Electronic Supplementary Information

Synthesis, Characterization, and Anticancer Potential of Pyrene-Appended Schiff Base Tin(IV) Complexes: Experimental and Computational Insights

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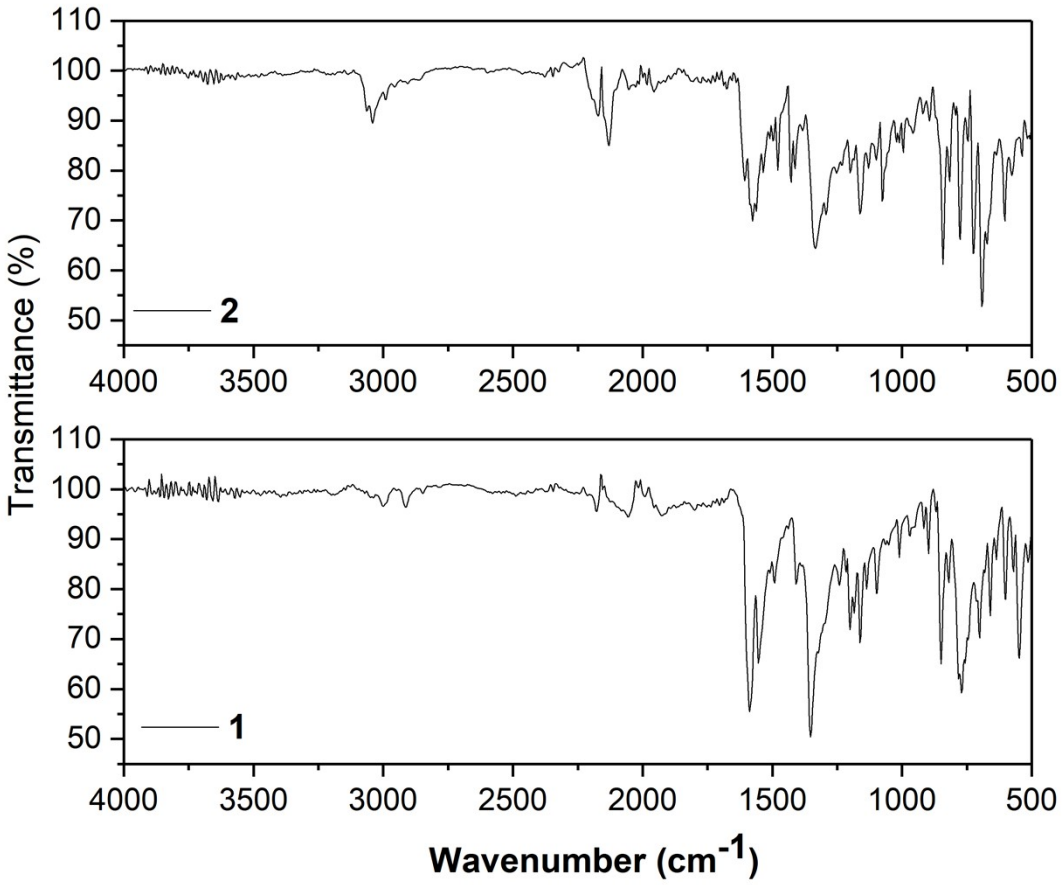


Figure S1: FT-IR spectra of **1** and **2**.

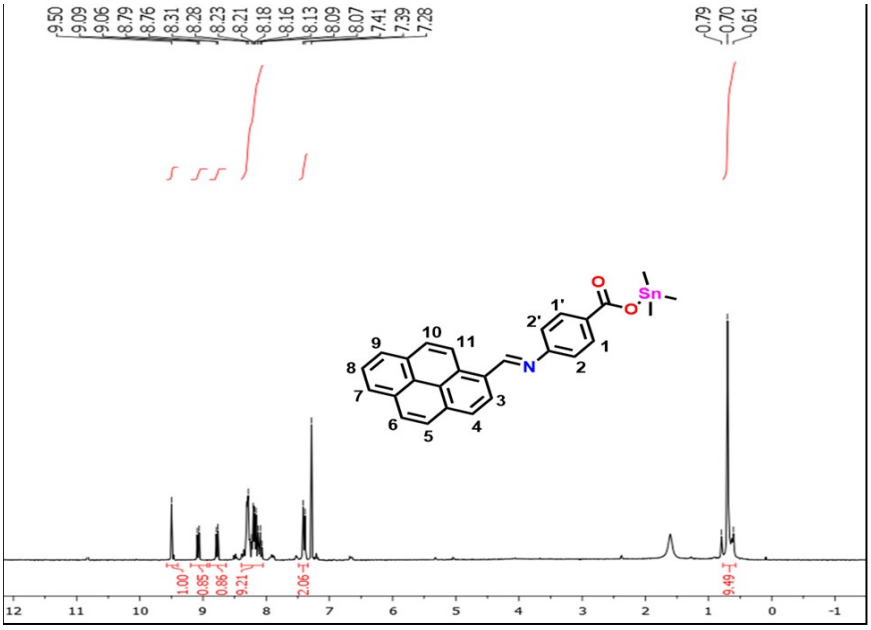


Figure S2. ^{1}H-NMR spectrum of **1** recorded in $CDCl_3$.

