

Design of Promising Heptacoordinated Organotin (IV) Complexes-PEDOT: PSS-Based Composite for New-Generation Optoelectronic Devices Applications

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Table S1. Characteristic IR stretching frequencies of carboxylate group.

Compound	$\nu_{\text{asym}}(\text{COO})$	$\nu_{\text{sym}}(\text{COO})$	$\Delta\nu (\text{COO})$
1a	1637	1351	286
1b	1639	1347	292
1c	1639	1348	291
1d	1643	1355	288

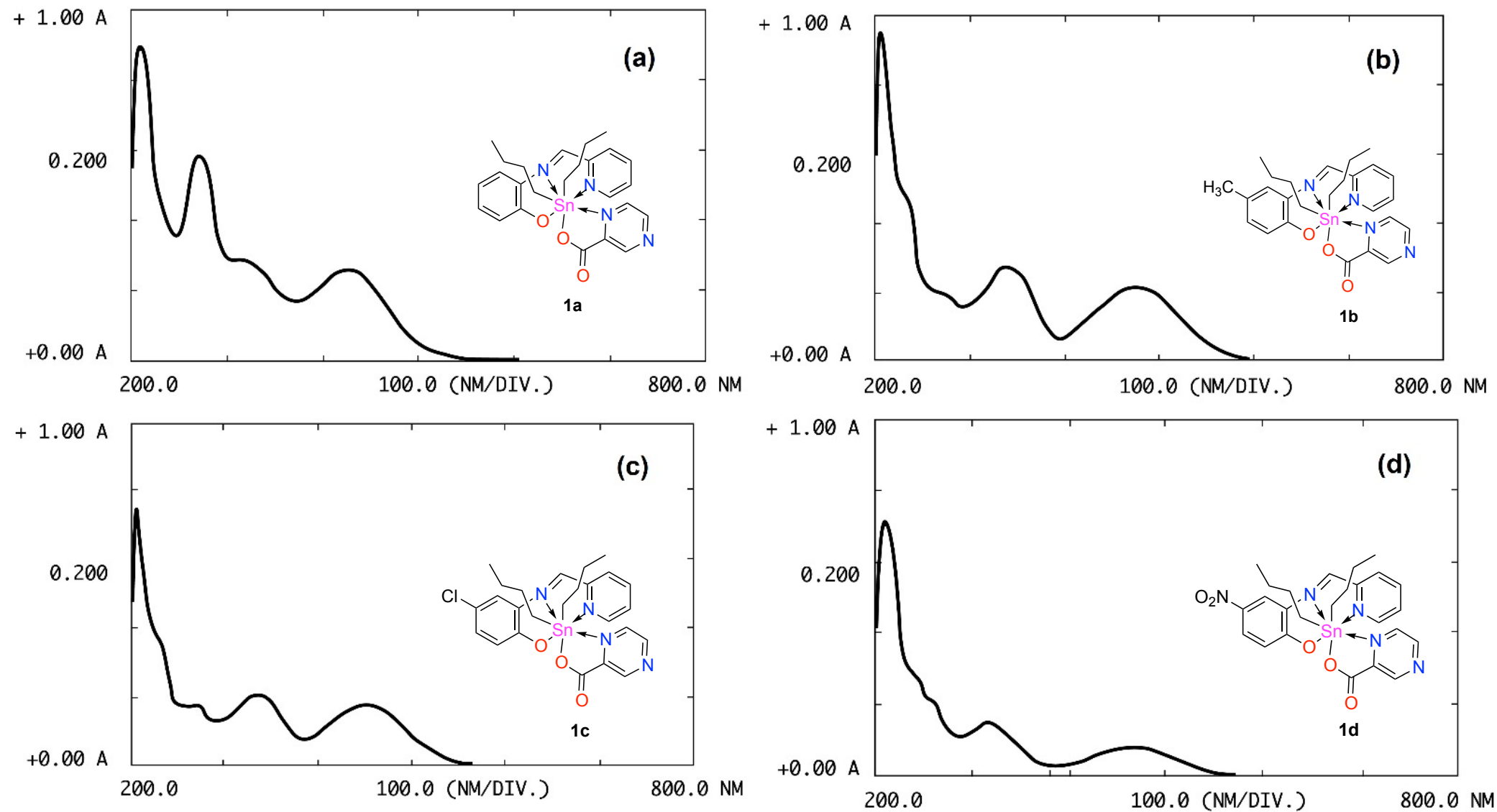


Figure S1. UV-vis absorbance in methanol of **1a-1c**.

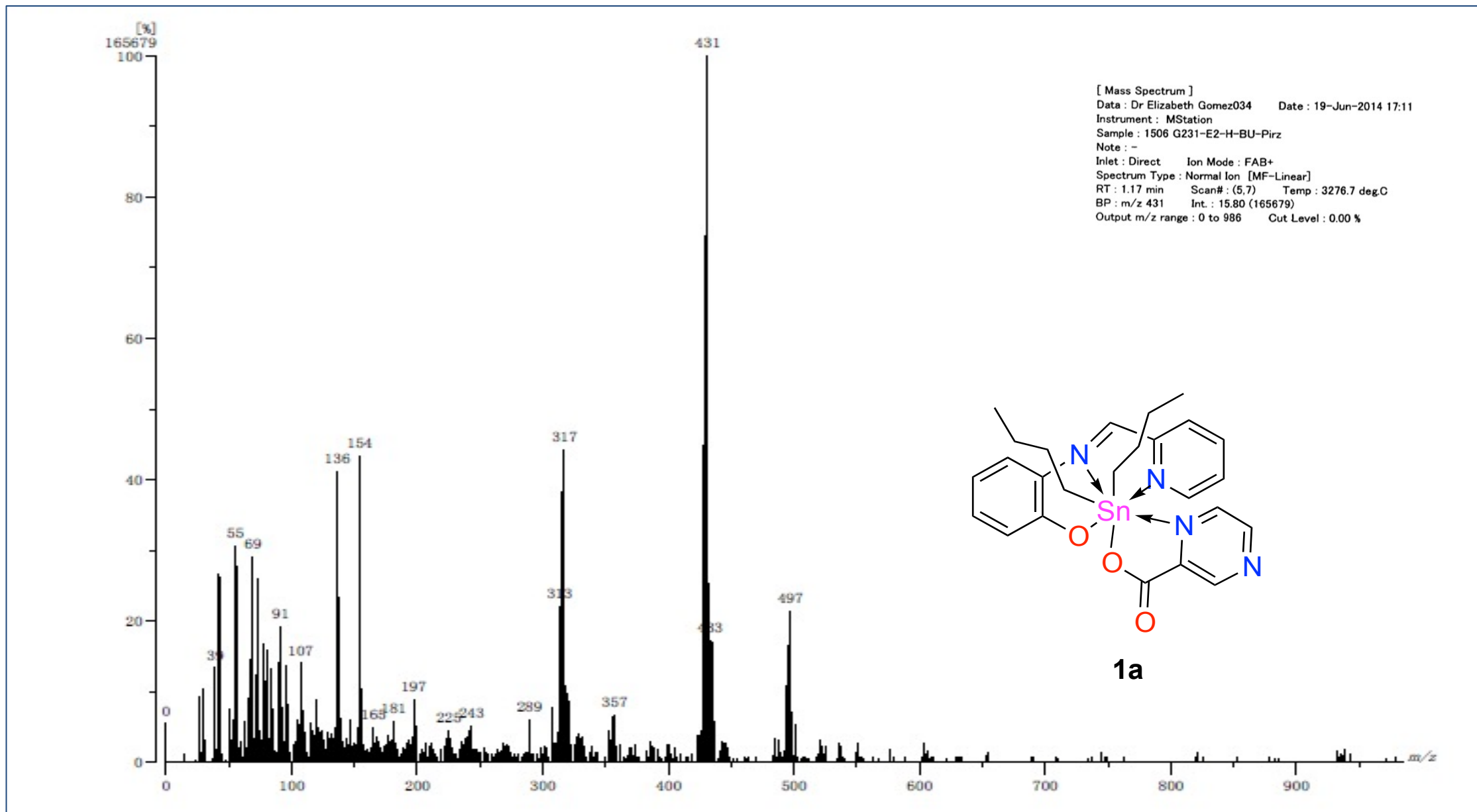


Figure S2. Mass spectrum FAB⁺ of 1a.

[Mass Spectrum]
Data : Dr Elizabeth Gomez039 Date : 19-Jun-2014 17:32
Instrument : MStation
Sample : 1507 G233-E3-Me-Bu-Pirz
Note : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.29 min Scan# : (2.6) Temp : 3276.7 deg.C
BP : m/z 154 Int. : 27.18 (285006)
Output m/z range : 0 to 738 Cut Level : 0.00 %

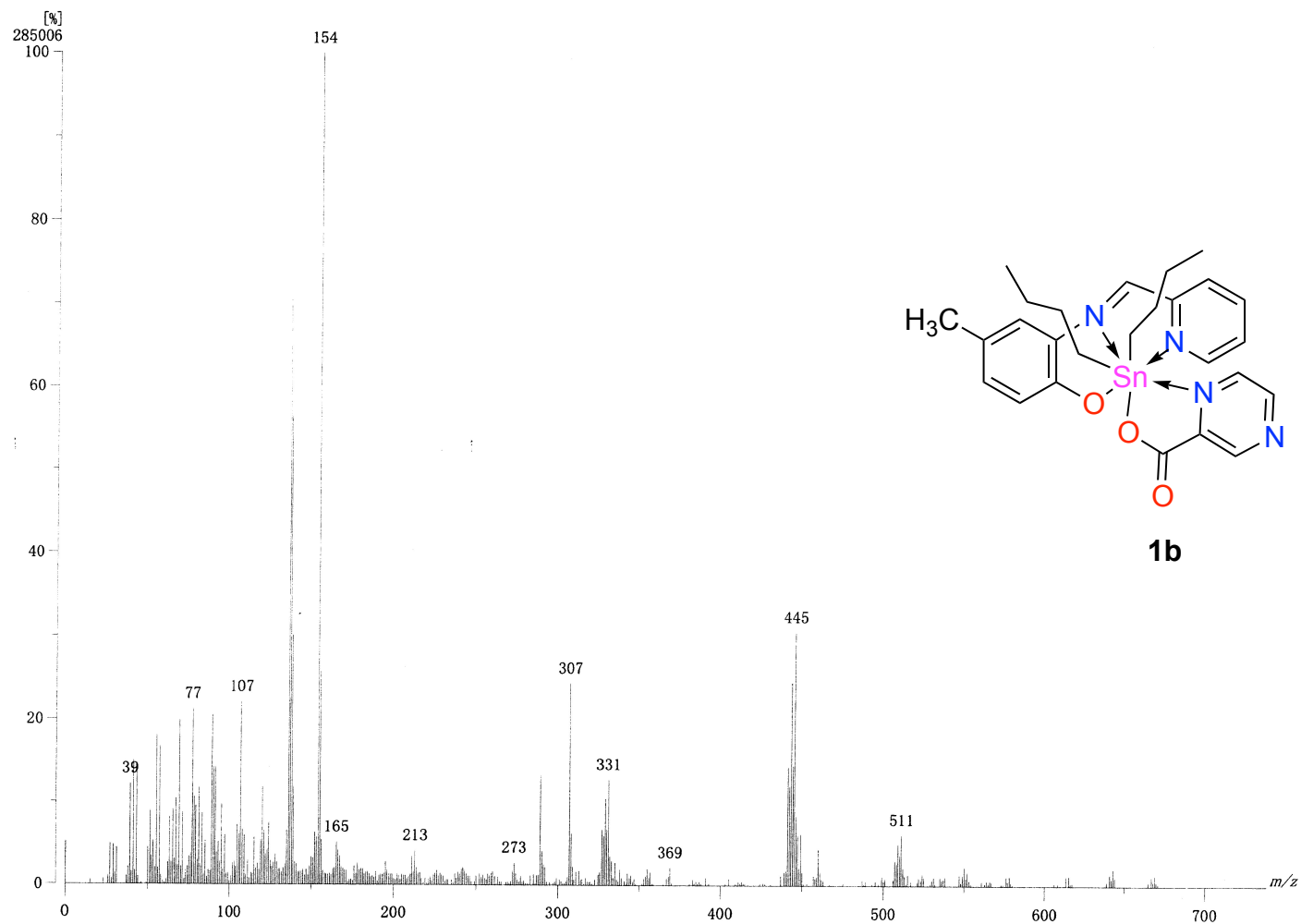


Figure S3. Mass spectrum FAB⁺ of **1b**.

