

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

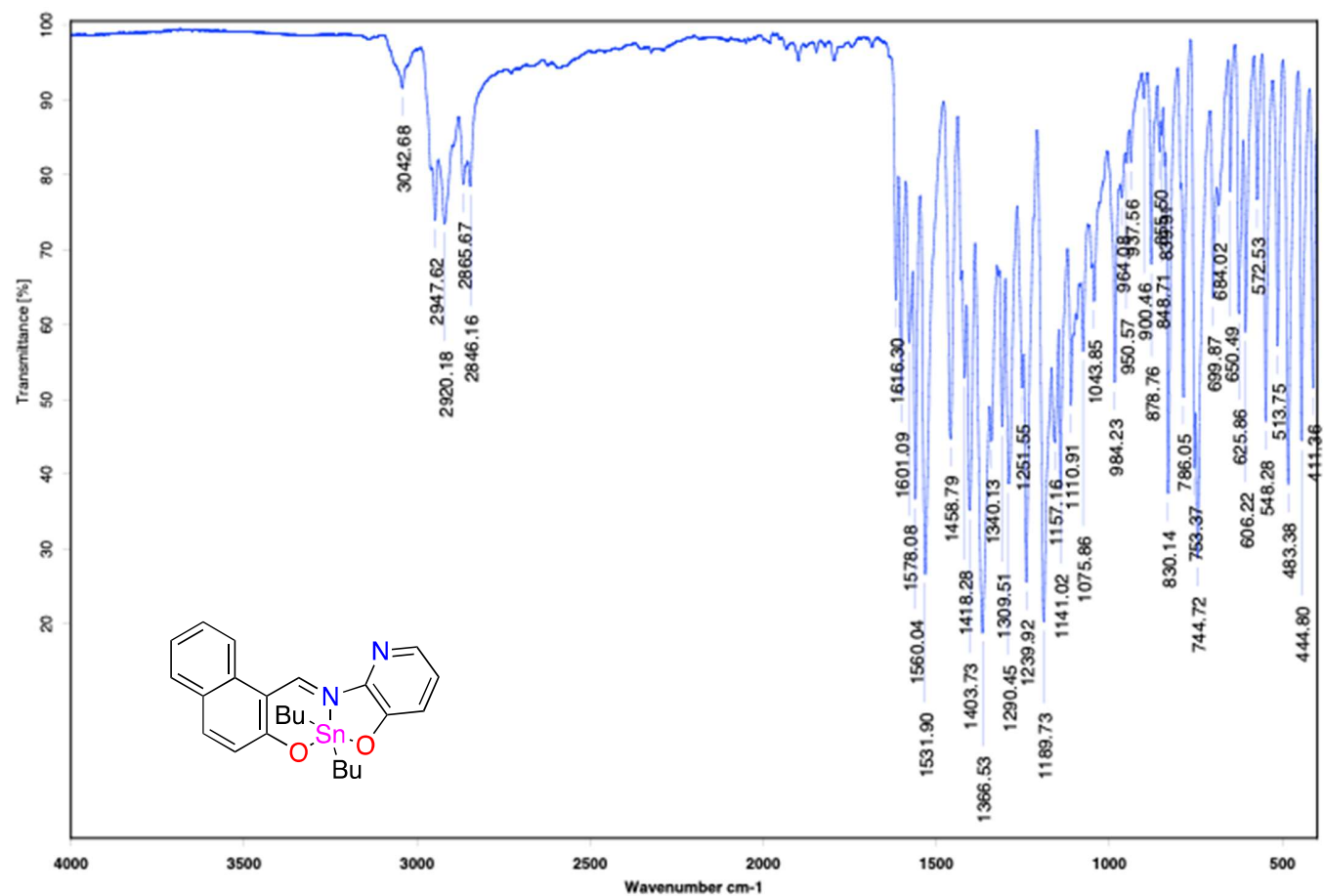


Figure S1. ATR-IR of complex **1a**

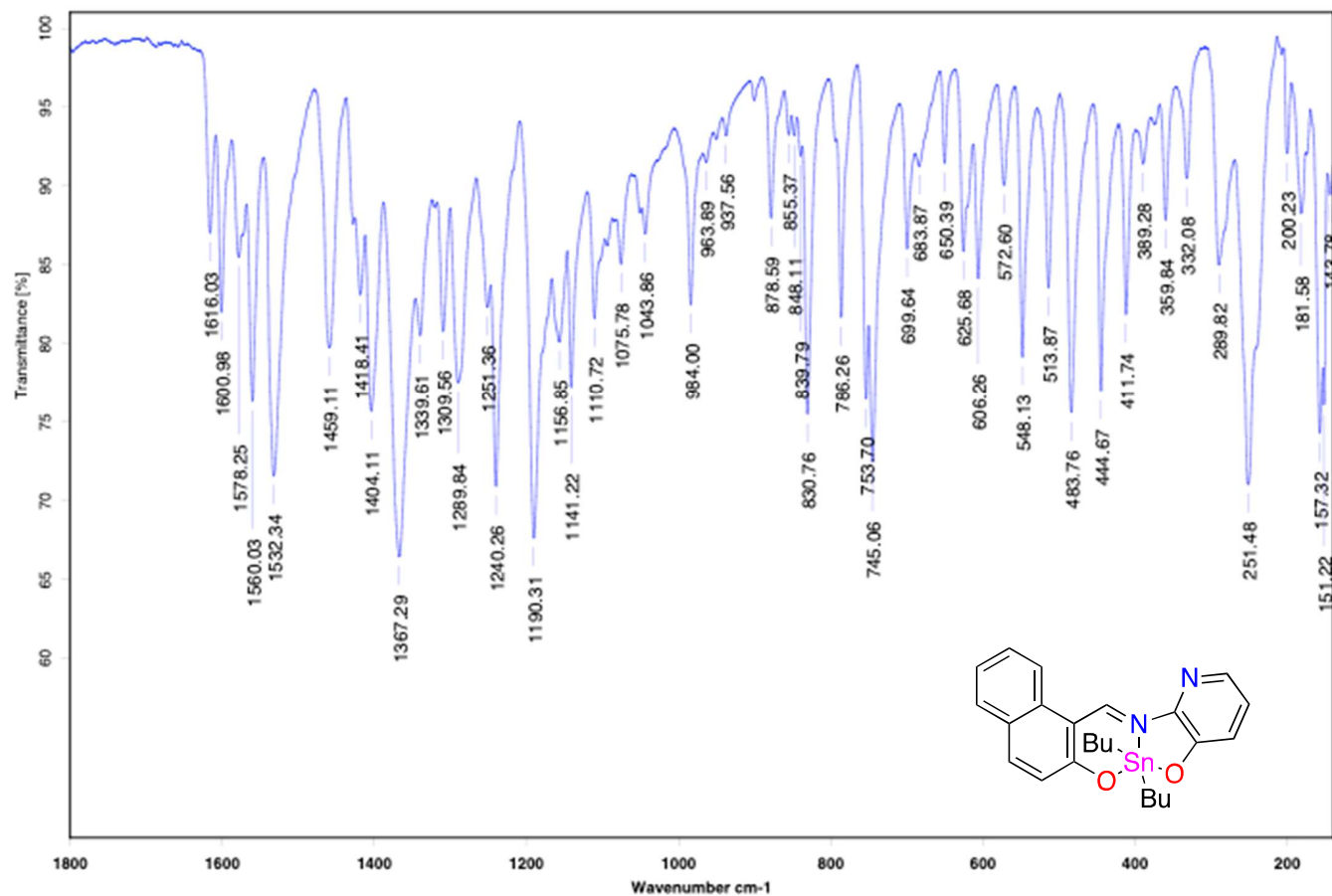


Figure S2. Far-IR of complex **1a**

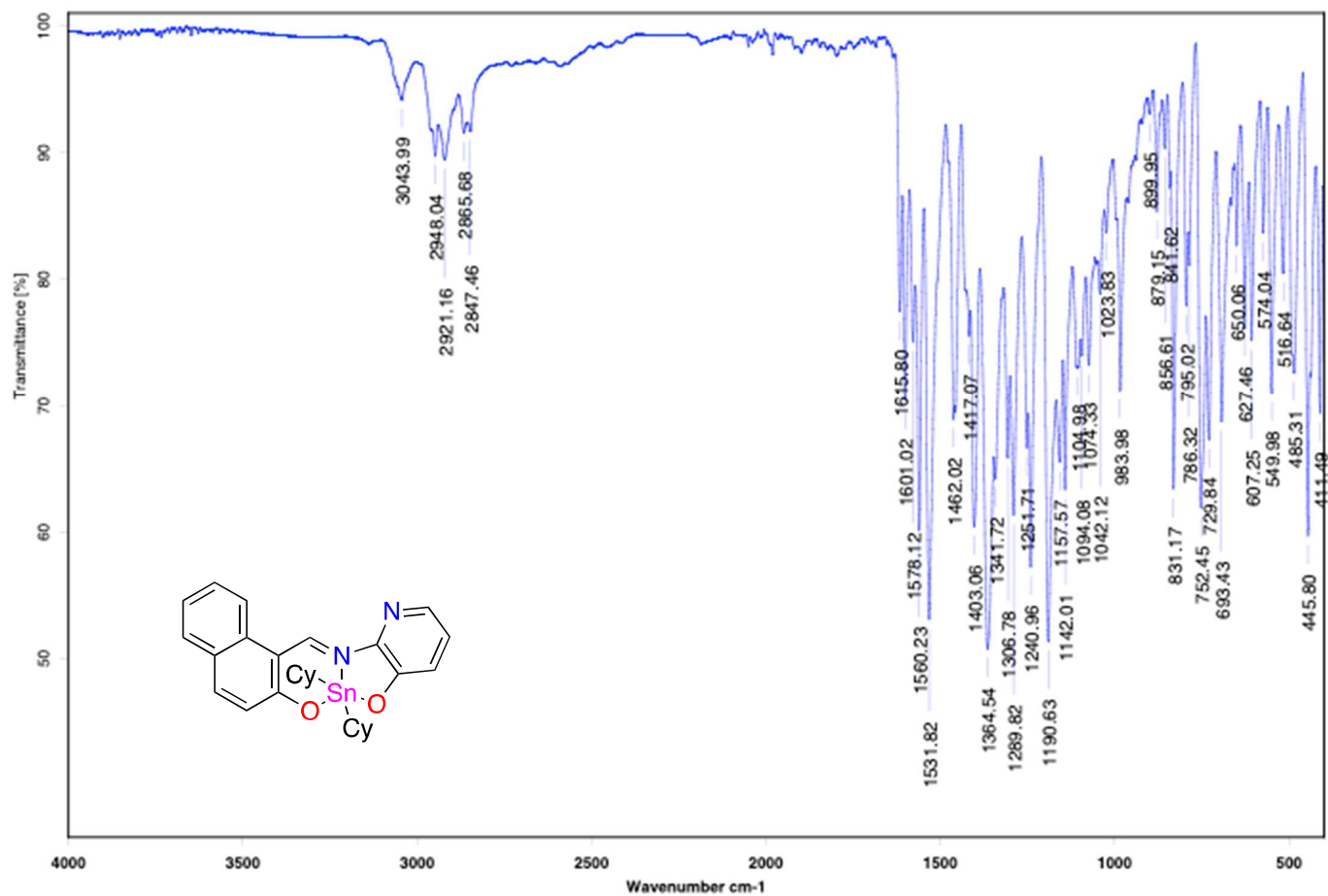


Figure S3. ATR-IR of complex **1b**

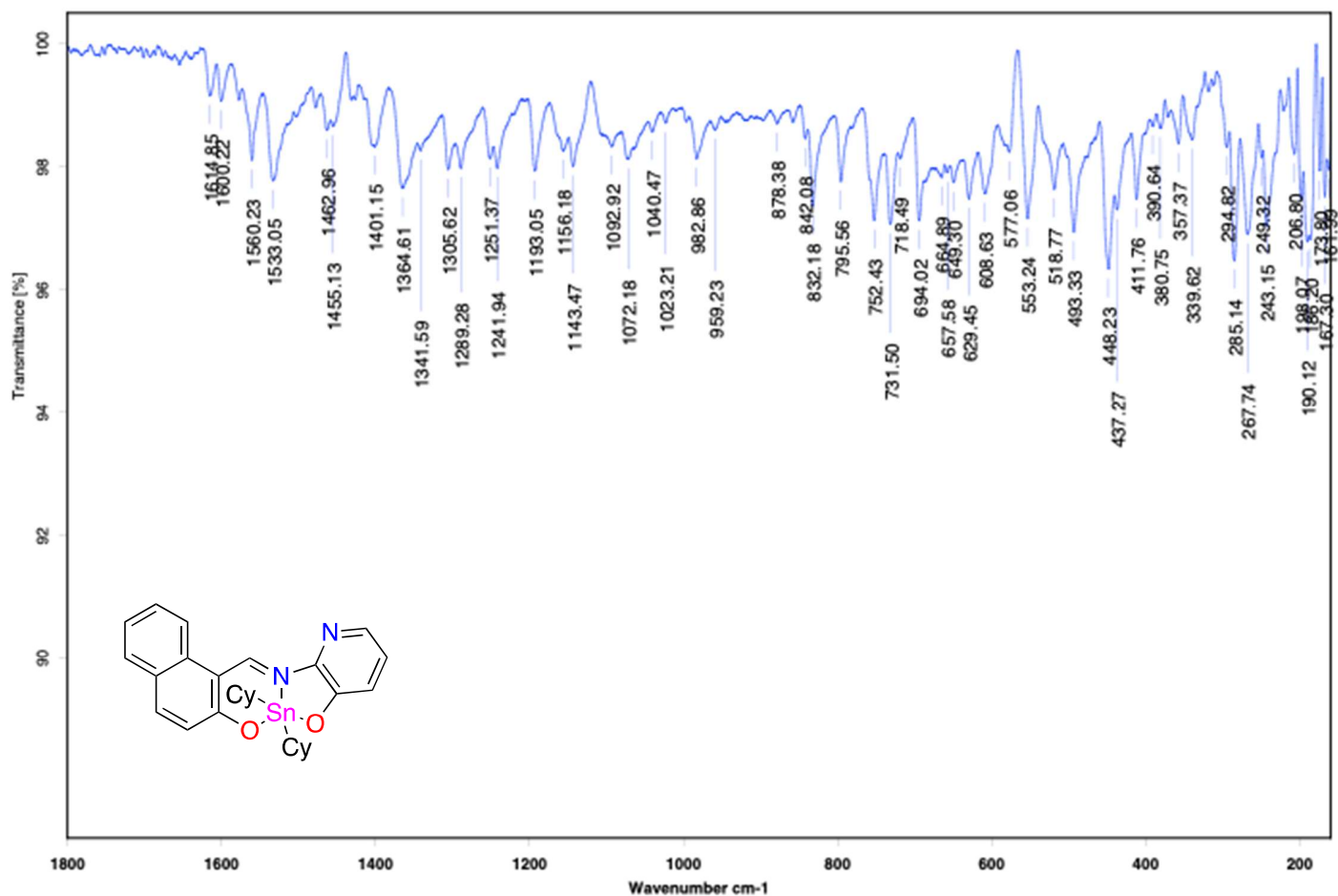


Figure S4. Far-IR of complex **1b**

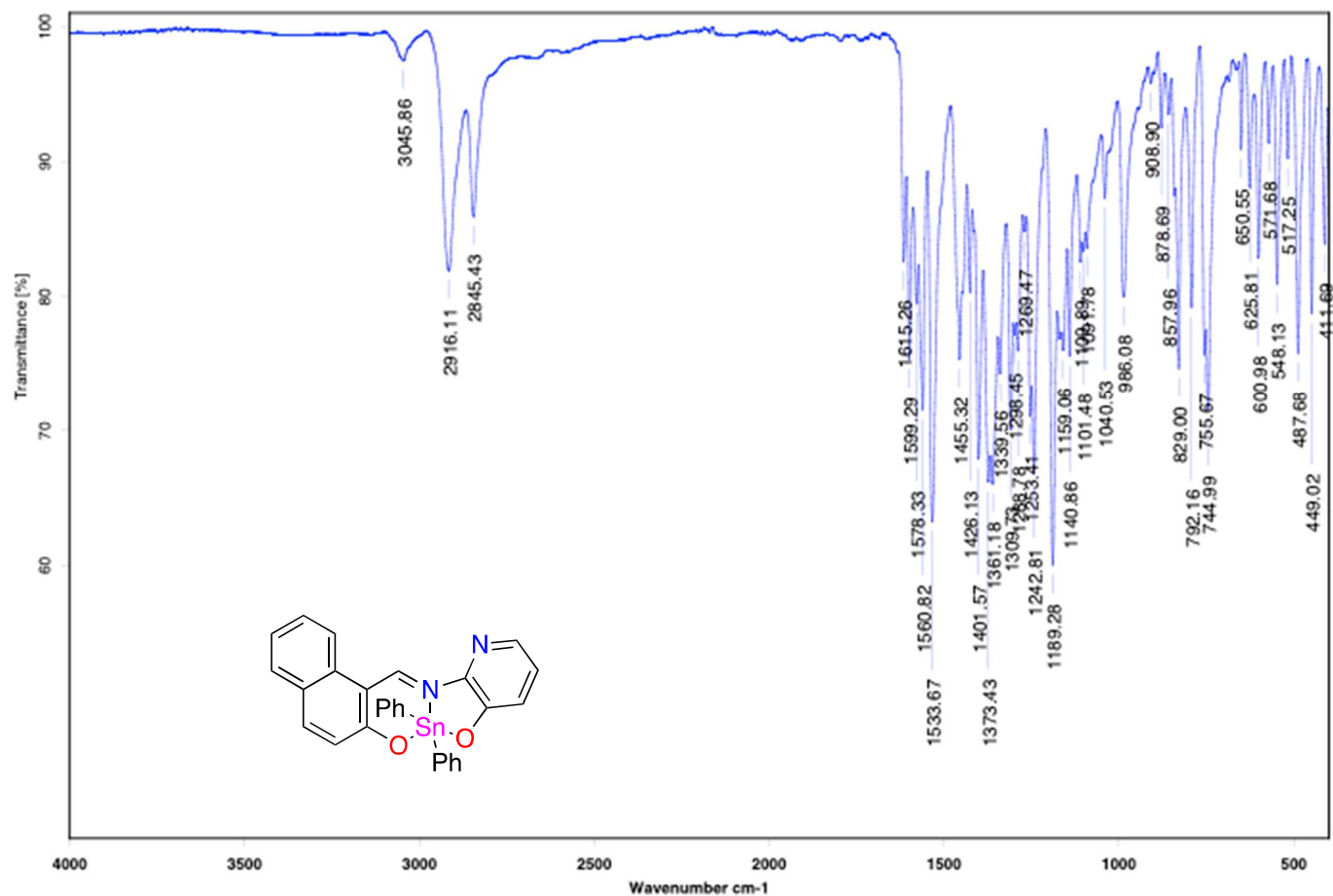


Figure S5. ATR-IR of complex 1c