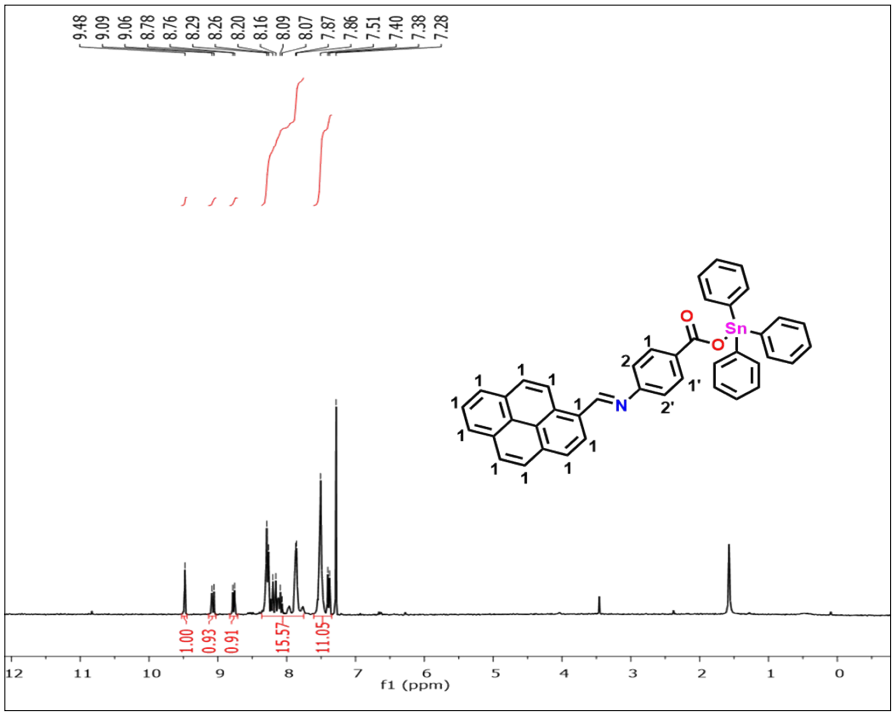


Figure S3. ^{1}H-NMR spectrum of **2** recorded in $CDCl_3$.

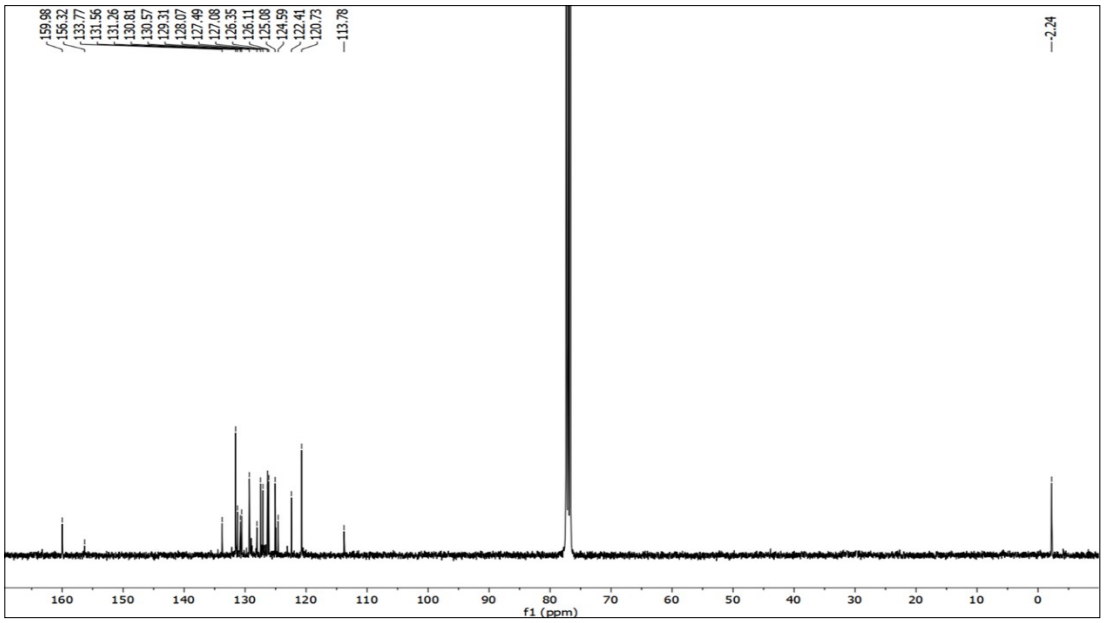


Figure S4. ^{13}C-NMR spectrum of **1** recorded in $CDCl_3$.

