

## Supplementary Materials

# Pentacoordinated Organotin(IV) Complexes as an Alternative in the Design of Highly Efficient Optoelectronic and Photovoltaic Devices: Synthesis and Photophysical Characterization

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Table S1. Characteristic IR stretching frequencies of compounds **1a-1d**

Compound	$\nu(\text{C}=\text{N})$	$\nu(\text{Sn}-\text{C})$	$\nu(\text{Sn}-\text{O})$	$\nu(\text{Sn}-\text{N})$
<b>1a</b>	1601	606	548	483
<b>1b</b>	1601	607	550	485
<b>1c</b>	1599	601	548	488
<b>1d</b>	1602	603	549	488



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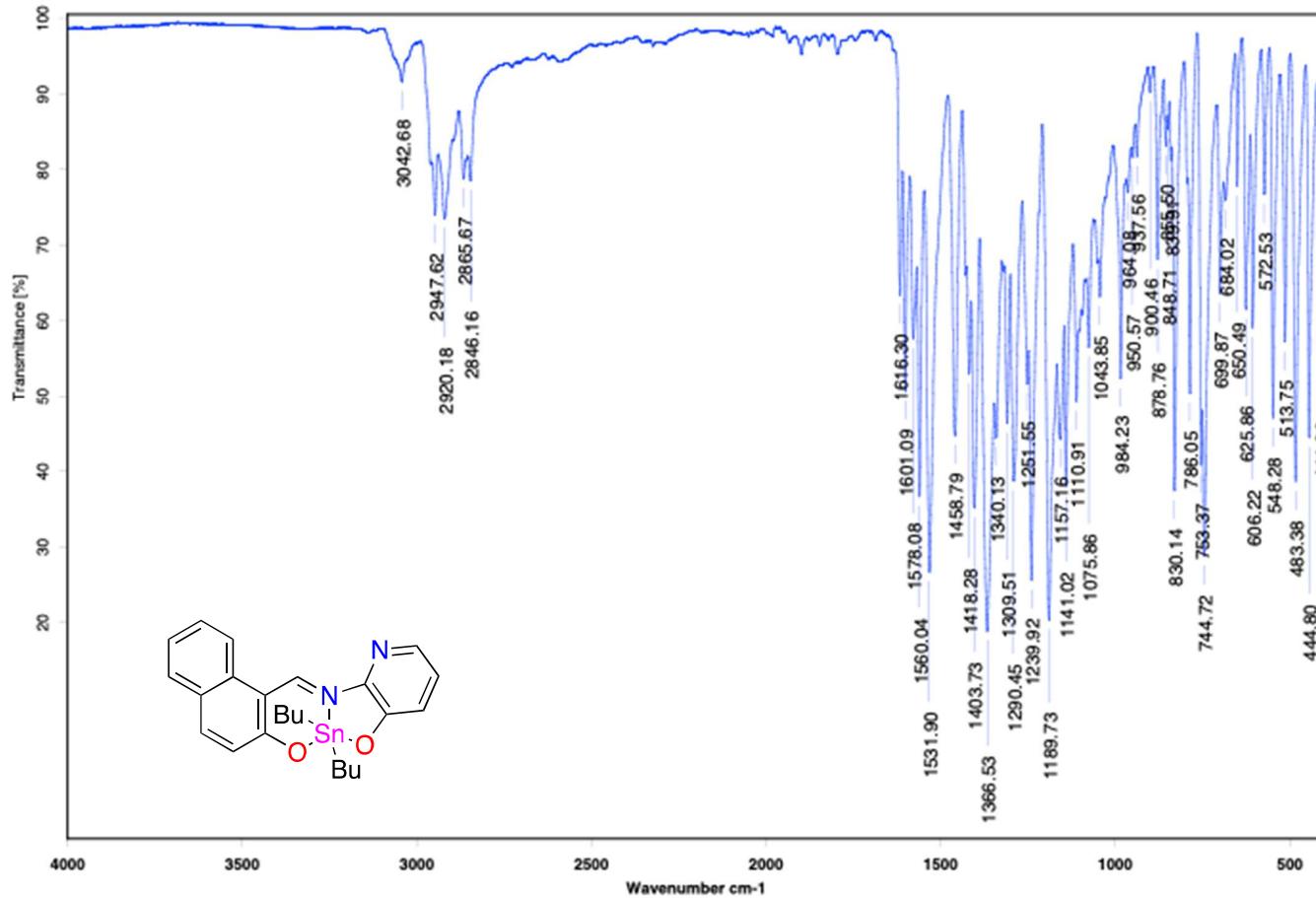


Figure S1. ATR-IR of complex **1a**



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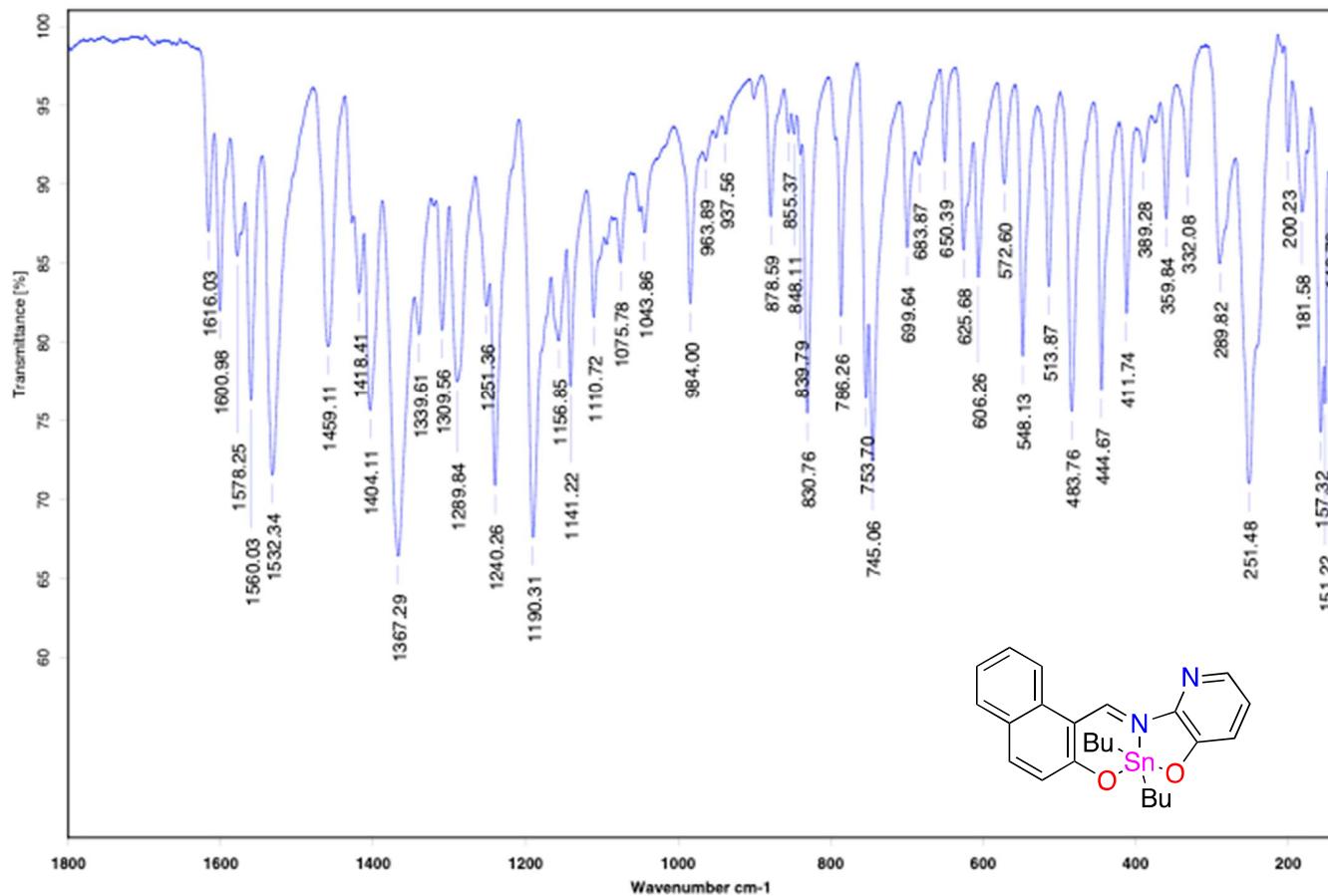


Figure S2. Far-IR of complex **1a**



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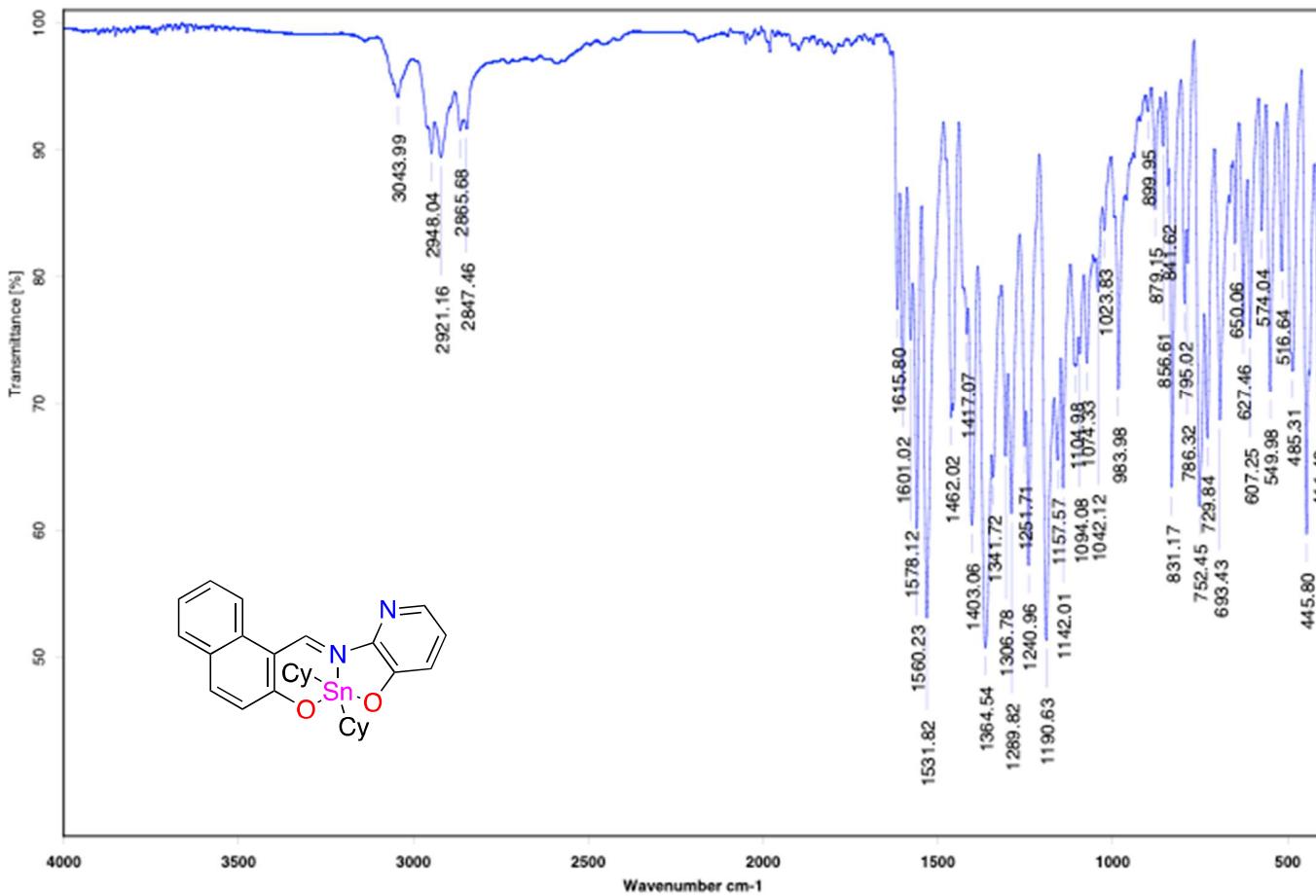


Figure S3. ATR-IR of complex **1b**



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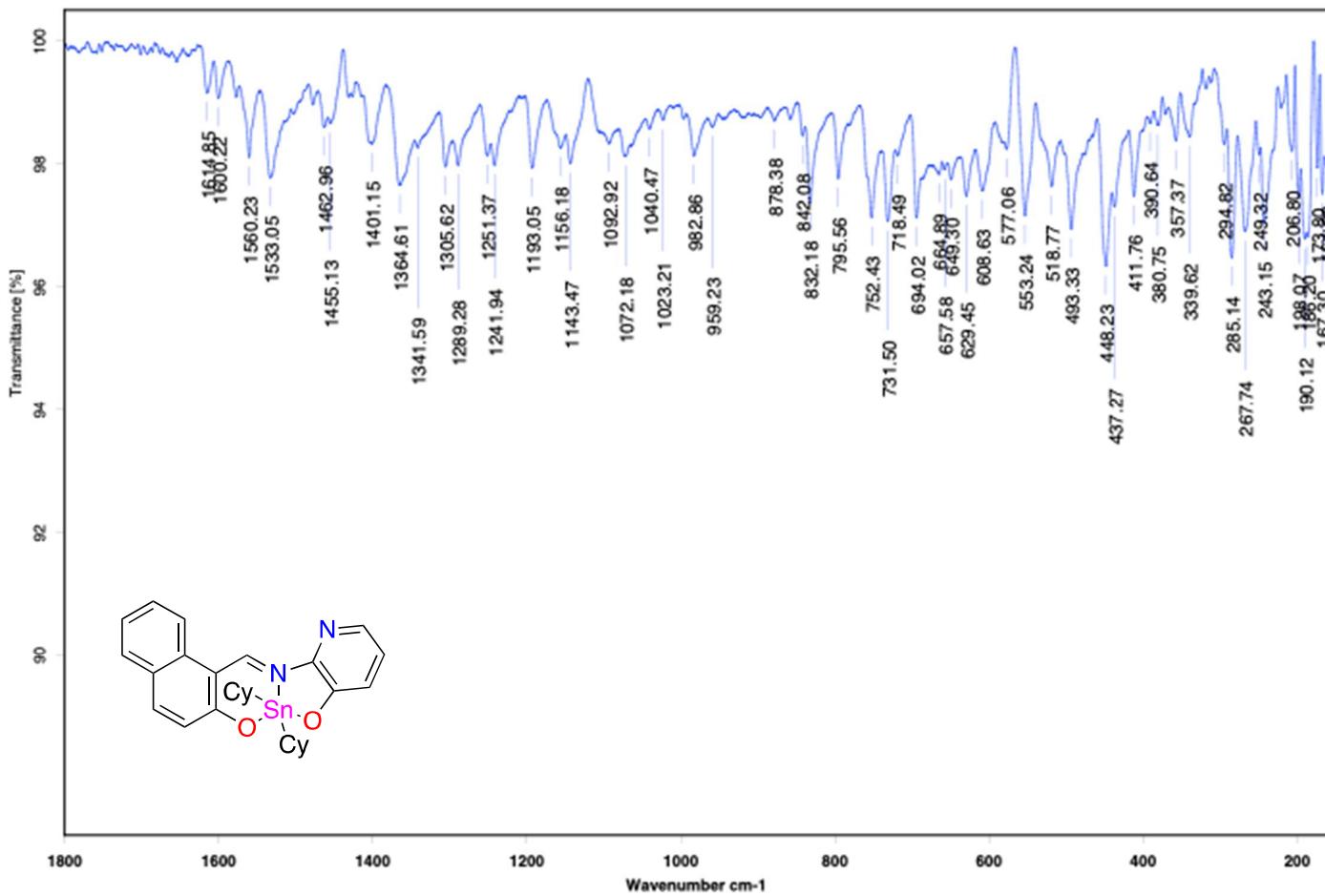


