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SUPPLEMENTARY DATA

Water stable fluorescent organotin(IV) compounds: Aggregation induced emission enhancement and recognition of lead ions in aqueous system

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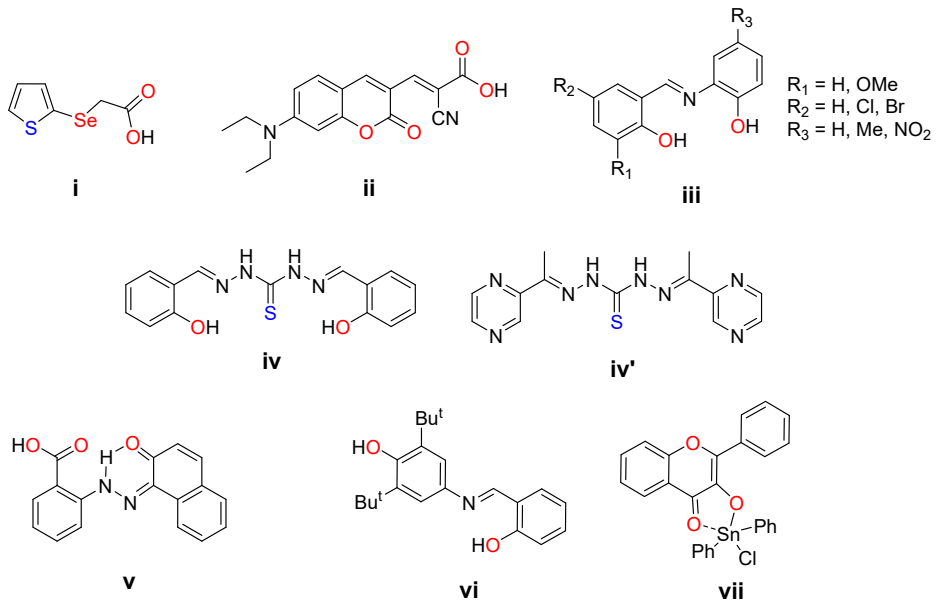


Chart S1. Some of the ligating systems for deriving organotin compounds (**i-vi**), and 3-hydroxy-4*H*-chromen-4-one based organotin compound (**vii**) for selective fluorometric detection of pyrophosphate.

1. Results and discussion

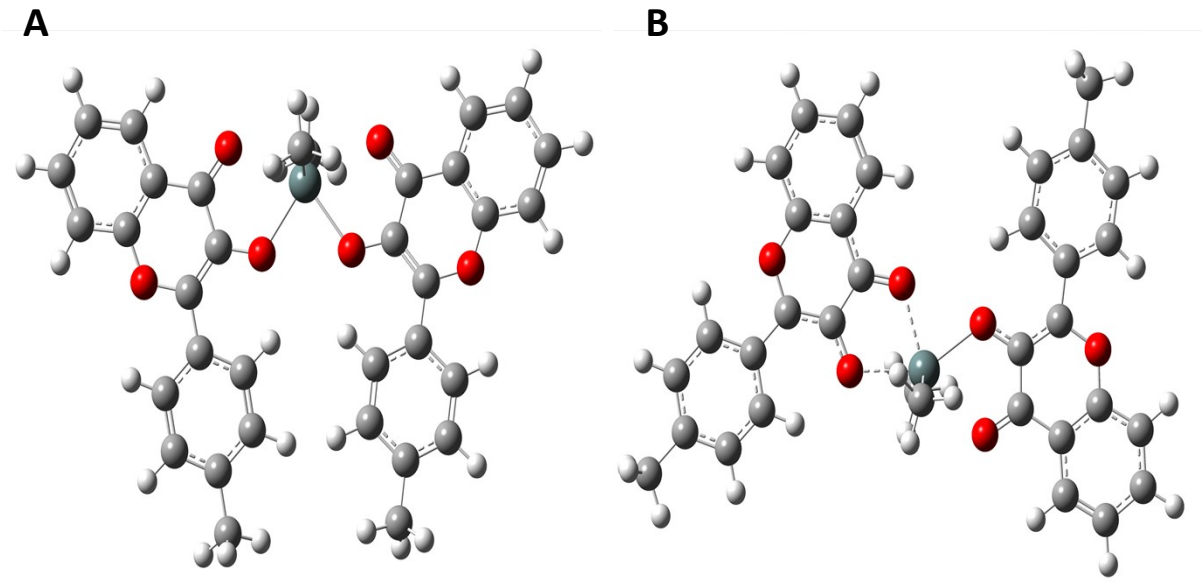


Figure S1. Geometry-optimized (B3LYP/DGDZVP) structures of compound **4b**. Sn-$O_{(keto)}$ and Sn-$O_{(hydroxyl)}$ bonds; (**A**) in *cis*-configuration (**B**) in *trans* configuration.

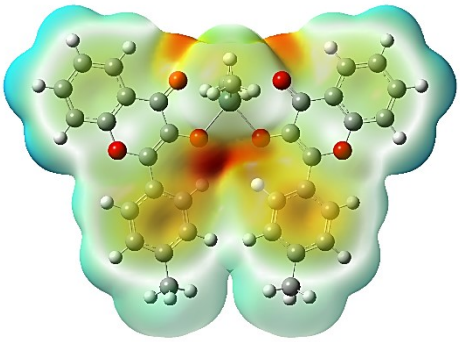


Figure S2. MEP diagram for 4b: The red, orange, yellow, green, and blue are standard colors for representing the magnitude of electrostatic potential. They are arranged in the order like, blue > green > yellow > orange > red, where the highest electropositive potential is indicated by blue region and most electronegative potential by red region.

Table S1. Calculated coordinates of **4b-(A)** *cis*-configured Sn-$O_{(keto)}$ and Sn-$O_{(hydroxyl)}$ bonds with B3LYP/DGDZVP on Sn, H, C, and O.
0,1

atom	x	y	z
Sn	0.0000326553	-1.9318220007	0.0001189831
O	-1.3623862026	-0.2864065701	0.0218632969
O	-4.9514985553	0.2581763729	-0.0051455026
O	1.3623827798	-0.2863585028	-0.0212046092
O	4.9515001644	0.2582257554	0.0050161796
O	-2.2816299754	-2.809039615	-0.1667913
O	2.2816663931	-2.8090044334	0.1667828555
C	3.3450069793	1.9610096077	-0.2676849178
C	-2.6707808095	-0.4974747563	-0.0118160729
C	-3.3450484262	1.9609463773	0.2678746746
C	2.6707886973	-0.4974185273	0.0121070658
C	-5.4239517465	-1.0030131841	-0.1531217801
C	-3.6039598001	0.5303233708	0.0774444966
C	-3.131366756	-1.8741673852	-0.1340511014
C	-4.5593496204	-2.1082537238	-0.2152828863
C	3.6039460967	0.5303859012	-0.0773122516
C	5.4239822025	-1.00297502	0.1527945489
C	3.1313989327	-1.874128247	0.1340554154
C	4.5593955006	-2.1082252373	0.214998672
C	-6.8177641853	-1.1626847039	-0.2327380827
H	-7.4572437753	-0.286345646	-0.179243849
C	5.1140131679	-3.4011401294	0.3594286602
H	4.4344025944	-4.2466742903	0.4066282896
C	-2.9116981877	4.7457444066	0.7022624505
C	4.4079683195	2.8899399614	-0.1875368411
H	5.410040558	2.5418323342	0.03711364
C	6.8178083268	-1.1626500398	0.2321620236
H	7.4572773523	-0.2863044588	0.1786479742
C	2.0581273014	2.4581406848	-0.5674195062
H	1.224754441	1.7712981653	-0.6363177869
C	-5.1139395533	-3.4011560895	-0.359937638
H	-4.4343178919	-4.2466831789	-0.4071034056
C	-4.4079221614	2.889921662	0.1871314456
H	-5.4098945128	2.541846901	-0.0380194795
C	-7.3388945779	-2.4410535499	-0.3756255902
H	-8.4158605619	-2.5748388063	-0.4378208951
C	-2.0583016998	2.4580229866	0.5682573502
H	-1.2249998311	1.7711396079	0.6376178459
C	-6.4865733067	-3.566680958	-0.4396481704
H	-6.9124120761	-4.5600719895	-0.5516355957
C	2.9115715316	4.7458124136	-0.7019872325
C	-1.8595336275	3.822428623	0.7859404545
H	-0.8588662488	4.1706442382	1.0341436616
C	-4.1901831777	4.2485543276	0.3962394567
H	-5.030673627	4.9370211728	0.3262826588
C	6.4866614095	-3.5666684858	0.4388904365

H	6.9125219963	-4.5600693021	0.5507074372
C	4.1901898976	4.2485716905	-0.3966042656
H	5.0307532222	4.9369978069	-0.3271212931
C	-0.1039499608	-2.6526072682	2.0326437321
H	0.7226145901	-2.2299320844	2.608418893
H	-0.0190502679	-3.7422388473	2.0359252807
H	-1.0585541476	-2.3625755534	2.4768401033
C	1.8593170955	3.822545991	-0.785063825
H	0.8585342544	4.170798357	-1.0327472704
C	0.1039477357	-2.6519988434	-2.0326294052
H	-0.7223455355	-2.2287032845	-2.6083434612
H	0.0184766365	-3.7415840855	-2.0363001091
H	1.0587354202	-2.3622953776	-2.476643529
C	7.3389671797	-2.4410317417	0.3748358244
H	8.4159442414	-2.5748181786	0.4368369415
C	2.6822455613	6.2255518194	-0.9105920809
H	2.6341907285	6.7555787918	0.0491406782
H	1.7431692265	6.4149738178	-1.4387894199
H	3.4937875791	6.6790095669	-1.4894447016
C	-2.6823983921	6.2254861383	0.9108809188
H	-3.4943363124	6.6790828007	1.4890666684
H	-2.6335694977	6.7553990766	-0.0488768764
H	-1.7437017607	6.4148843688	1.4397617187

Table S2. Calculated coordinates of **4b-(B)** *trans*-configured Sn-$O_{(keto)}$ and Sn-$O_{(hydroxyl)}$ bonds with B3LYP/DGDZVP on Sn, H, C, and O.

0,1

atom	**x**	**y**	**z**
Sn	0.0741172753	-1.0552787371	-0.0000073724
O	2.3817726802	-1.0139617577	0.0003253839
O	4.7233488728	1.7616385622	0.0001854272
O	-1.7813542803	0.0240048684	-0.0001214875
O	-5.3377408496	-0.6998493117	0.0003708514
O	0.7107236199	1.0642570472	-0.0000361216
O	-1.7764436355	-2.6735621679	-0.0002662421
C	-4.4145855956	1.4693747923	0.000380126
C	2.899434099	0.1844008165	0.0002239694
C	5.3710110817	-0.5042587511	0.0004865279
C	-2.934870262	-0.6259014335	0.0000408777
C	3.8817184719	2.8193035333	-0.0000037758
C	4.2753293688	0.462871501	0.0002956776
C	1.9731221677	1.3004489441	0.0000289969
C	2.4851520026	2.6431894804	-0.0000905687
C	-4.1657524537	0.024282942	0.0002588661
C	-5.3475933983	-2.0542643156	0.0002810558
C	-2.8939710338	-2.0835719263	-0.0000645869
C	-4.1557876159	-2.7975858848	0.0000553759
C	4.4559339652	4.1021721239	-0.0001124803
H	5.5376769039	4.199702375	-0.0000402152

C	-4.2327422325	-4.2097749401	-0.0000273922
H	-3.3038176166	-4.7720132415	-0.0001992859
C	7.5377898628	-2.3585752011	0.0008504815
C	-5.7393861884	1.9588739778	0.0006471011
H	-6.5702240601	1.2623640728	0.0007639349
C	-6.601788292	-2.6882557287	0.000420035
H	-7.5034801166	-2.082655938	0.0005907634
C	-3.3637345048	2.4163760386	0.0002484701
H	-2.3386780066	2.069848262	0.0000568361
C	1.6540166478	3.7915383687	-0.0002958644
H	0.5784523039	3.6451790792	-0.0003659837
C	6.7158516079	-0.0616681692	0.0005320165
H	6.9321974814	1.0009624957	0.0004247822
C	3.6212595973	5.2096939758	-0.0003118005
H	4.0552522029	6.2061994322	-0.0003990404
C	5.1368191002	-1.8969941577	0.0006280296
H	4.1172443869	-2.259106655	0.0005941116
C	2.2143984105	5.0559340945	-0.000405265
H	1.5771982315	5.9360909864	-0.0005639442
C	-4.9604644446	4.2700406609	0.0006348871
C	6.2059483014	-2.7949582331	0.0008047779
H	5.9933143409	-3.8622913355	0.0009082379
C	7.7680223859	-0.9704749217	0.0007090669
H	8.7909777347	-0.597565713	0.0007362827
C	-5.464905729	-4.8419492541	0.00011023
H	-5.5233917861	-5.9269952219	0.0000513072
C	-6.0004274199	3.3282197043	0.0007715983
H	-7.0337376758	3.669943795	0.0009851636
C	0.2400875005	-1.6669545104	-2.0642976436
H	-0.740188682	-1.6230532742	-2.5434336061
H	0.6153656175	-2.6928750322	-2.1043148716
H	0.945550285	-1.0113697432	-2.579787008
C	-3.643808326	3.7815083372	0.0003764618
H	-2.8141996419	4.48700969	0.0002796571
C	0.2396544182	-1.667043508	2.0643008111
H	0.9445456259	-1.011087252	2.5800992679
H	0.6155454132	-2.6927385887	2.1043618912
H	-0.7408123514	-1.6237550469	2.5430997286
C	-6.652214427	-4.0751797582	0.0003342481
H	-7.6177733651	-4.5745378708	0.0004406404
C	-5.2381962967	5.7562804542	0.0007047246
H	-4.804222728	6.2411599447	-0.8816629573
H	-4.8027323432	6.2413716263	0.8822155318
H	-6.3120078944	5.964282994	4,0.0015750127
C	8.6927739429	-3.3337144005	0.0010591455
H	9.3291315972	-3.1948874801	0.8830157943
H	9.3294790243	-3.1948601508	-0.8806404315
H	8.3428877238	-4.3698143643	0.0009777806

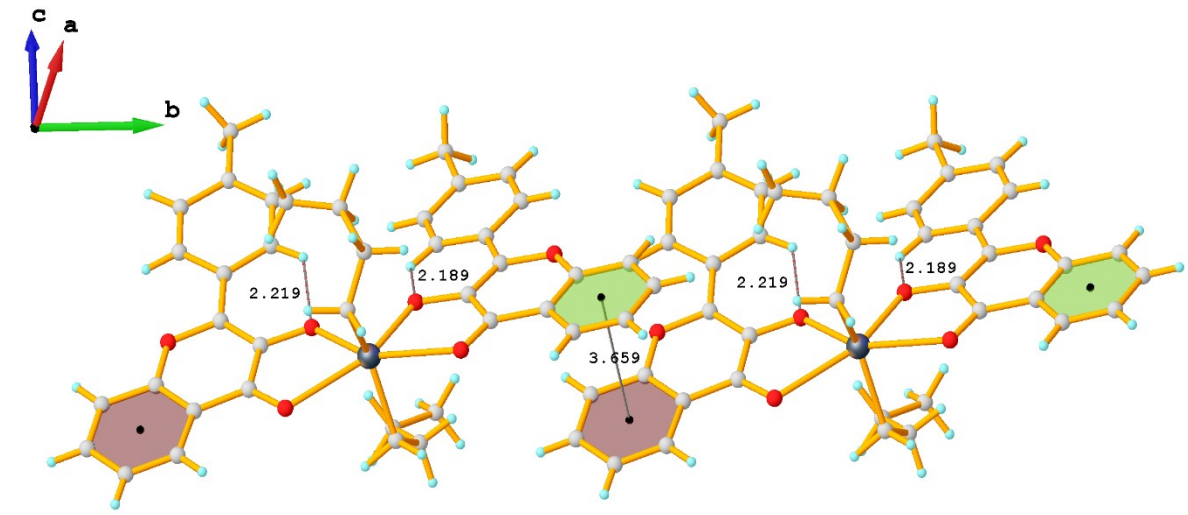


Figure S3. Intramolecular hydrogen bonding and π···π interactions in compound **4a**.

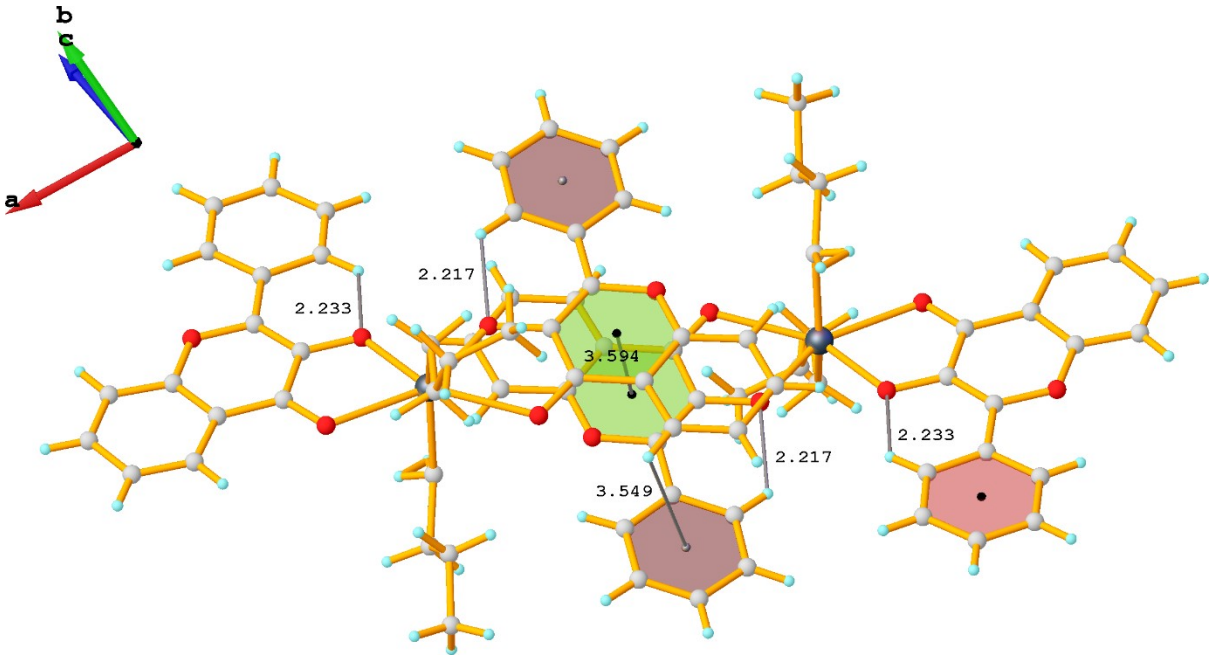


Figure S4. Intramolecular hydrogen bonding and non-covalent π···π, and C–H·····π interactions in the compound **5a**.

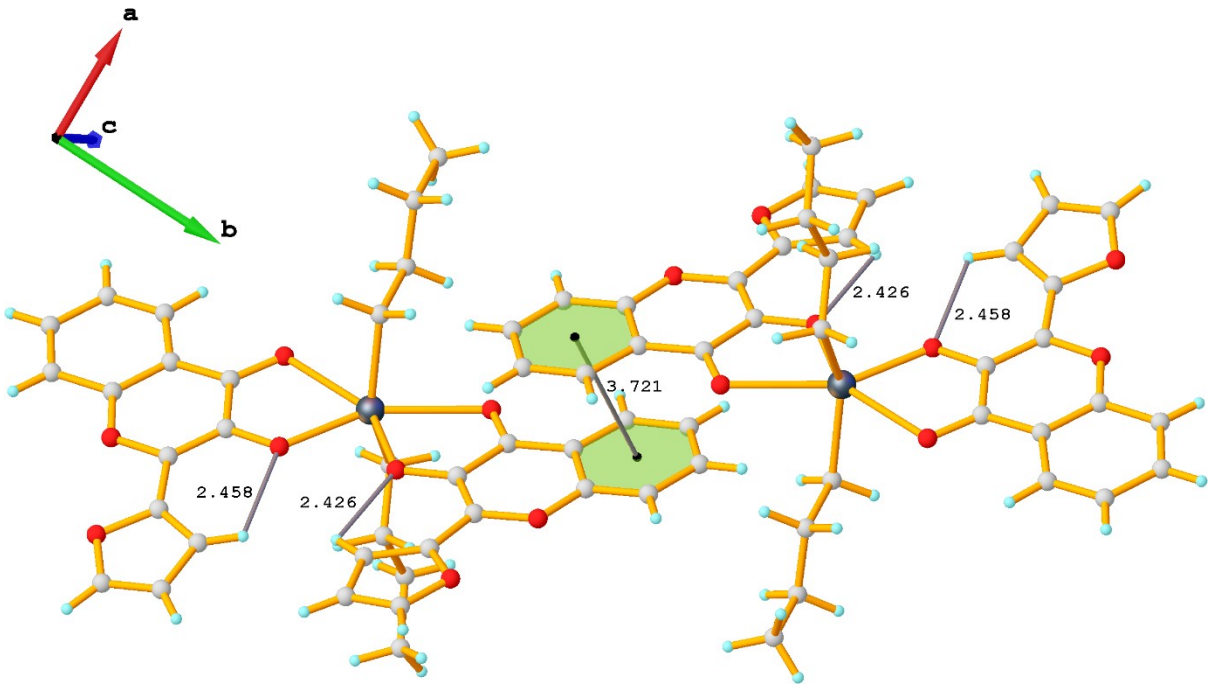


Figure S5. The crystalline lattice involving the Intramolecular H-bonding and π···π interactions in **6a**.

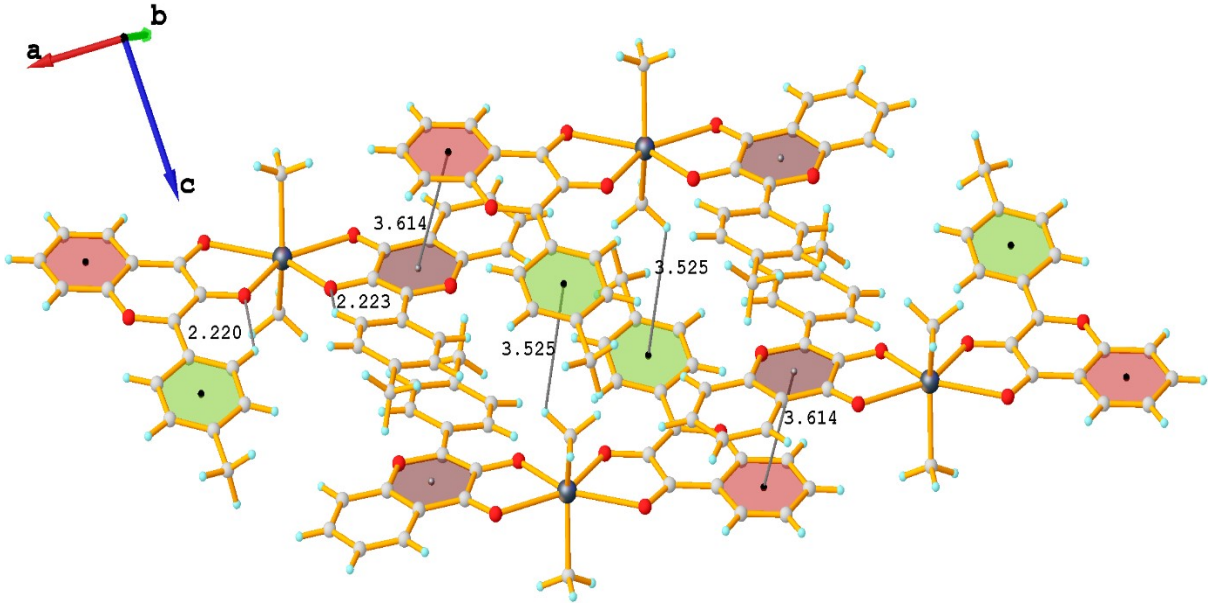


Figure S6. Intramolecular H-bonding, C-H·····π, and π···π interactions in the compound **4b**.