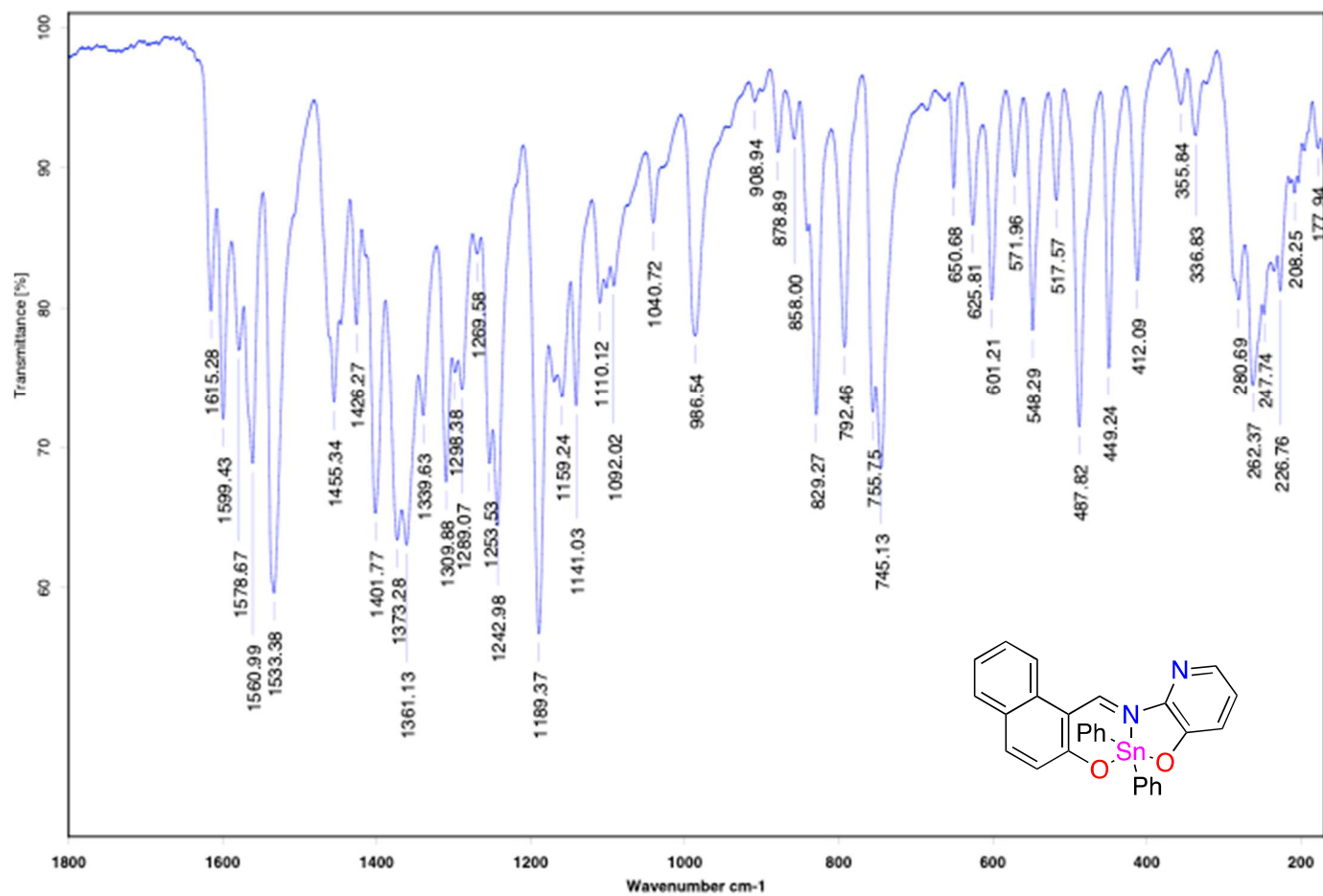


Figure S6. Far-IR of complex 1c

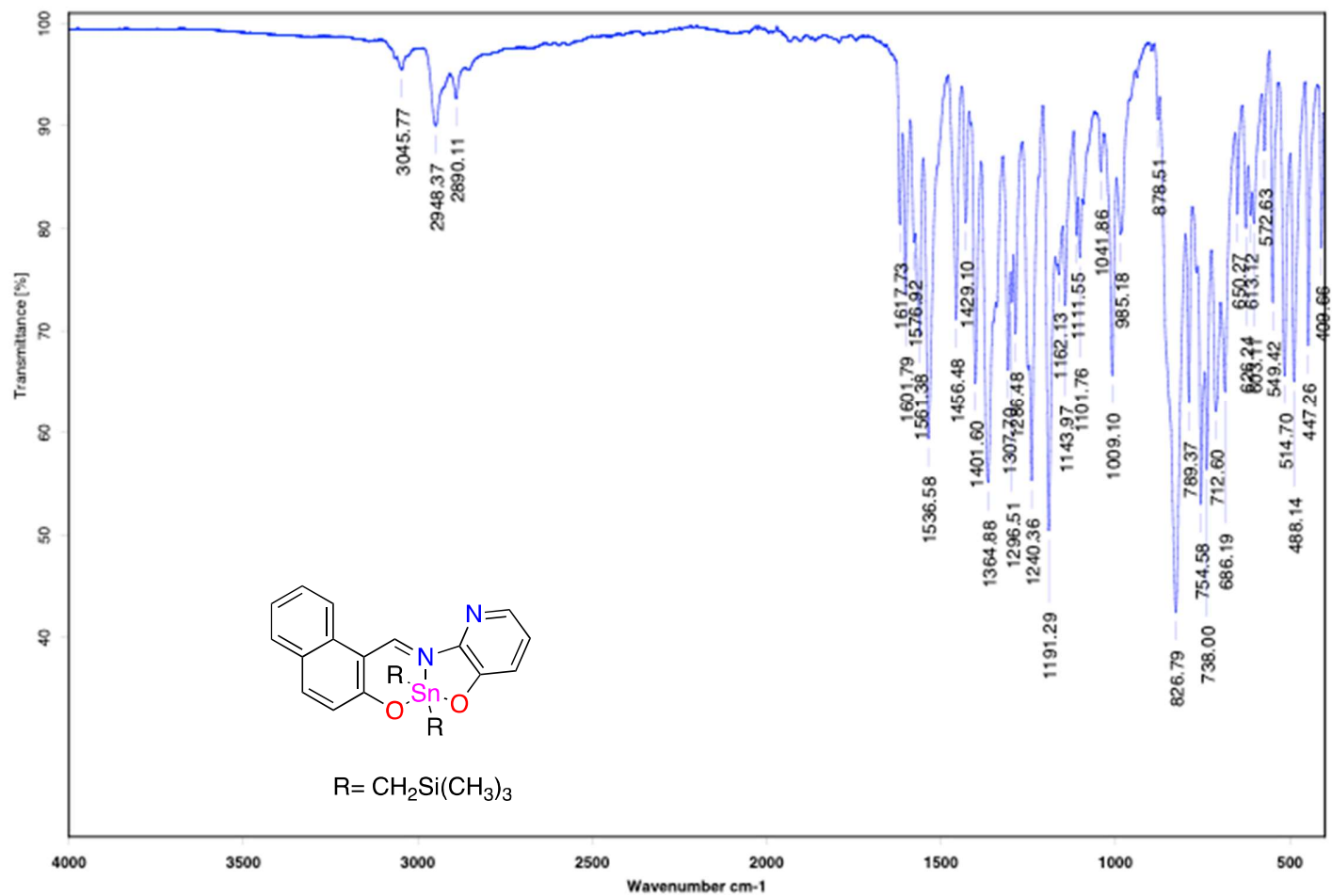


Figure S7. ATR-IR of complex **1d**



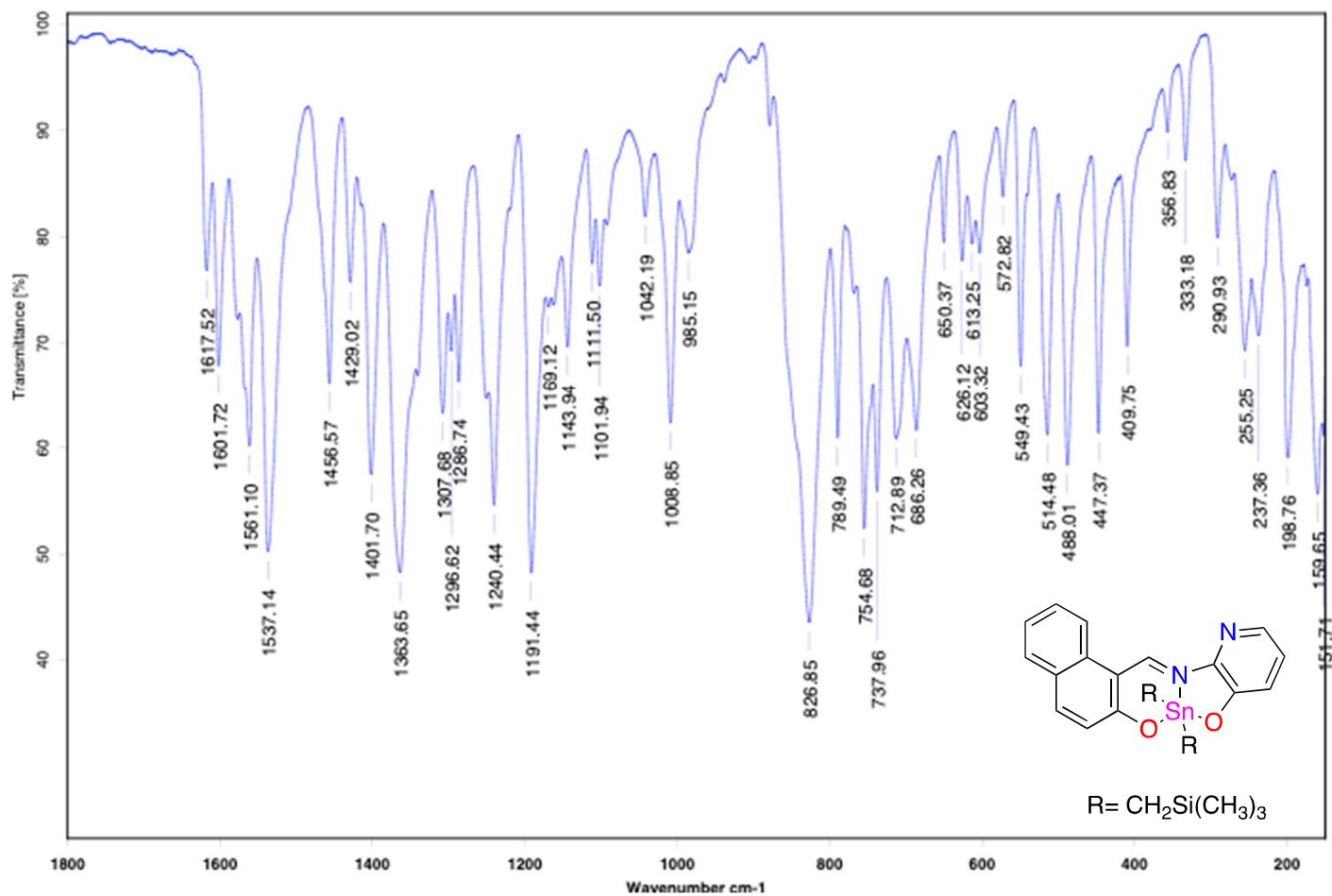


Figure S8. ATR-IR of complex **1d**

INSTITUTO DE QUIMICA, UNAM  
LABORATORIO DE ESPECTROMETRIA DE MASAS

Acq. Data Name: U-2992 SCP3a  
Creation Parameters: Average(MS[1] Time:3..3)  
Elizabeth Gomez / Samuel Cuenca

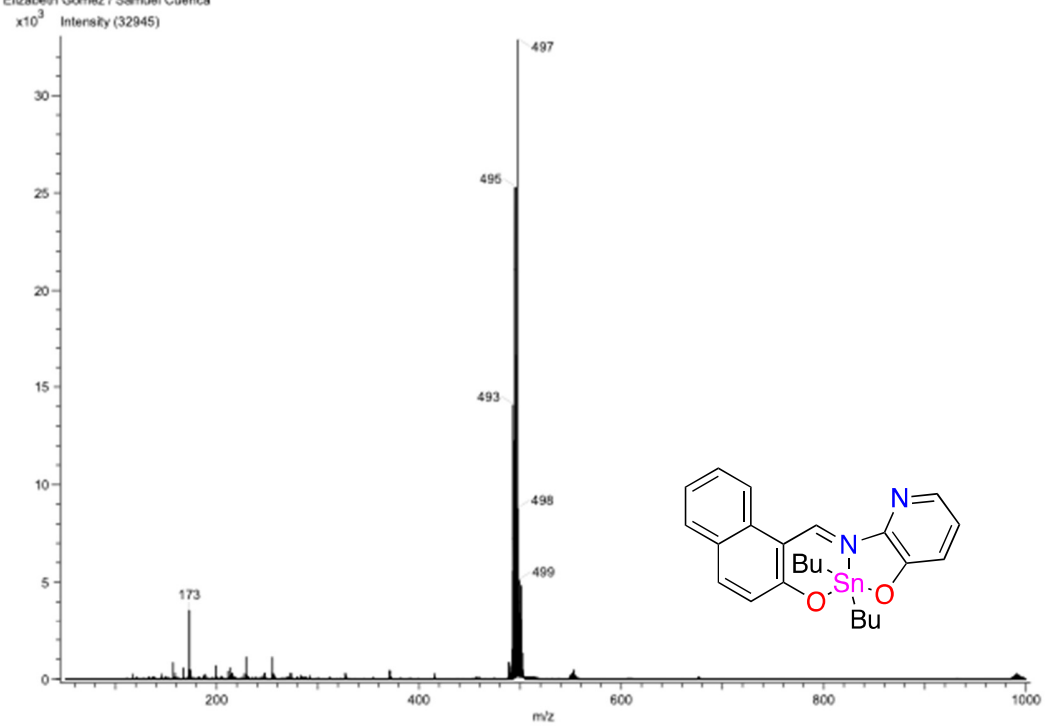


