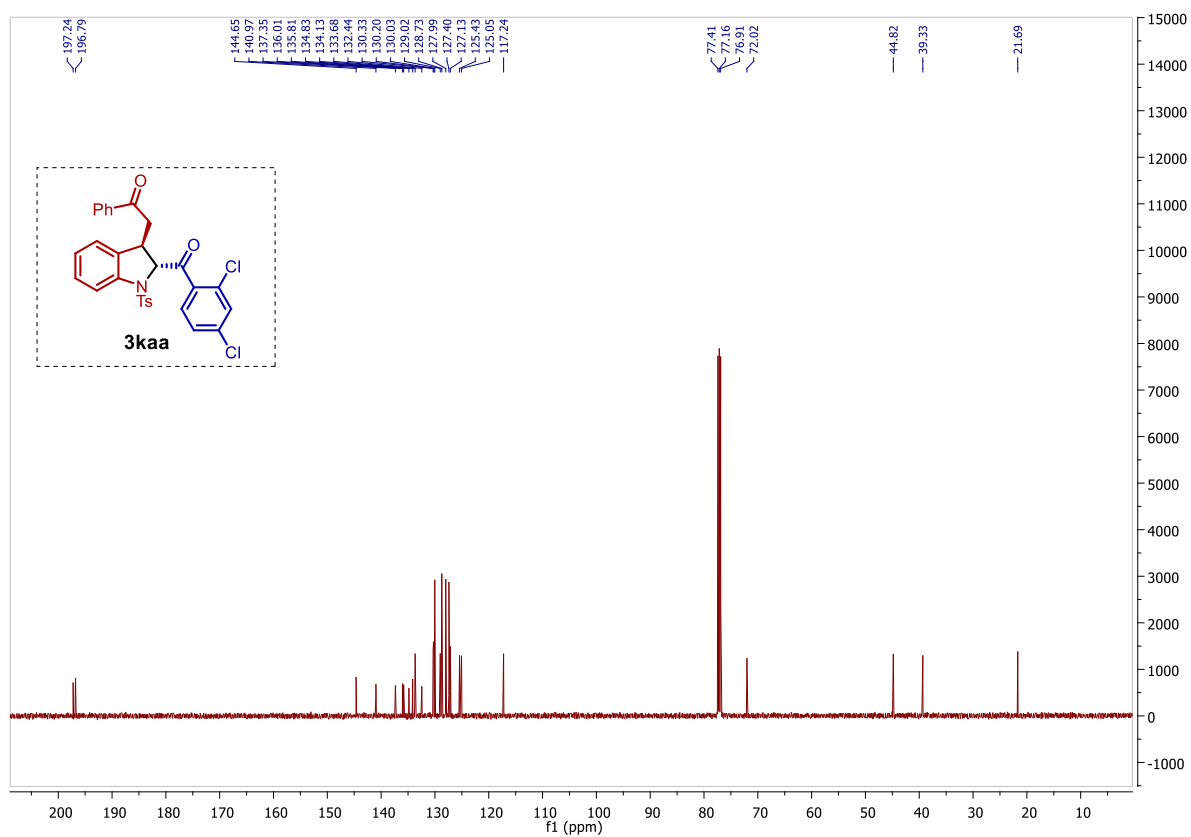
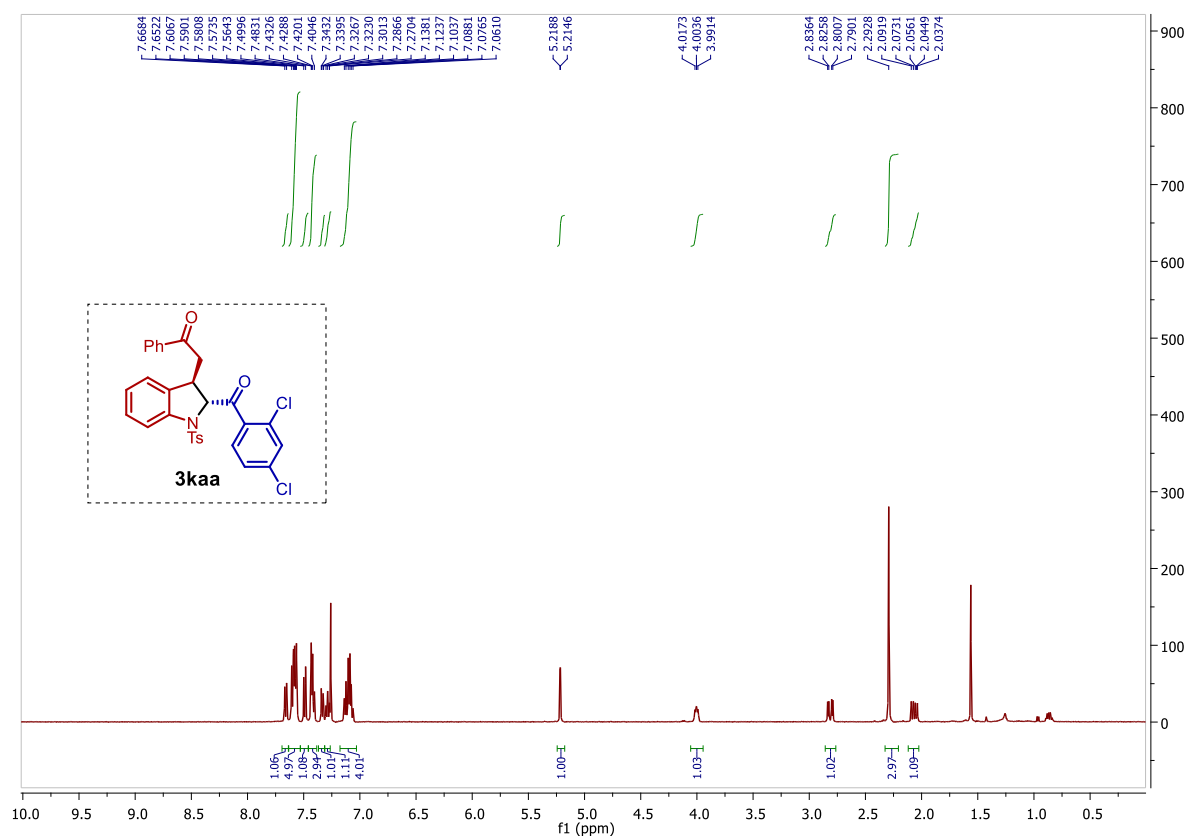
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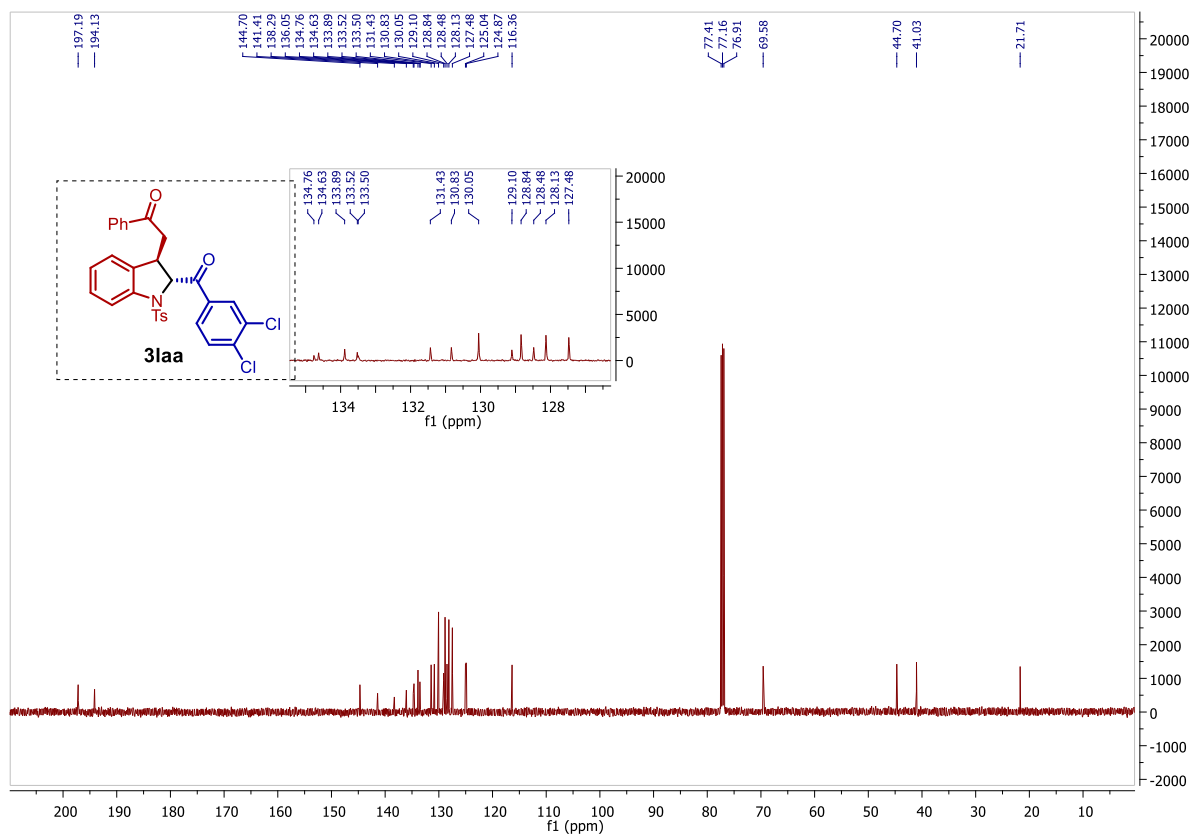
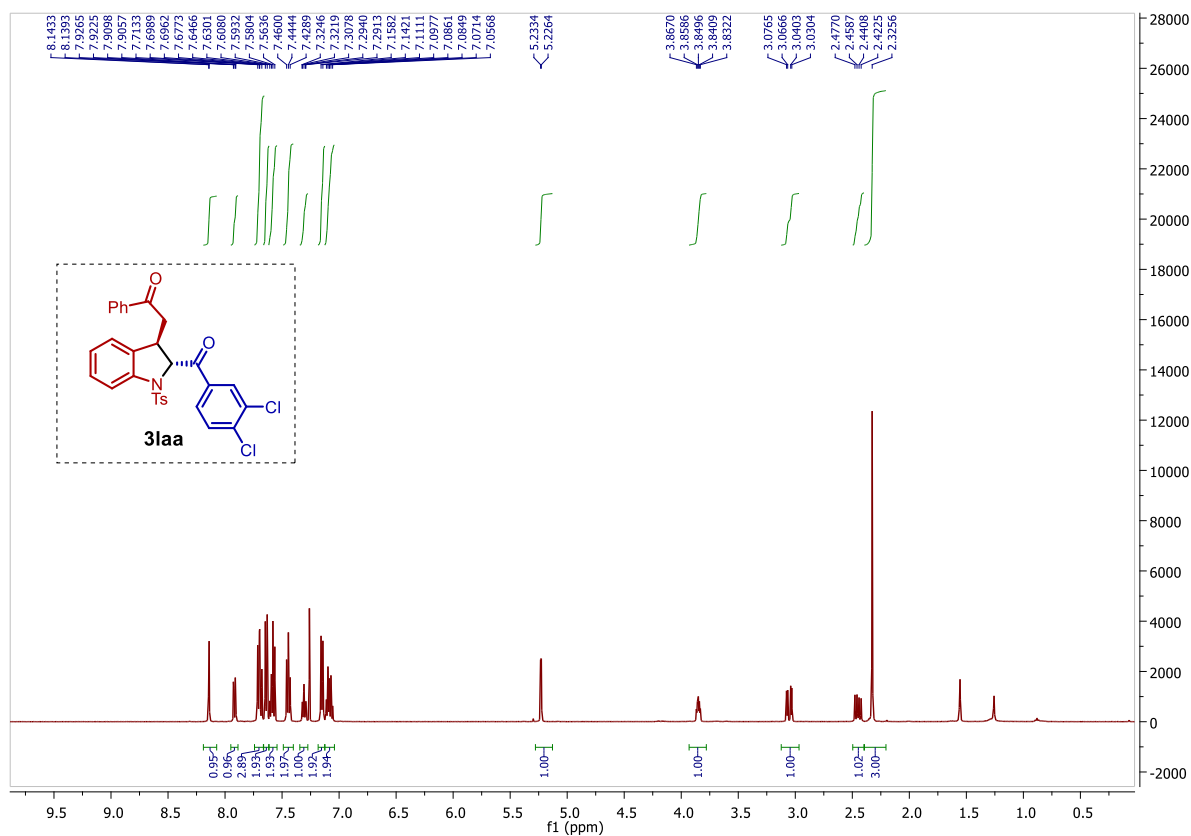


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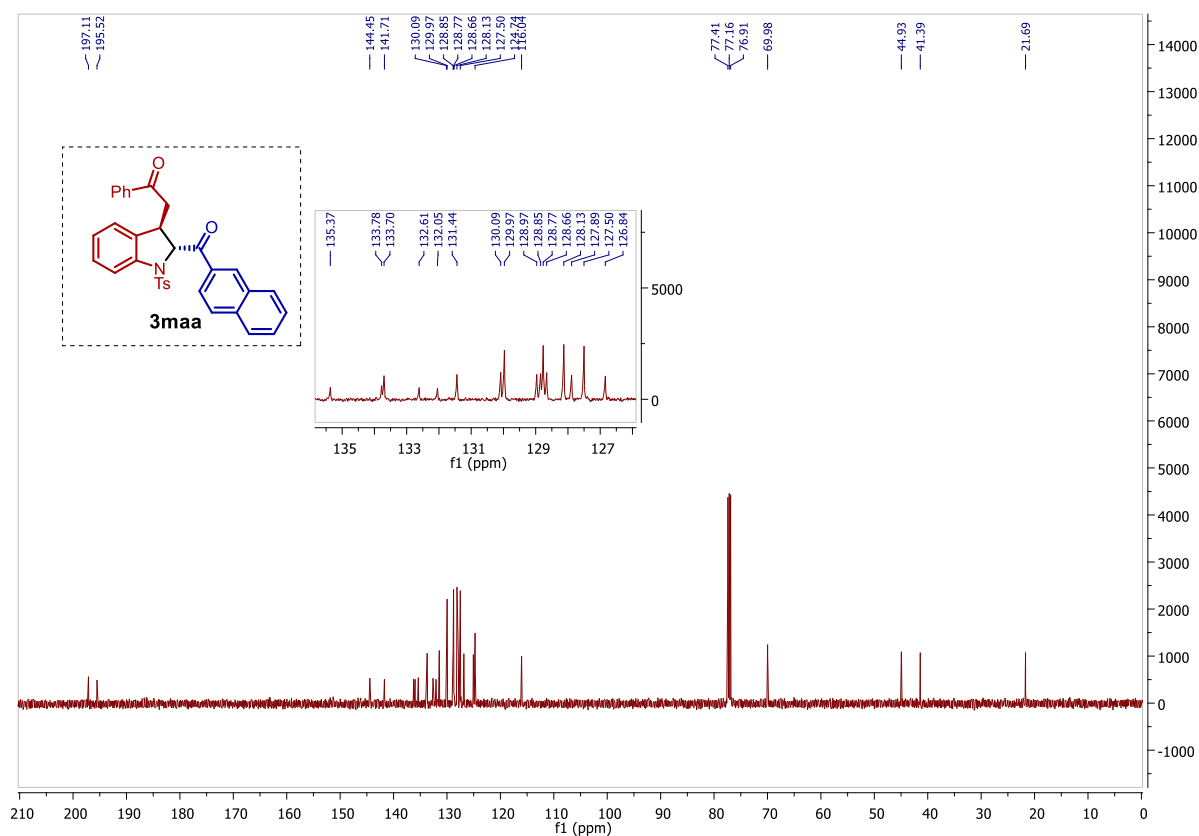
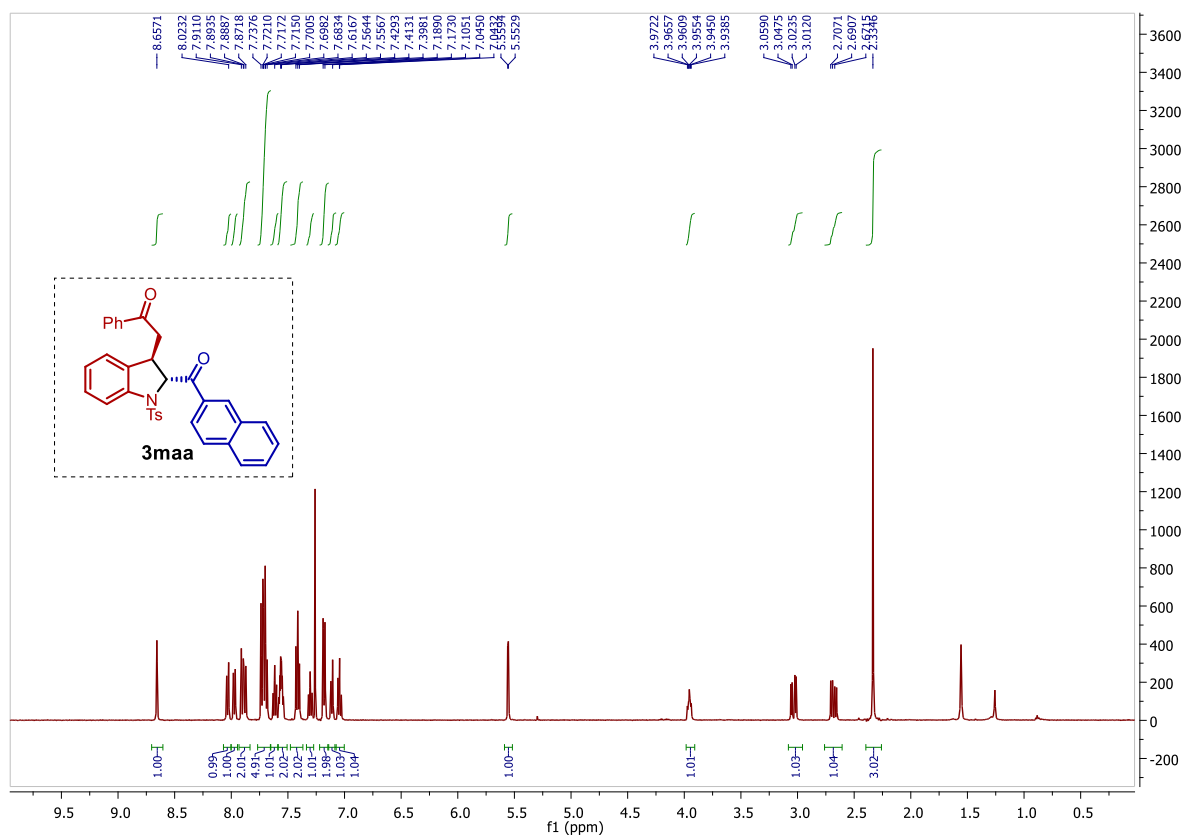


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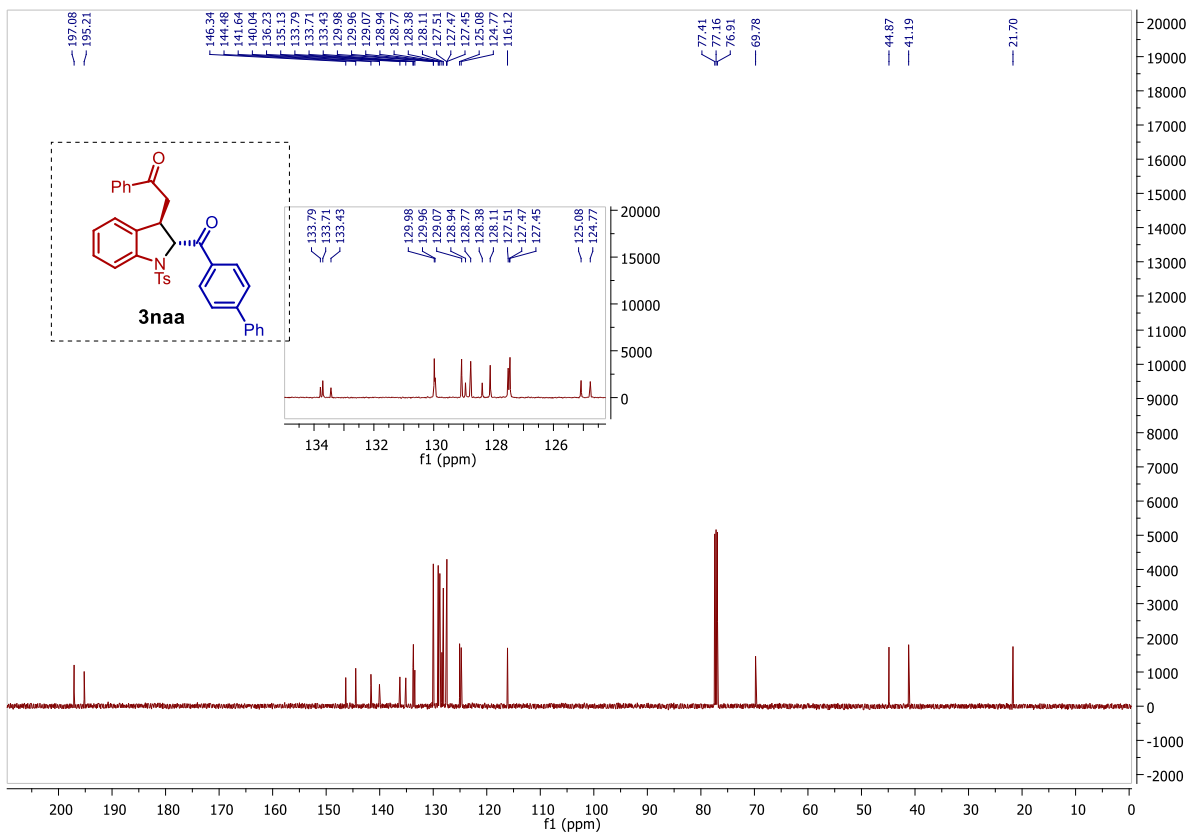
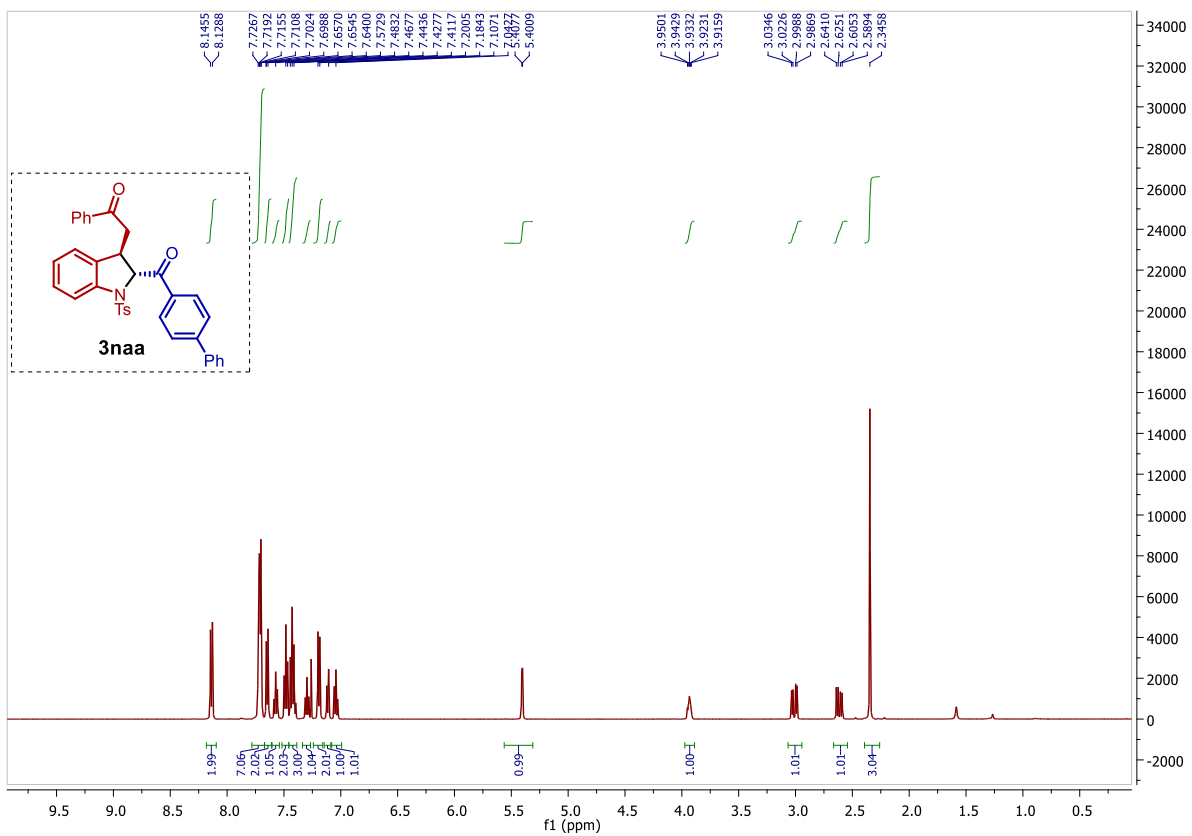