[Mass Spectrum]
Data : Dr Elizabeth Gomez041 Date : 19-Jun-2014 17:41
Instrument : MStation
Sample : 1509 G235-E5-Cl-Bu-Pirz
Note : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.88 min Scan# : (4,17) Temp : 3276.7 deg.C
BP : m/z 154 Int. : 39.40 (413111)
Output m/z range : 0 to 698 Cut Level : 0.00 %

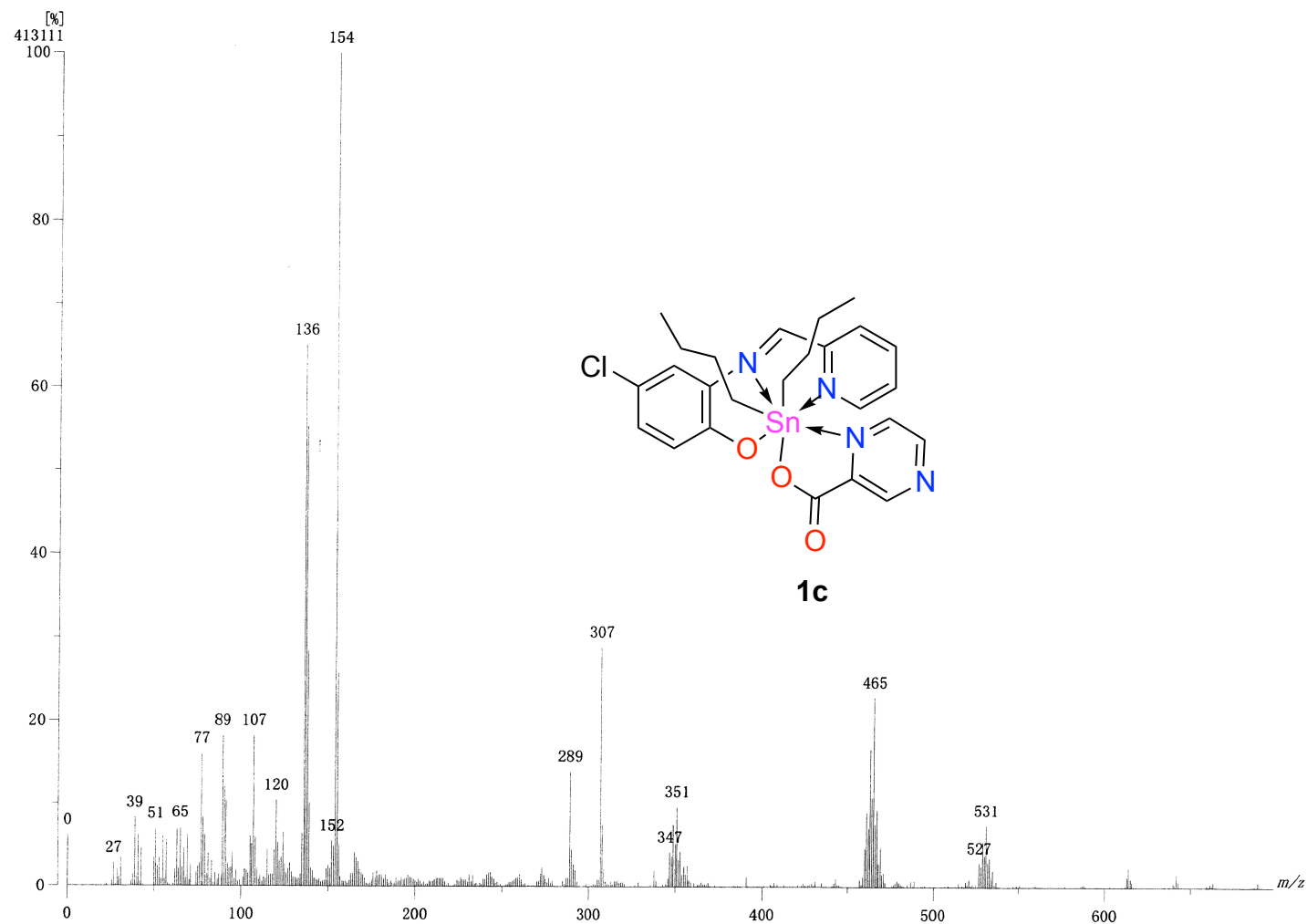


Figure S4. Mass spectrum FAB⁺ of **1c**.

[Mass Spectrum]
Data : Dr Elizabeth Gomez040 Date : 19-Jun-2014 17:35
Instrument : MStation
Sample : 1508 G234-E4-NO2-Bu-Pirz
Note : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.29 min Scan# : (2,10) Temp : 3276.7 deg.C
BP : m/z 154 Int. : 17.35 (181913)
Output m/z range : 0 to 684 Cut Level : 0.00 %

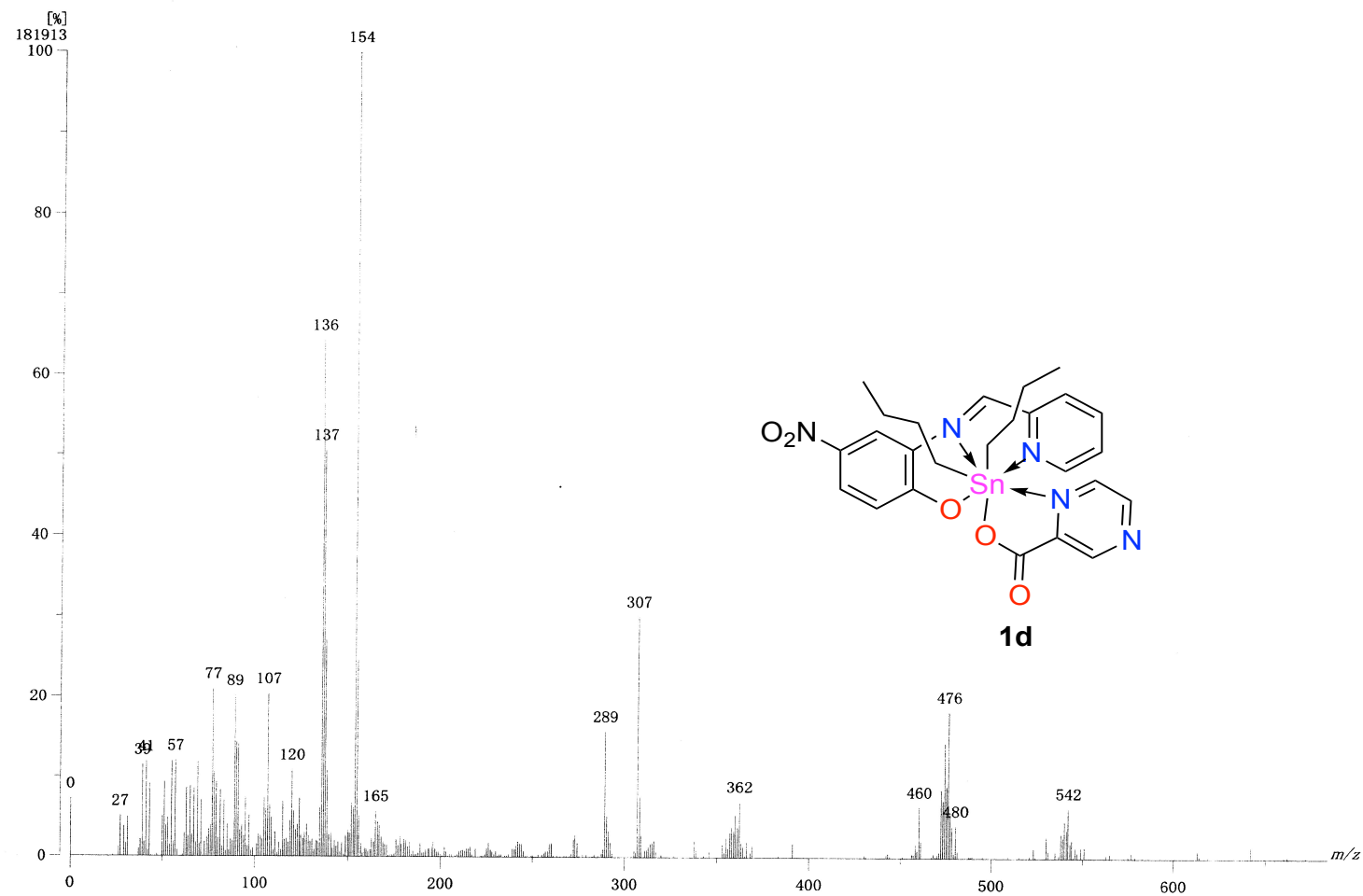


Figure S5. Mass spectrum FAB⁺ of 1d.

G231-E2-H-Bu-Pirz
COSY

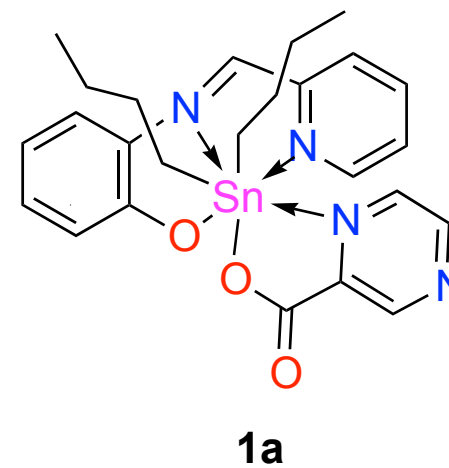
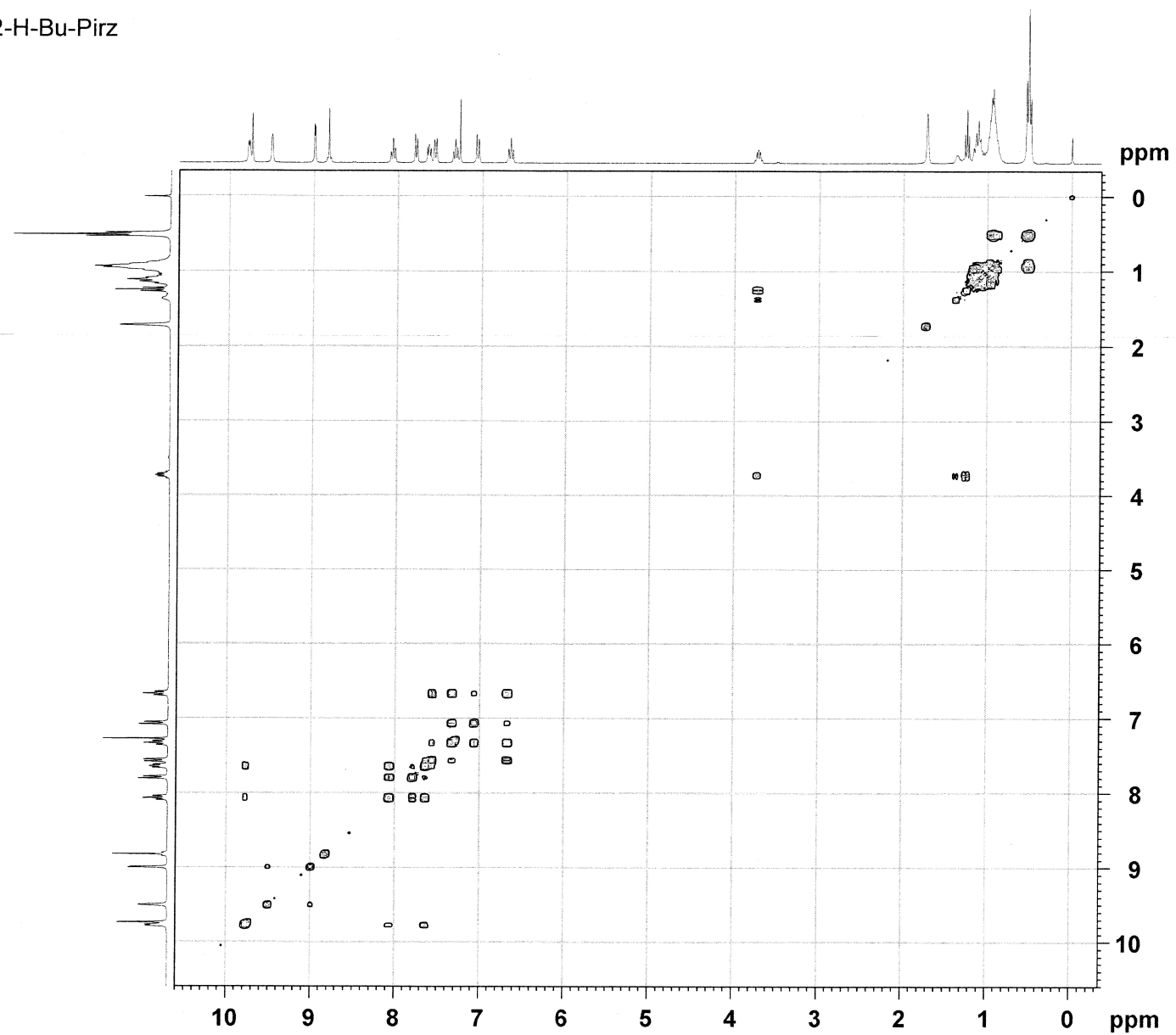