Figure S9. Mass Spectrometry (DART<sup>+</sup>) of complex **1a**



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

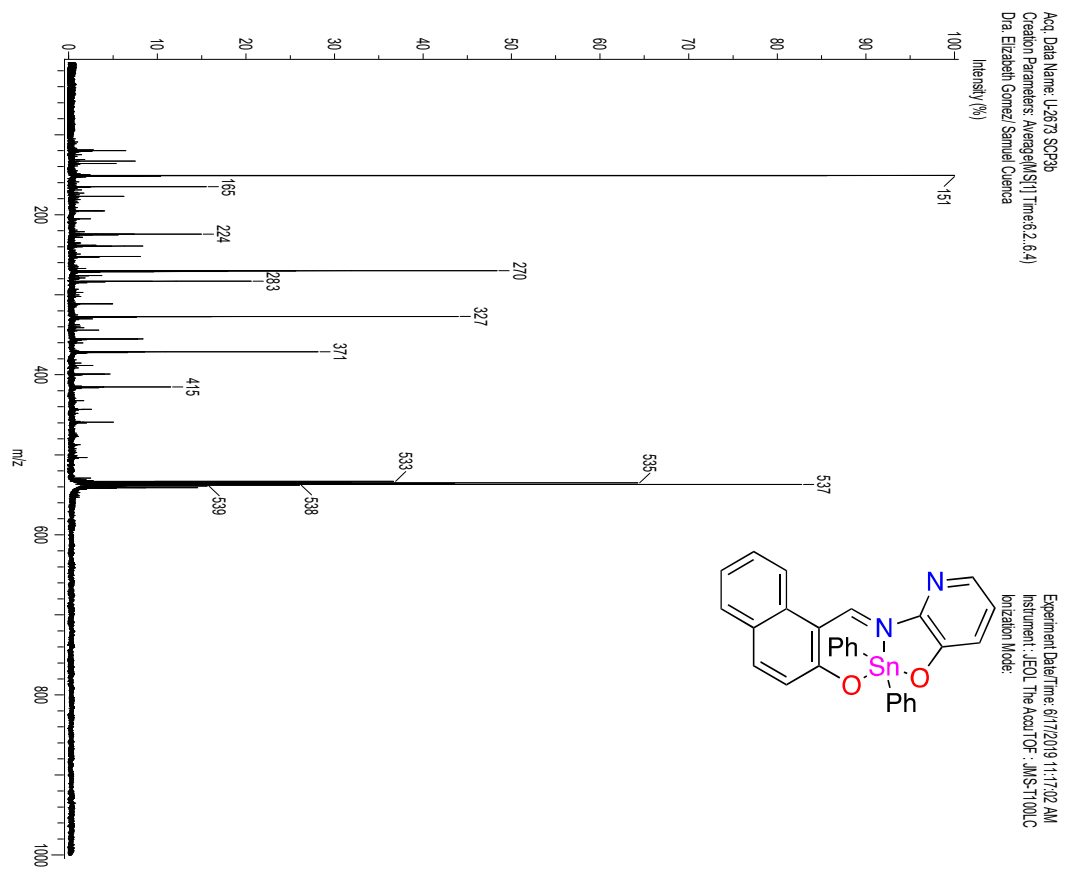


Figure S11. Mass Spectrometry (DART<sup>+</sup>) of complex **1c**

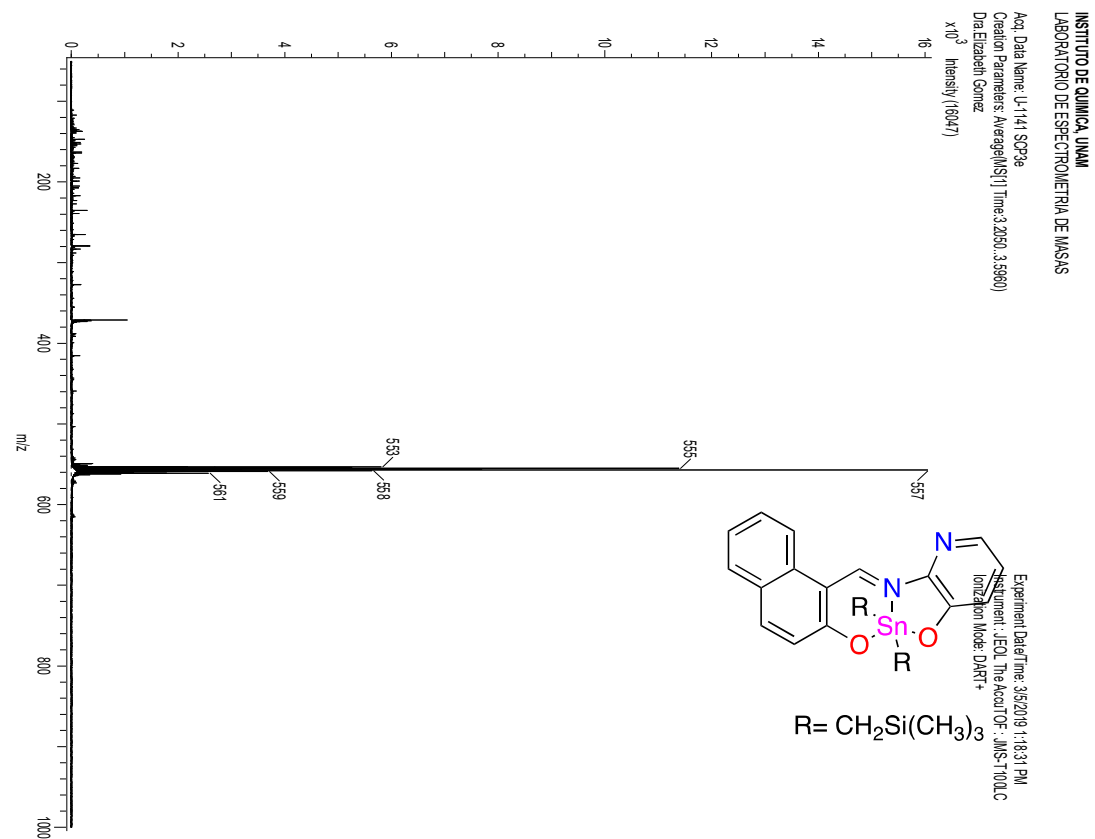


Figure S12. Mass Spectrometry (DART<sup>+</sup>) of complex **1d**

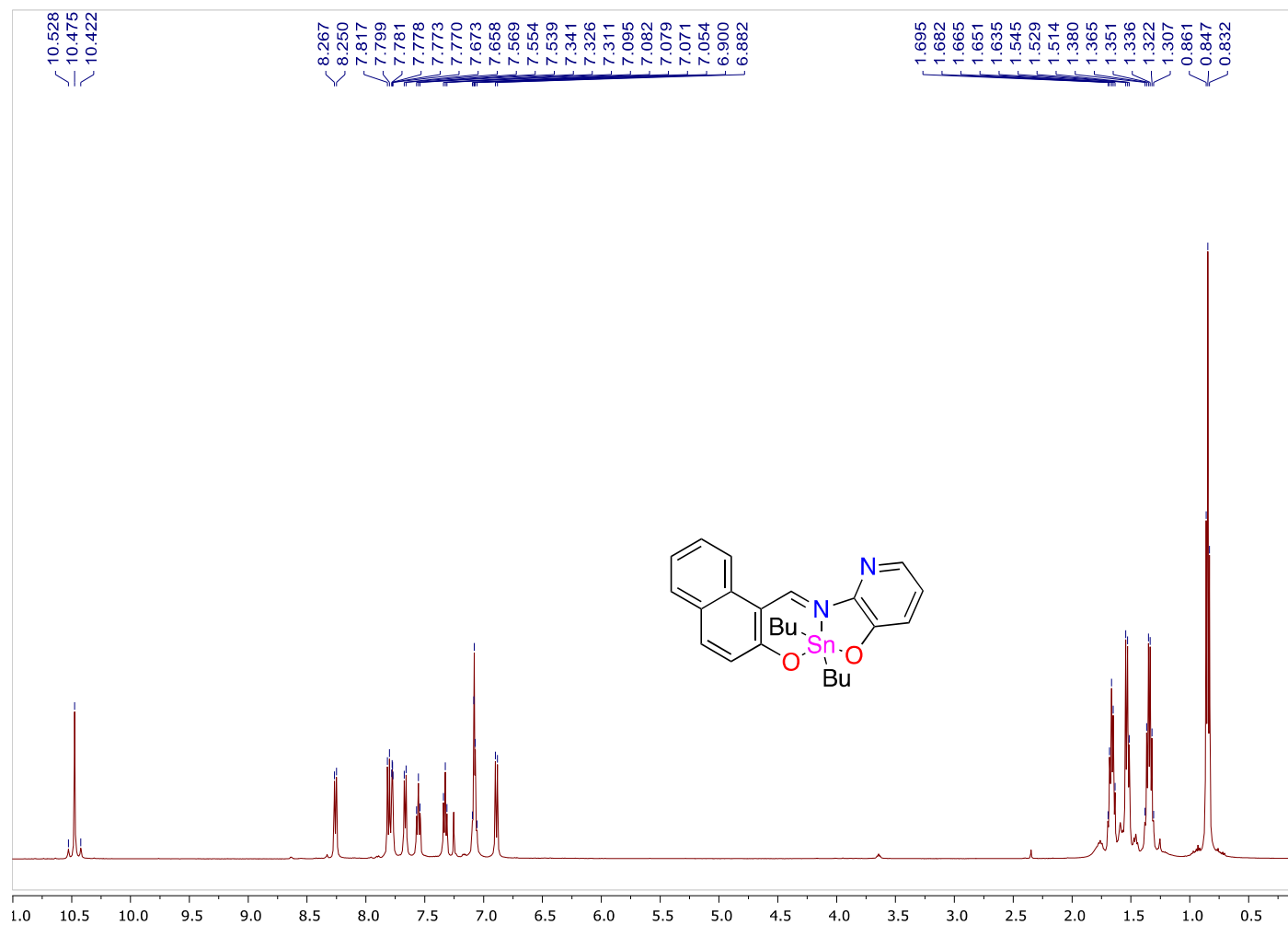


Figure S13.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz) of complex **1a**