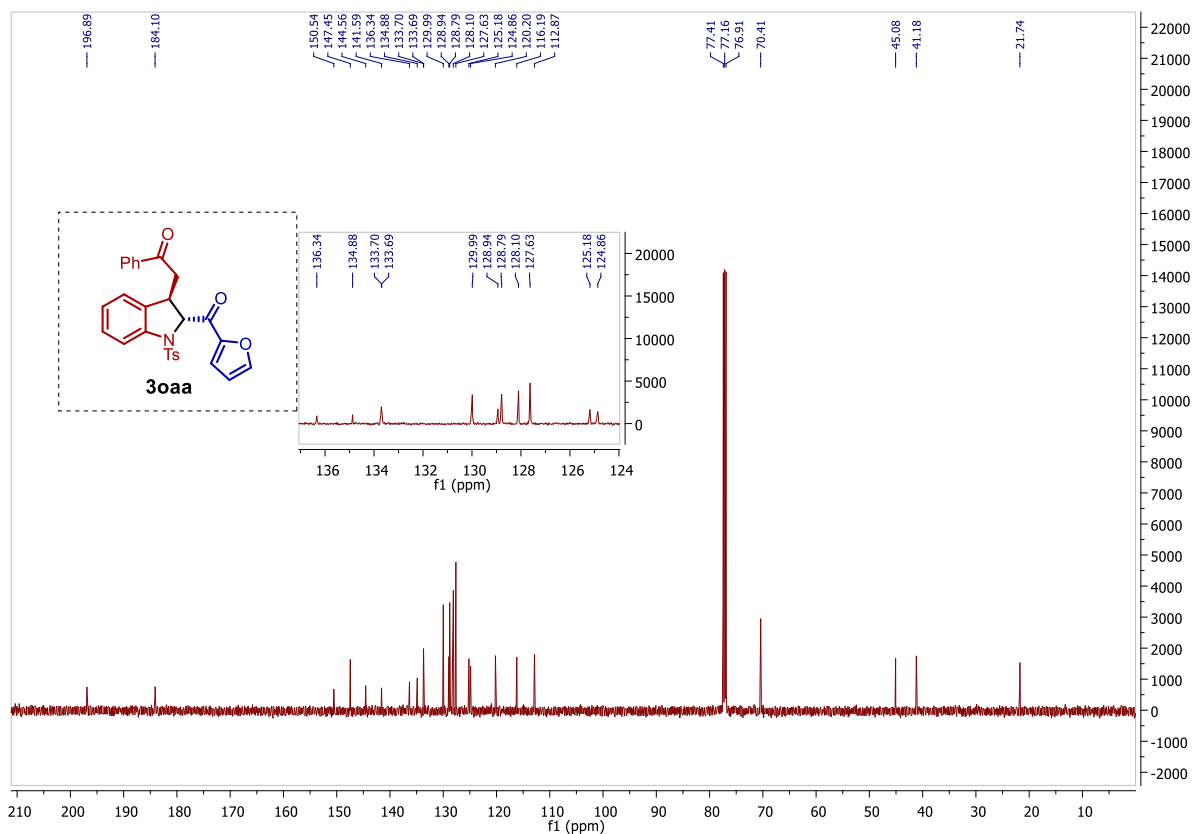
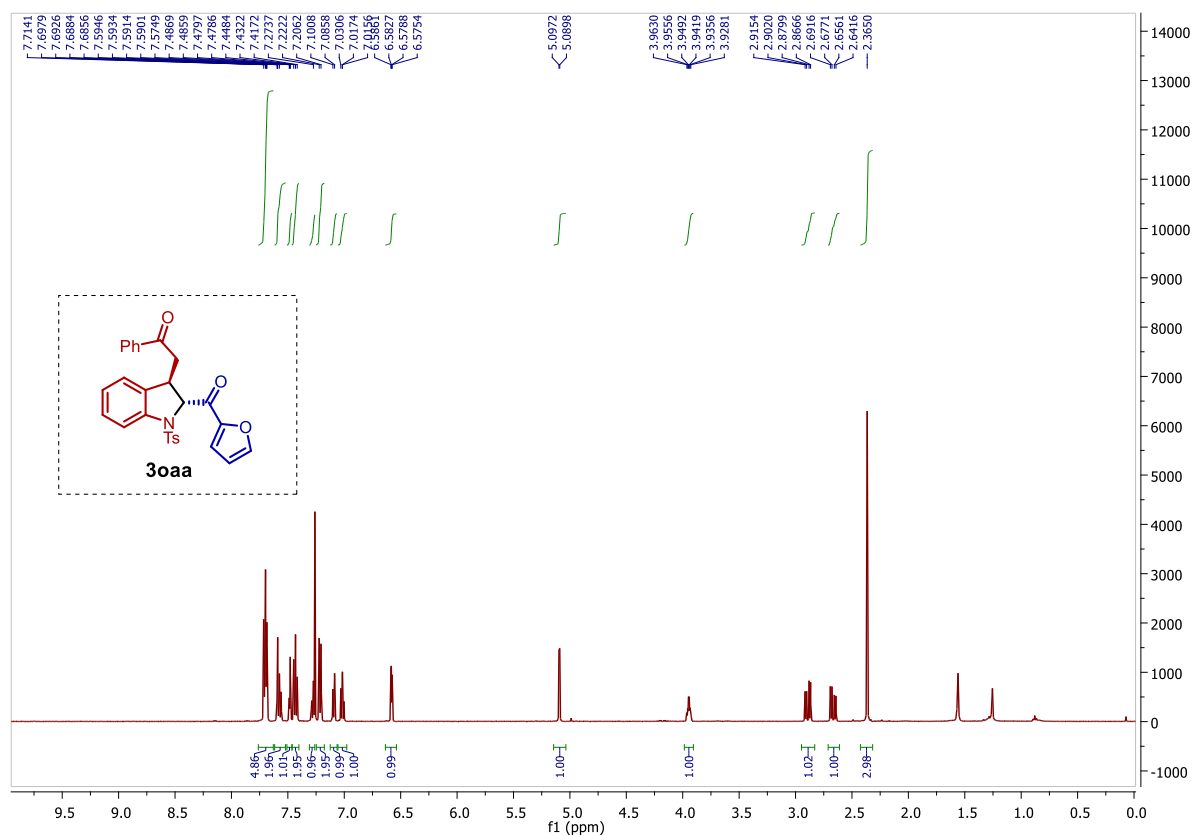
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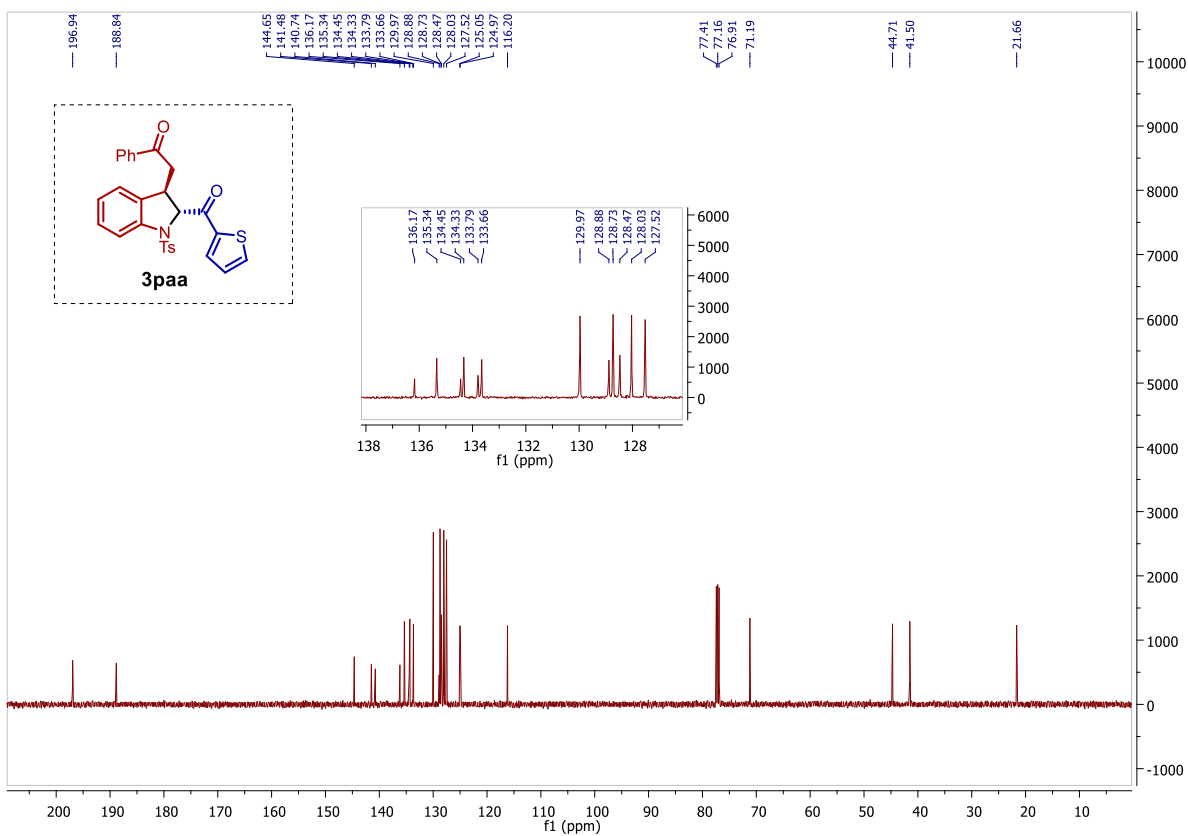
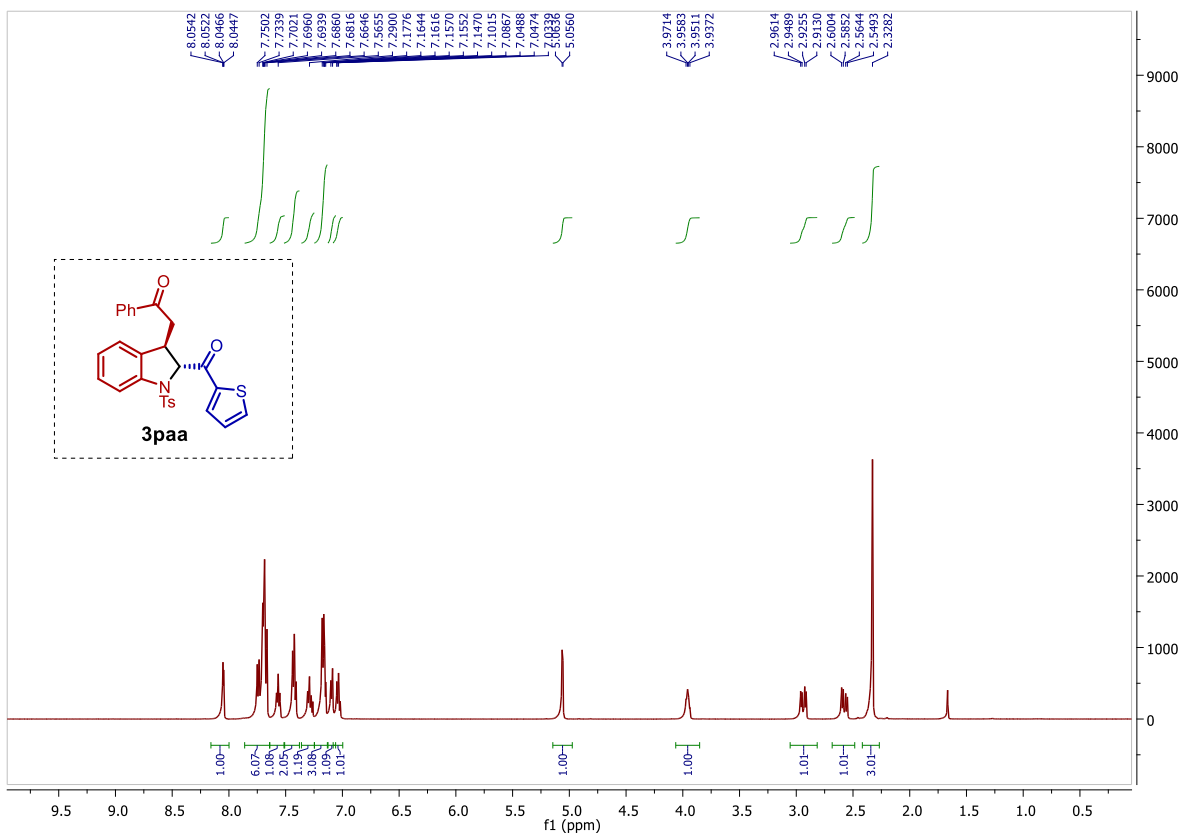
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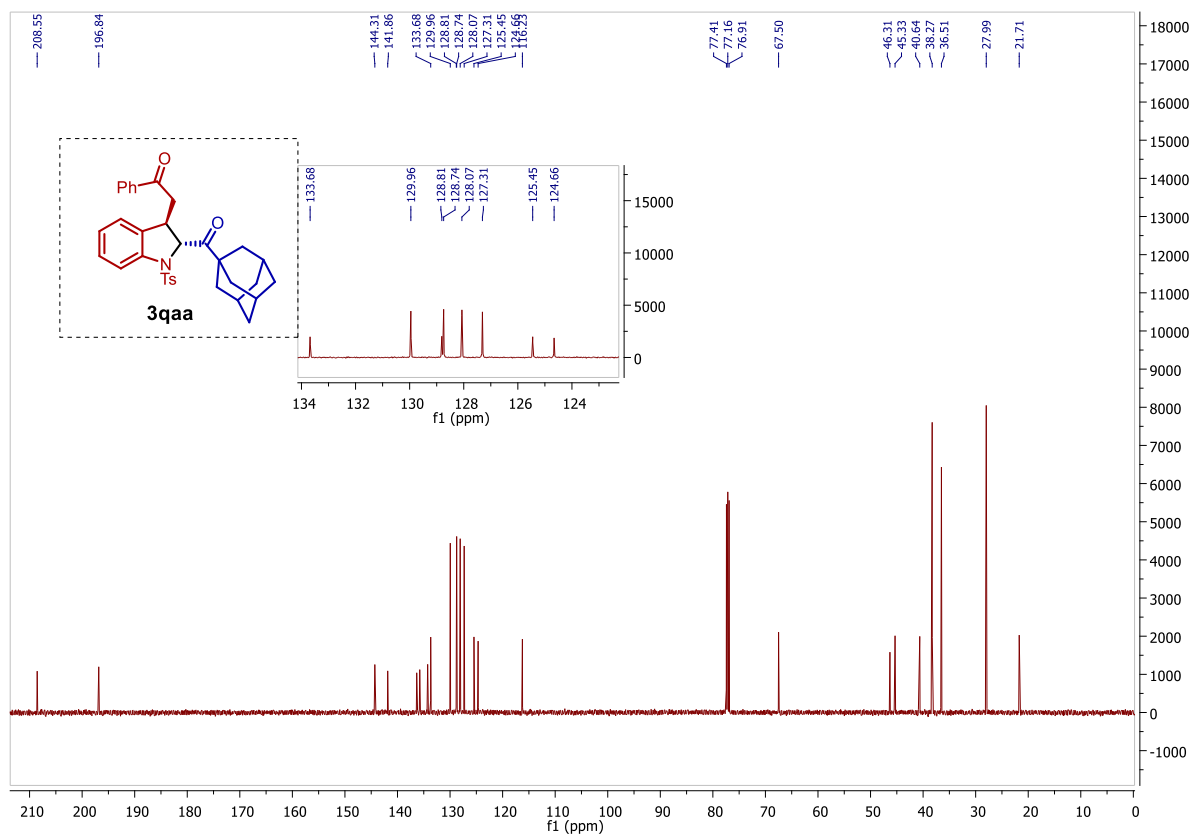
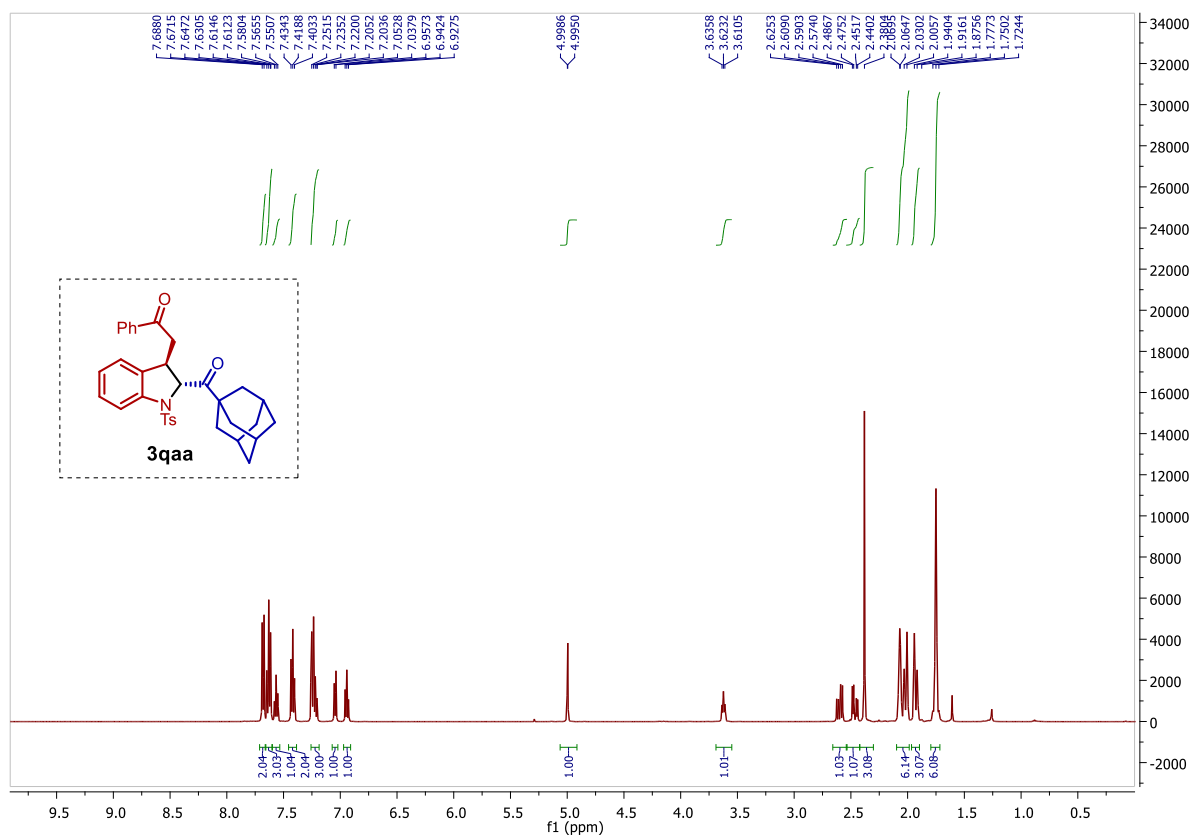
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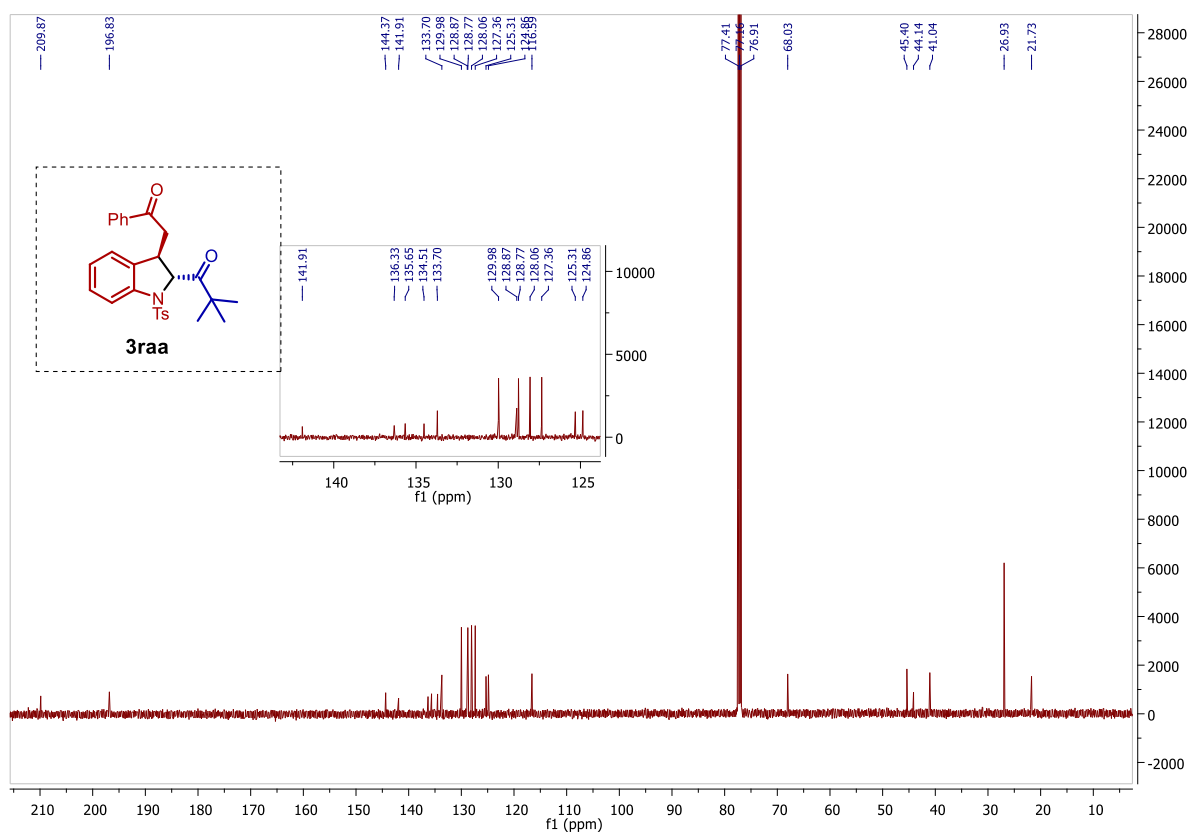
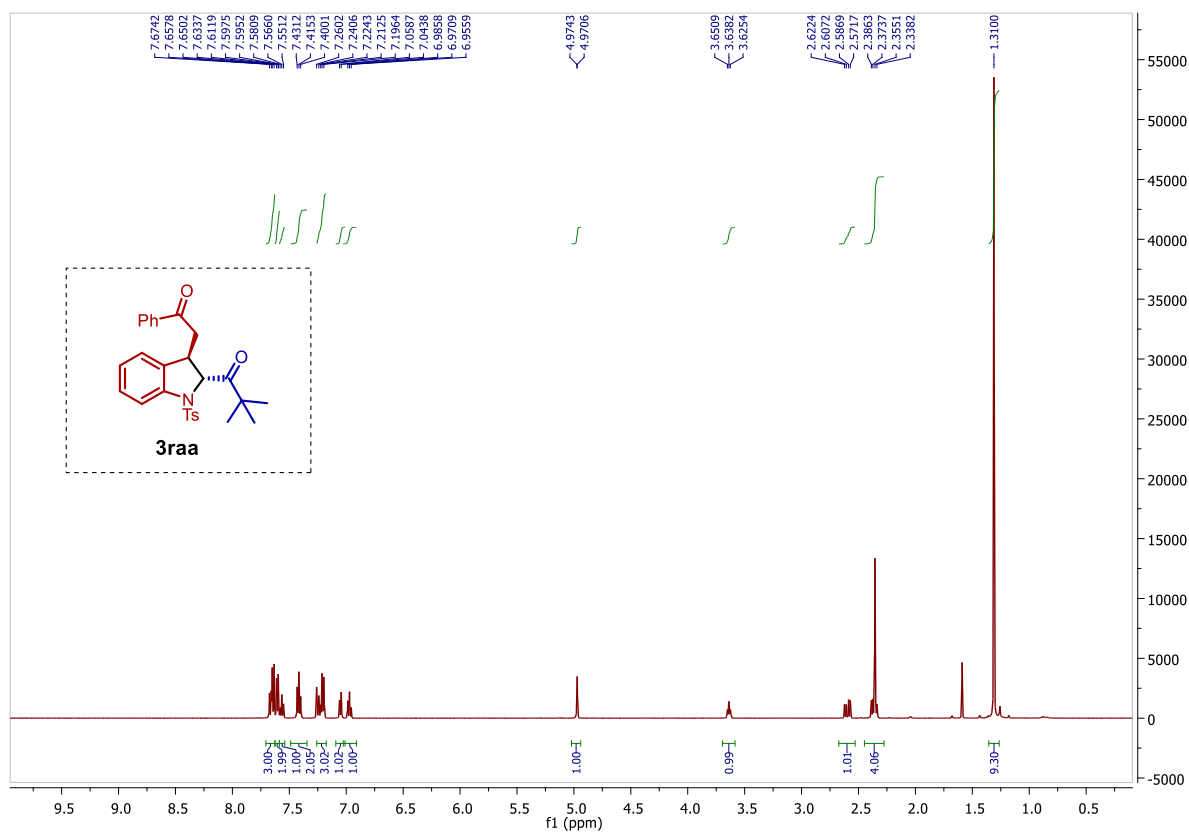
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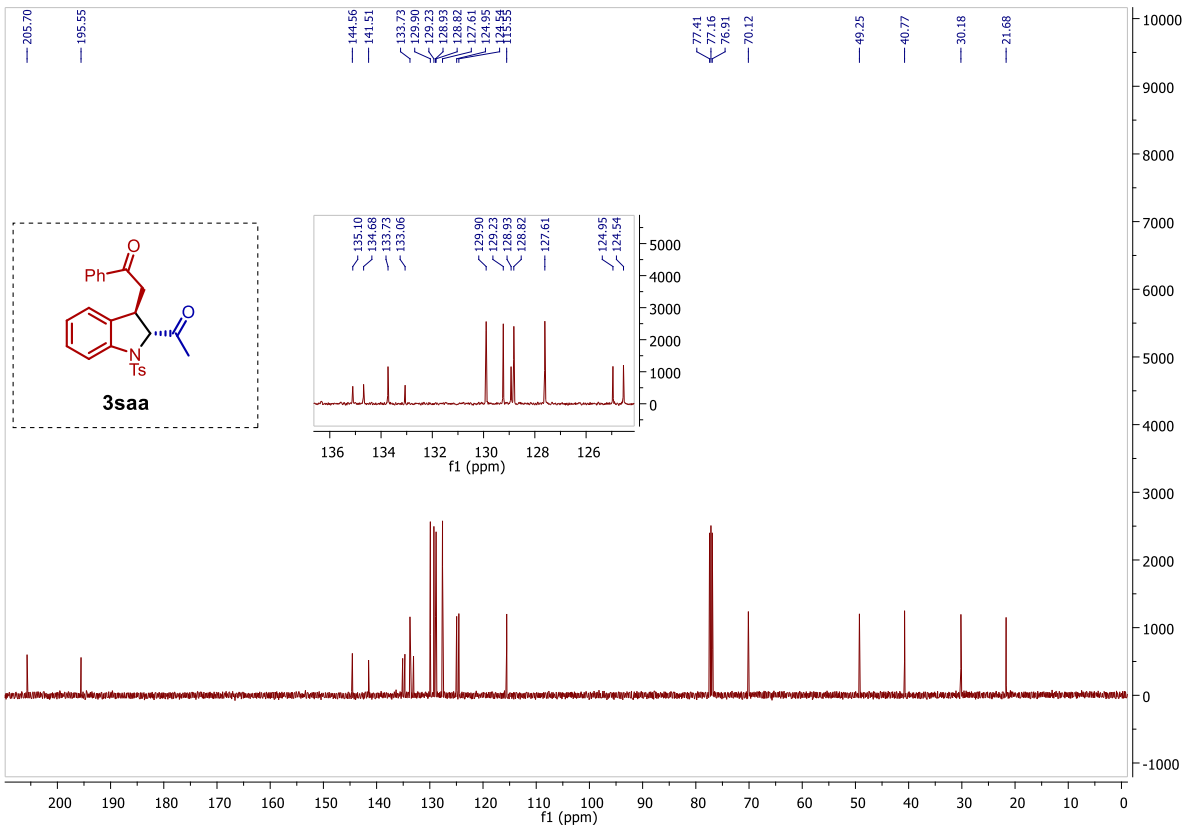
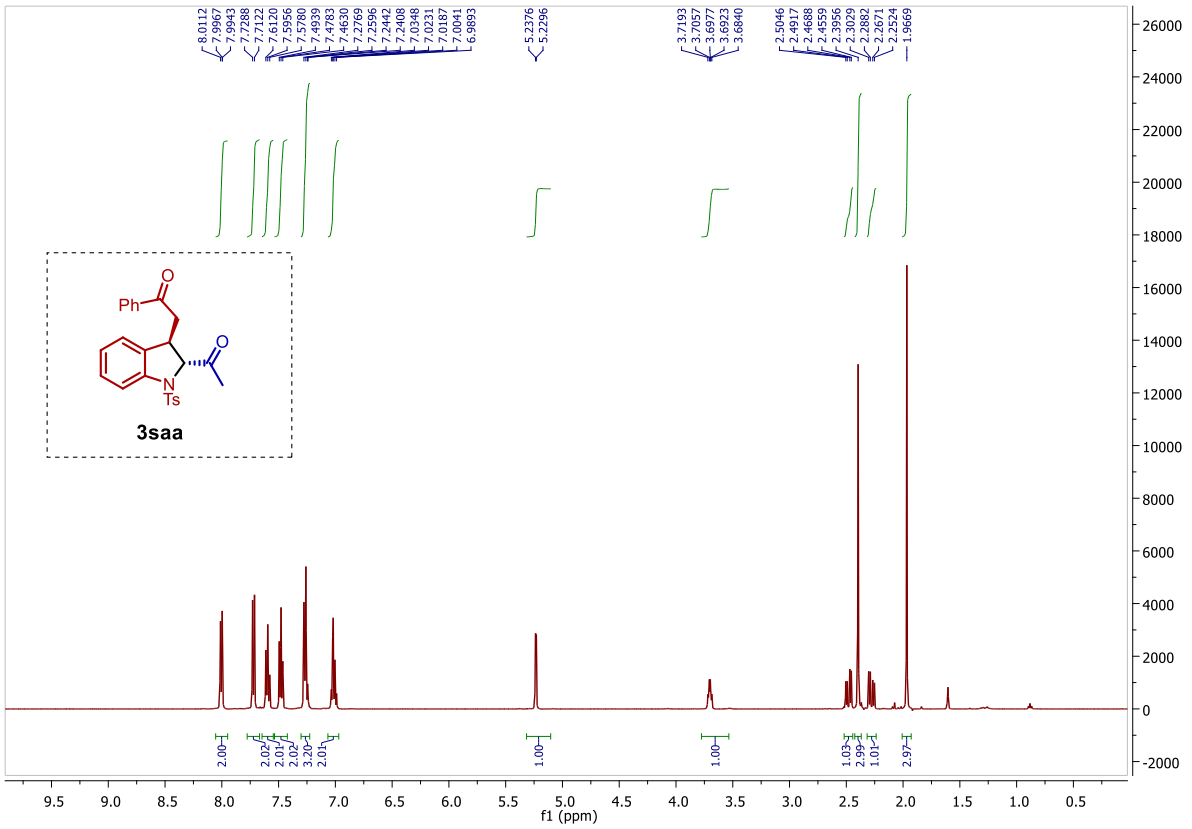
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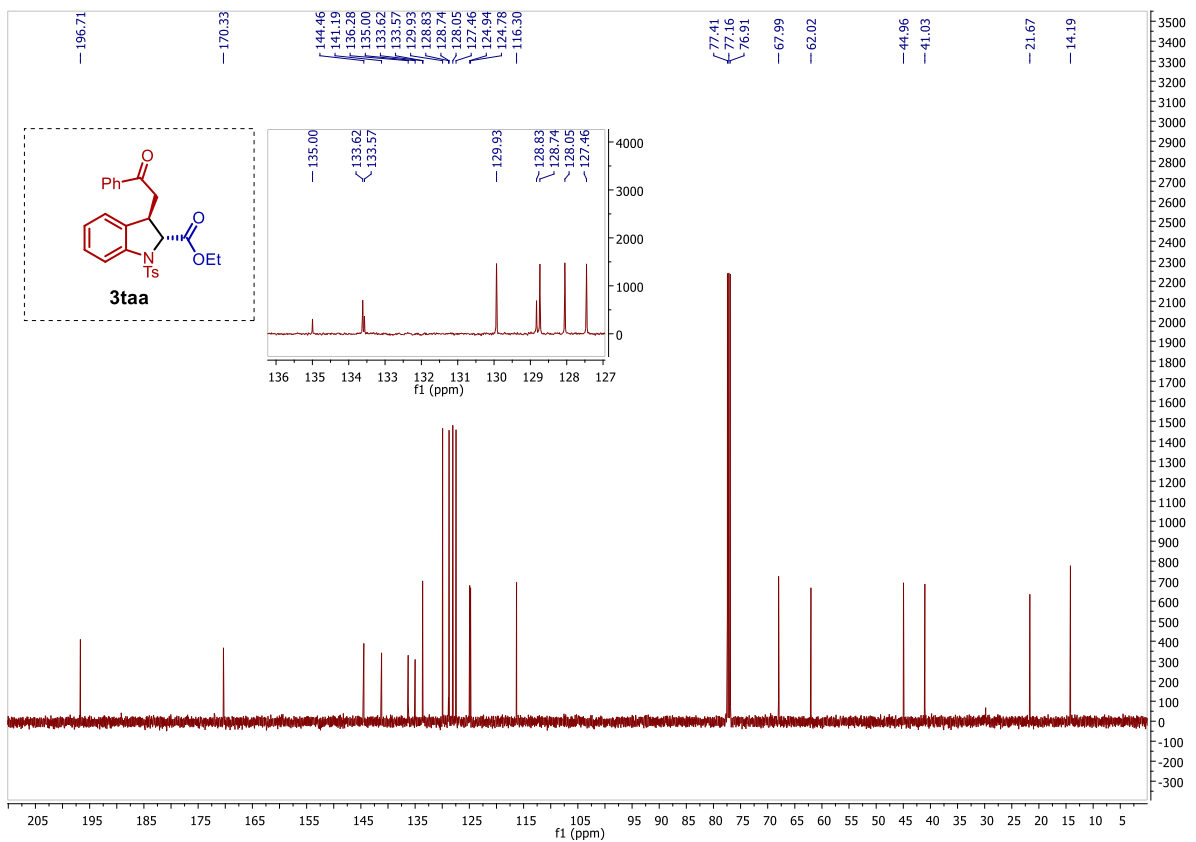
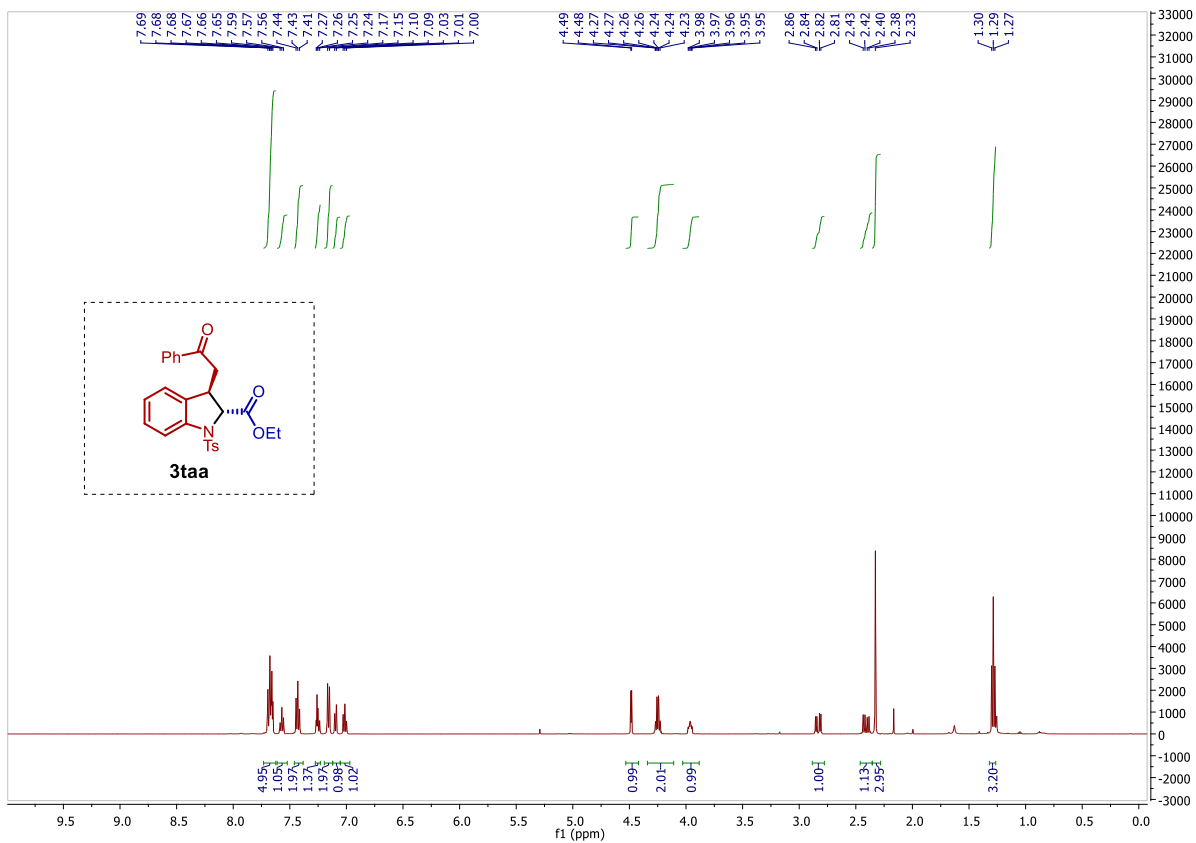