Figure S6. COSY spectrum of **1a**.

G231-E2-H-Bu-Pirz
HSQC

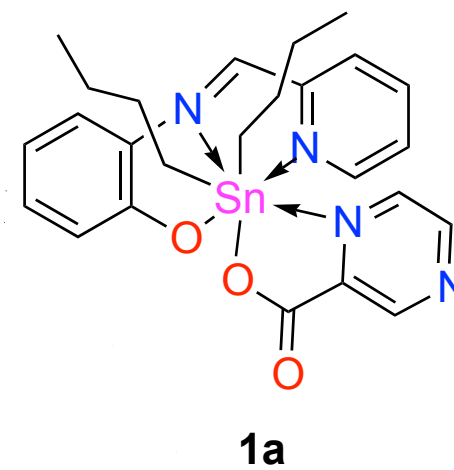
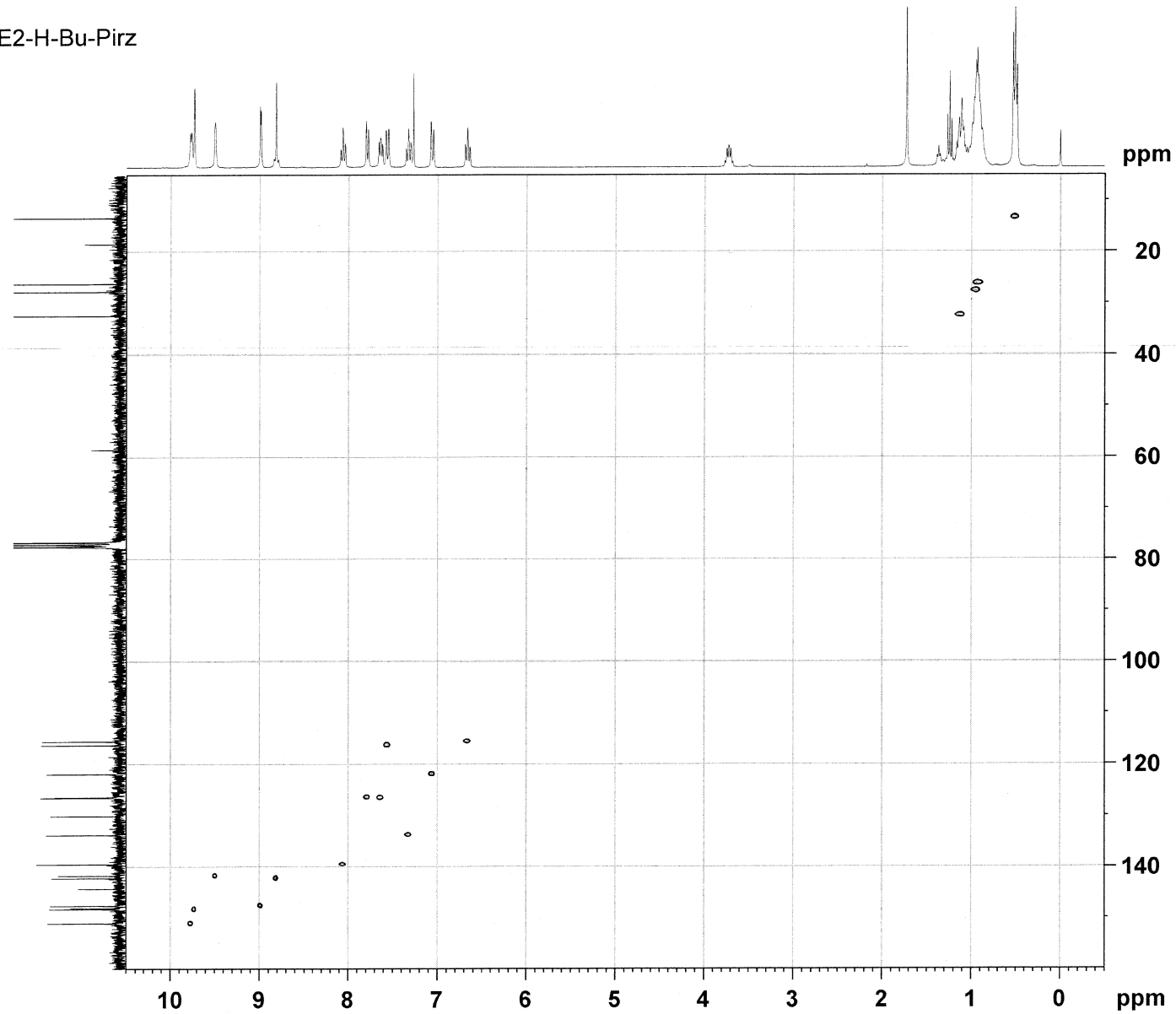


Figure S7. HSQC spectrum of **1a**.

G231-E2-H-Bu-Pirz
HMBC

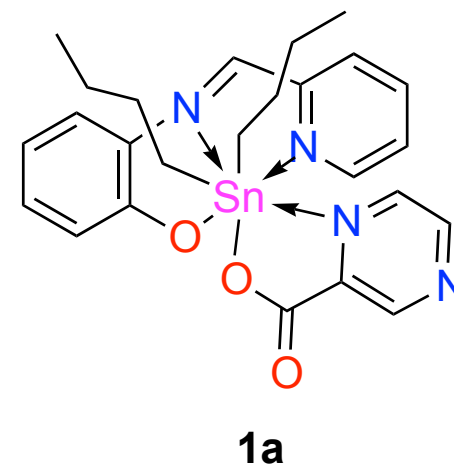
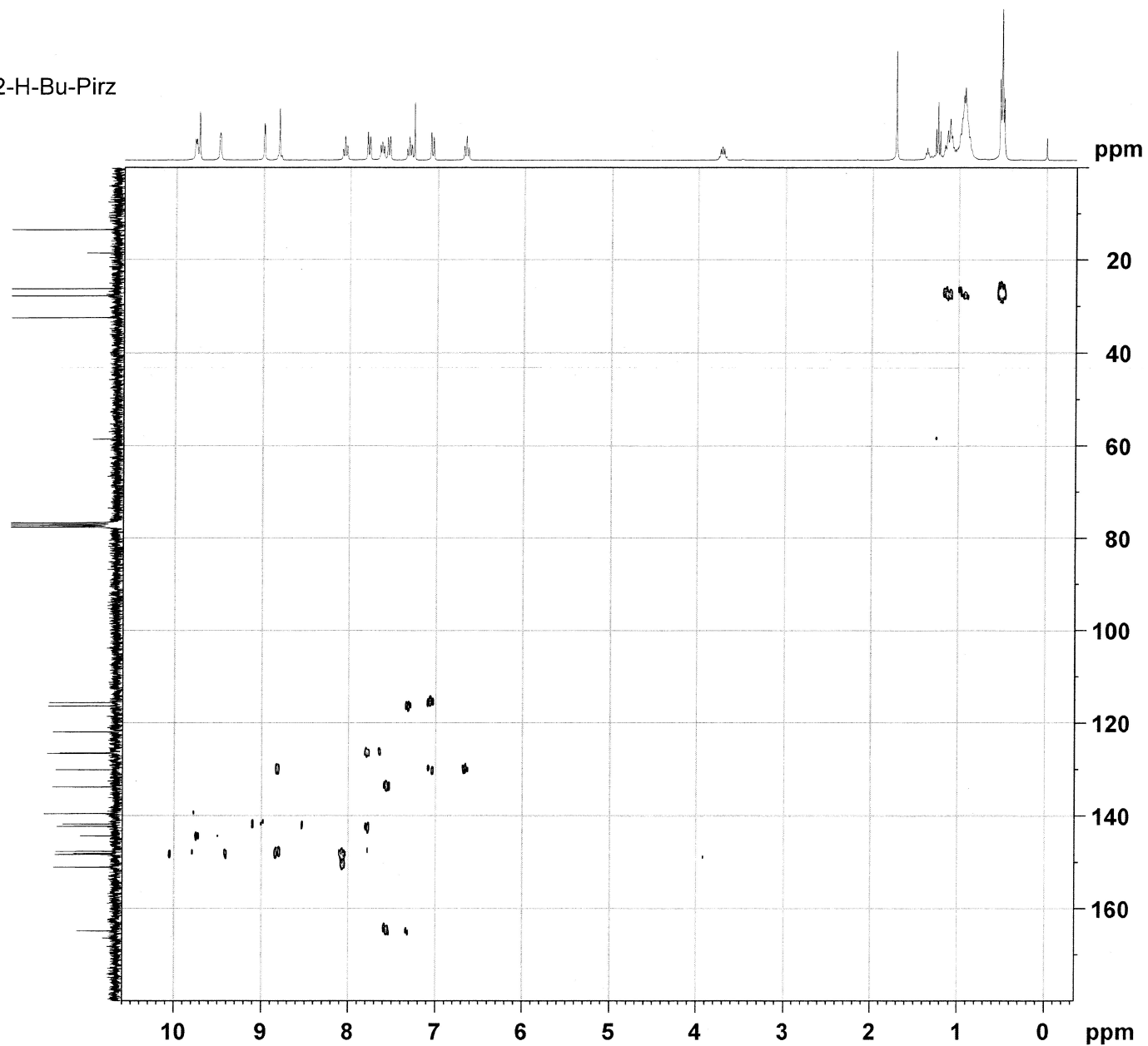