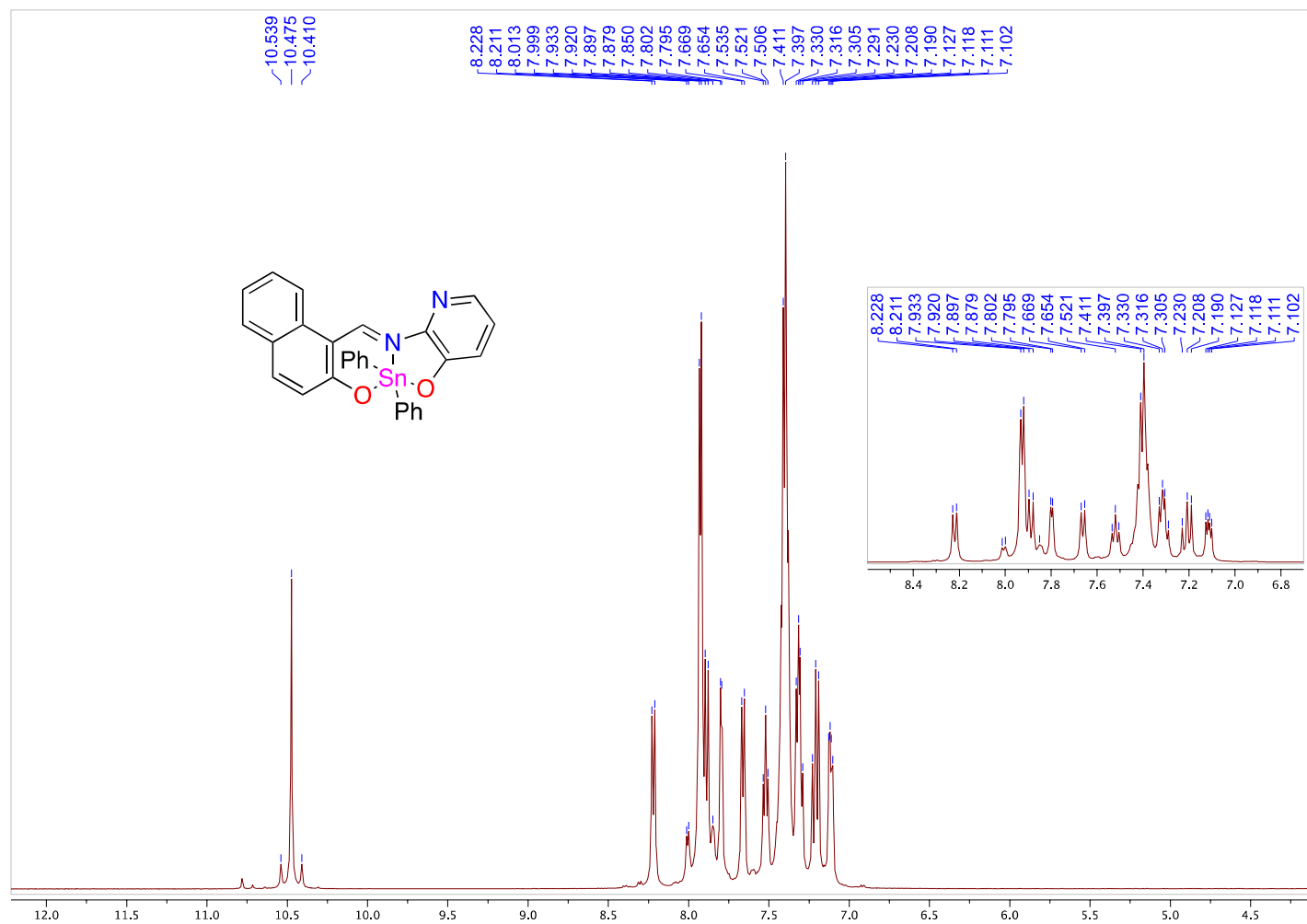


Fig. S15.  $^1\text{H}$  NMR (CDCl<sub>3</sub>, 500 MHz) of complex **1c**



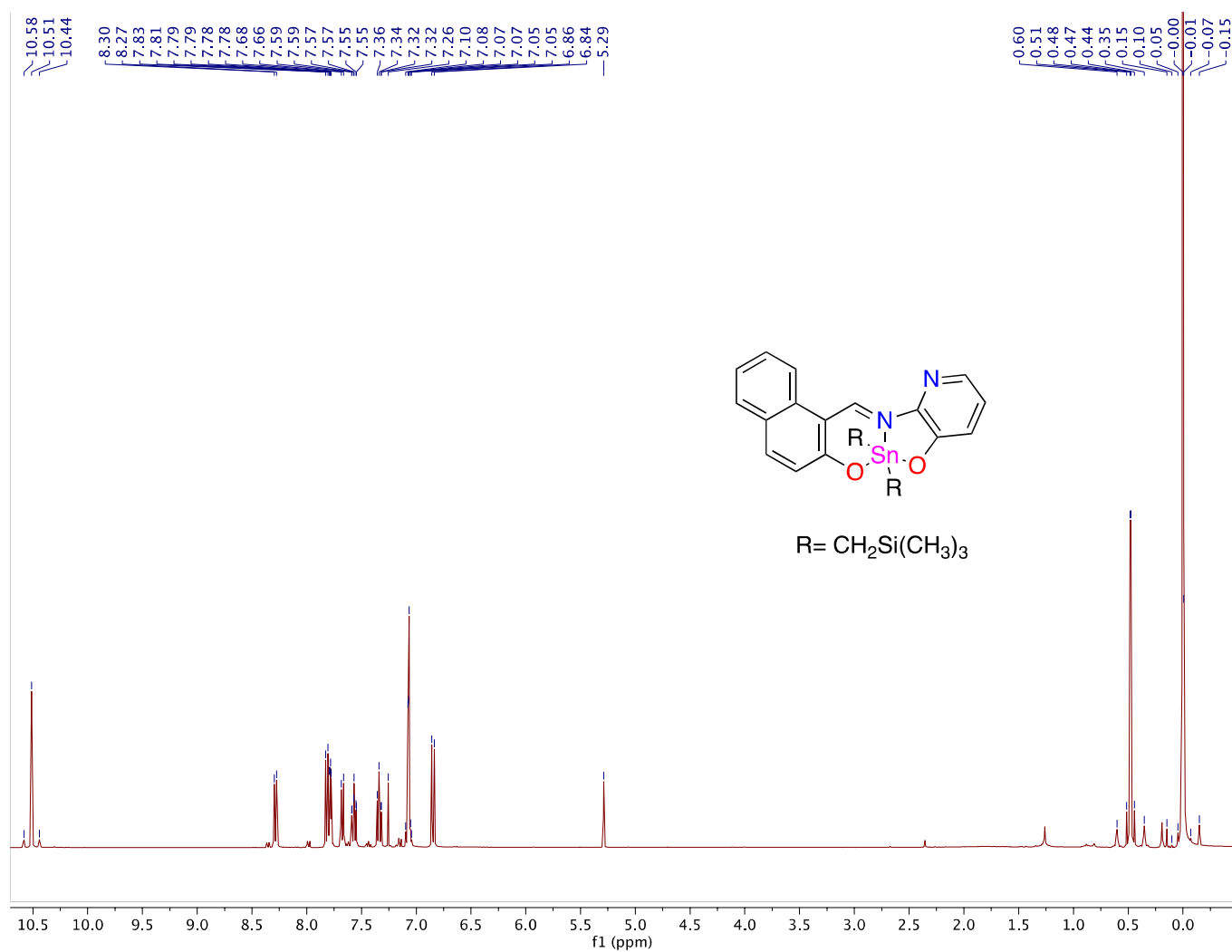


Figure S16.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) of complex **1d**