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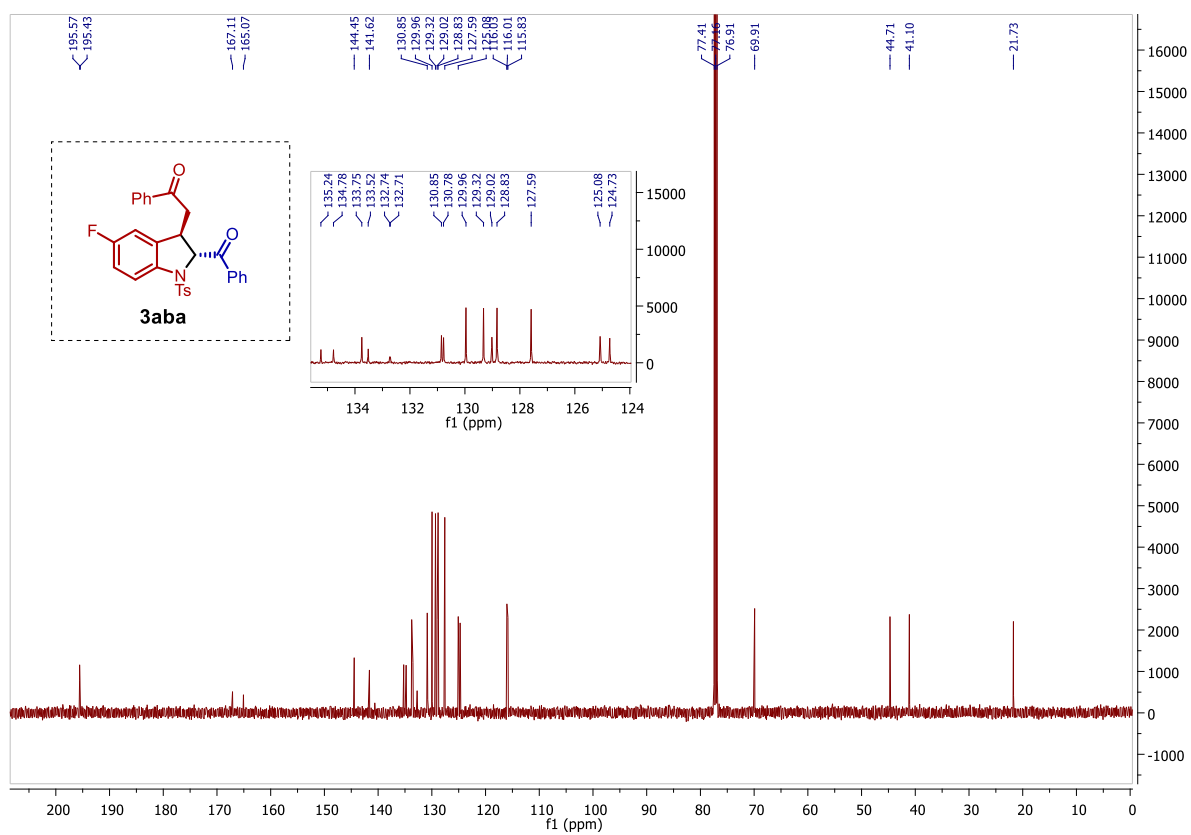
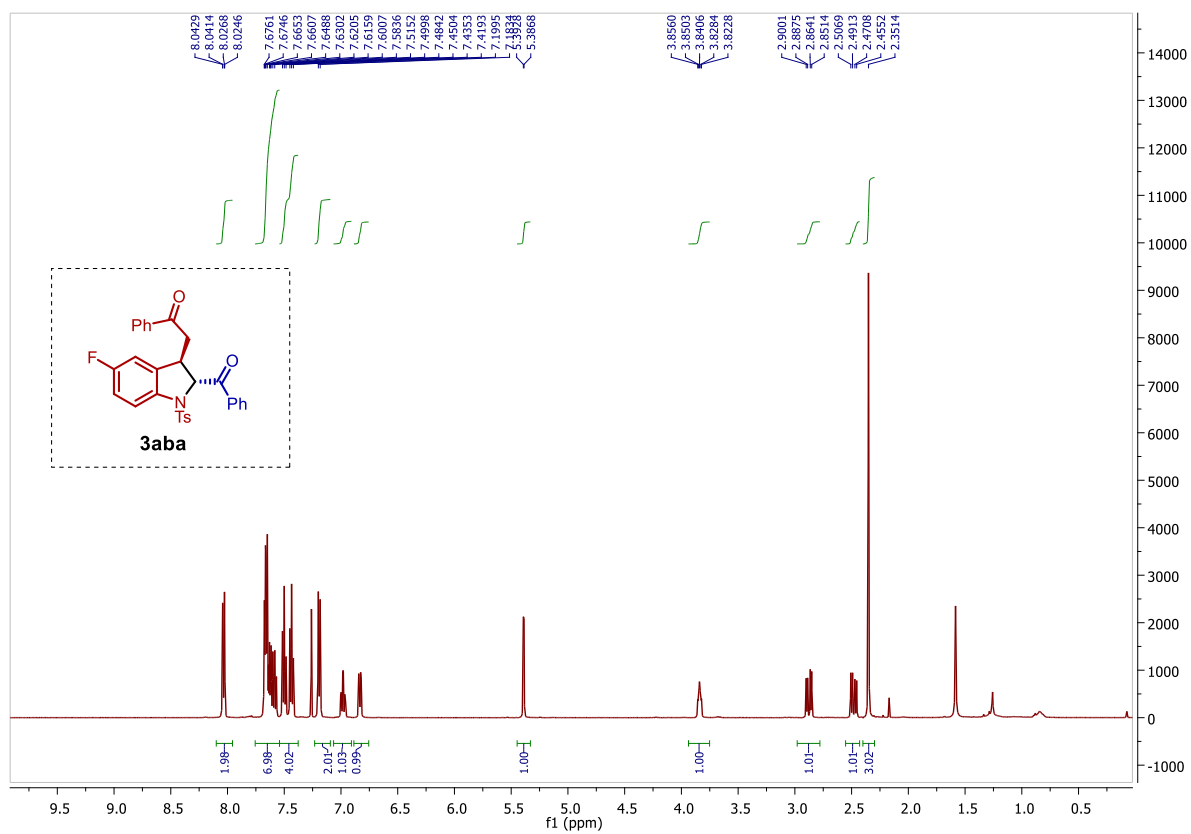


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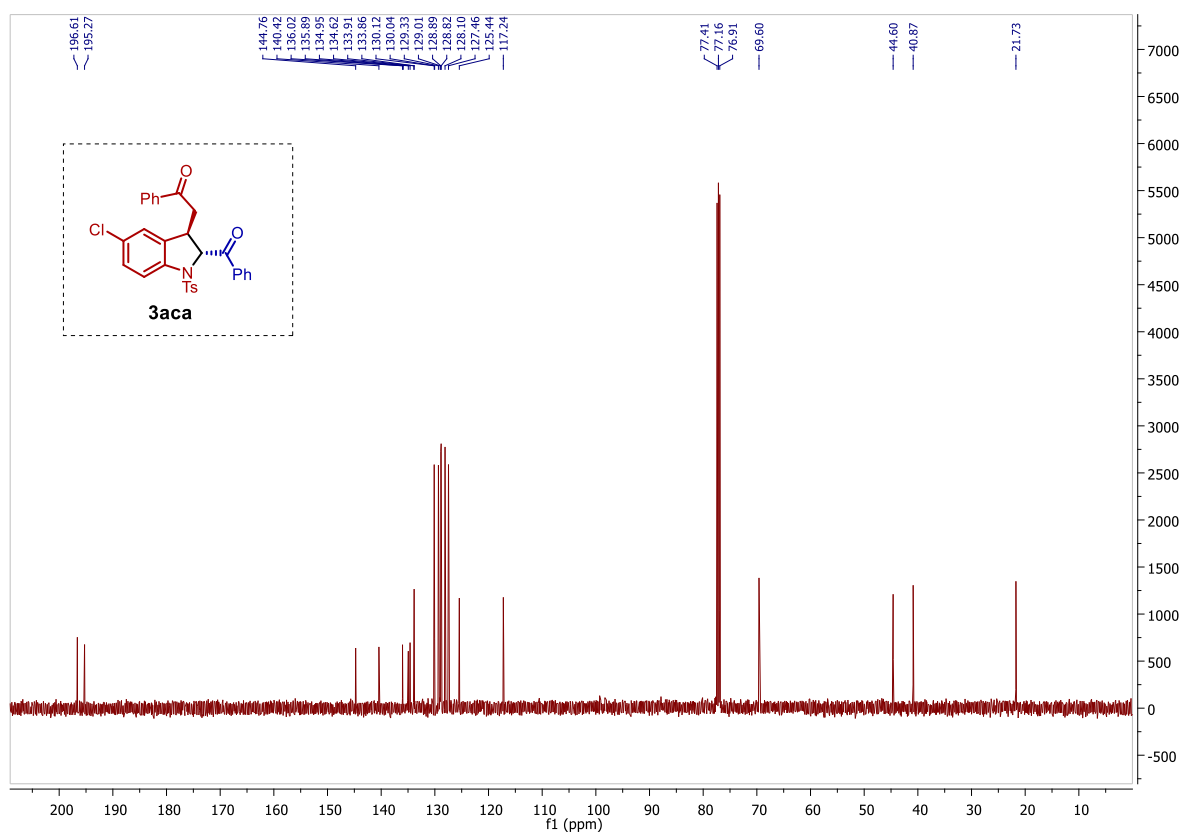
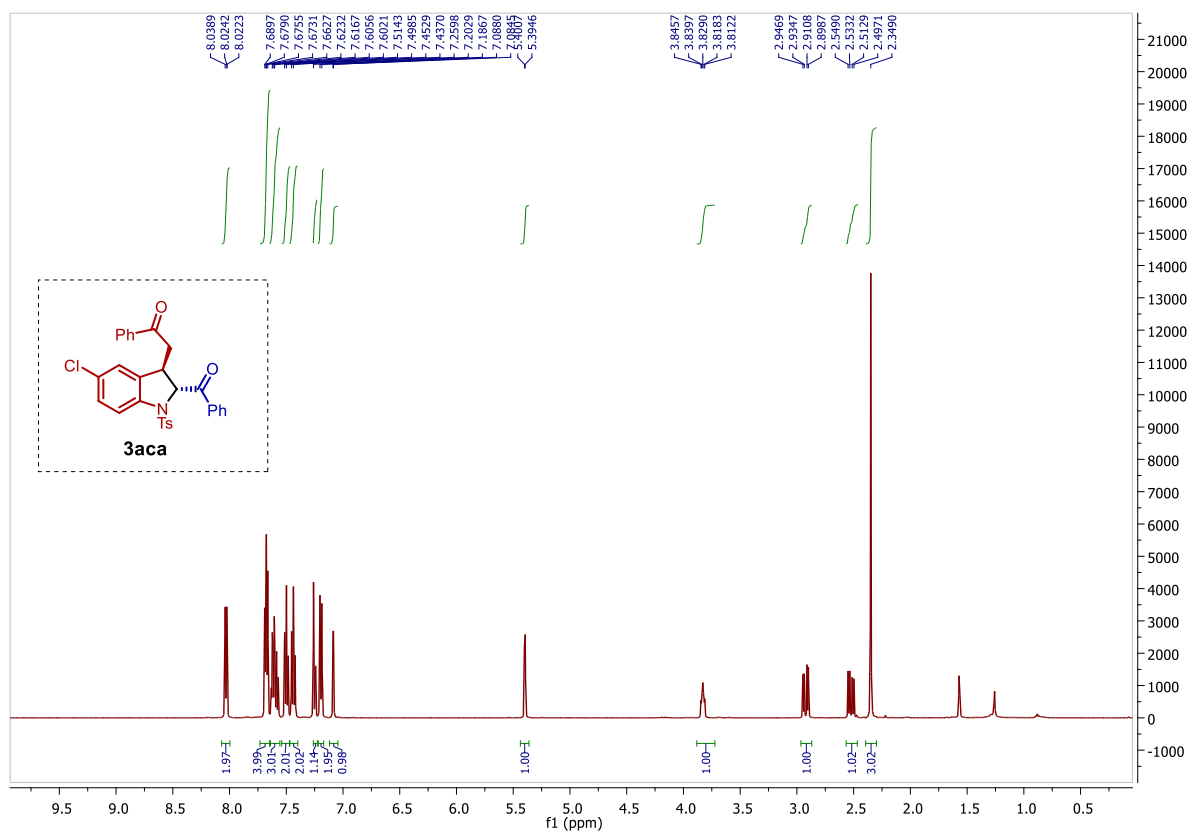