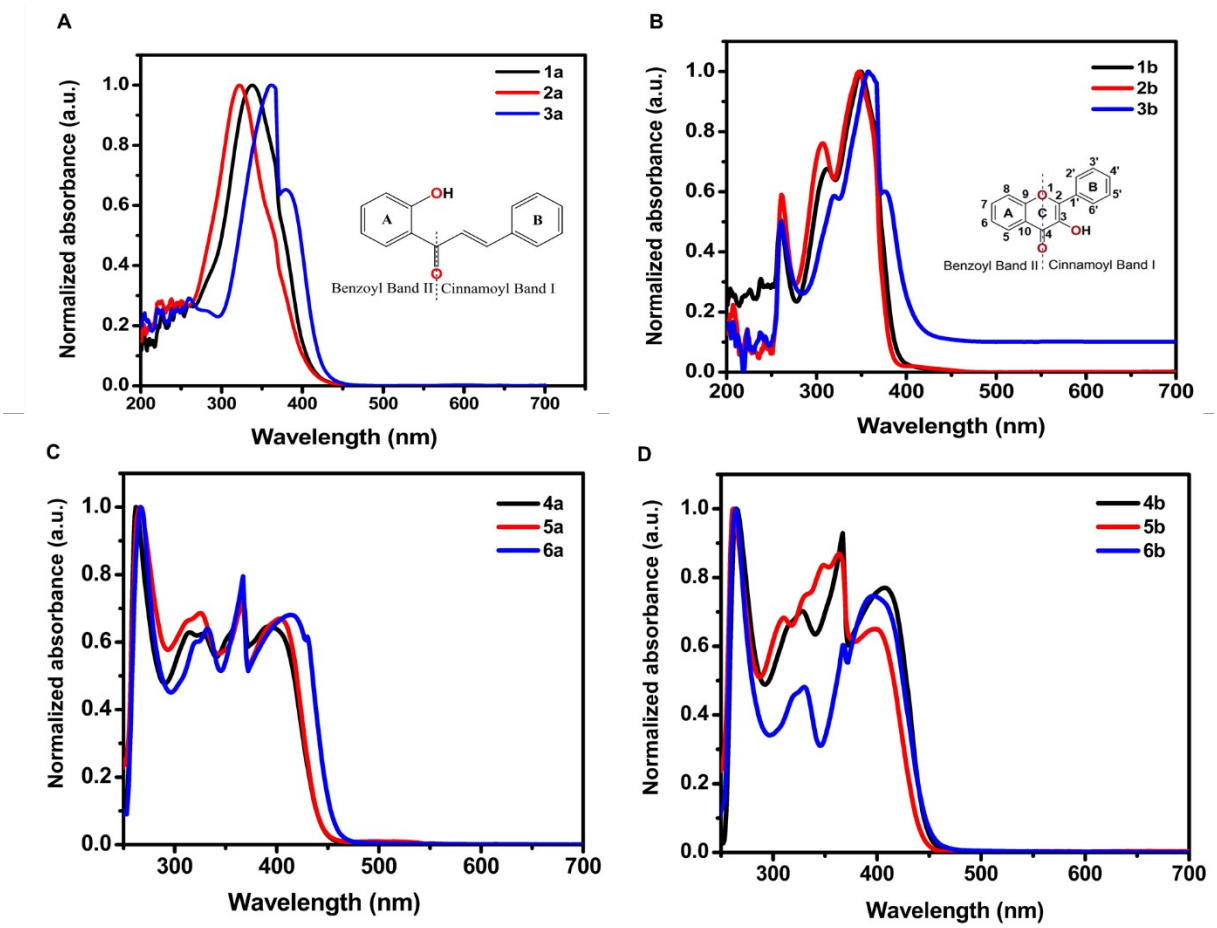
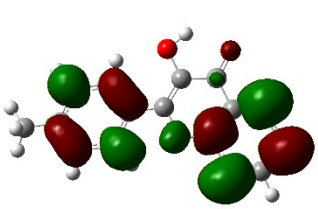
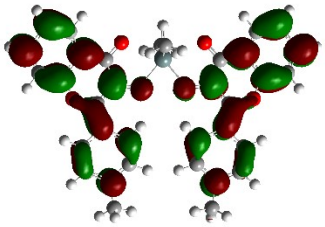
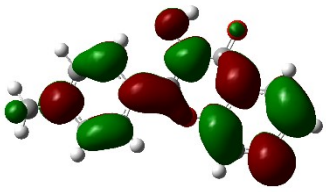
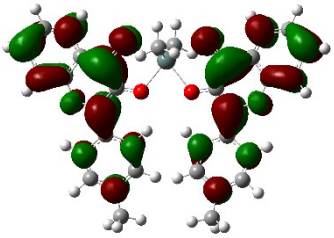
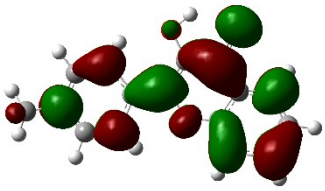
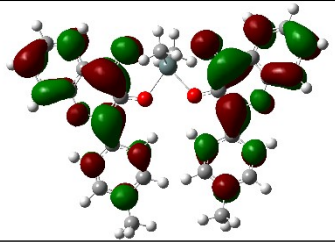
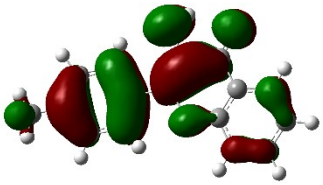
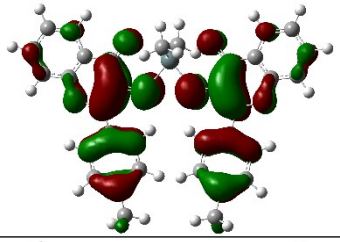
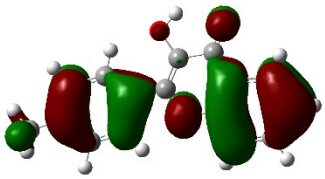
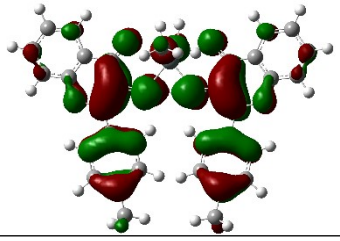
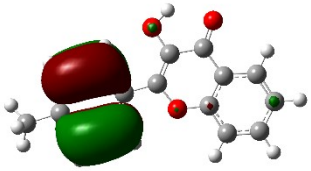
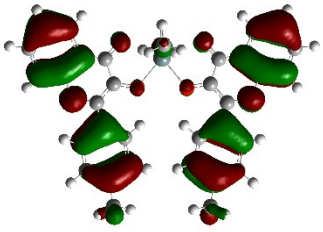
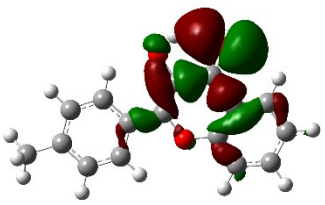
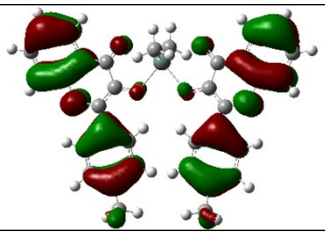


Figure S7. Normalized absorption spectra in MeOH of 0.12 mM (**A**) 2-hydroxychalcones (**1a-3a**), (**B**) 3-hydroxy-4*H*-chromen-4-ones (**1b-3b**), (**C**) organotin(IV) compounds (**4a-6a**) and (**D**) organotin(IV) compounds (**4b-6b**) (Inset: Divisions of bands I and II related to UV–Vis absorption of: Ring A (Band II) benzoyl system; Ring B (Band I) cinnamoyl system in chalcone and chromone structure).

Table S3. Calculated coordinates of **1b** with B3LYP/DGDZVP on H, C, and O.
0,1

atom	x	y	z
O	0.5636596434	-0.9116388651	-0.0040913203
O	-0.1064093614	2.6688238516	0.0035366071
H	0.6414072159	3.3129351298	0.0066347294
O	2.5146013589	2.6614009571	0.0073570841
C	-0.1564185226	0.2627777142	-0.0026270245
C	0.5154919539	1.4591200246	0.0011068851
C	1.9740794653	1.5378937705	0.0035047482
C	2.6805846034	0.2626474186	0.0017776955
C	4.0889839748	0.1771797519	0.0038367973
H	4.6559449009	1.1036142131	0.0067532184
C	4.7137589865	-1.0605446544	0.0021390001
H	5.798265983	-1.1268057989	0.0036939469
C	3.9382976258	-2.2397455002	-0.0016466534
H	4.4294362703	-3.2094856485	-0.0030067769
C	2.5504054197	-2.1791139008	-0.0036828217
H	1.9391955757	-3.0769798131	-0.0066440219
C	1.9260423362	-0.9216132723	-0.0019161802
C	-1.6067228042	0.0287994541	-0.00401251
C	-2.5400406624	1.0874633331	-0.0154515391
H	-2.1958474992	2.1129602182	-0.024938535
C	-3.909655186	0.8242812852	-0.0188034339
H	-4.6043750245	1.6619644797	-0.0315223245
C	-4.4100125998	-0.4866788091	-0.0091560036
C	-3.4783737269	-1.5373188712	-0.0012130828
H	-3.831276634	-2.5669215512	0.0002087156
C	-2.1072451062	-1.2910424624	0.0019723023
H	-1.417124735	-2.1271314464	0.0060523359
C	-5.8966256257	-0.7583945898	0.0205113155
H	-6.2616395708	-0.8227416011	1.0533762855
H	-6.1416438815	-1.7047932366	-0.4713708885
H	-6.4598423737	0.0381144192	-0.4752175507

Table S4. The frontier molecular orbitals of **1b** and **4b** estimated from TD-DFT calculations.

	1b	**4b**
LUMO + 2		
LUMO + 1		
LUMO		
HOMO		
HOMO - 1		
HOMO - 2		
HOMO - 3		

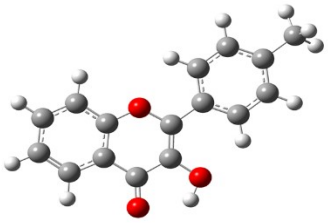
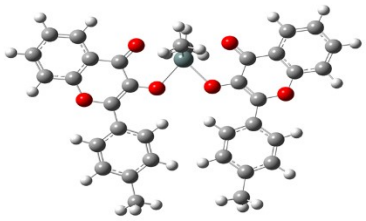
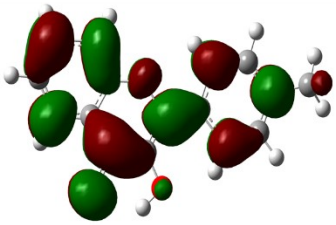
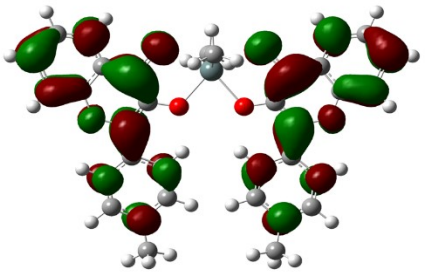
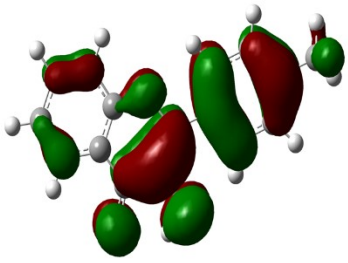
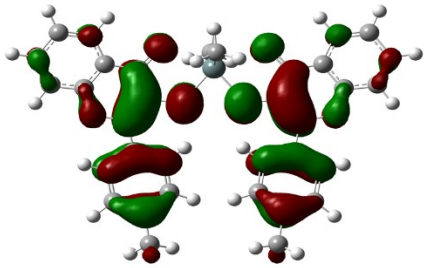
	1b	4b
Geometry-optimized structures		
	Electronic energy= -528801.0 kcal/mol	Electronic energy= -4887591.0 kcal/mol
LUMO		
	Energy= -52.2 kcal/mol	Energy= -12.4 kcal/mol
Energy gap	= 87.1 kcal/mol =3.777 eV	= 0.3 kcal/mol =0.012 eV
HOMO		
	Energy= -139.3 kcal/mol	Energy= -12.7 kcal/mol

Figure S8. Geometry-optimized structures and HOMO-LUMO band gap for **1b** and **4b**.

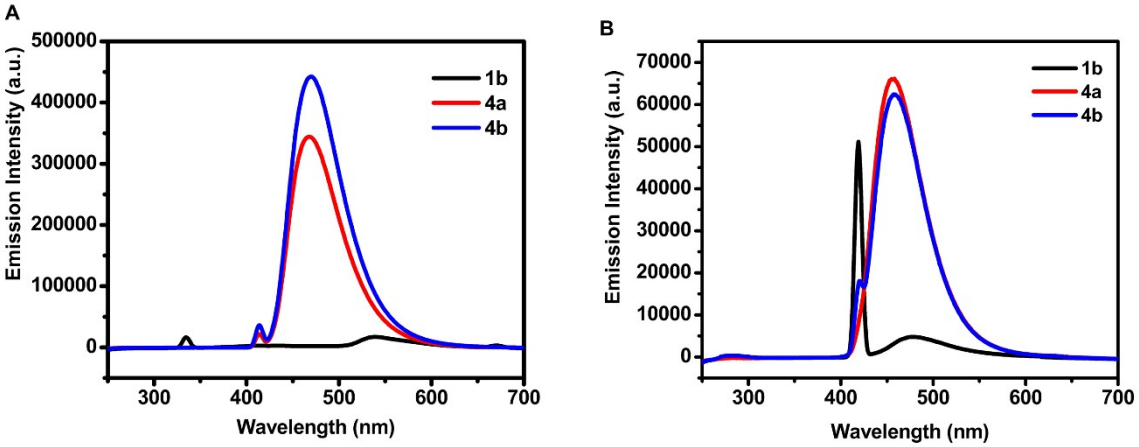


Figure S9. Fluorescence spectra of 18.54 μM (**A**) 3-hydroxy-4*H*-chromen-4-one **1b**, organotin(IV) compounds **4a**, **4b** in DMSO and (**B**) in MeOH at λ_{ex} = 415 nm.

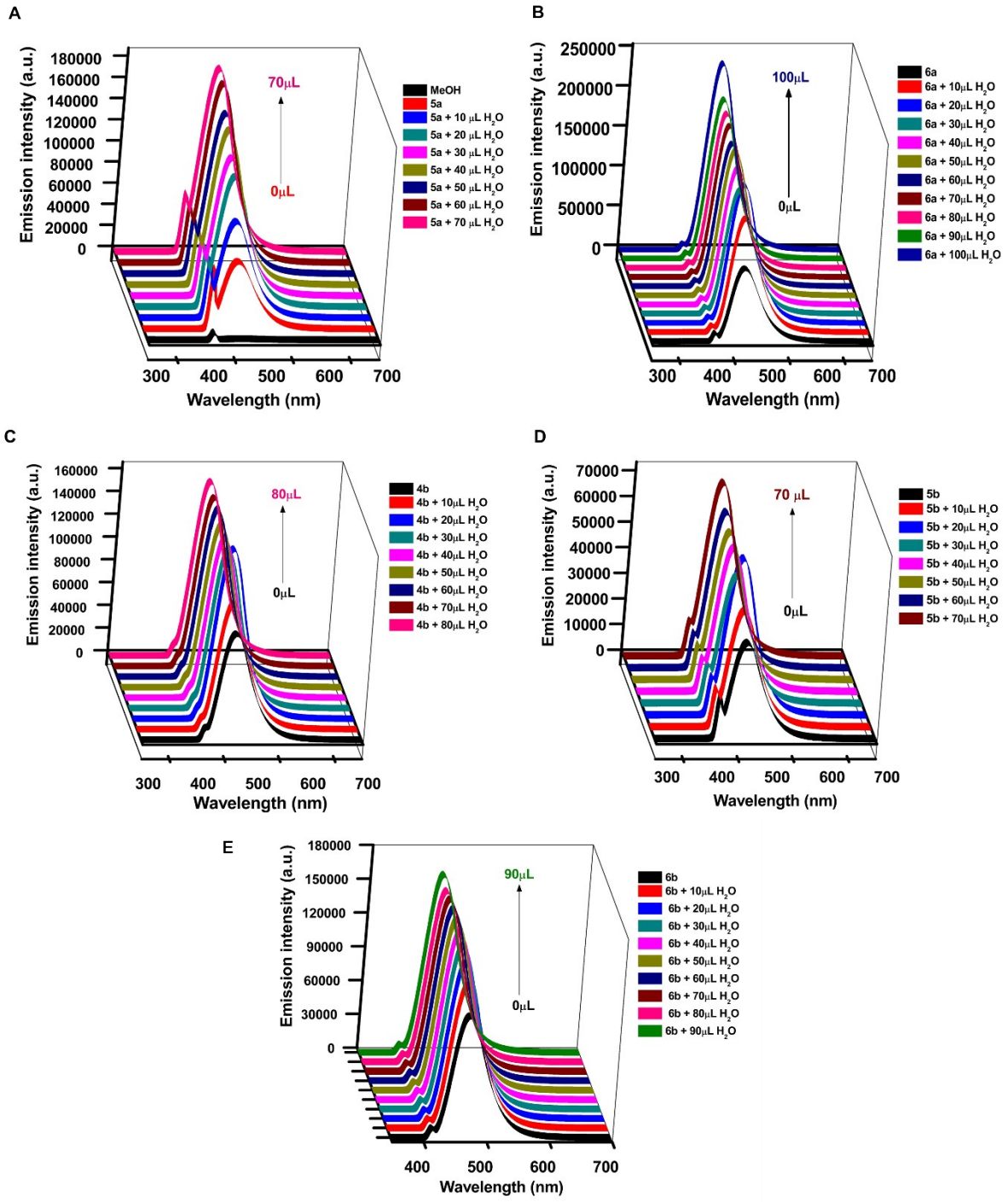


Figure S10. Fluorescence spectra of 18.54 μM organotin(IV) complexes in MeOH/H_2O mixtures, λ_{ex} = 415 nm, (**A**) of **5a**, (**B**) of **6a**, (**C**) of **4b**, (**D**) of **5b**, and (**E**) of **6b**.

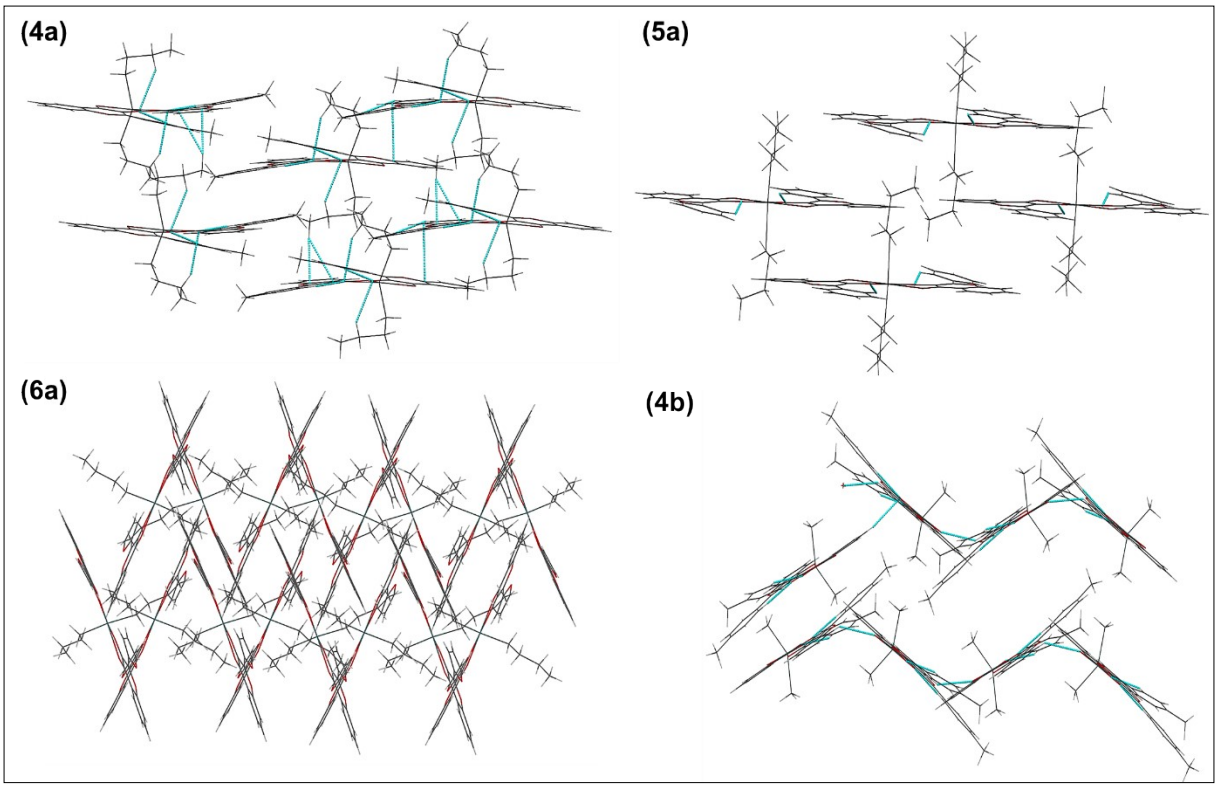


Figure S11. Wireframe representation (drawn with Mercury 4.2.0) of J-type stacking interactions; brickwork arrangement for **4a** and **5a**, herringbone stacking interactions in **6a** and **4b**.

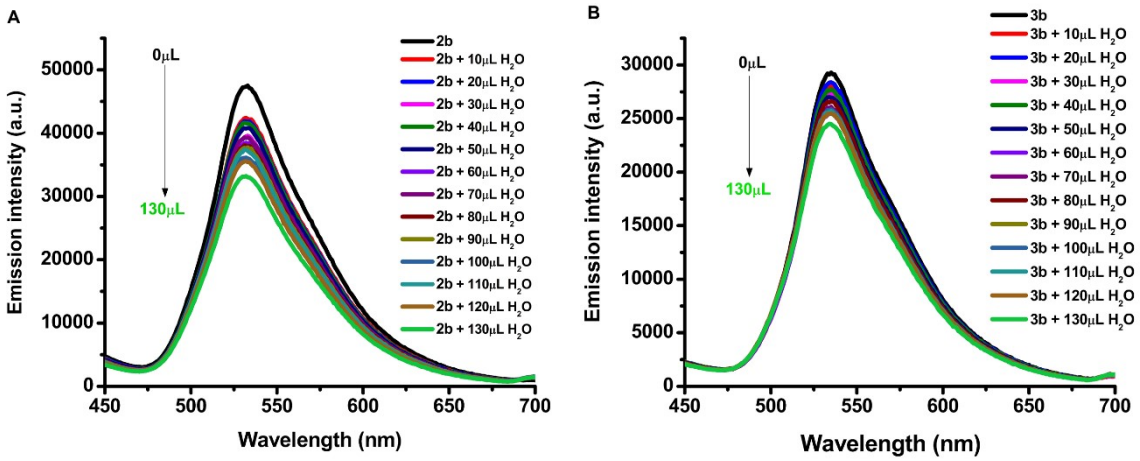


Figure S12. Fluorescence spectra of 18.54 μM ligands in MeOH/H_2O mixtures, λ_{ex} = 350 nm**,** (**A**) of **2b** and (**B**) of **3b**.