Figure S8. HMBC spectrum for **1a**

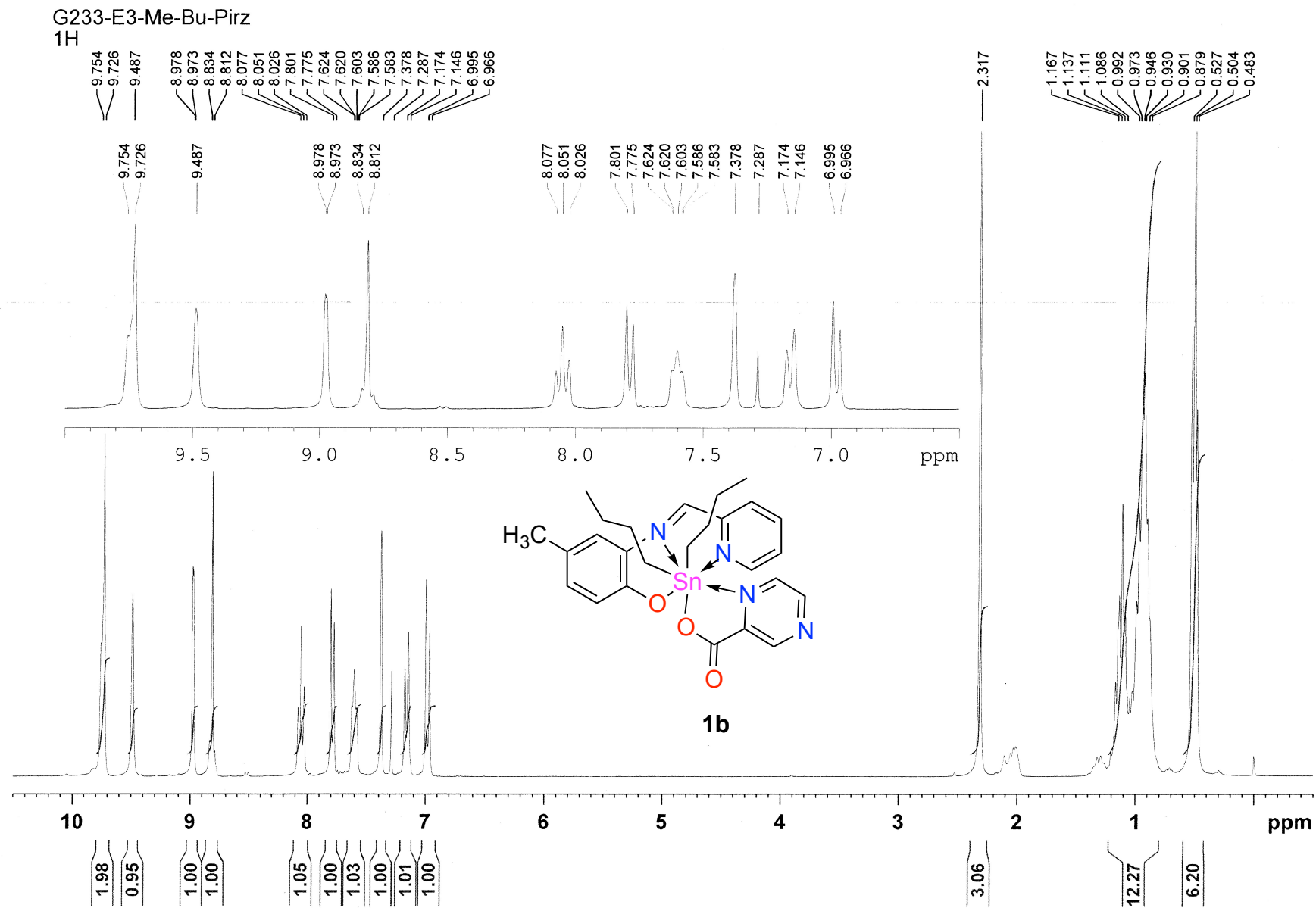


Figure S9. ^1H NMR spectrum of **1b**.

i233-E3-Me-Bu-Pirz
¹³C

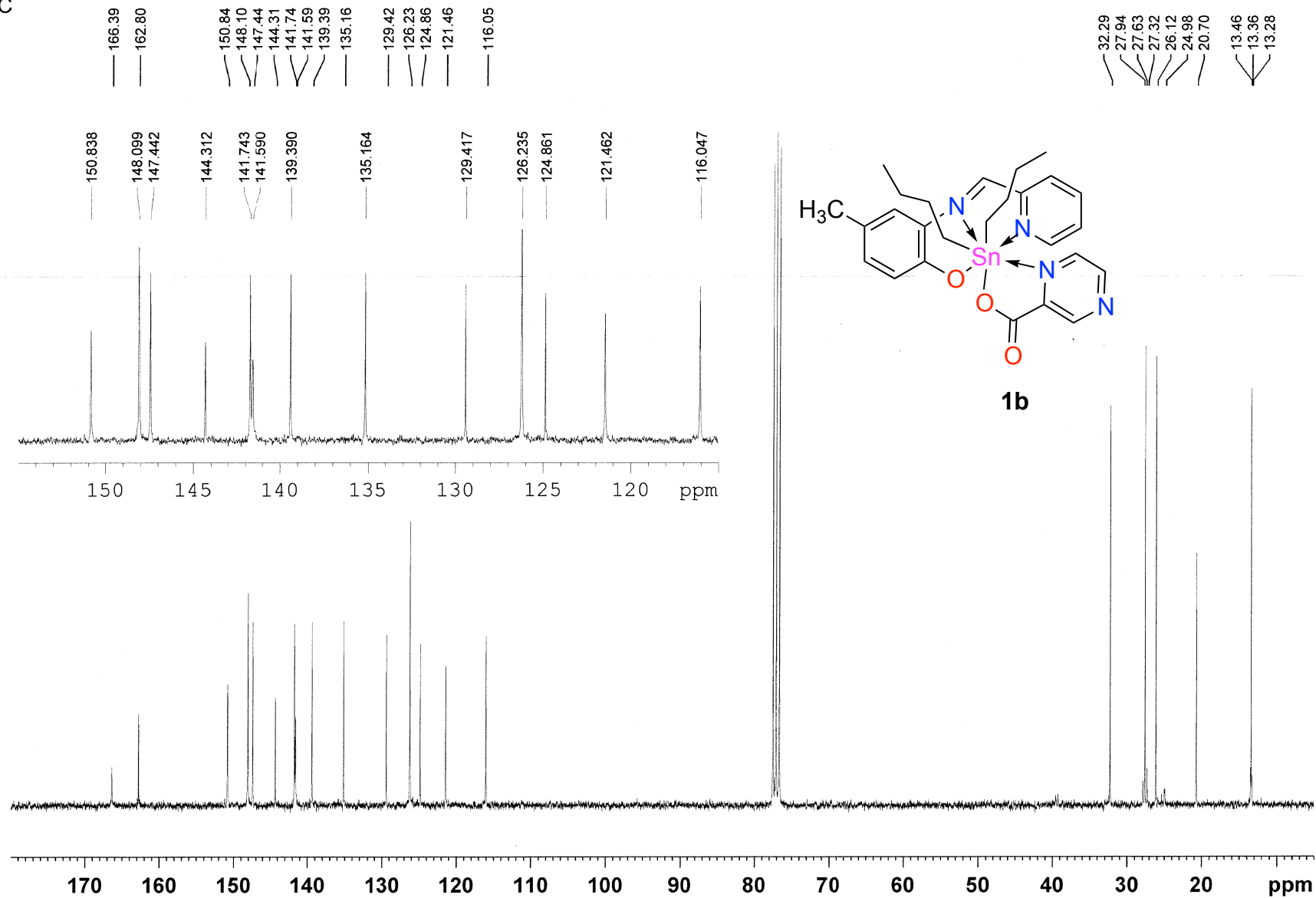


Figure 10. ¹³C NMR spectrum of **1b**.

COSY

3-E3-Me-Bu-Pirz

Y

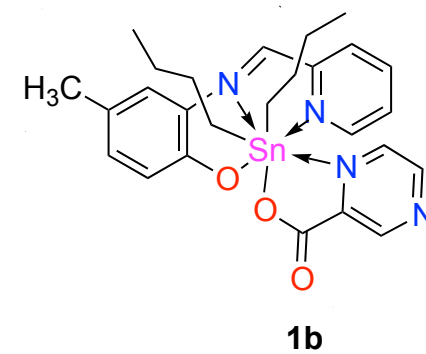
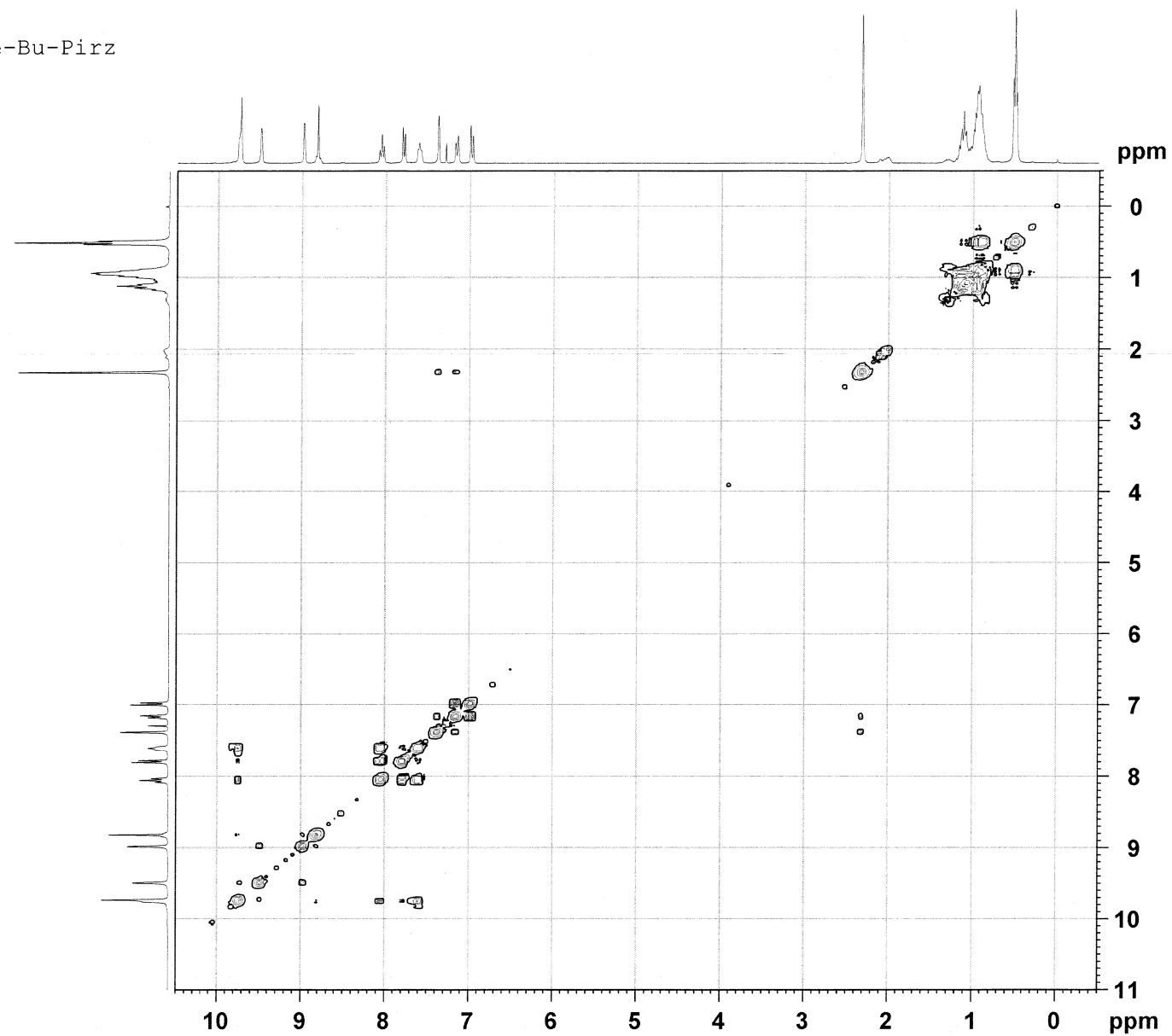


Figure S11. COSY spectrum of **1b**.