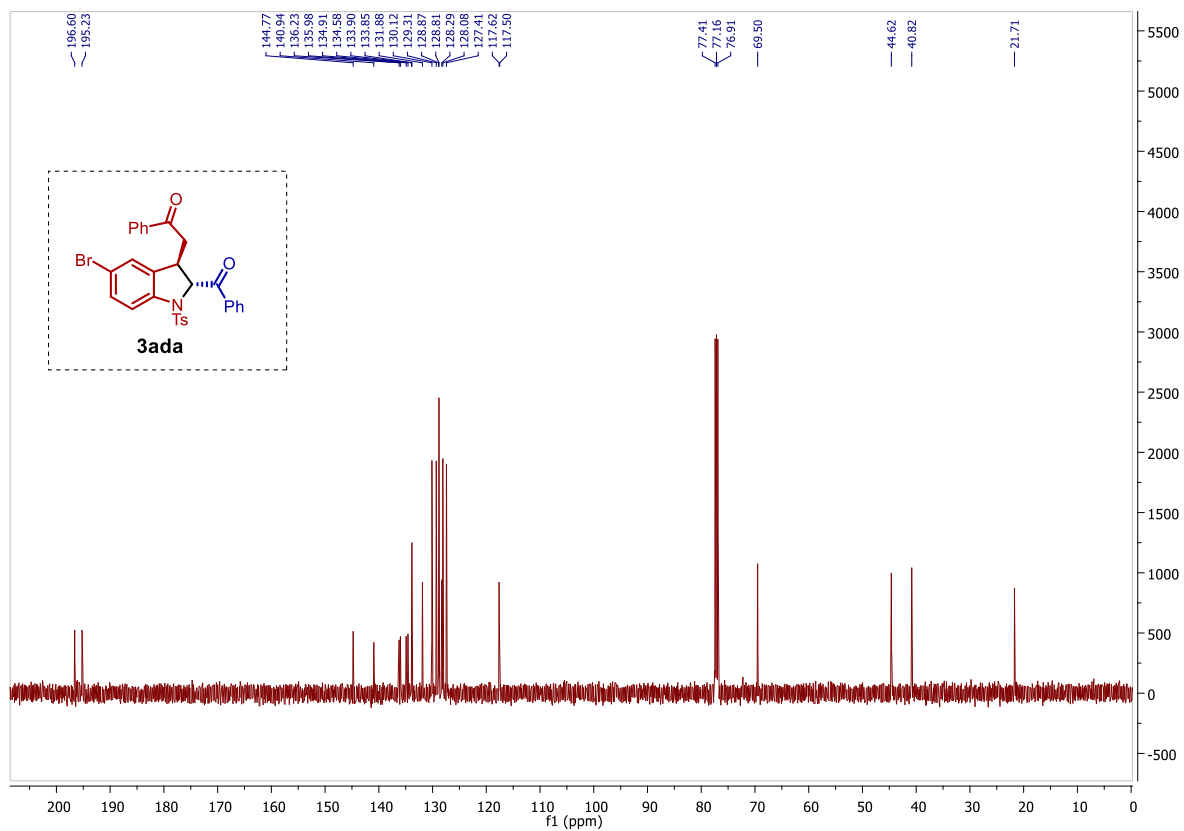
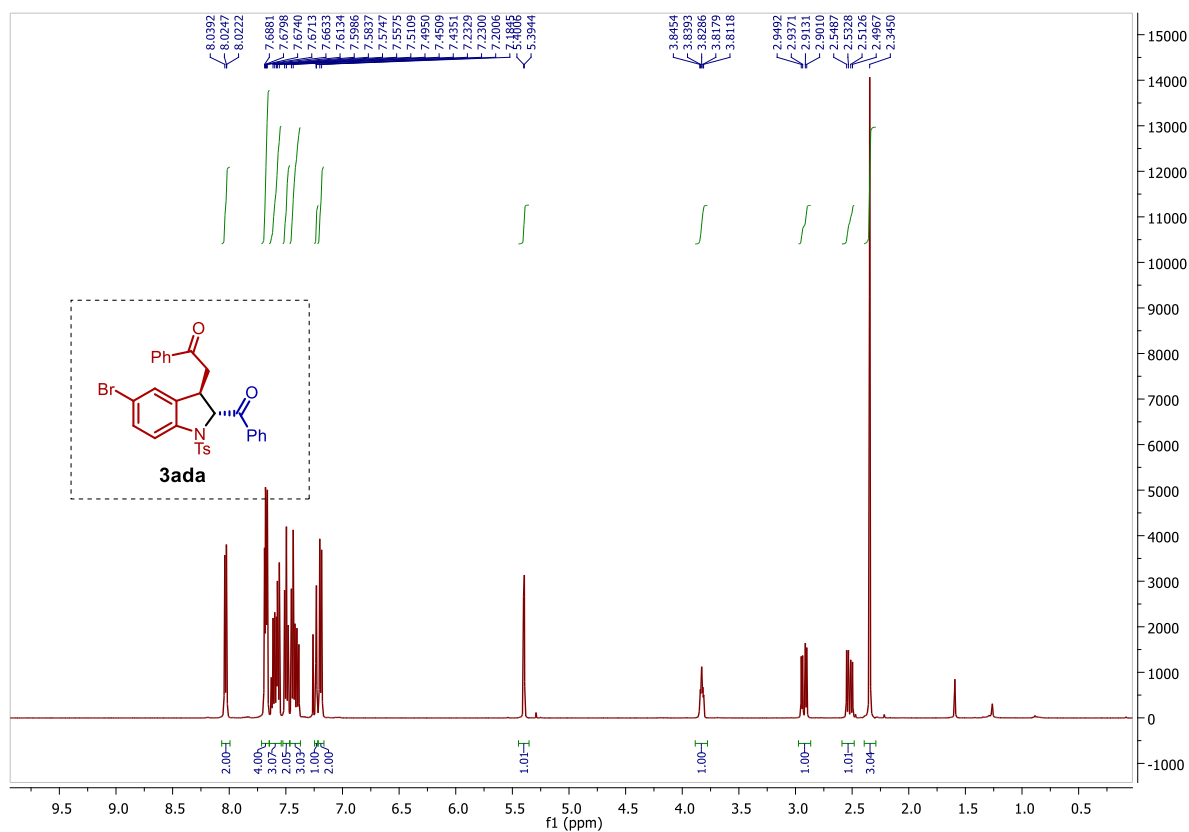
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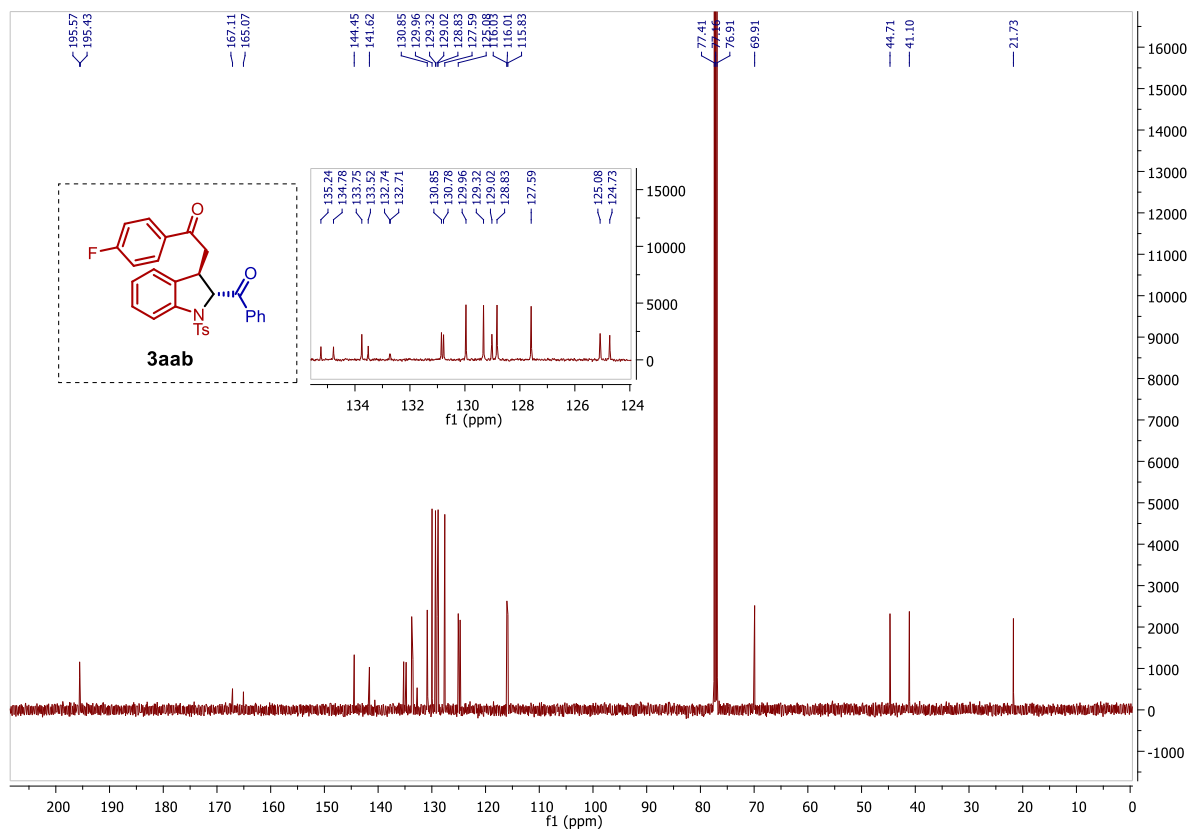
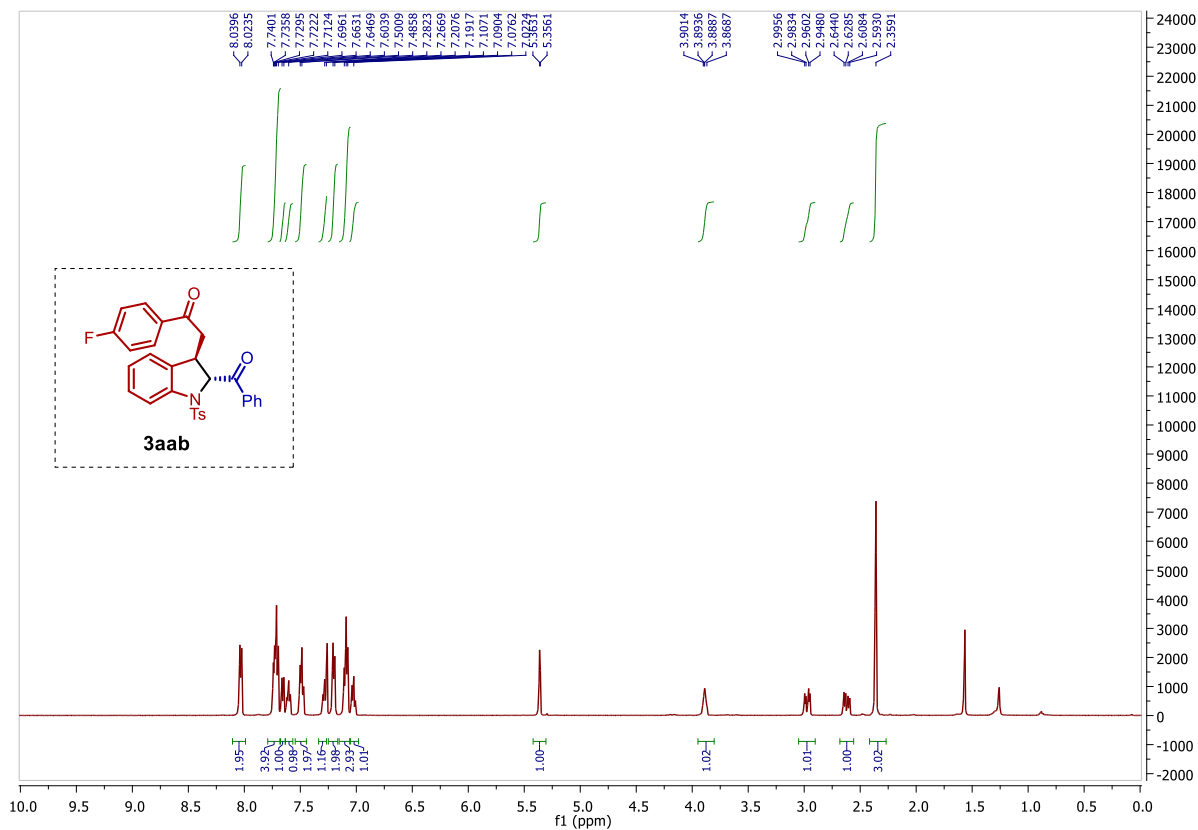
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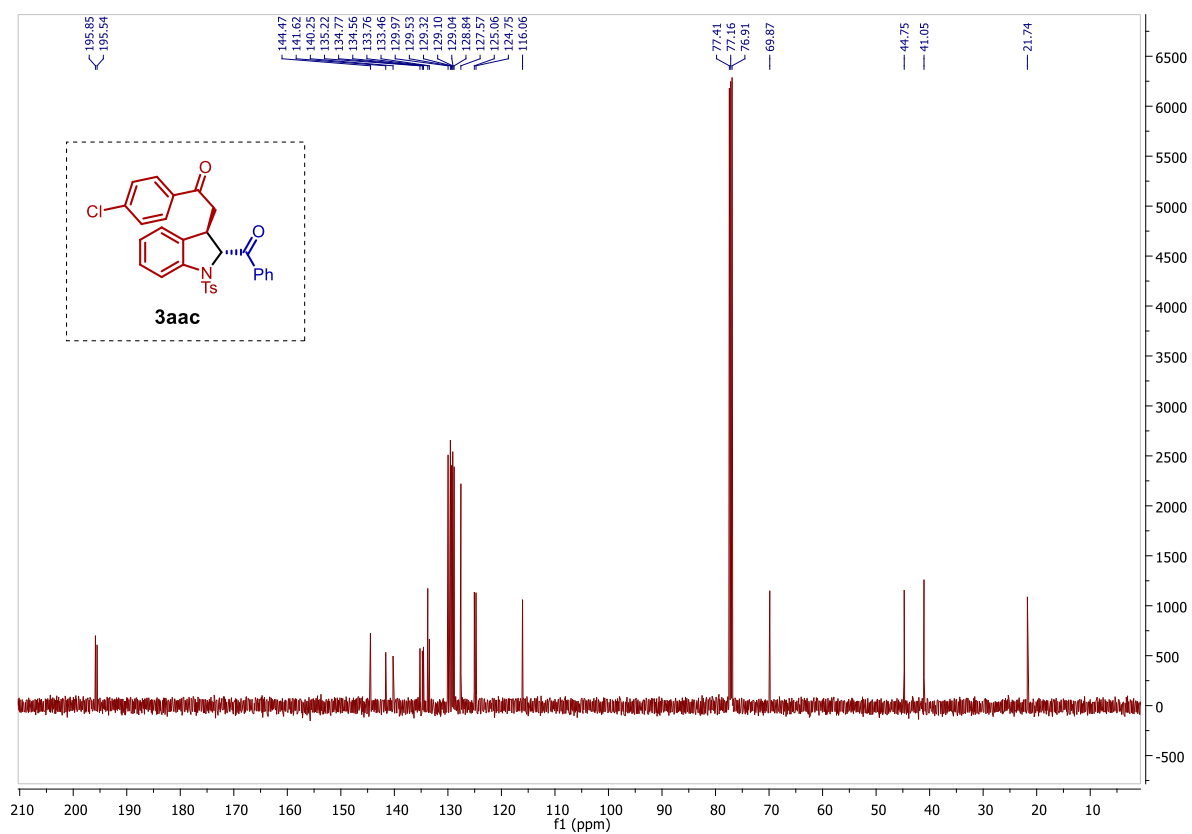
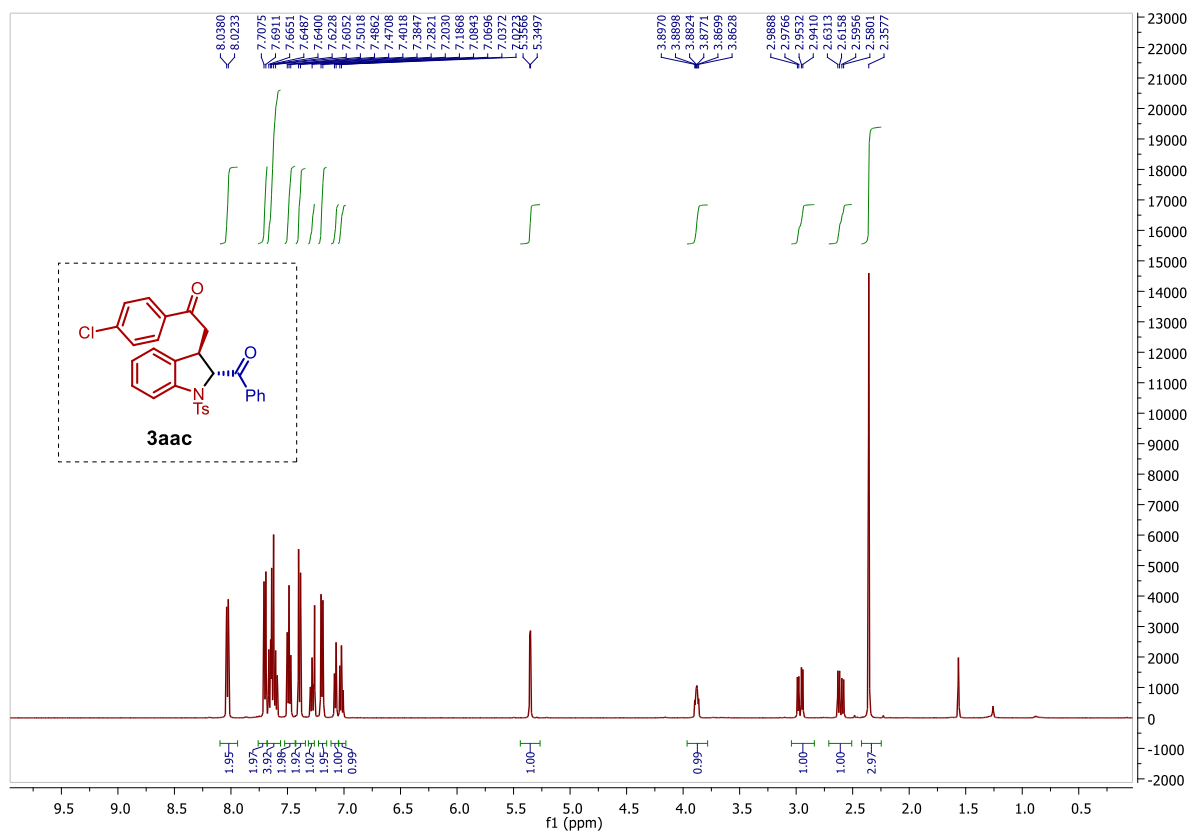
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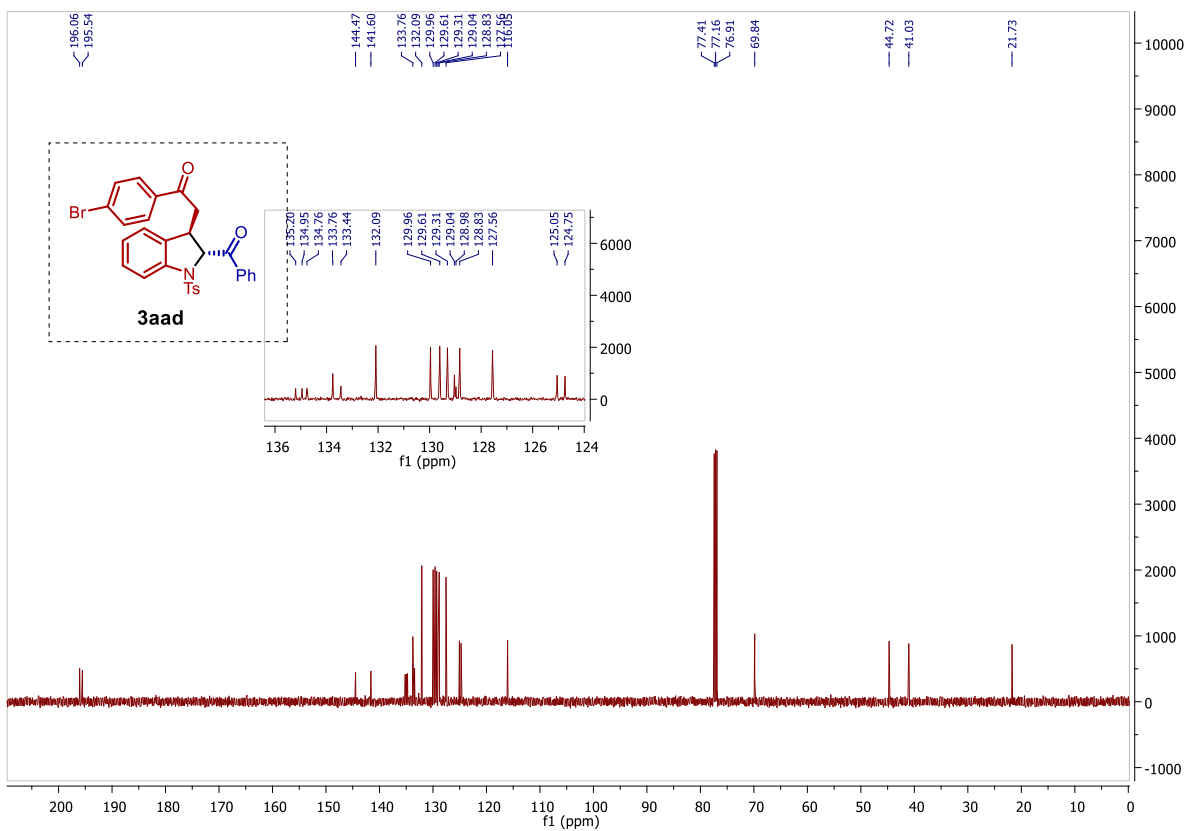
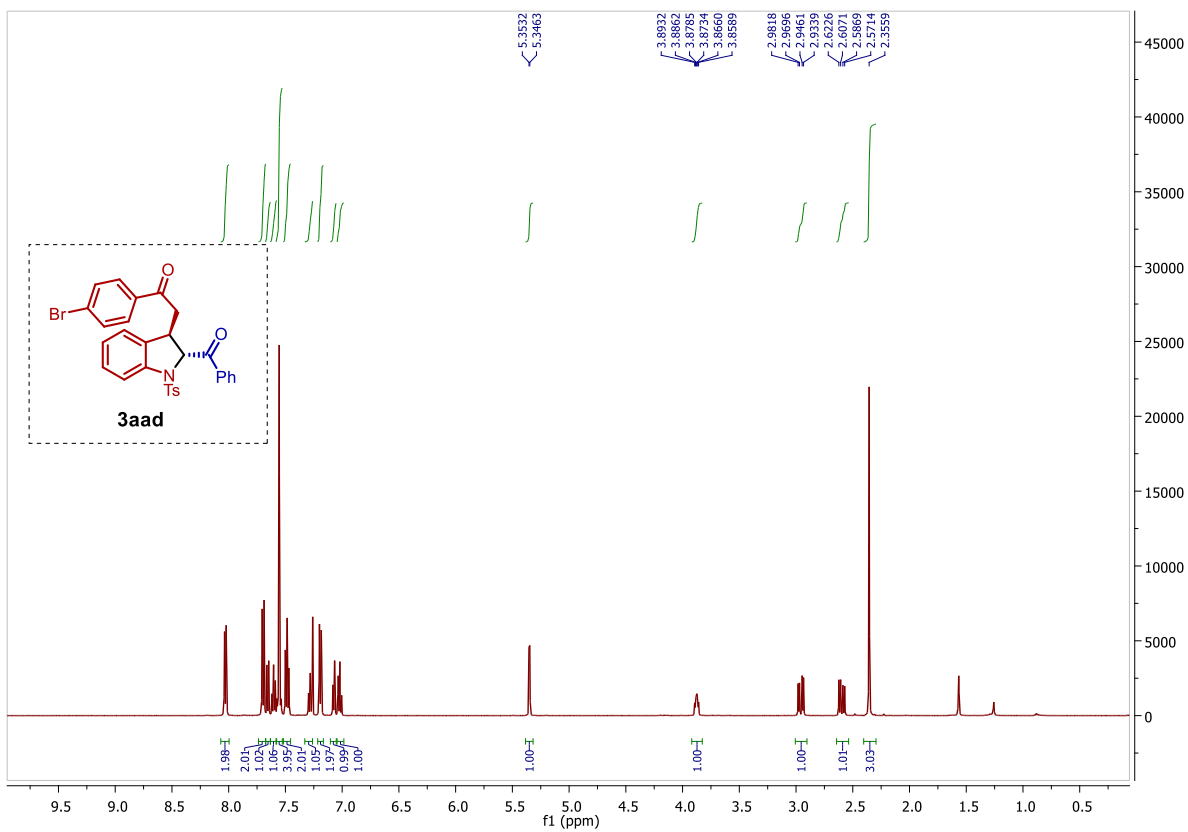
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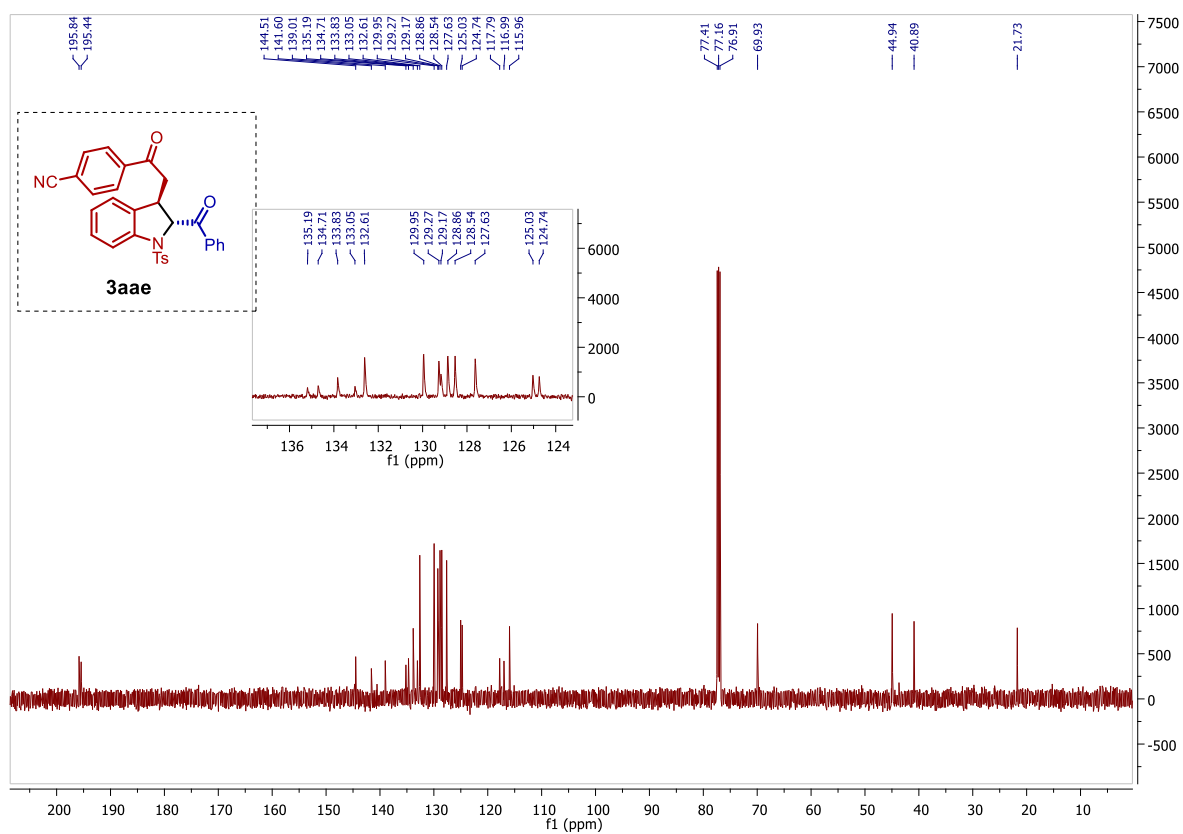
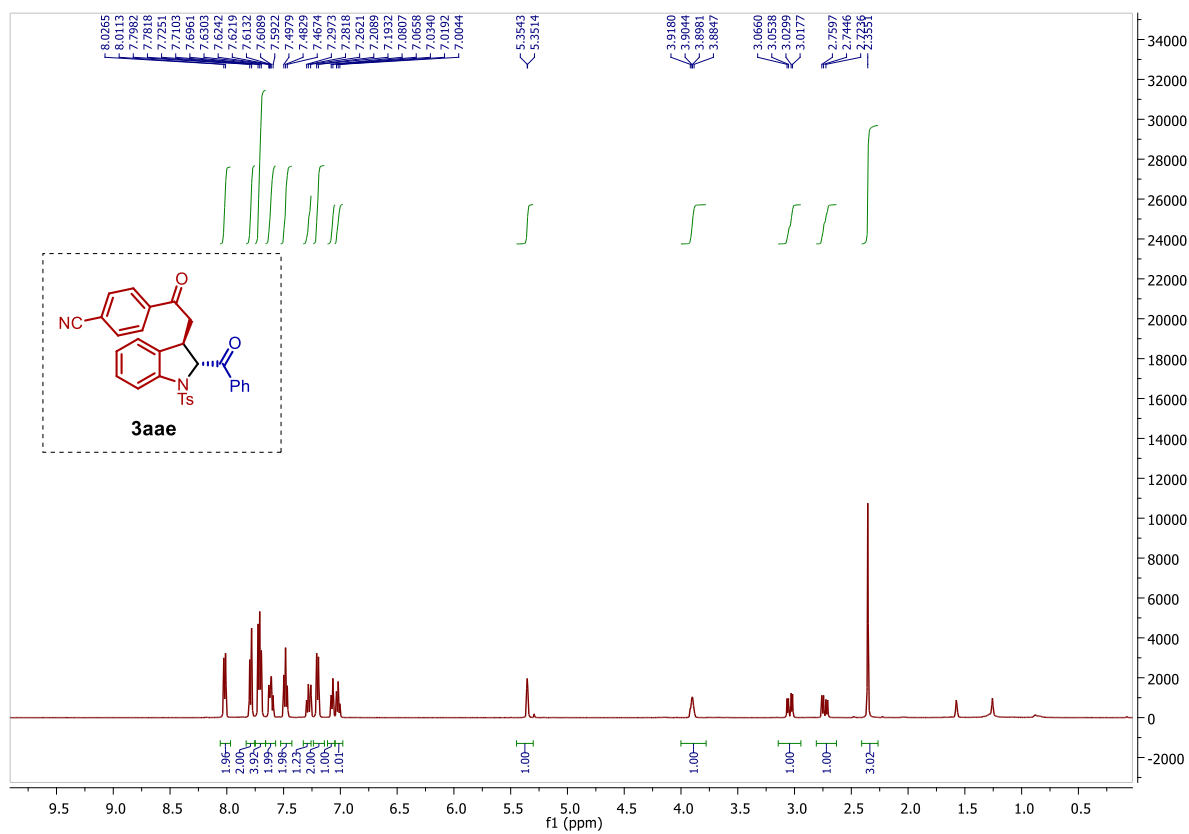
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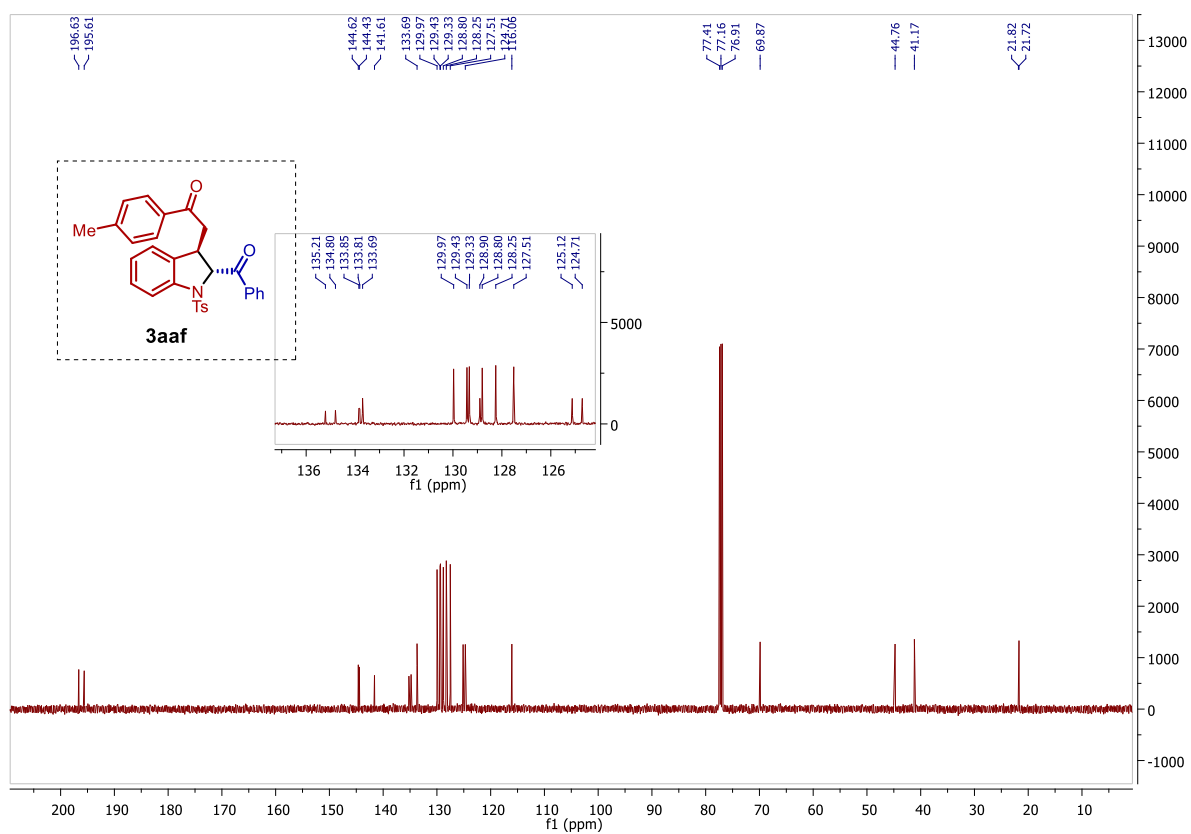
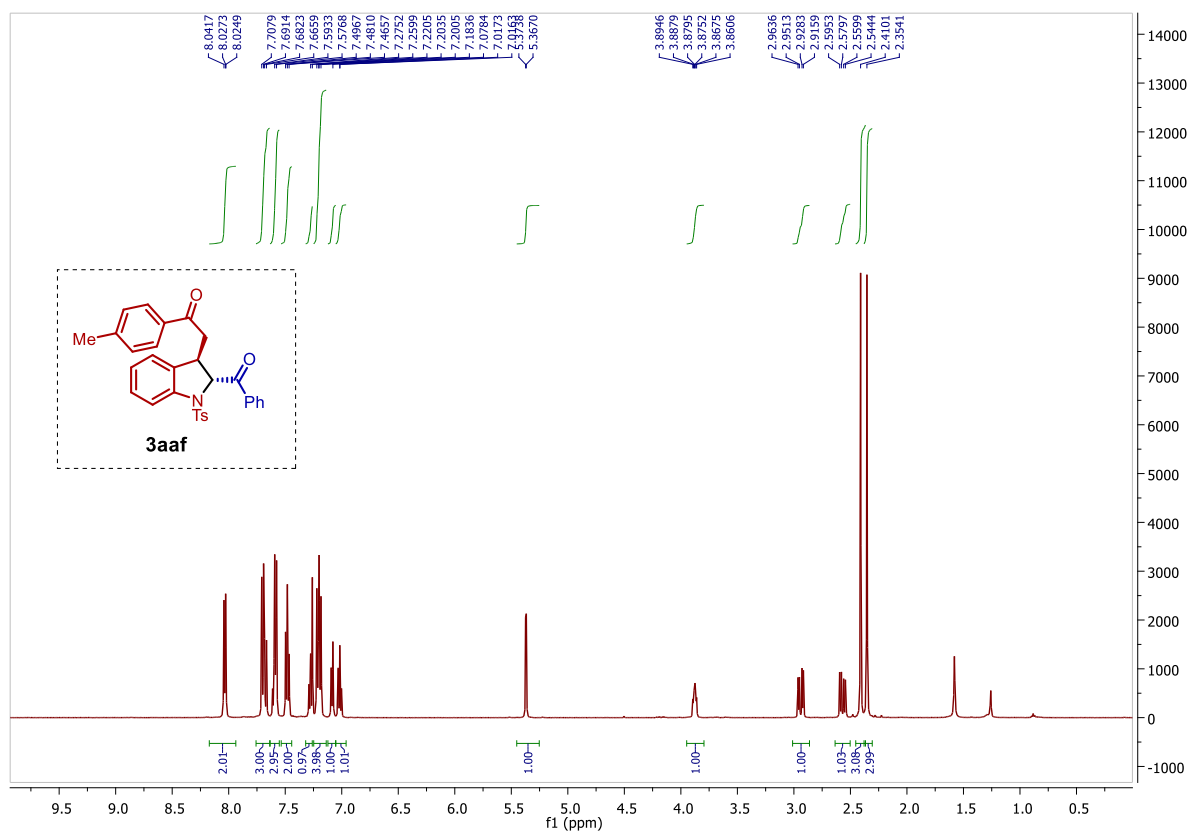


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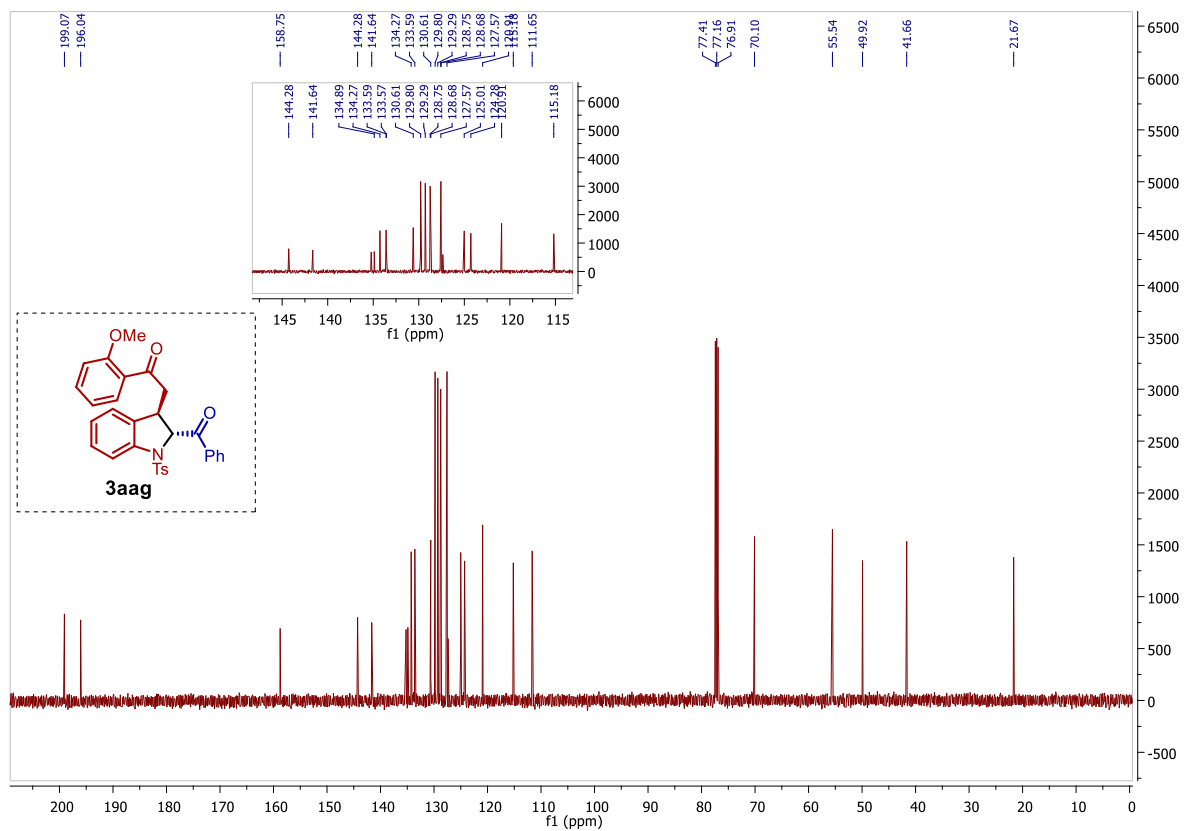
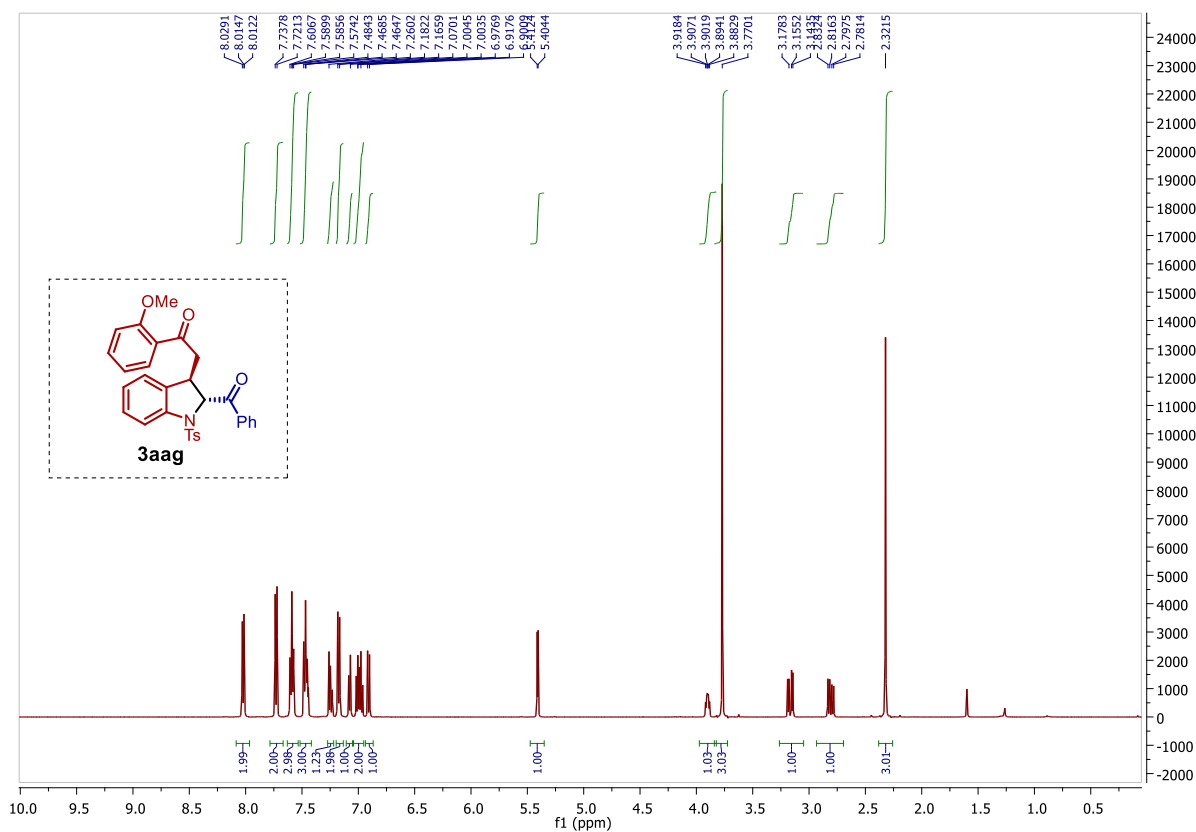