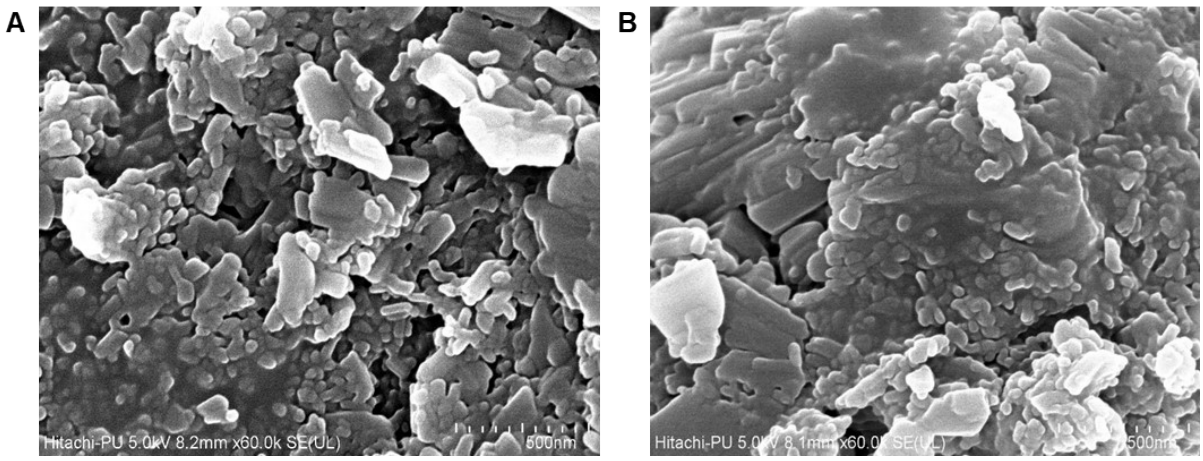


Figure S13. (**A**) and (**B**) FESEM images of **4a** at 4.76 % water fraction and 33.33% water fraction in MeOH, respectively.

Table S5. Similarities between crystallographic data and structure refinement parameters of **4a** and **4a'**.

Parameter	**4a**	**4a'**
Empirical formula	$C_{40}H_{40}O_6Sn$	$C_{40}H_{40}O_6Sn$
Formula weight	735.41	735.41
T(K)	293(2)	293(2)
Crystal system	triclinic	triclinic
Space group	*P*-1	*P*-1
a(Å)	8.2279(2)	8.2419(2)
b(Å)	12.1695(2)	12.1794(4)
c(Å)	18.0429(4)	18.0560(8)
α(°)	85.696(2)	85.726(3)
β(°)	89.597(2)	89.592(3)
γ(°)	75.392(2)	75.354(2)
V(Å^3)	1743.16(7)	1748.59(11)
Z	2	2
ρ_{calc}(g/cm^3)	1.401	1.397
μ(mm^{-1})	0.779	0.777
F(000)	756.0	756.0
Crystal size(mm^3)	0.33 × 0.24 × 0.13	0.12 × 0.1 × 0.07
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range	6.792 to 54.9	6.786 to 50.14
Index ranges	-10 ≤ h ≤ 10, -15 ≤ k ≤ 14, -23 ≤ l ≤ 22	-9 ≤ h ≤ 9, -14 ≤ k ≤ 14, 0 ≤ l ≤ 21
Reflections collected	24253	25944
Independent reflections	7414	6185
θ_{max}(°) and Completeness(%)	27.450 and 0.929	25.070 and 0.994
Absorption correction	Multi-scan	Multi-scan
T_{min} and T_{max}	0.783 and 0.906	0.912 and 0.949
Data/restraints/parameters	7414/15/428	6185/36/429
GOF on F^2	1.014	1.084
R_1, wR_2 [I>2σ (I)]	0.0659, 0.1742	0.0781, 0.1958
R_1, wR_2 [all data]	0.0775, 0.1874	0.0978, 0.2090
Largest diff. peak/ hole(e Å^{-3})	1.08/-1.42	1.35/-1.24

Table S6. Similarities between selected bond lengths (Å) and bond angles (°) of **4a** and **4a'**.

	4a	**4a'**
	Bond length (Å)	
Sn-O4	2.073(3)	2.077(5)
Sn-O3	2.066(3)	2.071(6)
Sn-O2	2.485(3)	2.475(7)
Sn-O1	2.437(3)	2.440(6)
Sn-C*	2.133(6)	2.135(12)
Sn-C**	2.129(6)	2.112(11)
	Bond angles (°)	
O4-Sn-O1	72.23(11)	72.2(2)
O4-Sn-O2	150.49(12)	150.7(2)
O4-Sn-C*	108.4(2)	108.1(4)
O4-Sn-C**	102.7(2)	102.0(4)
O3-Sn-O4	79.31(11)	79.6(2)
O3-Sn-O1	151.12(12)	151.3(2)
O3-Sn-O2	71.63(12)	71.5(2)
O3-Sn-C**	108.3(2)	108.2(4)
O3-Sn-C*	101.7(2)	102.2(4)
O1-Sn-O2	137.12(11)	137.0(2)
C*-Sn-O2	83.0(2)	82.3(5)
C*-Sn-O1	83.1(3)	83.2(5)
C**-Sn-O2	82.1(2)	83.5(4)
C**-Sn-O1	83.1(2)	82.4(4)
C**-Sn-C*	140.0(3)	140.4(5)
For **4a**= C*=C33, C**=C37,	For **4a'**= C*=C37, C**=C33	

Table S7. Readings of the emission measurements for **4a** in the absence of analyte.

Blank Readings (4a)	Fluorescence Intensity
1	533.4211
2	521.3424
3	513.9273
4	515.5544
5	511.2778
6	510.8295
7	509.4567
8	526.5432
9	596.5542
10	520.3423
Standard Deviation (σ)	25.95367

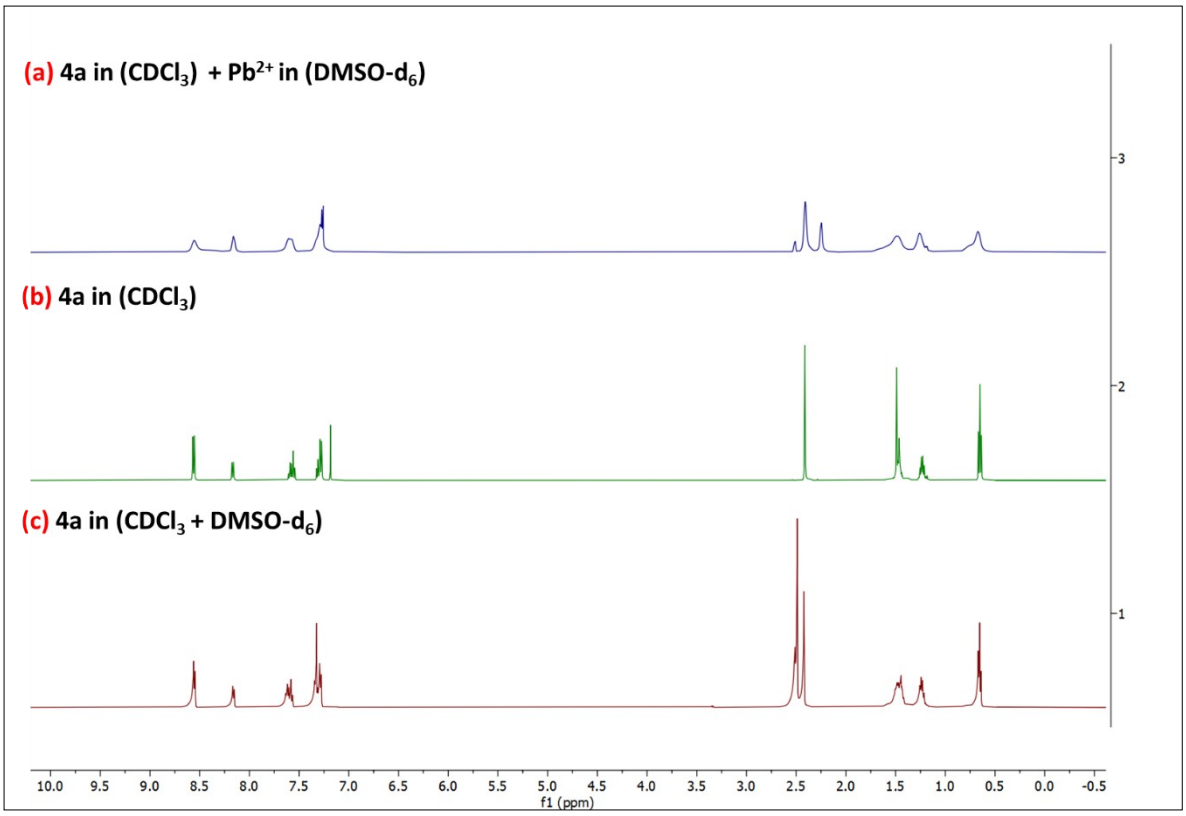


Figure S14. ^{1}H NMR spectrum **(a)** of **4a** (in $CDCl_3$) in the presence of 10 µL of $Pb(NO_3)_2$ (in DMSO-d_6), **(b)** of **4a** only (in $CDCl_3$), and **(c)** of **4a** in ($CDCl_3$ + DMSO-d_6 recording for comparison).

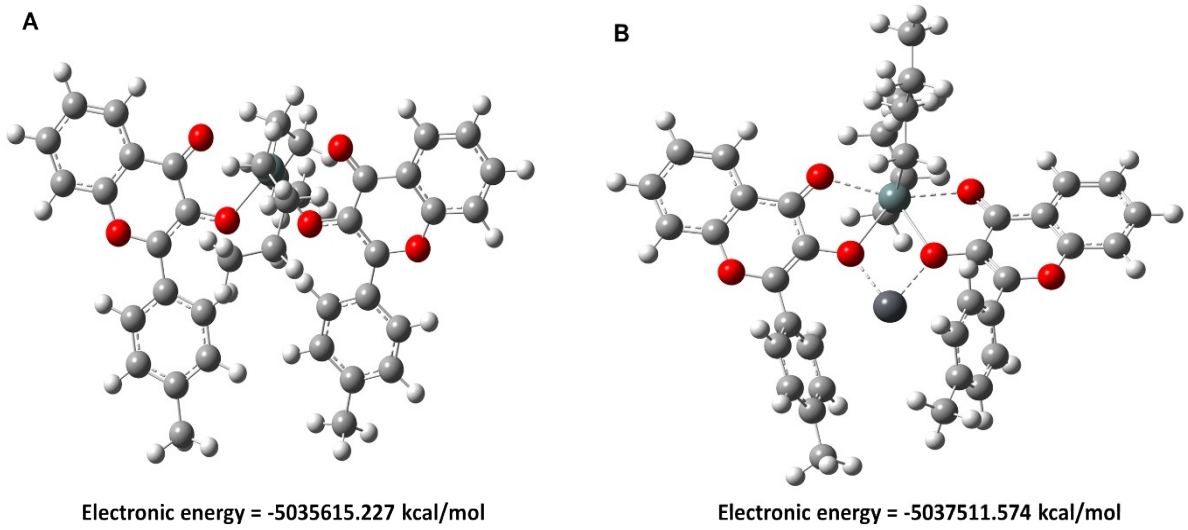


Figure S15. (**A**) Geometry-optimized (B3LYP/DGDZVP) structure of compound **4a** (**B**) Geometry-optimized (GenECP: Lanl2DZ for Pb and DGDZVP for Sn, H, C, O) structure of compound **4a**+**Pb**$^{2+}$.

Table S8. Calculated coordinates of **4a** with B3LYP/DGDZVP on Sn, H, C, and O.
0,1

atom	x	y	z
Sn	-0.019292	-1.81737	0.010214
O	-1.395913	-0.173853	-0.037226
O	1.329061	-0.148928	0.005696
O	.905974	0.473752	-0.072358
O	-4.983384	0.381398	0.058631
O	2.30135	-2.649868	-0.151594
O	-2.321678	-2.692887	0.197423
C	-2.704103	-0.38065	0.026267
C	3.553459	0.719204	0.017792
C	2.641828	-0.329936	-0.04001
C	-3.636807	0.648321	-0.055801
C	-4.594163	-1.982965	0.287665
C	-3.166945	-1.754951	0.17302
C	3.1314	-1.698493	-0.141153
C	-5.45659	-0.87609	0.231815
C	3.268872	2.148345	0.18204
C	4.563665	-1.903978	-0.231147
C	5.404536	-0.779666	-0.199094
C	-3.381448	2.076333	-0.270862
C	-7.370541	-2.305151	0.512778
H	-8.446278	-2.434732	0.600142
C	-6.848824	-1.030187	0.343881
H	-7.486693	-0.152442	0.294287
C	-5.149284	-3.272336	0.458918
H	-4.471293	-4.119495	0.500398
C	5.144632	-3.187218	-0.35573
H	4.483038	-4.047894	-0.379966
C	-6.520346	-3.432678	0.570754
H	-6.946486	-4.423421	0.70322
C	6.800709	-0.91079	-0.288687
H	7.421537	-0.020036	-0.258655
C	0.129137	-2.574606	2.053901
H	-0.889221	-2.809962	2.377438
H	0.671048	-3.521997	1.958478
C	-0.142082	-2.652212	-2.003598
H	0.165149	-3.69775	-1.885977
H	-1.204245	-2.662883	-2.262211
C	7.348095	-2.1803	-0.411228
H	8.427101	-2.292148	-0.480936
C	6.51979	-3.324957	-0.445123
H	6.965965	-4.311019	-0.541628
C	0.033198	-0.395806	3.430966
H	-0.950758	-0.695414	3.817789

H	-0.160312	0.190383	2.524717
C	1.975736	2.627718	0.482197
H	1.155405	1.927423	0.569051
C	0.32227	-0.530954	-3.446683
H	0.43472	0.103398	-2.559157
H	1.04618	-0.156519	-4.182625
C	-2.959497	4.85453	-0.757774
C	4.313856	3.095161	0.075629
H	5.320248	2.761388	-0.151172
C	-2.103671	2.568397	-0.613237
H	-1.272979	1.879883	-0.695572
C	1.753518	3.992155	0.676854
H	0.74852	4.326422	0.926112
C	2.787867	4.932575	0.568821
C	0.704624	-1.98051	-3.097232
H	0.62772	-2.58935	-4.011347
H	1.761637	-2.010281	-2.80904
C	-4.441143	3.007502	-0.173668
H	-5.436574	2.663556	0.084227
C	0.831282	-1.656312	3.067335
H	1.821308	-1.36345	2.69583
H	1.016086	-2.231013	3.98754
C	-1.093489	-0.367023	-4.01728
H	-1.278355	0.671721	-4.312826
H	-1.862295	-0.635616	-3.285467
H	-1.240307	-0.996964	-4.903766
C	-2.736883	6.330677	-0.997078
H	-3.54915	6.767379	-1.587885
H	-1.797533	6.513543	-1.527006
H	-2.694683	6.881601	-0.048973
C	-4.228923	4.362765	-0.408289
H	-5.066918	5.052767	-0.324528
C	-1.910478	3.929343	-0.85683
H	-0.917127	4.273026	-1.138149
C	0.74163	0.485082	4.468082
H	0.142527	1.368583	4.715639
H	1.710153	0.836778	4.093657
H	0.92521	-0.064016	5.399803
C	4.072872	4.453075	0.261306
H	4.900032	5.155311	0.171681
C	2.534948	6.411361	0.755846
H	1.573186	6.594848	1.243577
H	2.522294	6.934112	-0.208863
H	3.317223	6.877209	1.364703

Table S9. Calculated coordinates of **4a+Pb^{2+}** with GenECP: Lanl2DZ for Pb and DGDZVP for Sn, H, C, and O.
2,1

atom	x	y	z
Sn	-0.361890421	-1.9681214993	-0.1847891161
O	1.1978542656	-0.2375111055	-0.0501817661
O	4.8404512592	-0.1333712881	-0.0121867891
O	-1.2856316214	0.1798773436	-0.0618316263
O	-4.701490082	21.4450967638	0.0304904552
O	1.780554941	-2.8306571599	0.2763183582
O	-2.6688731833	-2.0334264954	-0.6761502947
C	-2.731088892	2.6371959287	0.6490375465
C	2.5140936885	-0.6189198388	0.0003797053
C	3.3813653083	1.6890093665	-0.4870365792
C	-2.6534708671	0.247422232	-0.1185859868
C	5.1464227092	-1.4447307883	0.2572585626
C	3.5551336005	0.2569724501	-0.1546687832
C	2.7591972037	-2.0282378841	0.2215356595
C	4.1396090487	-2.4276246565	0.3660850565
C	-3.359231823	1.3849546088	0.1663526452
C	-5.4116792696	0.3404684506	-0.3710969076
C	-3.3370662206	-0.973537138	-0.4922163247
C	-4.7727356907	-0.8912638032	-0.6286597356
C	6.5018345548	-1.7611489598	0.3984893441
H	7.2500581357	-0.9802488372	0.3023582669
C	-5.5644148039	-1.9974041874	-1.0199156209
H	-5.0733177773	-2.9449522412	-1.2175666658
C	3.0240345855	4.4279888036	-1.1581562344
C	-2.6750211753	3.7861728151	-0.1586206458
H	-3.1229066387	3.7757723145	-1.1494422586
C	-6.7970648605	0.4910021603	-0.4947396893
H	-7.255160608	1.4524431863	-0.2833913878
C	-2.1675588741	2.6845750235	1.9409108026
H	-2.2472389288	1.8213695903	2.5984959101
C	4.5220417983	-3.7657622057	0.6234094485
H	3.7473510537	-4.5213943553	0.7073256164
C	3.7785362168	2.7006198182	0.4037581618
H	4.2427177034	2.437979603	1.3512473193
C	6.8487207727	-3.0820963502	0.6535635892
H	7.8969974567	-3.3445220146	0.7646449217
C	2.8072718774	2.0564531291	-1.7222785887
H	2.5504657764	1.2887791932	-2.4494176778
C	5.8607616789	-4.0861975281	0.7662012442
H	6.1578029395	-5.11161574	0.9646034744
C	-1.4995174876	5.0147812297	1.602794402
C	2.6320619869	3.4064377644	-2.0465917583
H	2.223352838	3.6699542466	-3.0197428772

C	3.5929754798	4.047203624	0.0696391239
H	3.9189753872	4.8140052139	0.7684691589
C	-6.9352210452	-1.8559522376	-1.1460475432
H	-7.5453005693	-2.7023014651	-1.4470005225
C	-2.0610987367	4.9519529974	0.3154477114
H	-2.0422466444	5.8343307386	-0.3199181193
C	-0.0515105474	-2.3436179263	-2.3039639087
H	-0.425337702	-1.4512503174	-2.8185143542
H	1.0334965432	-2.3890622466	-2.4403192362
C	-1.5608797675	3.8575509171	2.4046240702
H	-1.1639456522	3.8851153528	3.4170928576
C	-0.8437097004	-2.5312469364	1.8535946193
H	-0.0173721937	-2.1604227835	2.4695353284
H	-1.7499962336	-1.9784709052	2.1221423904
C	-7.5492290244	-0.61057242	-0.8832112837
H	-8.626320367	-0.5105297556	-0.9829740491
C	-0.9107231313	6.2982298964	2.13519232
H	-0.507124076	6.9224828397	1.3337265551
H	-0.1186614887	6.1103042945	2.8650457786
H	-1.6868614975	6.8831240274	2.6425971932
C	2.9003170796	5.8819879016	-1.5425223881
H	3.8093047247	6.2107477121	-2.0598935962
H	2.7769807993	6.5237312471	-0.6662291126
H	2.0615233207	6.0530736035	-2.2226459645
C	-1.0396721204	-4.0450297198	2.0539015996
H	-0.1344258472	-4.5836419171	1.7490410482
H	-1.8535954677	-4.40732234	1.4135338782
C	-1.3625843075	-4.3940096293	3.518378683
H	-2.2668703321	-3.8537589323	3.8277030776
H	-0.5502971544	-4.0324371775	4.1623269293
C	-1.5626046449	-5.8988745342	3.7392343777
H	-1.7890014859	-6.1125993108	4.7881206754
H	-2.3918126008	-6.2845584385	3.1358247384
H	-0.6631769021	-6.4647151415	3.472170802
C	-0.7366956983	-3.6141919013	-2.830624745
H	-1.8241585131	-3.4910441039	-2.7907518505
H	-0.4764667764	-3.7119348716	-3.8931878836
C	-0.3343706942	-4.9005344465	-2.0971536713
H	0.7590661601	-4.9960689671	-2.0956604022
H	-0.6340789766	-4.8264298944	-1.0377432425
C	-0.9633976142	-6.1619645579	-2.700650464
H	-0.648778853	-6.2995640247	-3.7405817398
H	-0.6673178971	-7.0560194083	-2.1439274273
H	-2.0574597994	-6.1071928236	-2.6878373054
Pb	0.2528333933	1.7660878221	0.1011777176

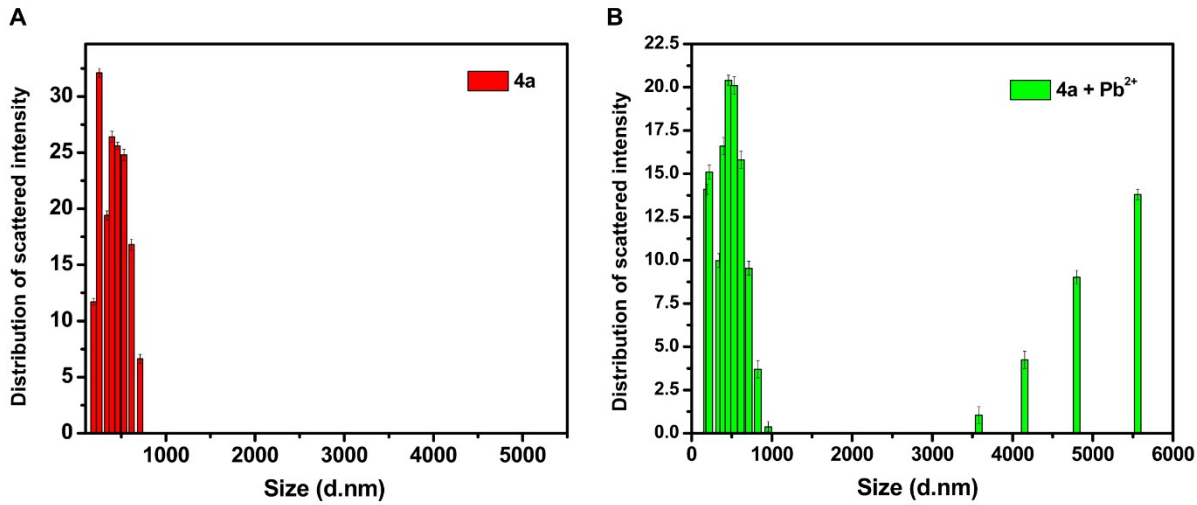


Figure S16. Distribution of intensity of scattered light for 0.2 mM **4a** (in Triton X-100) in the (**A**) absence and (**B**) presence of 50 μL of 10 mM $Pb(NO_3)_2$.