Figure S4. Far-IR of complex **1b**



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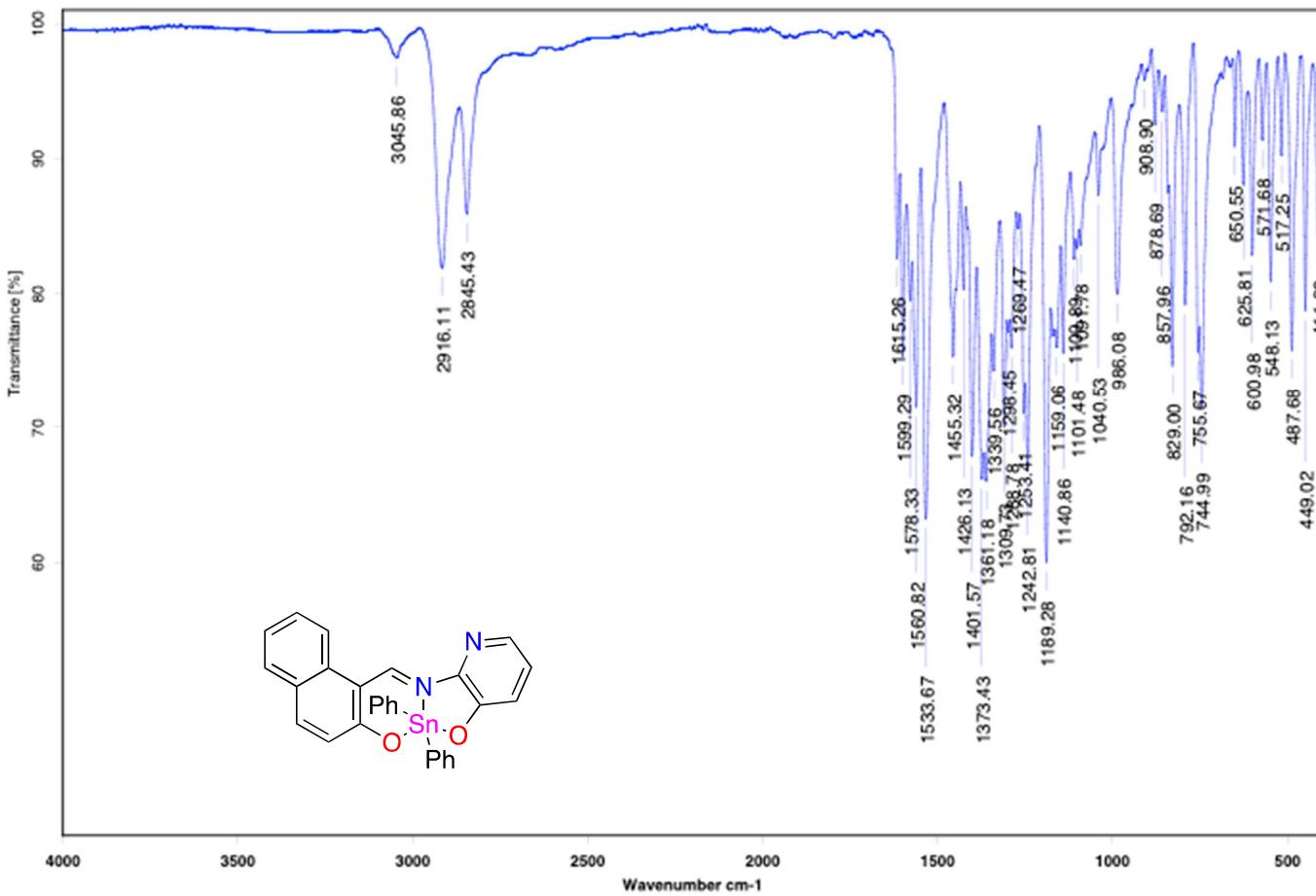


Figure S5. ATR-IR of complex **1c**



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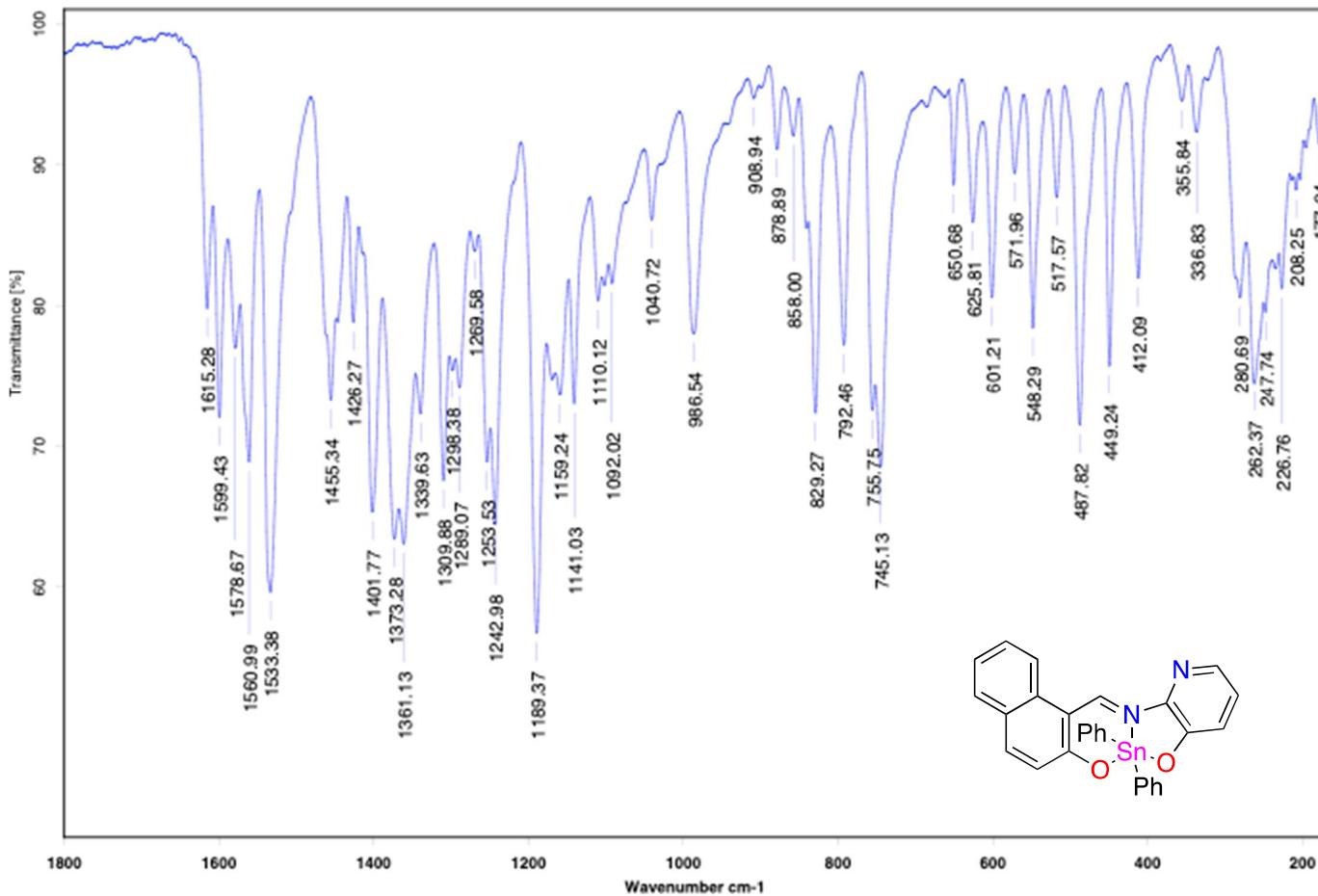


Figure S6.Far-IR of complex **1c**



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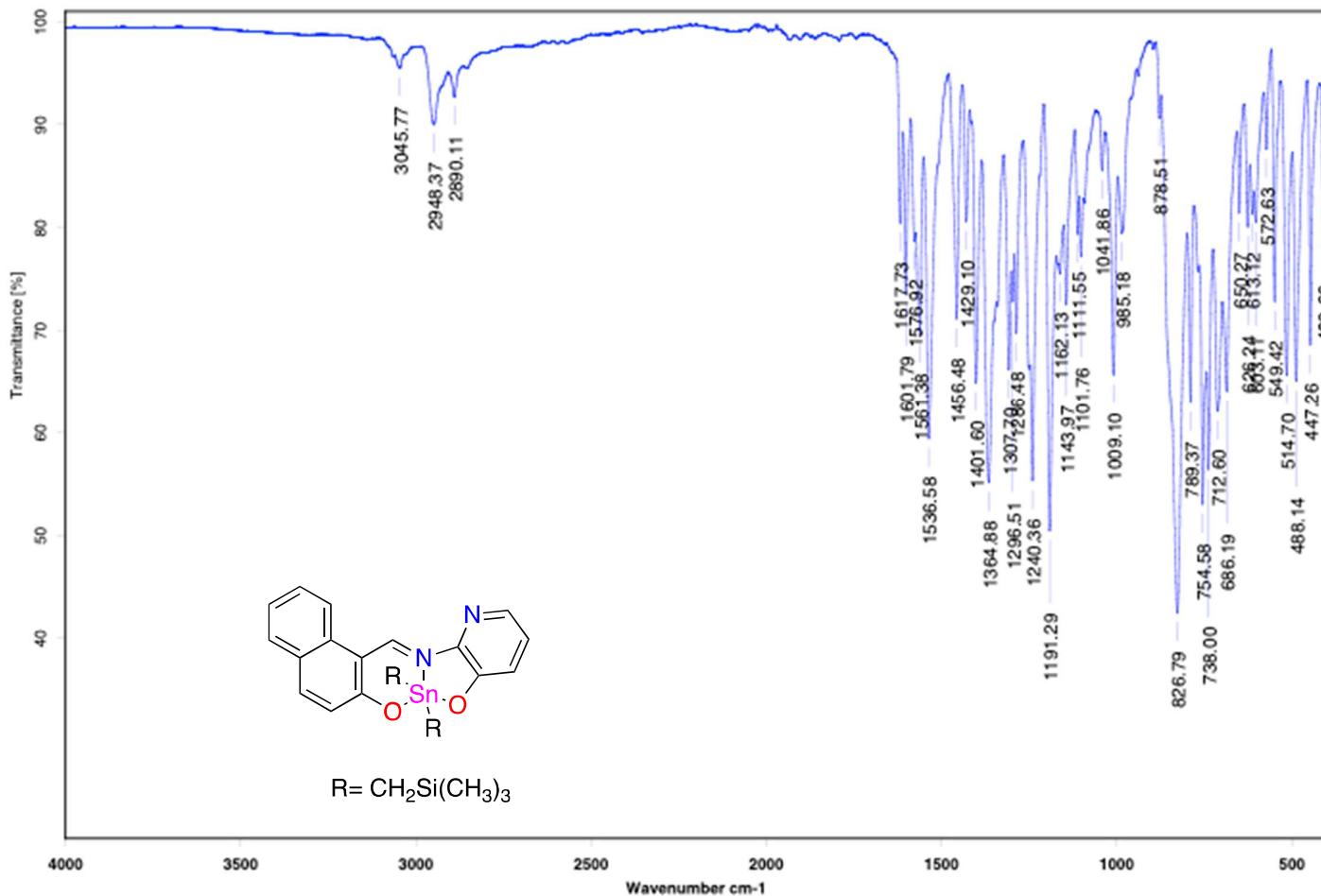


Figure S7. ATR-IR of complex **1d**



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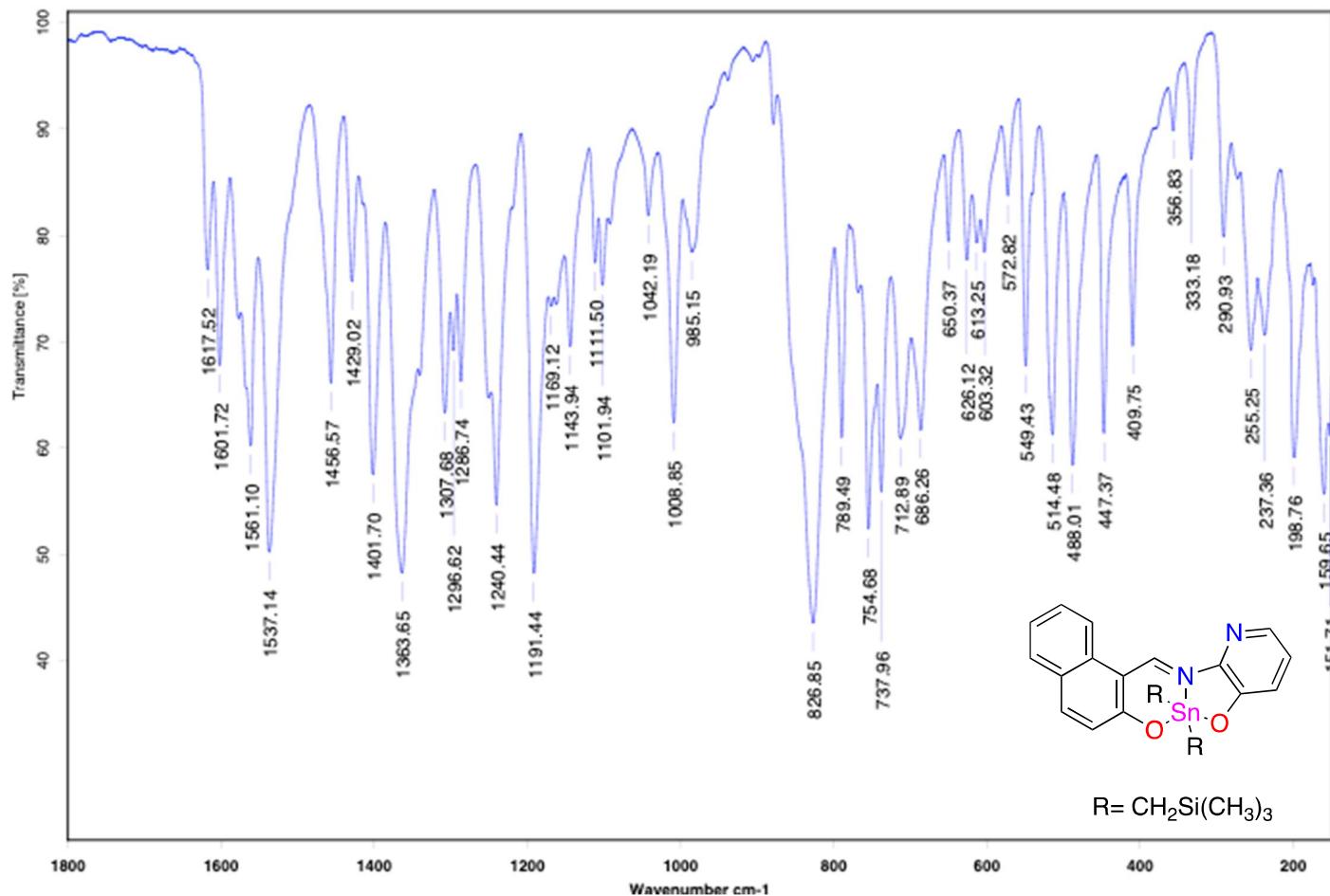