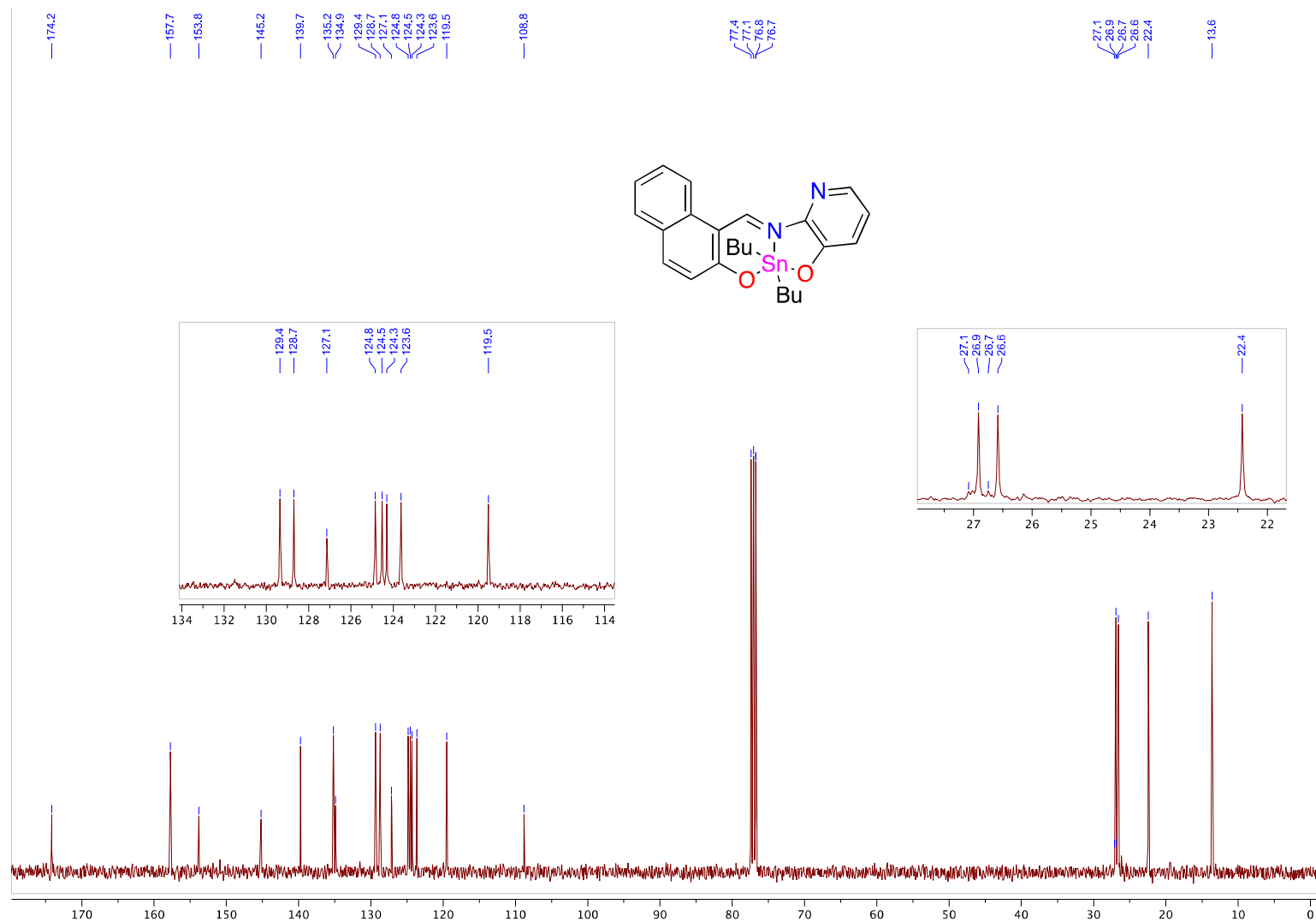


Figure S17. <sup>13</sup>CNMR (CDCl<sub>3</sub>, 100 MHz) of complex **1a**

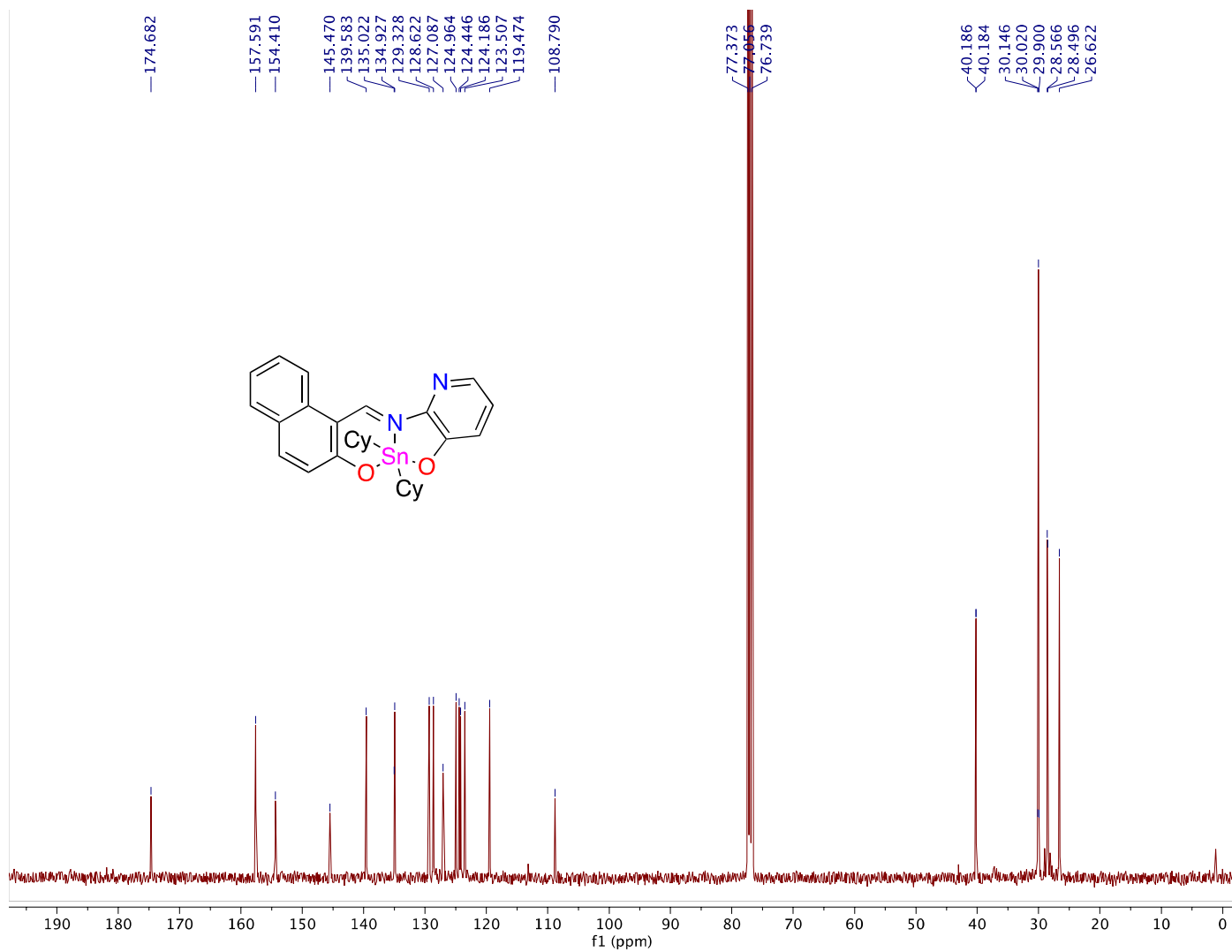


Figure S18.  $^{13}\text{C}$ NMR ( $\text{CDCl}_3$ , 100 MHz) of complex **1b**

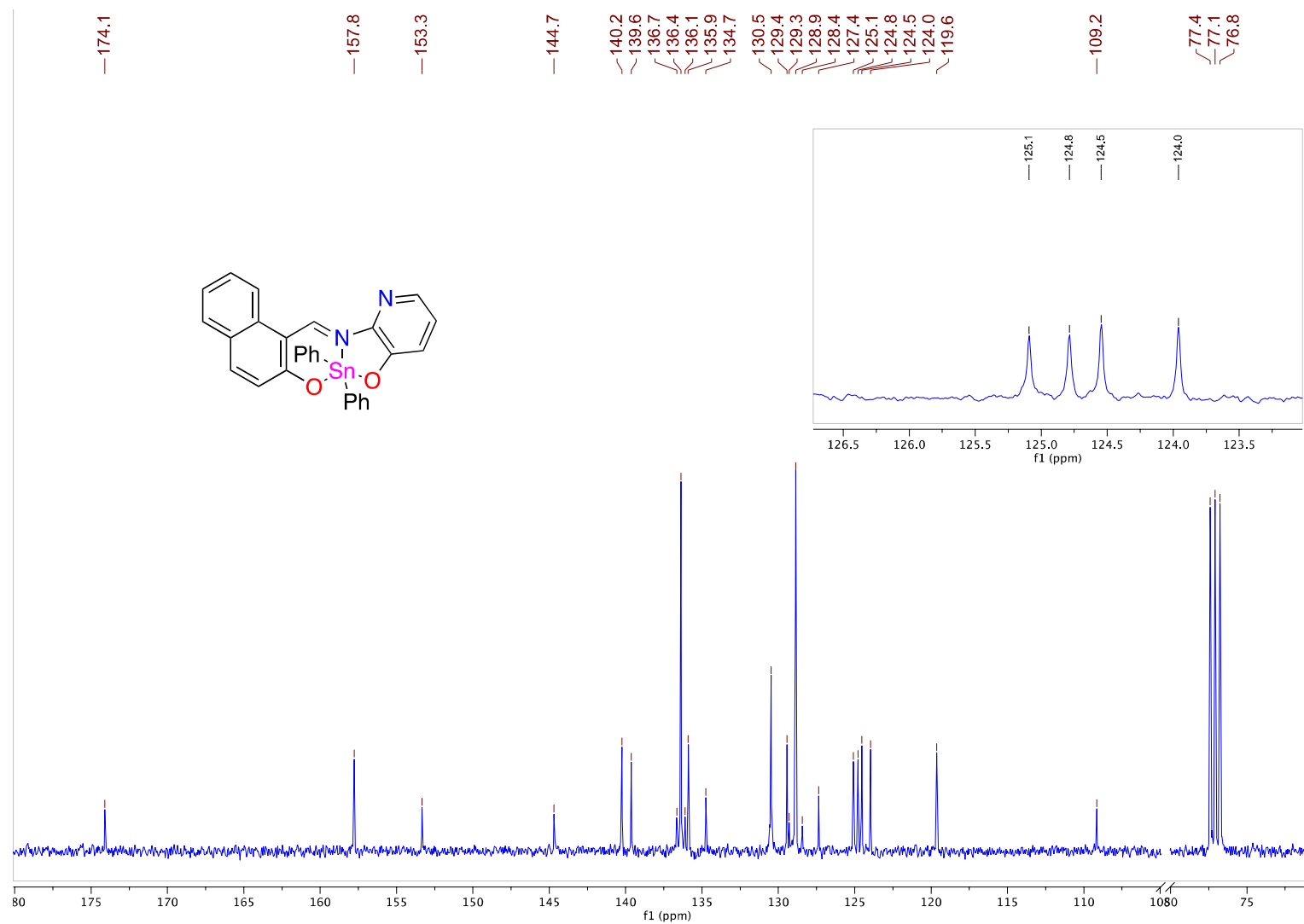


Figure S19. <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) complex **1c**