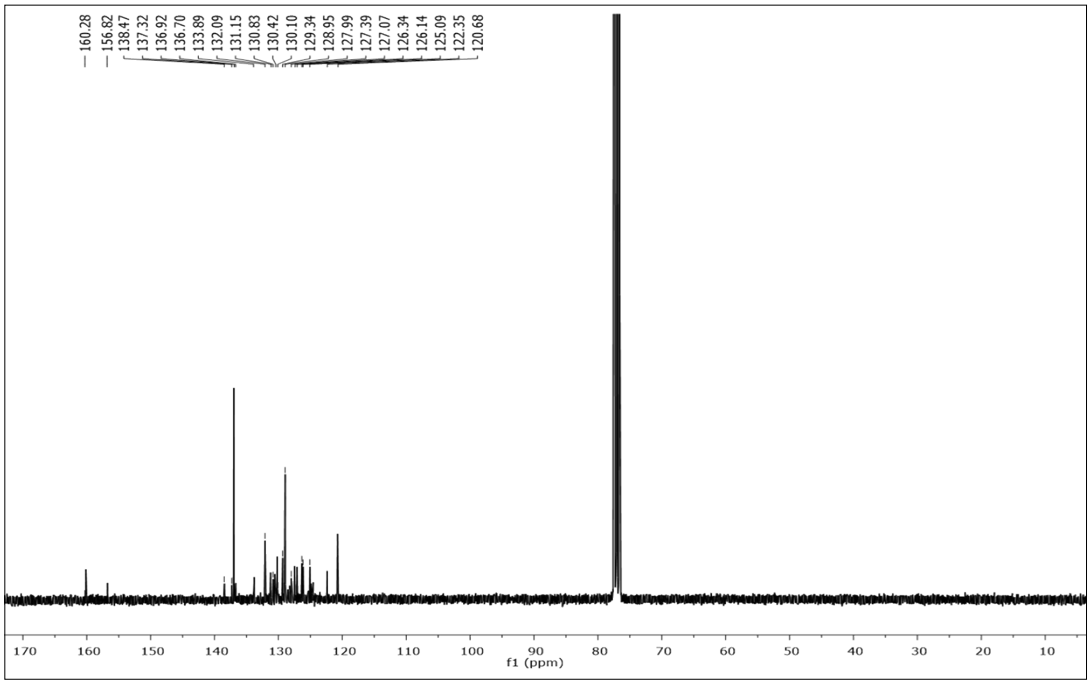


Figure S5. ^{13}C-NMR spectrum of **2** recorded in $CDCl_3$.

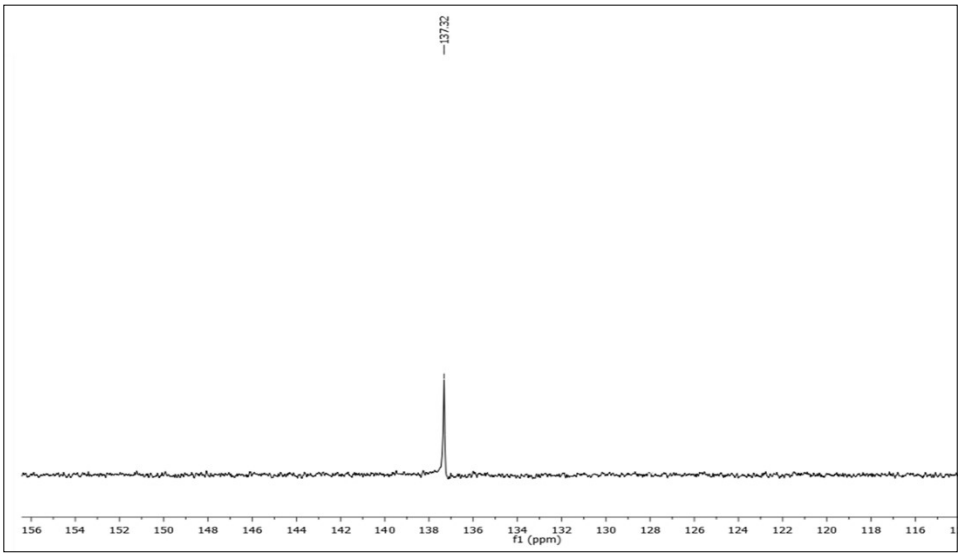


Figure S6. ^{119}Sn-NMR spectrum of **1** recorded in $CDCl_3$.

