New Journal of Chemistry

Synthesis, structural characterization and *in vitro* antiproliferative effects on carcinoma cells of novel organotin(IV) compounds with nicotinate and isonicotinate moieties.

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ELECTRONIC SUPPLEMENTARY INFORMATION

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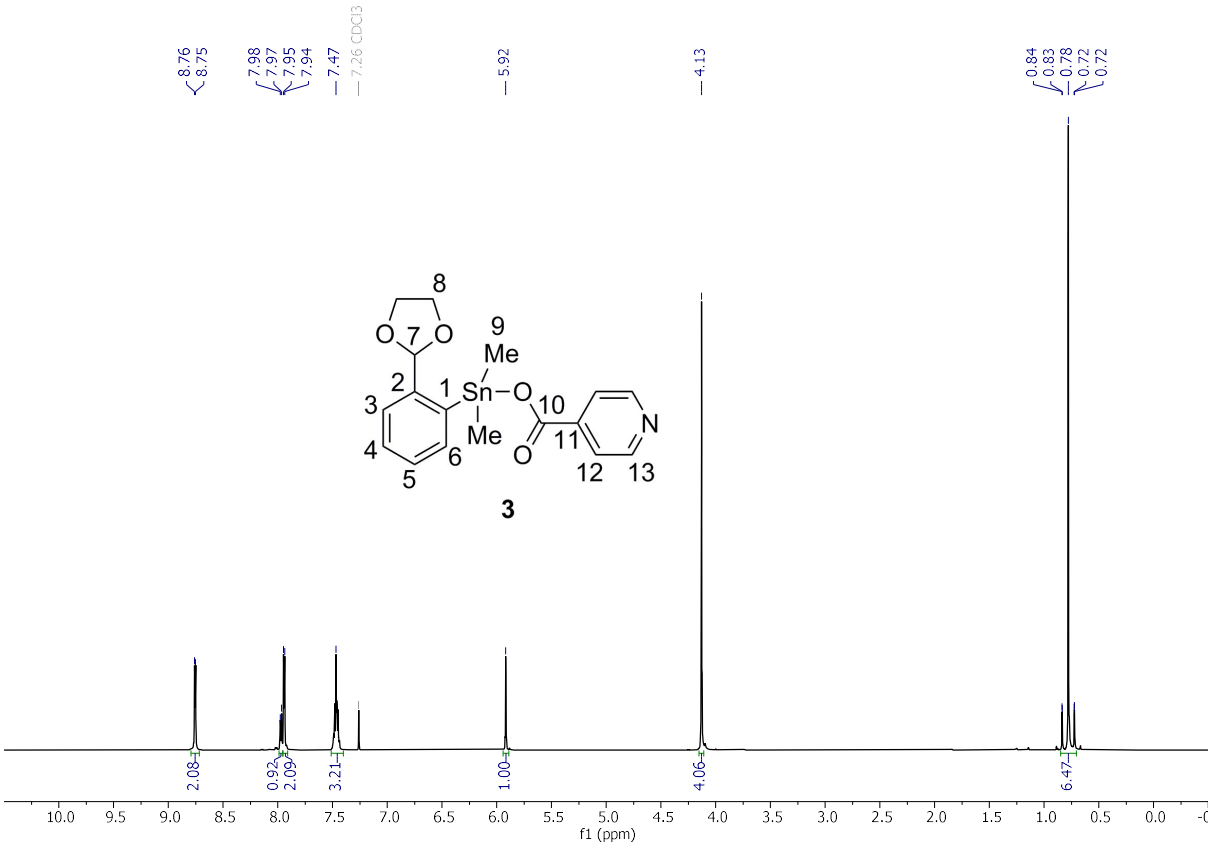

Figure S1. ^{1}H NMR spectra ($CDCl_3$, 600.1 MHz, 22 °C) of compound **3**.

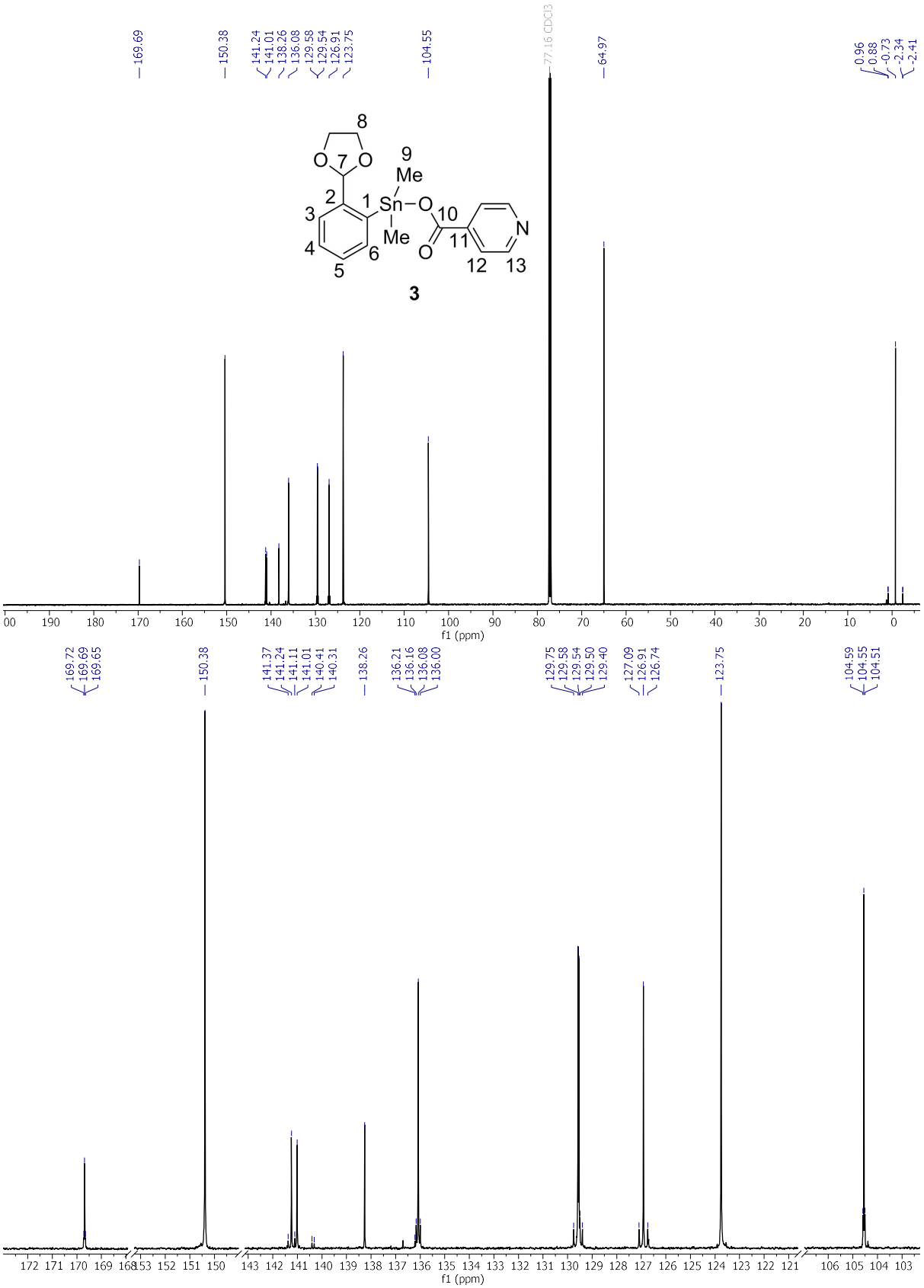

Figure S2. ^{13}C NMR spectra ($CDCl_3$, 150.9 MHz, 22 °C) of compound **3** and details of the aromatic region.

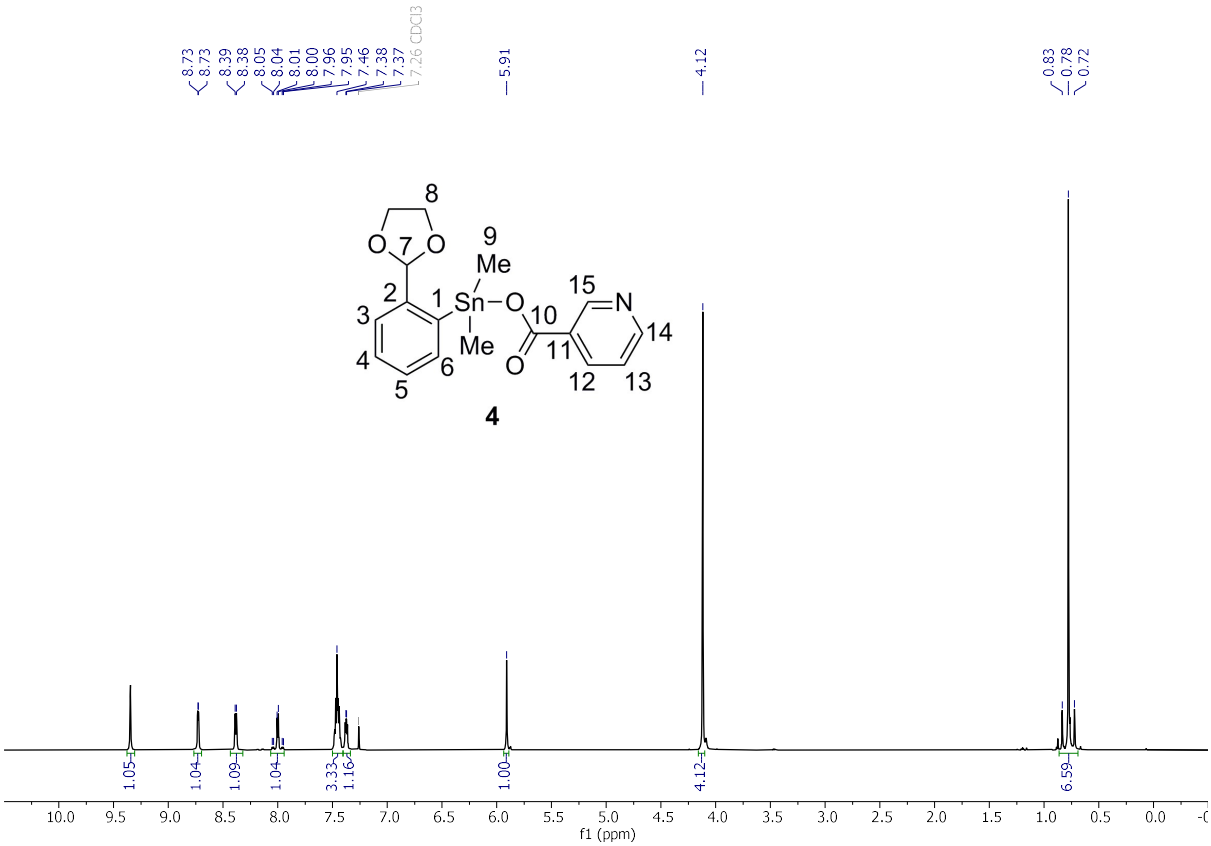

Figure S3. ^{1}H NMR spectra ($CDCl_3$, 600.1 MHz, 22 °C) of compound **4**.

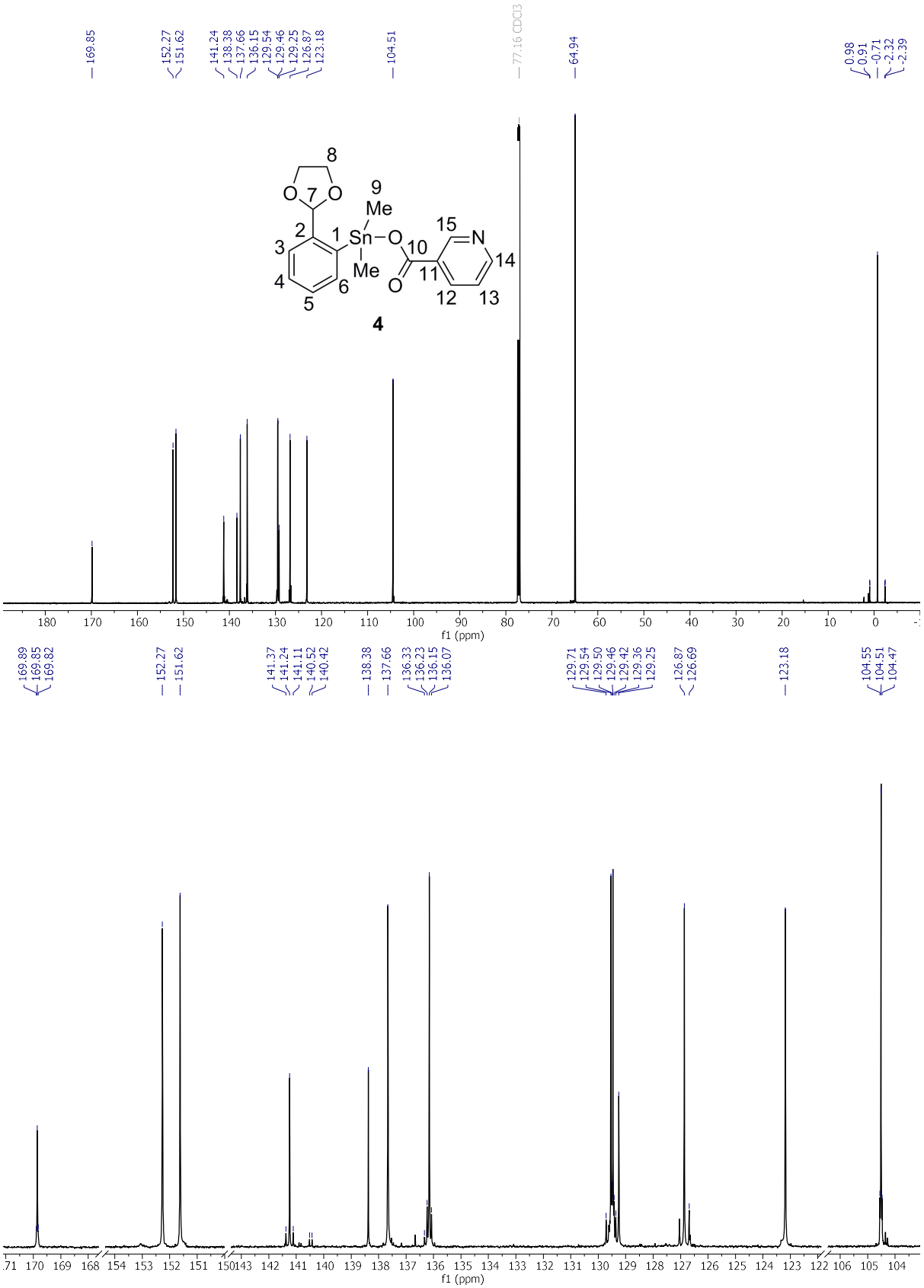

Figure S4. ^{13}C NMR spectra ($CDCl_3$, 150.9 MHz, 22 °C) of compound **4** and details of the aromatic region.