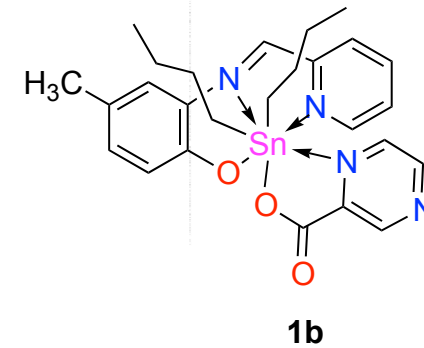
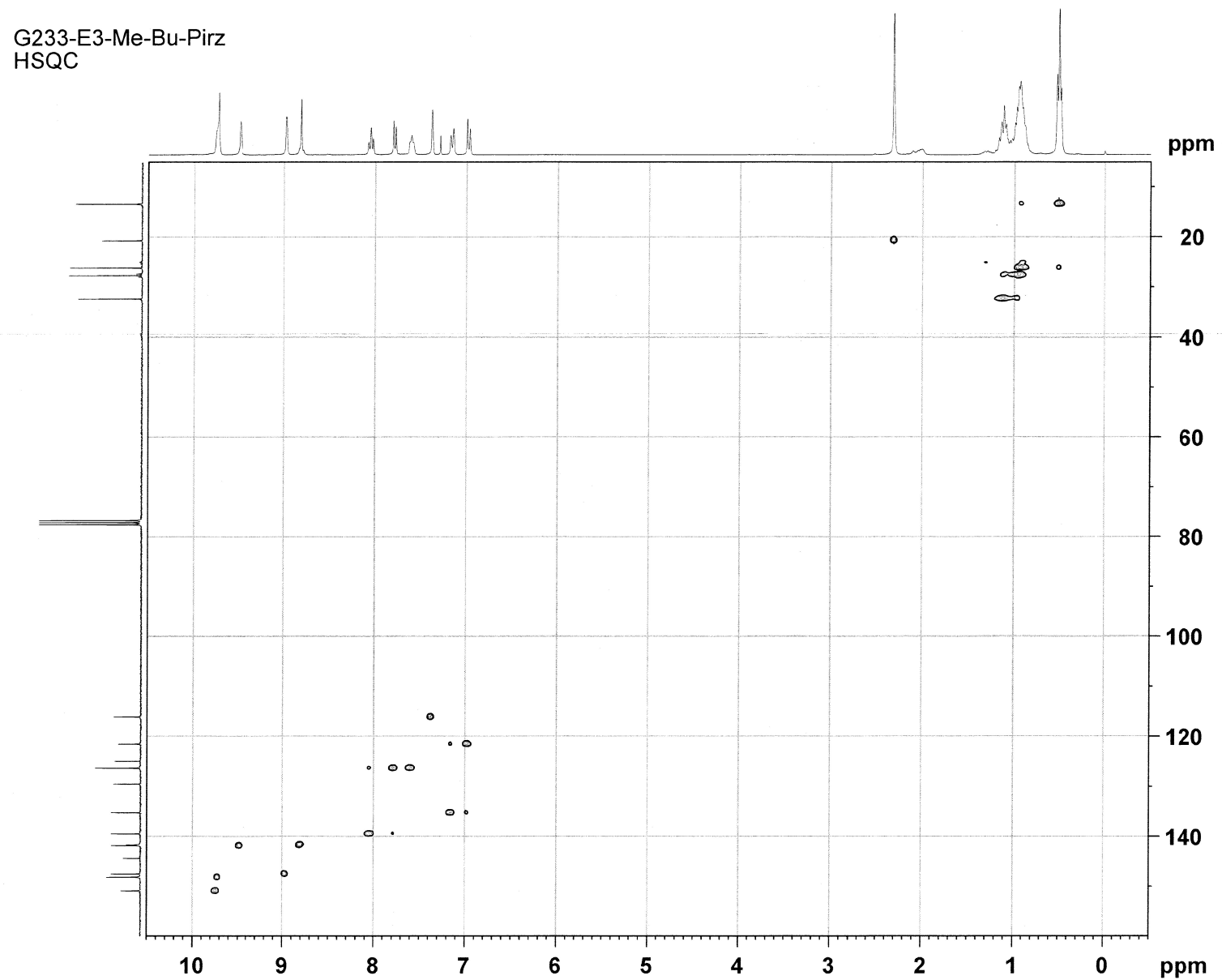


Figure S12. HSQC spectrum of **1b**.

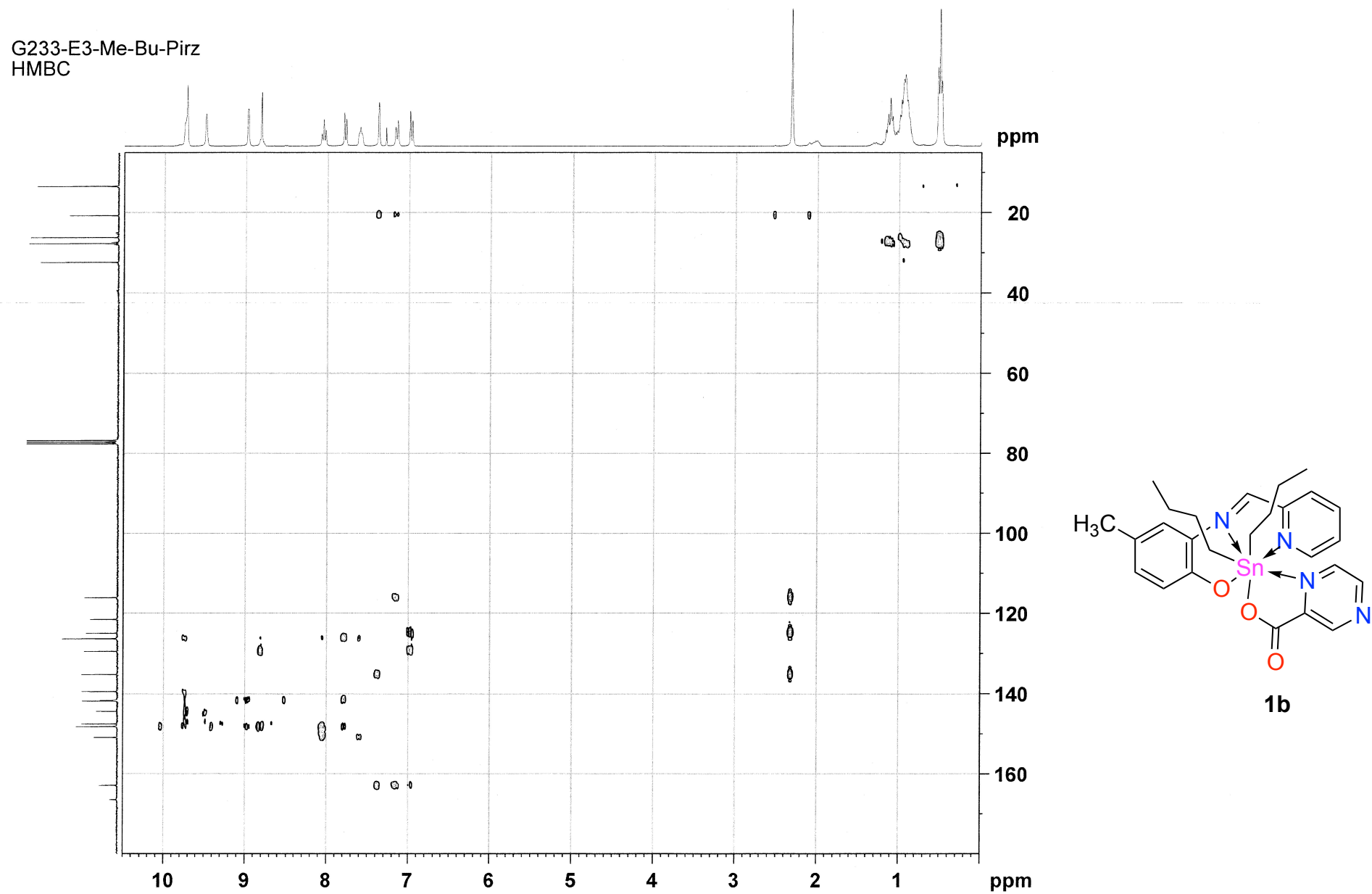


Figure S13. HMBC spectrum of **1b**.

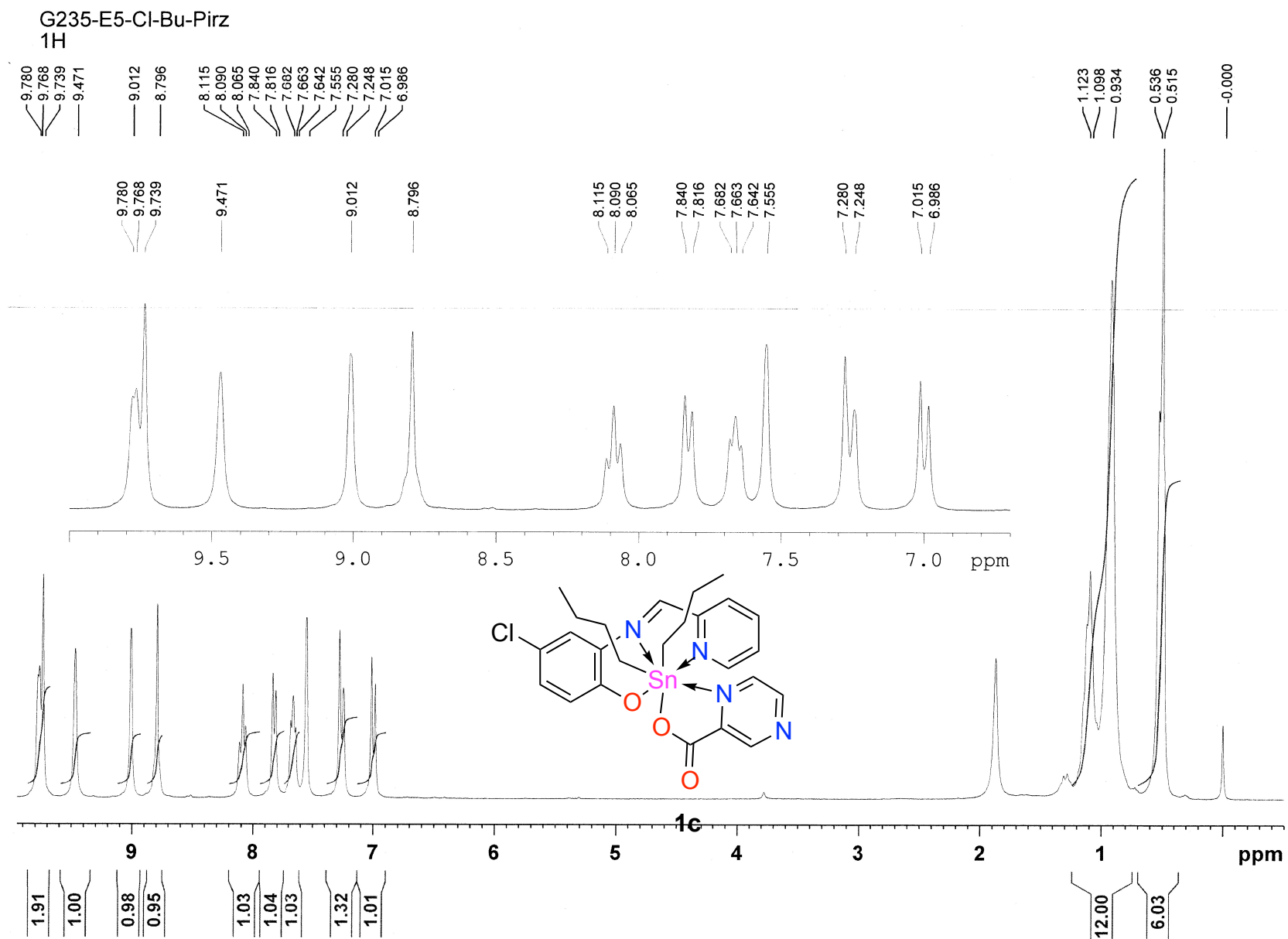


Figure S14. ^1H NMR spectrum of **1c**.