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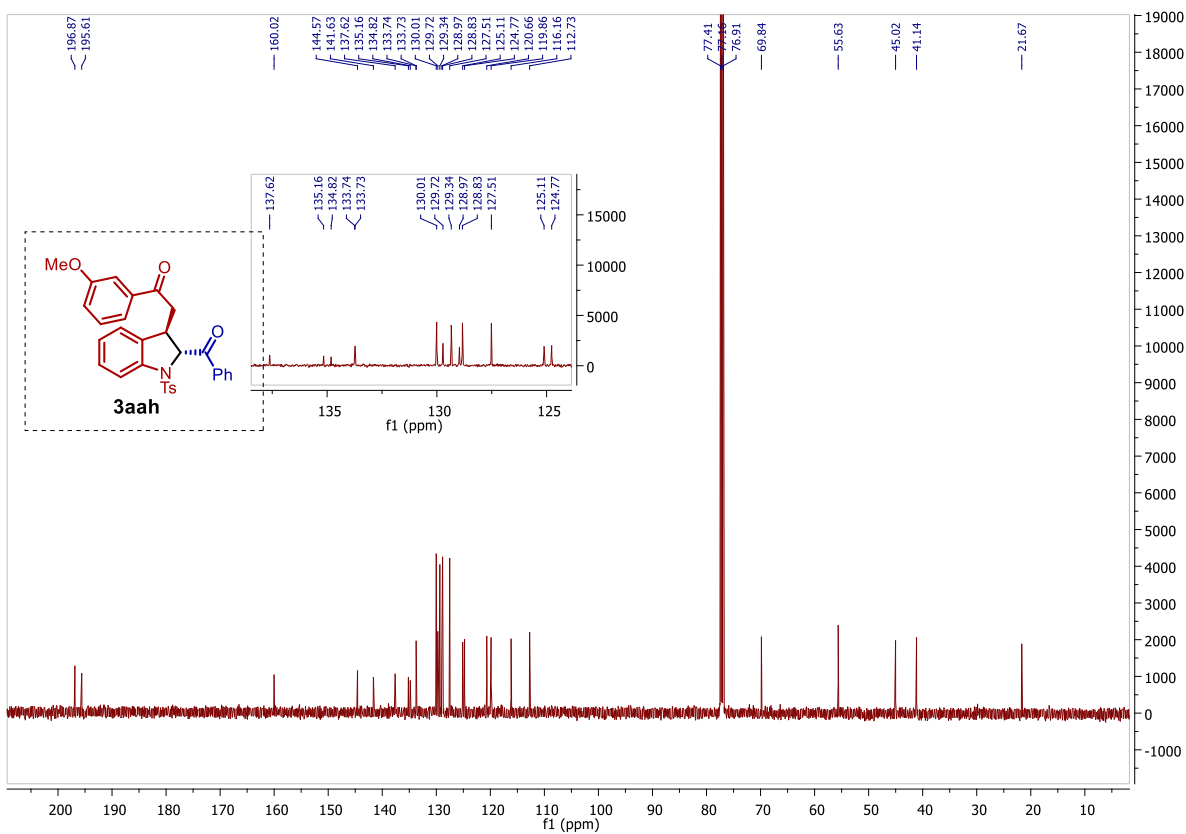
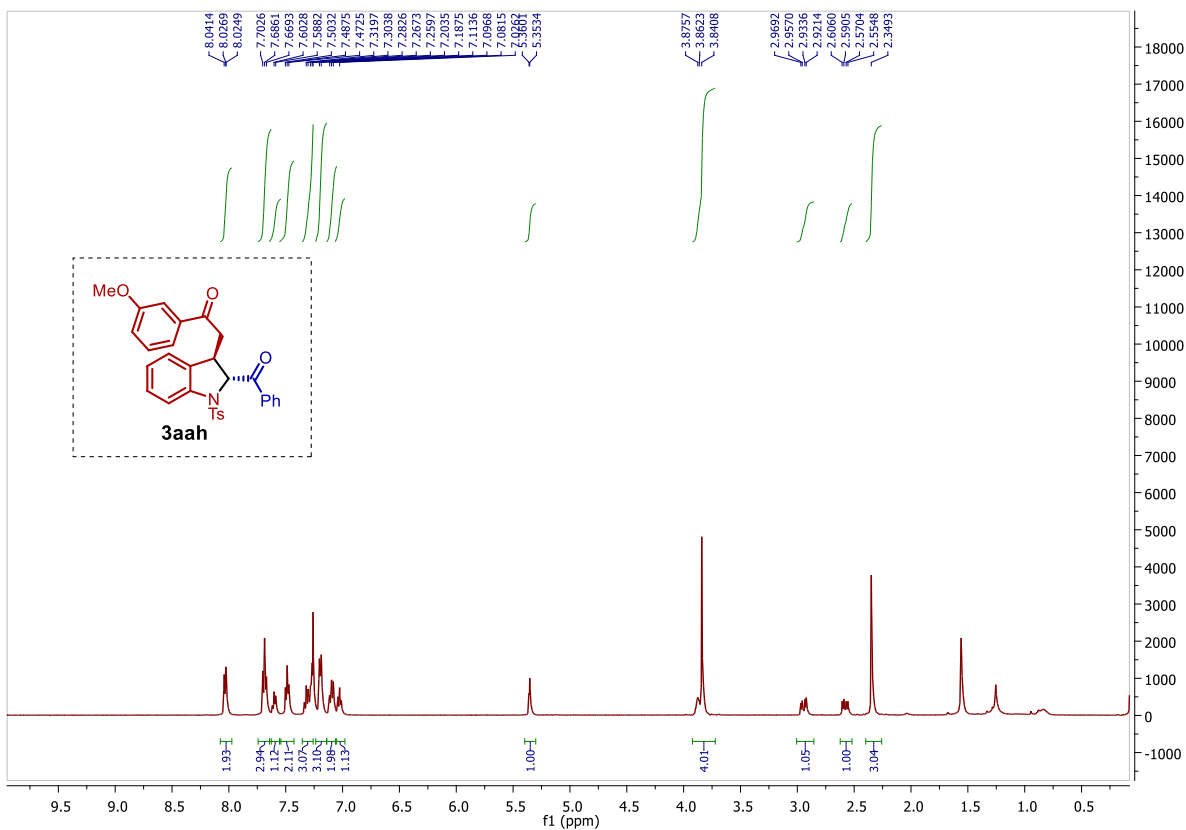




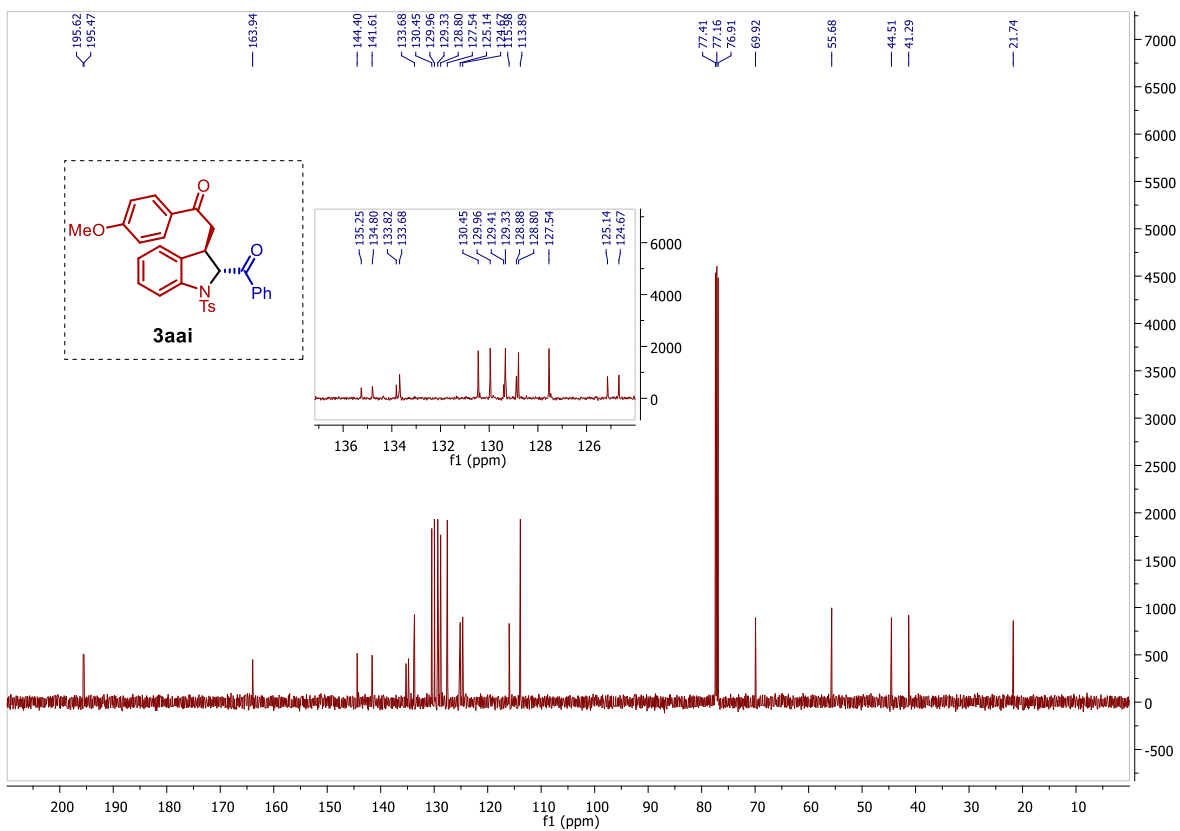
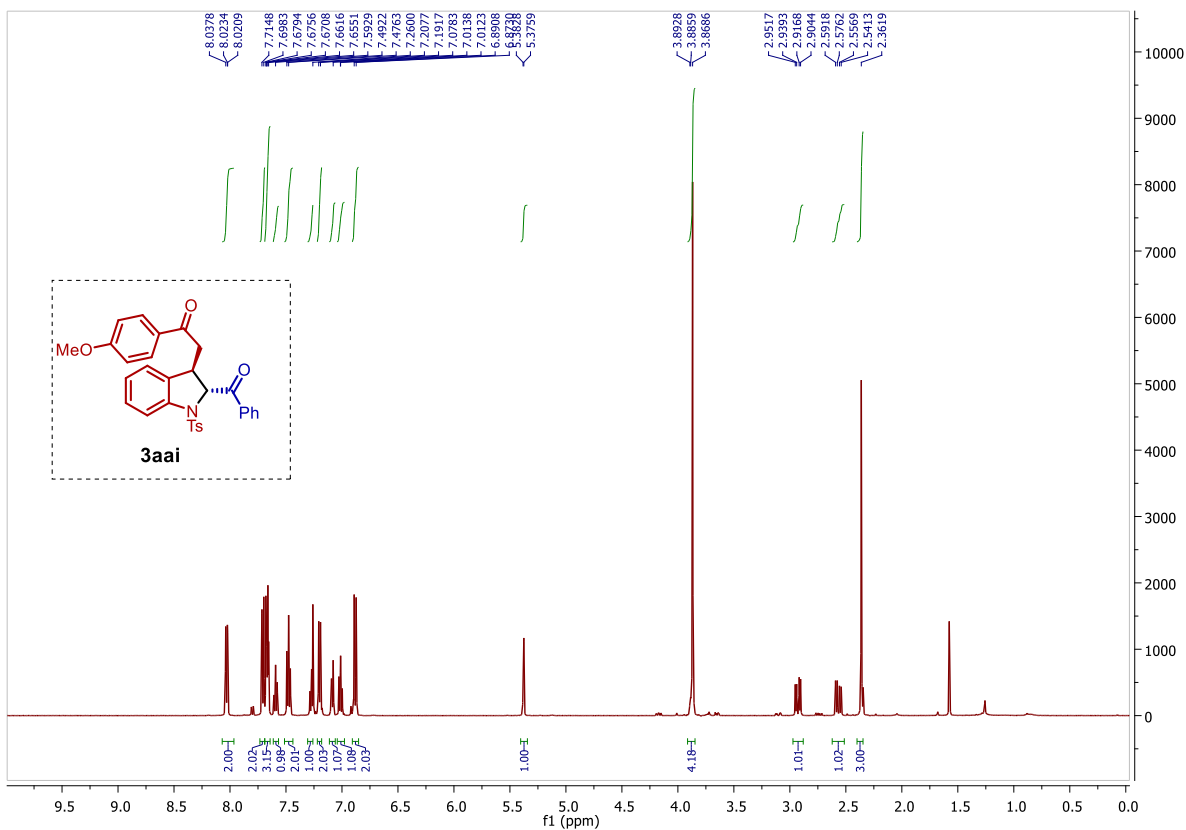
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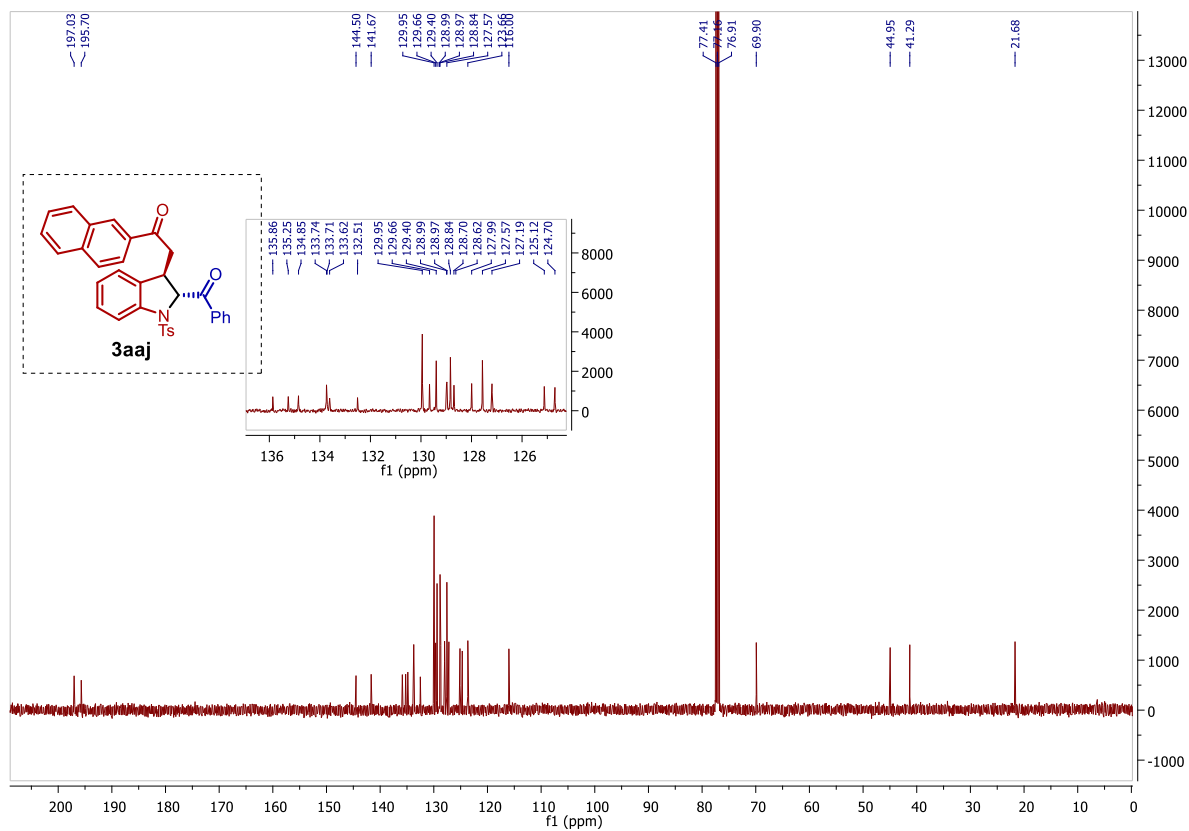
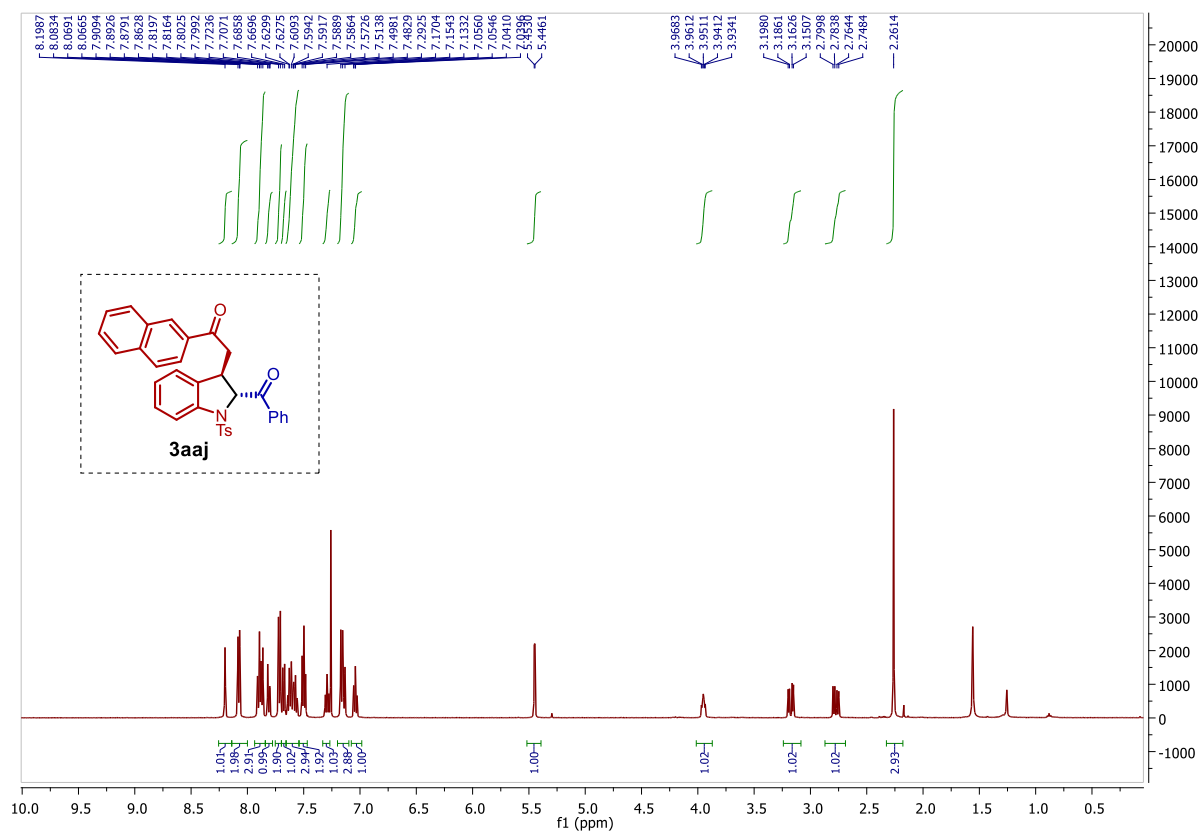
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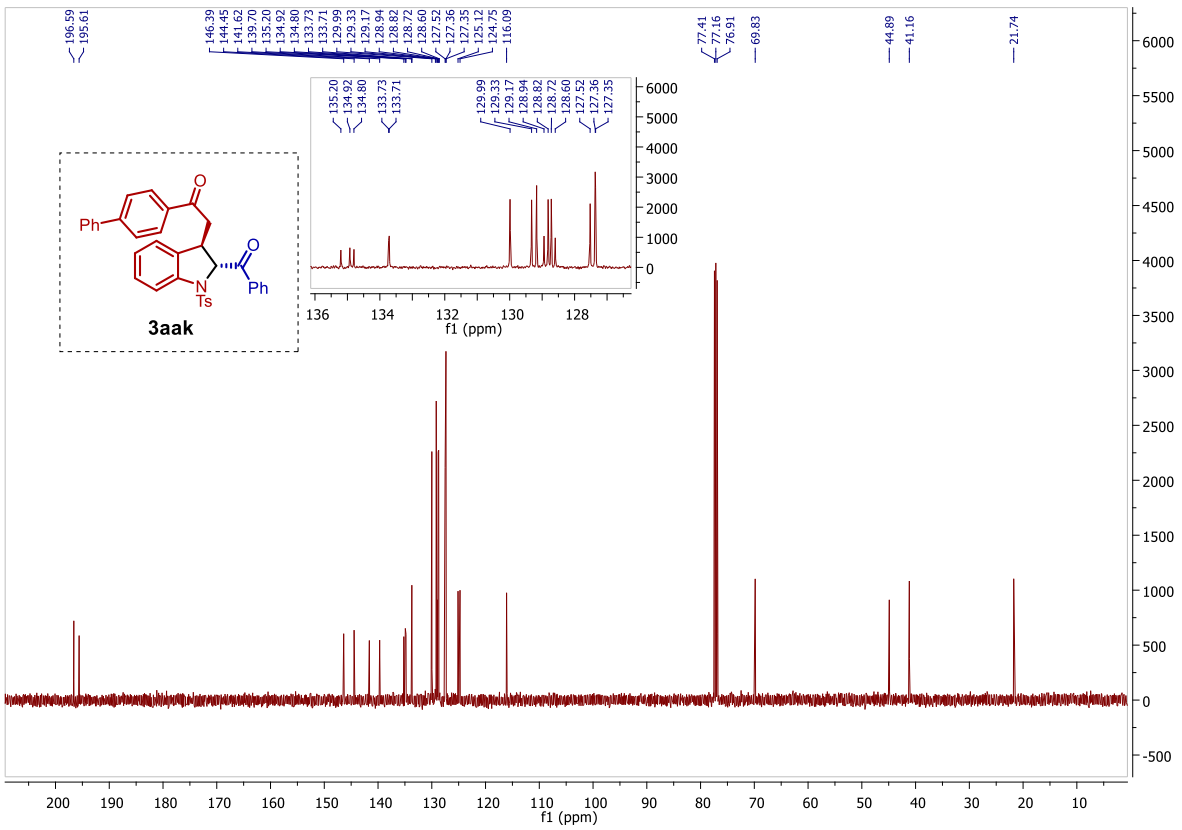
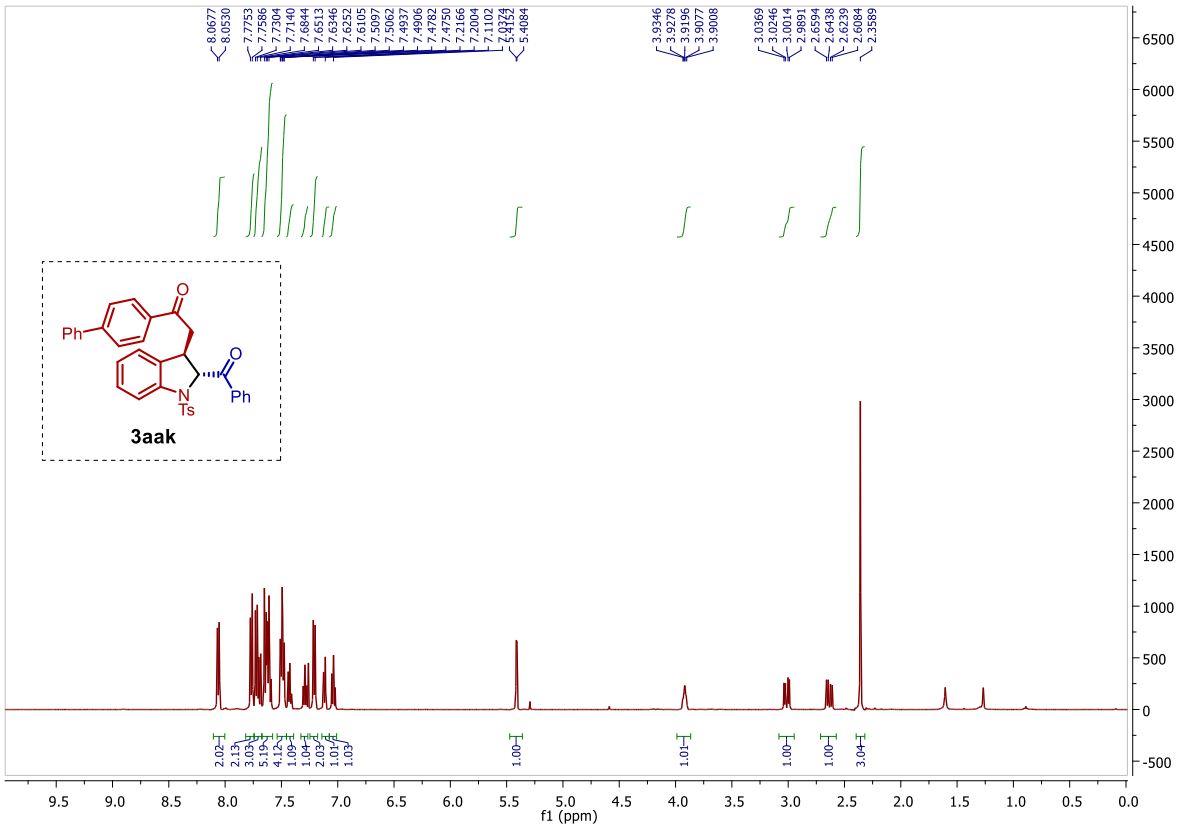
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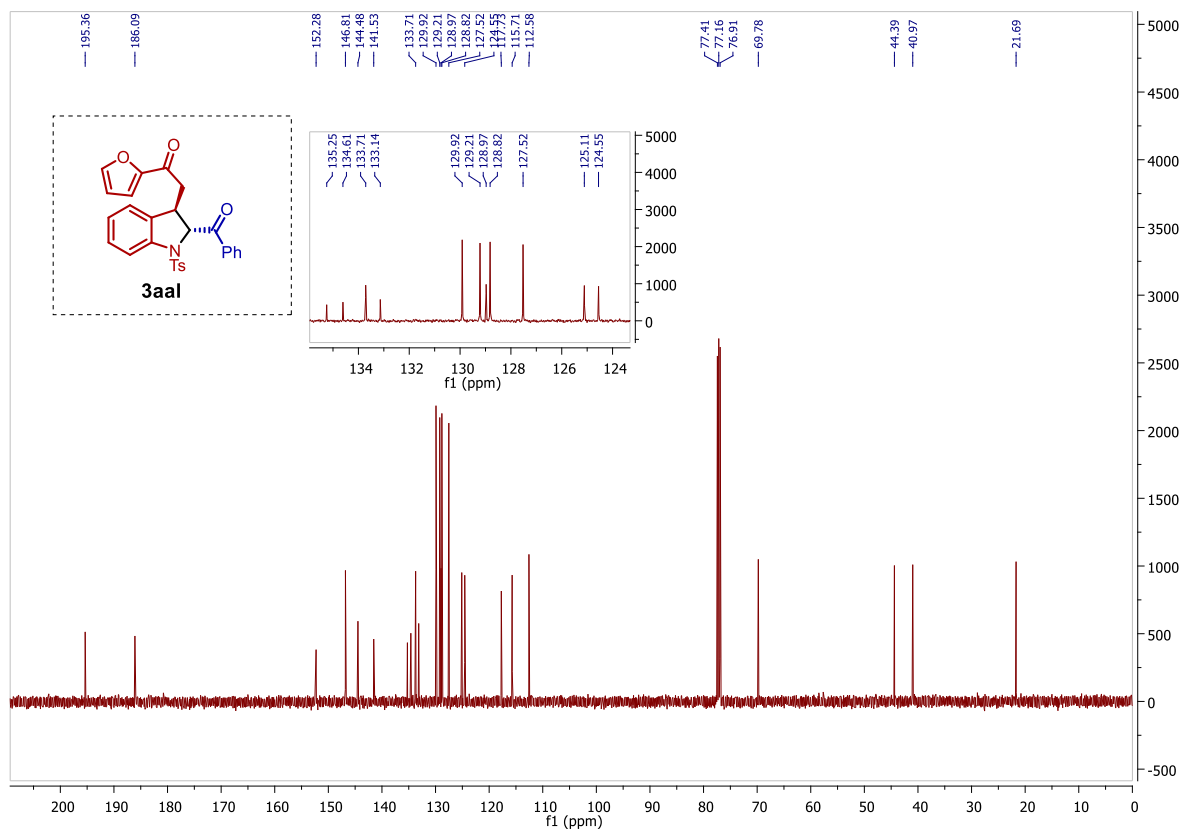
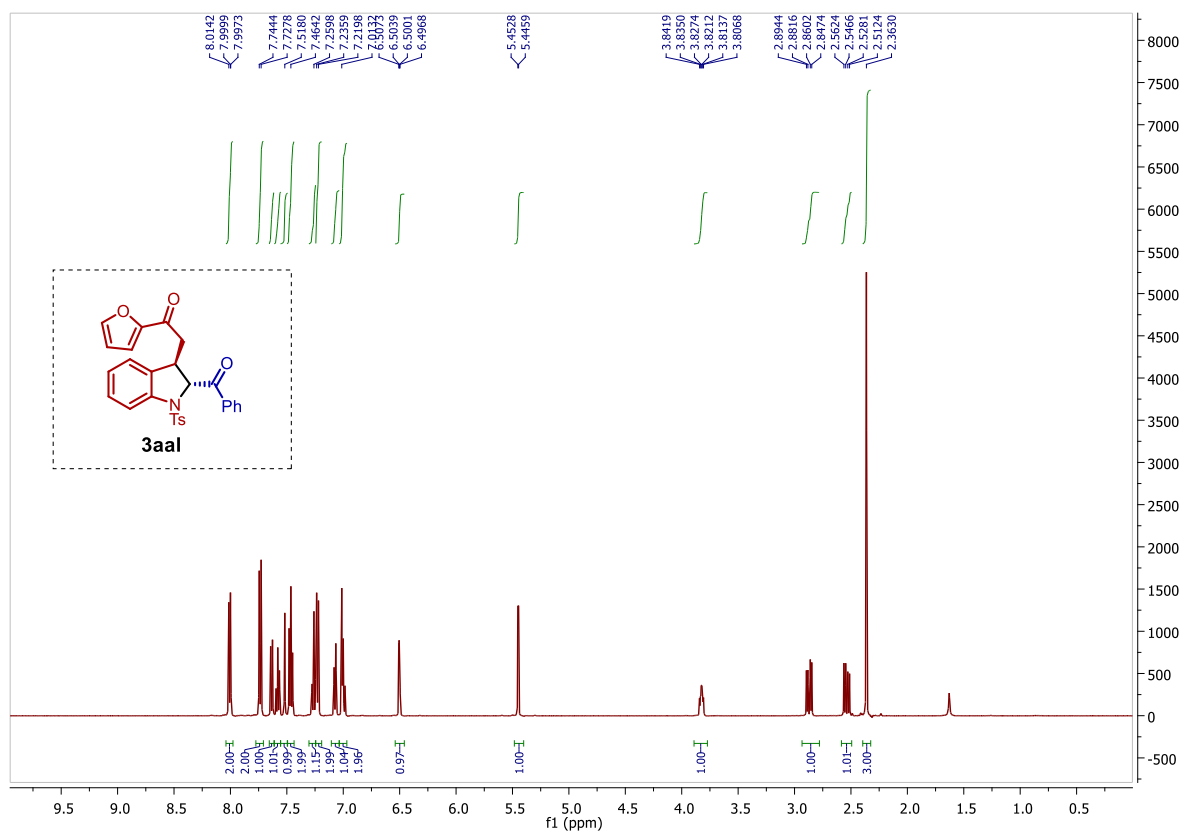
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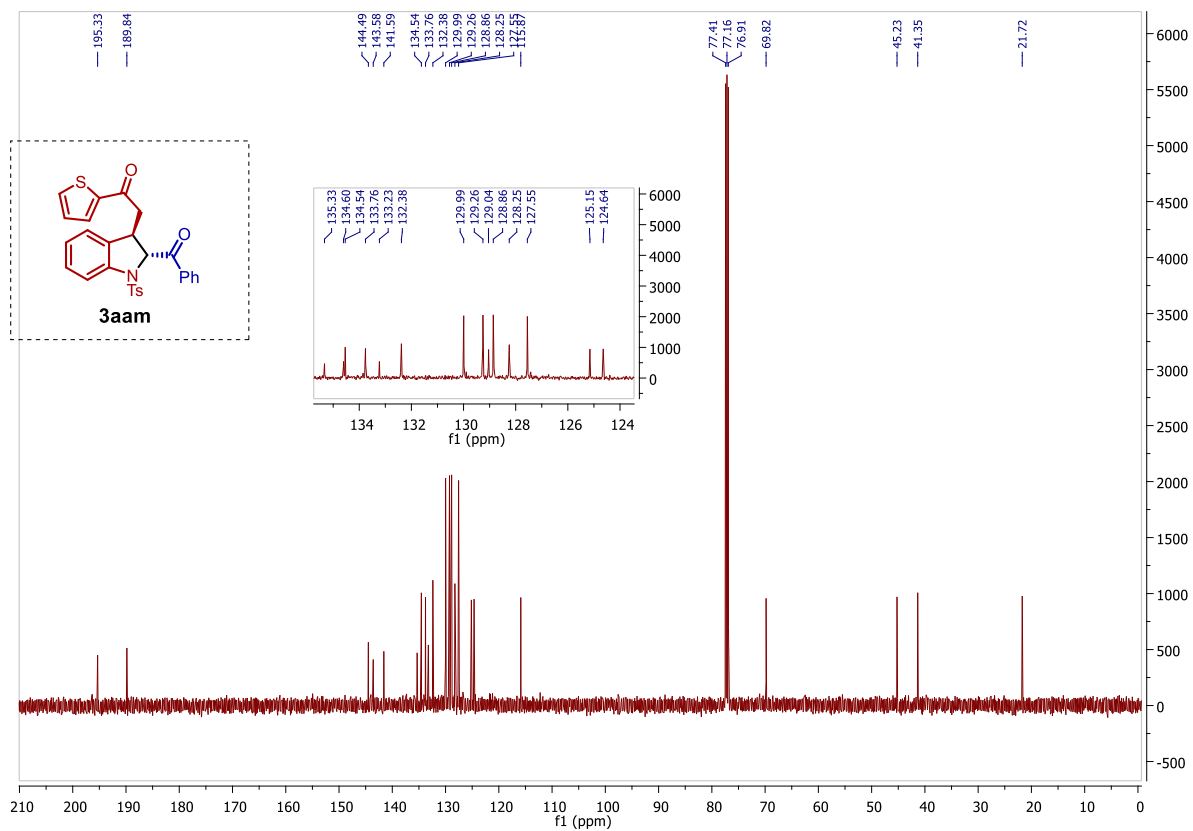
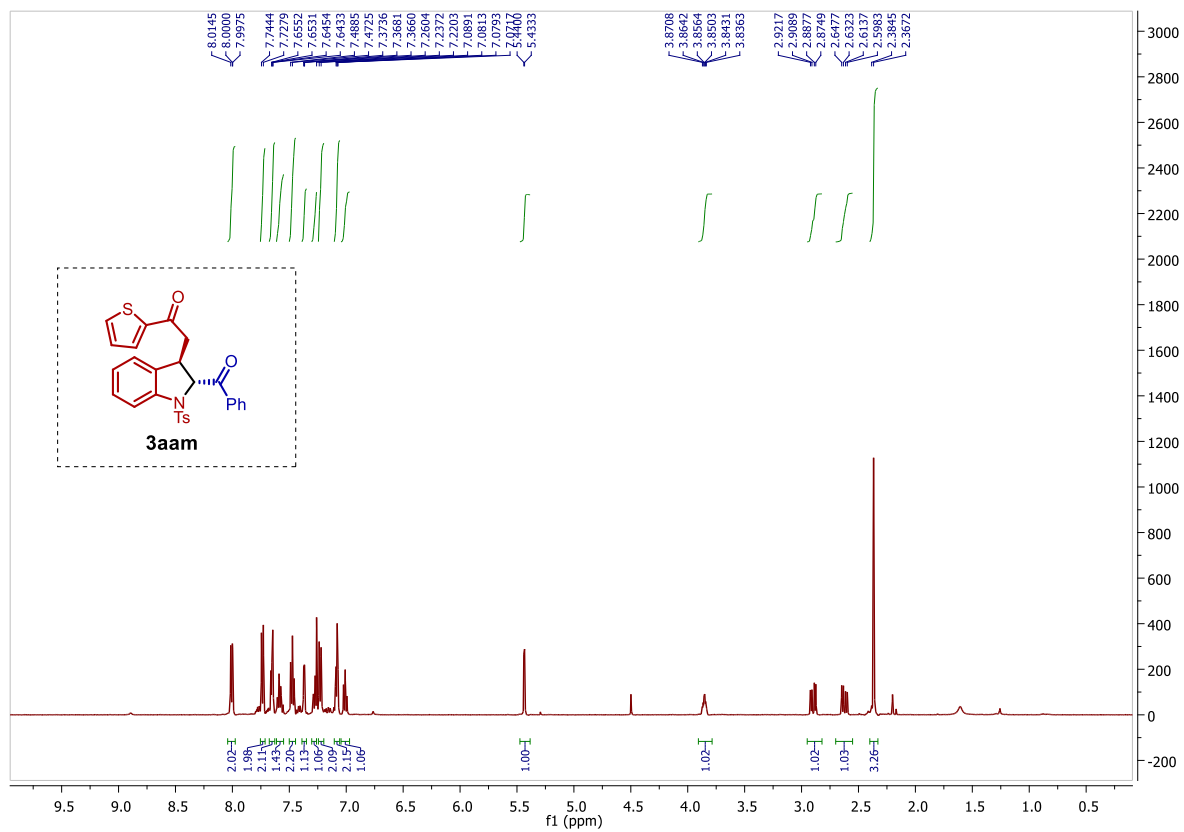
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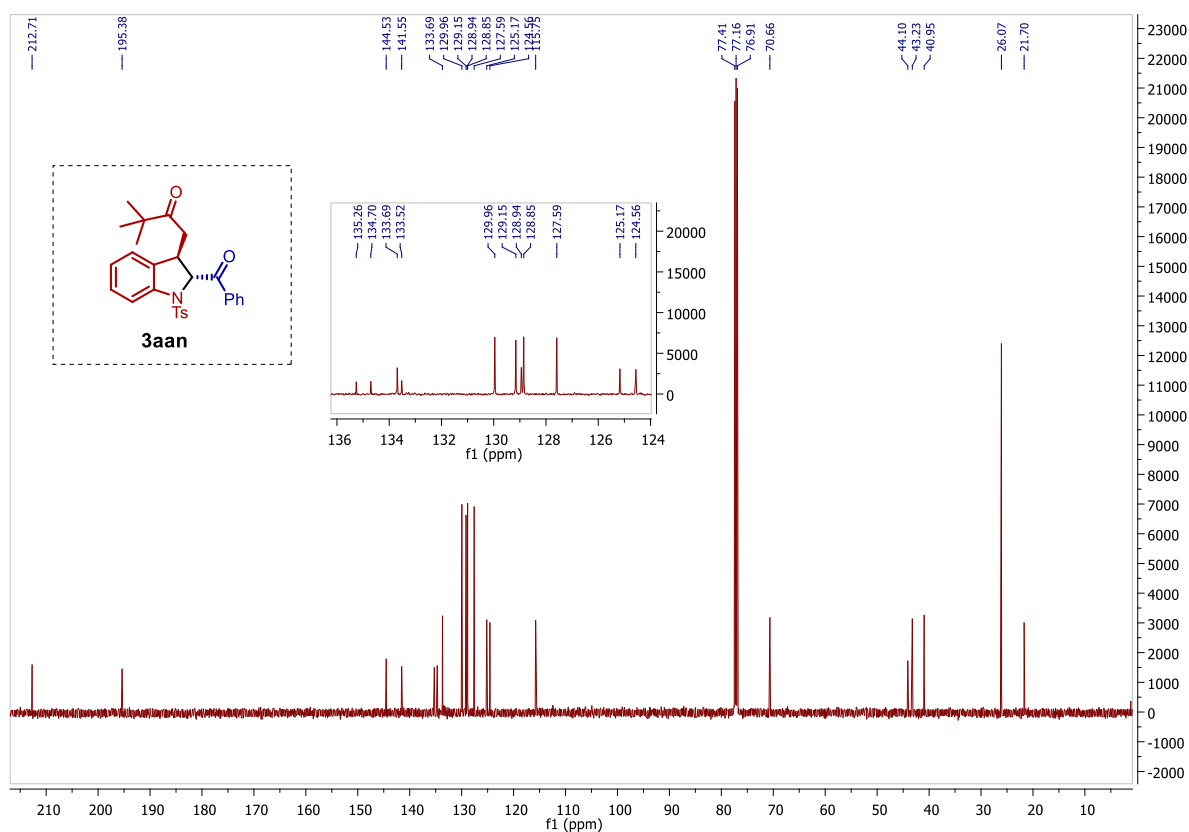
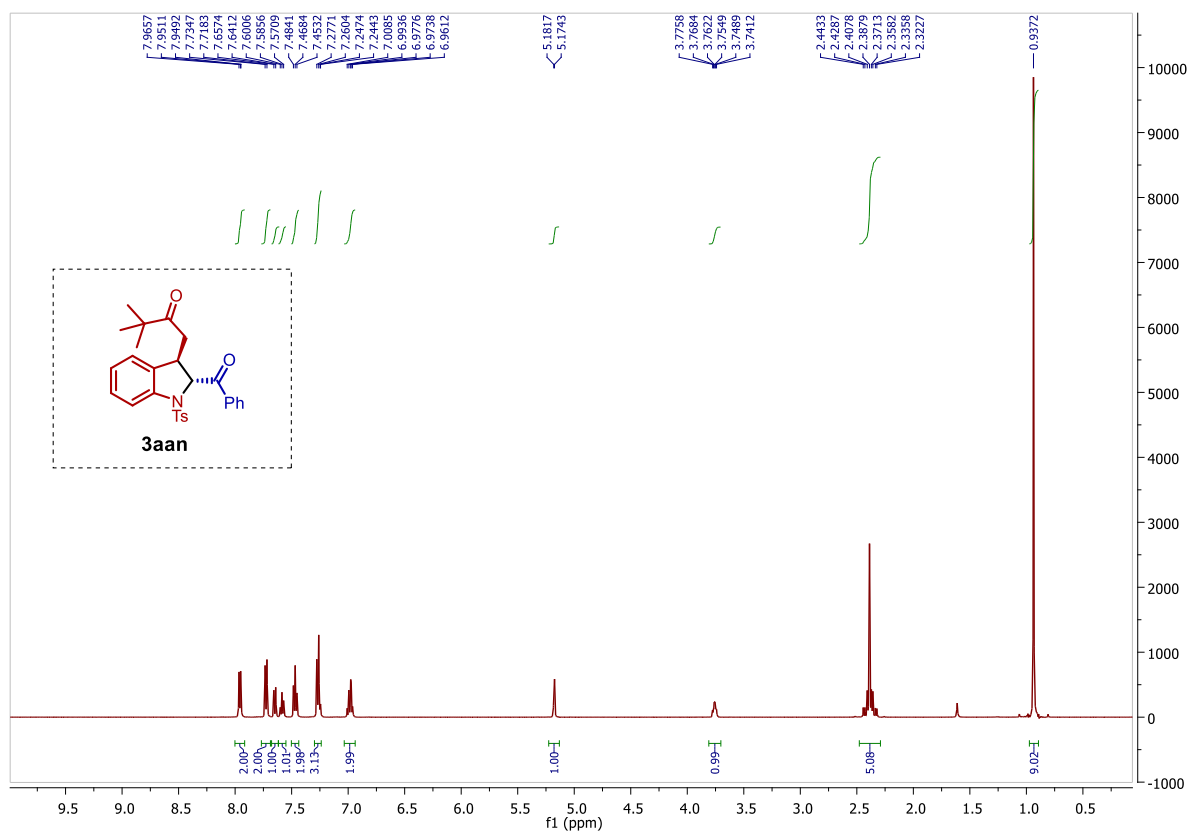