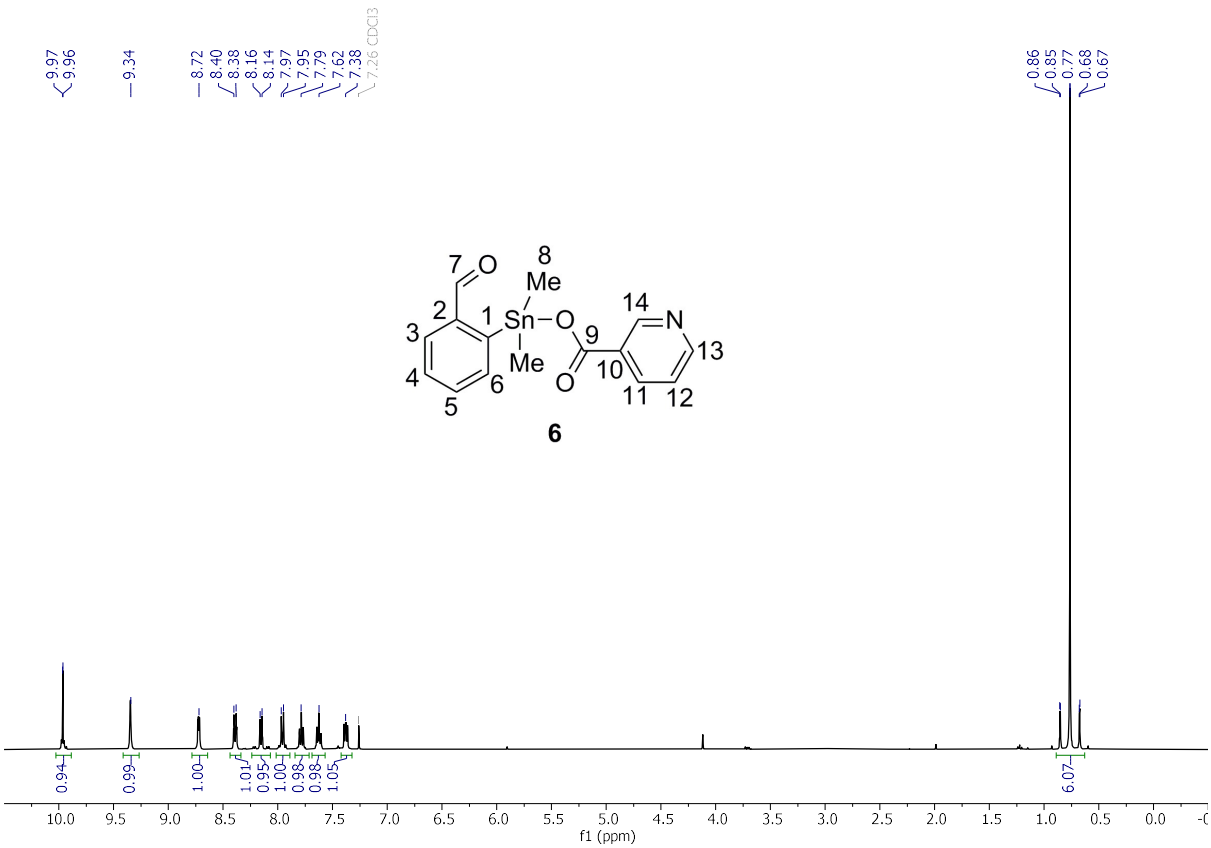

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Figure S5. ^{1}H NMR spectra ($CDCl_3$, 400.1 MHz, 21 °C) of compound **6**.

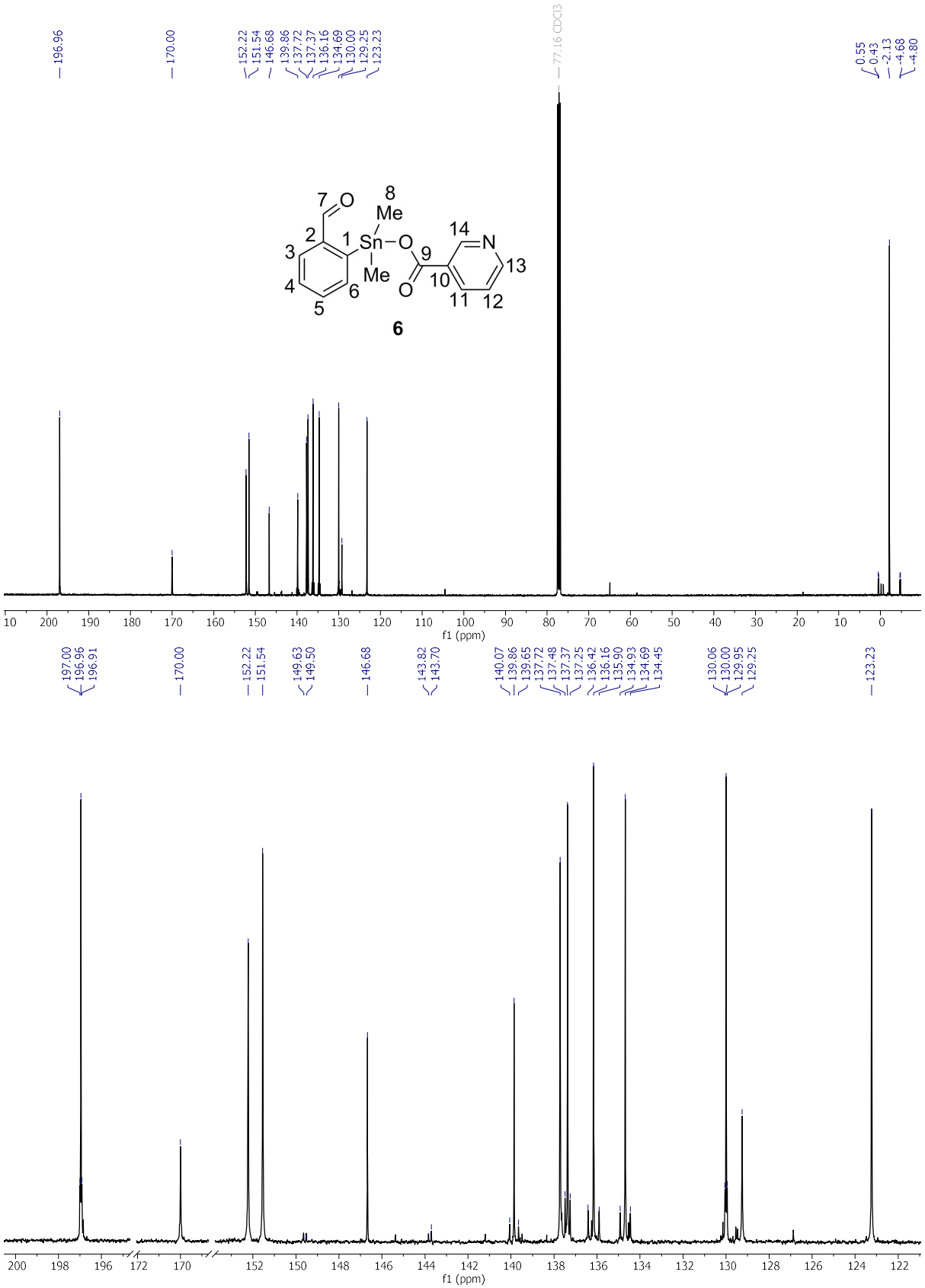

Figure S6. ^{13}C NMR spectra ($CDCl_3$, 100.6 MHz, 21 °C) of compound **6** and details of the aromatic region.

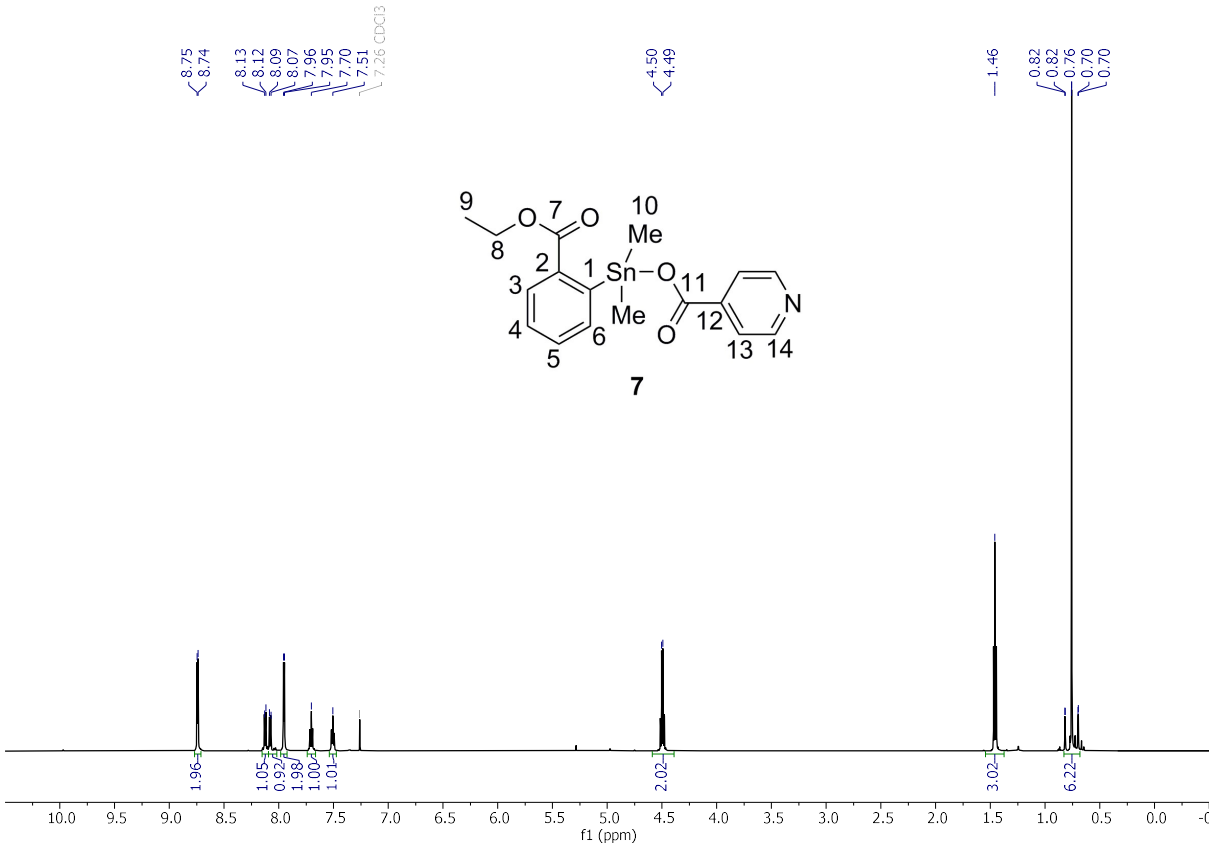

Figure S7. ^{1}H NMR spectra ($CDCl_3$, 600.1 MHz, 23 °C) of compound **7**.