Figure S8. ATR-IR of complex **1d**

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LABORATORIO DE ESPECTROMETRIA DE MASAS

Acq. Data Name: U-2992 SCP3a

Creation Parameters: Average(MS[1] Time:3..3)

Elizabeth Gomez / Samuel Cuencas

x10<sup>-3</sup> Intensity (32945)

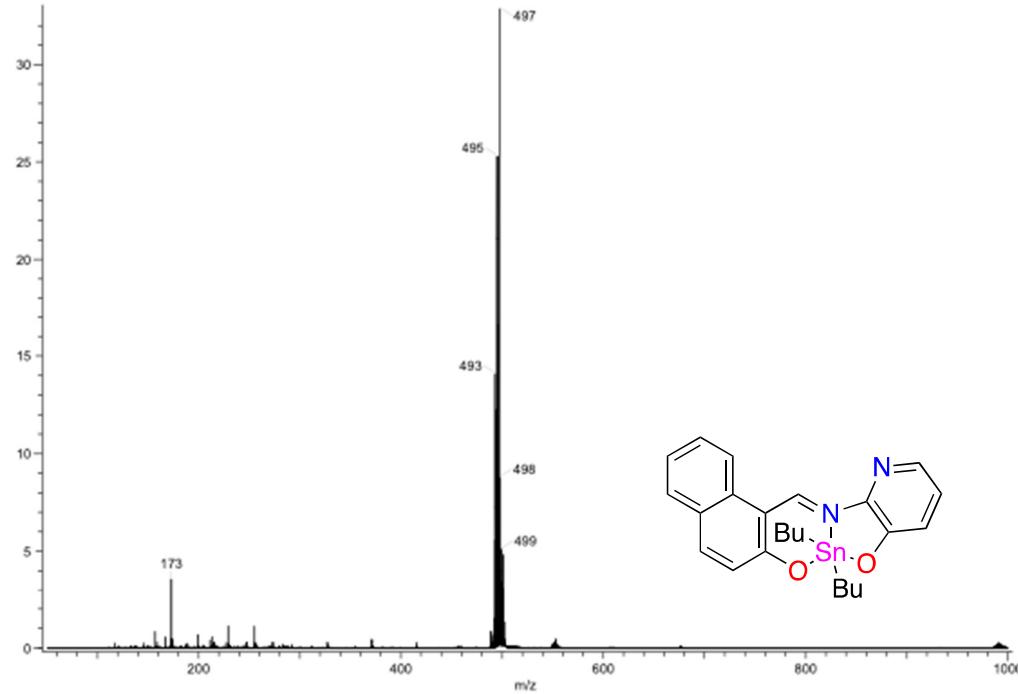


Figure S9. Mass Spectrometry (DART<sup>+</sup>) of complex **1a**

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LABORATORIO DE ESPECTROMETRÍA DE MASAS

Acq. Data Name: U-2085.SOP.d

Creation Parameters: Average[51] Time[3..3]

SAMUEL CUENCA

x10<sup>3</sup> Intensity(17/24)

Experiment Date/Time: 4/8/2019 1:17:55 PM  
Instrument: IED The AccuTOF-JMS-T100LC  
Ionization Mode: DART<sup>+</sup>

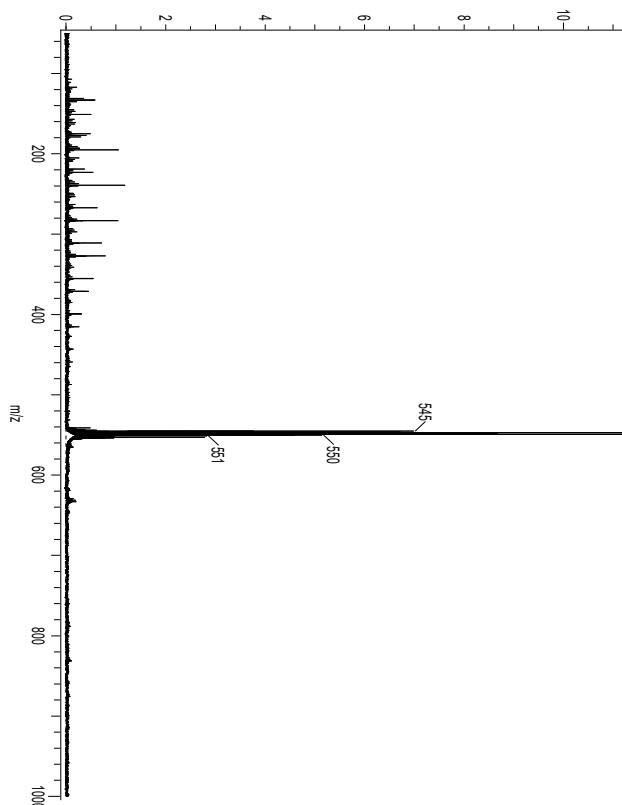
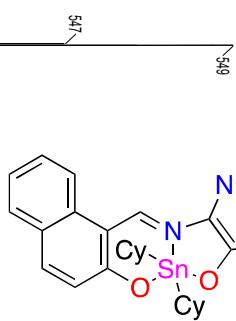


Figure S10. Mass Spectrometry (DART<sup>+</sup>) of complex **1b**

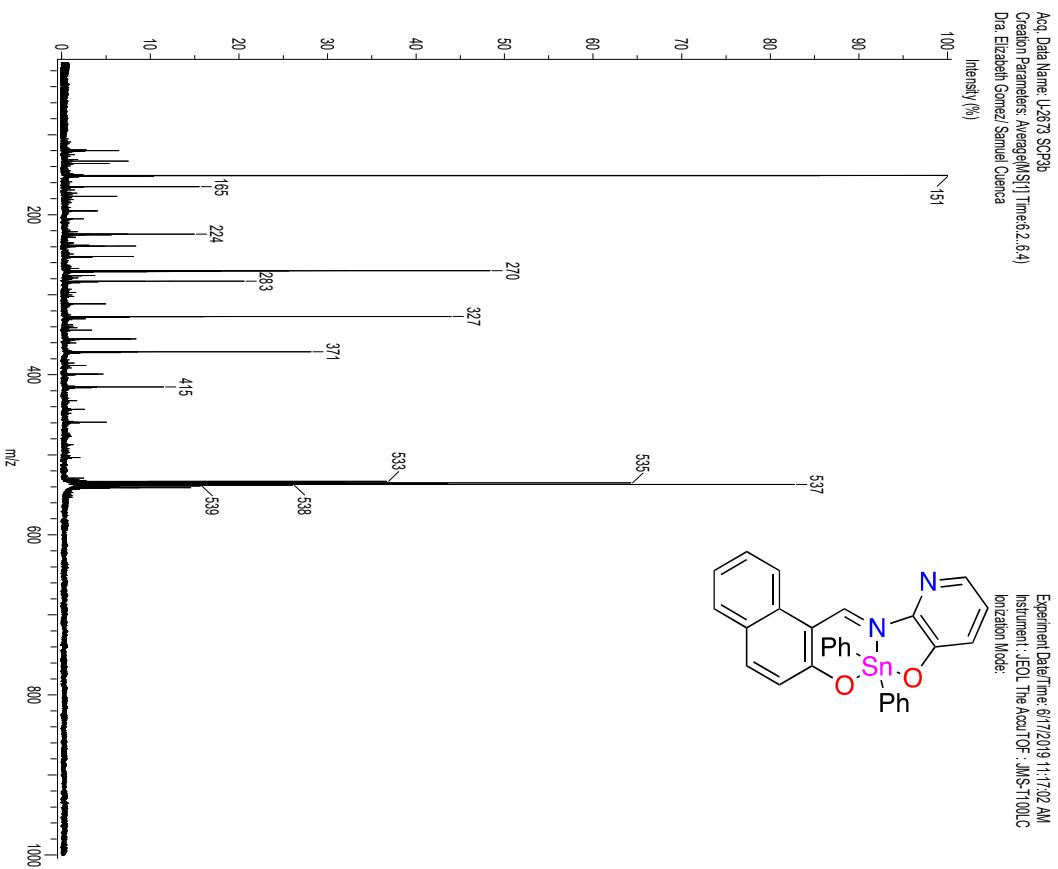


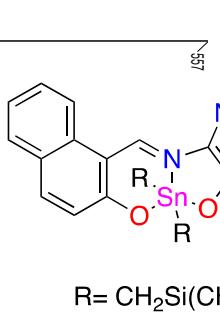
Figure S11. Mass Spectrometry (DART<sup>+</sup>) of complex **1c**

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LABORATORIO DE ESPECTROMETRÍA DE MASA

Acq. Data Name: U-141\_SOPe  
Creation Parameters: Average[MS1] Time:3.2150.3.5960)  
Dr. Elizabeth Gomez

$\times 10^3$   
Intensity (16047)

Experiment Date/Time: 3/5/2019 1:48:31 PM  
Instrument: IFC1 ThermoFisher JMS-T104C  
Ionization Mode: DART<sup>+</sup>



R=  $\text{CH}_2\text{Si}(\text{CH}_3)_3$

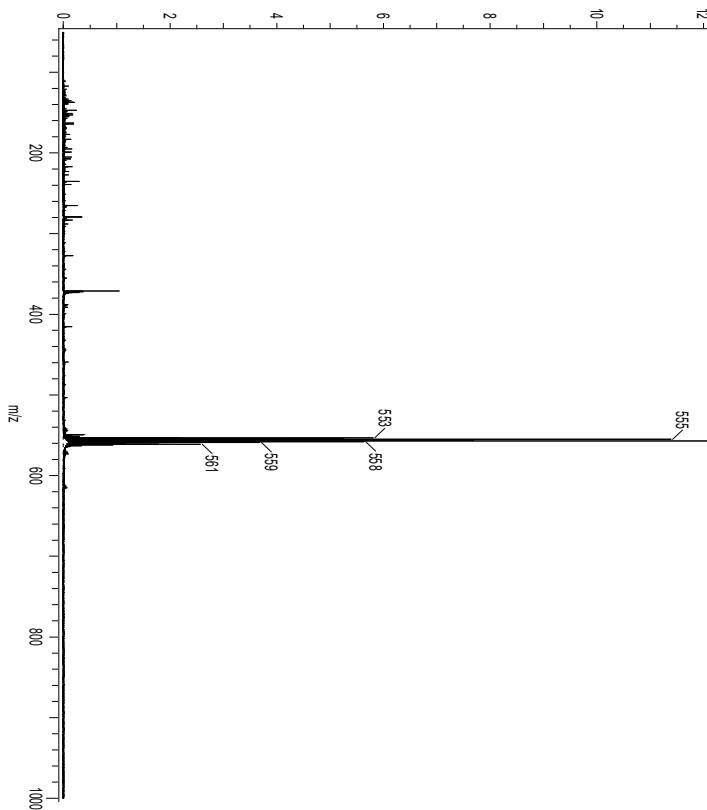


Figure S12. Mass Spectrometry (DART<sup>+</sup>) of complex **1d**

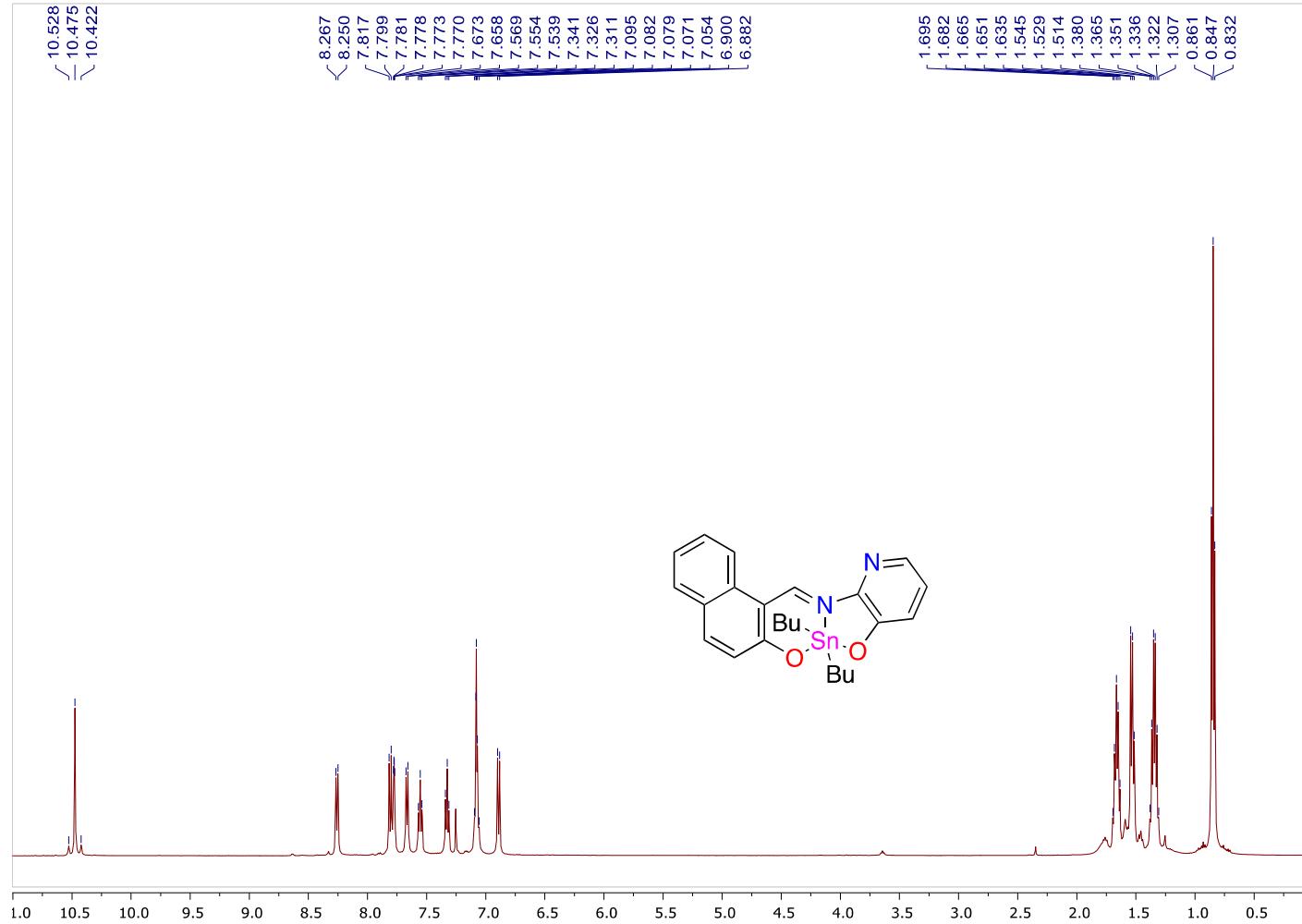


Figure S13.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz) of complex **1a**