2. Spectral data

2.1. FT-IR spectra of compounds

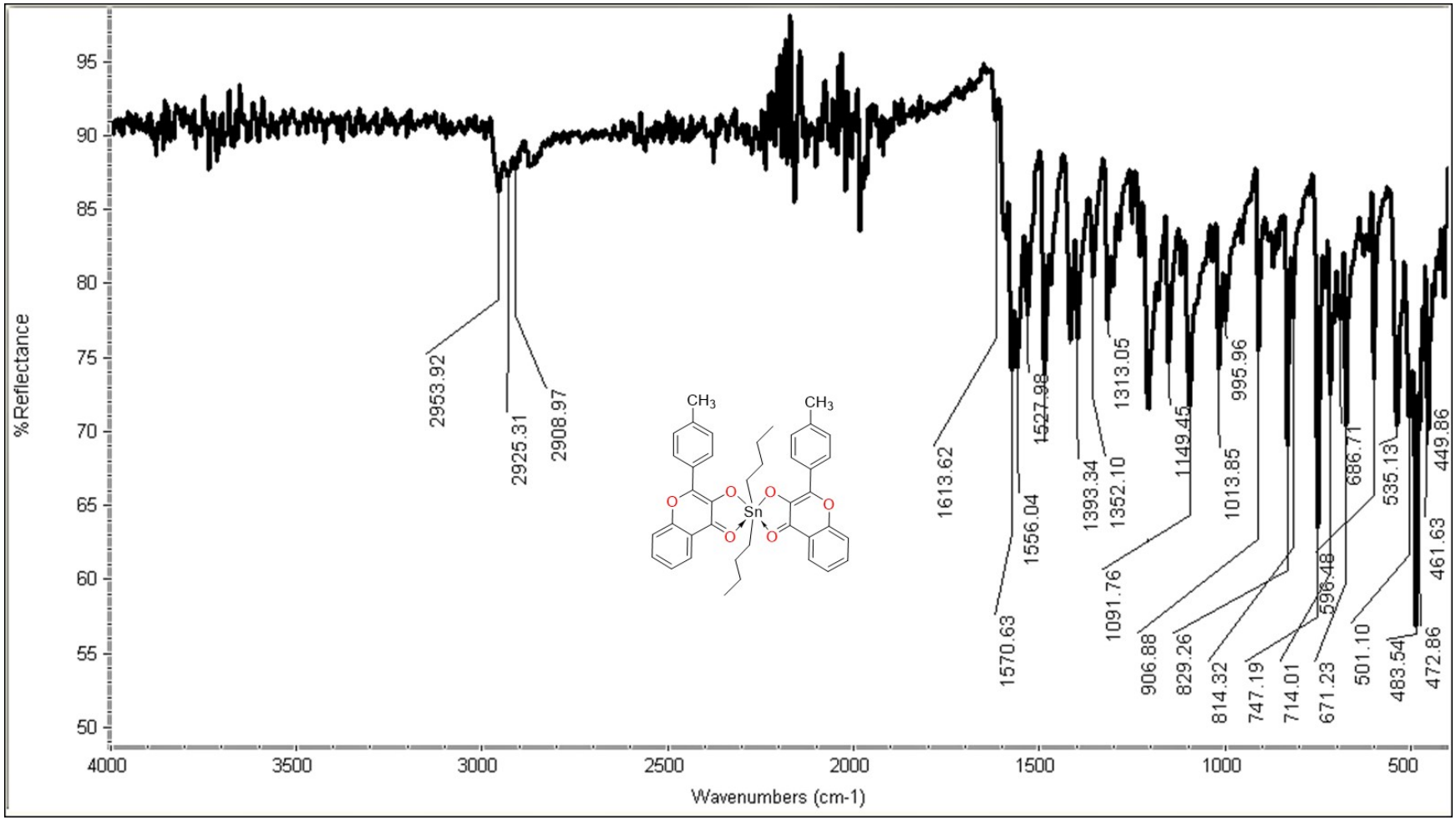


Figure S17. FT-IR spectrum of compound **4a**.

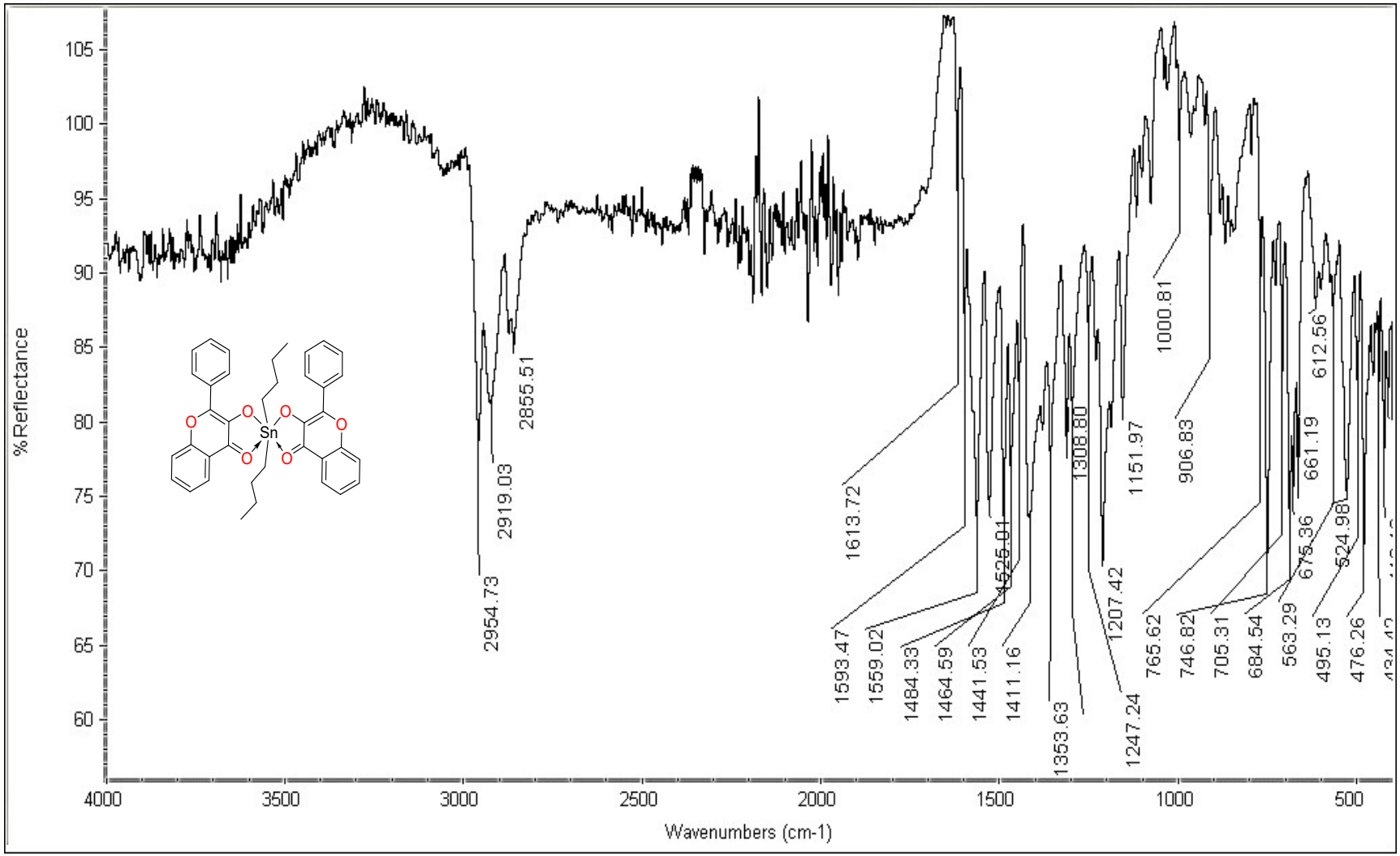


Figure S18. FT-IR spectrum of compound **5a**.

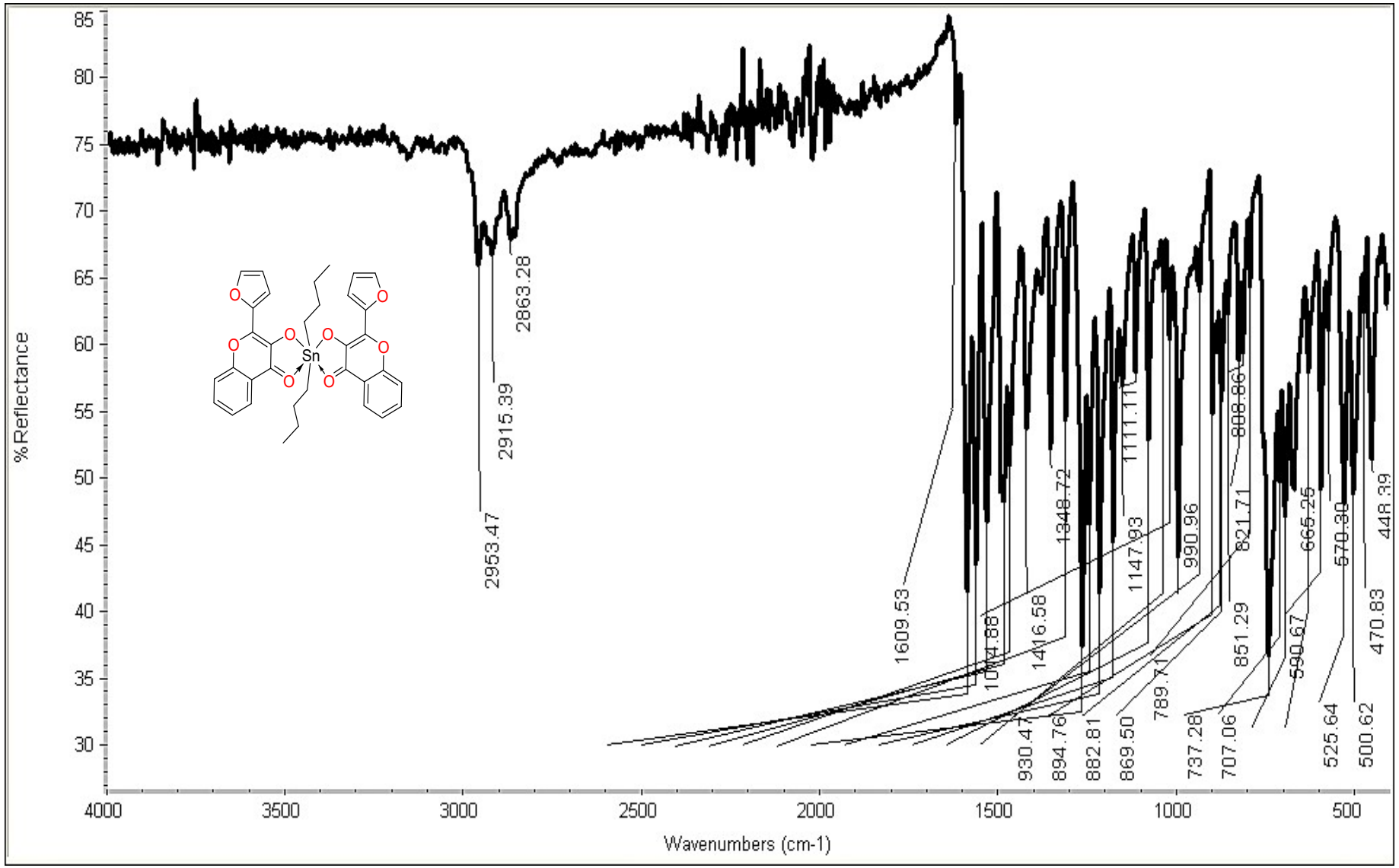


Figure S19. FT-IR spectrum of compound **6a**.

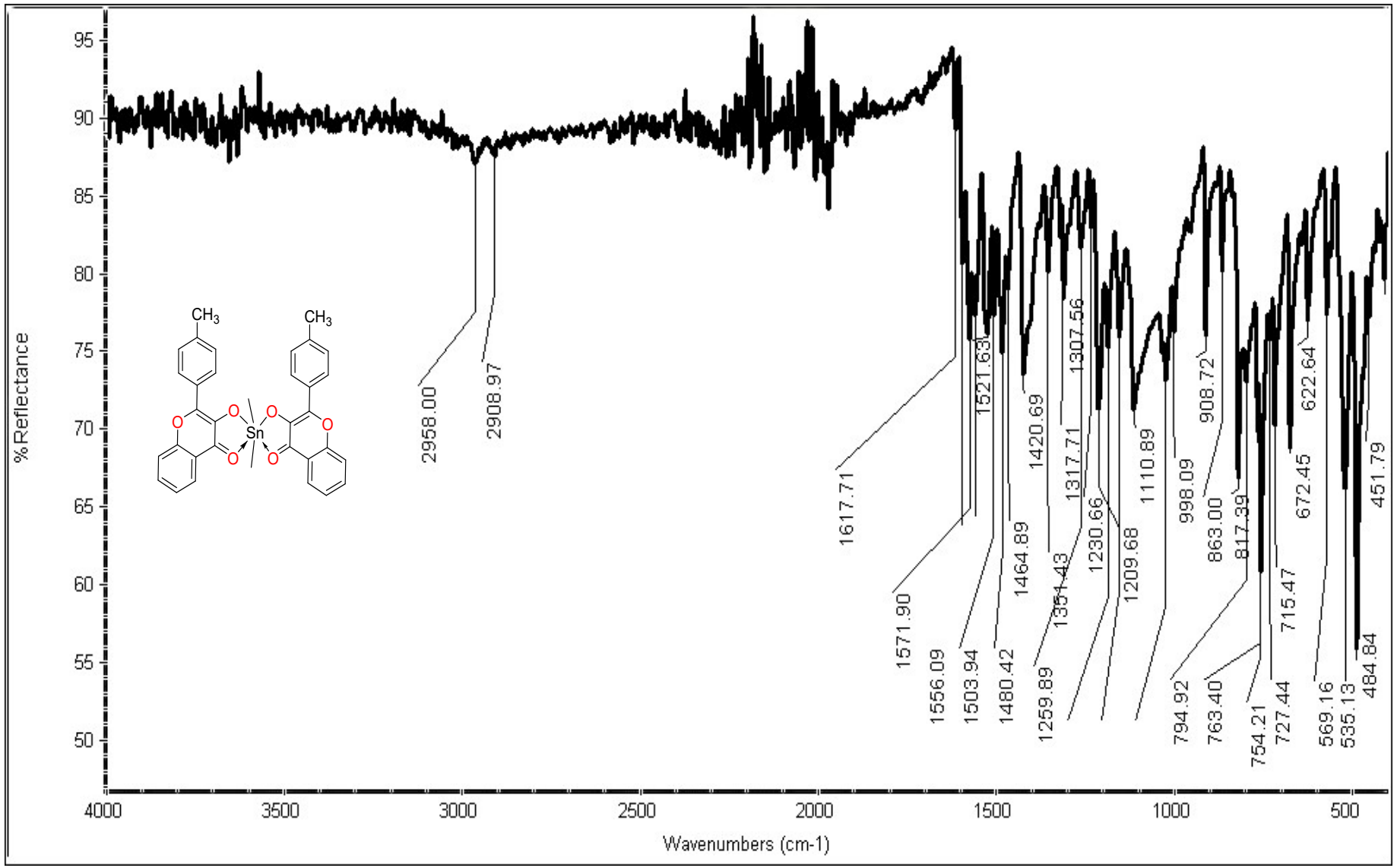


Figure S20. FT-IR spectrum of compound **4b**.

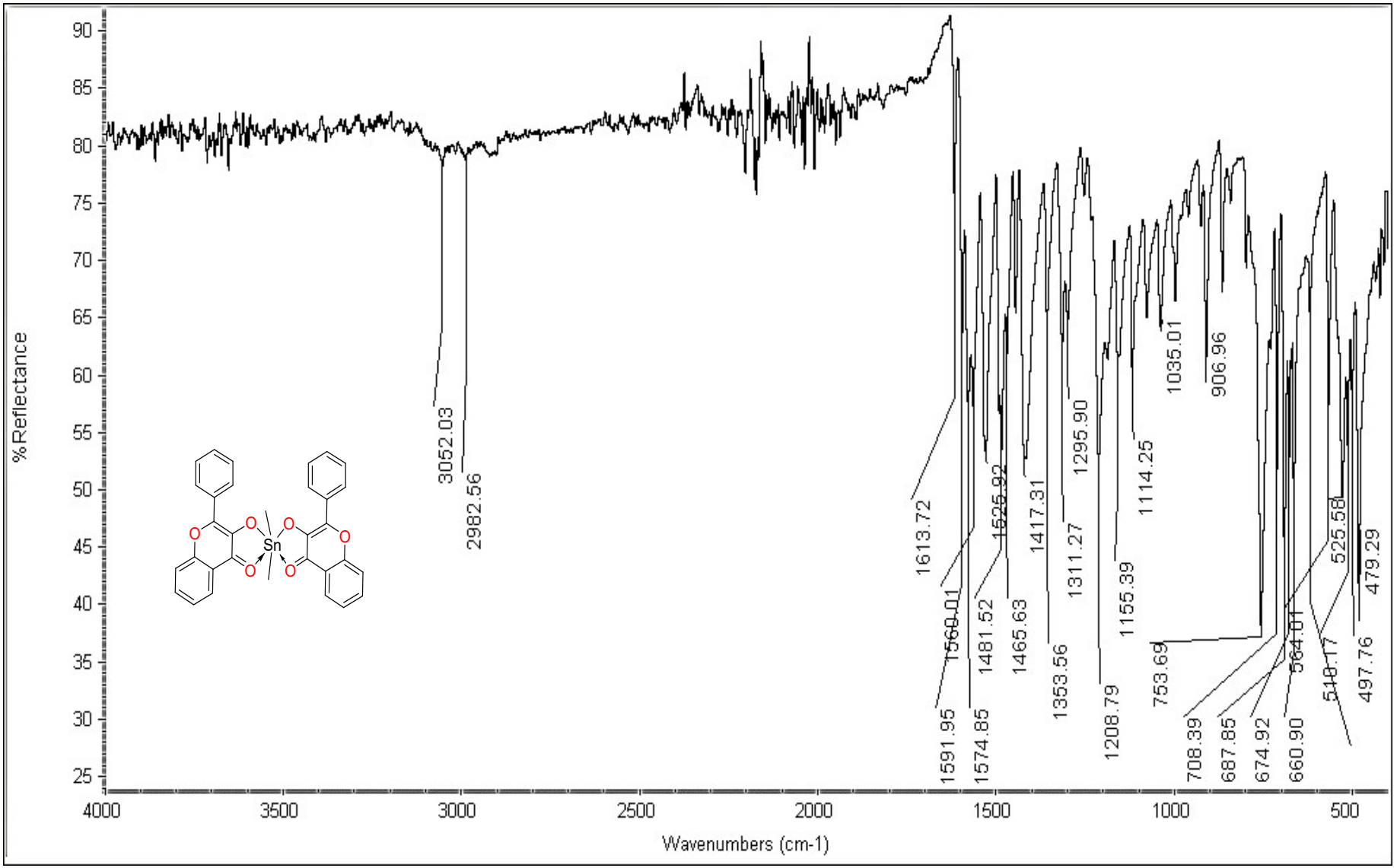


Figure S21. FT-IR spectrum of compound **5b**.

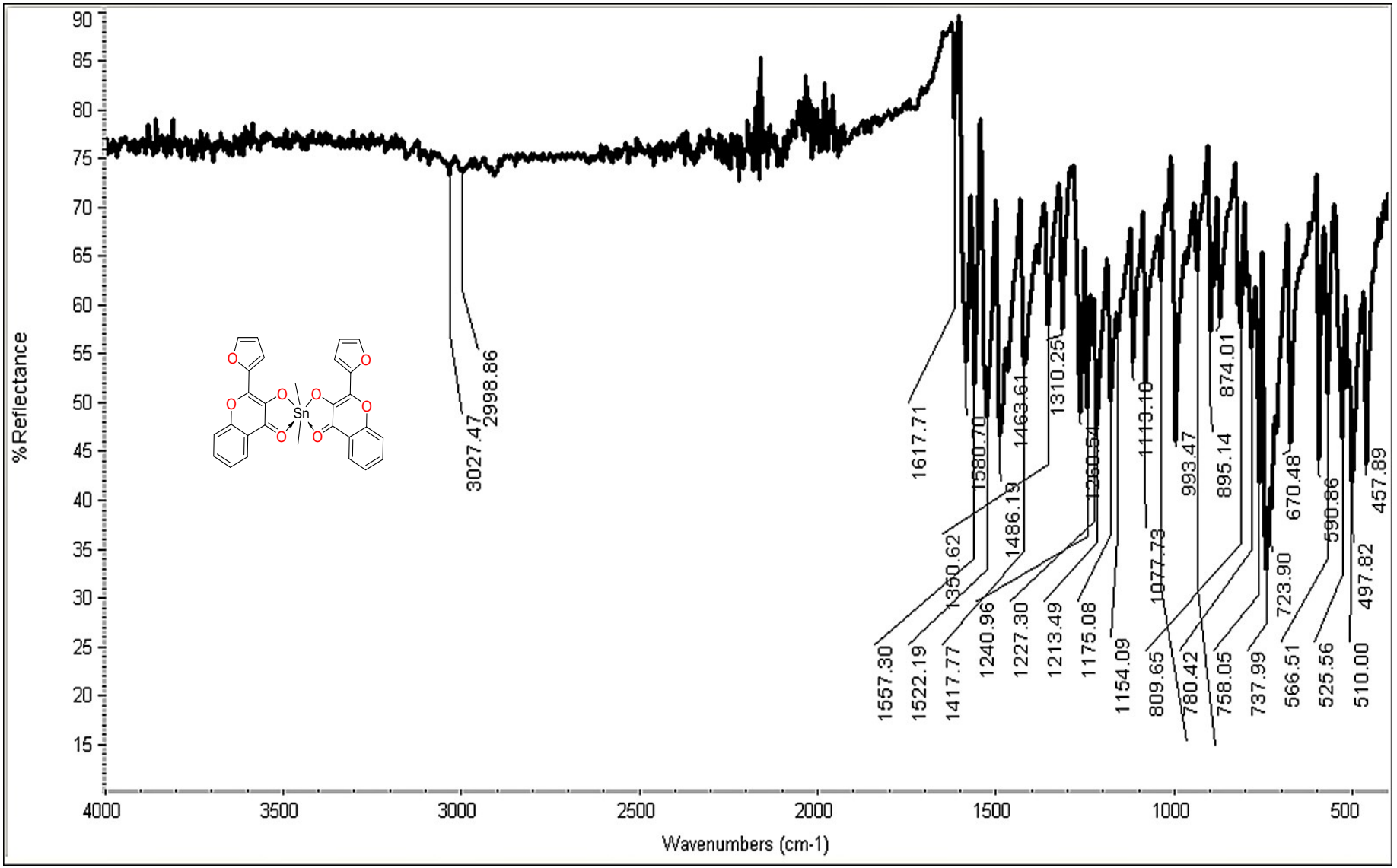


Figure S22. FT-IR spectrum of compound **6b**.