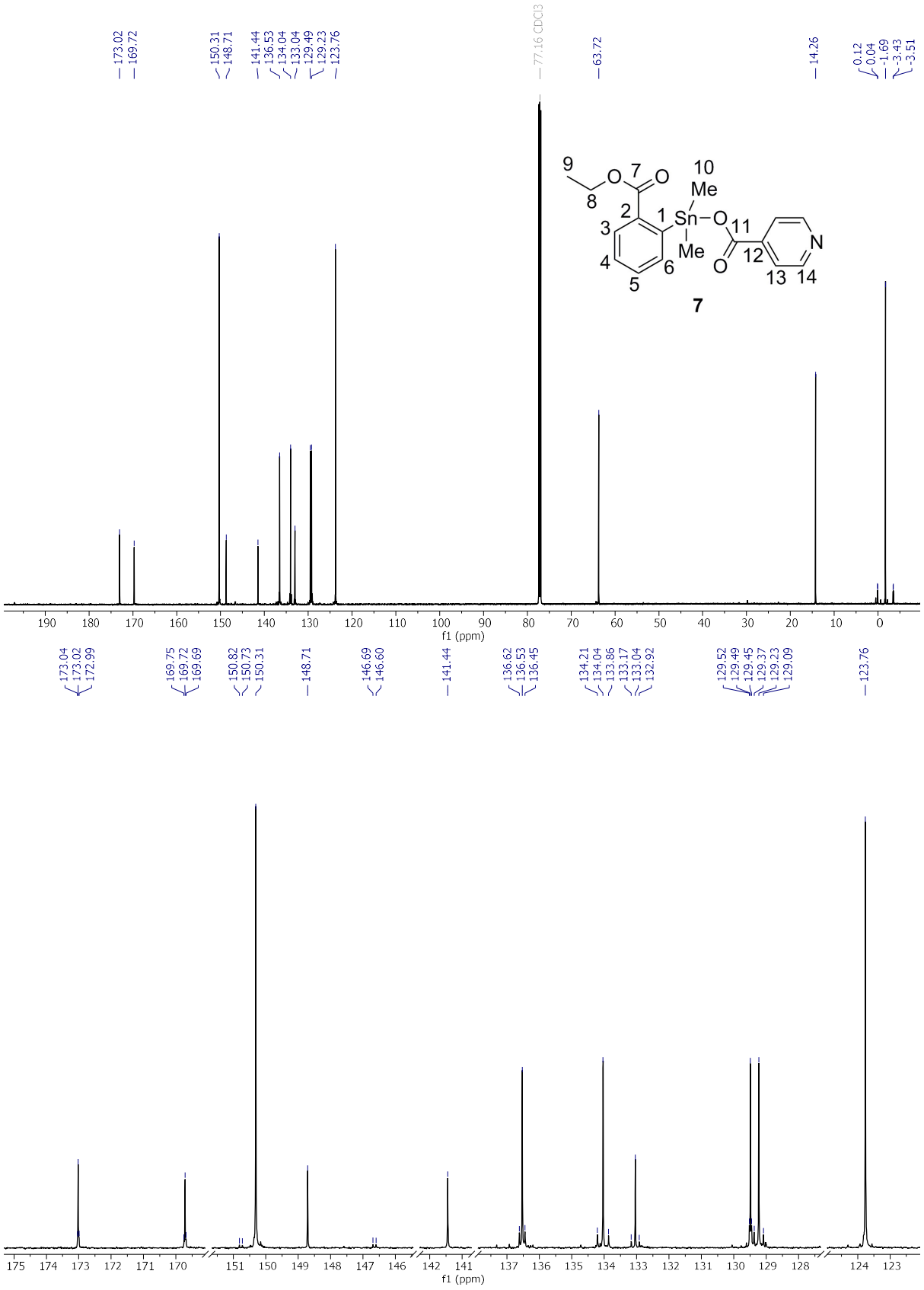

Figure S8. ^{13}C NMR spectra ($CDCl_3$, 150.9 MHz, 23 °C) of compound **7** and details of the aromatic region.

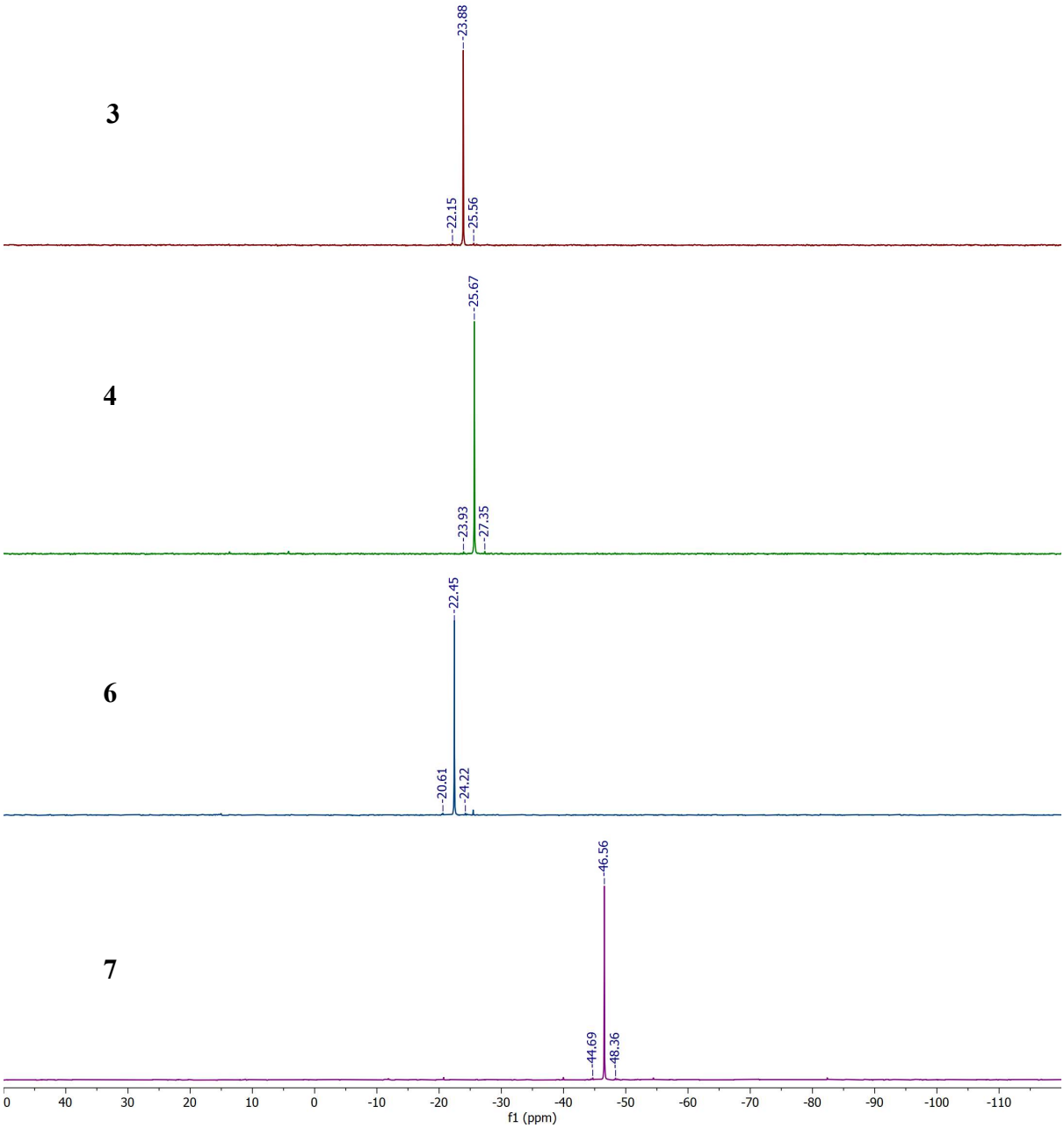

Figure S9. ^{119}Sn NMR ($CDCl_3$, 149.2 MHz, 21 °C) stacked spectra of compounds **3**, **4**, **6** and **7**.

Table S1. X-ray crystal data and structure refinement for compounds **3**, **4**, **5** and **7**.

	3	**4**	**5**	**7**
Empirical formula	$C_{17}H_{19}NO_4Sn$	$C_{17}H_{19}NO_4Sn$	$C_{15}H_{15}NO_3Sn$	$C_{17}H_{19}NO_4Sn$
Formula weight	420.02	420.02	375.97	420.02
Temperature (K)	297(2)	297(2)	100(2)	297(2)
Crystal system	triclinic	orthorhombic	orthorhombic	triclinic
Space group	*P*-1	*Pbca*	*P*212121	*P*-1
a (Å)	9.142(2)	11.6366(11)	7.2969(6)	8.942(2)
b (Å)	9.455(2)	11.8098(11)	10.3968(8)	10.955(2)
c (Å)	11.142(3)	25.255(2)	19.3079(12)	11.156(3)
α (º)	104.291(4)	90	90	118.128(4)
β (º)	107.472(4)	90	90	98.558(4)
γ (º)	91.291(4)	90	90	105.645(4)
Volume (Å^3)	885.3(3)	3470.7(6)	1464.78(19)	877.8(3)
Z	2	8	4	2
D_{calc} (g cm^{-3})	1.576	1.608	1.705	1.589
Absorption coefficient (mm^{-1})	1.461	1.491	1.705	1.474
F(000)	420	1680	744	420
Crystal size (mm)	0.18x0.19x0.25	0.29x0.28x0.15	0.06x0.08x0.11	0.2x0.26x0.28
θ range for data collection (º)	1.988 to 25.00	2.38 to 25.089	2.23 to 28.31	2.16 to 25.1
Reflections collected	8642	31704	19773	8608
Independent reflections	3118 [R_{int}= 0.034]	3084 [R_{int} =0.0625]	3644 [R_{int} =0.0259]	3126 [R_{int} =0.0452]
Absorption correction	Multi-scan[1]	Multi-scan[1]	Multi-scan[1]	Multi-scan[1]
Data / restraints / parameters	3118/0/210	3084/0/210	3644/0/184	3126/0/211
Goodness-of-fit on F^2	1.051	1.081	1.072	1.001
Final *R* indices [$I>2\sigma(I)$]	R_1= 0.0327 wR_2=0.0778	R_1= 0.0389 wR_2=0.0940	R_1= 0.0136 wR_2=0.0336	R_1= 0.0393 wR_2=0.0920
R indices (all data)	R_1= 0.0367 wR_2= 0.0808	R_1= 0.0553 wR_2= 0.1068	R_1= 0.0141 wR_2= 0.0339	R_1= 0.0494 wR_2= 0.0991
Largest difference peak and hole (e Å^{-3})	0.77 and –0.28	1.20 and –0.32	0.44 and –0.27	0.81 and –0.32
CCDC No.	2004064	2004065	2004066	2004067

[1]G. M. Sheldrick, *SADABS, Program for area detector adsorption correction*, Institute for Inorganic Chemistry, University of Göttingen, Germany, 1996.

CCDC 2004064, 2004065, 2004066 and 2004067 for **3**, **4**, **5** and **7**, respectively, contain the supplementary crystallographic data for this contribution. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

[2-{(CH$_2$O)$_2$CH}C$_6$H$_4$]Me$_2$Sn[O(O)CC$_5$H$_4$N-4] (3)

- the crystal contains a 1:1 mixture of *p*$R_{O(1)}$-$R_{O(1)}$-$S_{C(7)}$- and *p*$S_{O(1)}$-$S_{O(1)}$-$R_{C(7)}$-**3** isomers

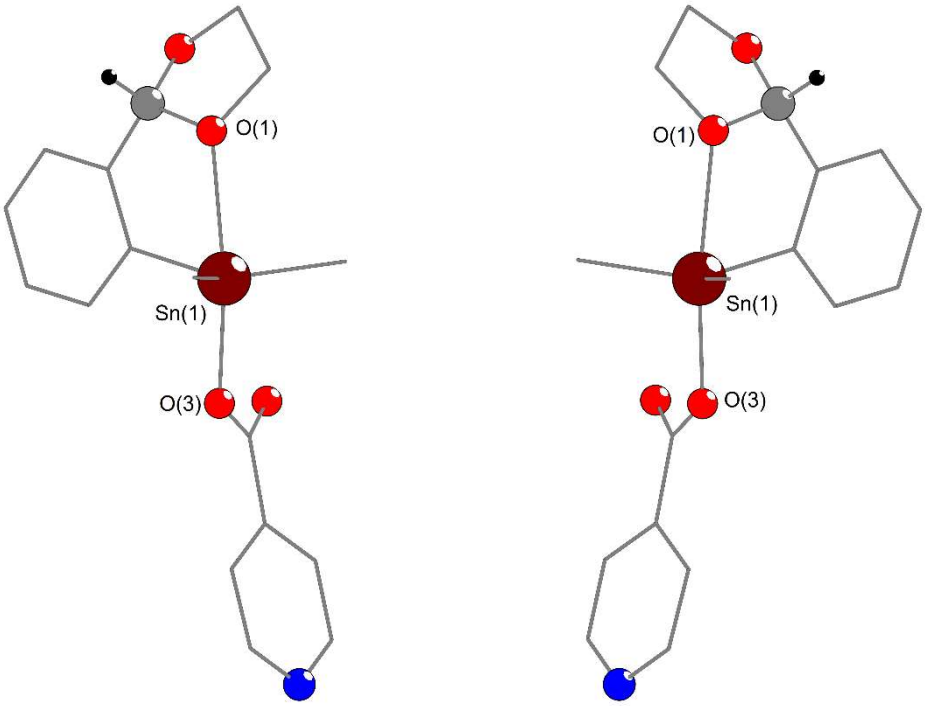

Figure S10. Molecular structure of *p*$R_{O(1)}$-$R_{O(1)}$-$S_{C(7)}$-**3** isomer (*left)* and *p*$S_{O(1)}$-$S_{O(1)}$-$R_{C(7)}$-**3** isomer (*right*) in the crystal of **3** (only methyne hydrogens are shown).

[2-{(CH$_2$O)$_2$CH}C$_6$H$_4$]Me$_2$Sn[O(O)CC$_5$H$_4$N-3] (4)

- the crystal contains a 1:1 mixture of *pR*$_{O(1)}$-*S*$_{O(1)}$-*R*$_{C(7)}$- and *pS*$_{O(1)}$-*R*$_{O(1)}$-*S*$_{C(7)}$-**4** isomers

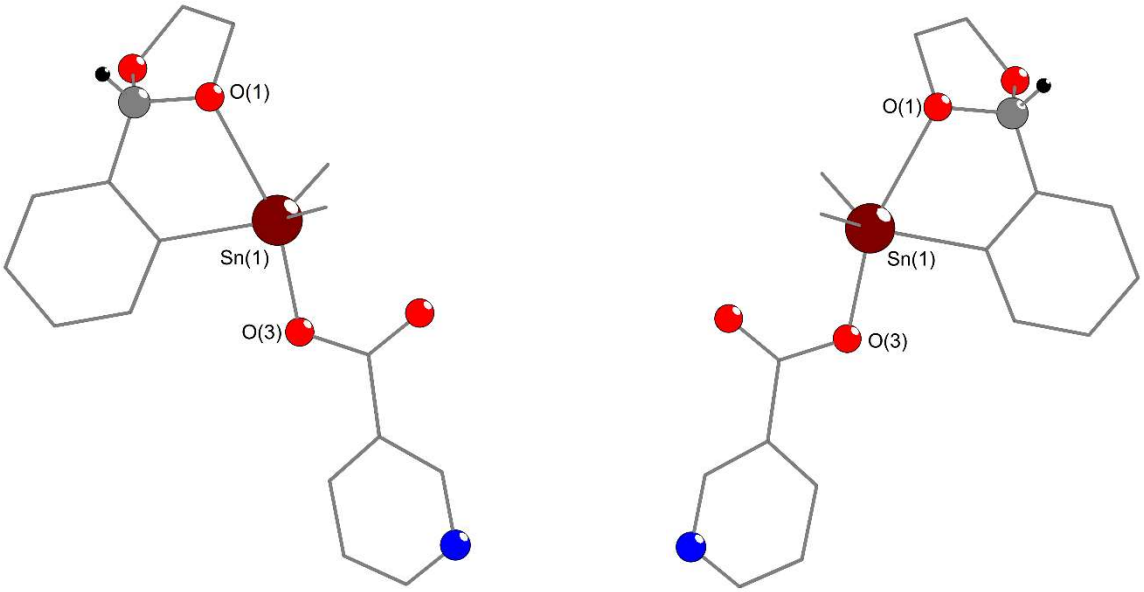

Figure S11. Molecular structure of *pR*$_{O(1)}$-*S*$_{O(1)}$-*R*$_{C(7)}$-**4** isomer (*left)* and *pS*$_{O(1)}$-*R*$_{O(1)}$-*S*$_{C(7)}$-**4** isomer (*right*) in the crystal of **4** (only methyne hydrogens are shown).