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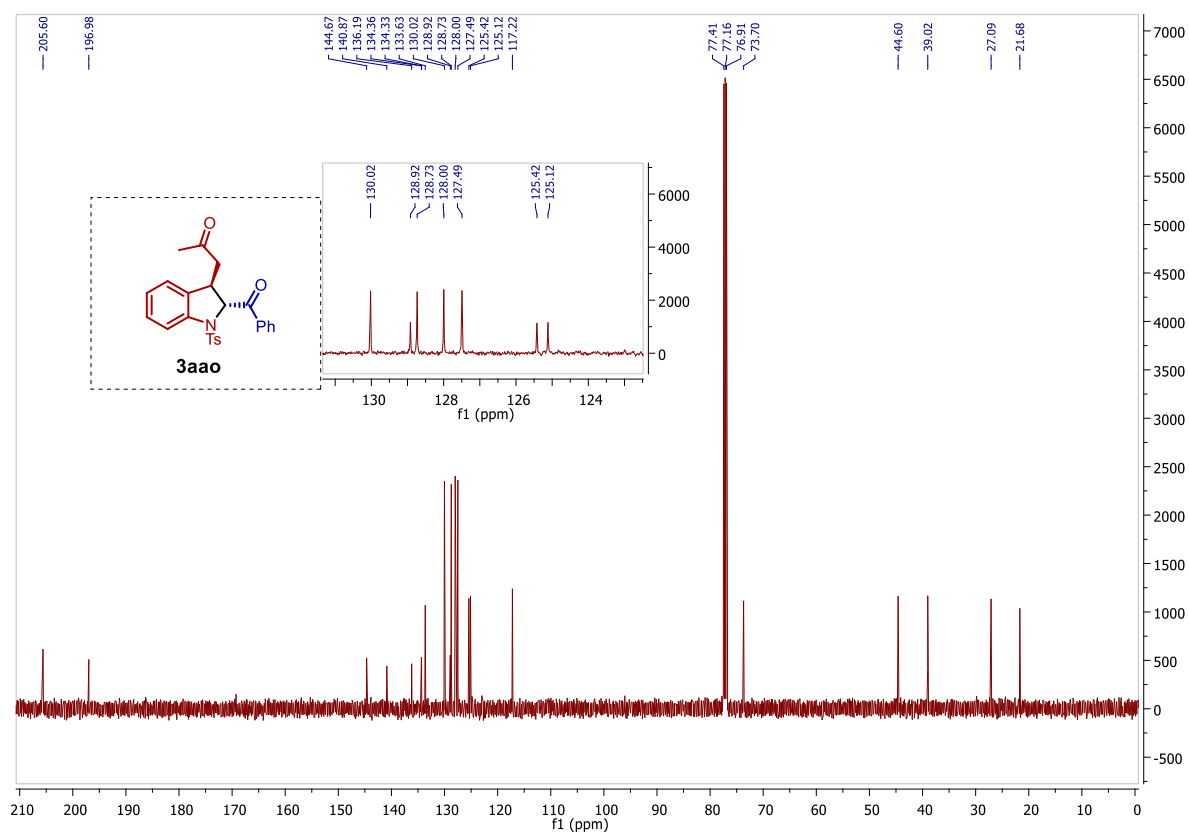
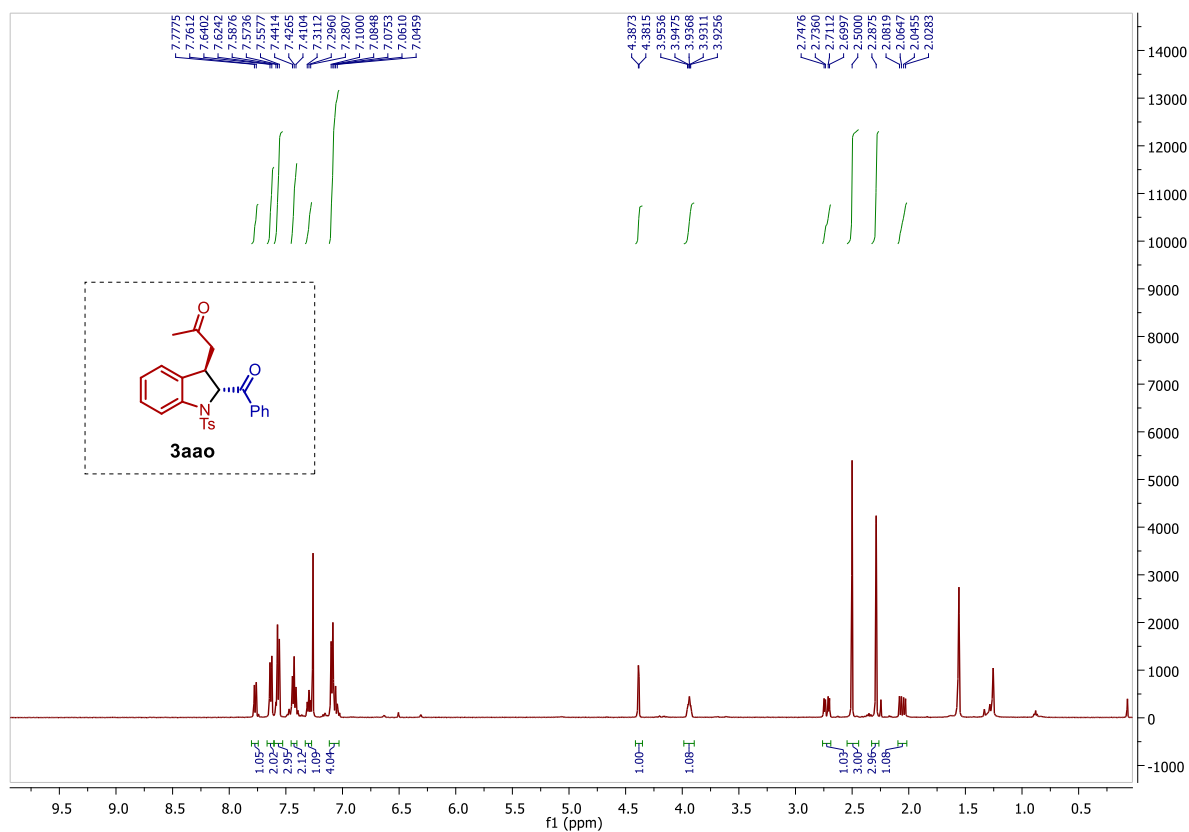


CDCl<sub>3</sub>, 500 MHz <sup>1</sup>H NMR and 125 MHz <sup>13</sup>C{<sup>1</sup>H} NMR Spectra of **3aam**

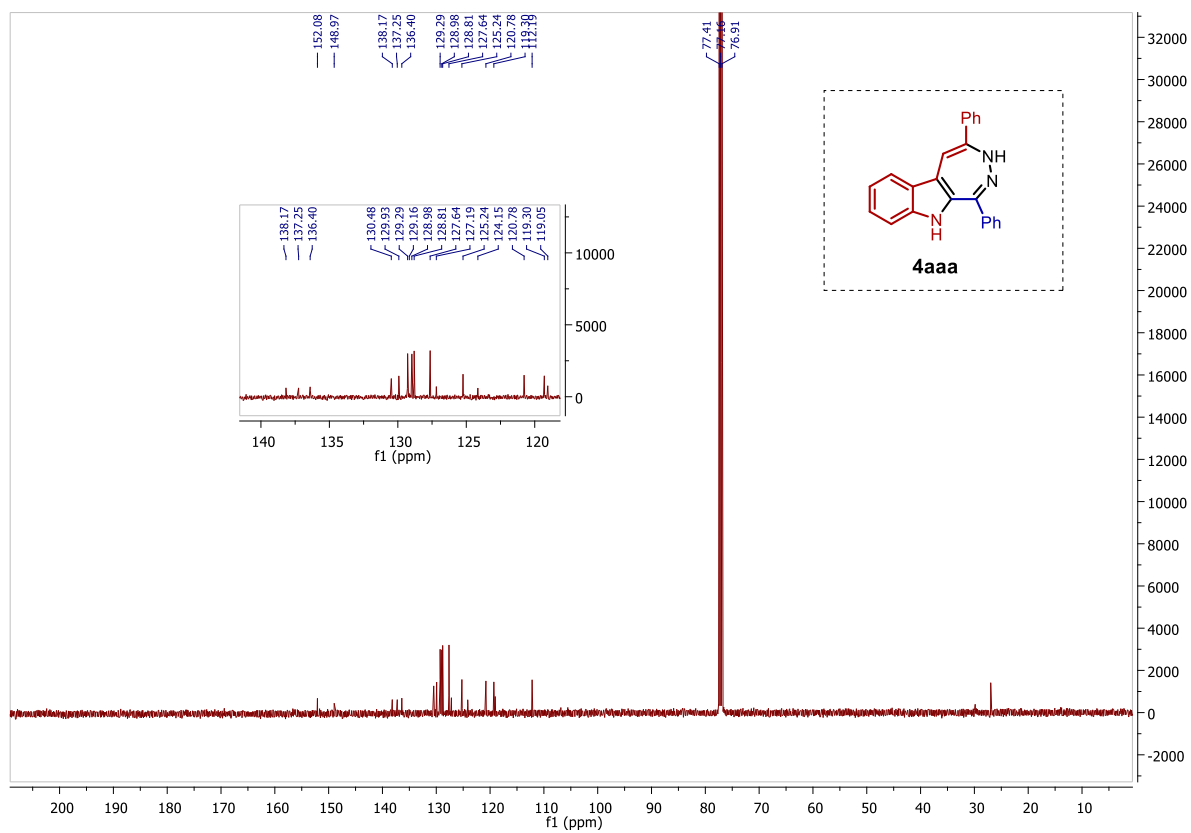
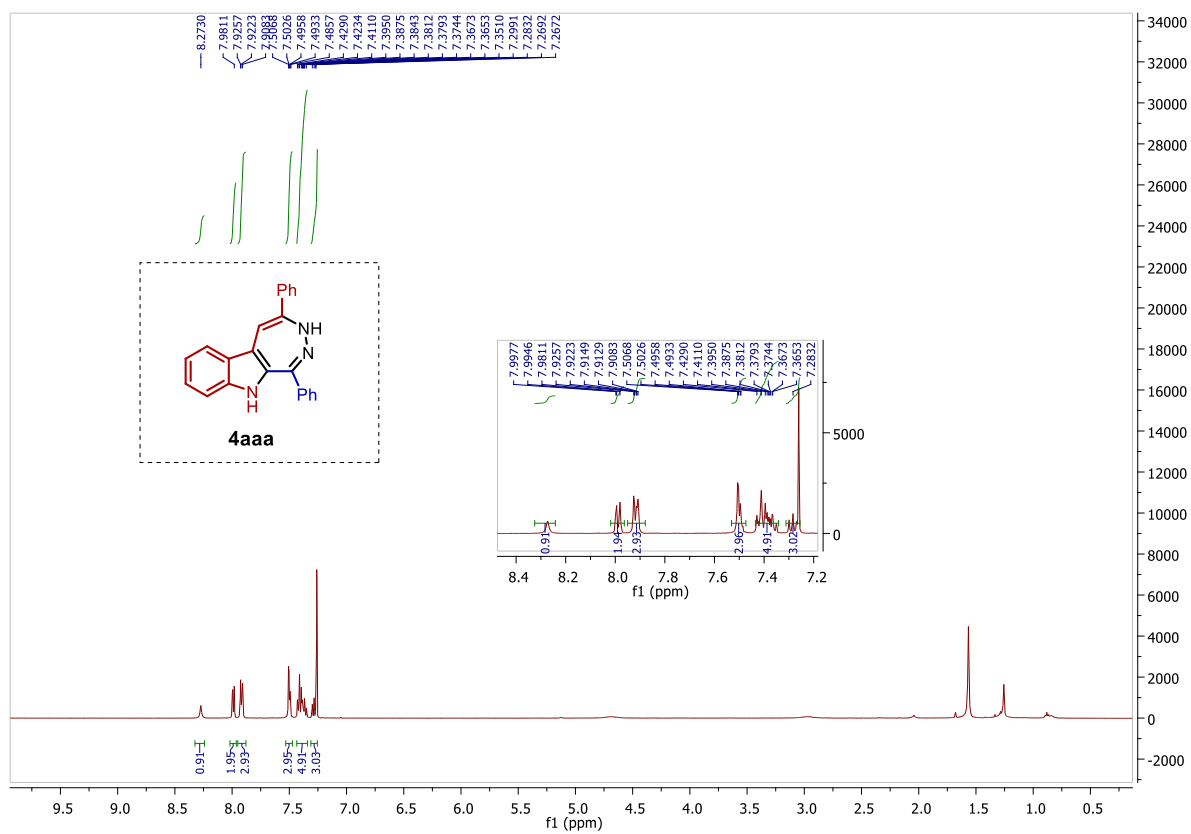