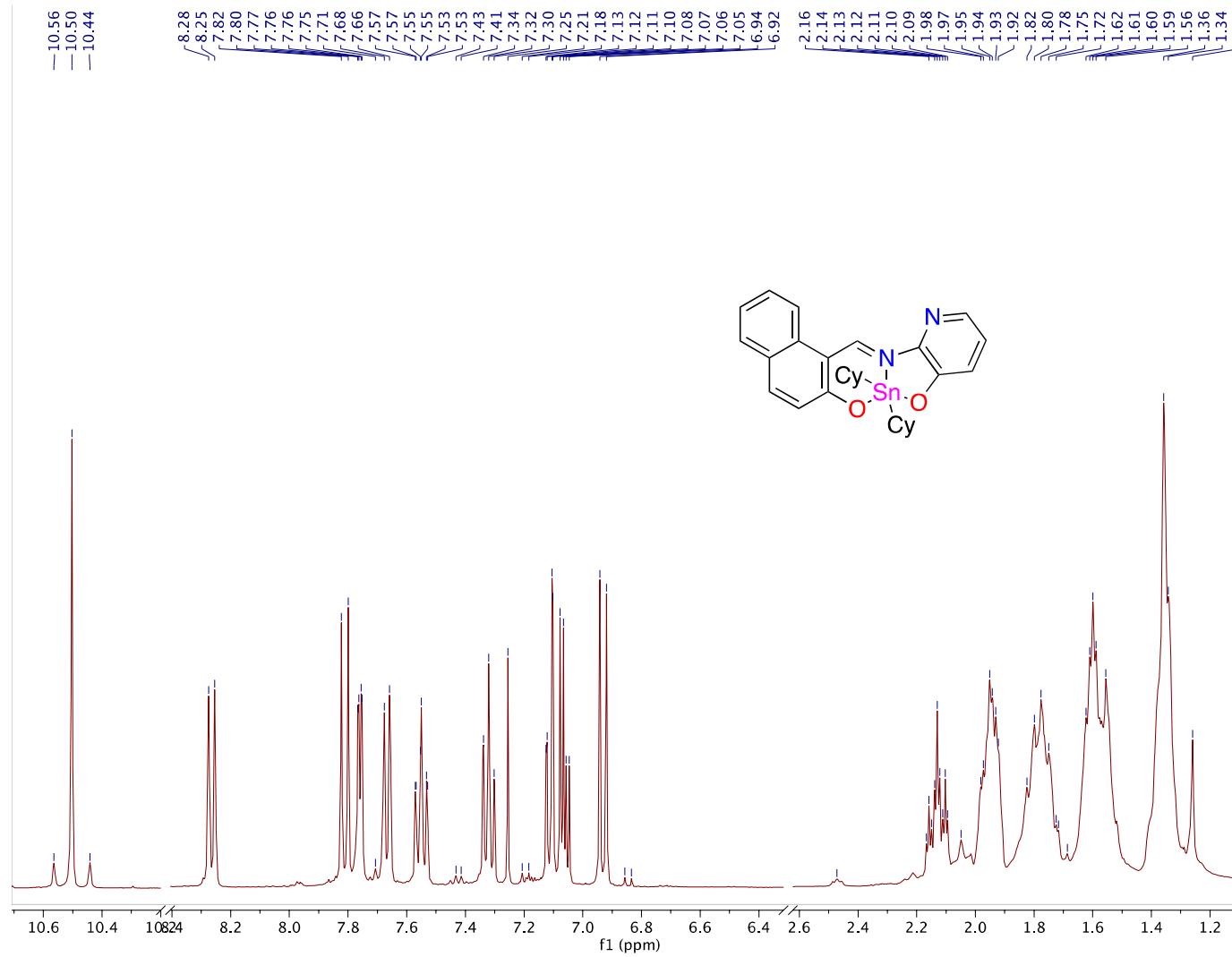


Figure S14.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) of complex **1b**

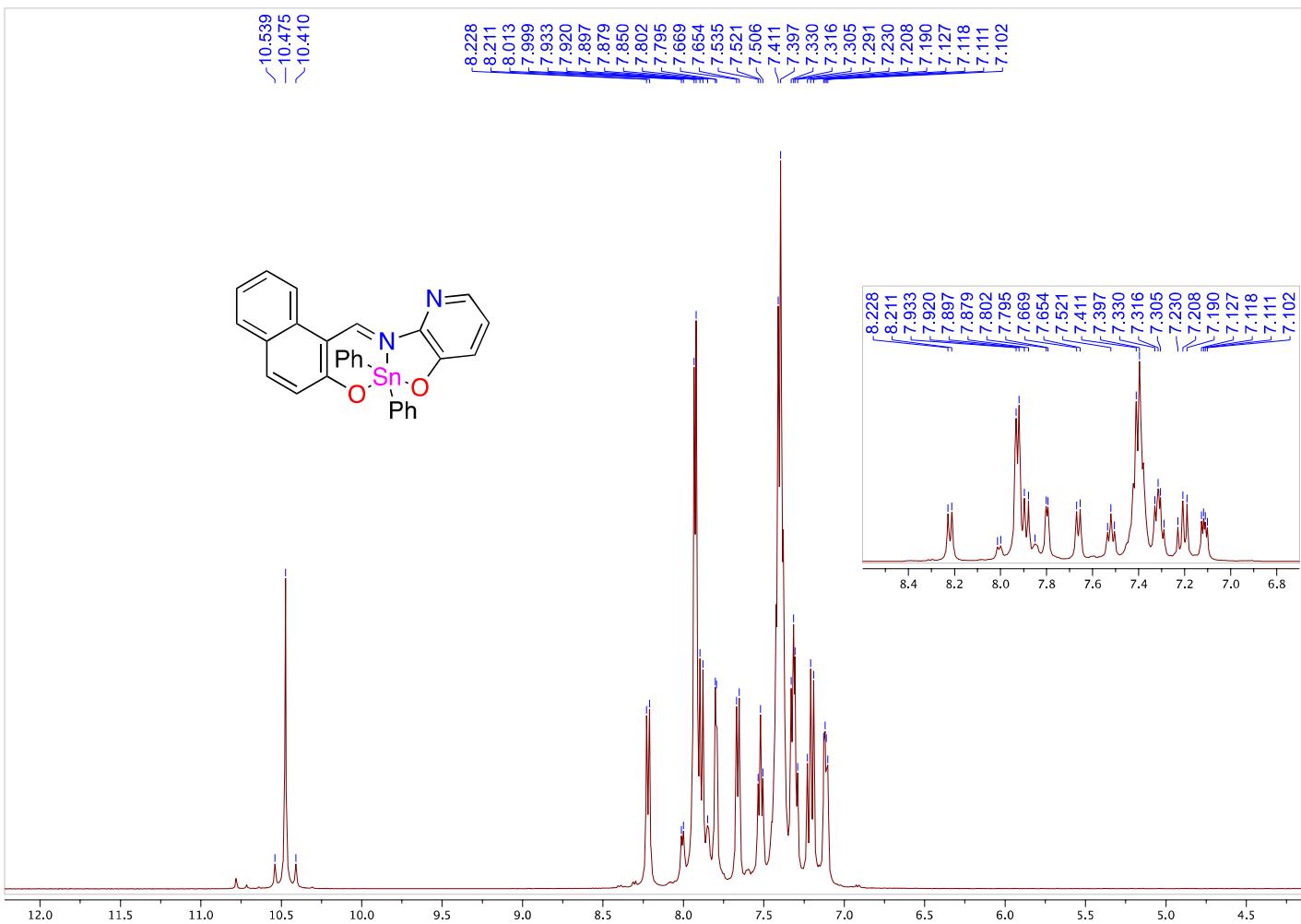


Fig. S15.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz) of complex **1c**

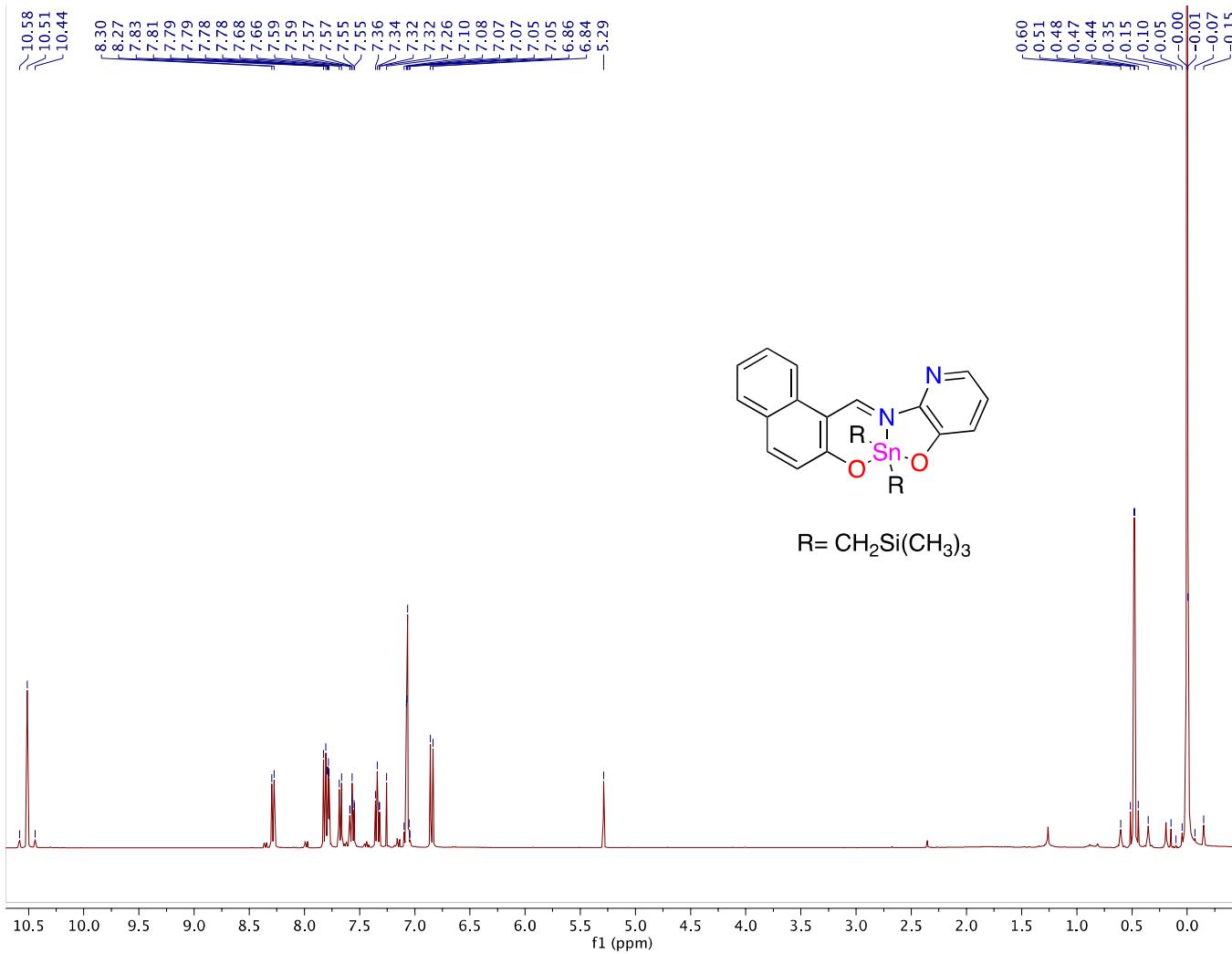


Figure S16.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) of complex **1d**