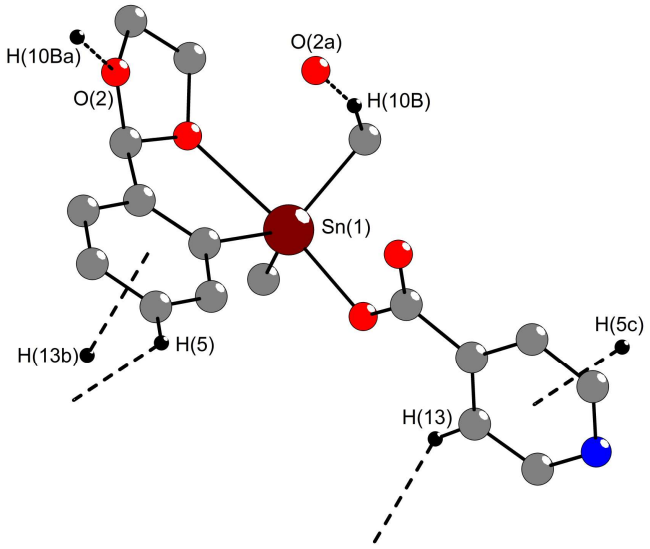

Figure S12. C–H···O and C–H···π interactions in the crystal of **3** [symmetry equivalent atoms (*–x,1–y, 1–z*), (*1–x, 1–y, 2–z*) and (*x, –1+y, z*) are given by "a", "b" and "c", respectively].

Intermolecular C–H···O interactions

C(10)–H(10B)···O(2a)	2.56 Å	Σr_{cov}(O,H) = 0.96 Å
		Σr_{vdW}(O,H) = 2.60 Å

Intermolecular C–H···π interactions

C(13)–H(13)···$Ph_{centroid}${C(1b)–C(6b)}	2.80 Å	γ = 5.0°
C(5c)–H(5c)···$Py_{centroid}$ {N(1),C(13)–C(17)}	3.02	γ = 9.4°

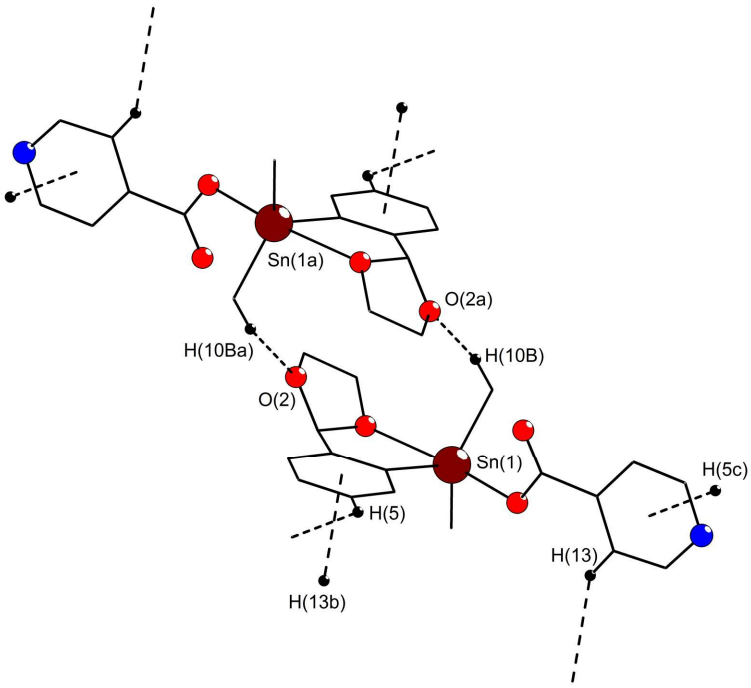

Figure S13. Dimer association in the crystal of **3** [symmetry equivalent atoms (*–x, 1–y, 1–z*), (*1–x, 1–y, 2–z)* and (*x, –1+y, z*) are given by "a", "b" and "c", respectively].

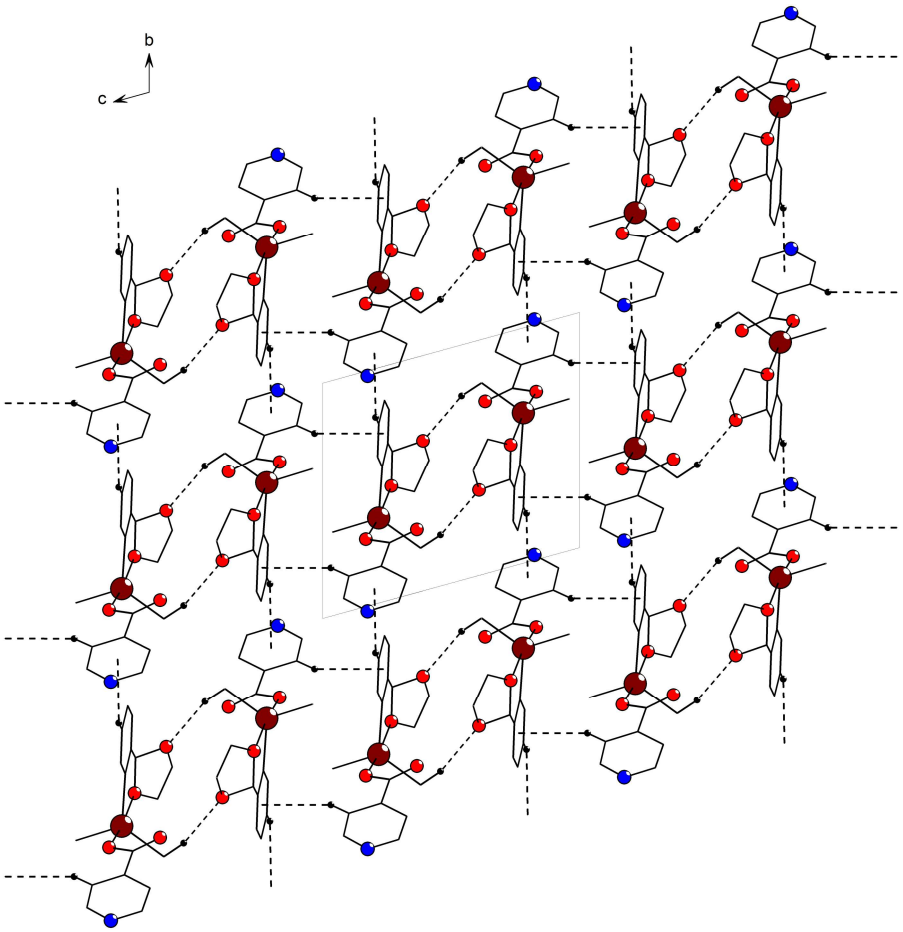

Figure S14. View along *a* axis in the packing of **3** showing a 2D layer (only hydrogen atoms involved in the intermolecular contacts are shown).

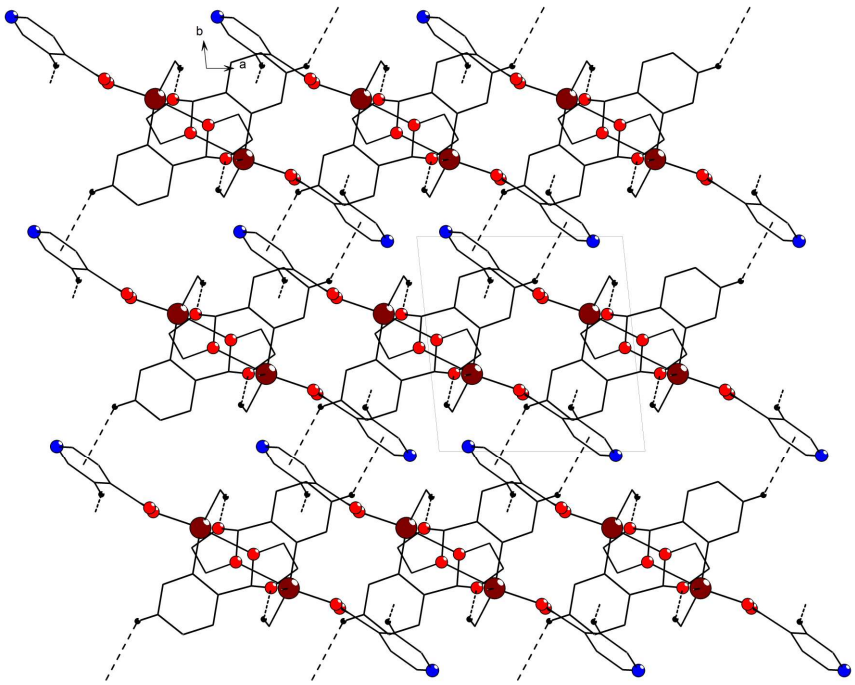

Figure S15. View along *c* axis in the packing of **3** showing a 2D layer (only hydrogen atoms involved in the intermolecular contacts are shown).

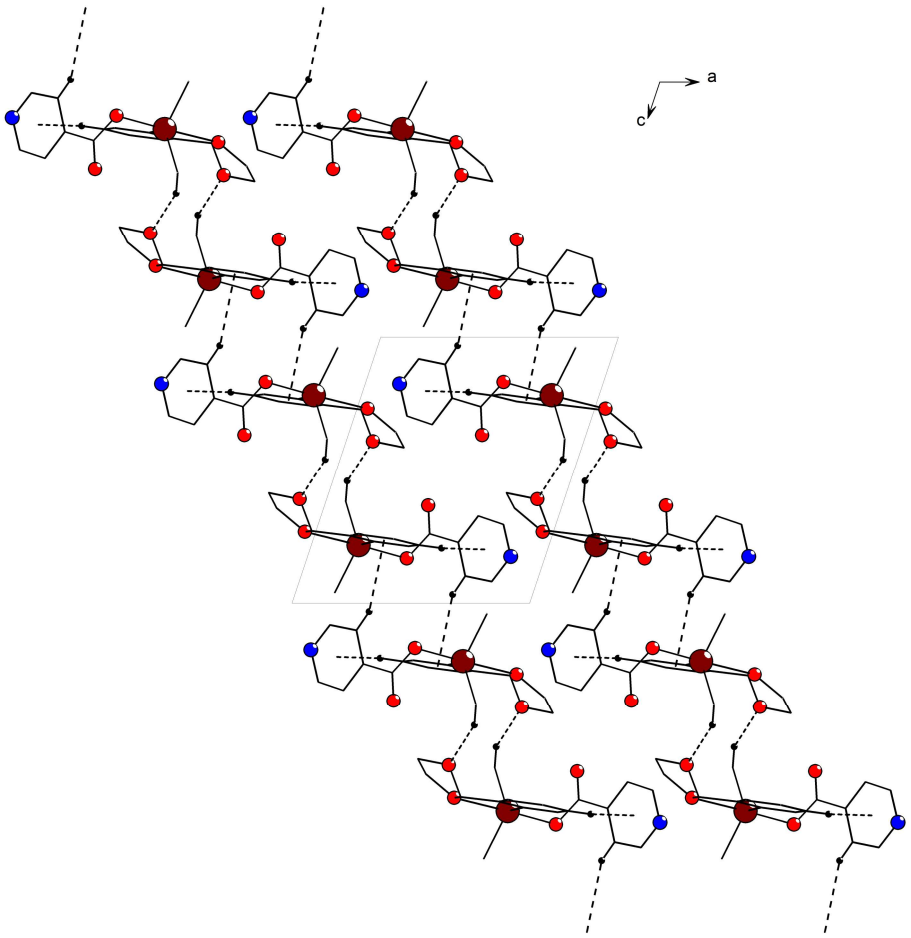

Figure S16. View along *b* axis in the packing of **3** showing parallel 2D layers (only hydrogen atoms involved in the intermolecular contacts are shown).

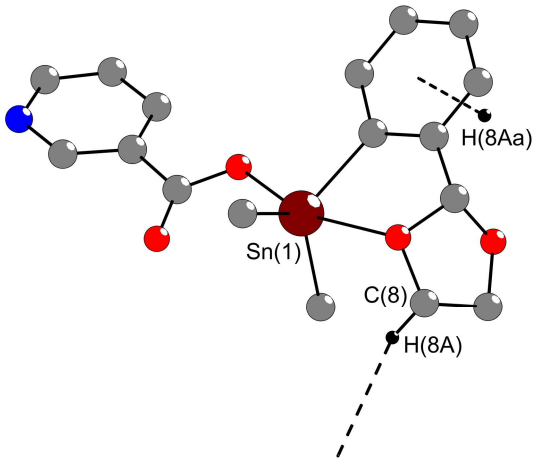

Figure S17. C–H···π interactions in the crystal of **4** [symmetry equivalent atom (*0.5–x, 0.5+y, z*) is given by "a"].