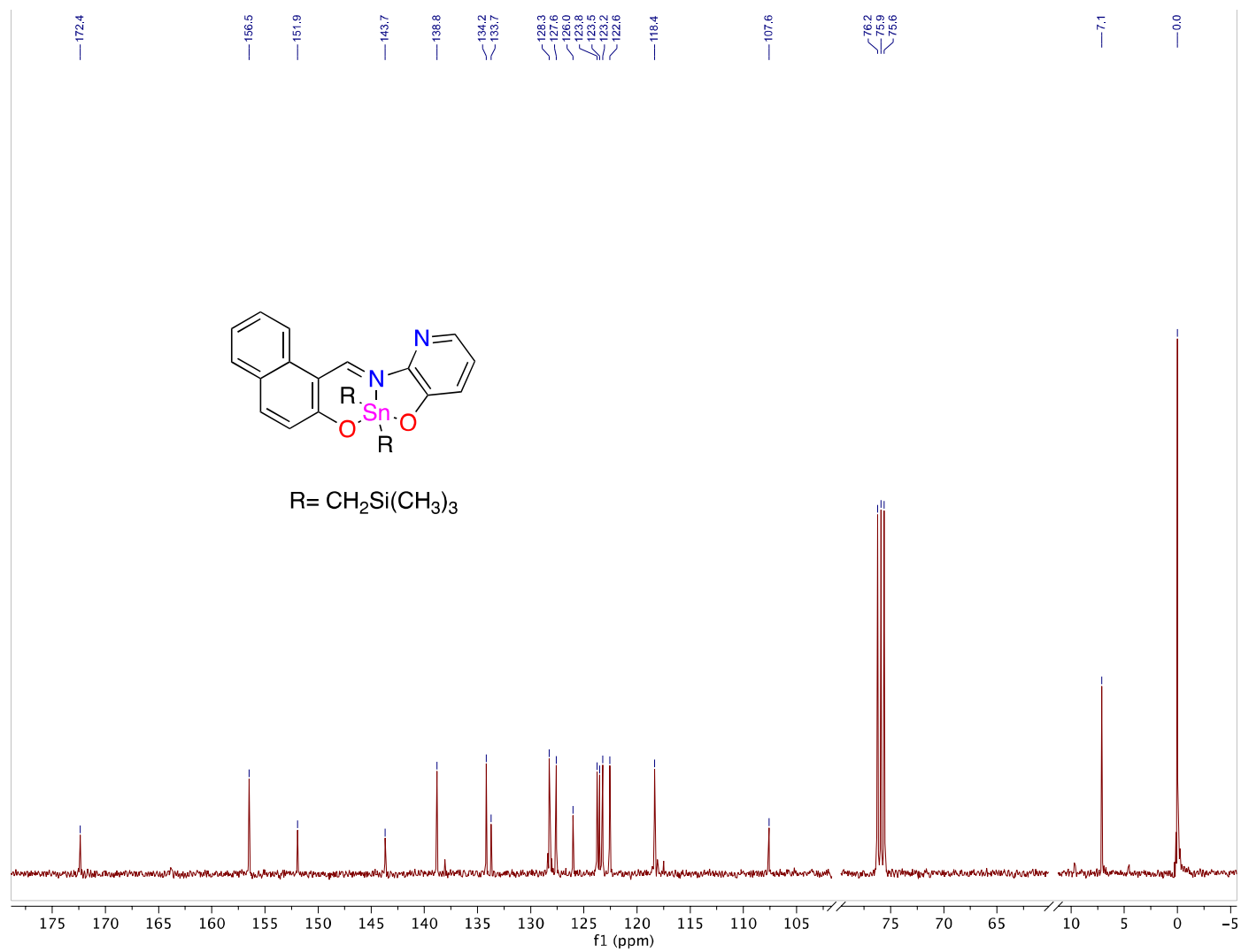


Figure S20.  $^{13}\text{C}$  NMR (CDCl<sub>3</sub>, 100 MHz) of complex **1d**

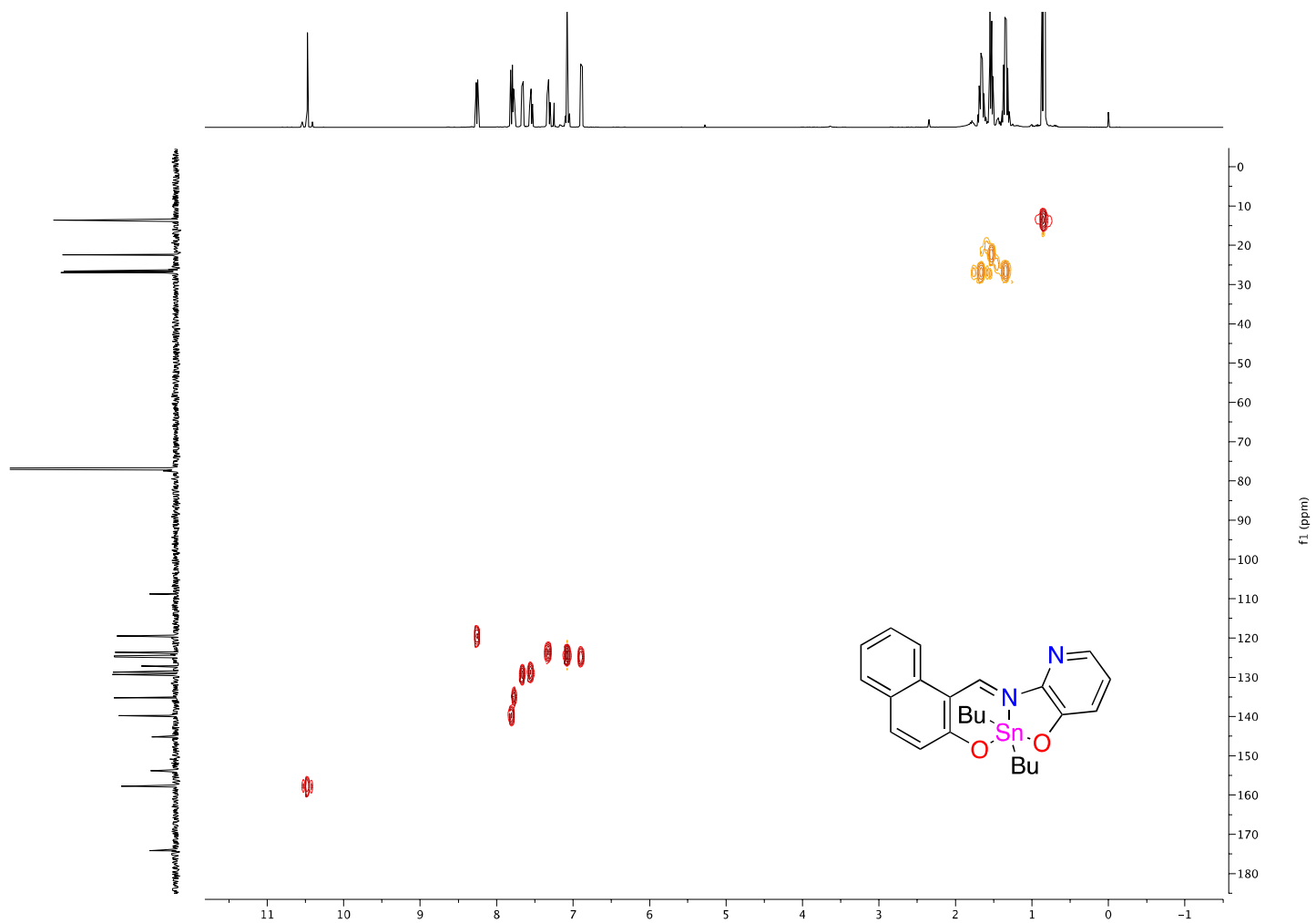


Figure S21. HSQC (CDCl<sub>3</sub>) of complex **1a**

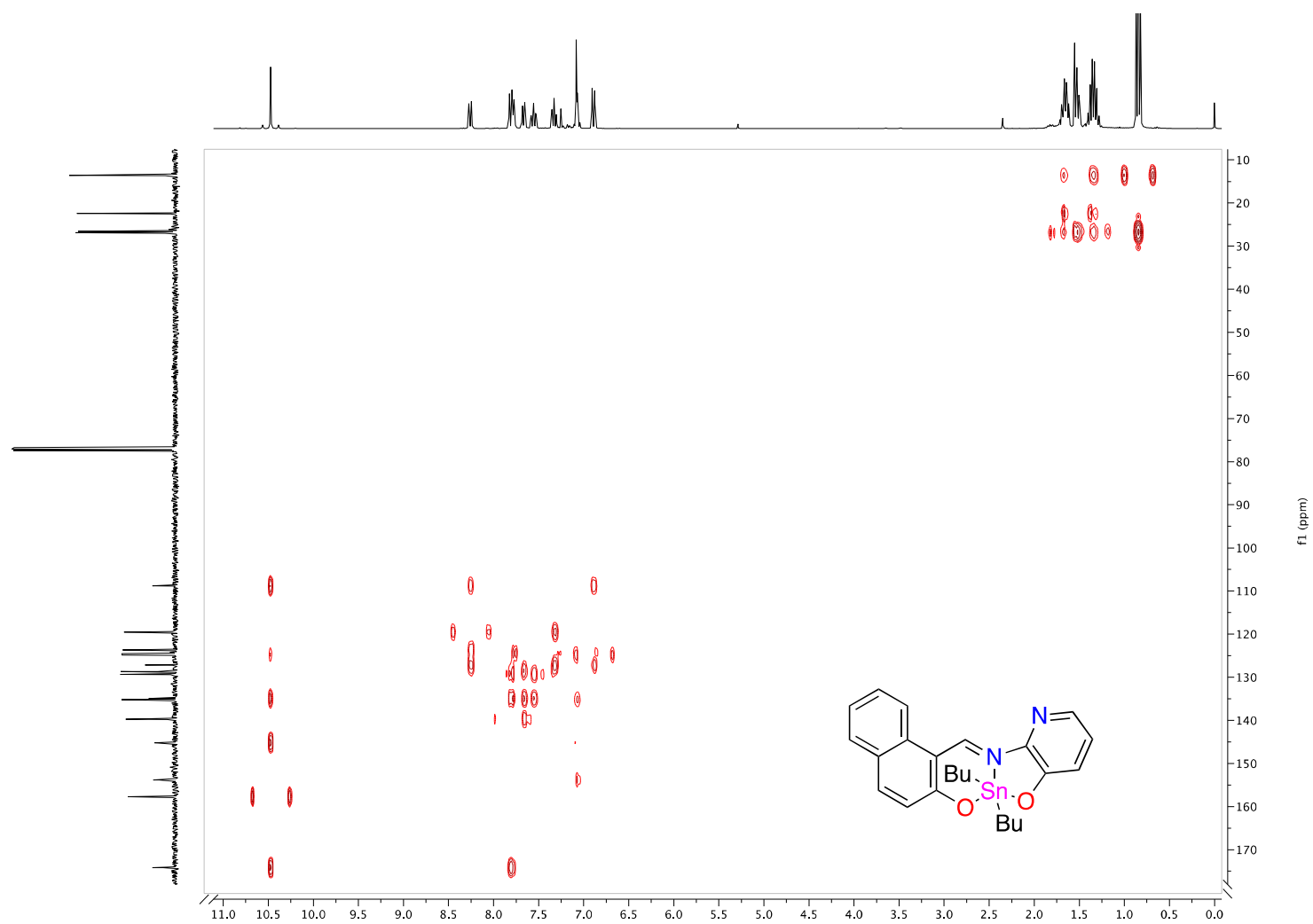


Figure S22. HMBC (CDCl<sub>3</sub>) of complex **1a**

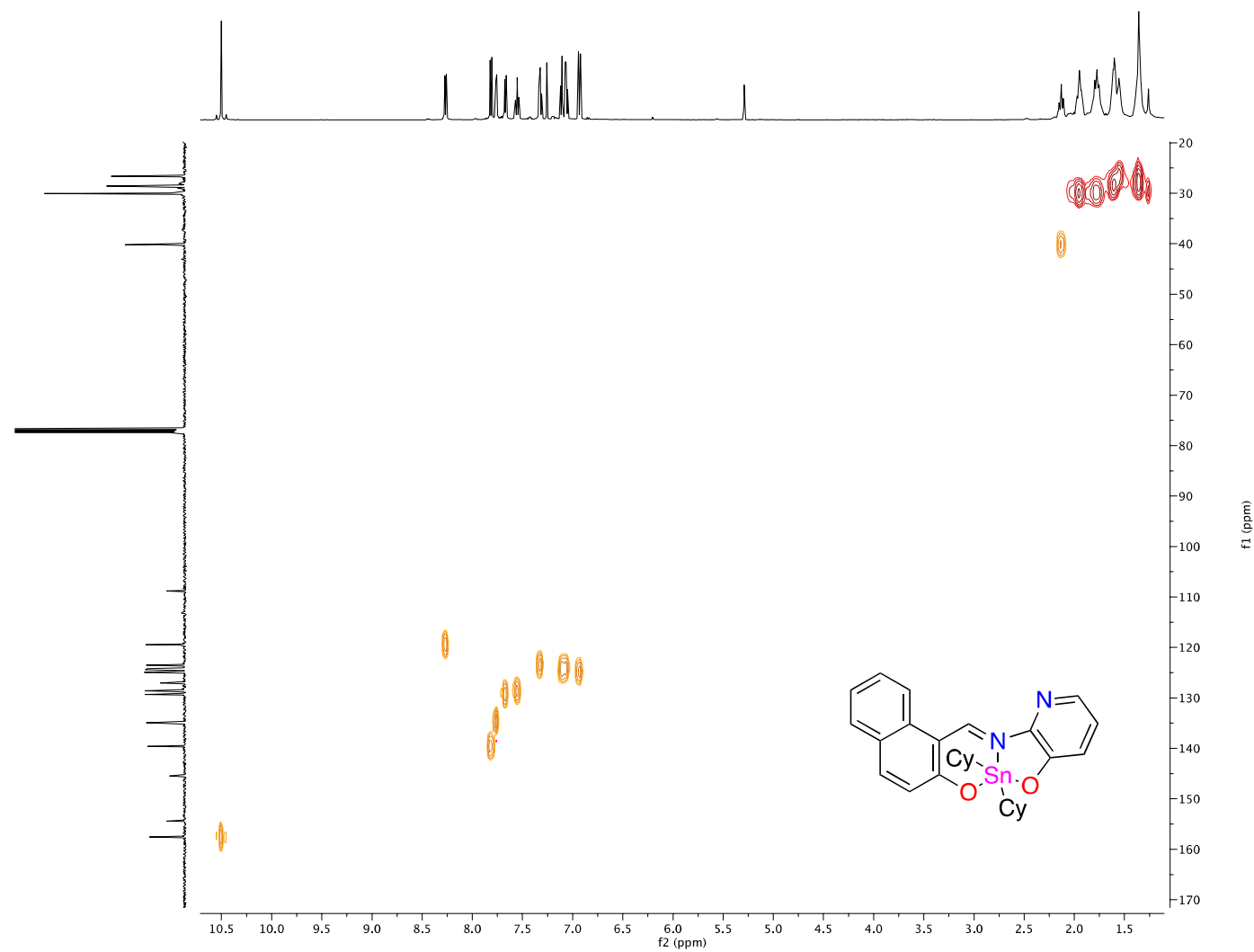


Figure S23. HSQC (CDCl<sub>3</sub>) of complex **1b**



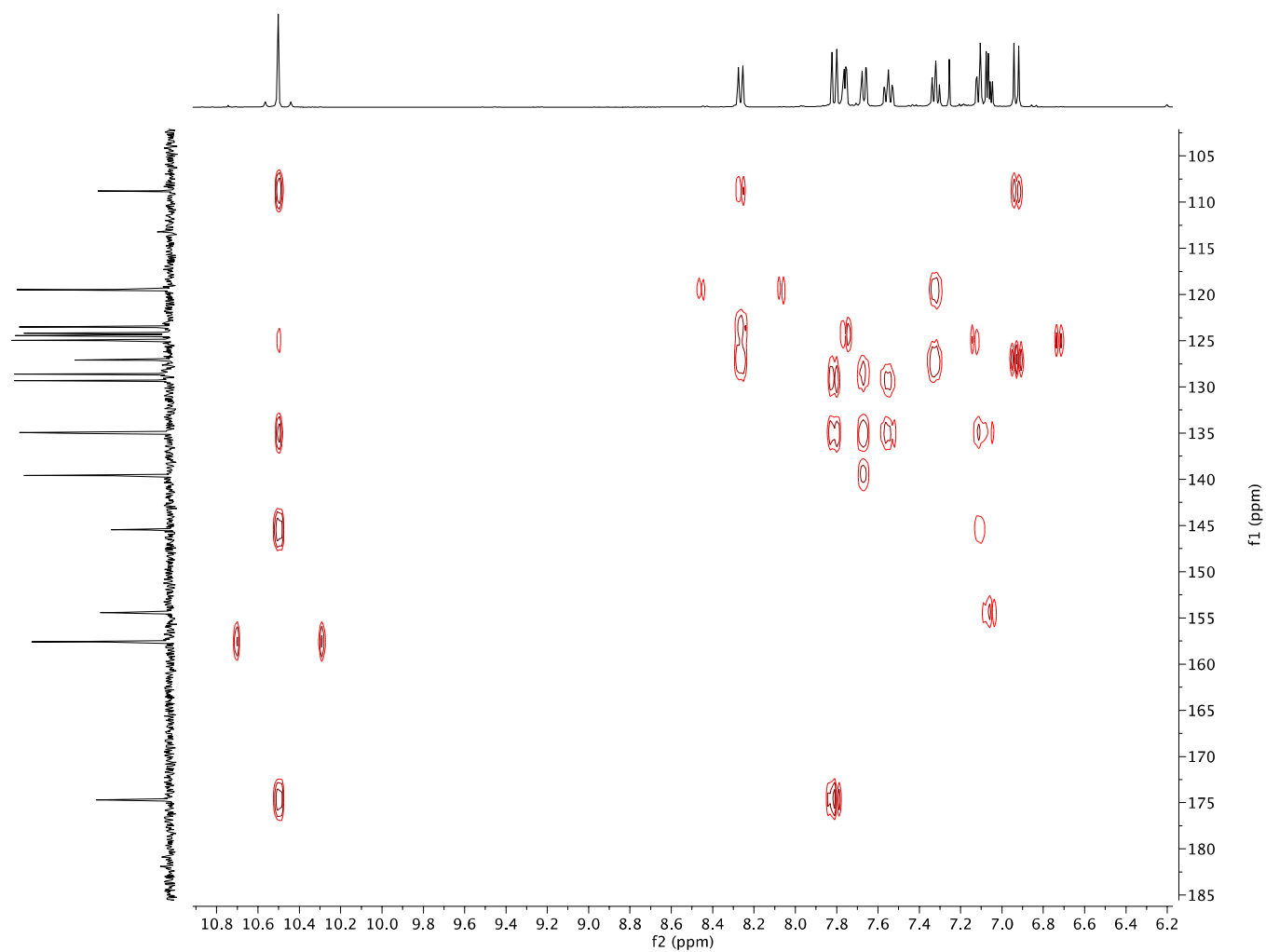