2.2. ^{1}H-NMR spectra of compounds

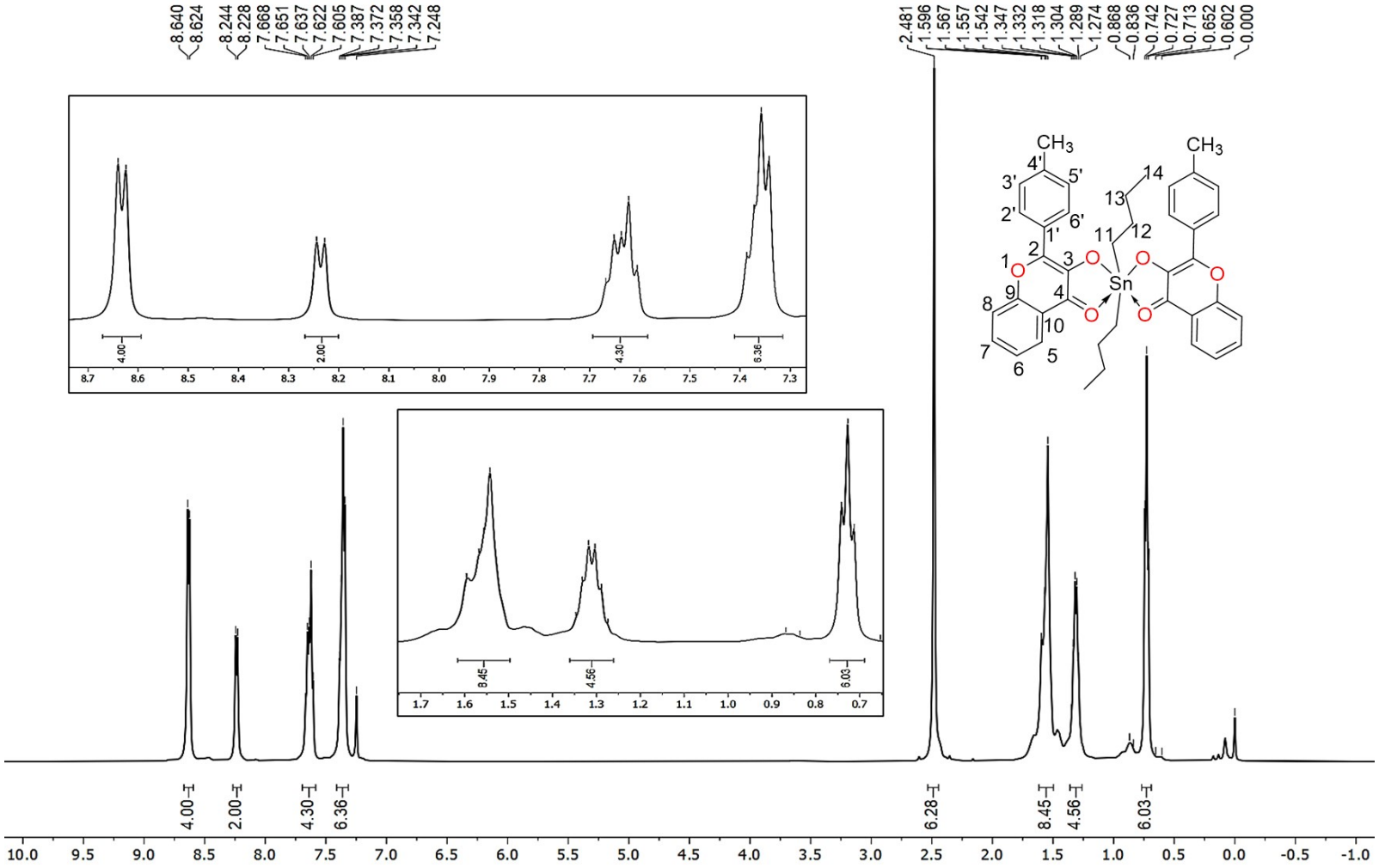
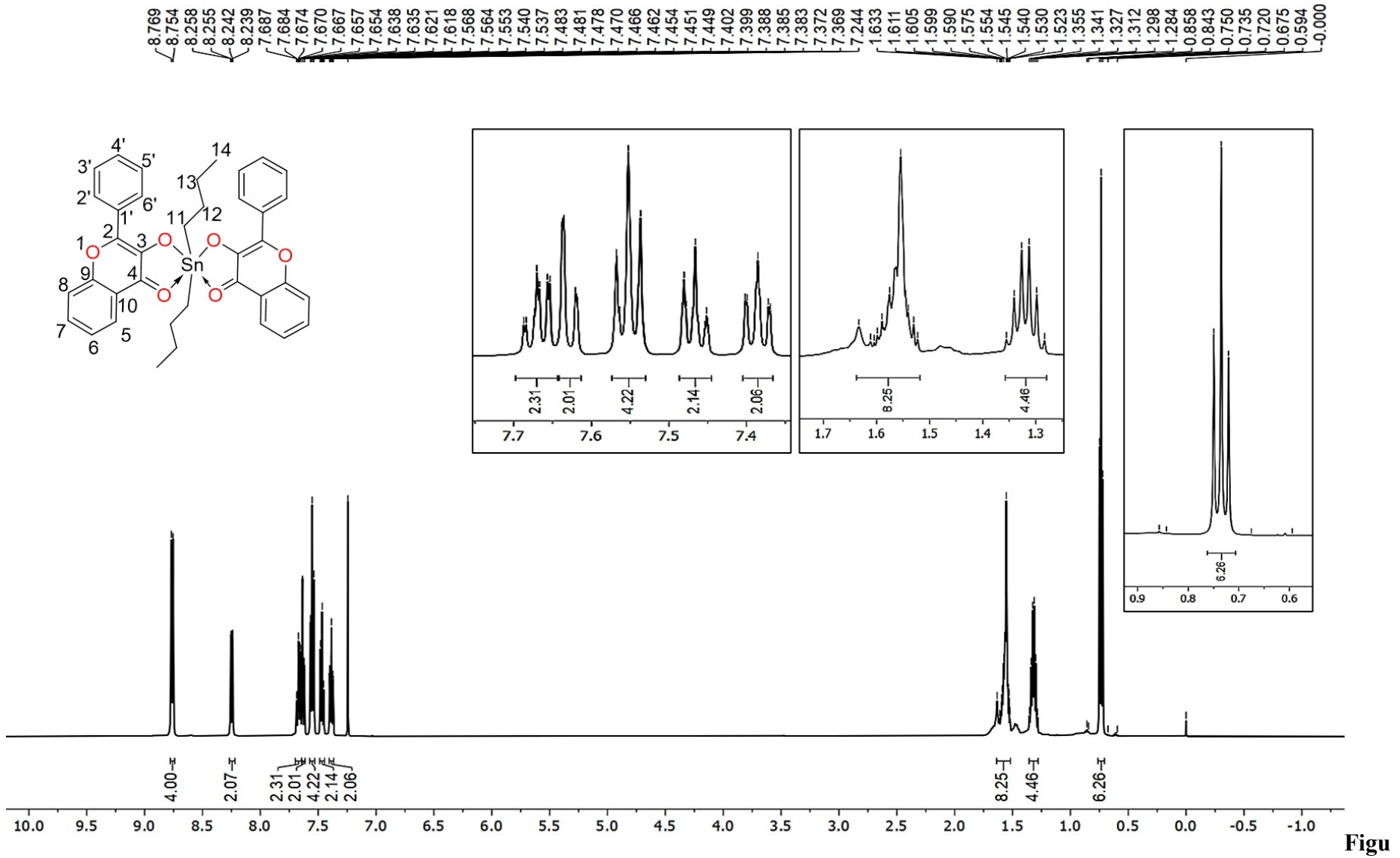


Figure S23. ^{1}H-NMR spectrum of compound **4a**.


8.769
8.754
8.258
8.255
8.242
8.239
7.687
7.684
7.674
7.670
7.667
7.657
7.654
7.638
7.635
7.621
7.618
7.568
7.564
7.553
7.540
7.537
7.483
7.481
7.478
7.470
7.466
7.462
7.454
7.451
7.449
7.402
7.399
7.388
7.385
7.383
7.372
7.369
7.244
1.633
1.611
1.605
1.599
1.590
1.575
1.554
1.545
1.540
1.530
1.523
1.355
1.341
1.327
1.312
1.298
1.284
0.858
0.843
0.750
0.735
0.720
0.675
0.594
-0.000
Sn
2.31
2.01
4.22
2.14
2.06
8.25
4.46
6.26
4.00
2.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0

Figu

re S24. ^{1}H-NMR spectrum of compound **5a**.

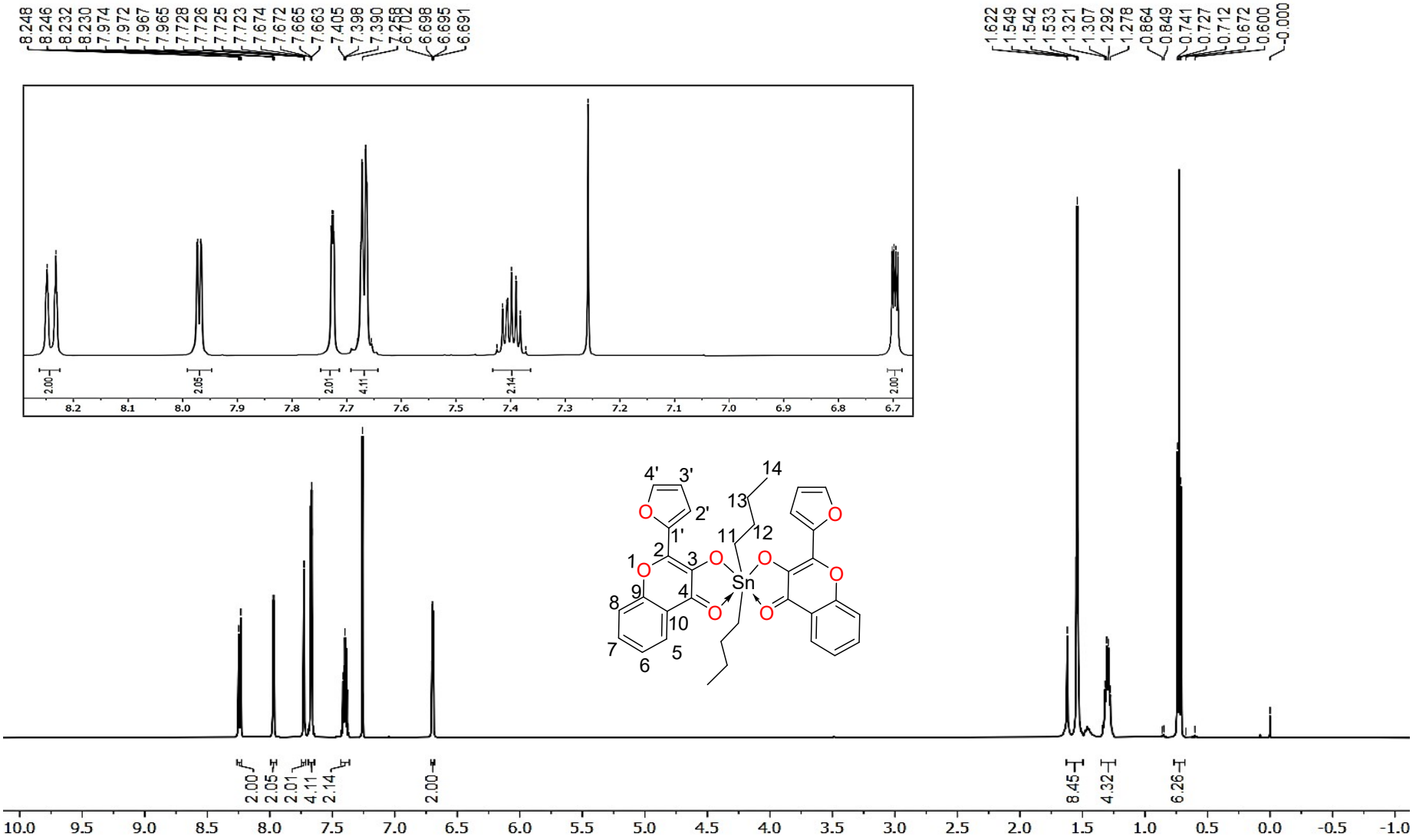


Figure S25. ^{1}H-NMR spectrum of compound **6a**.

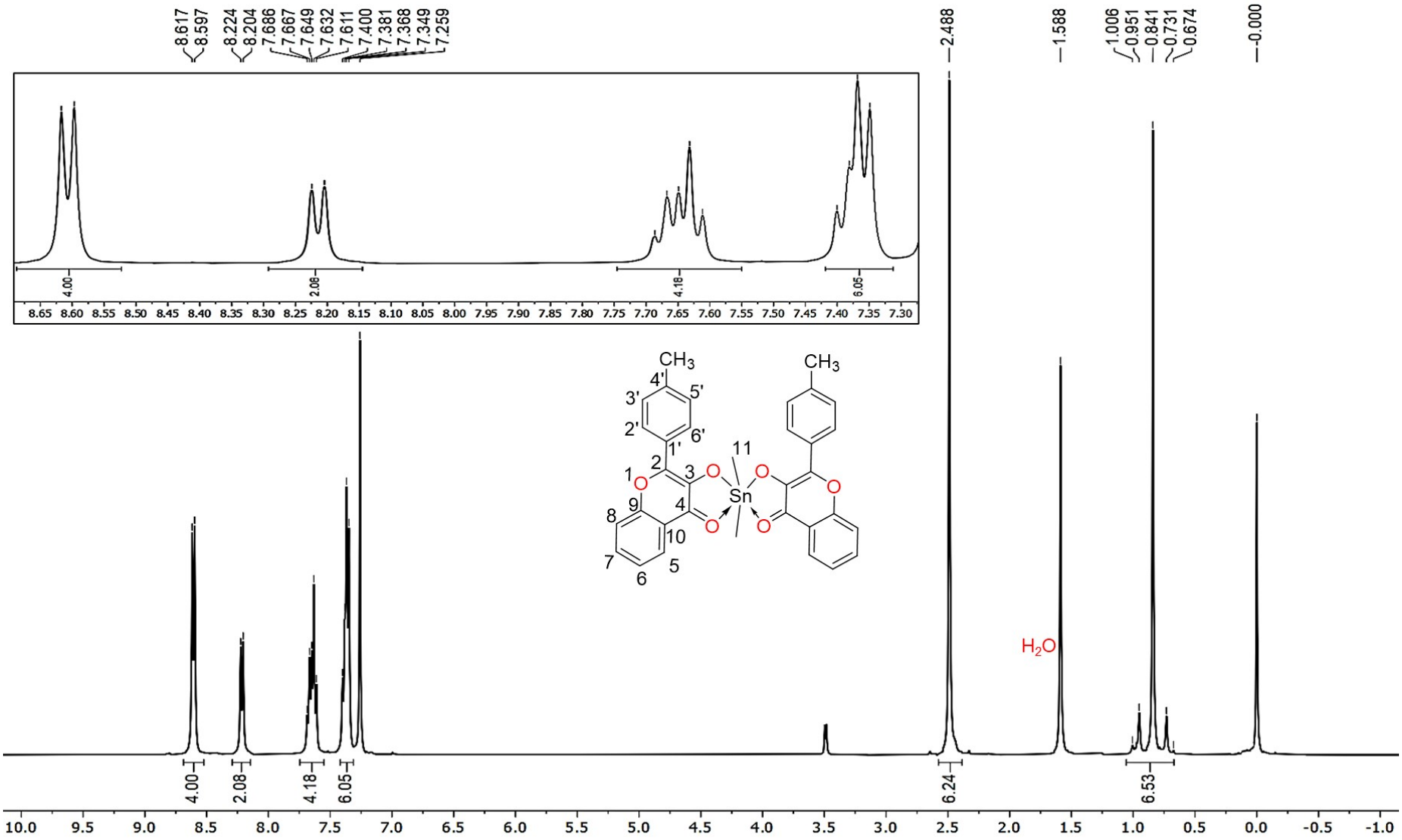


Figure S26. [1]H-NMR spectrum of compound **4b**.

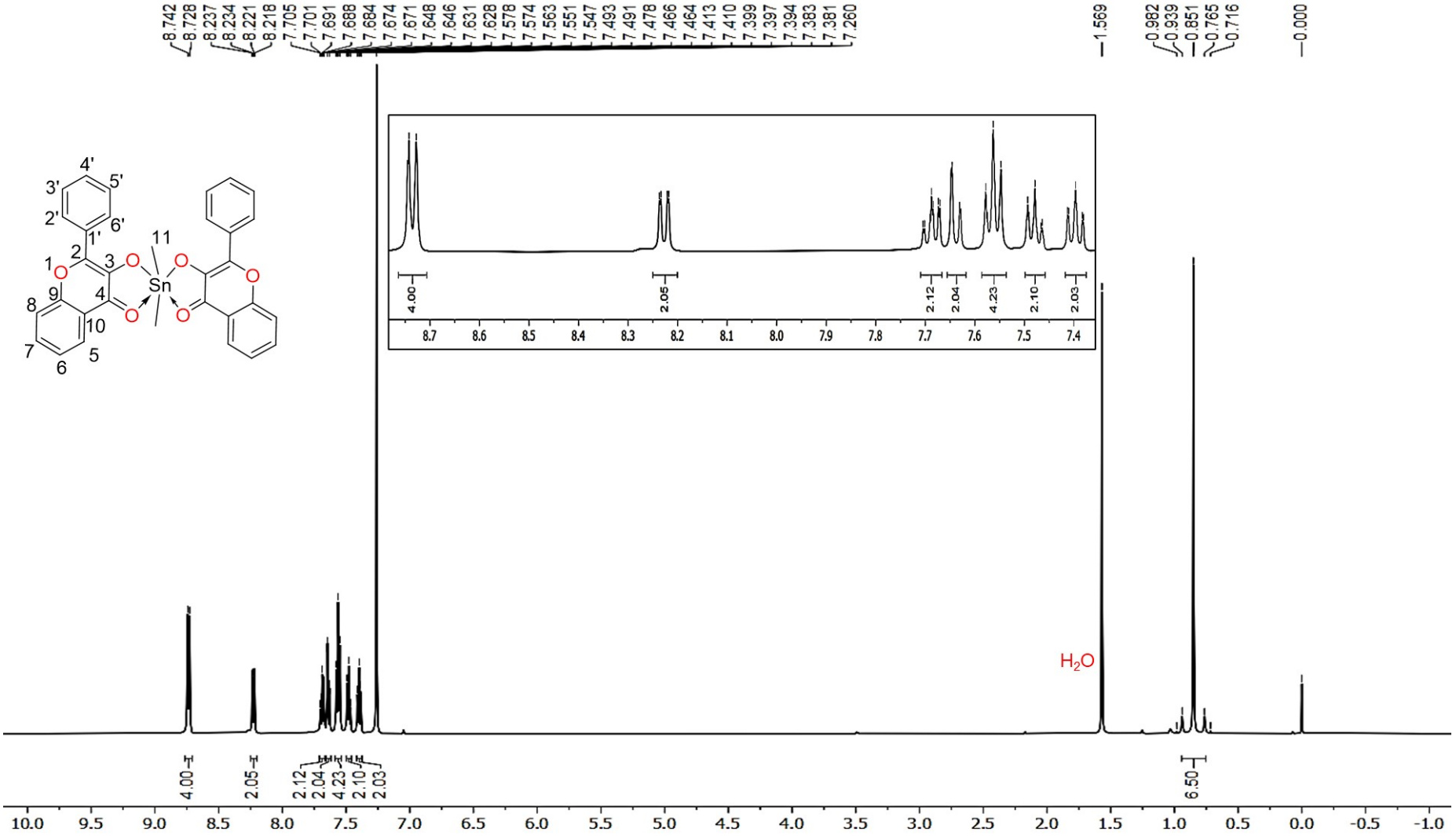


Figure S27. [1]H-NMR spectrum of compound **5b**.

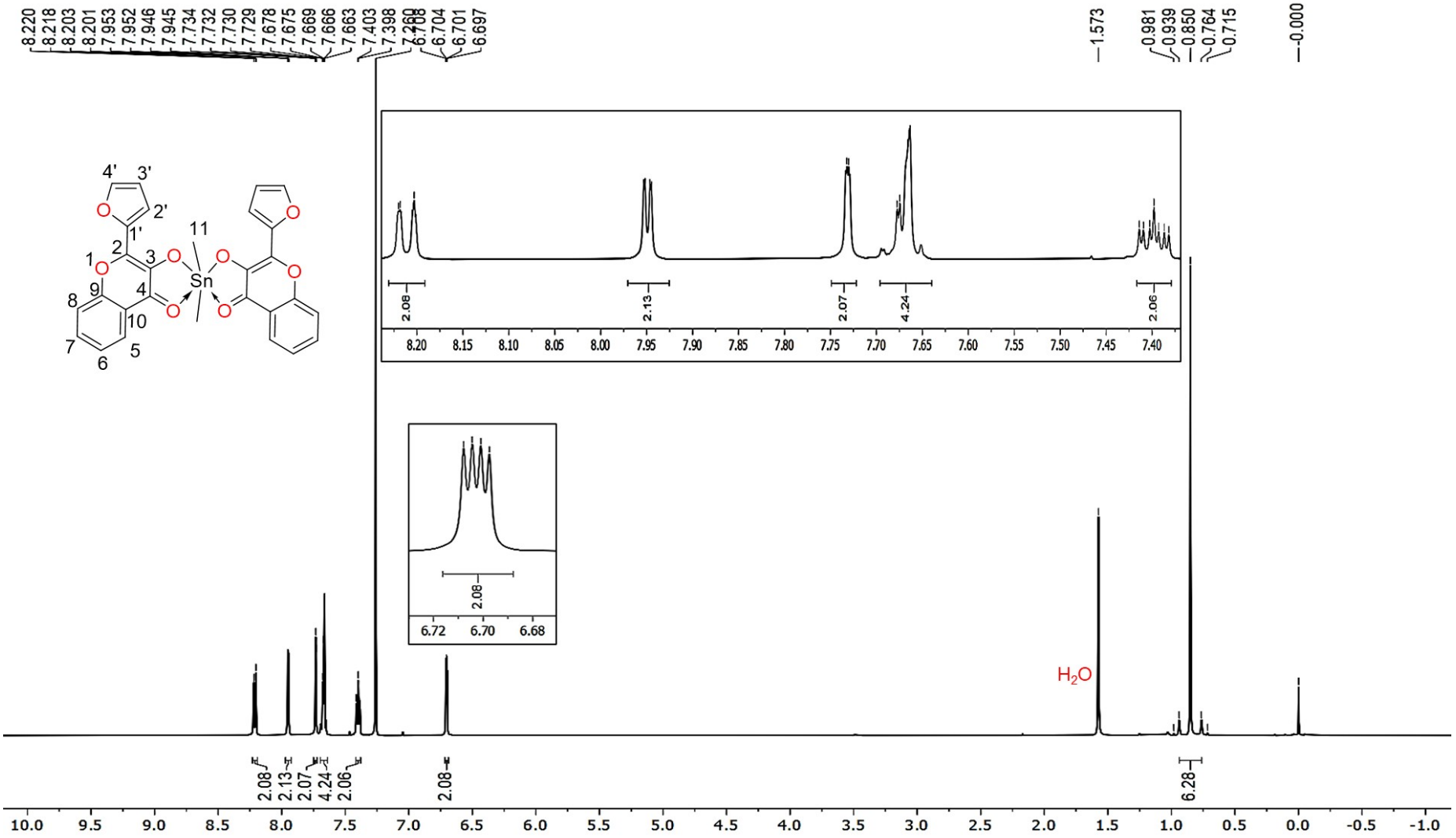


Figure S28. [1]H-NMR spectrum of compound **6b**.