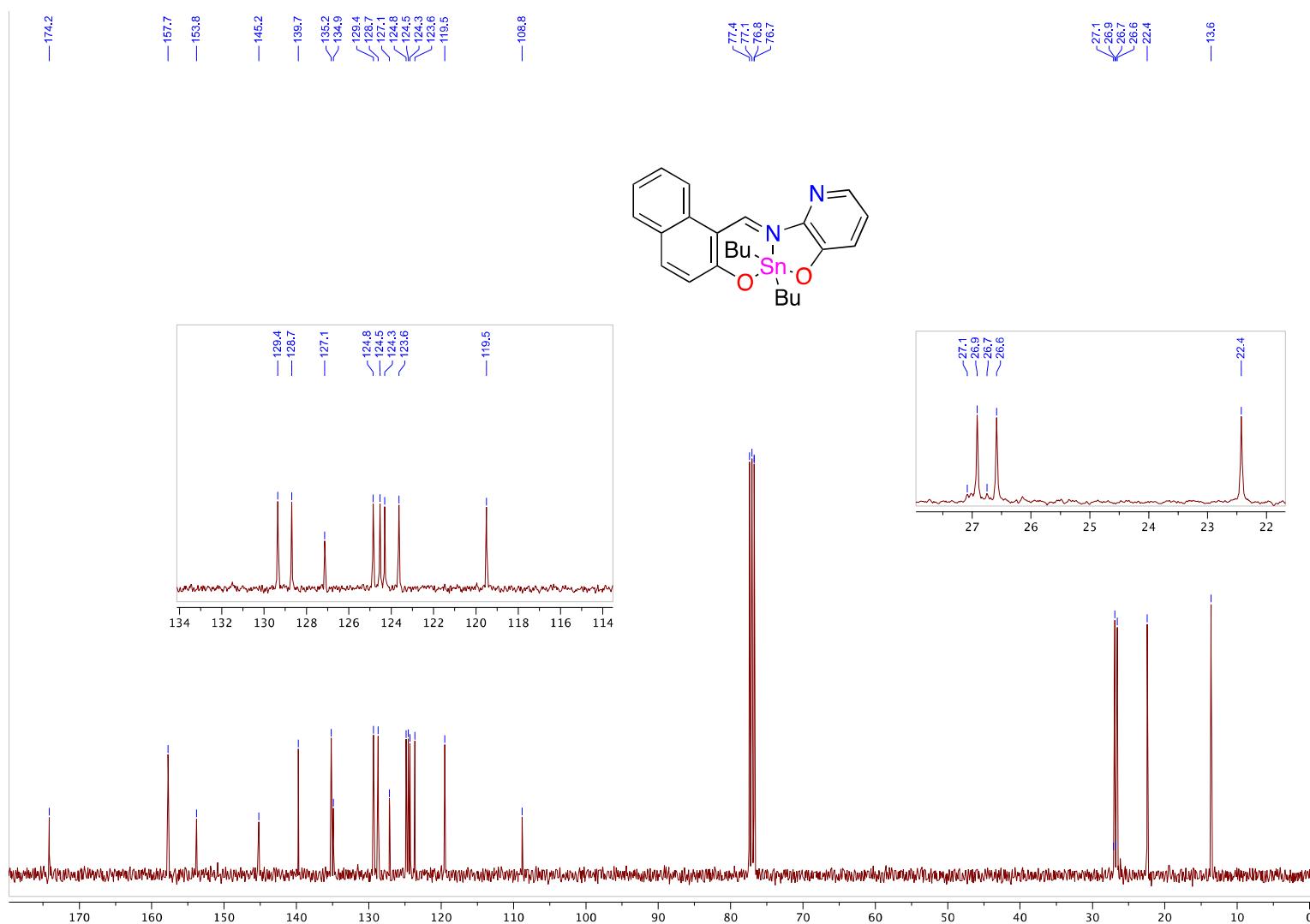


Figure S17.  $^{13}\text{C}$ NMR ( $\text{CDCl}_3$ , 100 MHz) of complex **1a**

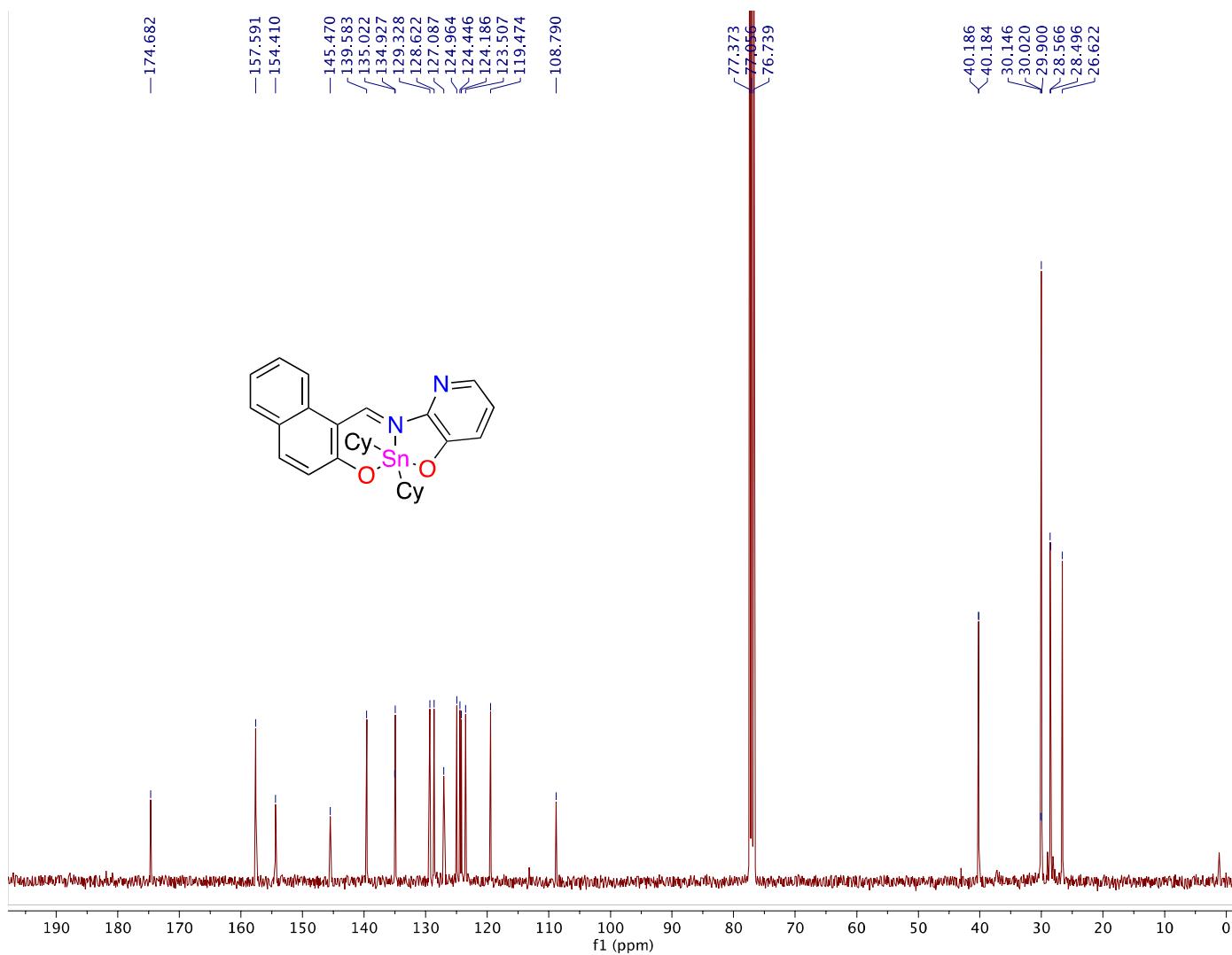


Figure S18.  $^{13}\text{C}$ NMR ( $\text{CDCl}_3$ , 100 MHz) of complex **1b**

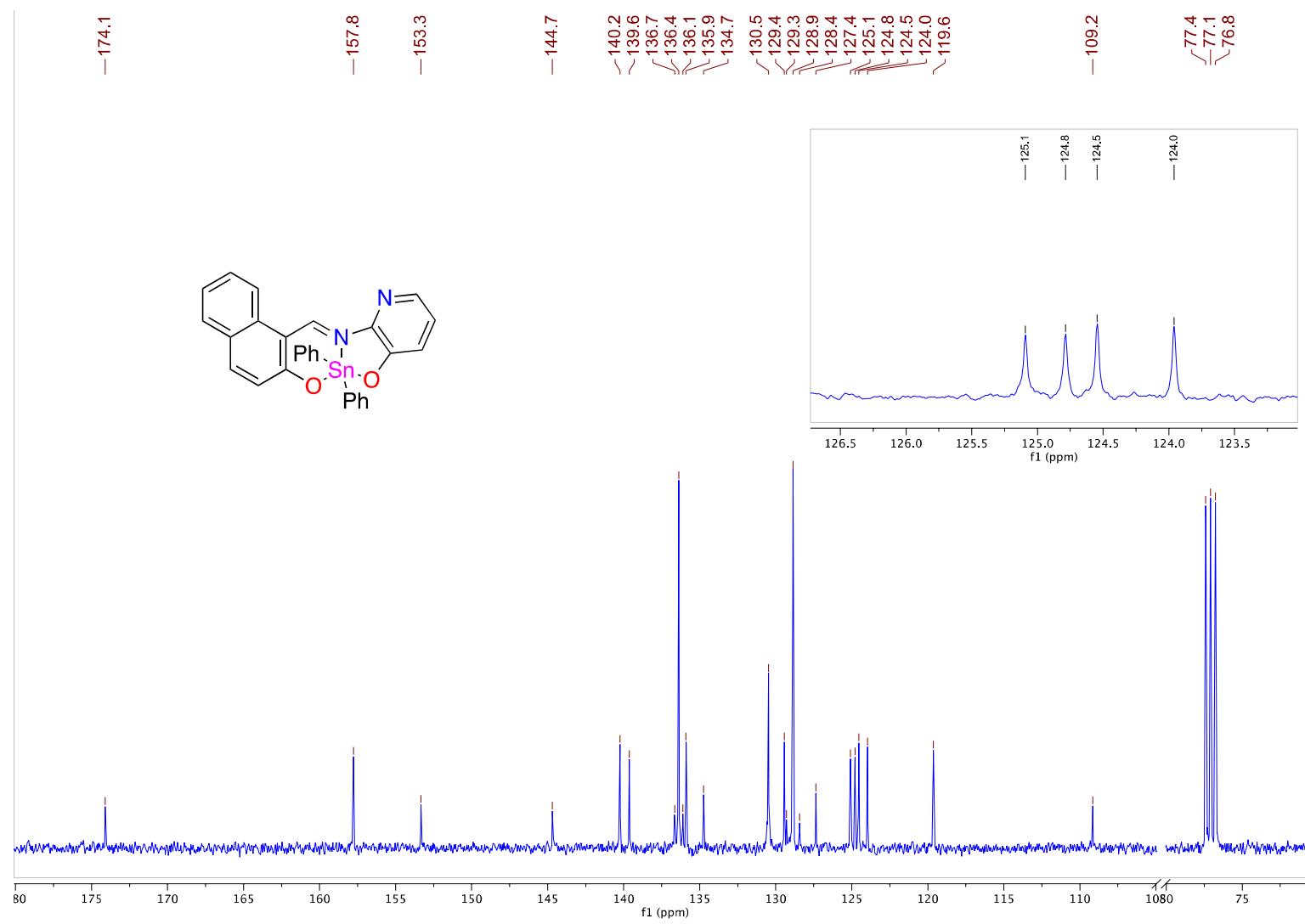


Figure S19.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) complex **1c**

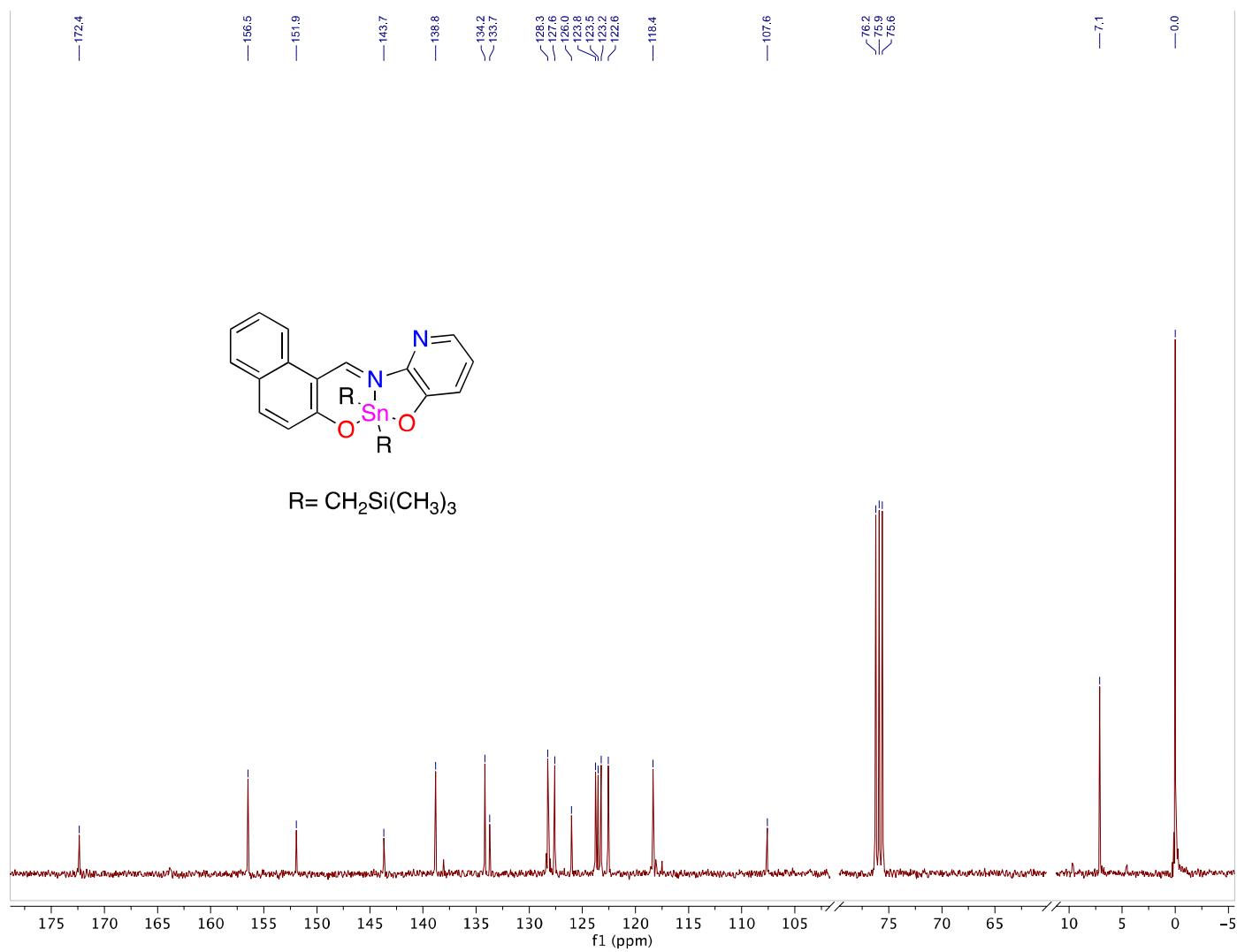


Figure S20.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) of complex **1d**