Figure S24. HMBC (CDCl<sub>3</sub>) of complex **1b**

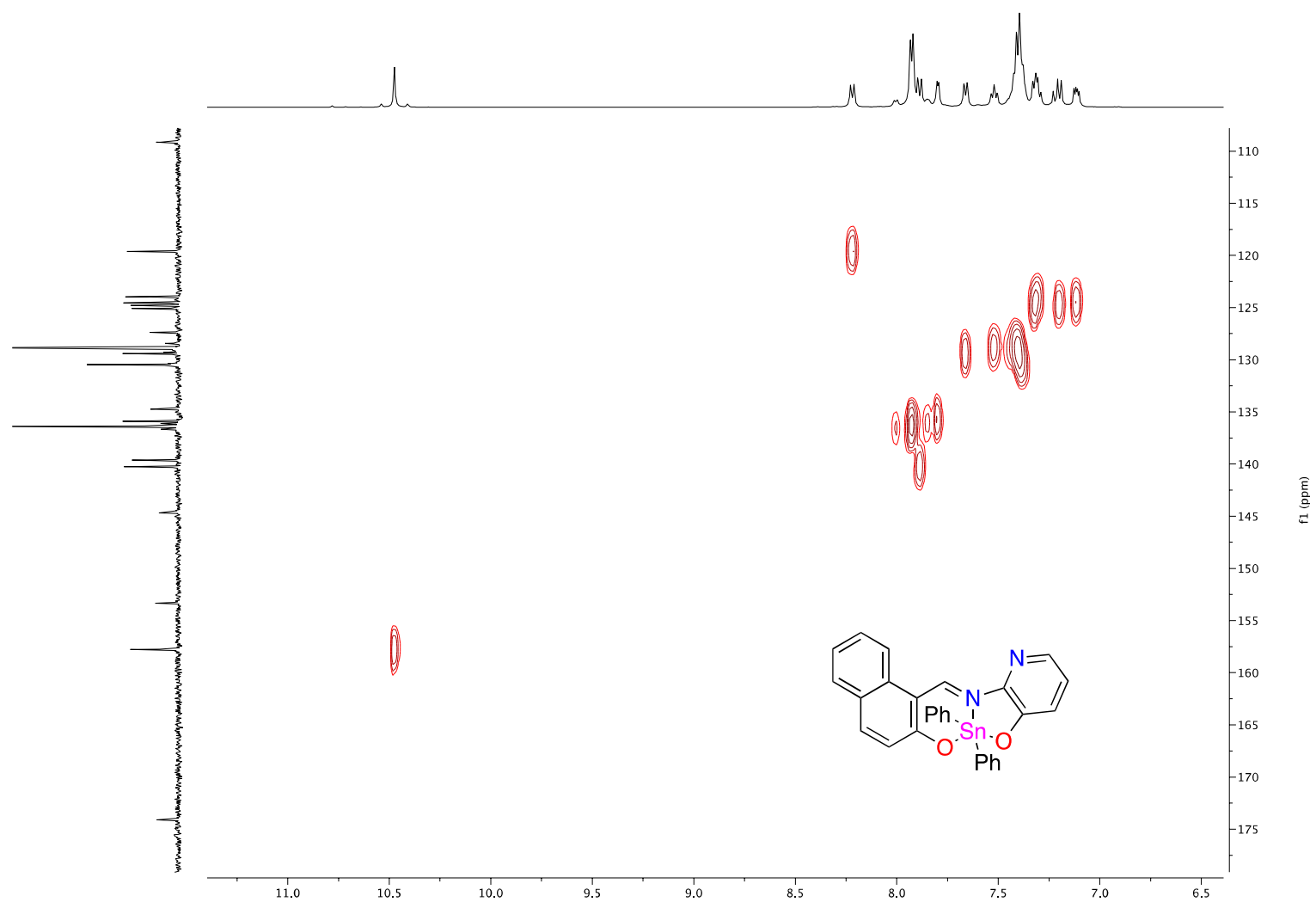


Figure S25. HSQC (CDCl<sub>3</sub>) of compound **1c**

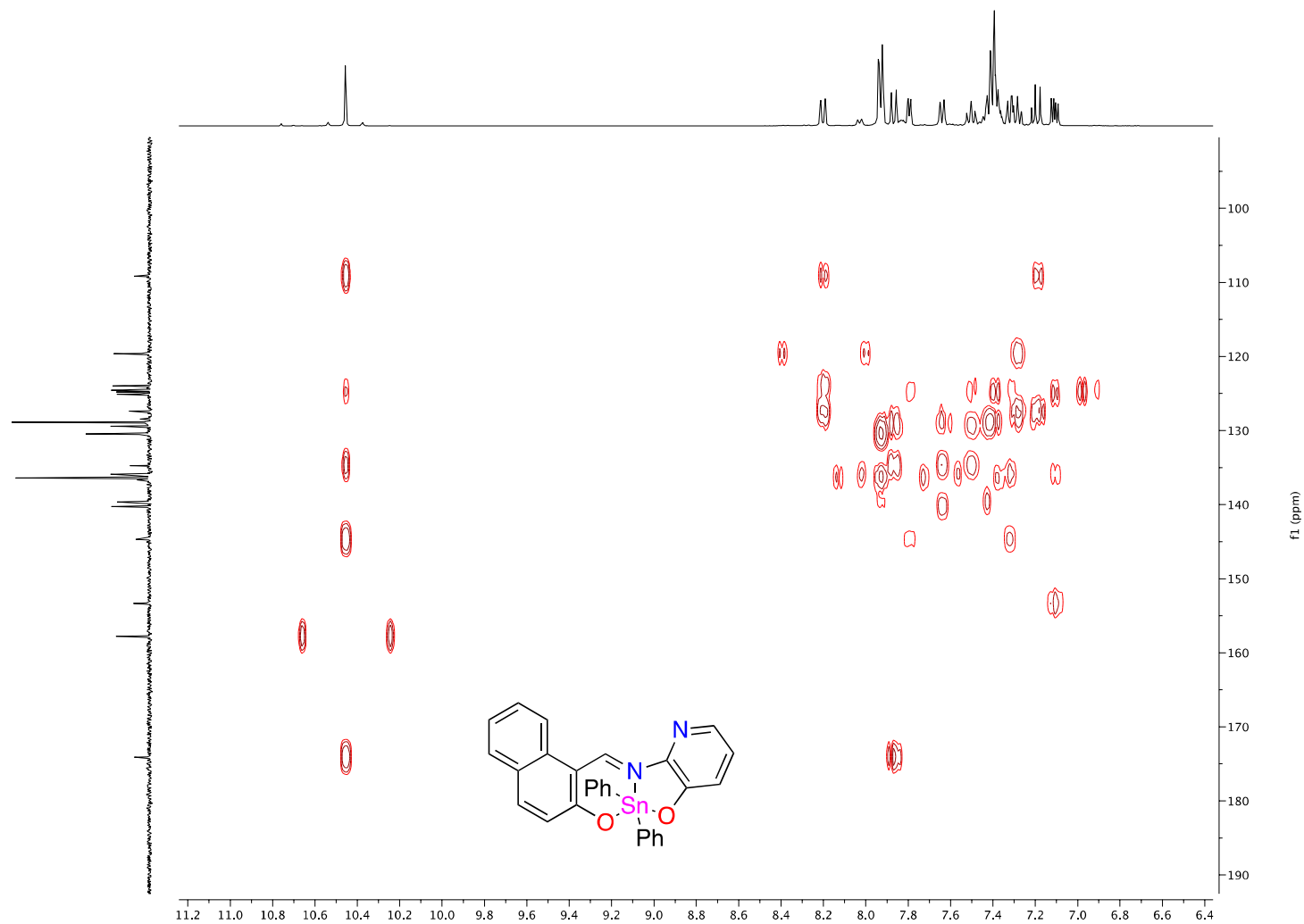


Figure S26. HMBC (CDCl<sub>3</sub>) of compound **1c**

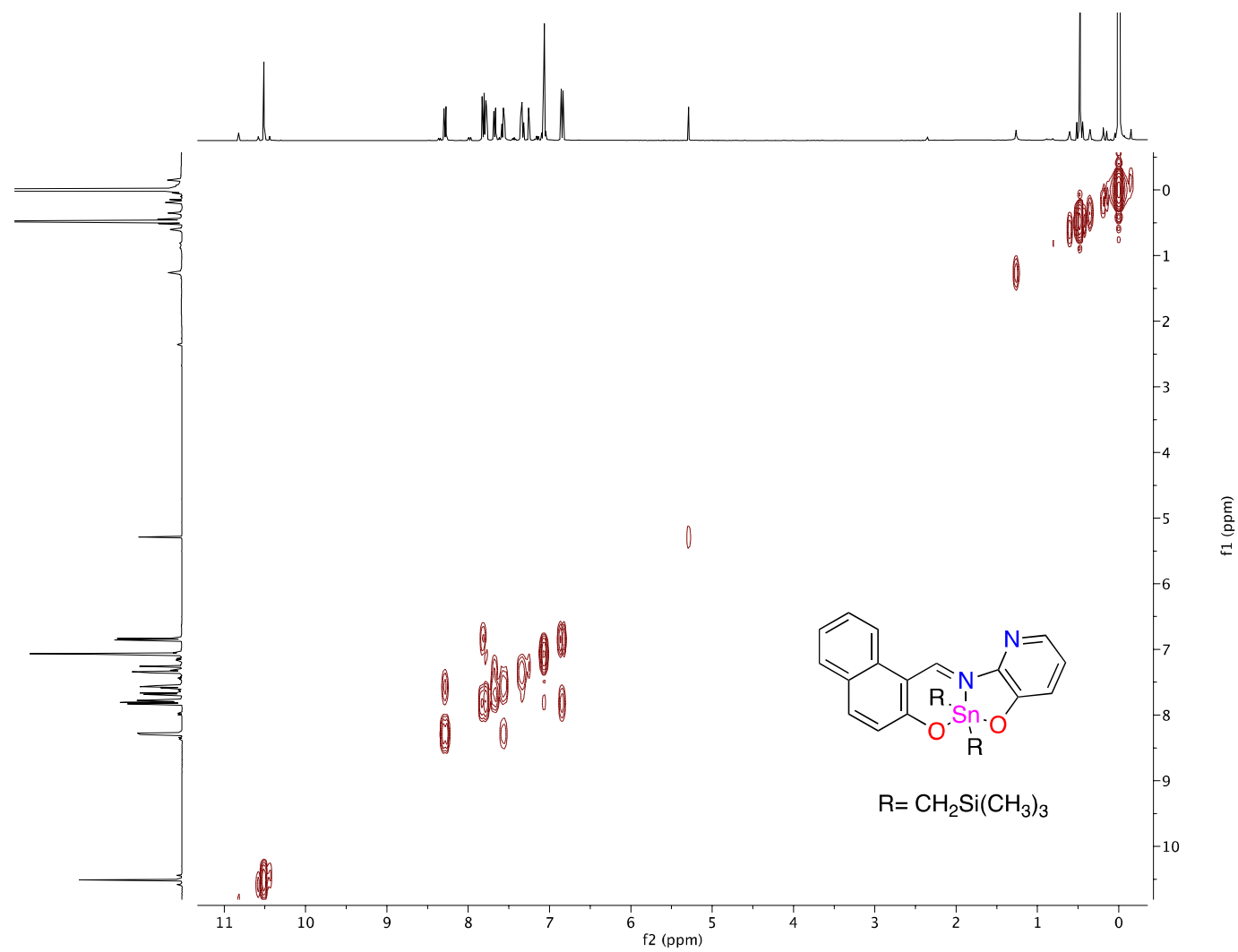


Figure S27. HSQC ( $\text{CDCl}_3$ ) of complex **1d**

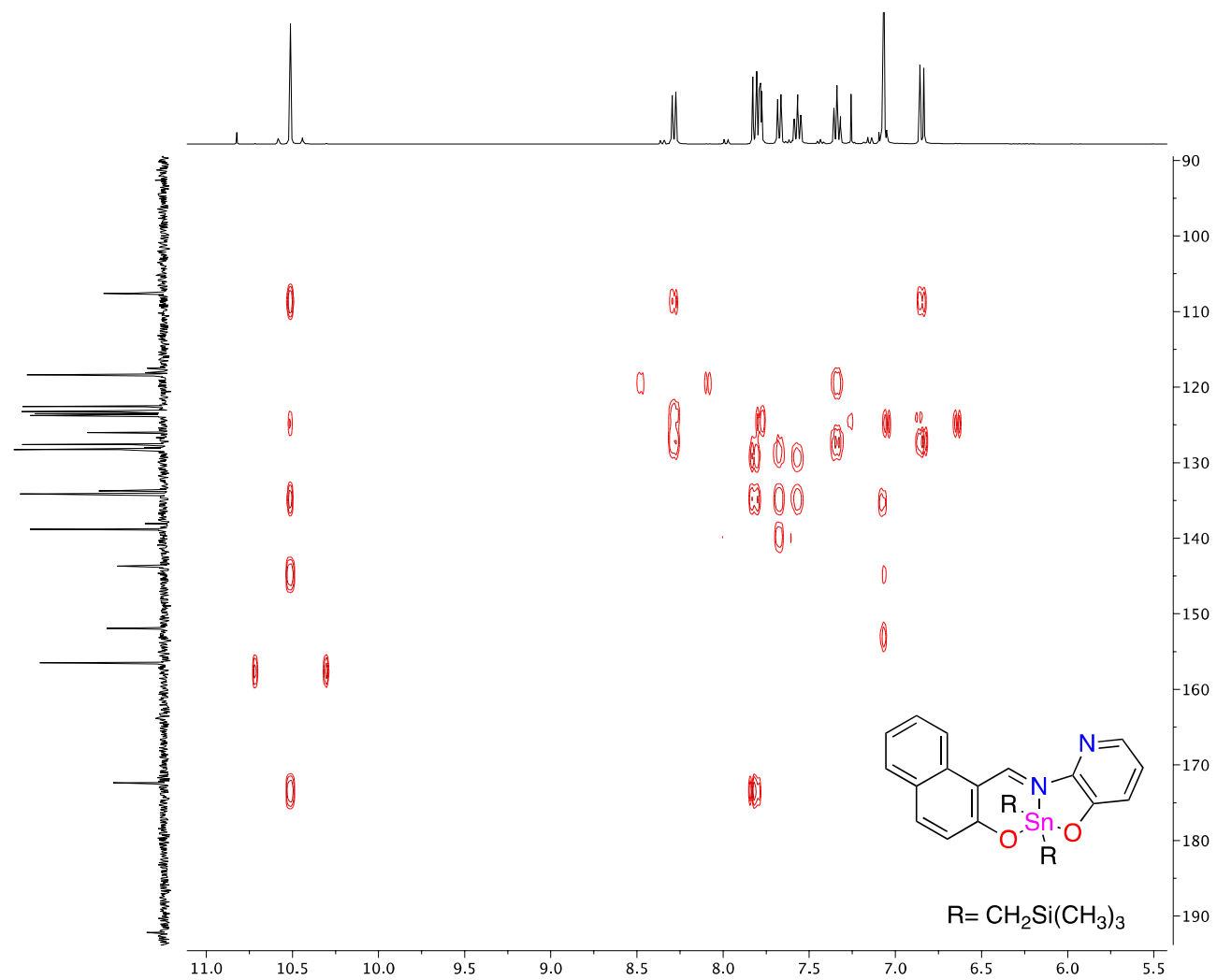


Figure S28. HMBC ( $\text{CDCl}_3$ ) of complex **1d**

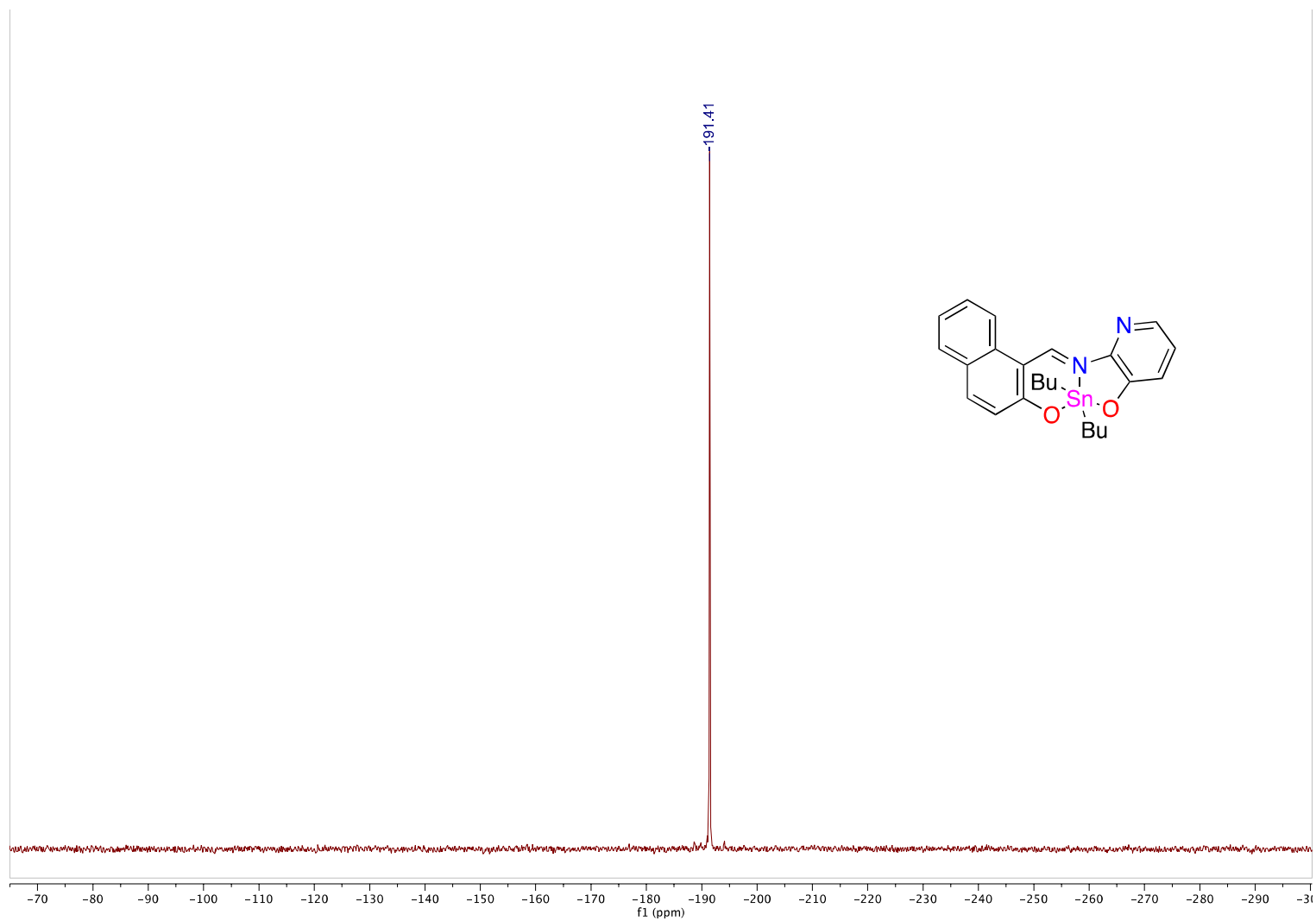