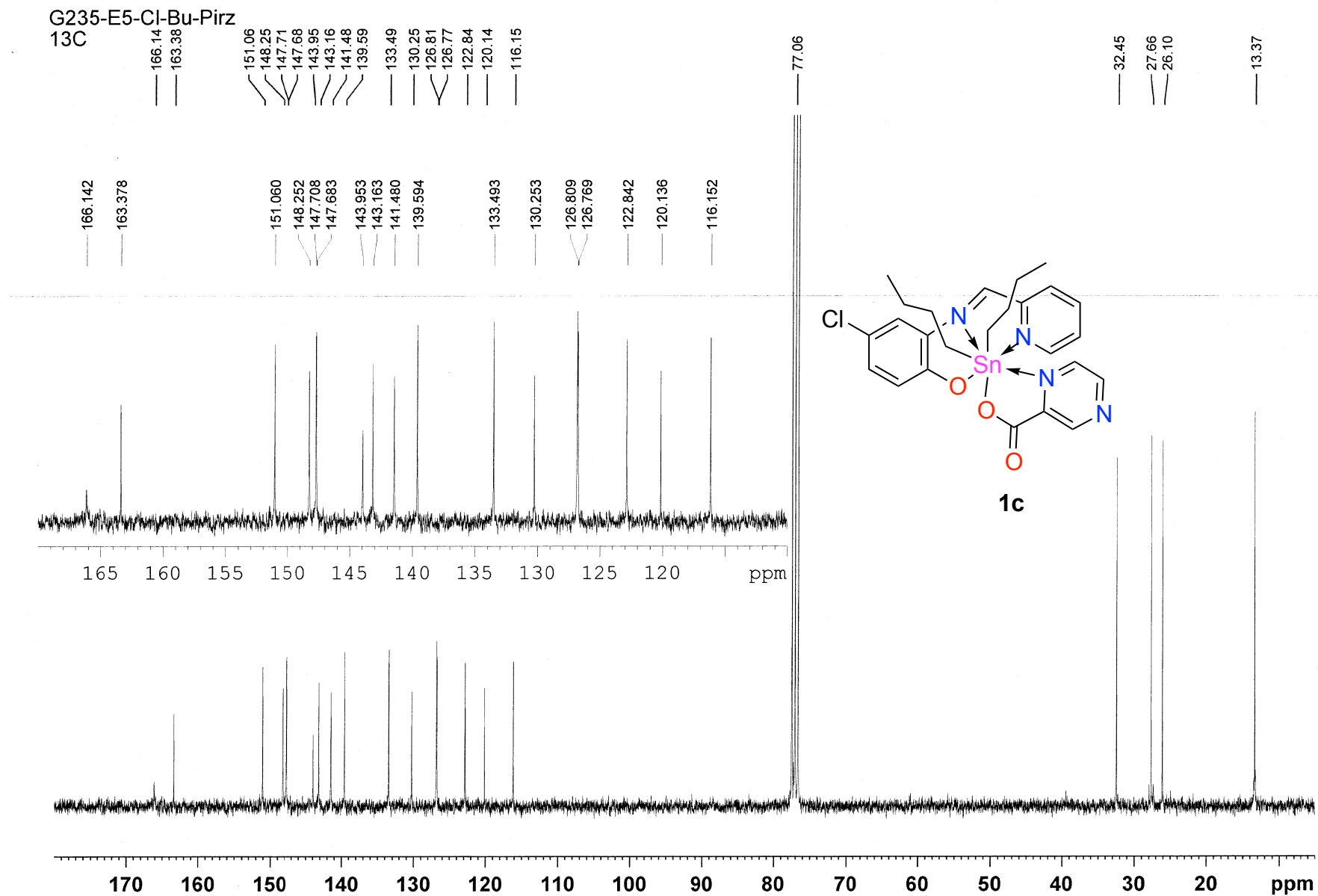


Figure S15. ¹³C NMR spectrum of **1c**.

G235-E5-Cl-Bu-Pirz
COSY

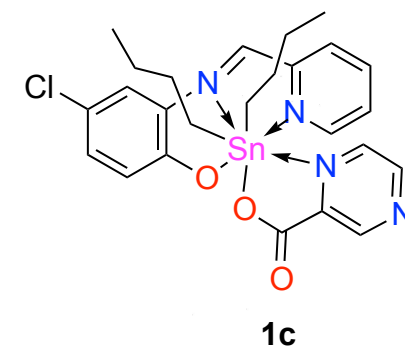
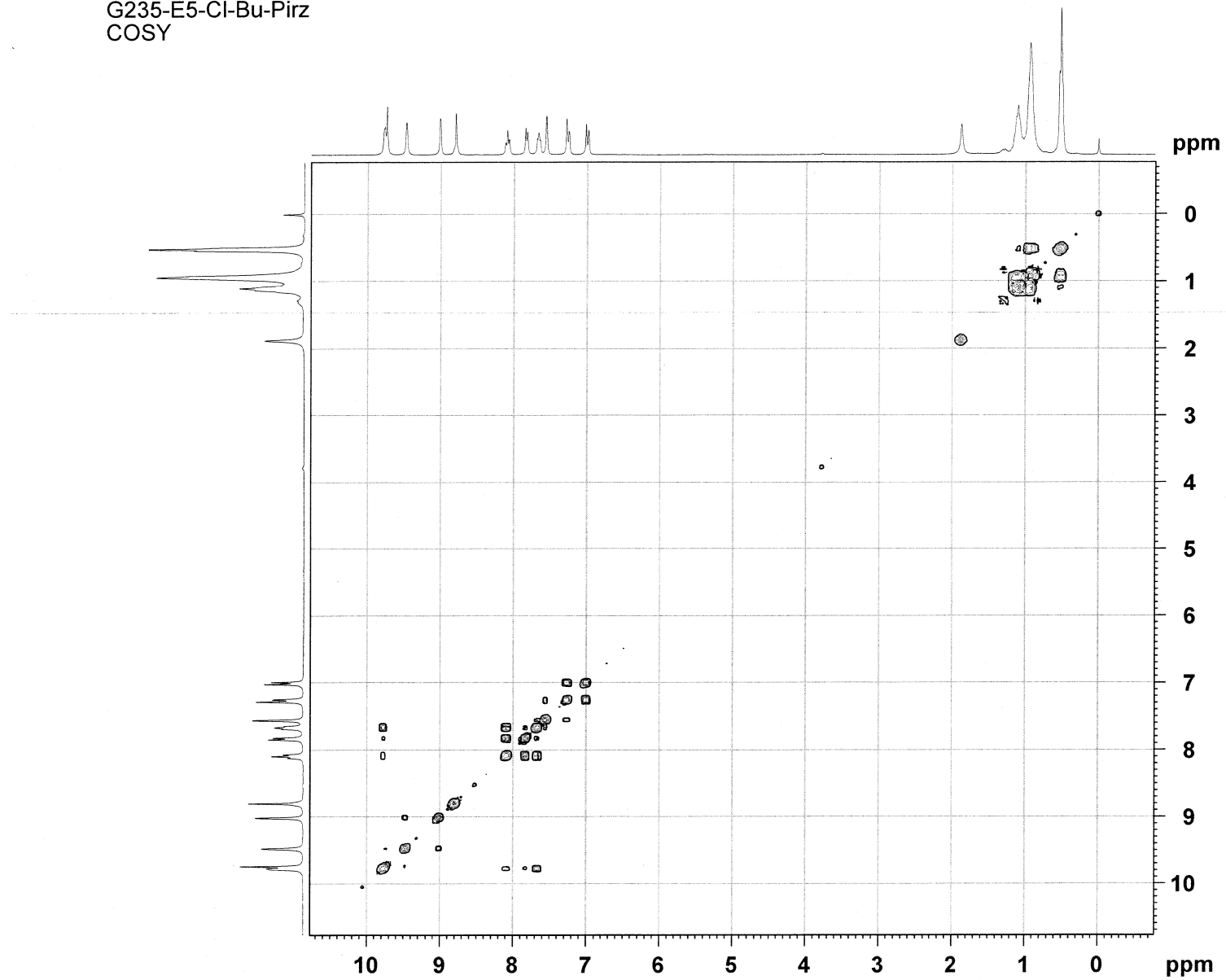


Figure S16. COSY spectrum of 1c.

G235-E5-Cl-Bu-Pirz
HSQC

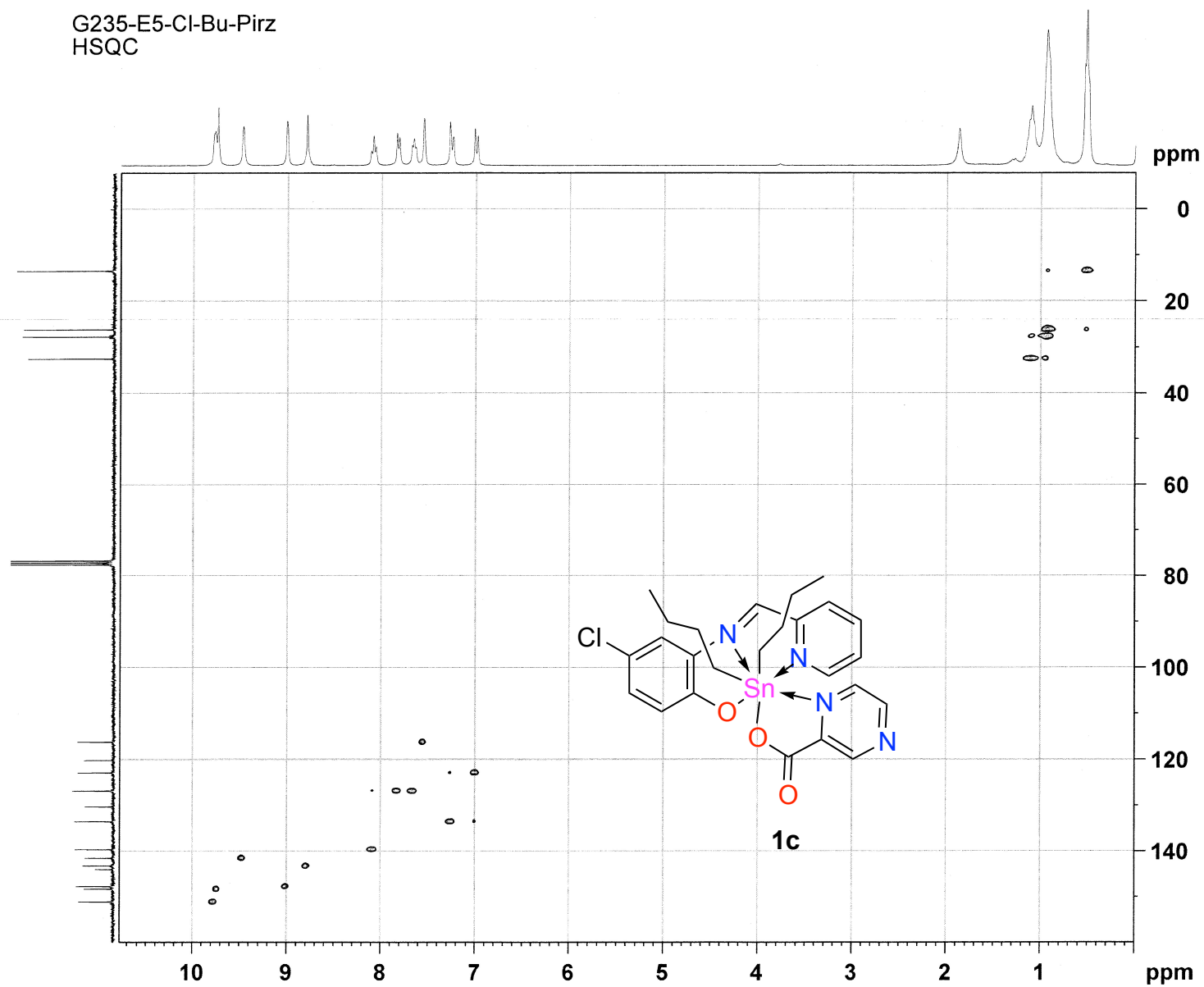


Figure S17. HSQC spectrum of 1c.