2.3. ^{13}C-NMR spectra of compounds

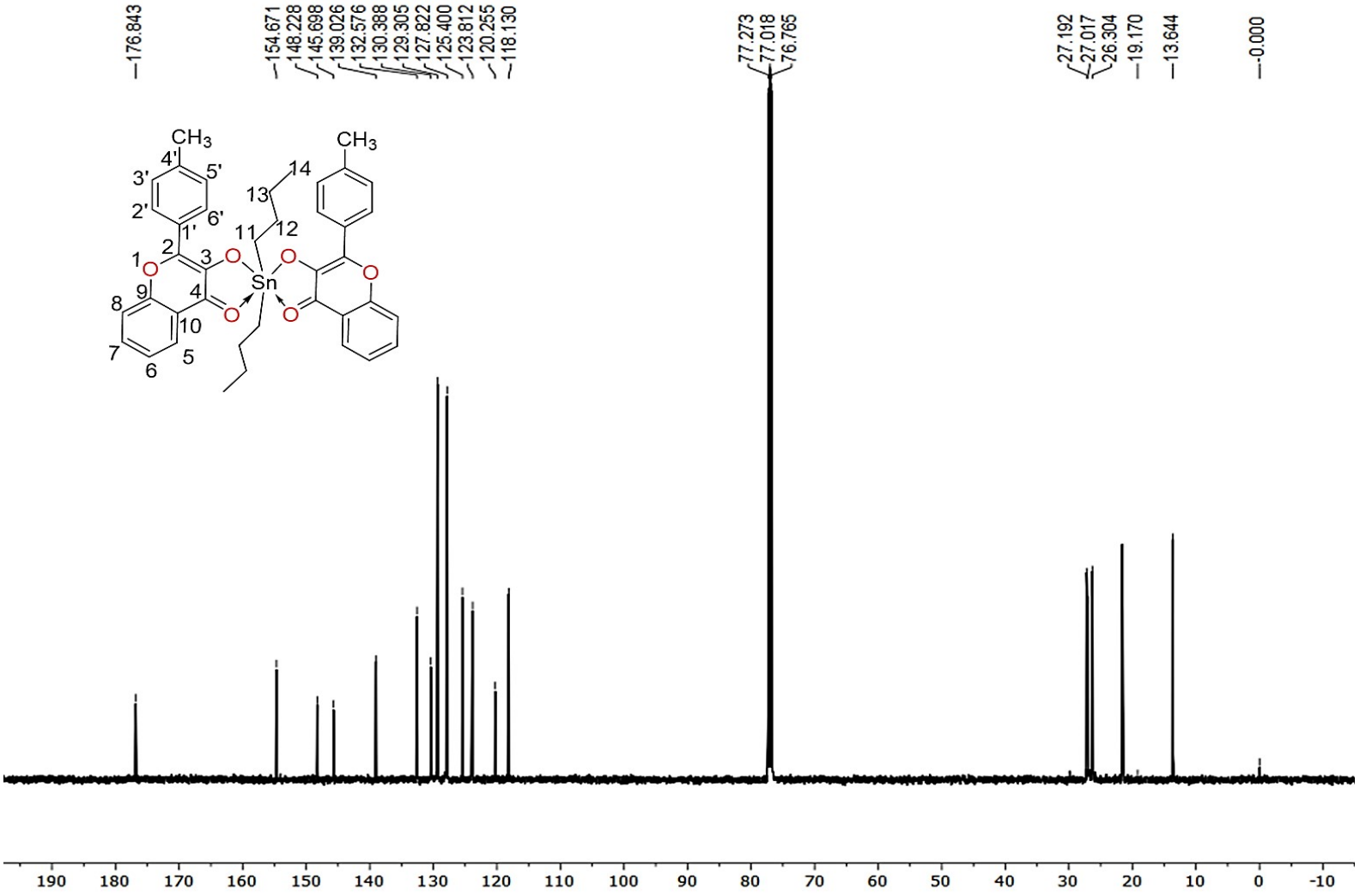


Figure S29. ^{13}C-NMR spectrum of compound **4a**.

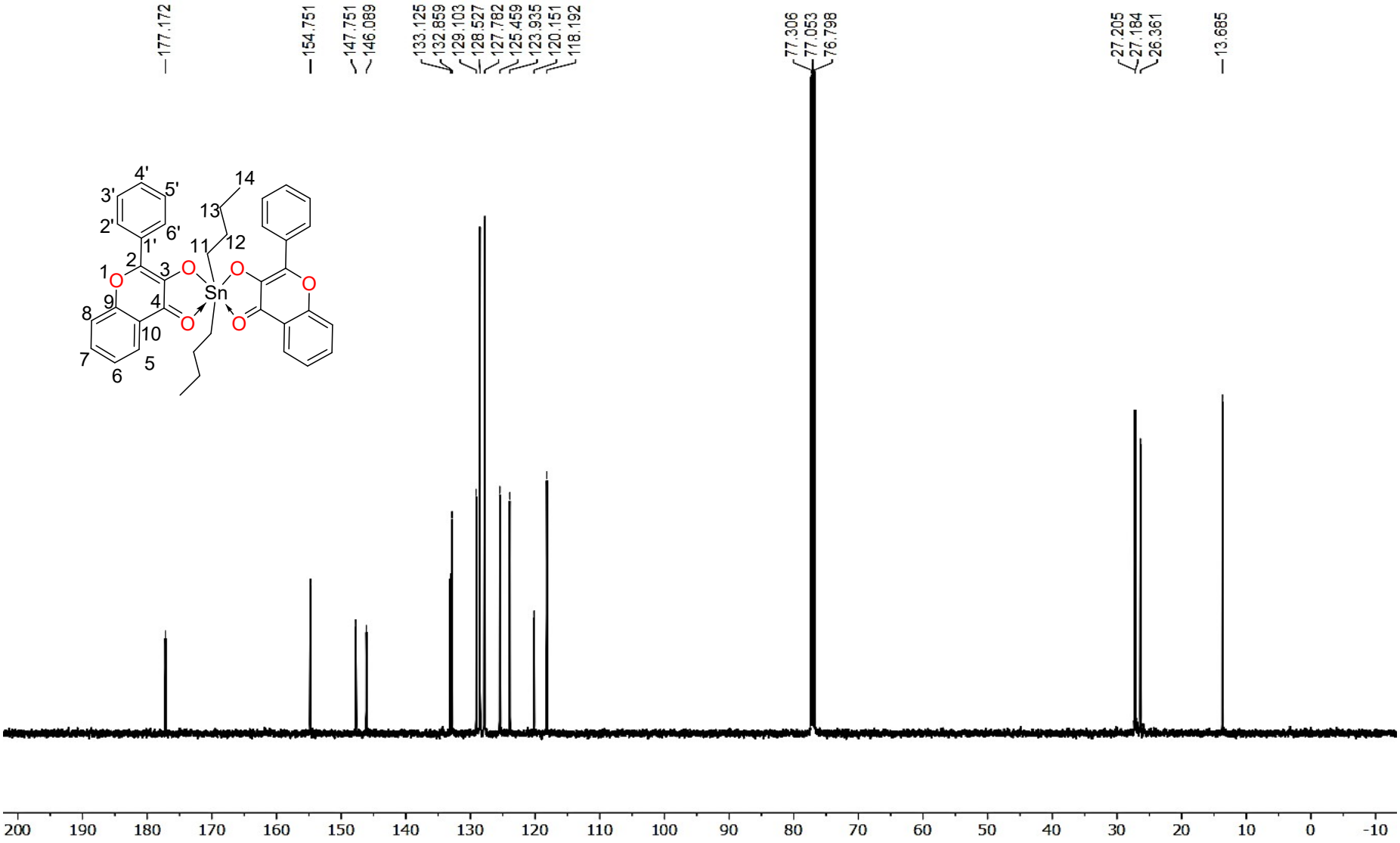


Figure S30. ^{13}C-NMR spectrum of compound **5a**.

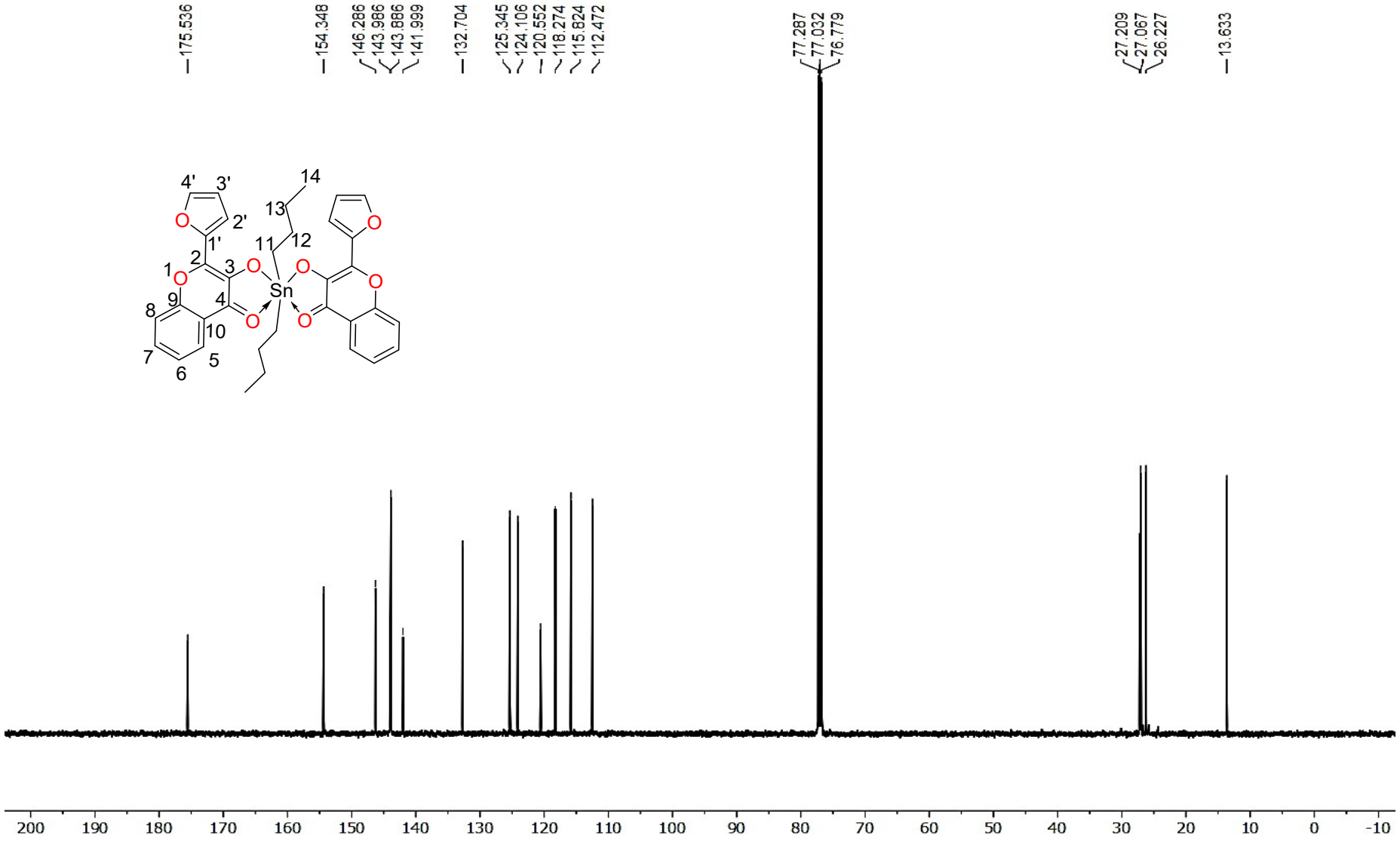


Figure S31. ^{13}C-NMR spectrum of compound **6a**.

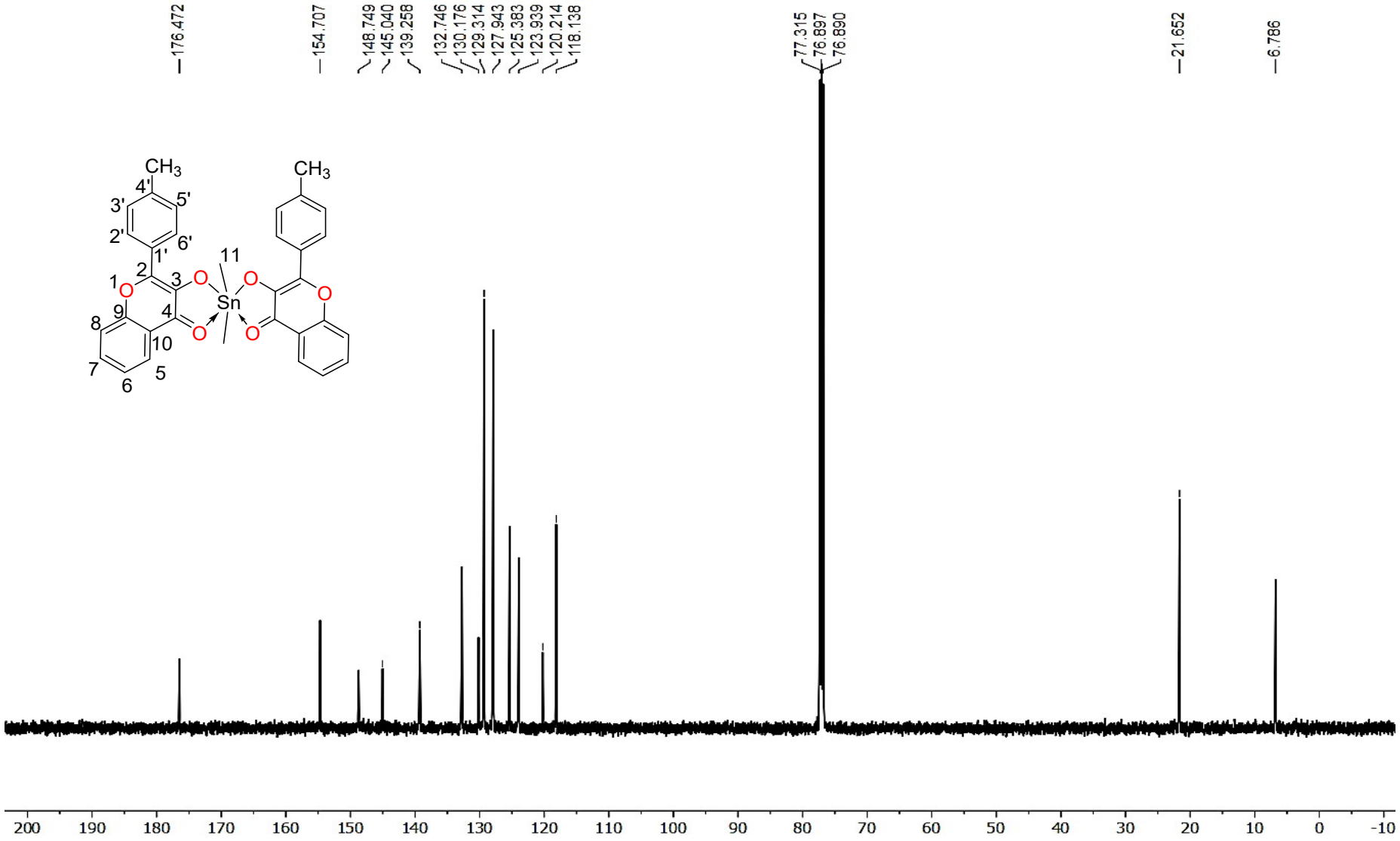


Figure S32. ^{13}C-NMR spectrum of compound **4b**.

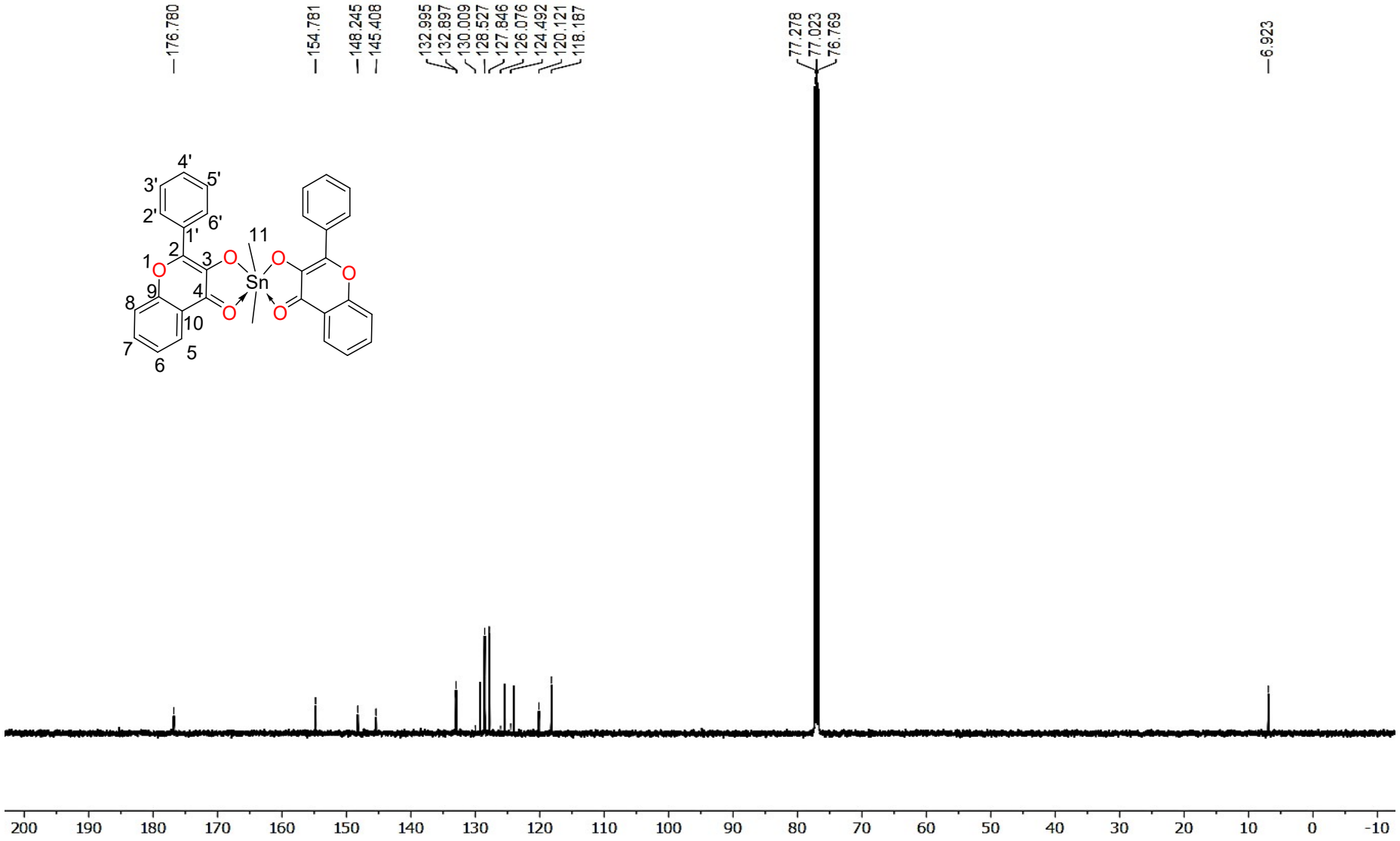


Figure S33. ^{13}C-NMR spectrum of compound **5b**.

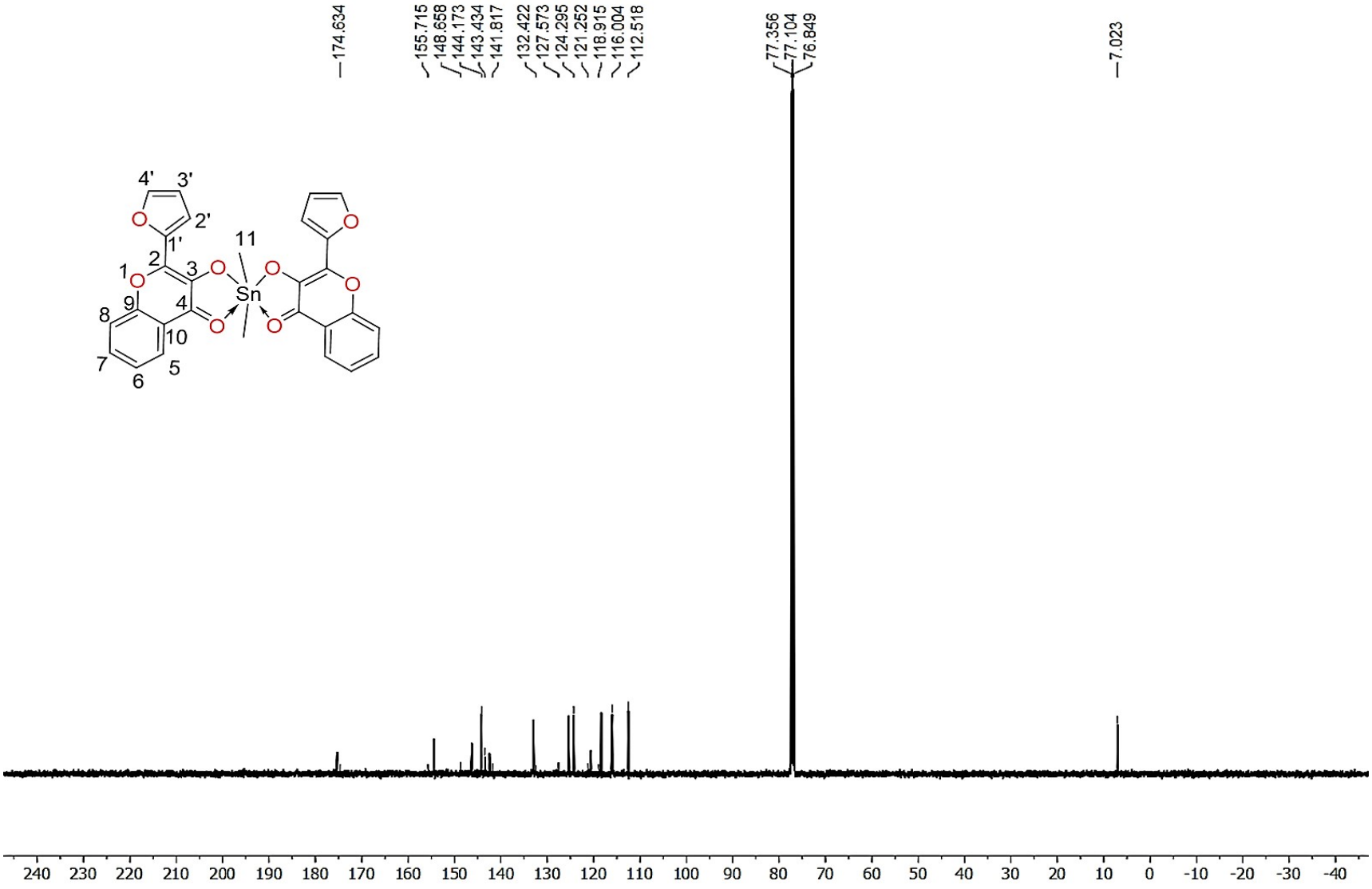


Figure S34. ^{13}C-NMR spectrum of compound **6b**.