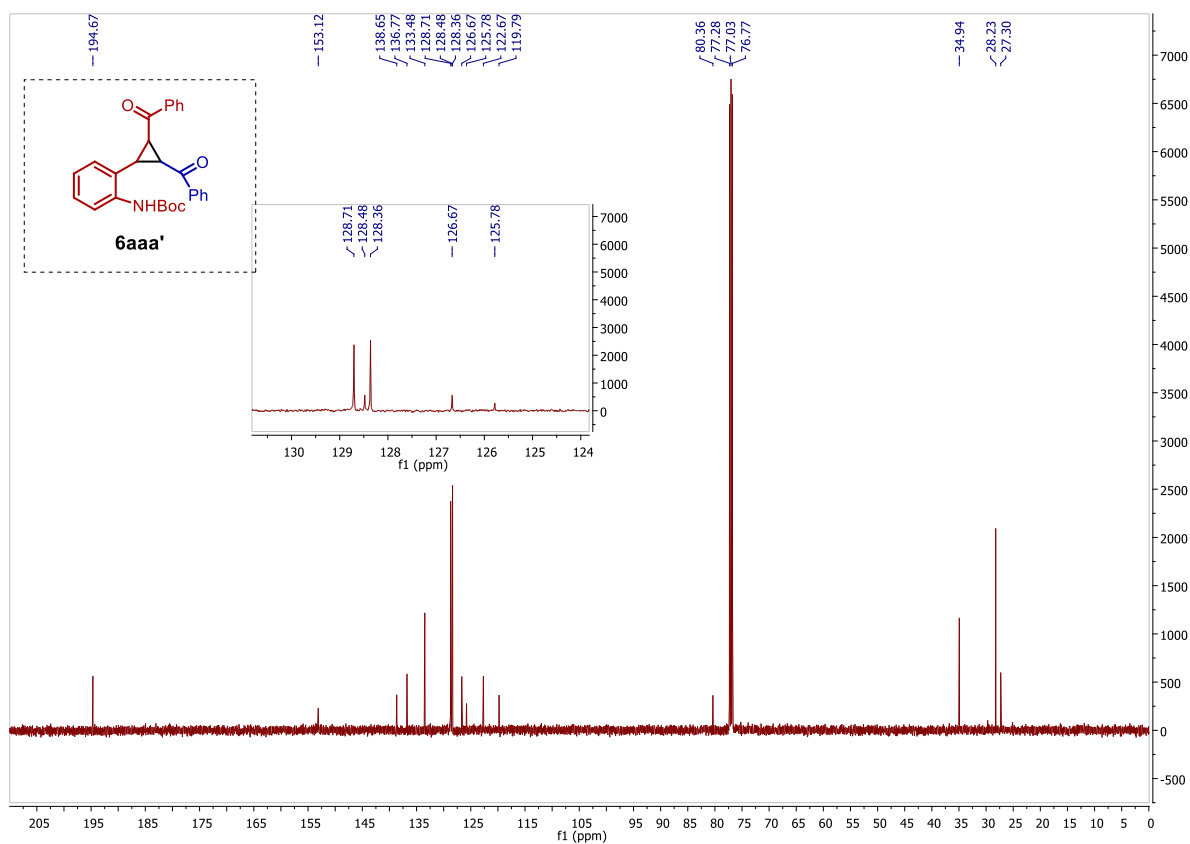
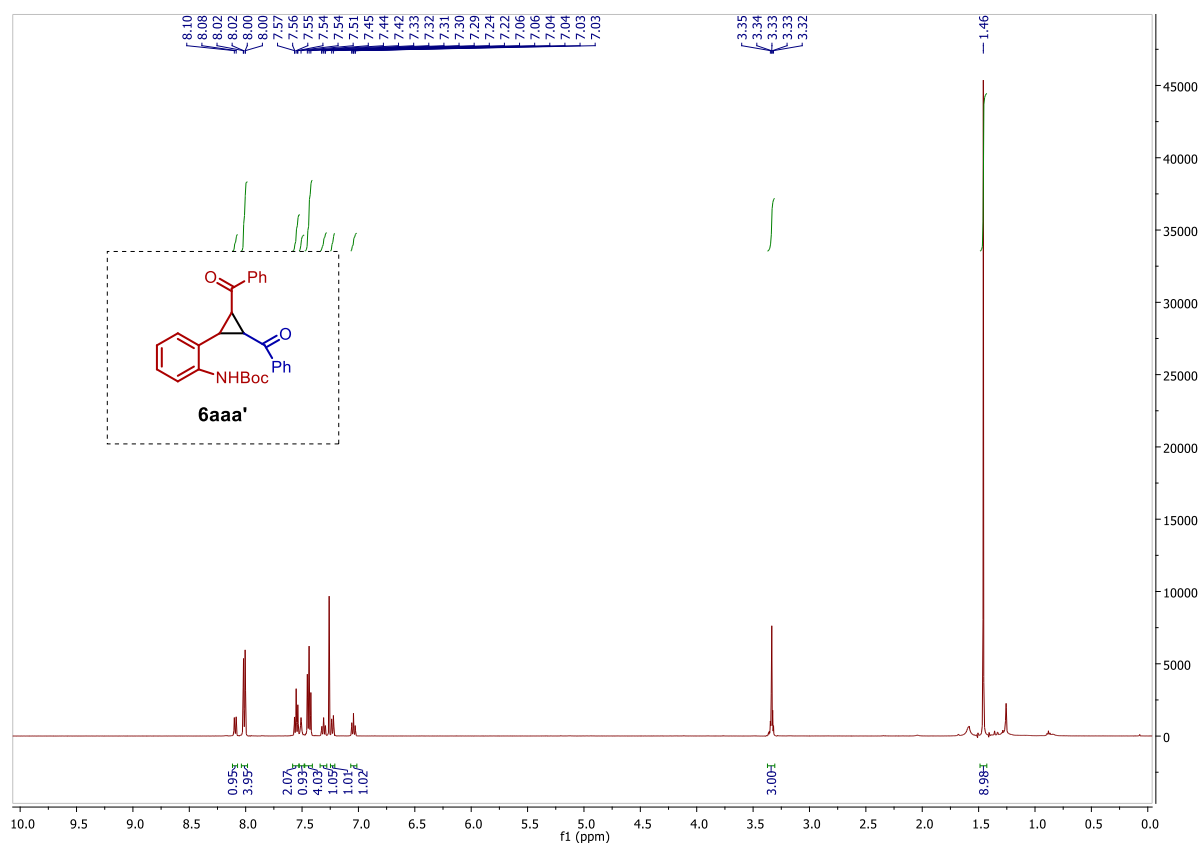
CDCl<sub>3</sub>, 500 MHz <sup>1</sup>H NMR and 125 MHz <sup>13</sup>C{<sup>1</sup>H} NMR Spectra of **3aan**



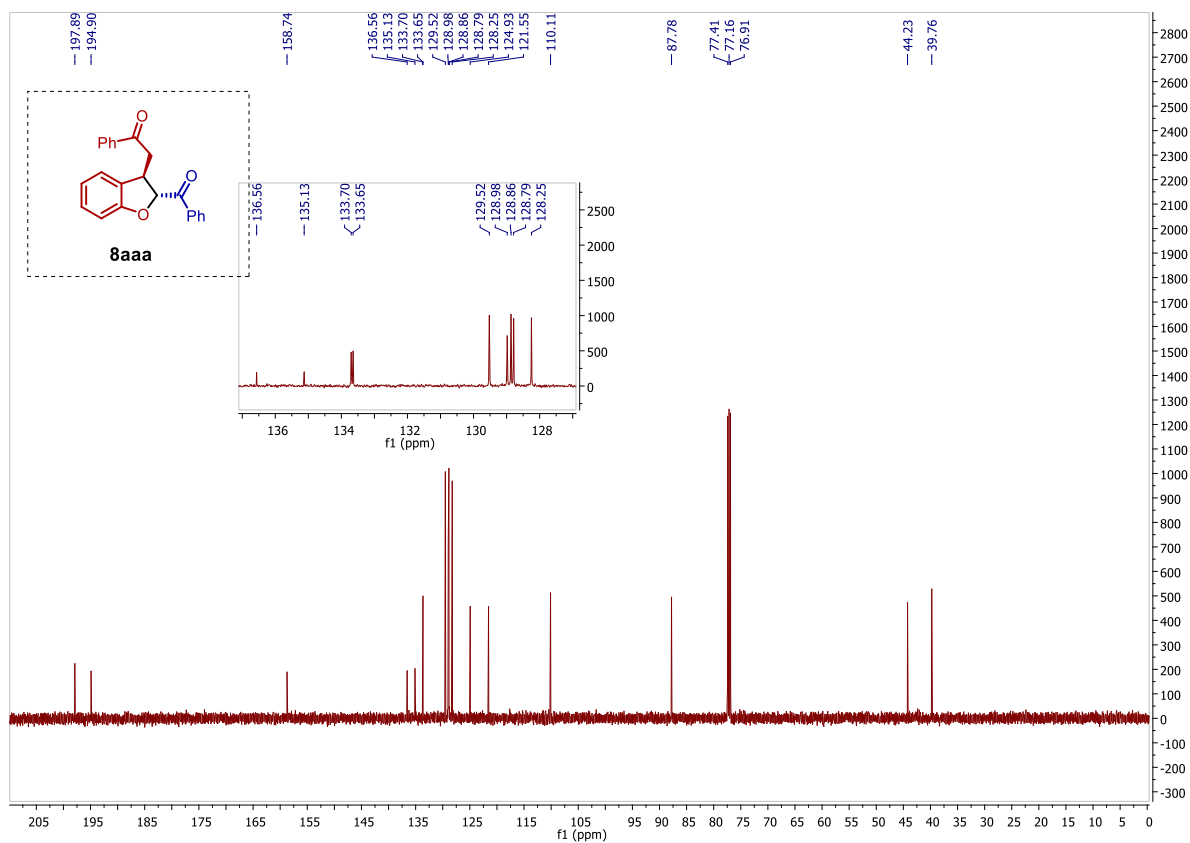
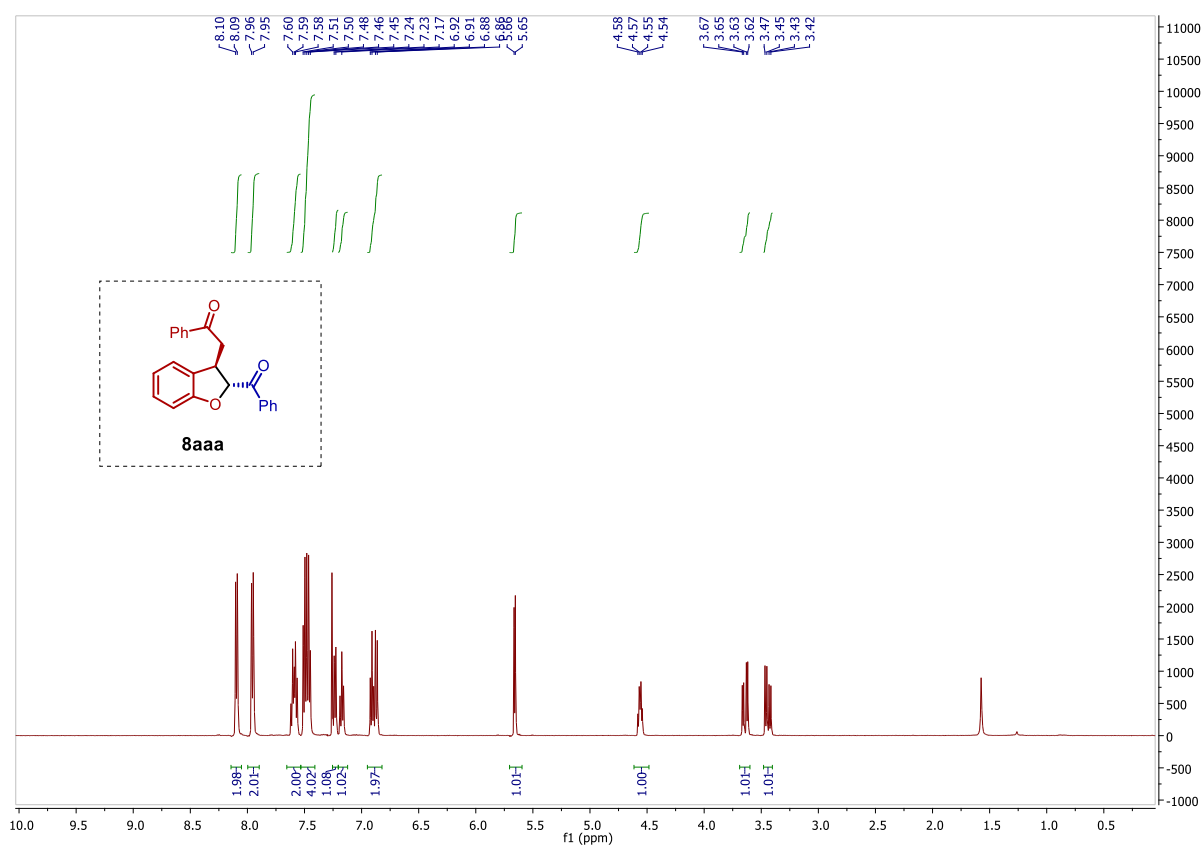
CDCl<sub>3</sub>, 500 MHz <sup>1</sup>H NMR and 125 MHz <sup>13</sup>C{<sup>1</sup>H} NMR Spectra of 3ao



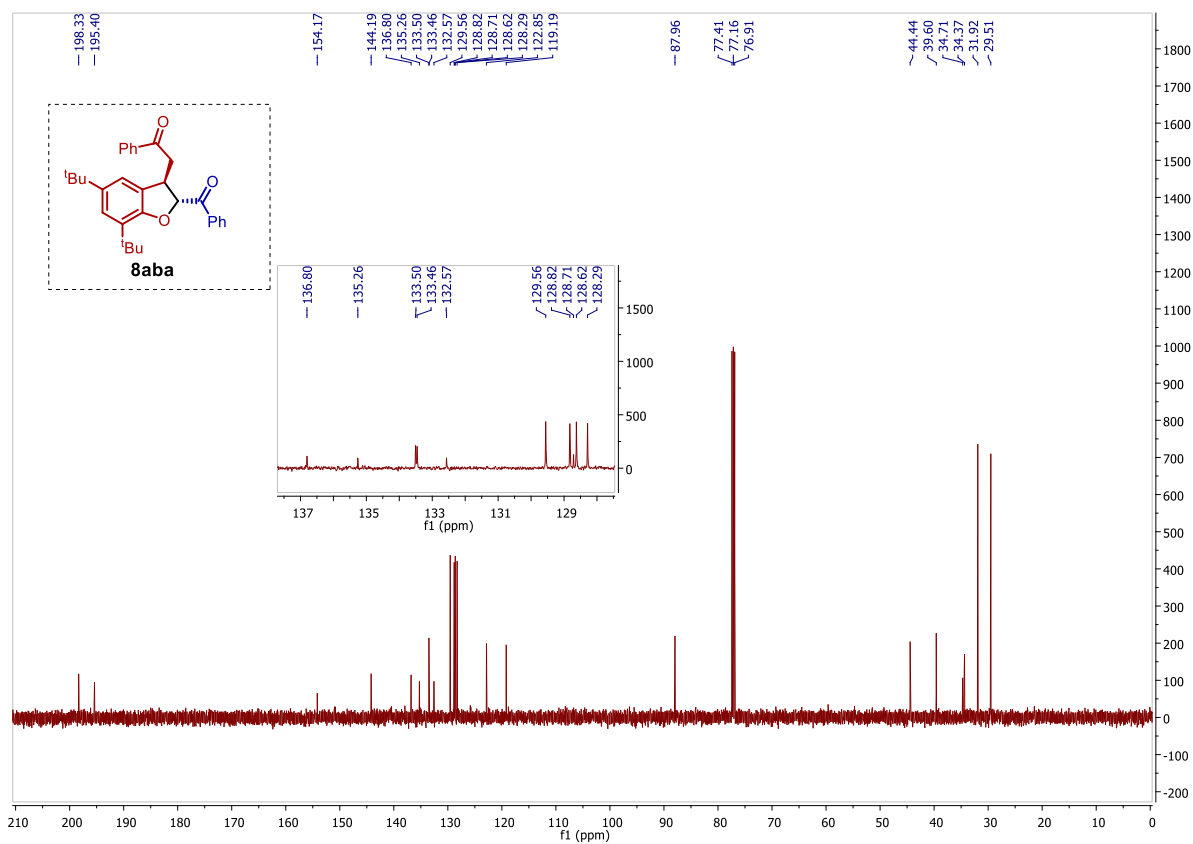
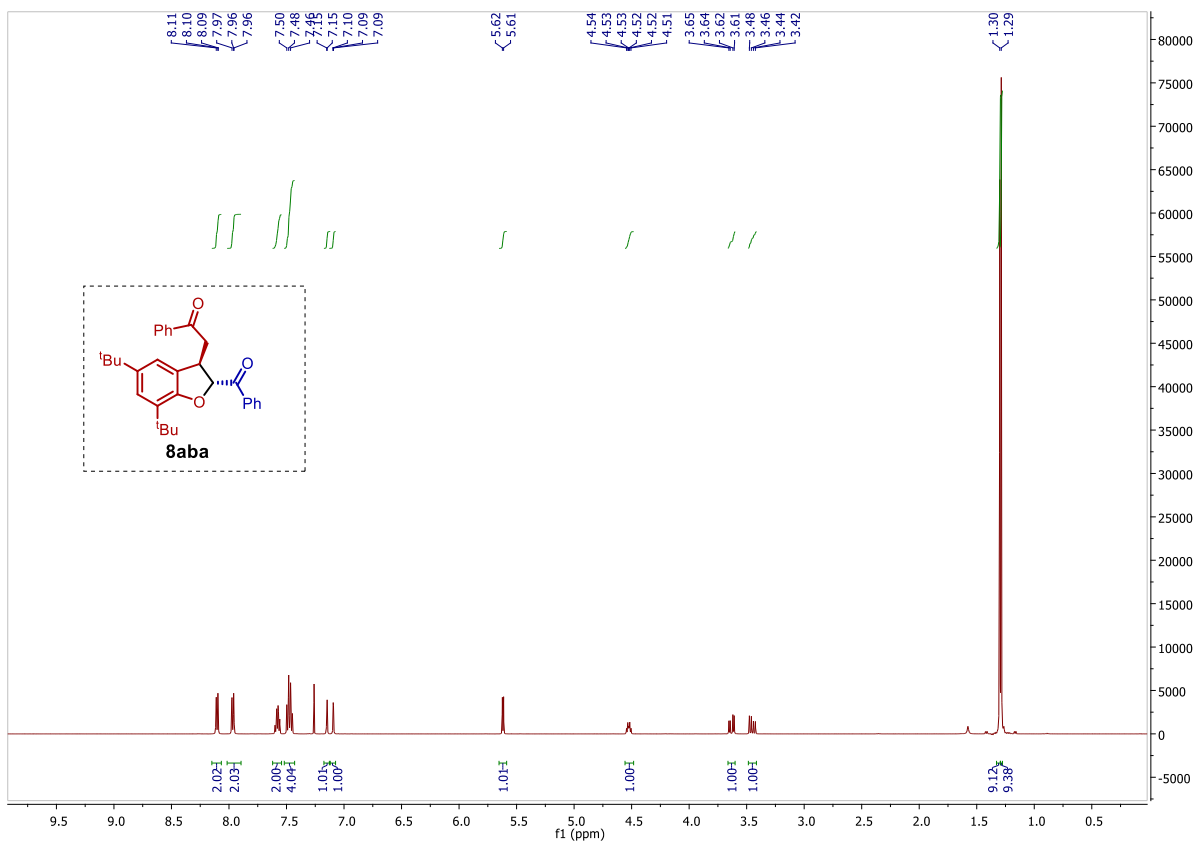
$\text{CDCl}_3$ , 500 MHz  $^1\text{H}$  NMR and 125 MHz  $^{13}\text{C}\{^1\text{H}\}$  NMR Spectra of **4aaa**



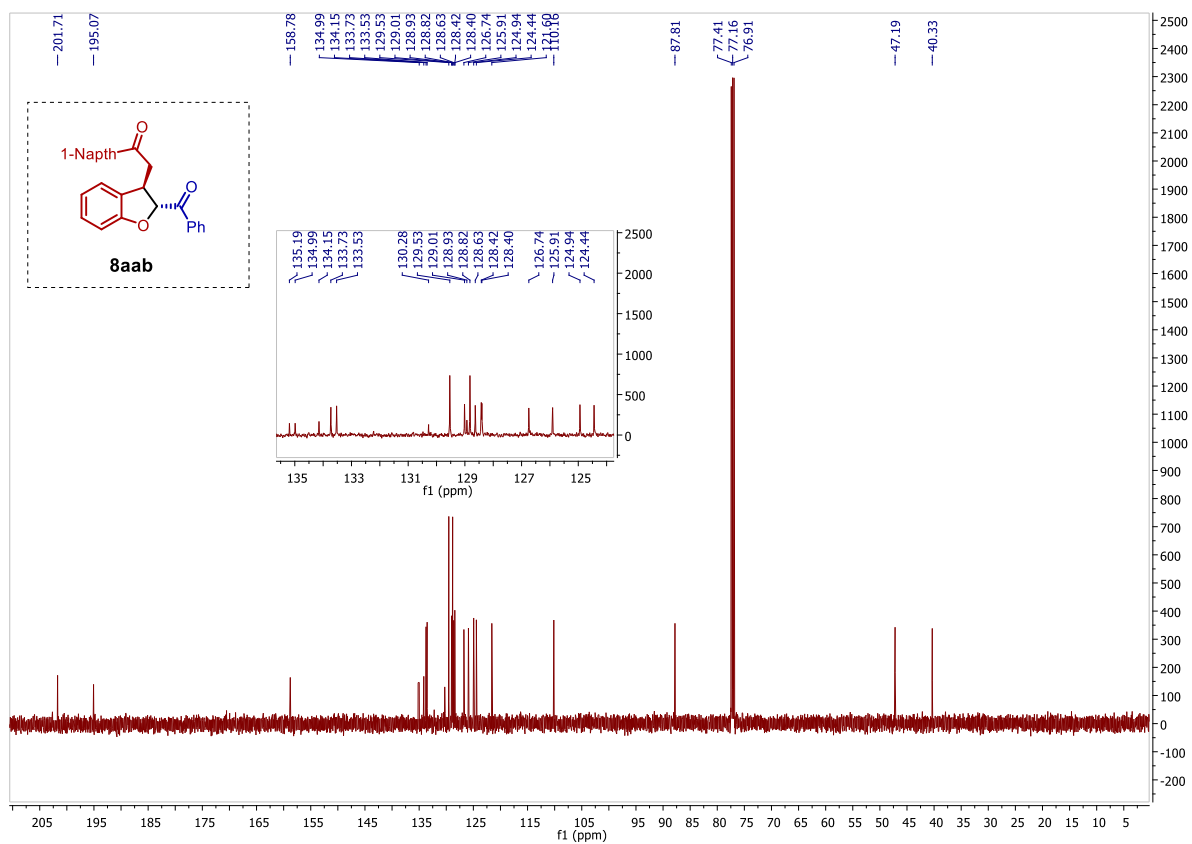
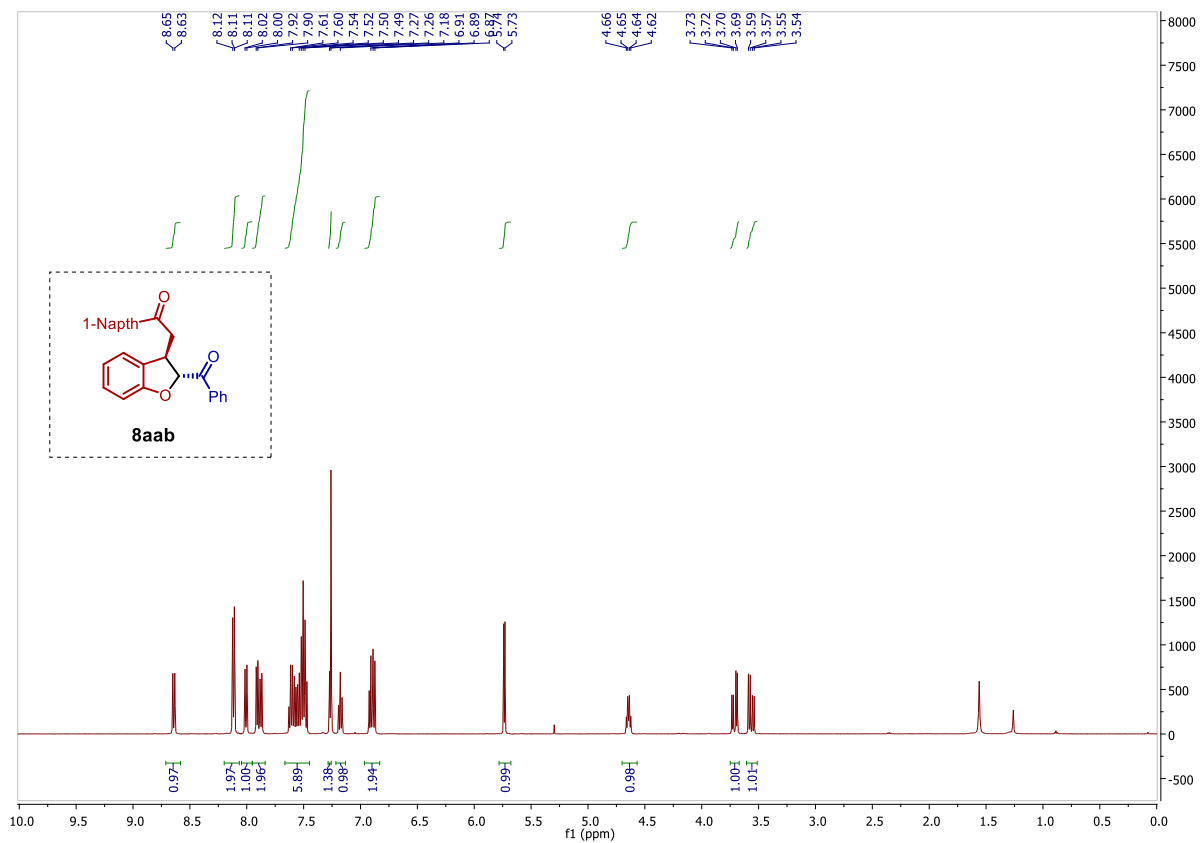
CDCl<sub>3</sub>, 500 MHz <sup>1</sup>H NMR and 125 MHz <sup>13</sup>C{<sup>1</sup>H} NMR Spectra of **6aaa'**