G235-E5-Cl-Bu-Pirz
HMBC

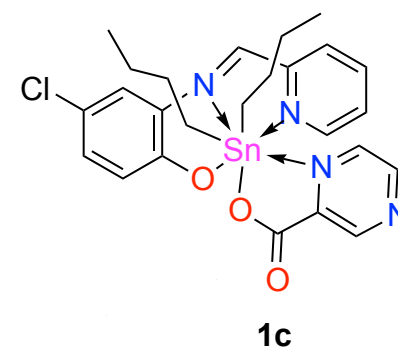
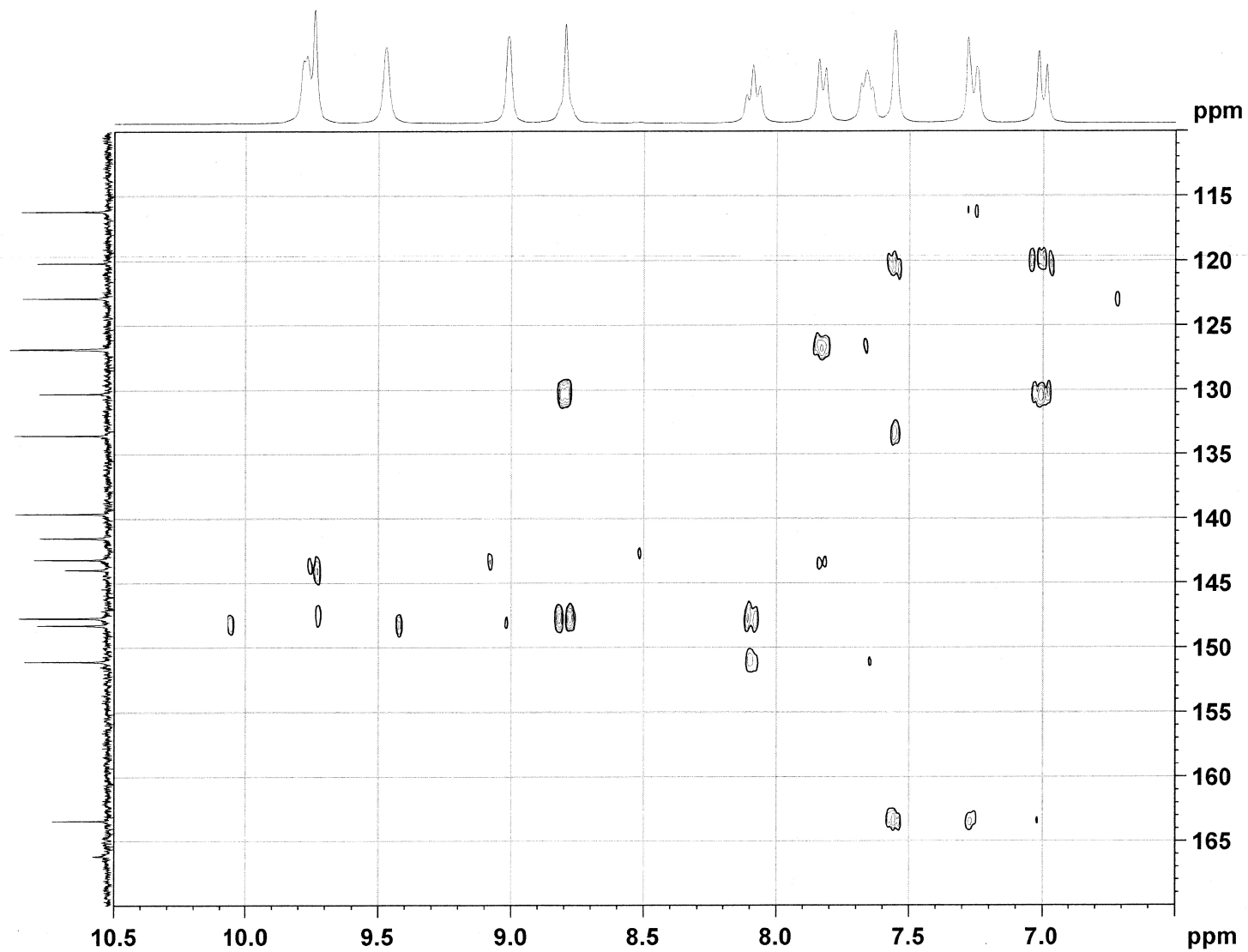


Figure S18. HMBC spectrum of **1c**.

G234-E4-NO₂-Bu-Pirz
¹H

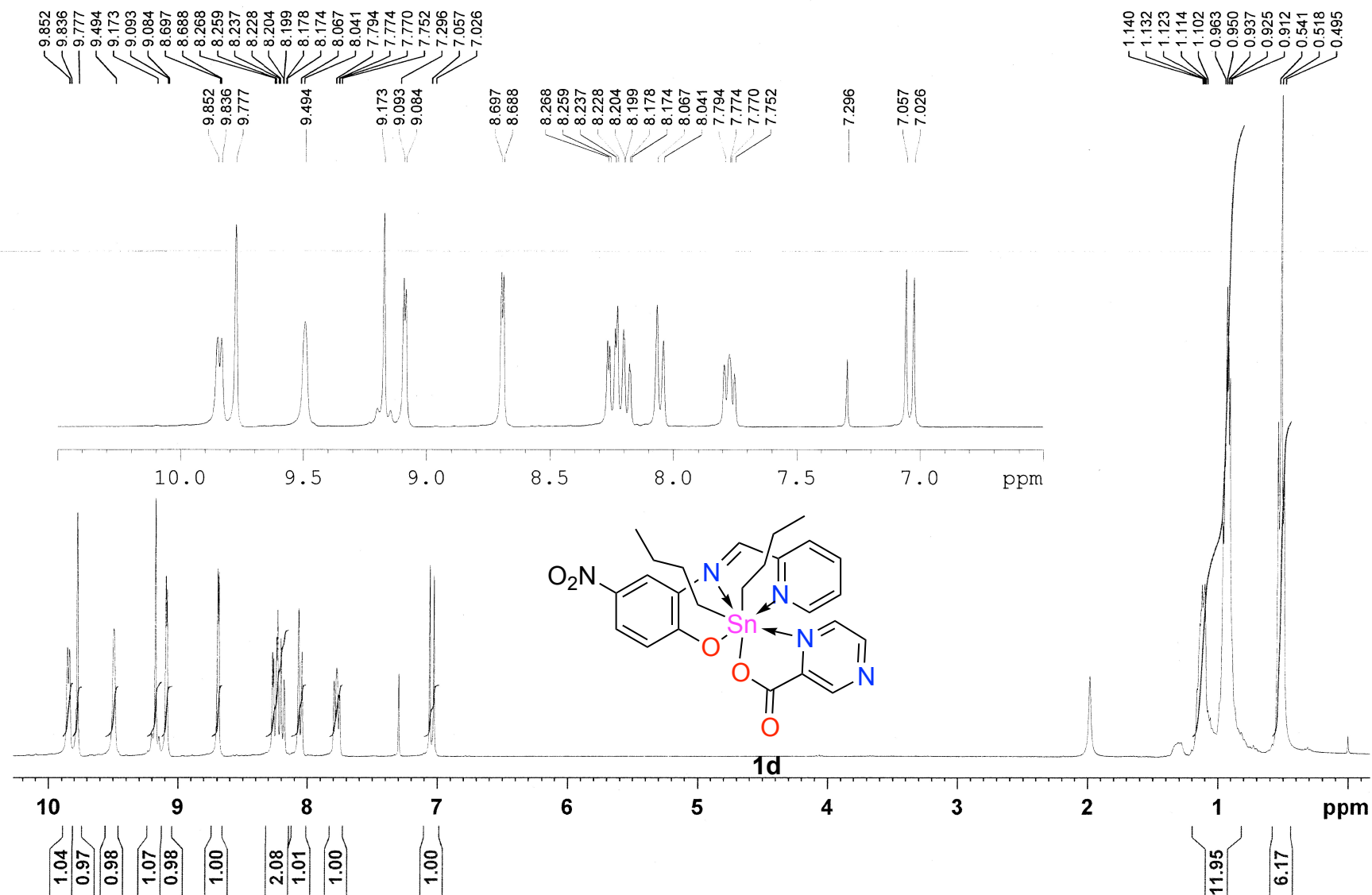


Figure S19. ¹H NMR spectrum of **1d**.

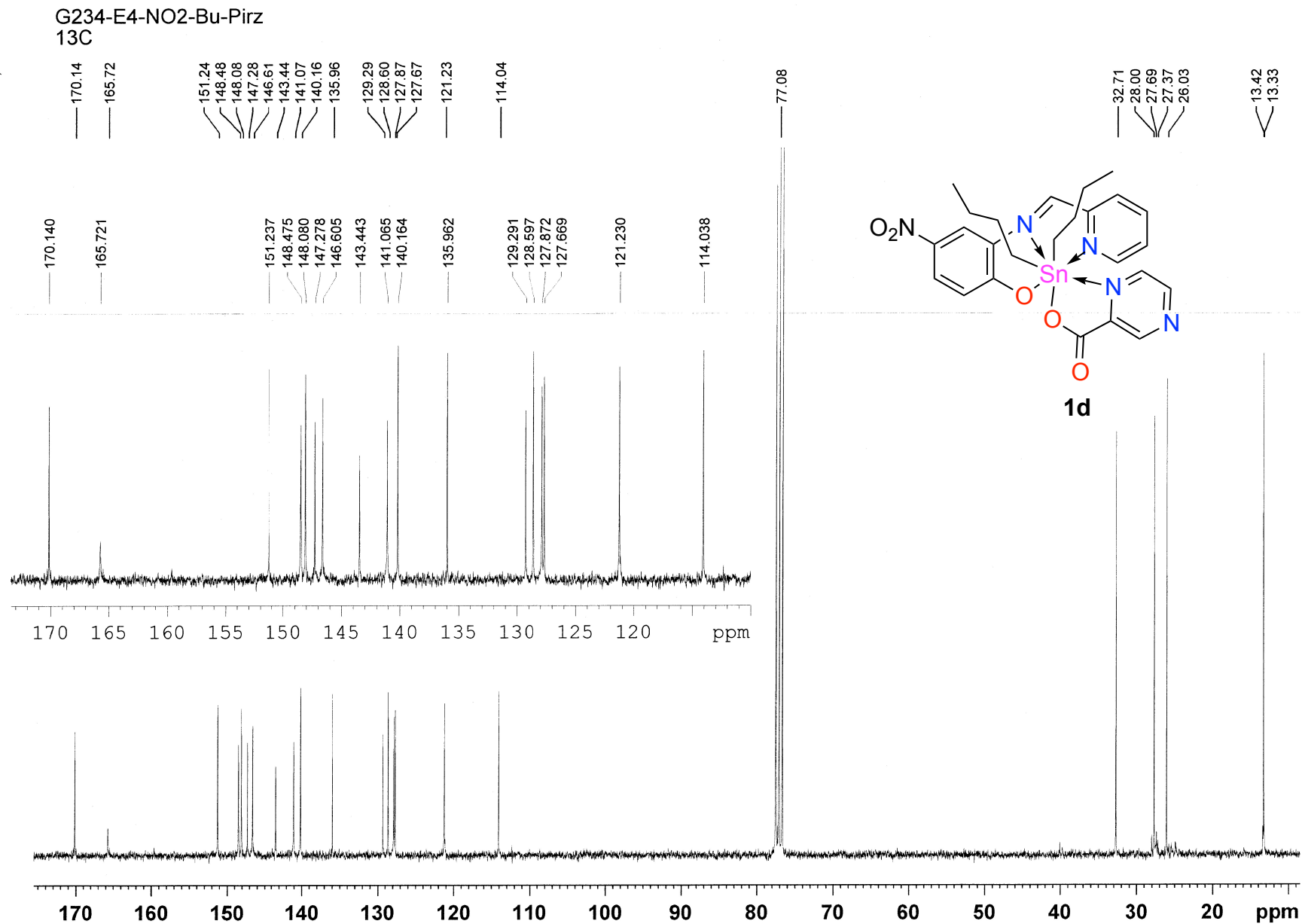


Figure S20. ¹³C NMR spectrum of **1d**.