2.4. ^{119}Sn-NMR spectra of compounds

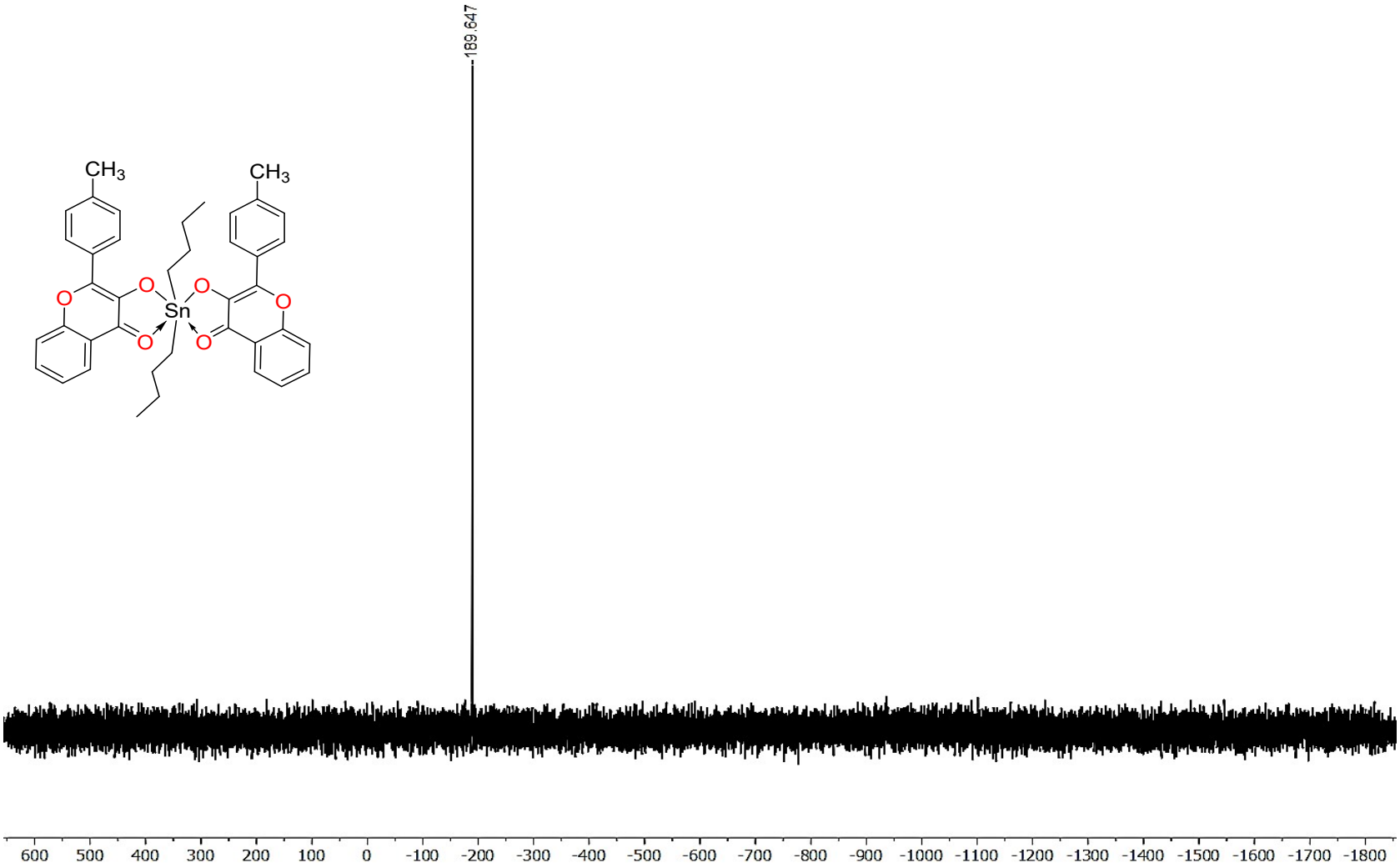


Figure S35. ^{119}Sn-NMR spectrum of compound **4a**.

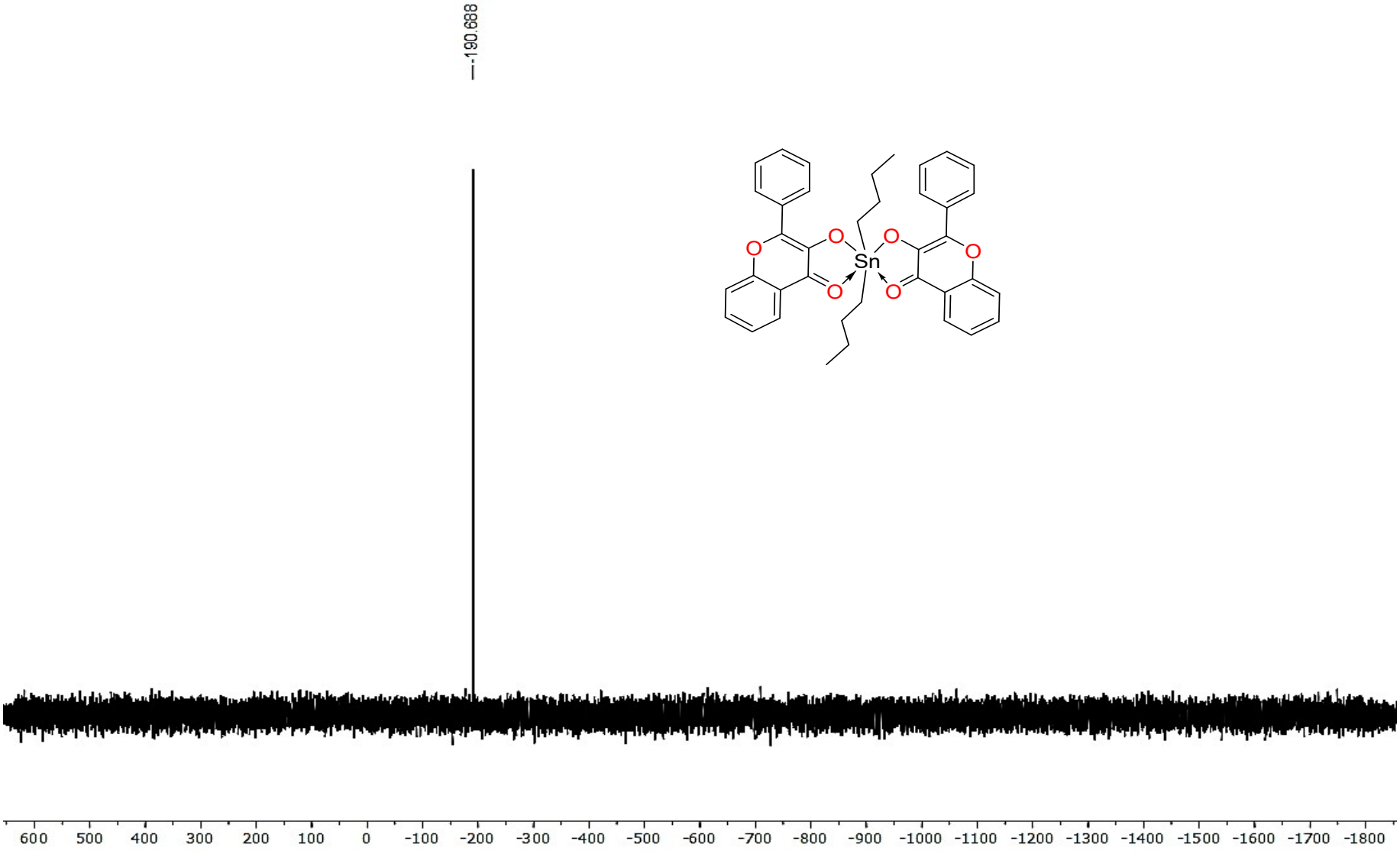


Figure S36. ^{119}Sn-NMR spectrum of compound **5a**.

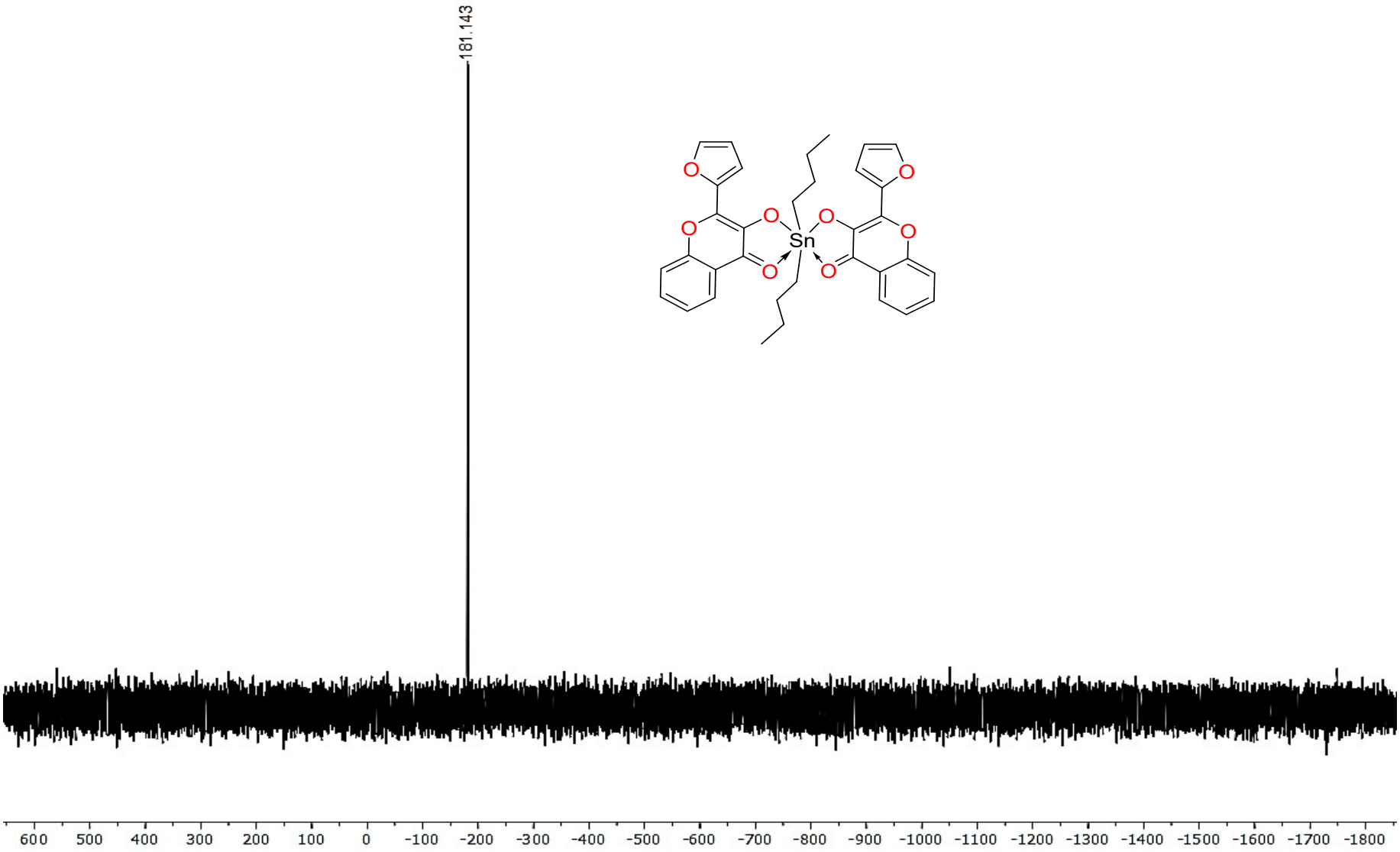


Figure S37. ^{119}Sn-NMR spectrum of compound **6a**.

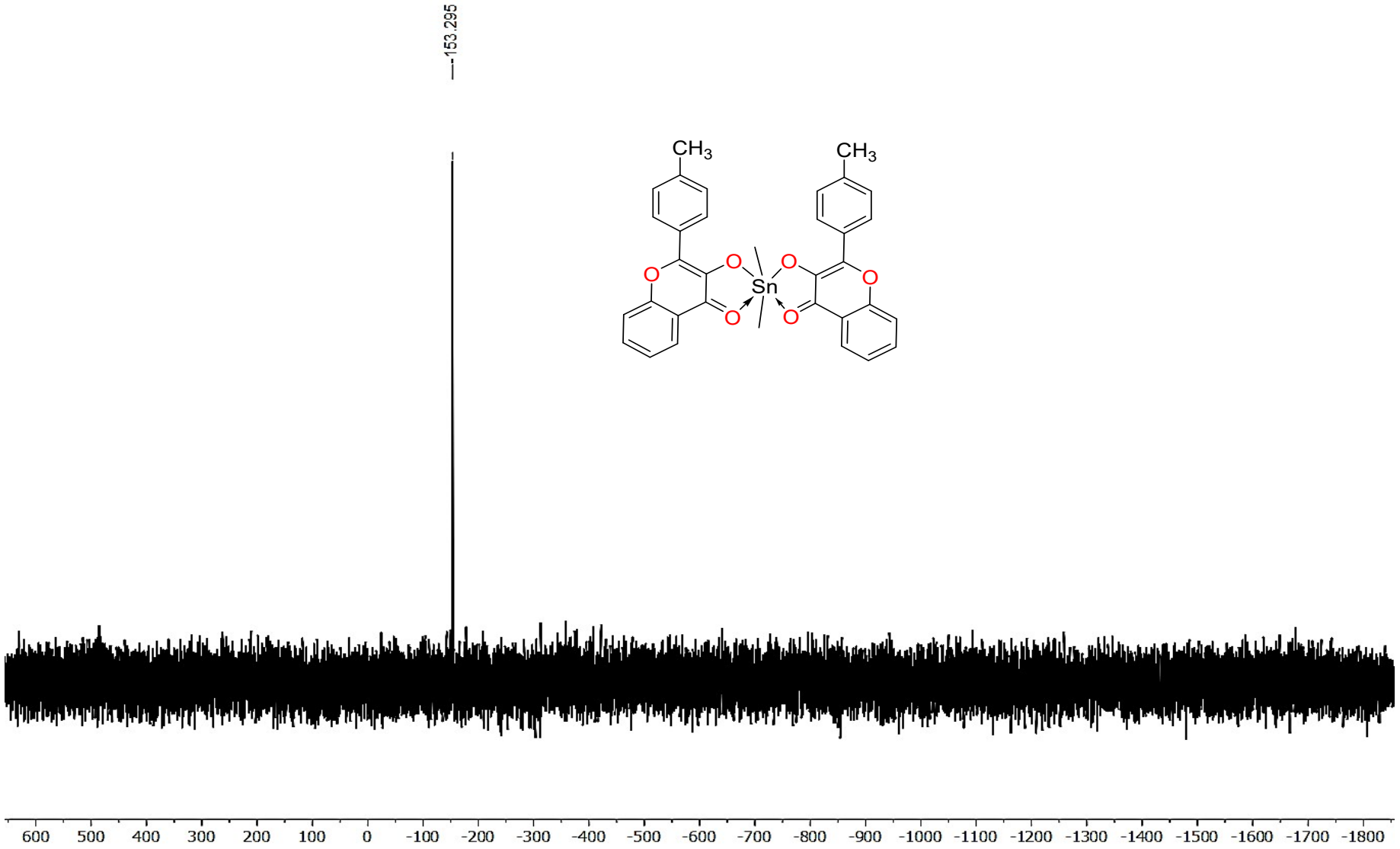


Figure S38. ^{119}Sn-NMR spectrum of compound **4b**.

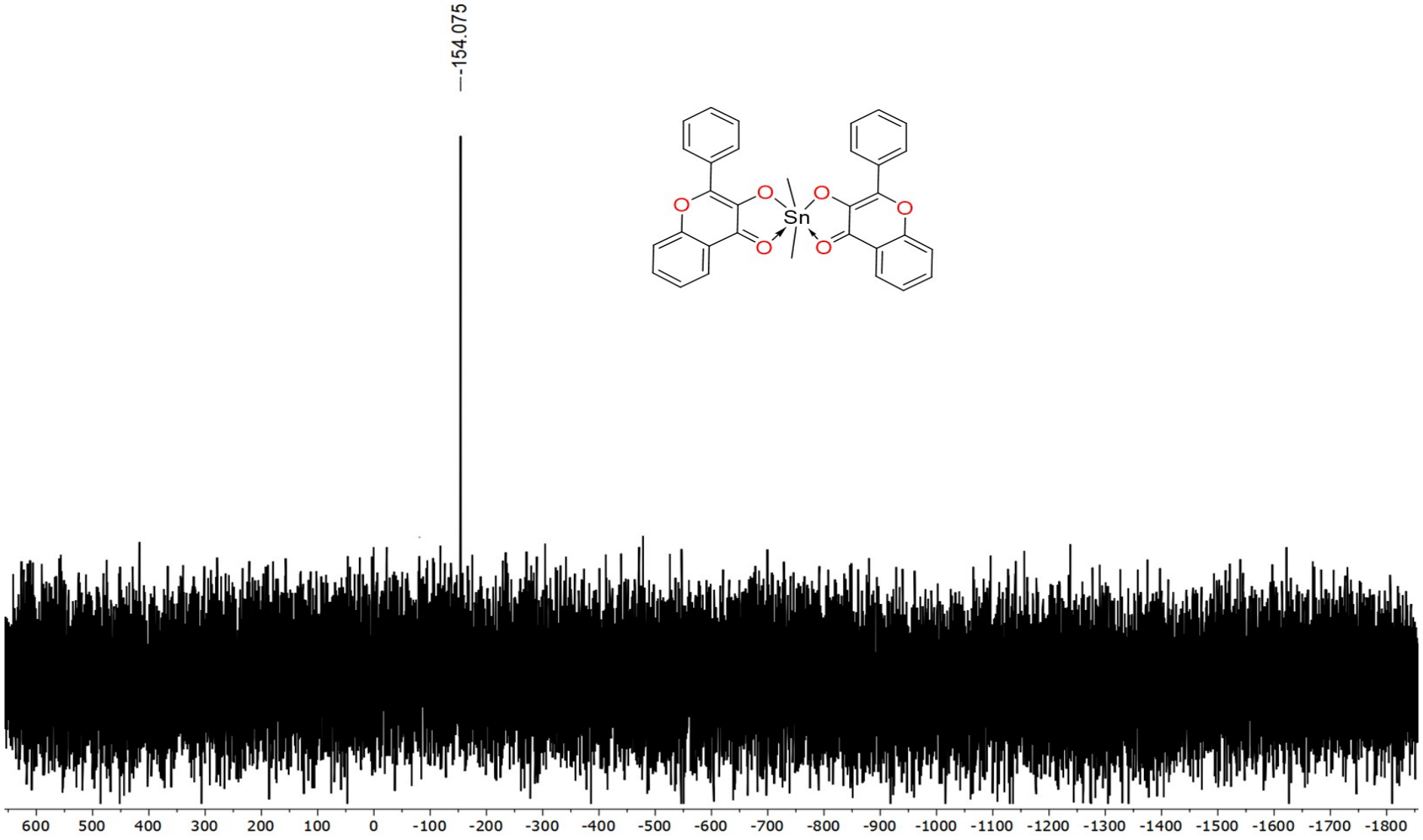


Figure S39. ^{119}Sn-NMR spectrum of compound **5b**.

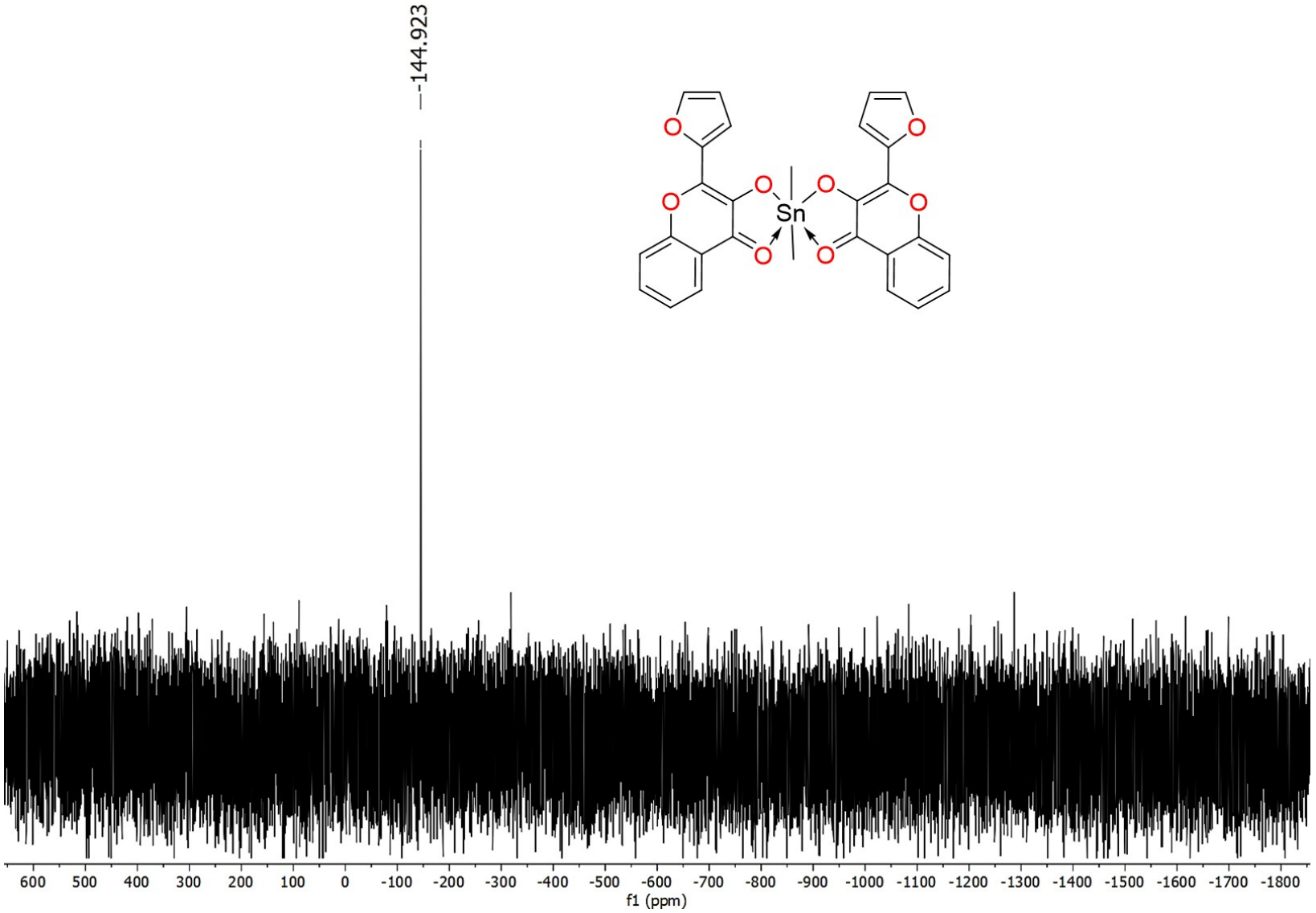


Figure S40. ^{119}Sn-NMR spectrum of compound **6b**.