Intermolecular C–H···π interactions

C(8a)–H(8Aa)···$Ph_{centroid}${C(1)–C(6)}	2.73 Å	γ = 6.4°

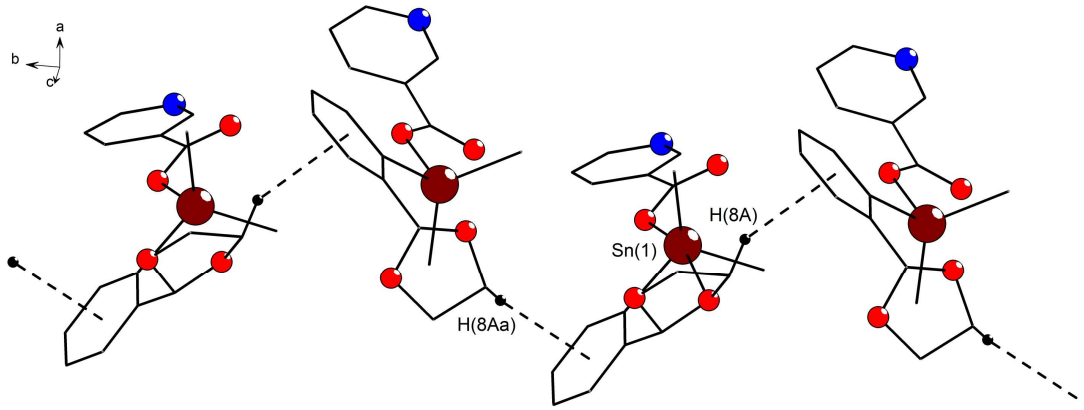

Figure S18. Zig-zag chain in the crystal of **4** [symmetry equivalent atom (*0.5–x, 0.5+y, z*) is given by "a"].

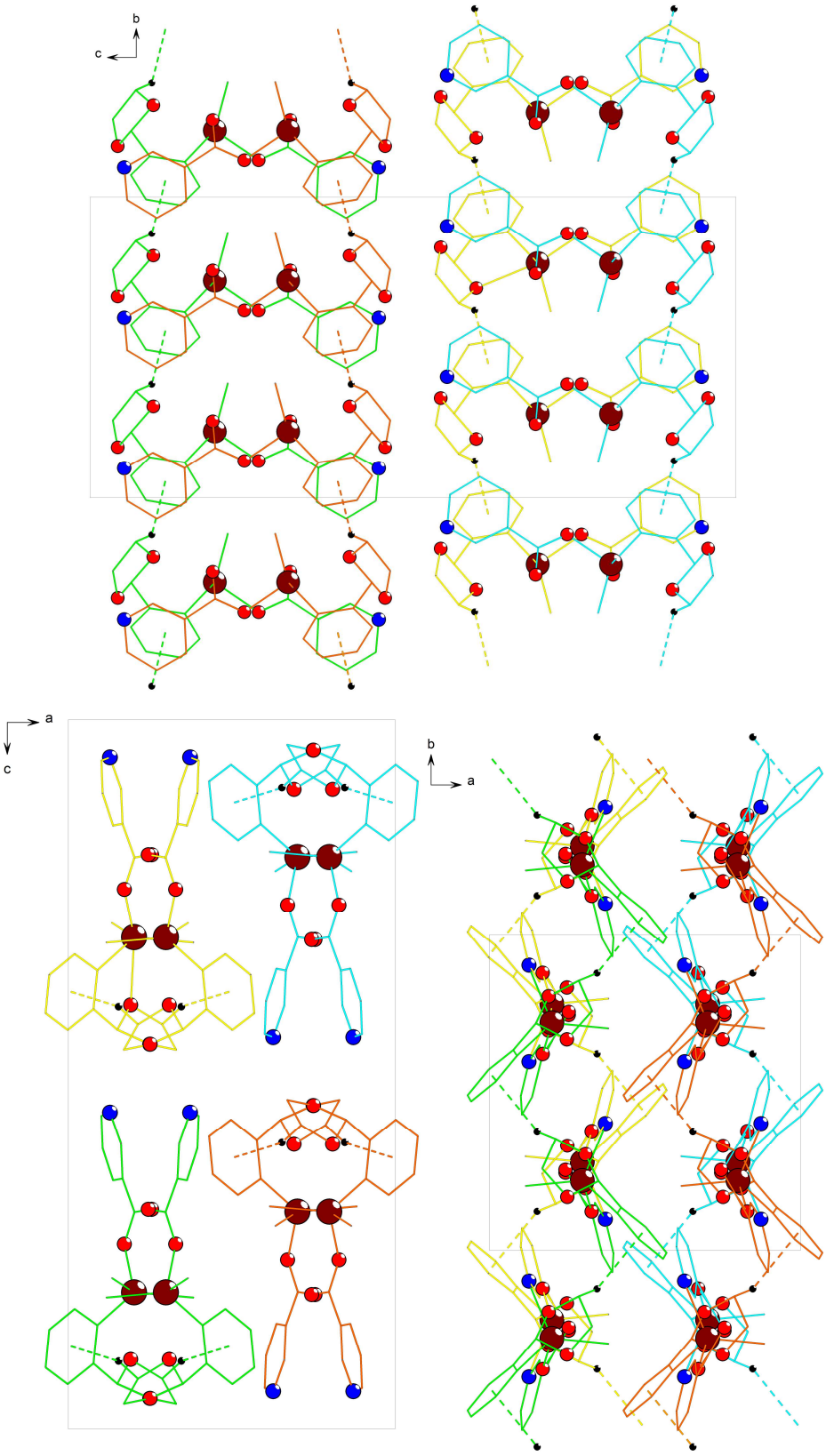

Figure S19. Parallel zig-zag chains in the crystal of **4**. View along *a*, *b* and *c* axis.

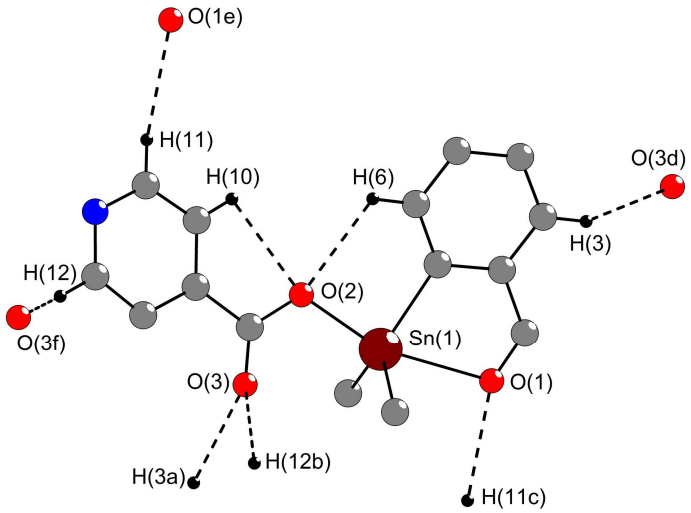

Figure S20. C–H···O intra- and intermolecular interactions in the crystal of **5** [symmetry equivalent atoms (*0.5–x, 1–y, –0.5+z*), (*1–x, 0.5+y, 0.5–z*), (*x, 1+y, z*), (*0.5–x, 1–y, 0.5+z*), (*x, –1+y, z*) and (*1–x, –0.5+y, 0.5–z*) are given by "a", "b", "c", "d", "e" and "f", respectively].

Intramolecular C–H···O interactions		
C(10)–H(10)···O(2)	2.48 Å	
C(6)–H(6)···O(2)	2.49 Å	
Intermolecular C–H···O interactions		
C(3)–H(3)···O(3d)	2.48 Å	Σr_{cov}(O,H) = 0.96 Å
C(12)–H(12)···O(3f)	2.49 Å	Σr_{vdW}(O,H) = 2.60 Å
C(11)–H(11)···O(1e)	2.54 Å	

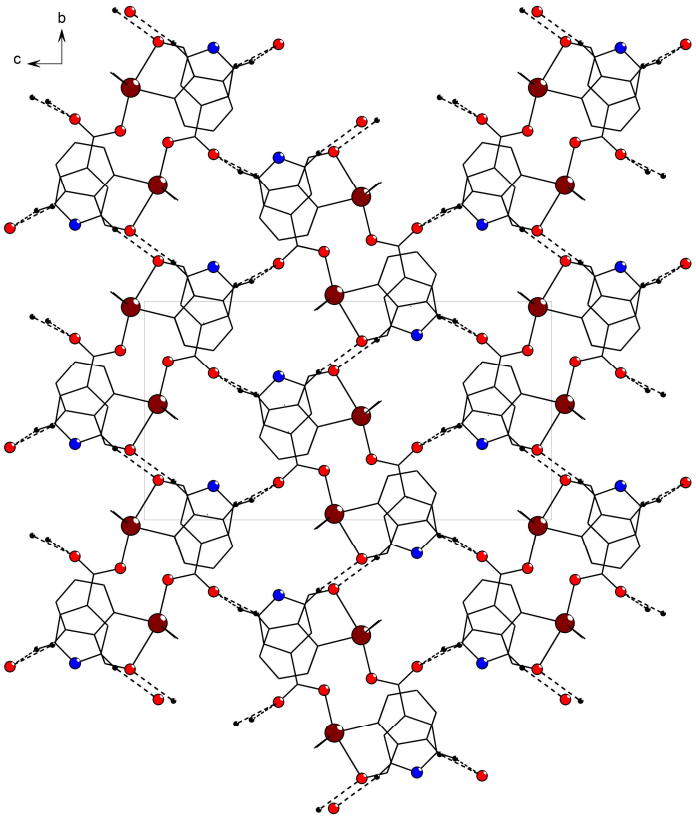

Figure S21. View along *a* axis of the crystal packing in **5**.

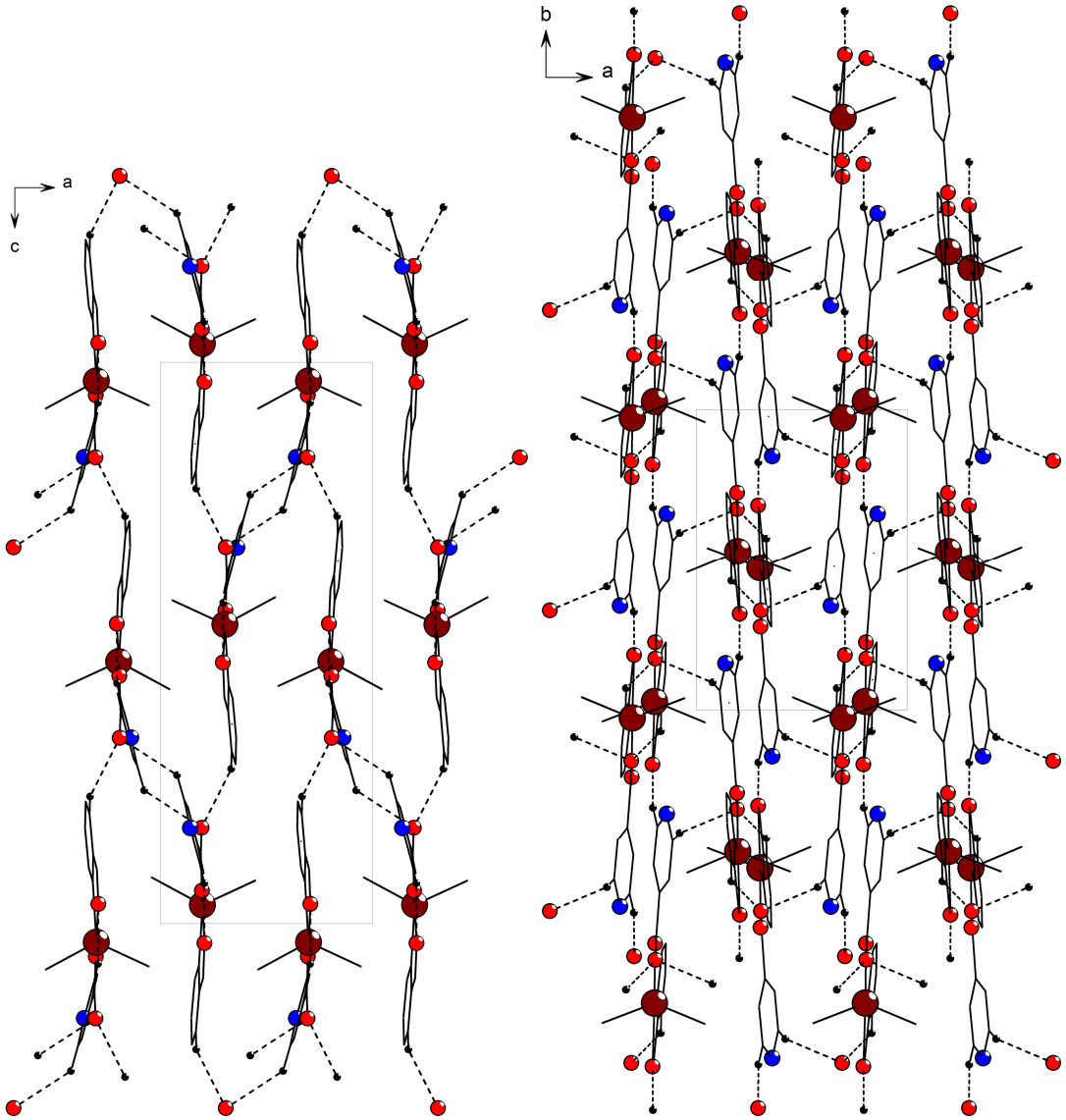

Figure S22. View along *b* and *c* axis of the 3D supramolecular architecture in the crystal of **5**.