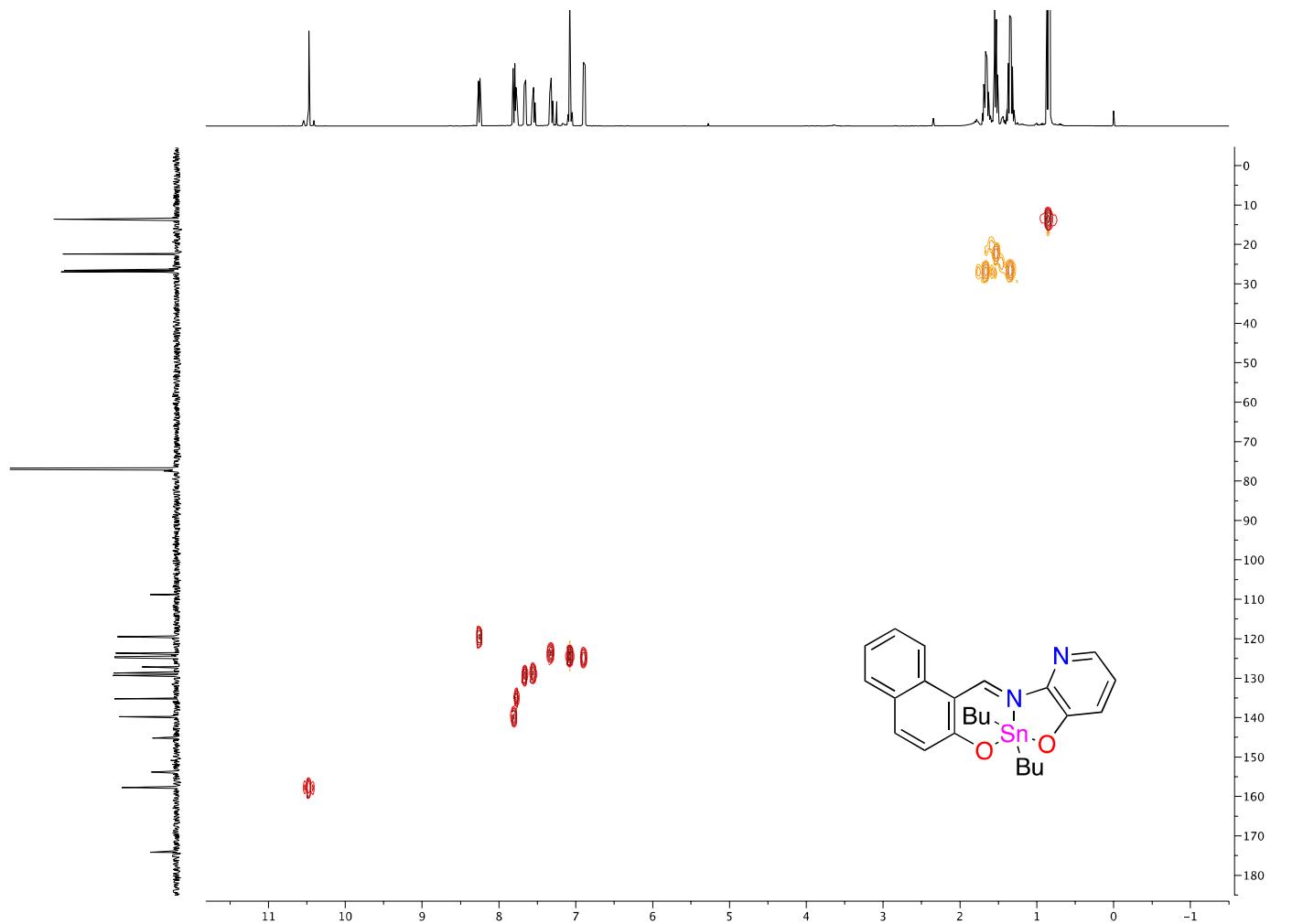


Figure S21. HSQC ( $\text{CDCl}_3$ ) of complex **1a**

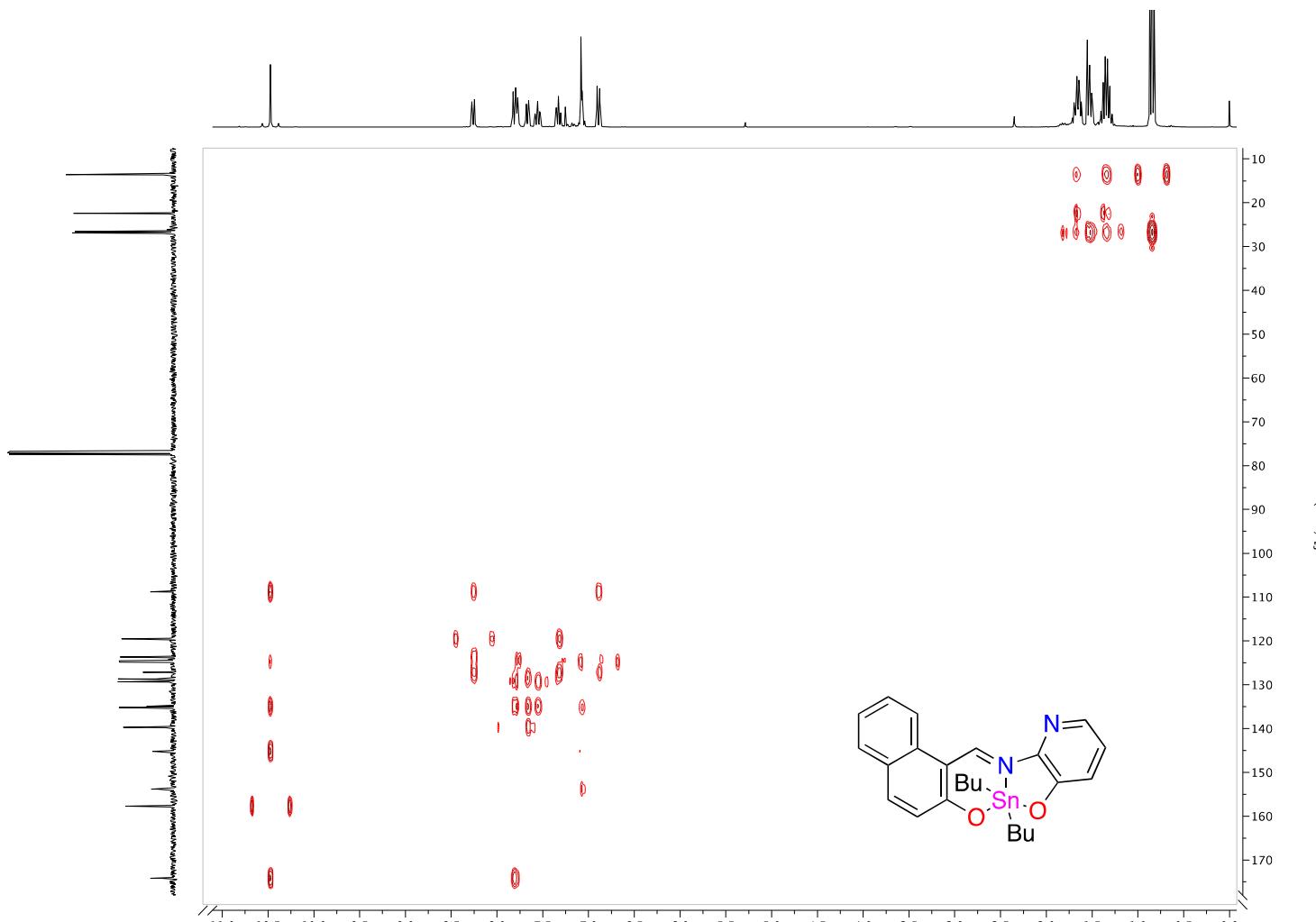


Figure S22. HMBC ( $\text{CDCl}_3$ ) of complex **1a**

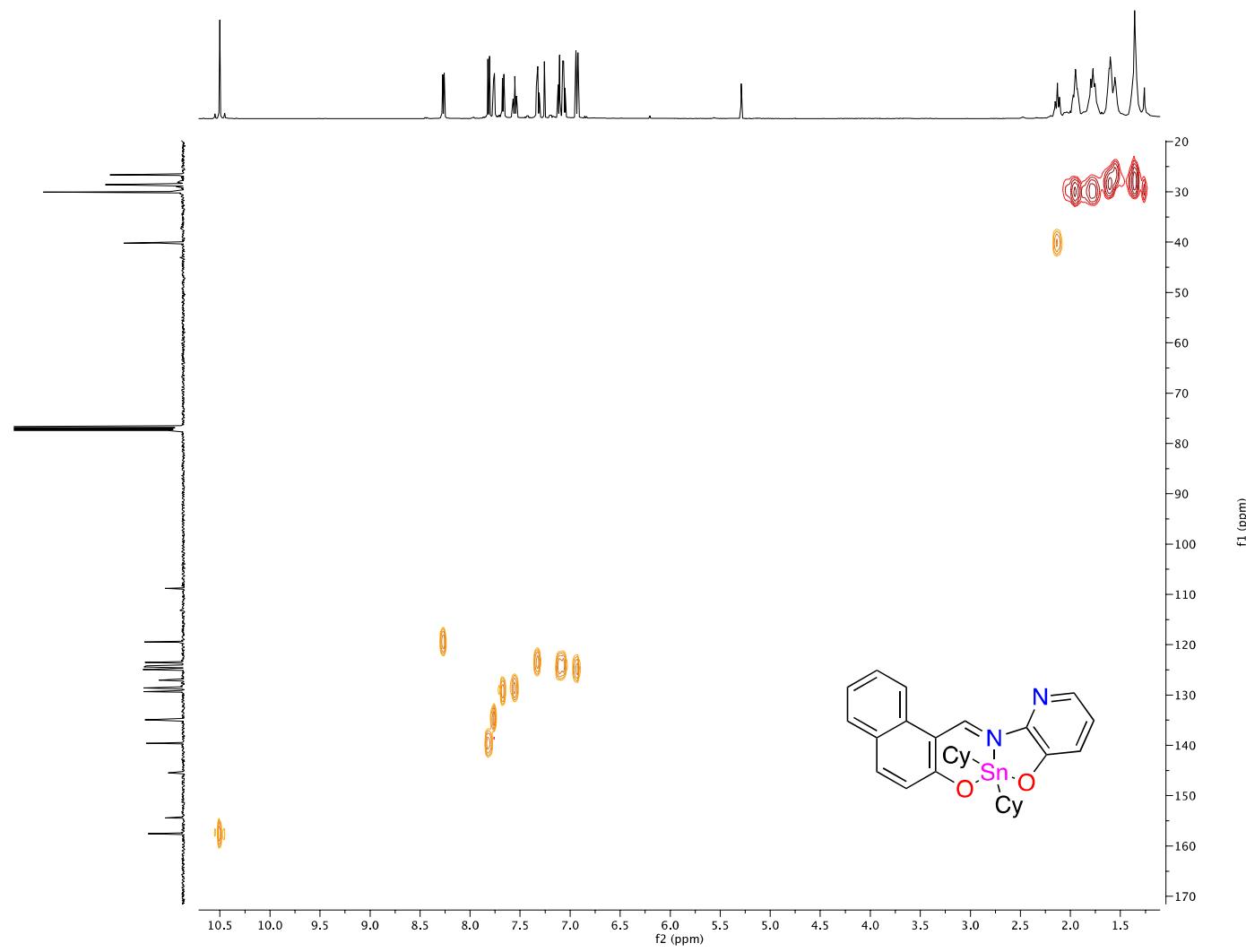


Figure S23. HSQC ( $\text{CDCl}_3$ ) of complex **1b**

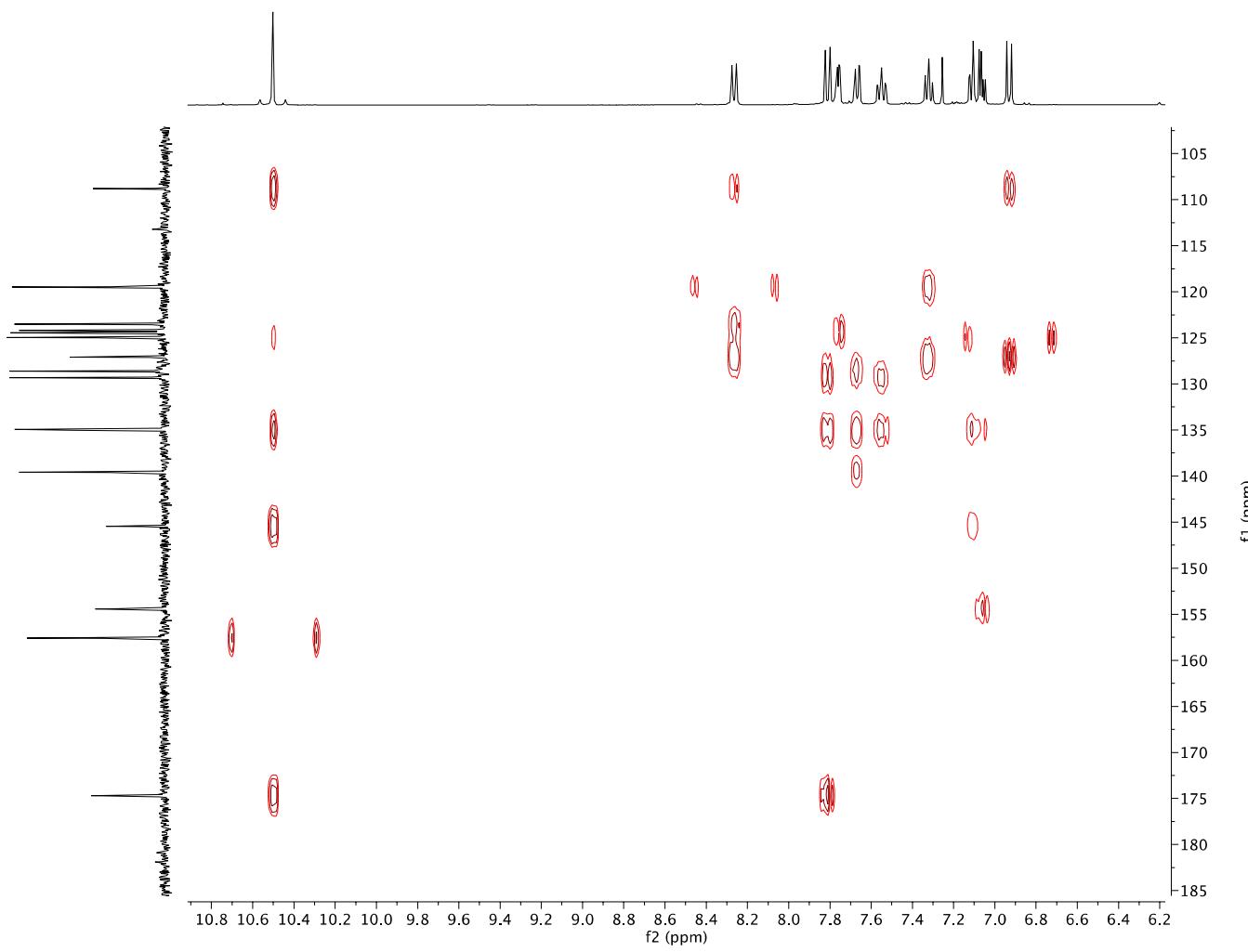


Figure S24. HMBC ( $\text{CDCl}_3$ ) of complex **1b**

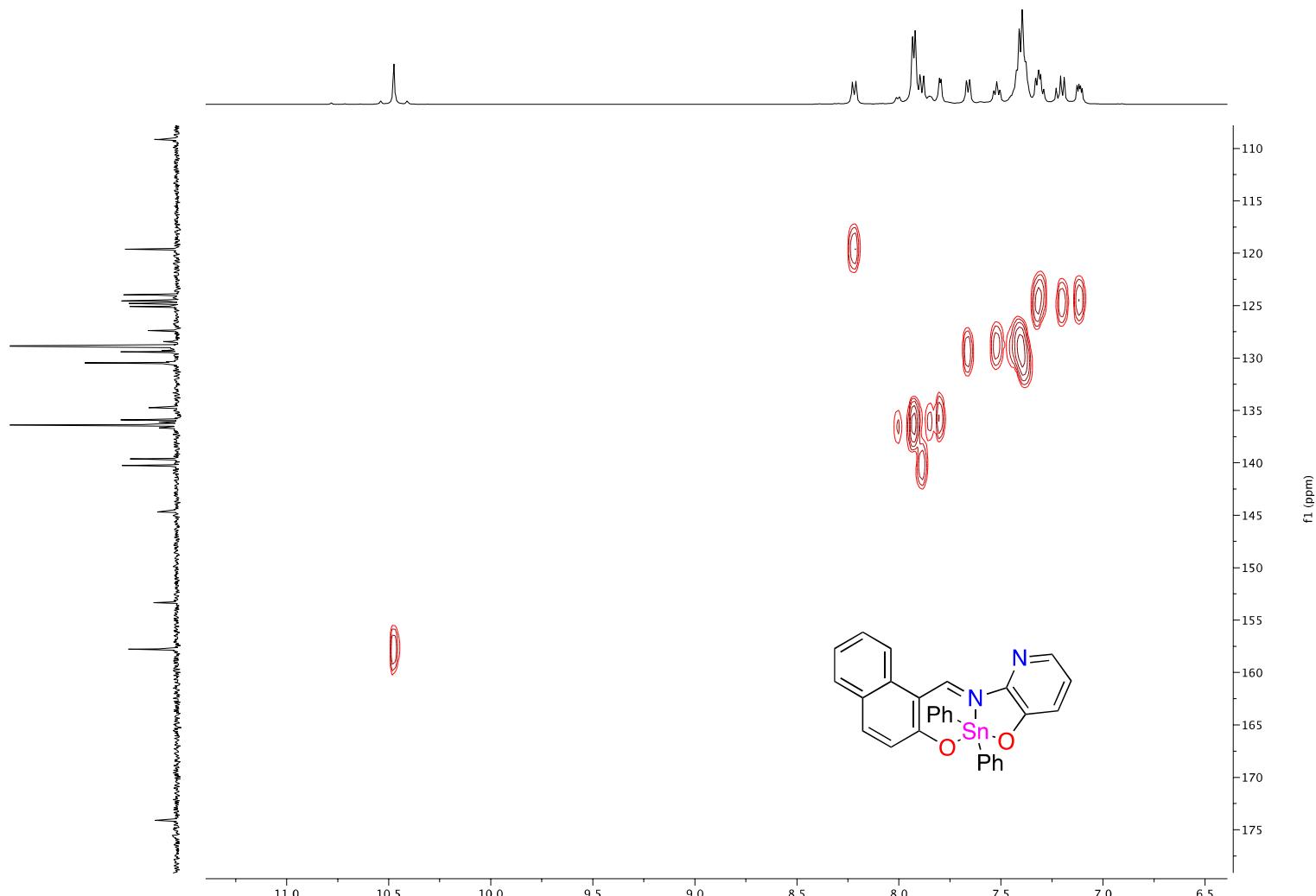