2.5. ESI-MS spectra of compounds

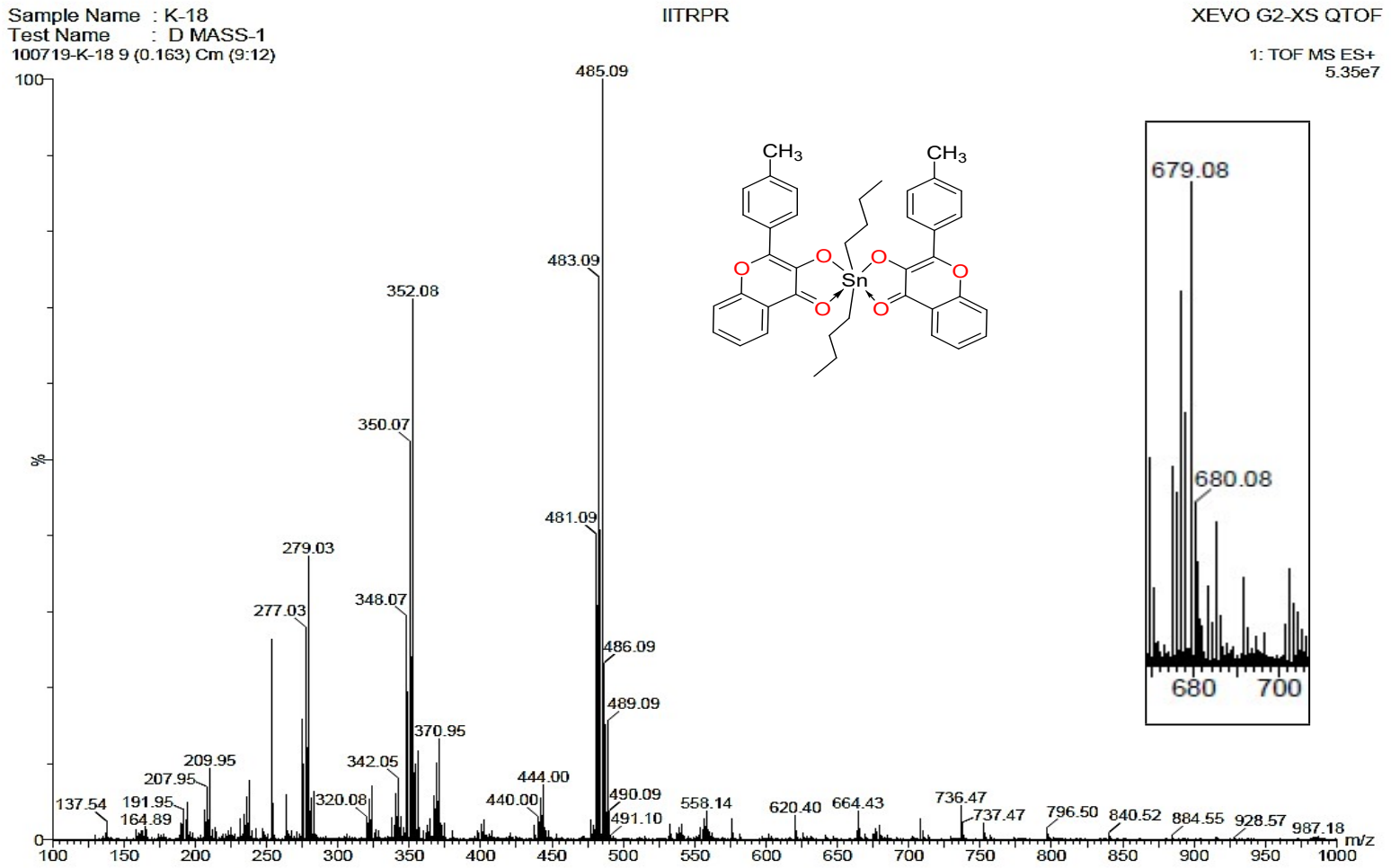


Figure S41. ESI-MS spectrum of compound **4a**; **Inset**: Cutout of the expanded spectrum.

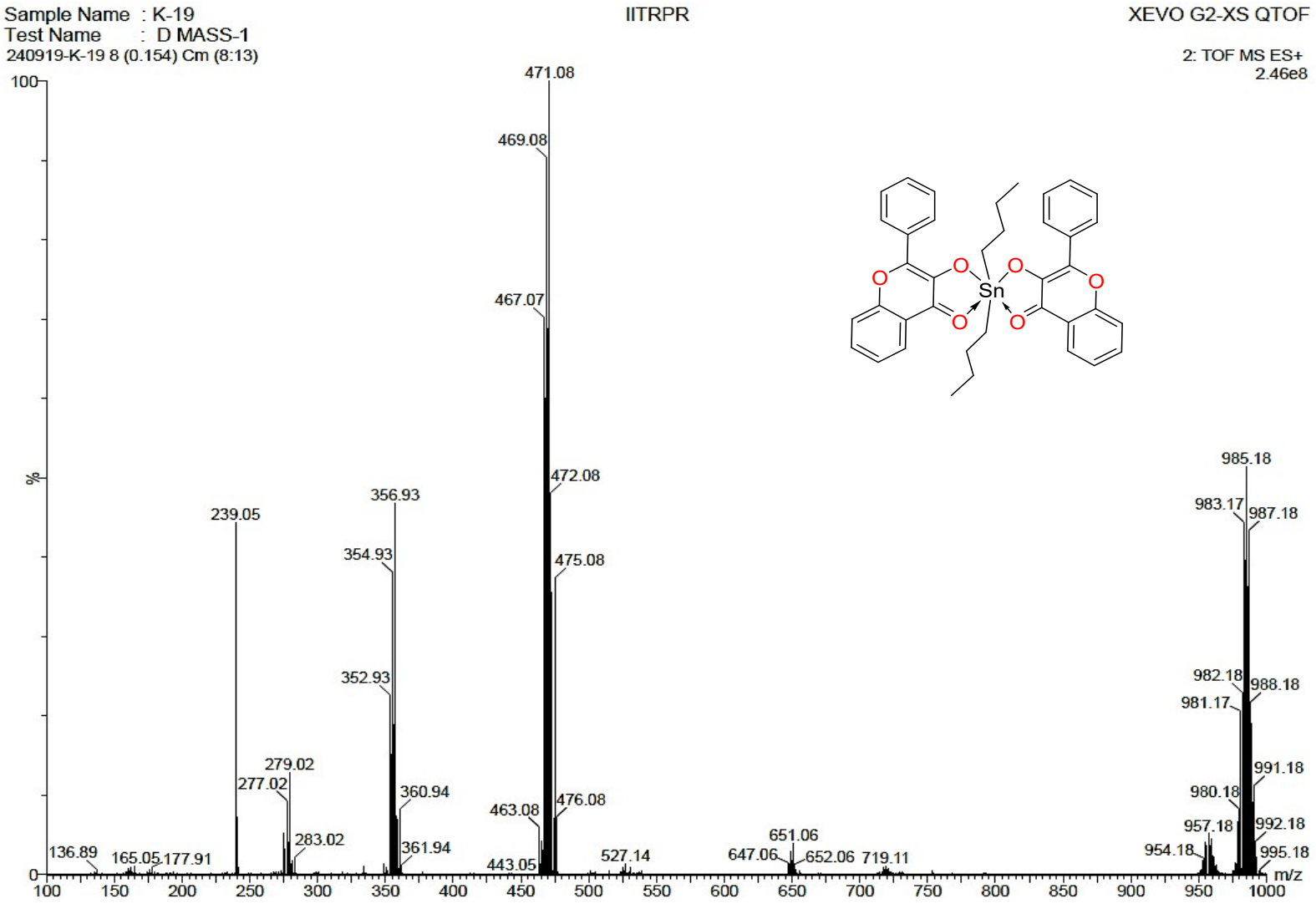


Figure S42. ESI-MS spectrum of compound **5a**.

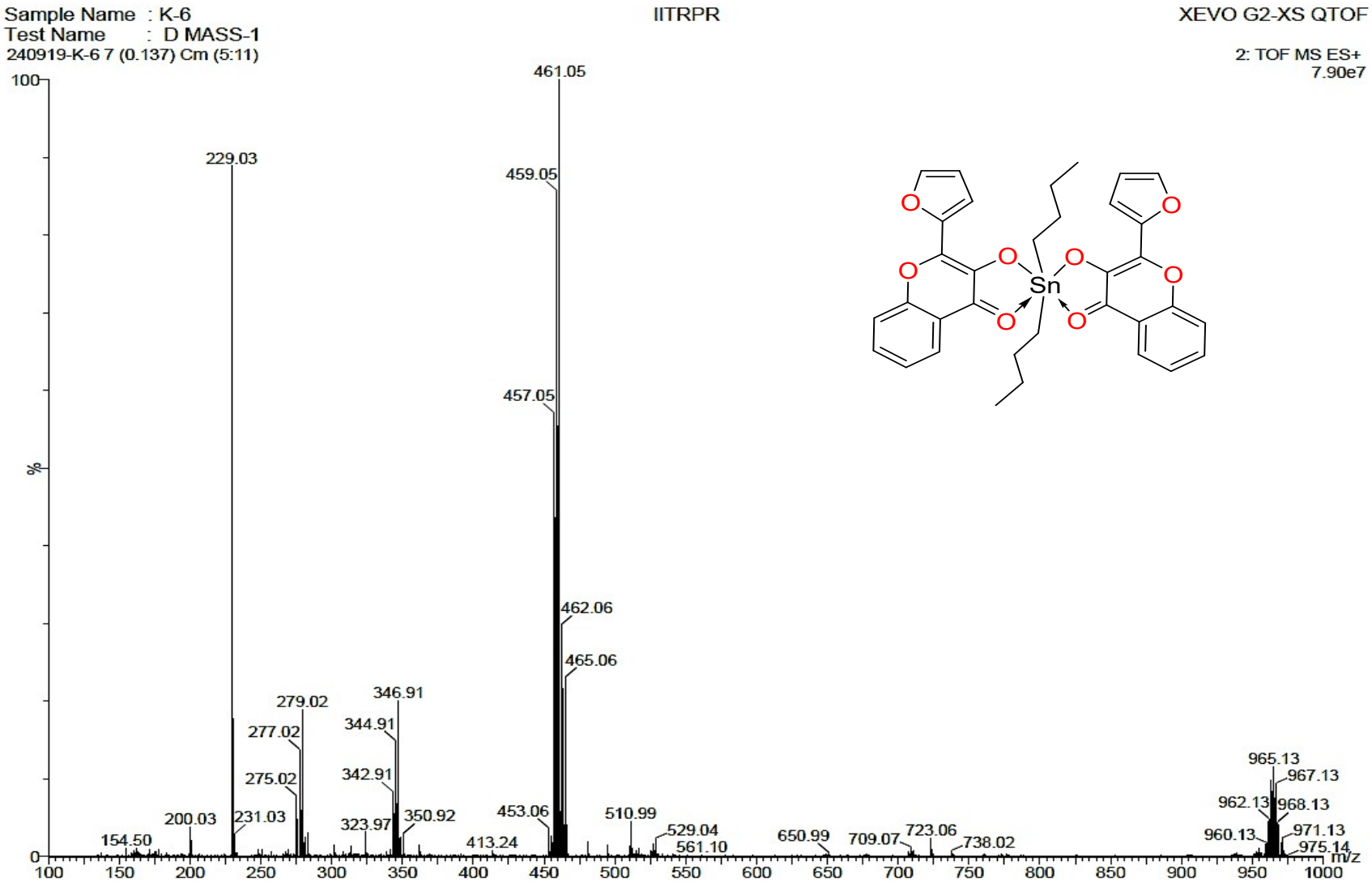


Figure S43. ESI-MS spectrum of compound **6a**.

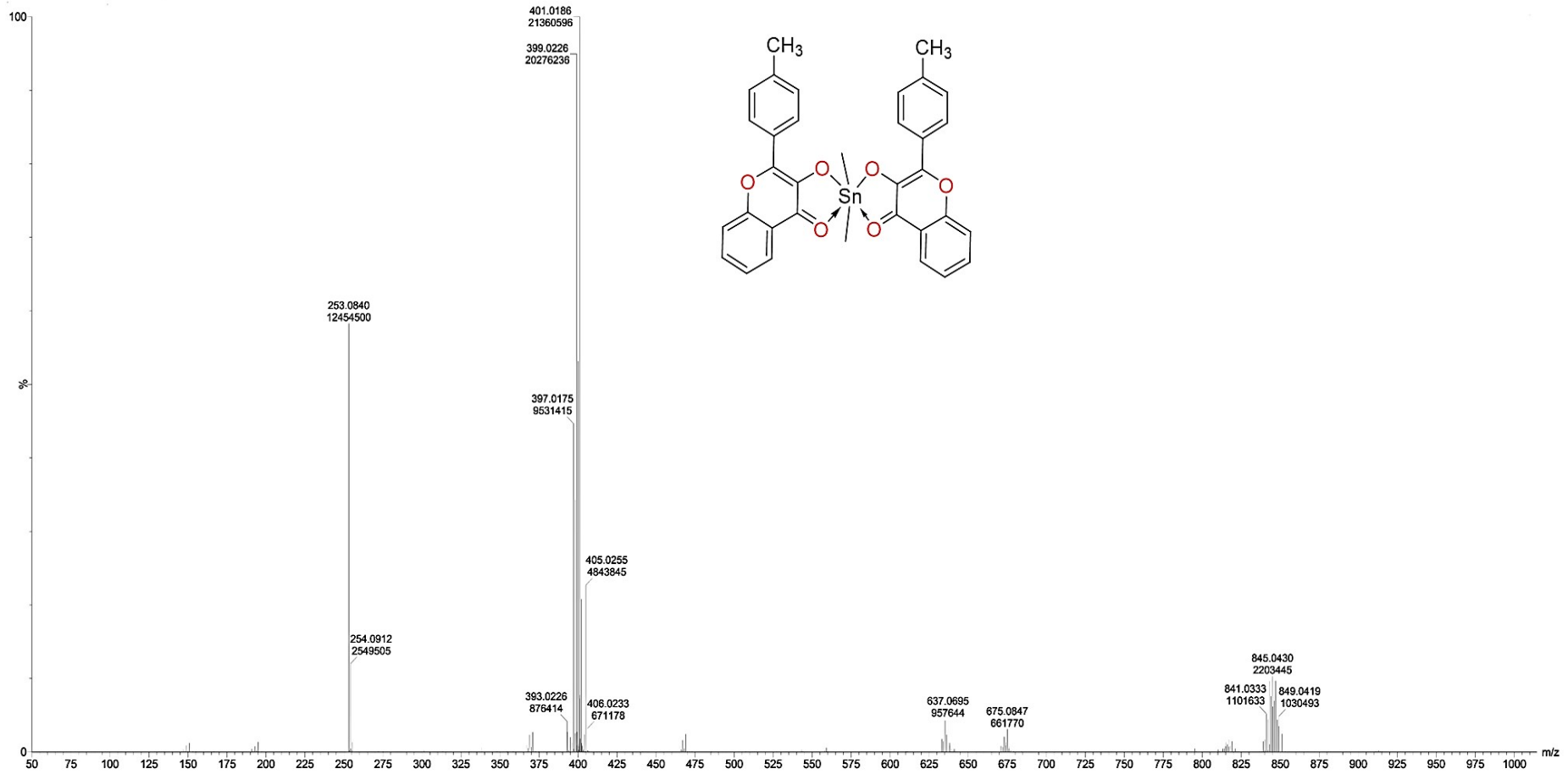


Figure S44. ESI-MS spectrum of compound **4b**.

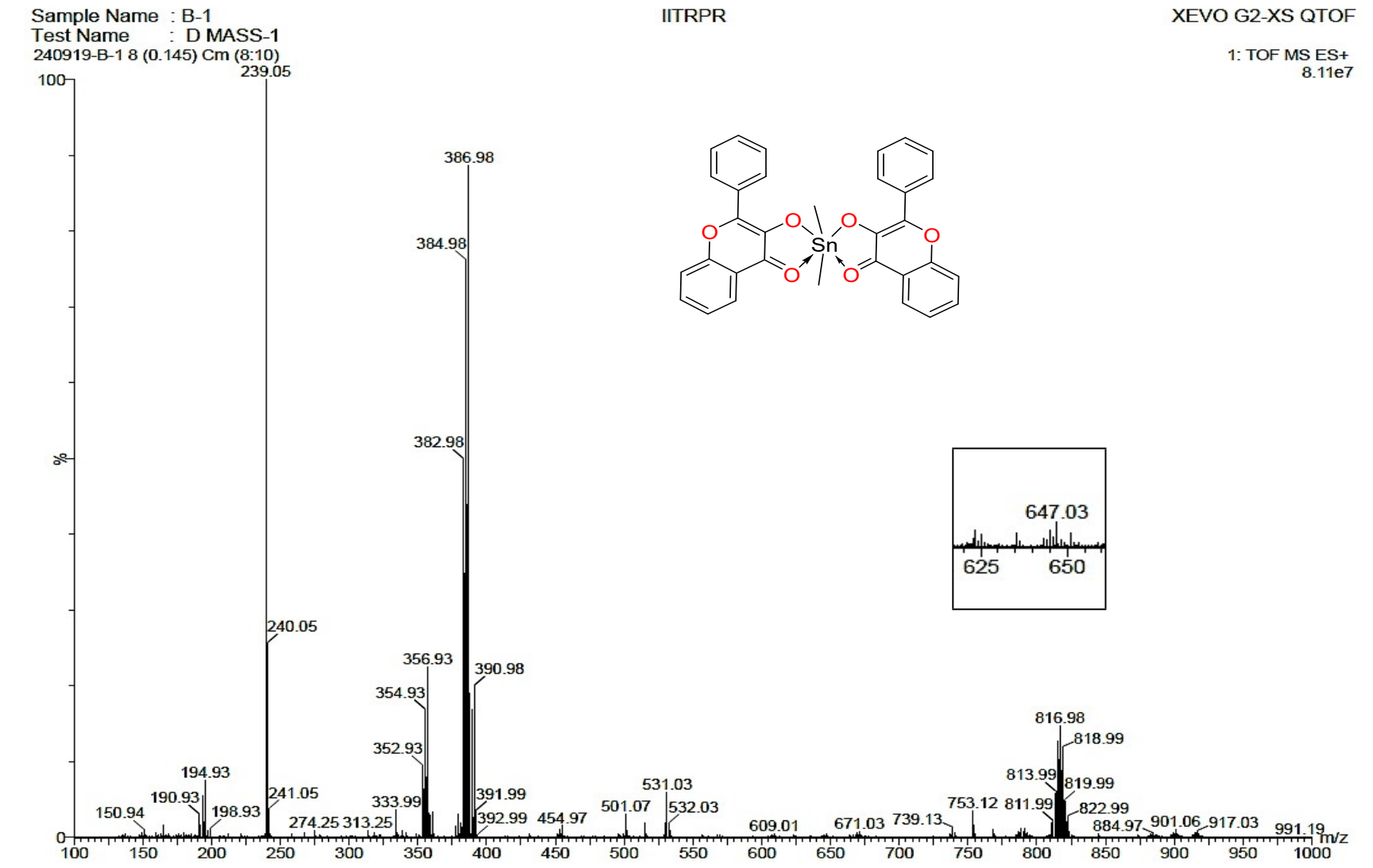


Figure S45. ESI-MS spectrum of compound **5b**; **Inset**: Cutout of the expanded spectrum.

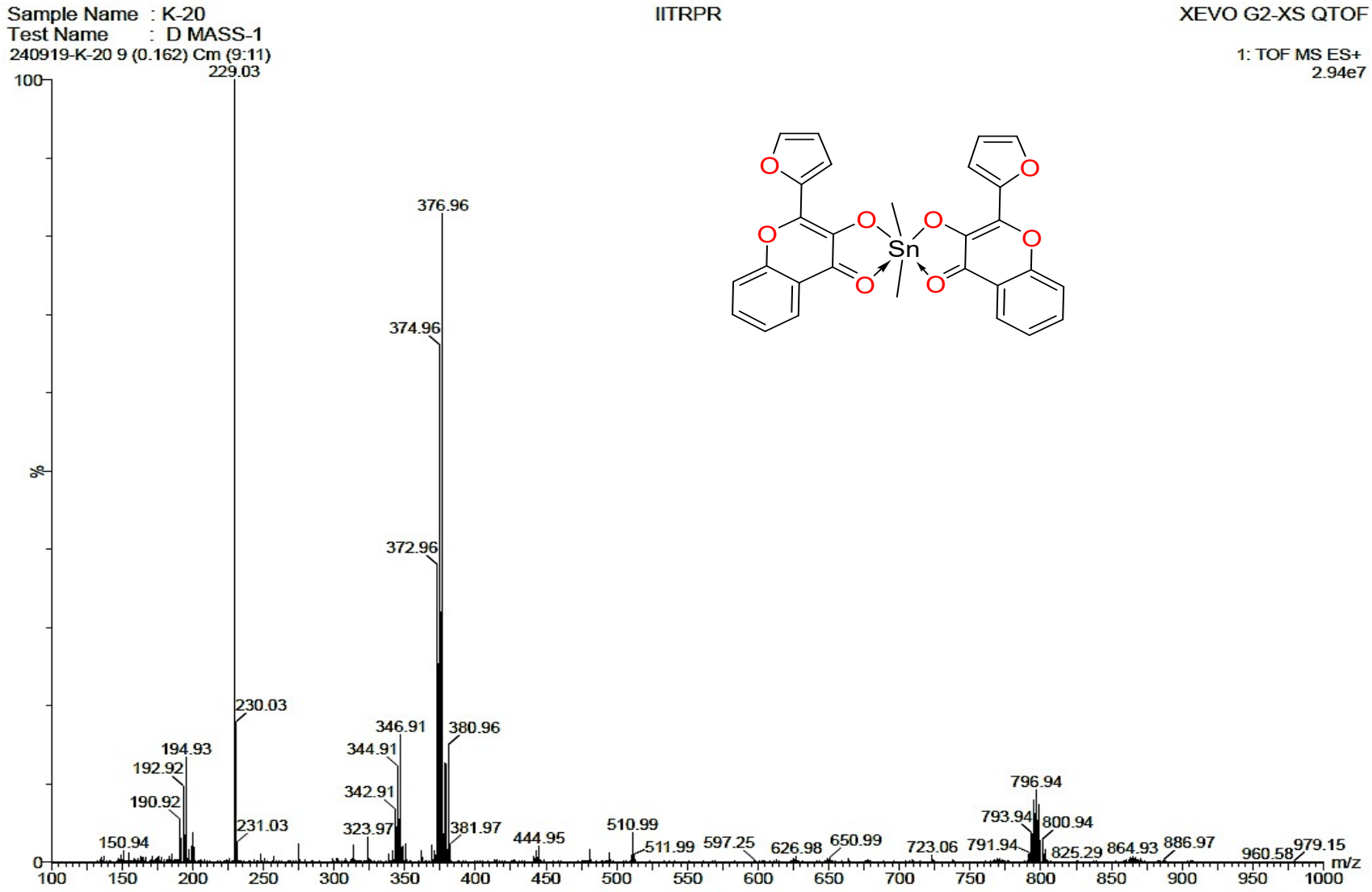


Figure S46. ESI-MS spectrum of compound **6b**.