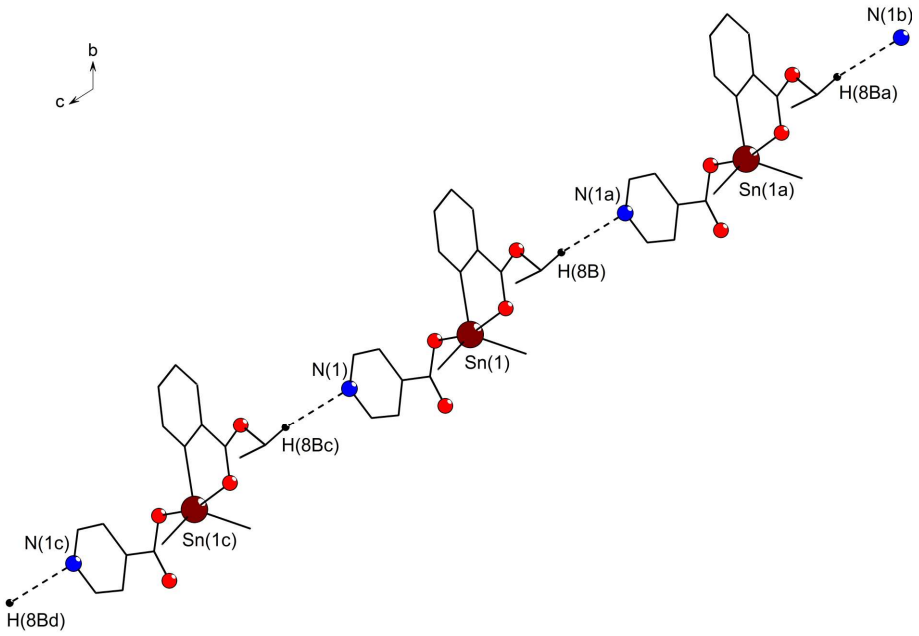

Figure S23. Polymer chain formed *via* C–H···N interactions in the crystal of **7** [symmetry equivalent atoms (*1+x, y, –1+z*), (*2+x, y, –2+z*), (*–1+x, y, 1+z*) and (*–2+x, y, 2+z*) are given by "a", "b", "c" and "d", respectively].

C(8)–H(8B)···N(1a)	2.64 Å	Σr_{cov}(N,H) = 1.00 Å	Σr_{vdW}(N,H) = 2.75 Å

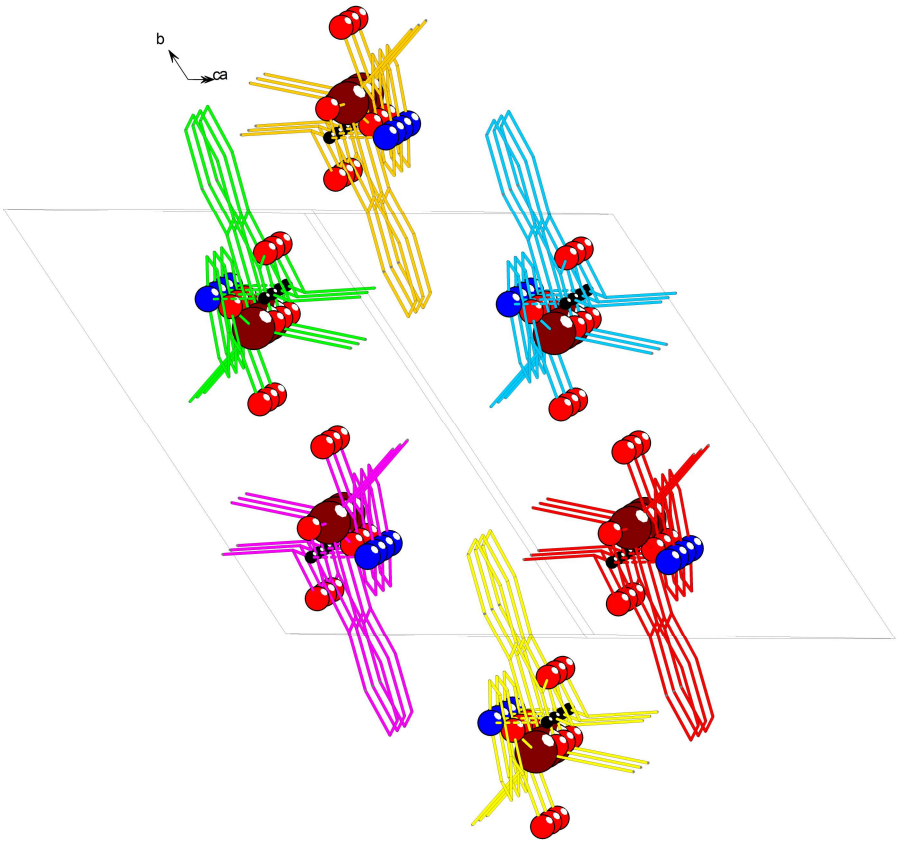

Figure S24. Parallel chains in the crystal packing of **7**.

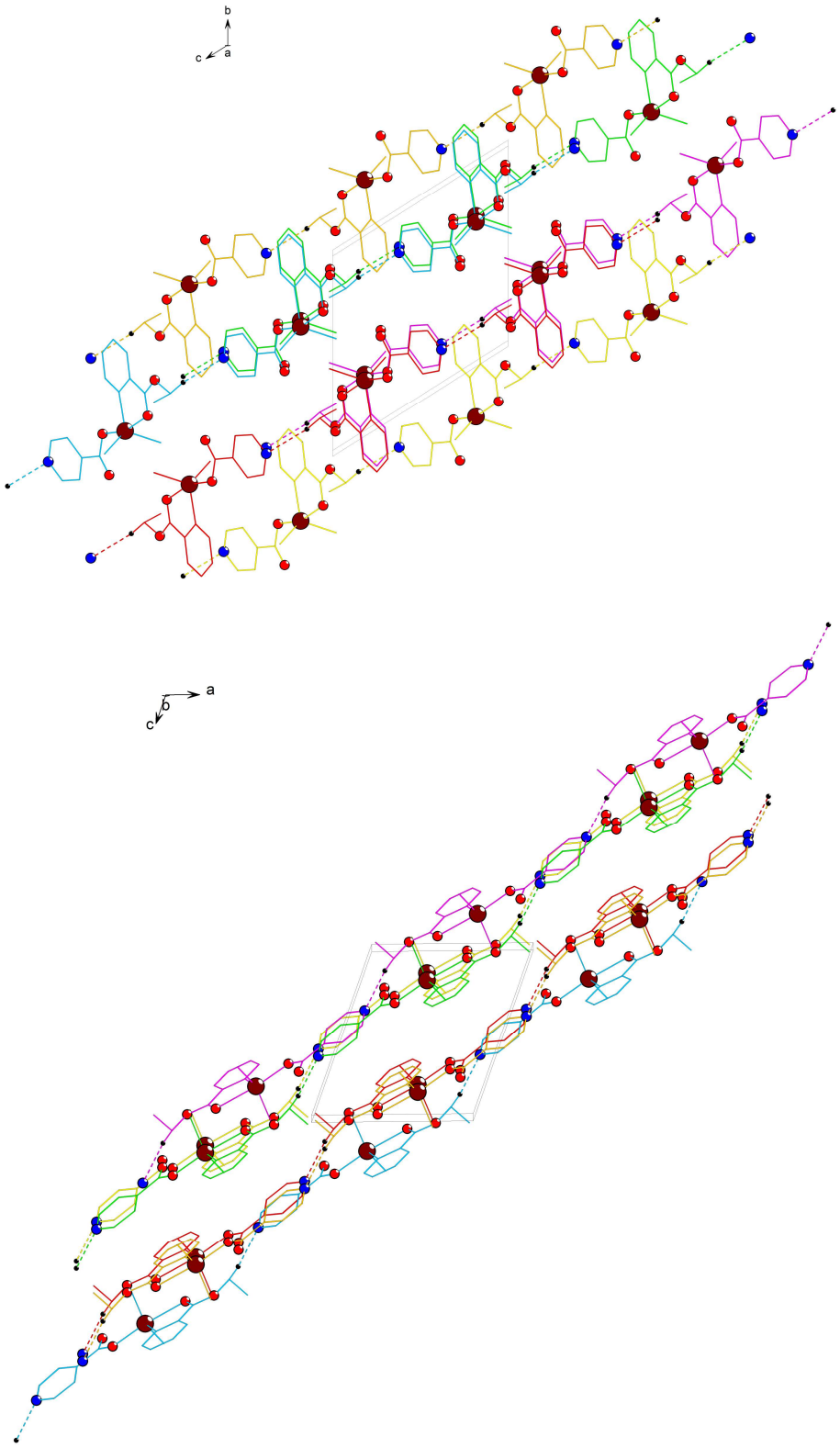

Figure S25. View along *a* and *b* axis in the crystal packing of **7**.

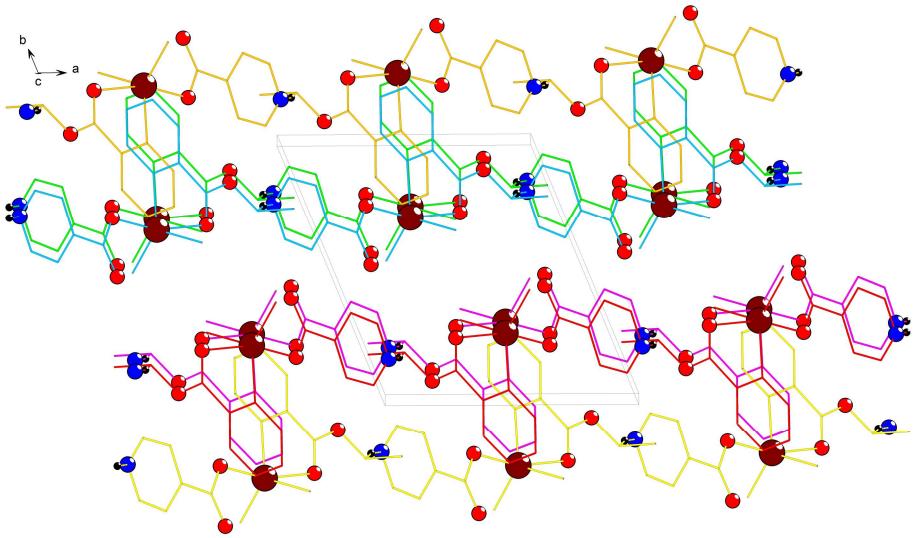

Figure S26. View along *c* axis in the crystal packing of **7**

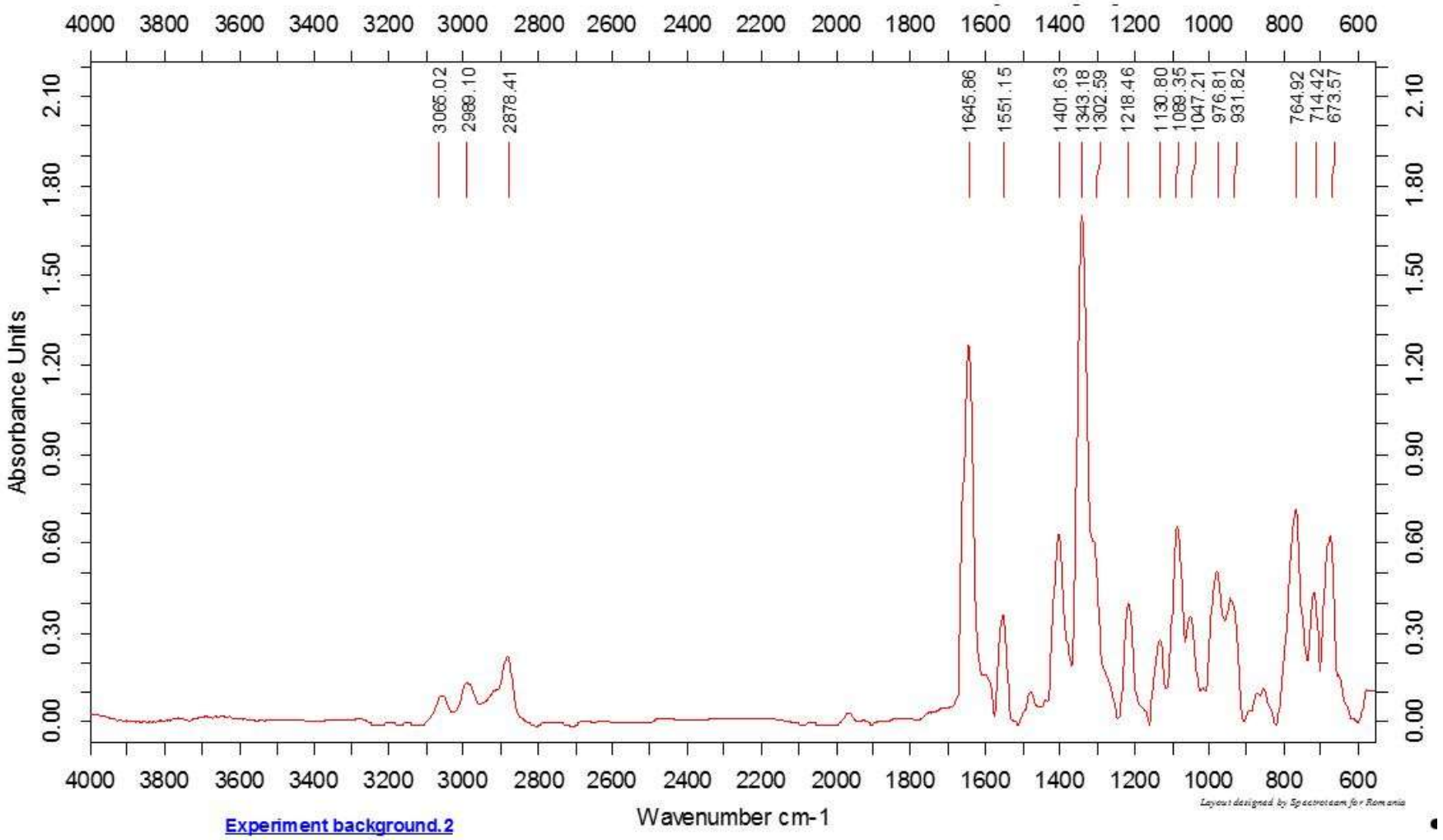

Figure S27. IR spectrum of compound **3**.