Figure S25. HSQC ( $\text{CDCl}_3$ ) of compound **1c**

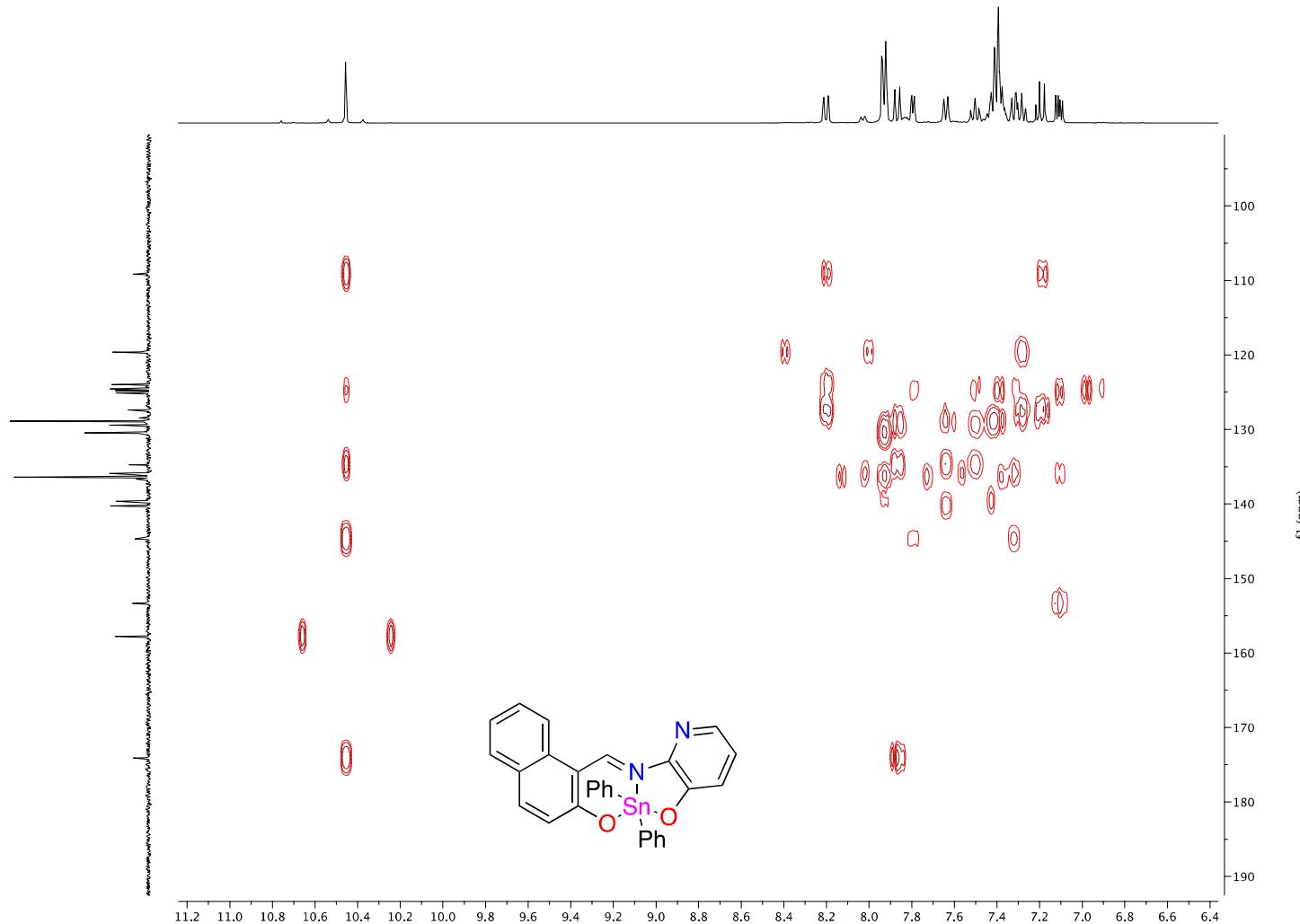


Figure S26. HMBC ( $\text{CDCl}_3$ ) of compound **1c**

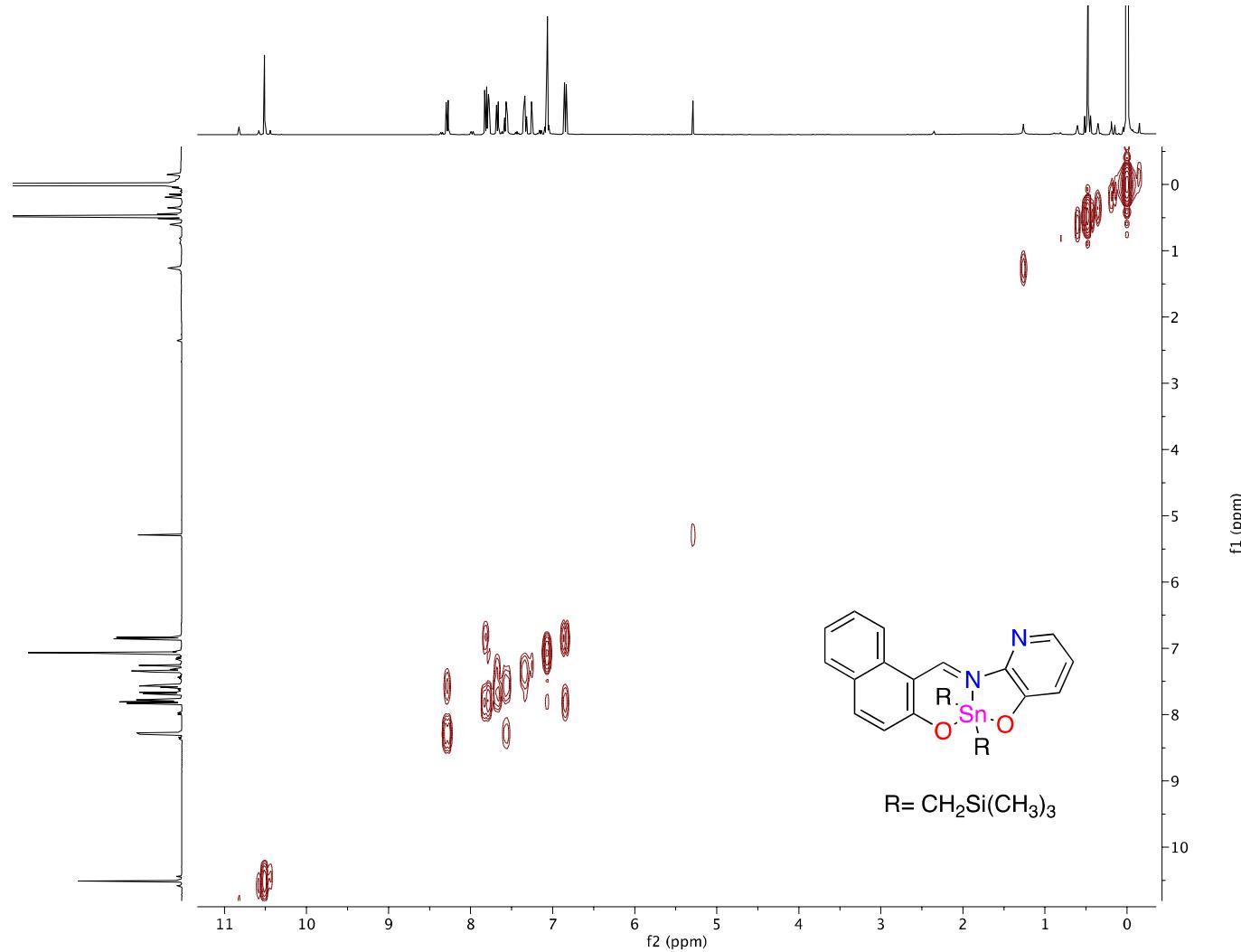


Figure S27. HSQC ( $\text{CDCl}_3$ ) of complex **1d**

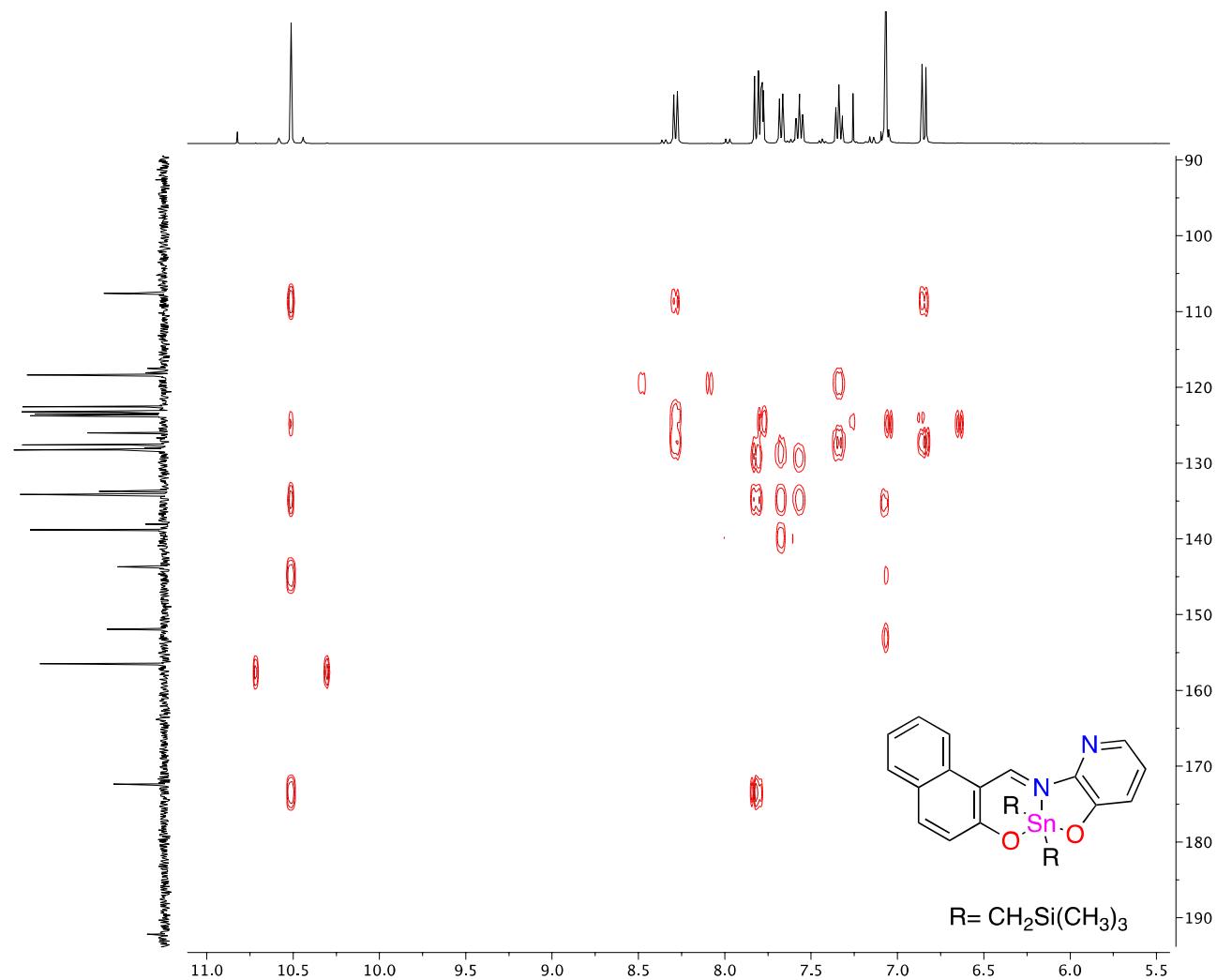


Figure S28. HMBC ( $\text{CDCl}_3$ ) of complex **1d**

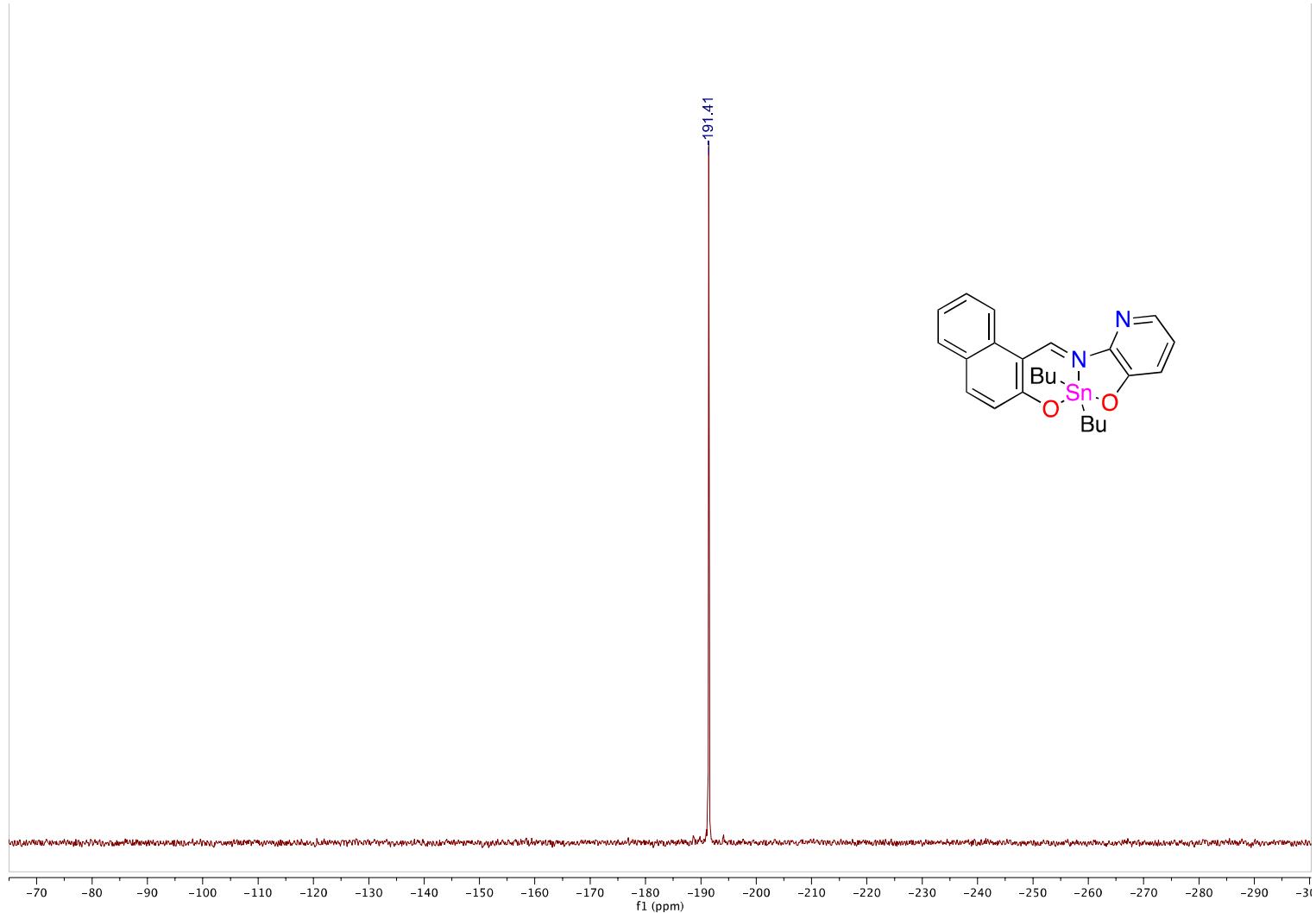