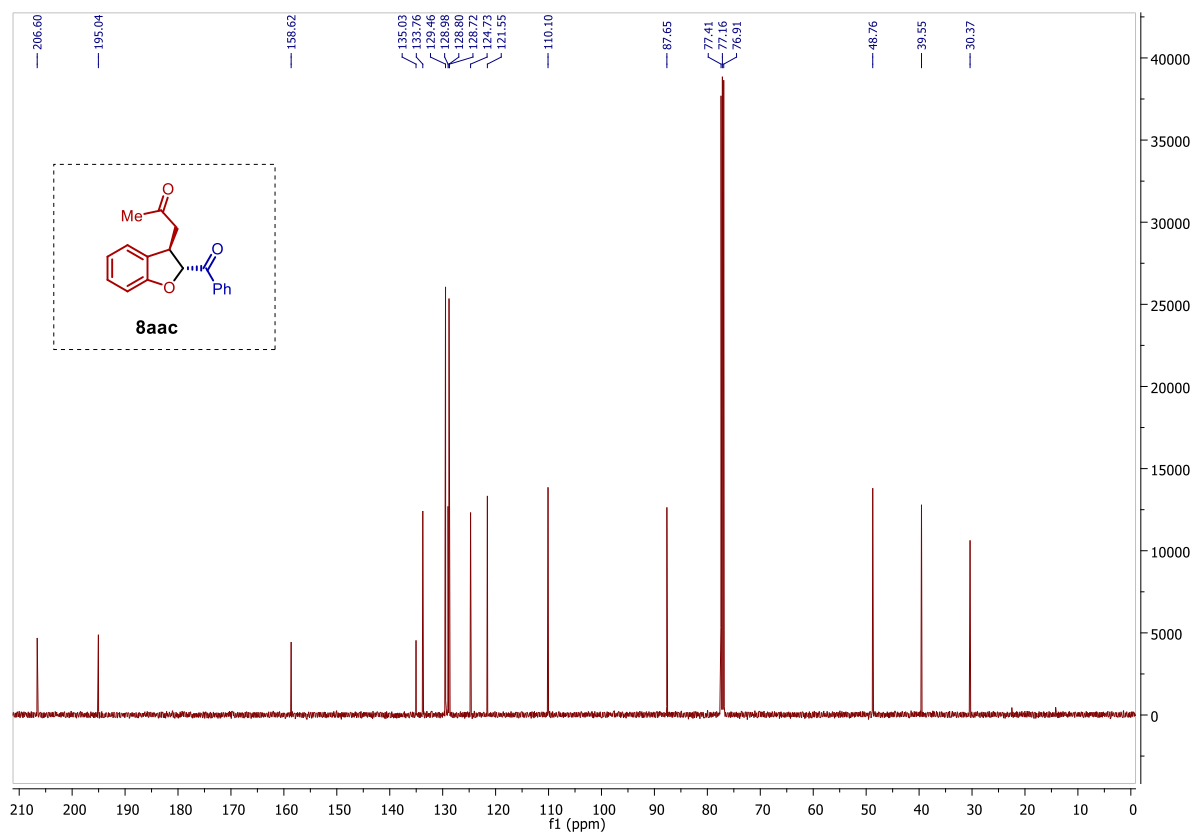
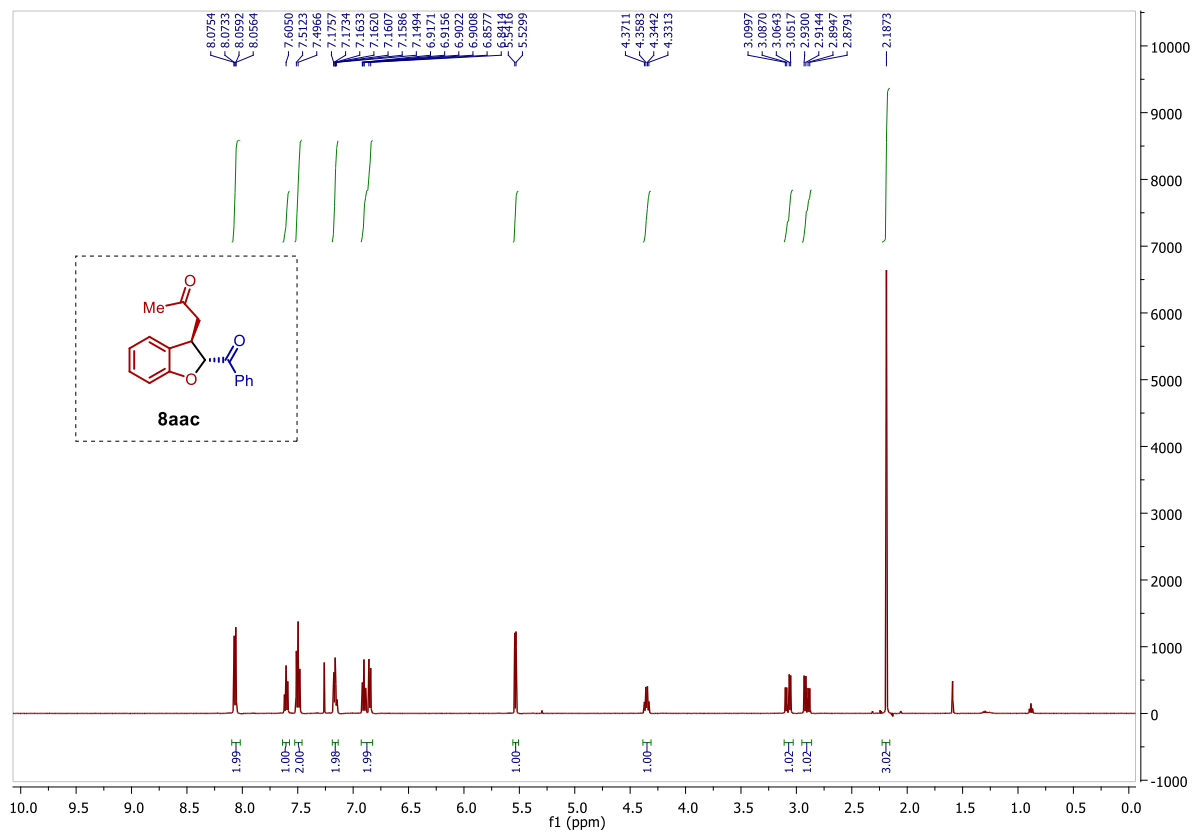
CDCl<sub>3</sub>, 500 MHz <sup>1</sup>H NMR and 125 MHz <sup>13</sup>C{<sup>1</sup>H} NMR Spectra of **8aaa**



CDCl<sub>3</sub>, 500 MHz <sup>1</sup>H NMR and 125 MHz <sup>13</sup>C{<sup>1</sup>H} NMR Spectra of 8aba

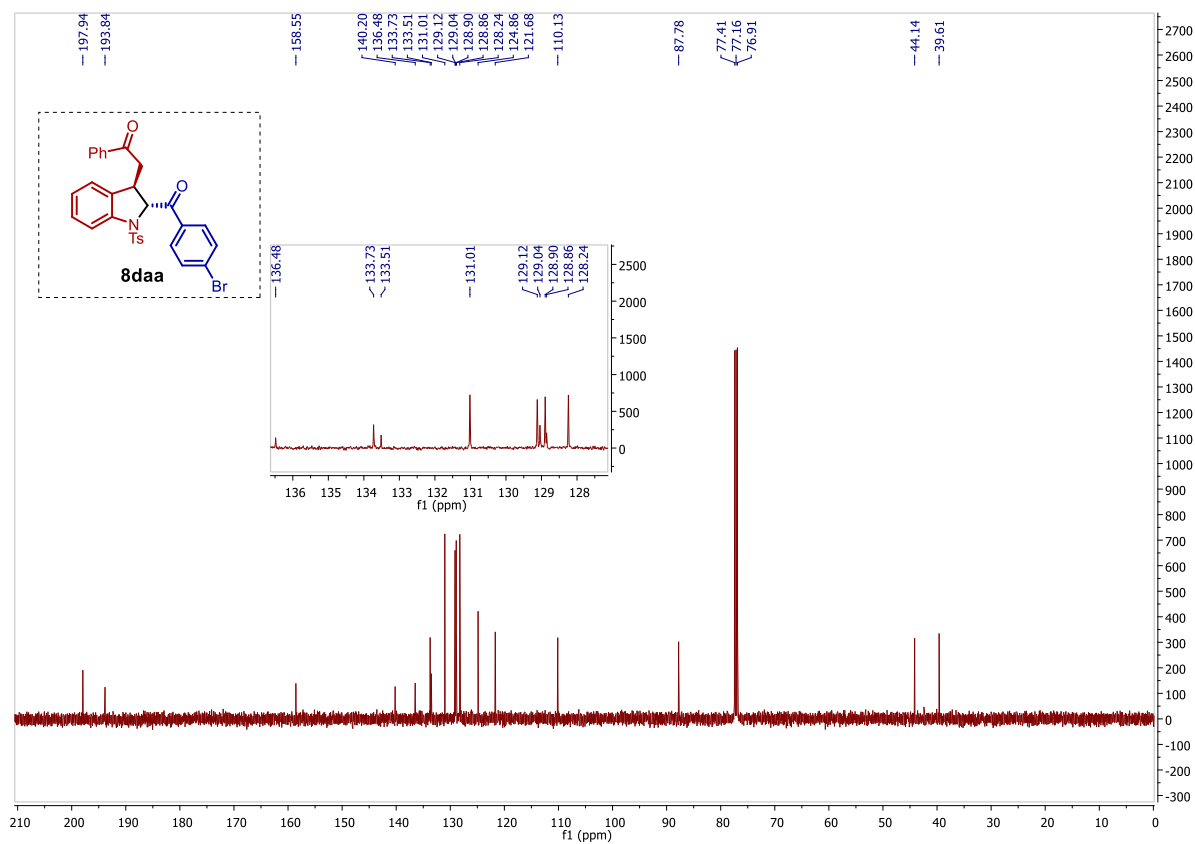
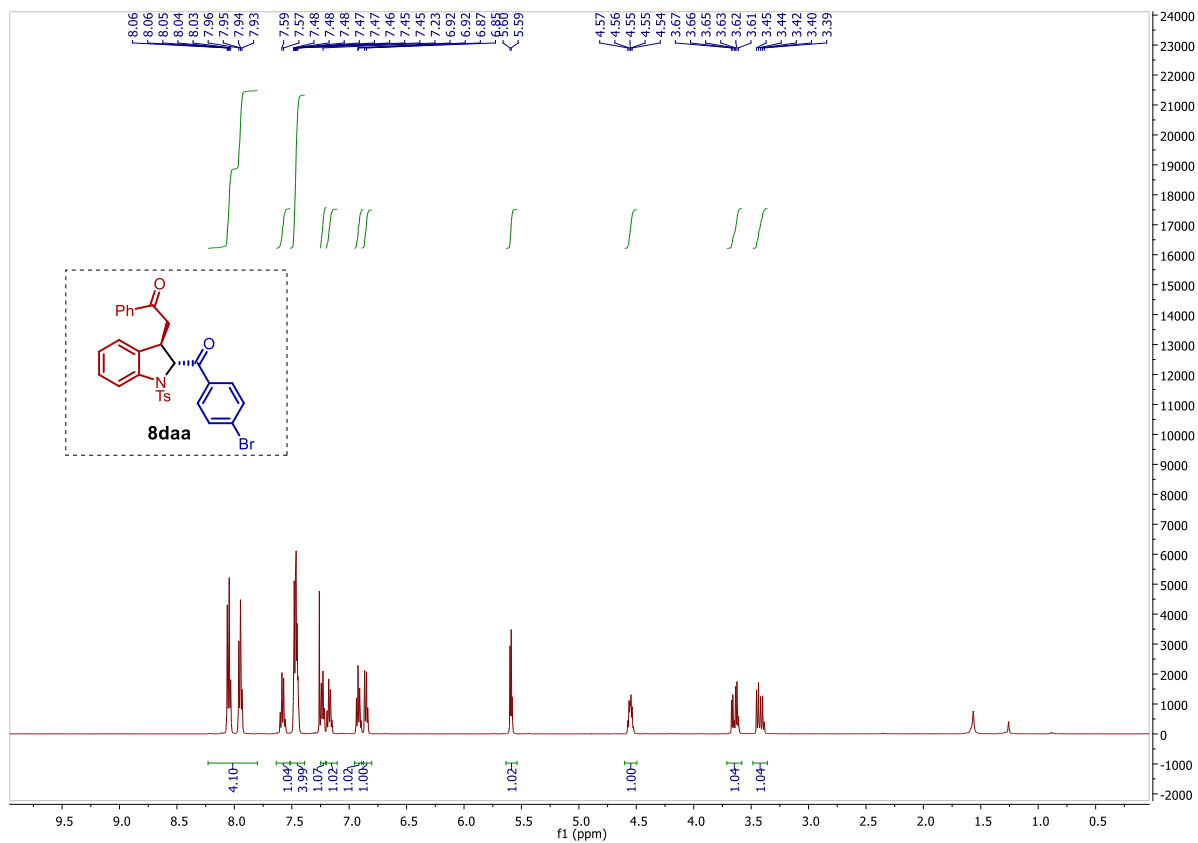


CDCl<sub>3</sub>, 500 MHz <sup>1</sup>H NMR and 125 MHz <sup>13</sup>C{<sup>1</sup>H} NMR Spectra of **8aab**



CDCl<sub>3</sub>, 500 MHz <sup>1</sup>H NMR and 125 MHz <sup>13</sup>C{<sup>1</sup>H} NMR Spectra of 8aac





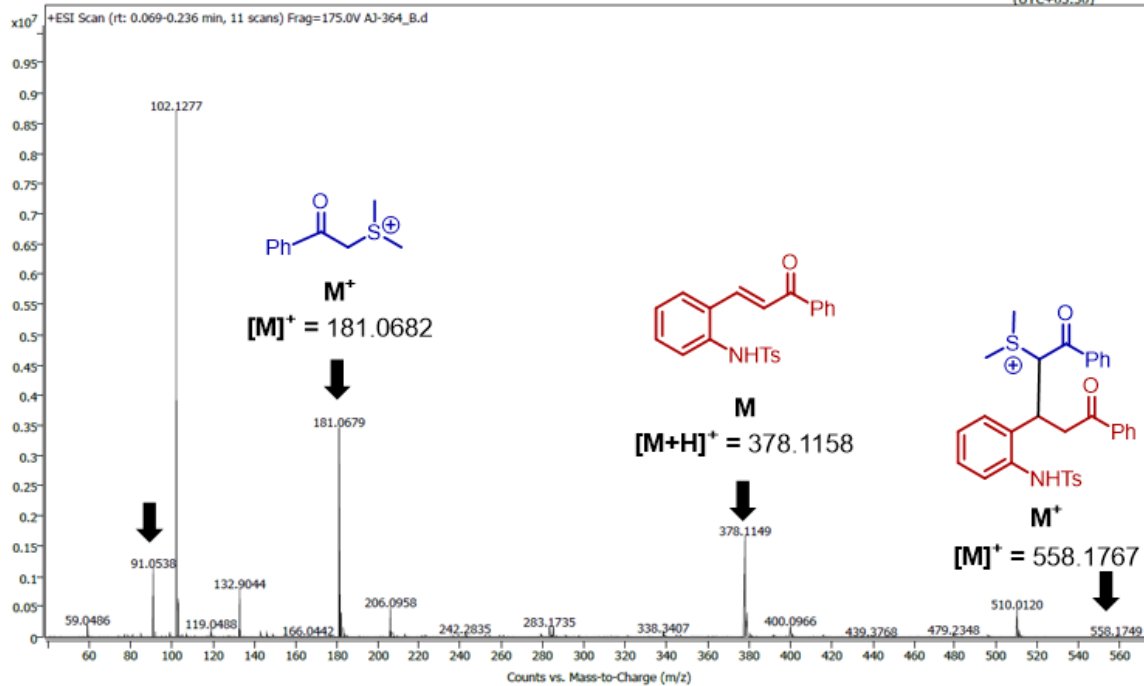
CDCl<sub>3</sub>, 500 MHz <sup>1</sup>H NMR and 125 MHz <sup>13</sup>C{<sup>1</sup>H} NMR Spectra of 8daa

## 2. HRMS Data

### Spectrum Plot Report



Name	AJ-364_B	Rack Pos.	Instrument	Instrument 1	Operator
Inj. Vol. (ul)	1	Plate Pos.	IRM Status	Success	
Data File	AJ-364_B.d	Method (Acq)	KAMAL Method.m	Comment	Acq. Time (Local)
					23-11-2023 17:13:41 (UTC+05:30)



Page 1 of 1

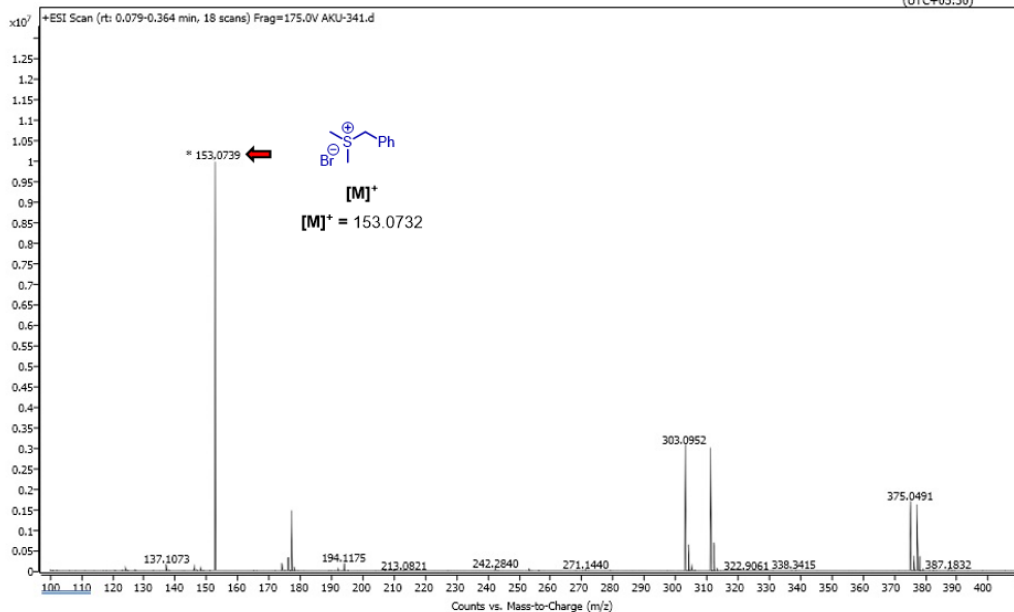
Generated at 17:18 on 23-11-2023

## HRMS data of Crude reaction mixture

### Spectrum Plot Report



Name	AKU-341	Rack Pos.	Instrument	Instrument 1	Operator
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Data File	AKU-341.d	Method (Acq)	KAMAL Method.m	Comment	Acq. Time (Local)
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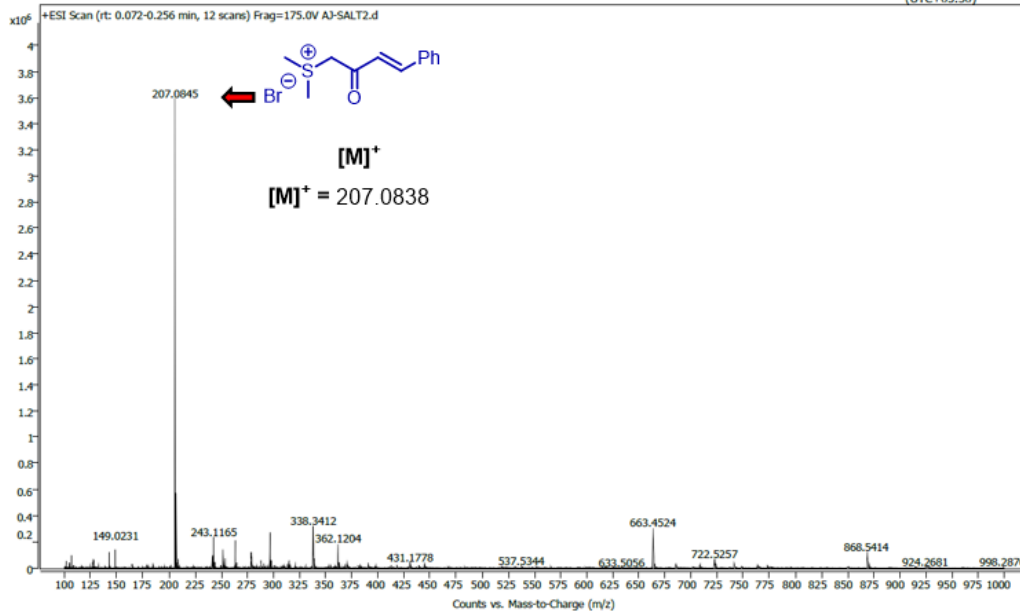


# HRMS data of 1u

## Spectrum Plot Report



Name	AJ-SALT2	Rack Pos.	Instrument	Instrument 1	Operator
Inj. Vol. (µl)	1	Plate Pos.	IRM Status	Success	
Data File	AJ-SALT2.d	Method (Acq)	KAMAL Method.m		Acq. Time (Local)
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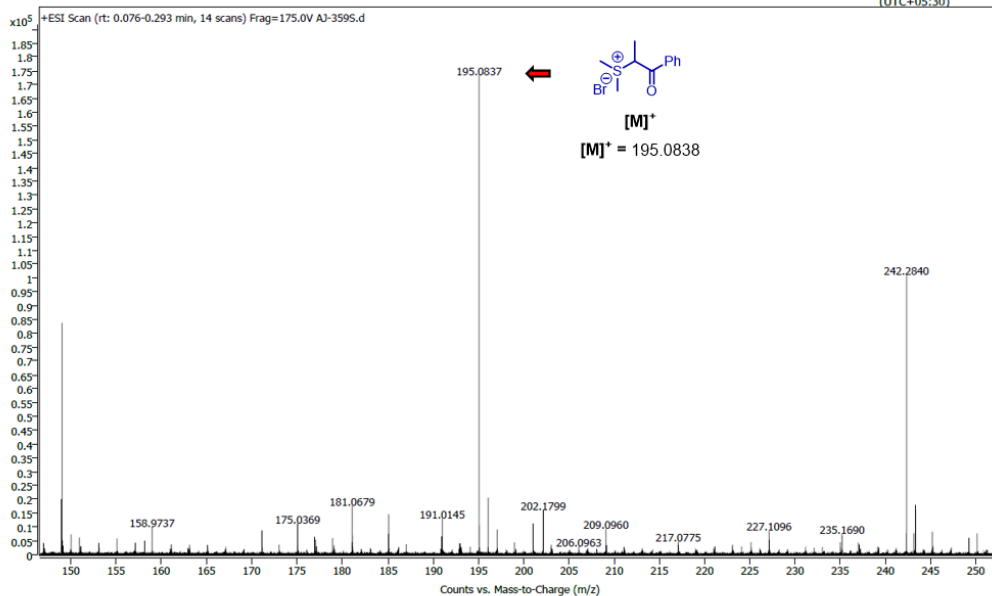


# HRMS data of 1v

## Spectrum Plot Report



Name	AJ-3595	Rack Pos.	Instrument	Instrument 1	Operator
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Data File	AJ-3595.d	Method (Acq)	KAMAL Method.m		Acq. Time (Local)
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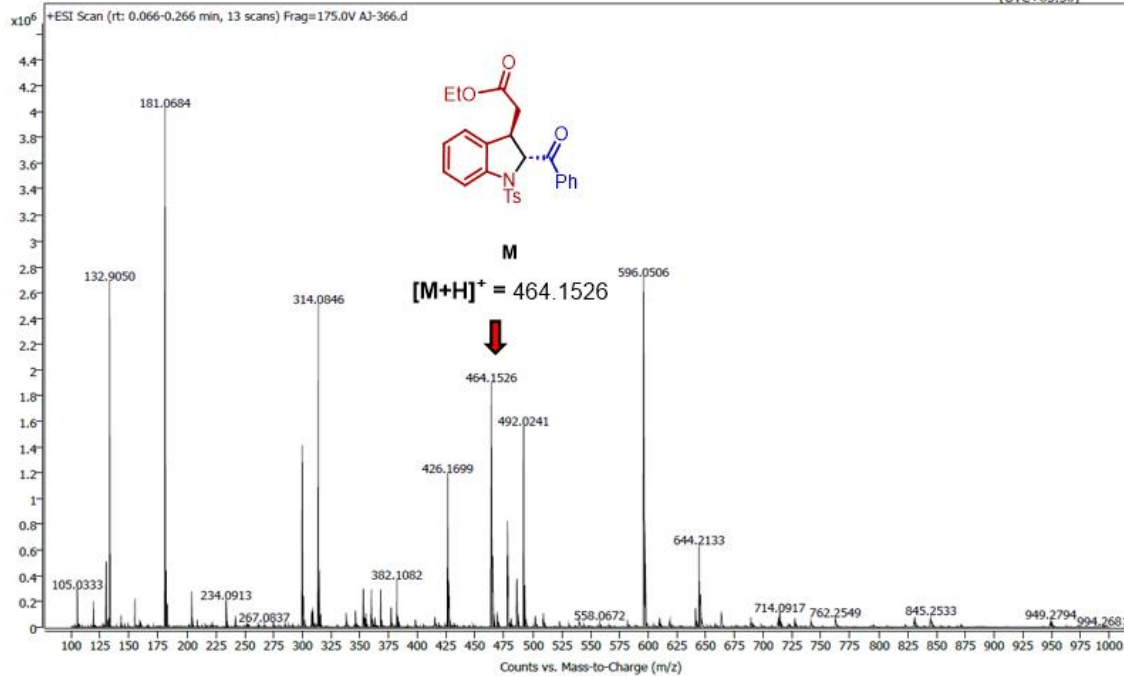


# HRMS data of 1w

## Spectrum Plot Report

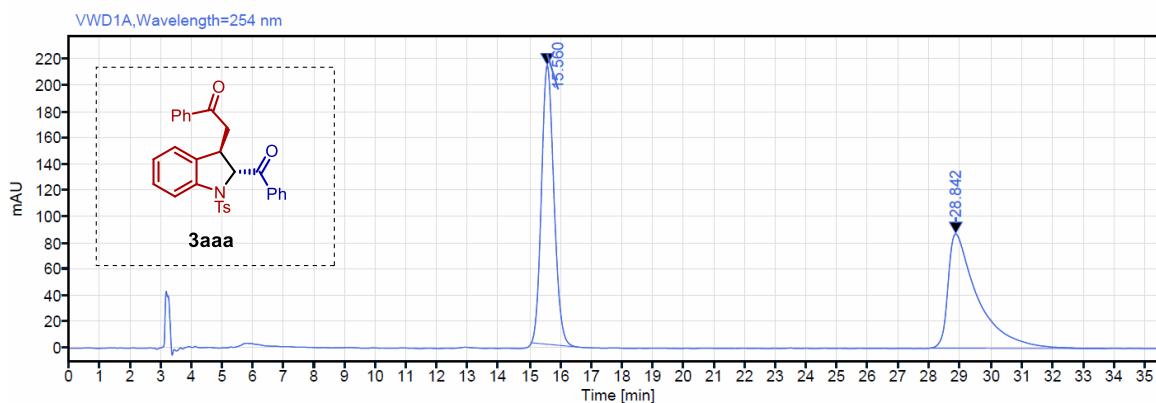


Name	AJ-366	Rack Pos.		Instrument	Instrument 1	Operator	
Inj. Vol. (ul)	1	Plate Pos.		IRM Status	Success		
Data File	AJ-366.d	Method (Acq)	KAMAL Method.m	Comment		Acq. Time (Local)	20-11-2023 17:02:17 (UTC+05:30)



# HRMS data of 3aap

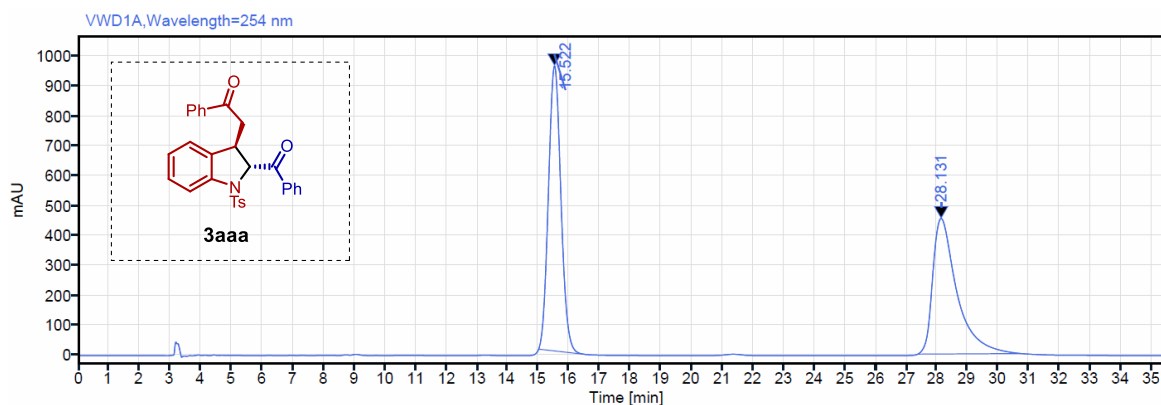
### 3. HPLC graph



Signal: VWD1A,Wavelength=254 nm

RT [min]	Type	Width [min]	Area	Height	Area%	Name
15.560	BB	1.56	5980.13	212.72	50.55	
28.842	MM	5.72	5848.87	87.21	49.45	
<b>Sum</b>			<b>11829.00</b>			

#### HPLC graph of racemic 3aaa

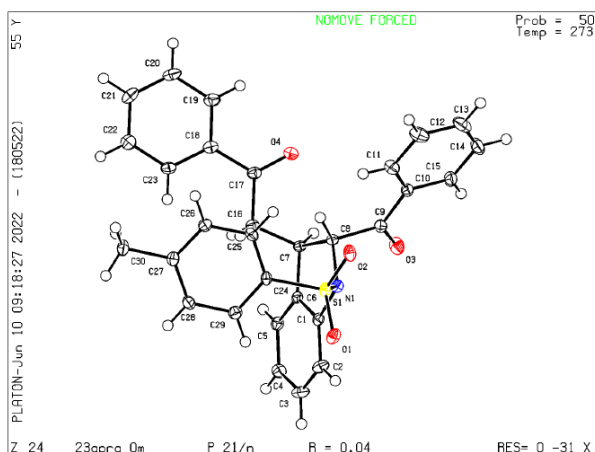


Signal: VWD1A,Wavelength=254 nm

RT [min]	Type	Width [min]	Area	Height	Area%	Name
15.522	IB	1.55	26850.43	952.79	52.04	
28.131	BB	3.36	24748.37	452.84	47.96	
<b>Sum</b>			<b>51598.80</b>			

#### HPLC graph of enantioenriched 3aaa

#### 4. X-ray crystal analysis of structure **3aaa**.



**Figure S1:** ORTEP Diagram of **3aaa** (CCDC 2178470)

**Table S1:** Crystal data and structure refinement for **3aaa**.

Identification code	<b>3aaa</b>
Empirical formula	C <sub>30</sub> H <sub>25</sub> NO <sub>4</sub> S
Formula weight	495.57
Temperature/K	273.15
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
a/Å	8.1168(14)
b/Å	17.929(3)
c/Å	16.686(3)
α/°	90
β/°	94.685(6)
γ/°	90
Volume/Å <sup>3</sup>	2420.1(7)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.360
μ/mm <sup>-1</sup>	0.172
F(000)	1040.0
Crystal size/mm <sup>3</sup>	0.2 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)

2 $\theta$ range for data collection/ $^{\circ}$	5.524 to 56.784
Index ranges	$-10 \leq h \leq 10$ , $-23 \leq k \leq 23$ , $-22 \leq l \leq 22$
Reflections collected	35876
Independent reflections	5987 [ $R_{\text{int}} = 0.0403$ , $R_{\text{sigma}} = 0.0293$ ]
Data/restraints/parameters	5987/0/326
Goodness-of-fit on $F^2$	1.188
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1 = 0.0444$ , $wR_2 = 0.1426$
Final R indexes [all data]	$R_1 = 0.0527$ , $wR_2 = 0.1522$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.45/-0.40