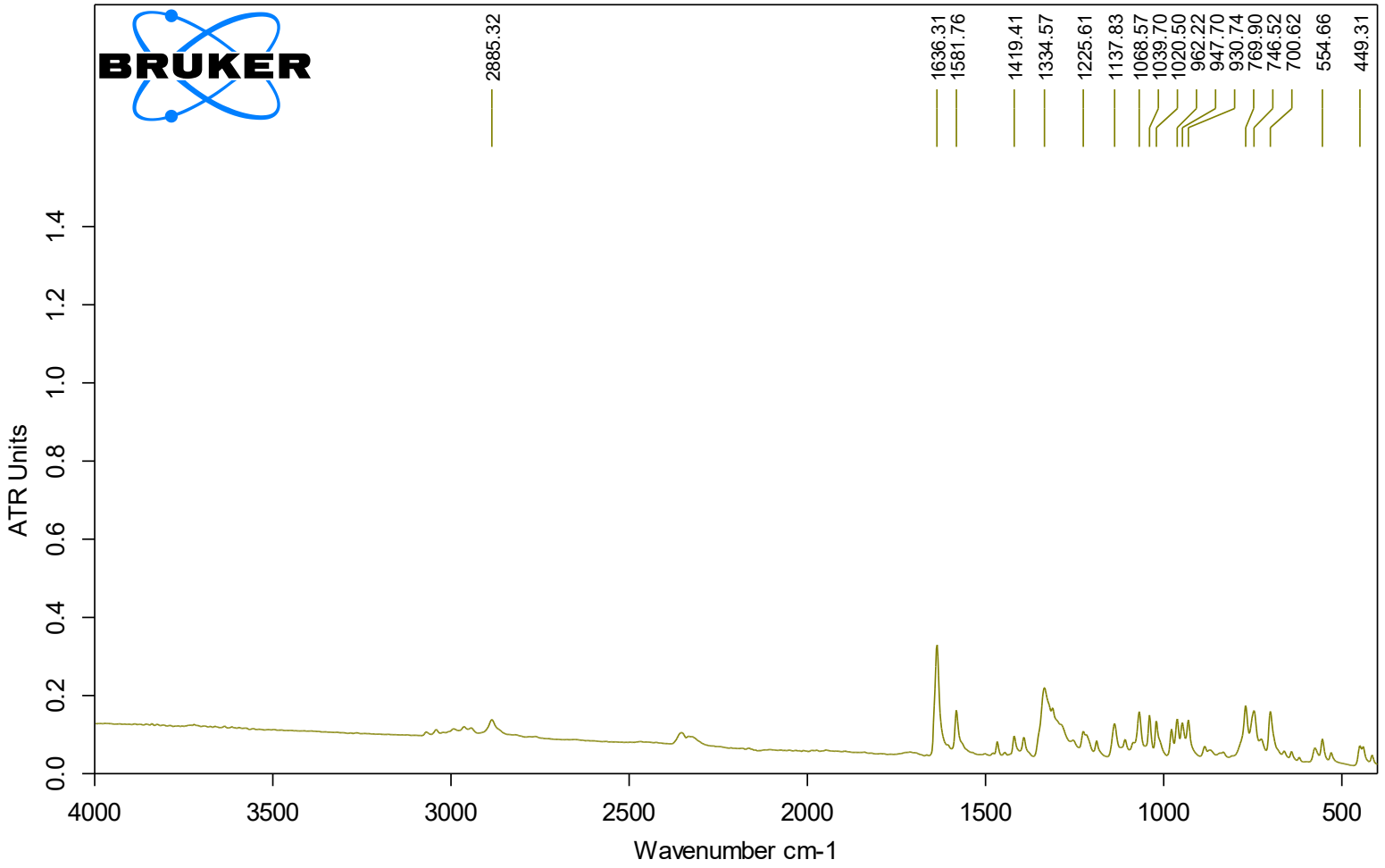

Figure S28. ATR-IR spectrum of compound **4**.

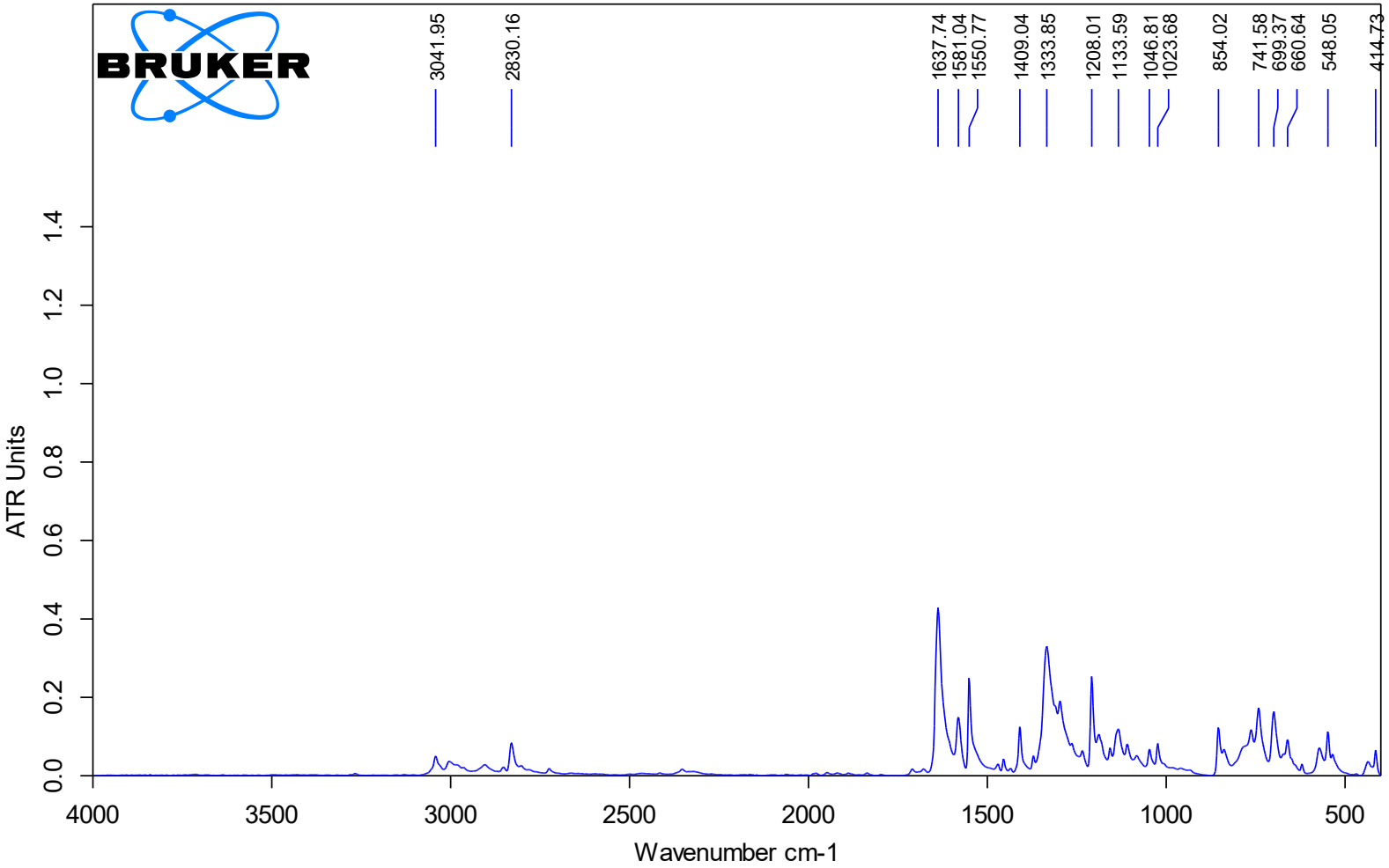

Figure S29. ATR-IR spectrum of compound **6**.

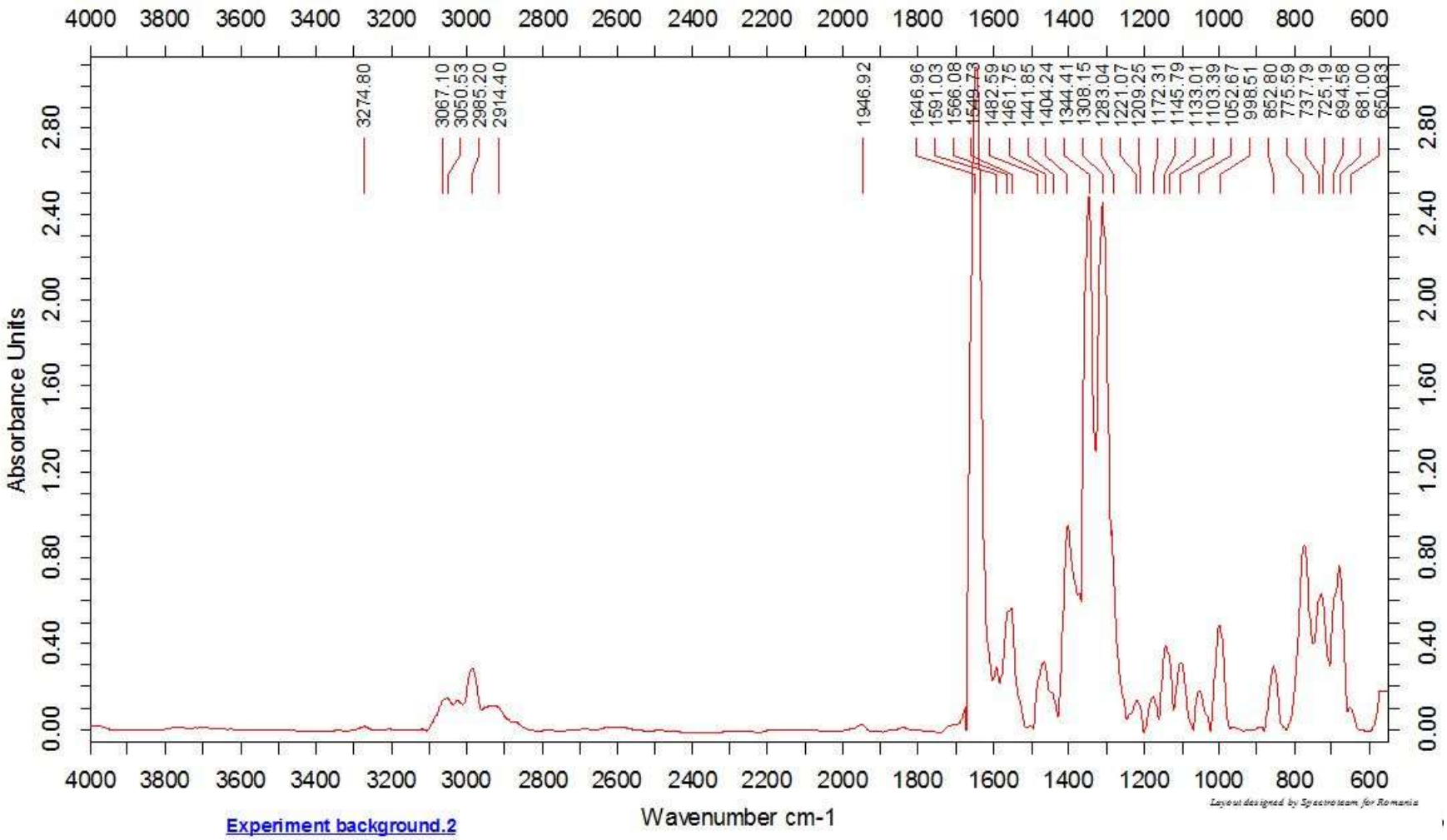

Figure S30. IR spectrum of compound **7**.