Figure S29.  $^{119}\text{Sn}$  NMR ( $\text{CDCl}_3$ , 112 MHz) of complex **1a**

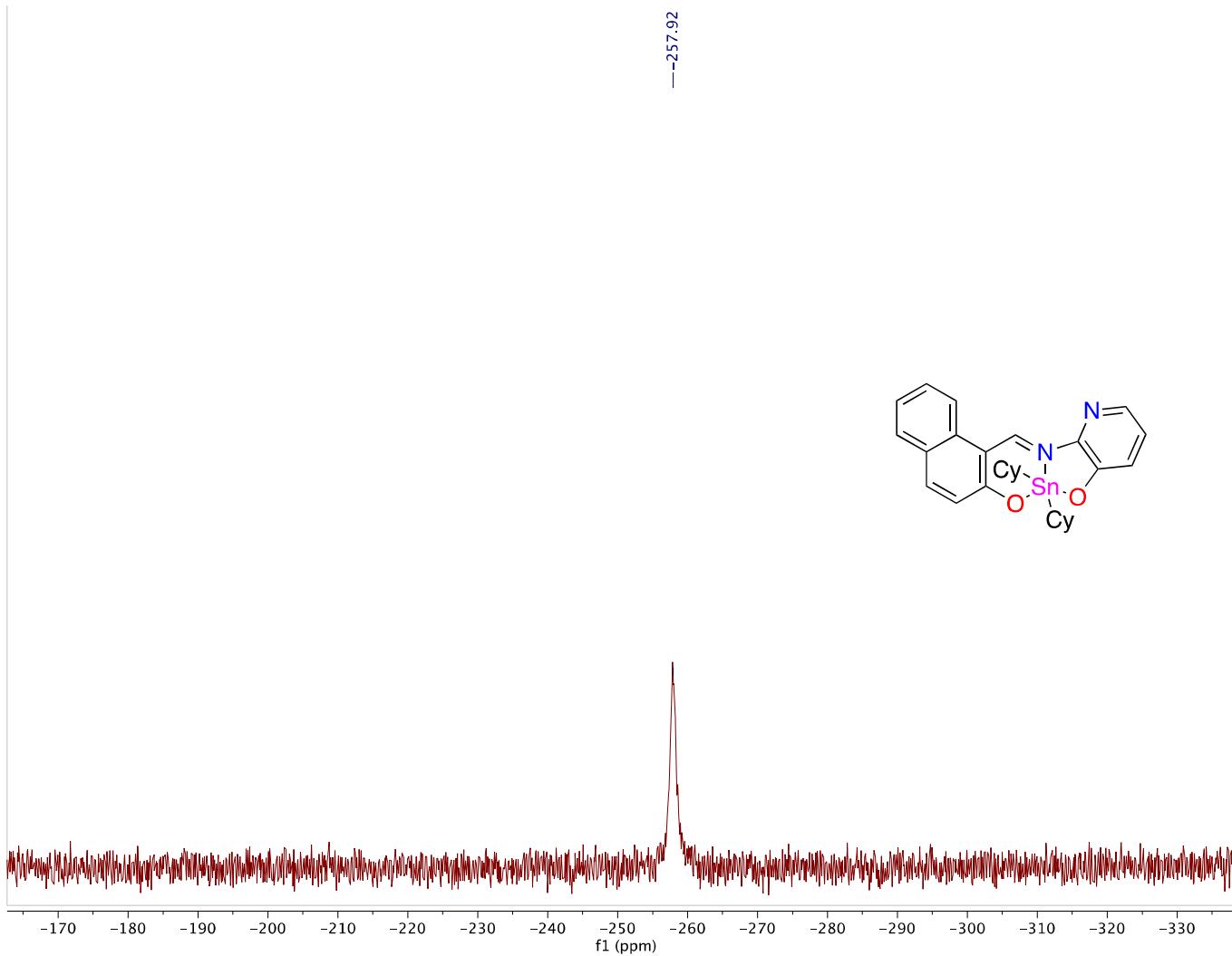


Figure S30.  $^{119}\text{Sn}$  NMR ( $\text{CDCl}_3$ , 112 MHz) of complex **1b**

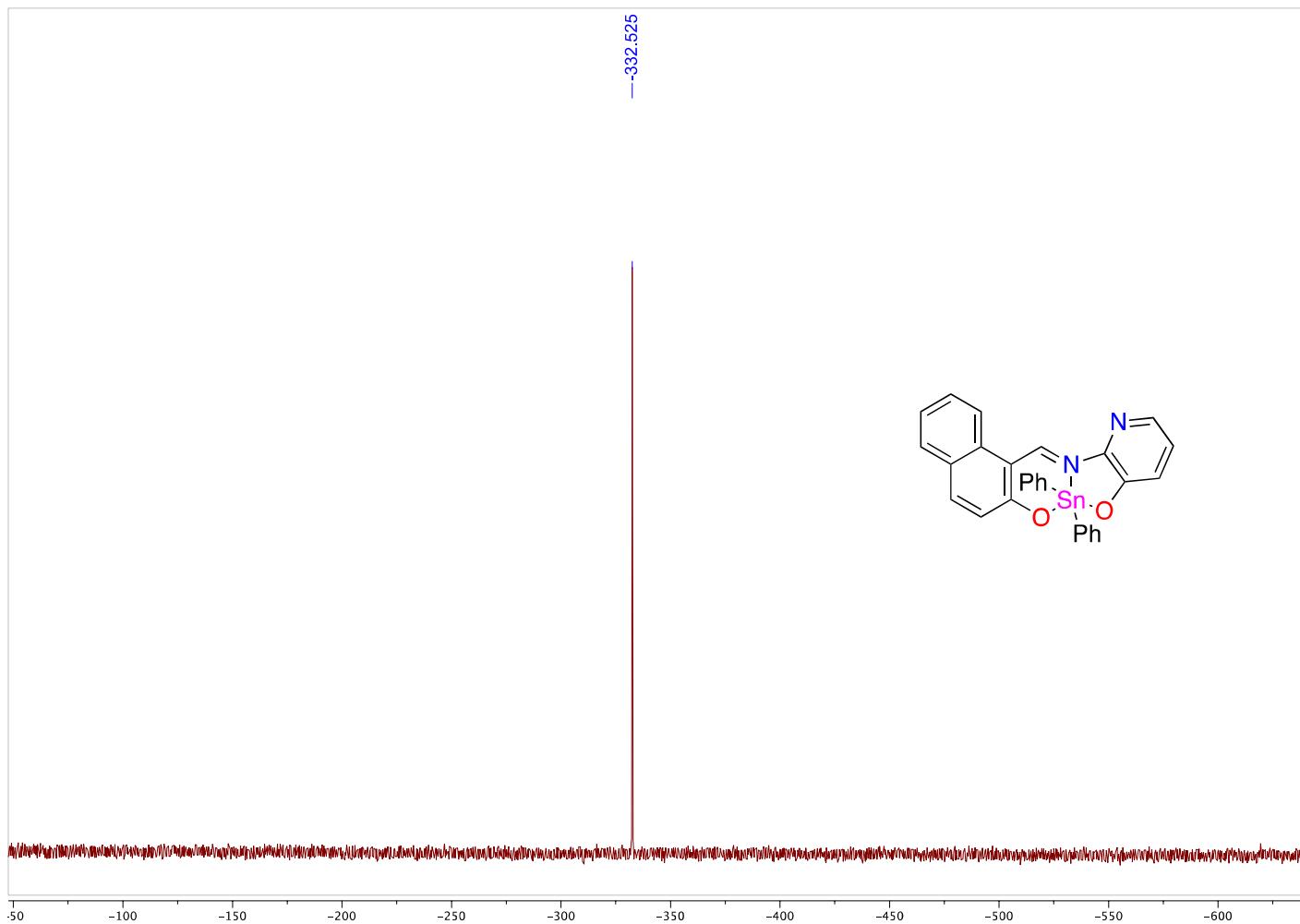


Figure S31.  $^{119}\text{Sn}$  NMR ( $\text{CDCl}_3$ , 112 MHz) of complex **1c**

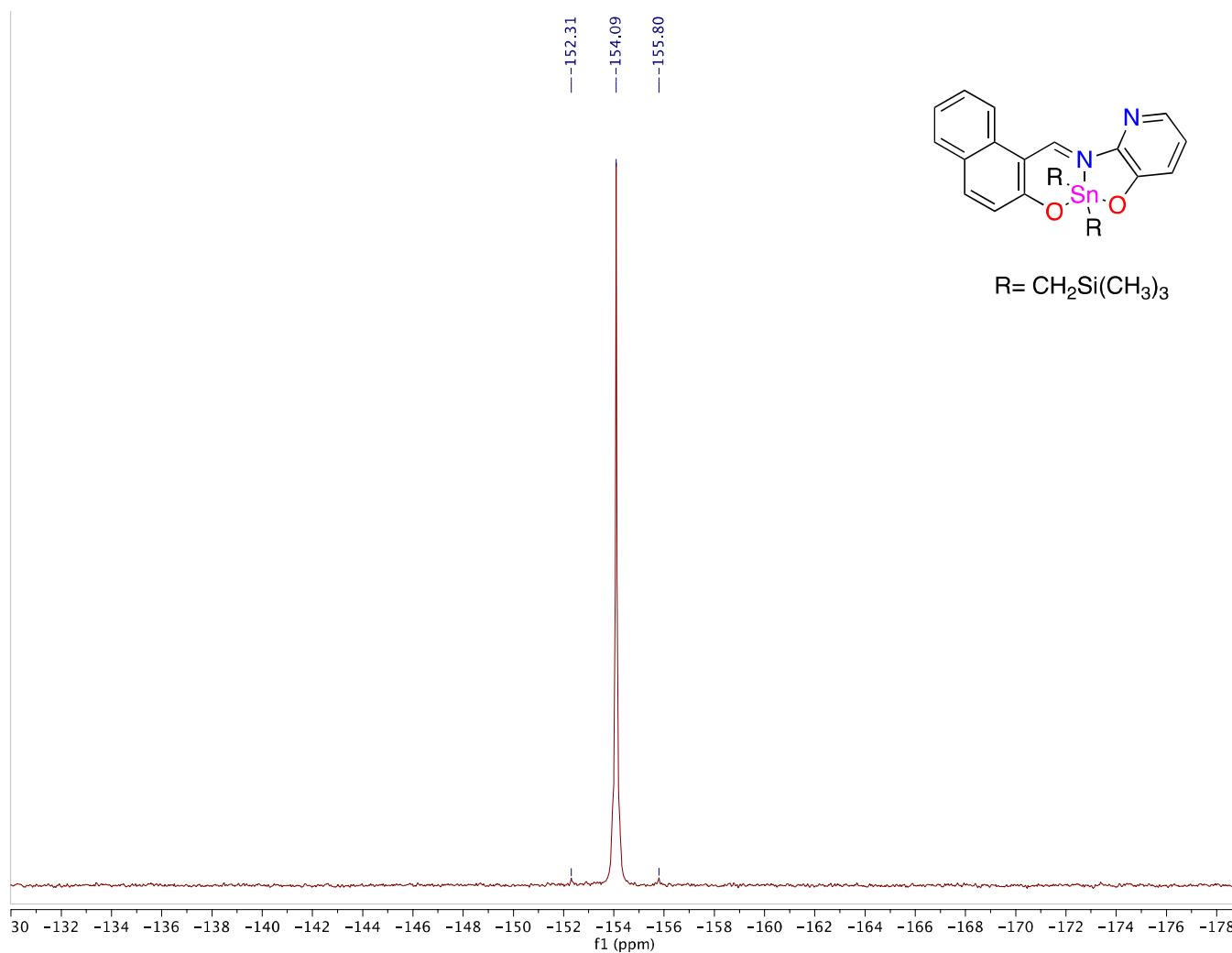


Figure S32.  $^{119}\text{Sn}$  NMR ( $\text{CDCl}_3$ , 112 MHz) of complex **1d**