G234-E4-NO₂-Bu-Pirz
COSY

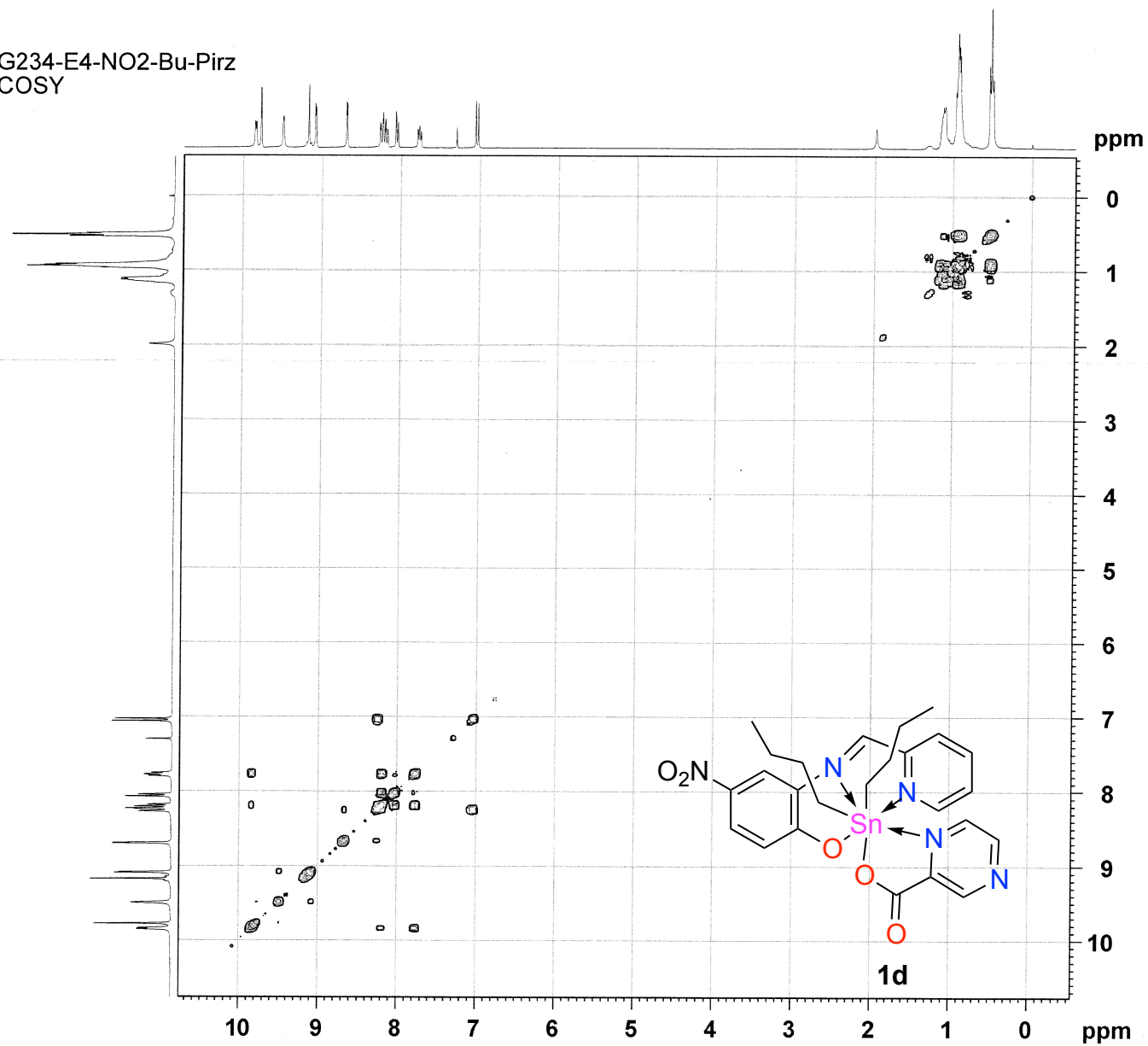


Figure S21. COSY spectrum of **1d**.

-E4-NO2-Bu-Pirz

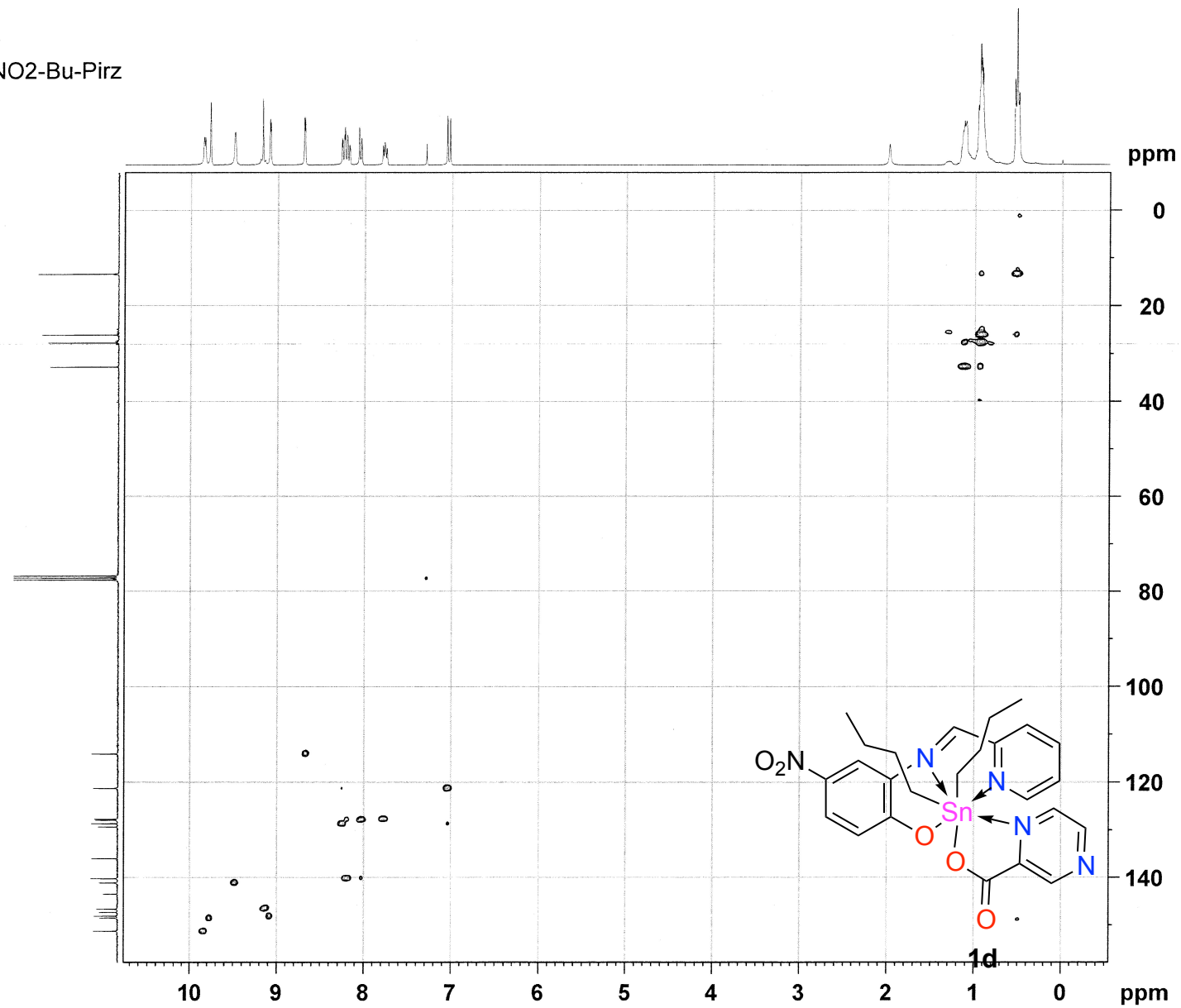


Figure S22. HMBC spectrum of **1d**.

G233-E3-Me-Bu-Pirz
119Sn

— 423.72

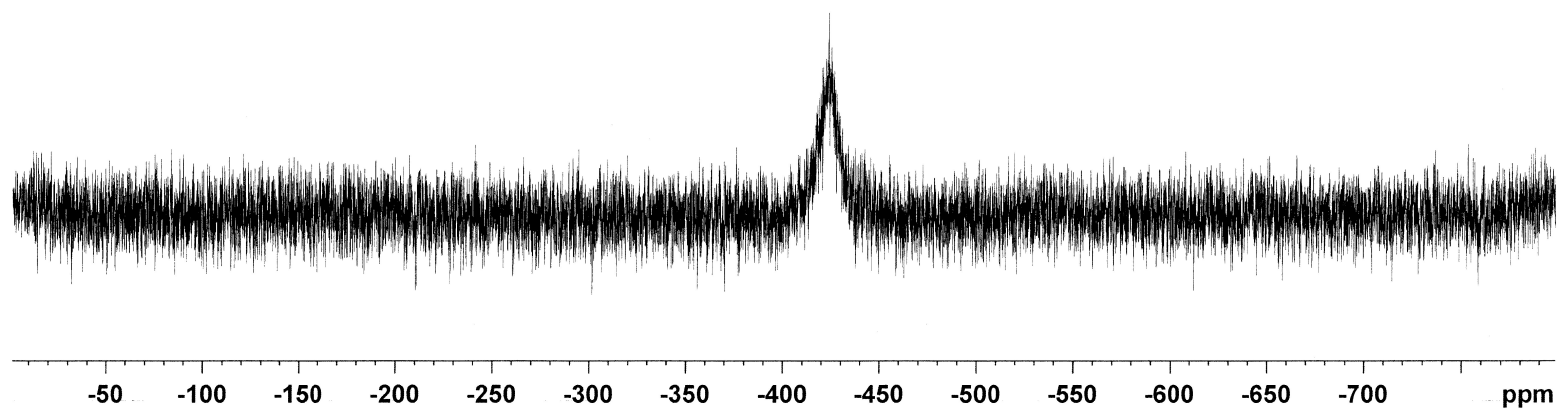
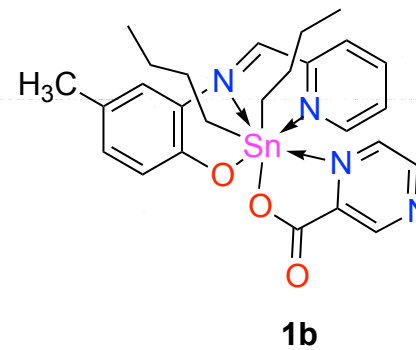


Figure S23. ^{119}Sn NMR in CDCl_3 solution of **1b**.