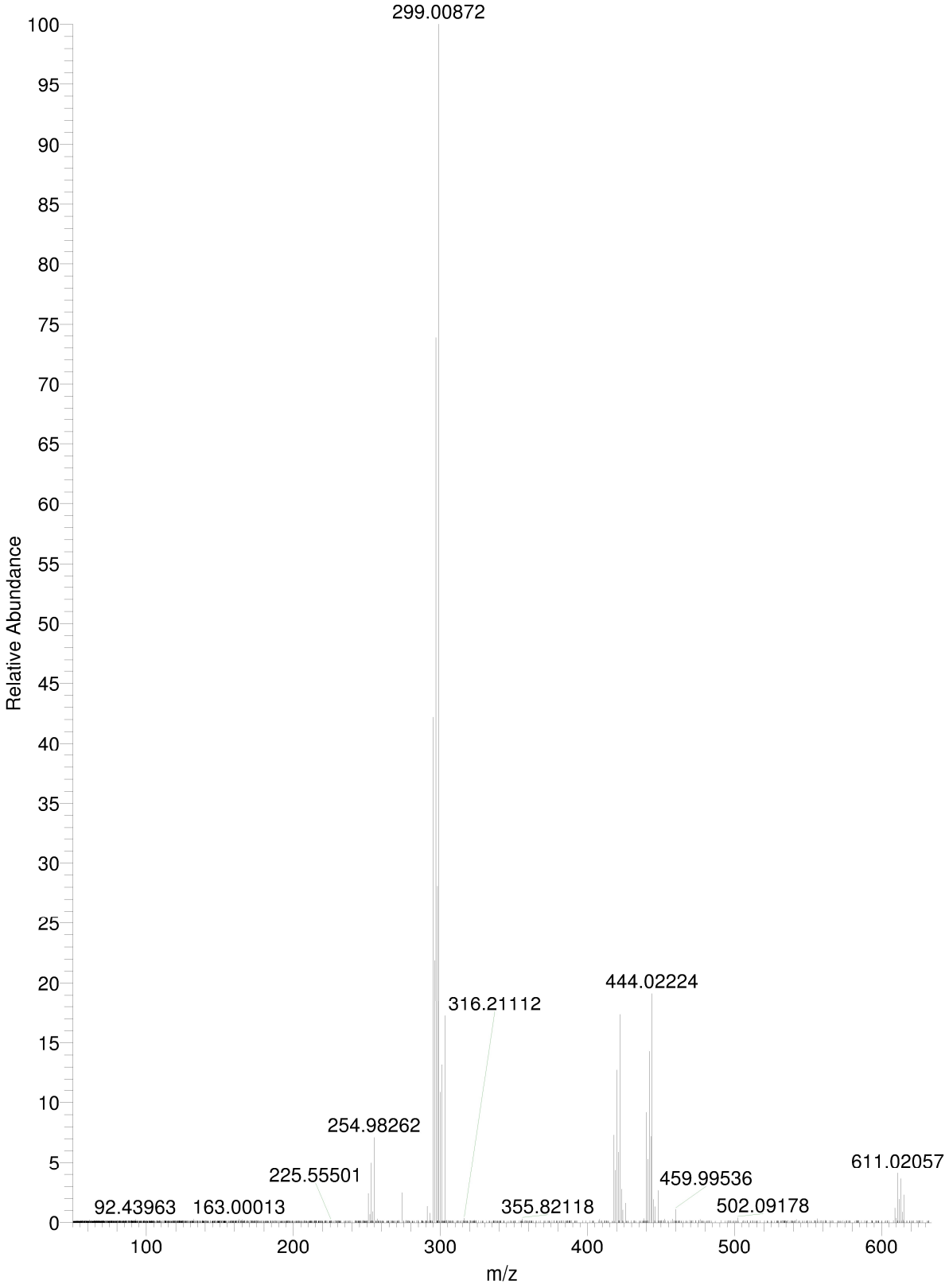

Figure S31. HRMS spectrum of compound **3**.

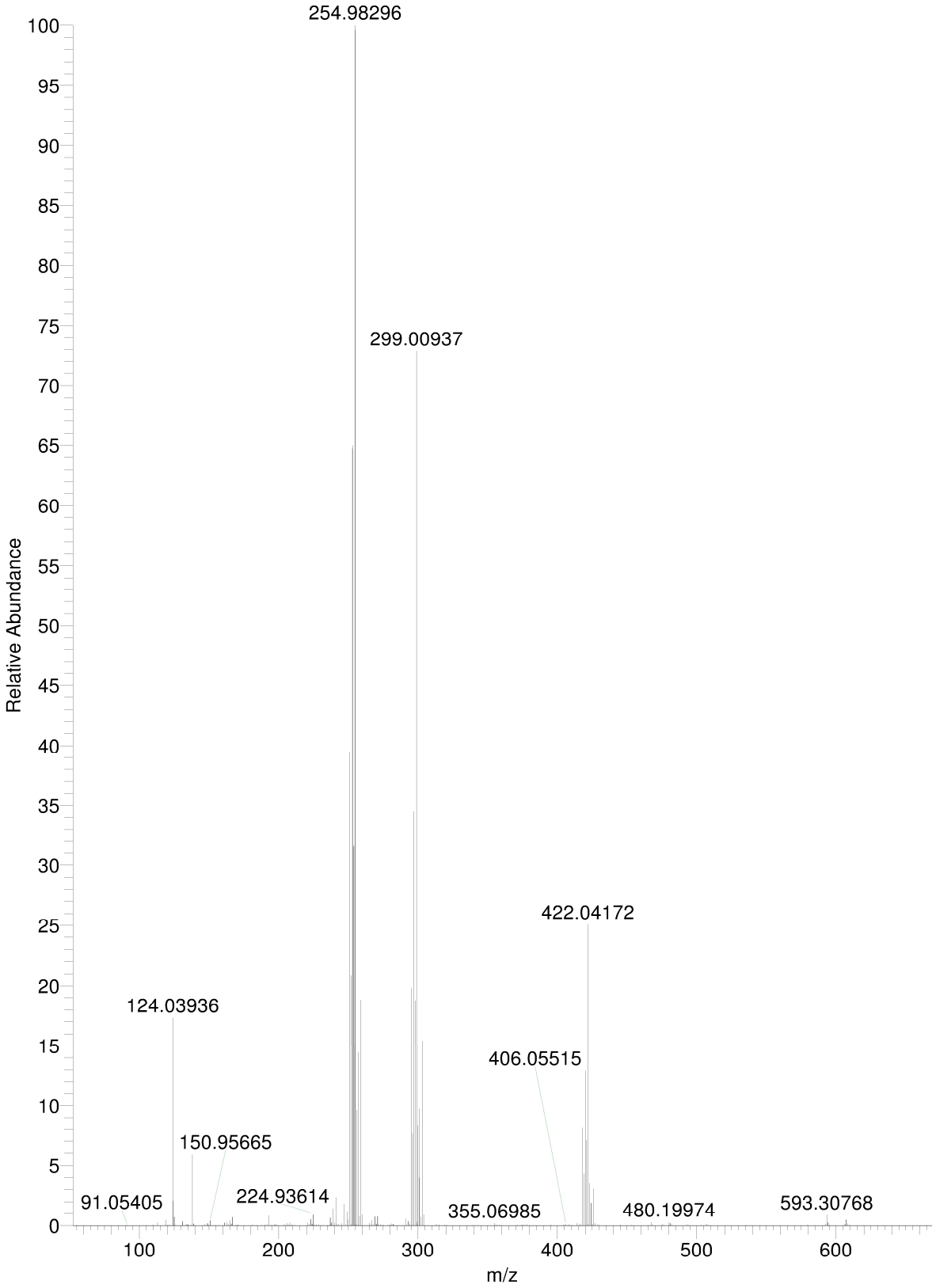

Figure S32. HRMS spectrum of compound **4**.

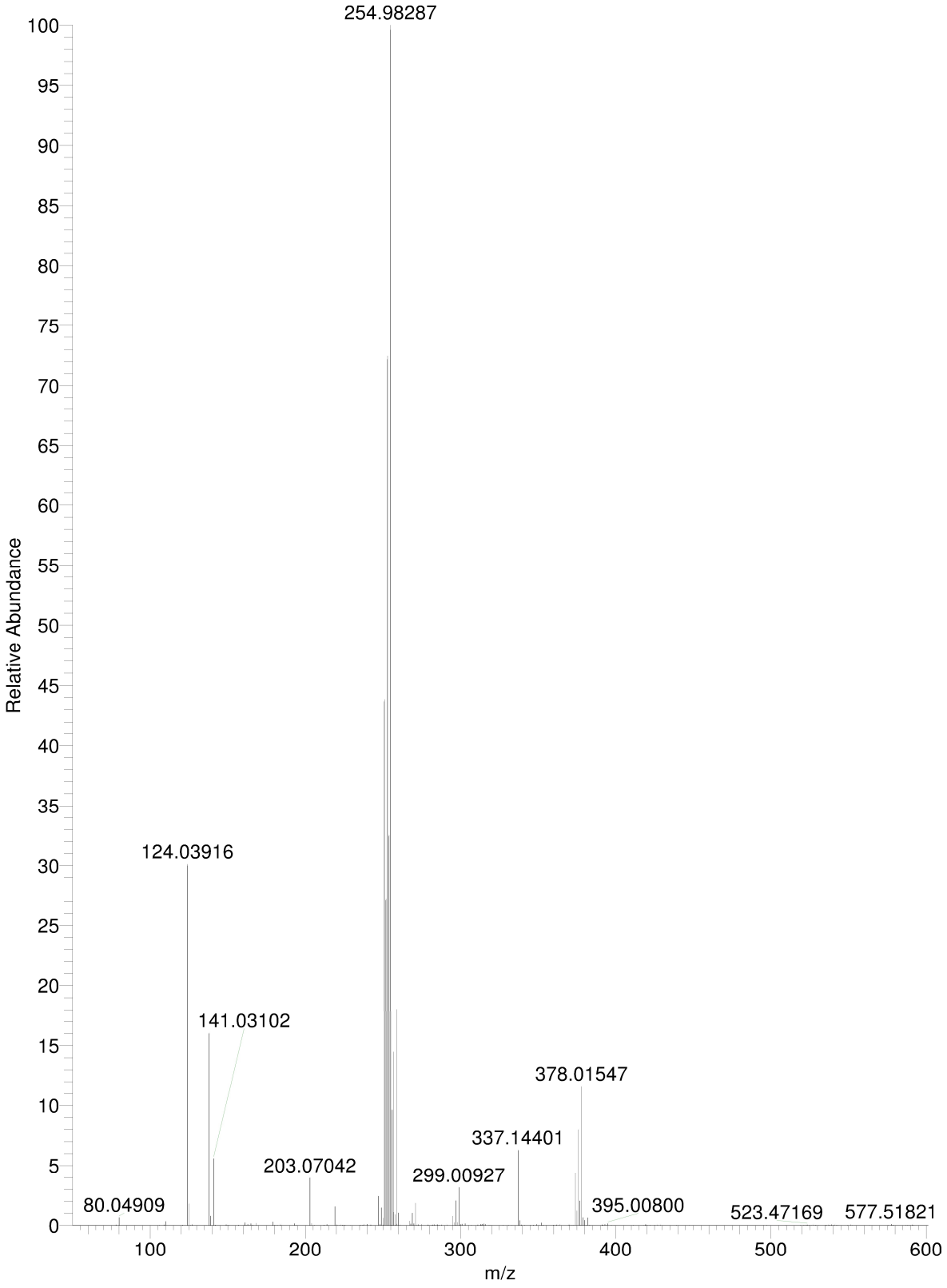

Figure S33. HRMS spectrum of compound **6**.

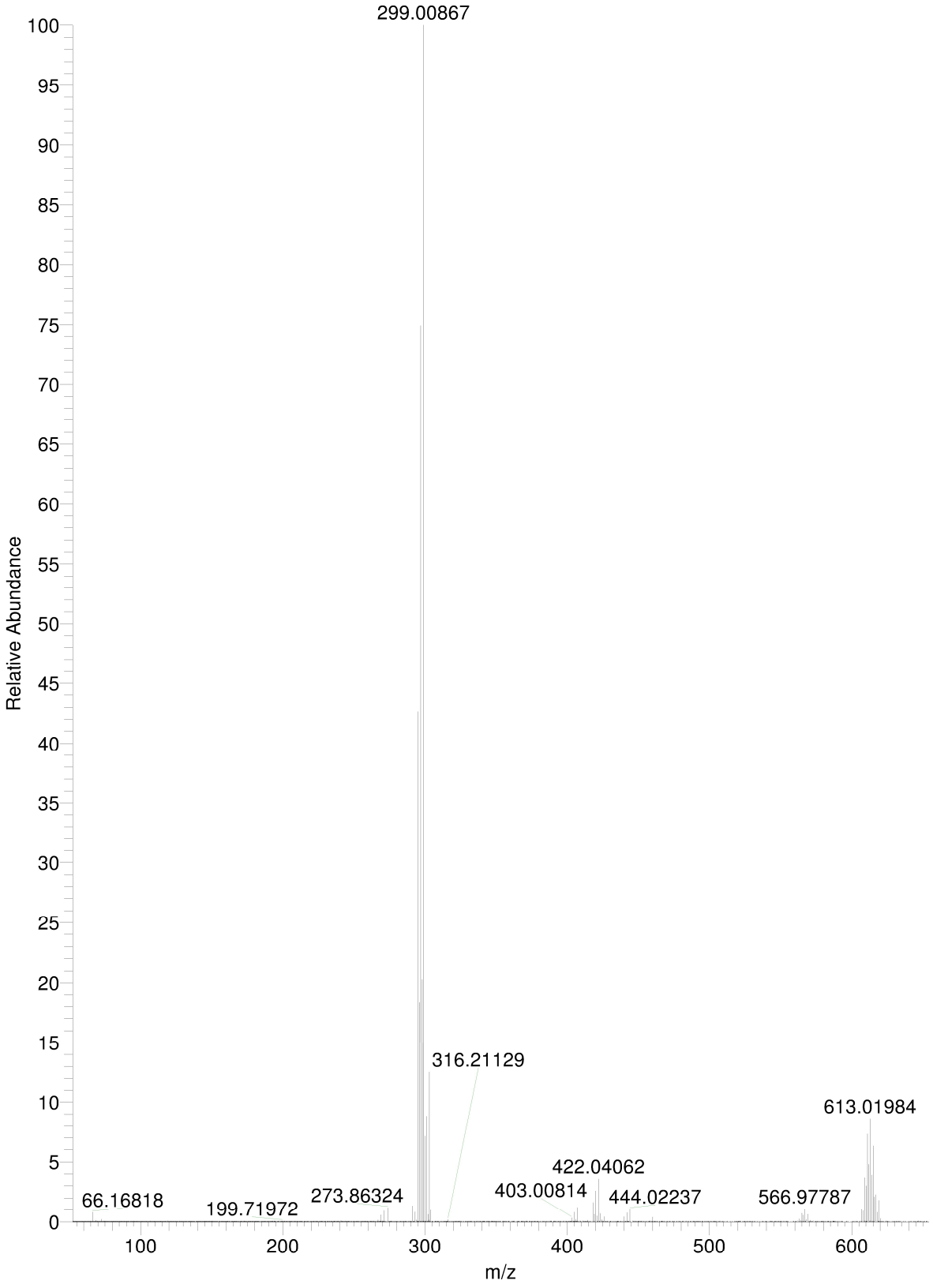

Figure S34. HRMS spectrum of compound **7**.