Figure S29.  $^{119}\text{Sn}$  NMR ( $\text{CDCl}_3$ , 112 MHz) of complex **1a**

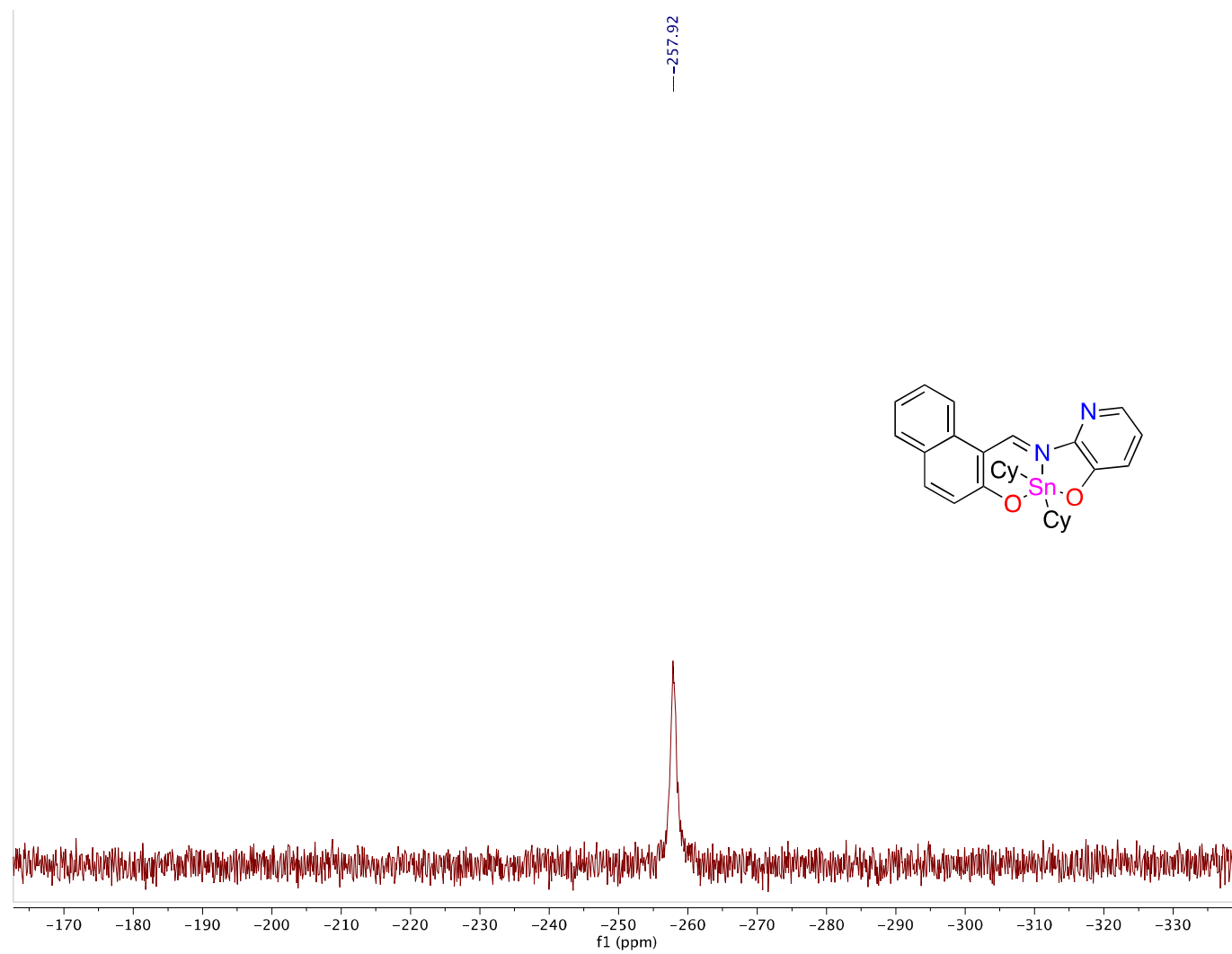


Figure S30.  $^{119}\text{Sn}$  NMR ( $\text{CDCl}_3$ , 112 MHz) of complex **1b**

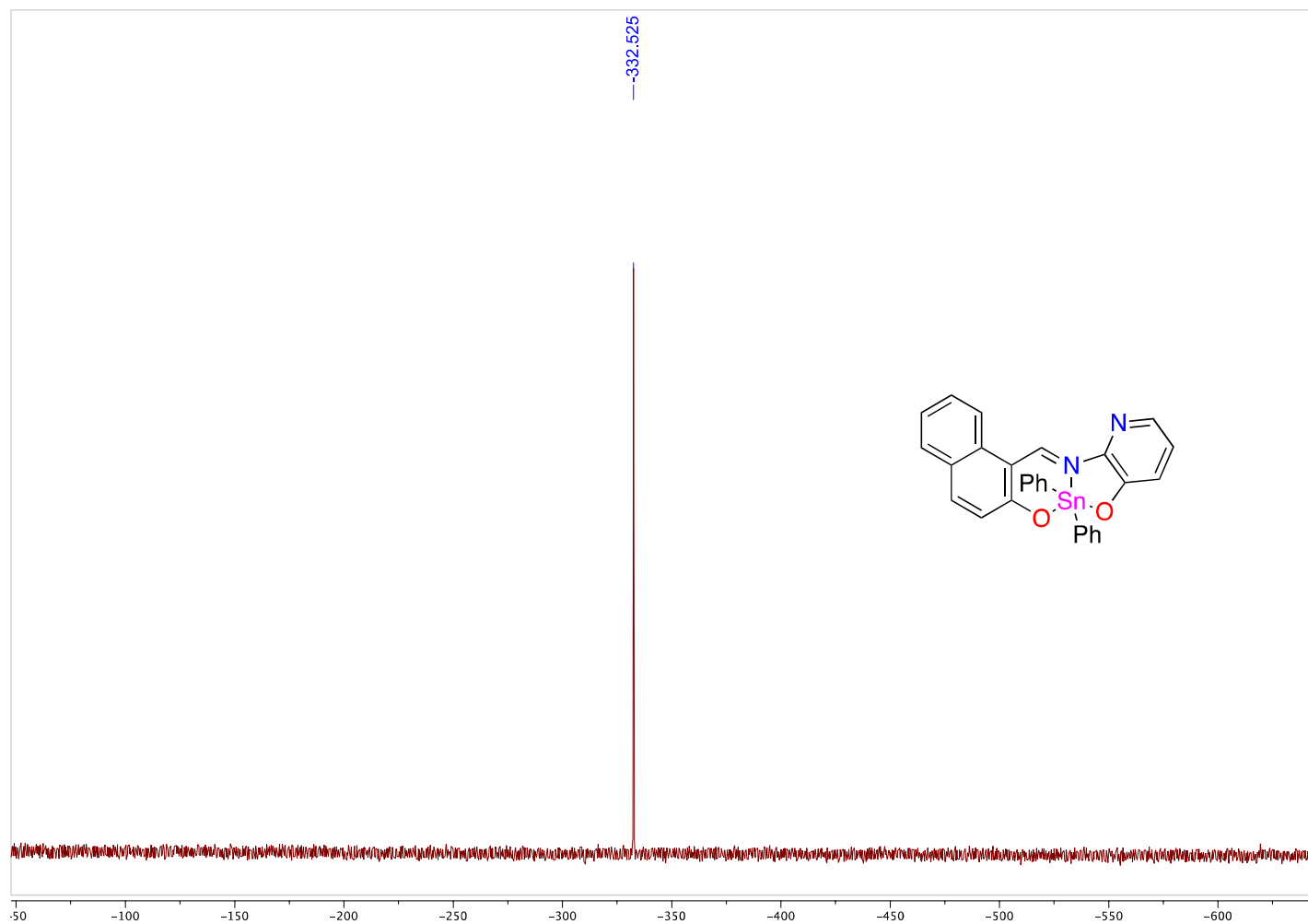


Figure S31.  $^{119}\text{Sn}$  NMR ( $\text{CDCl}_3$ , 112 MHz) of complex **1c**



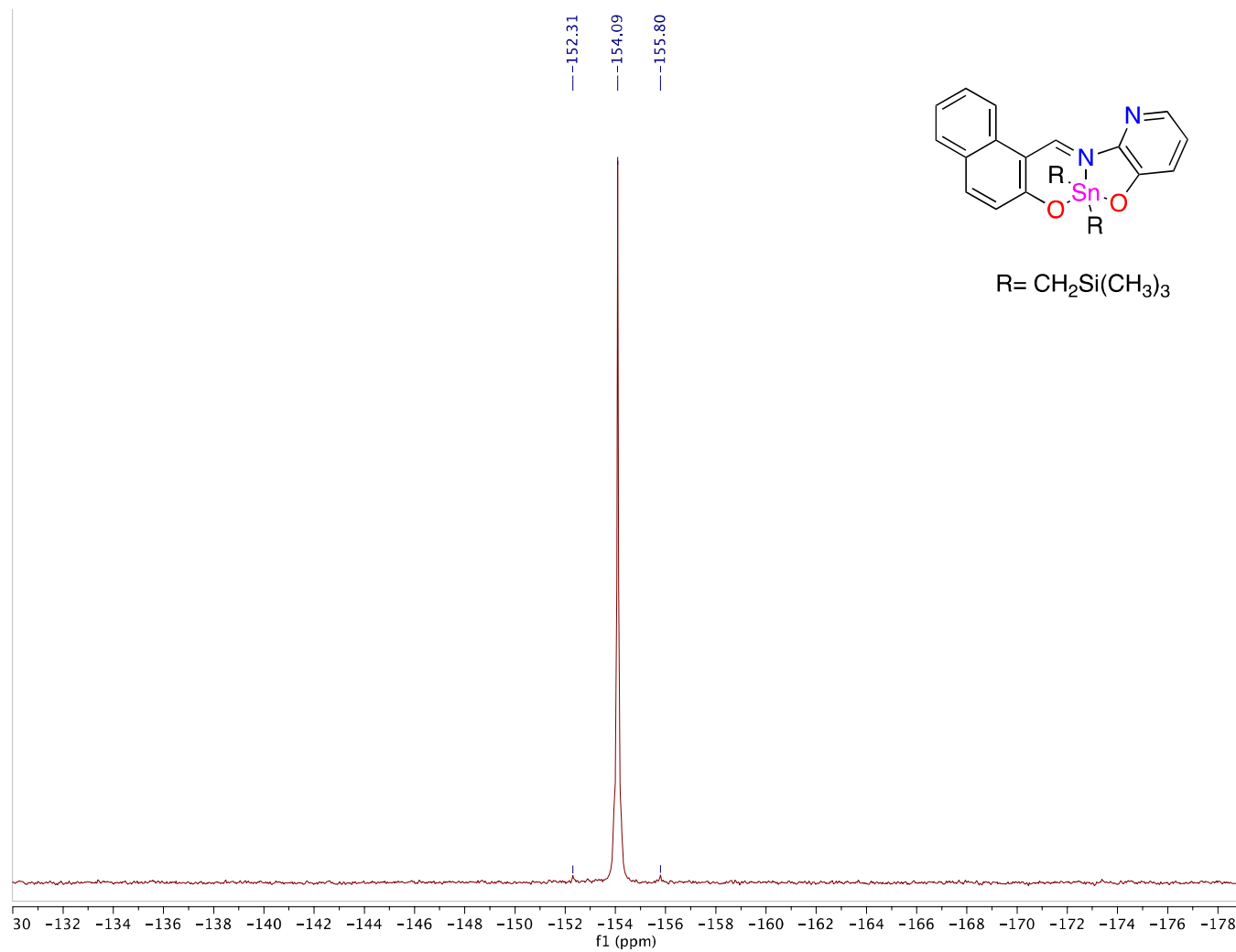


Figure S32.  $^{119}\text{Sn}$  NMR ( $\text{CDCl}_3$ , 112 MHz) of complex **1d**