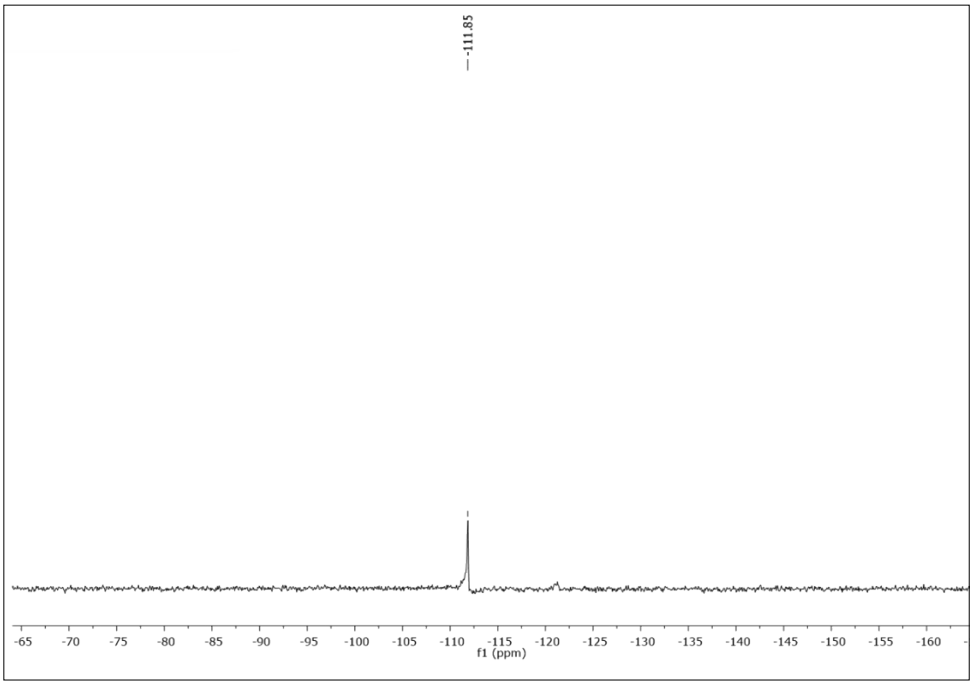


Figure S7. ^{119}Sn-NMR spectrum of **2** recorded in $CDCl_3$.

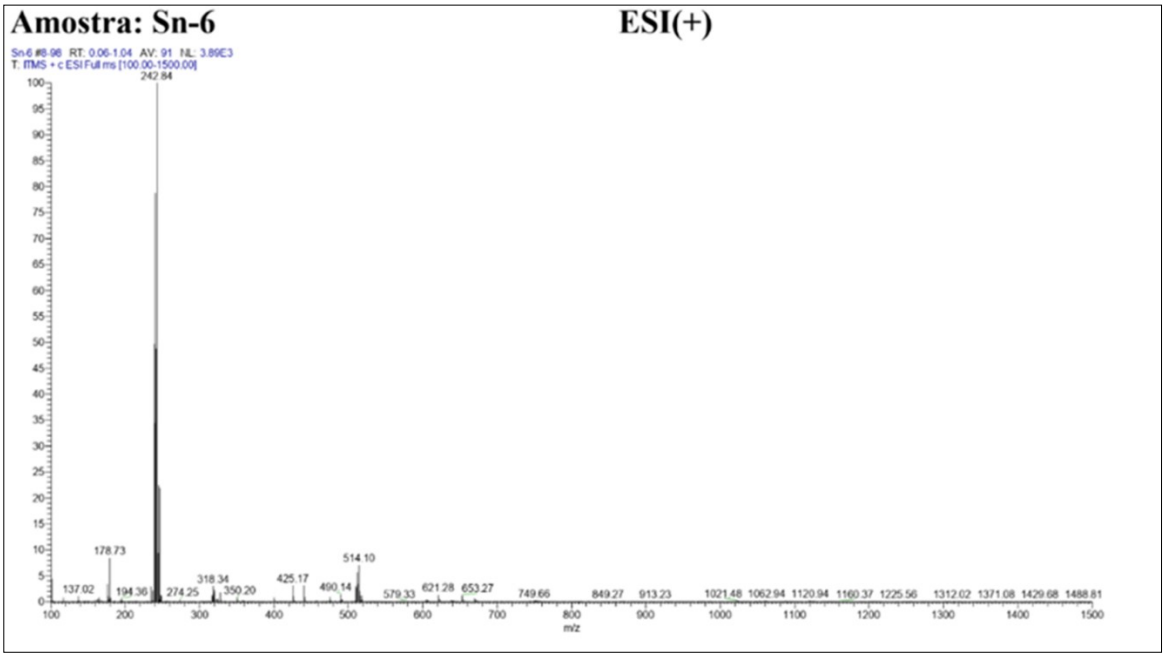


Figure S8. ESI-MS spectrum of **1** recorded in MeOH.

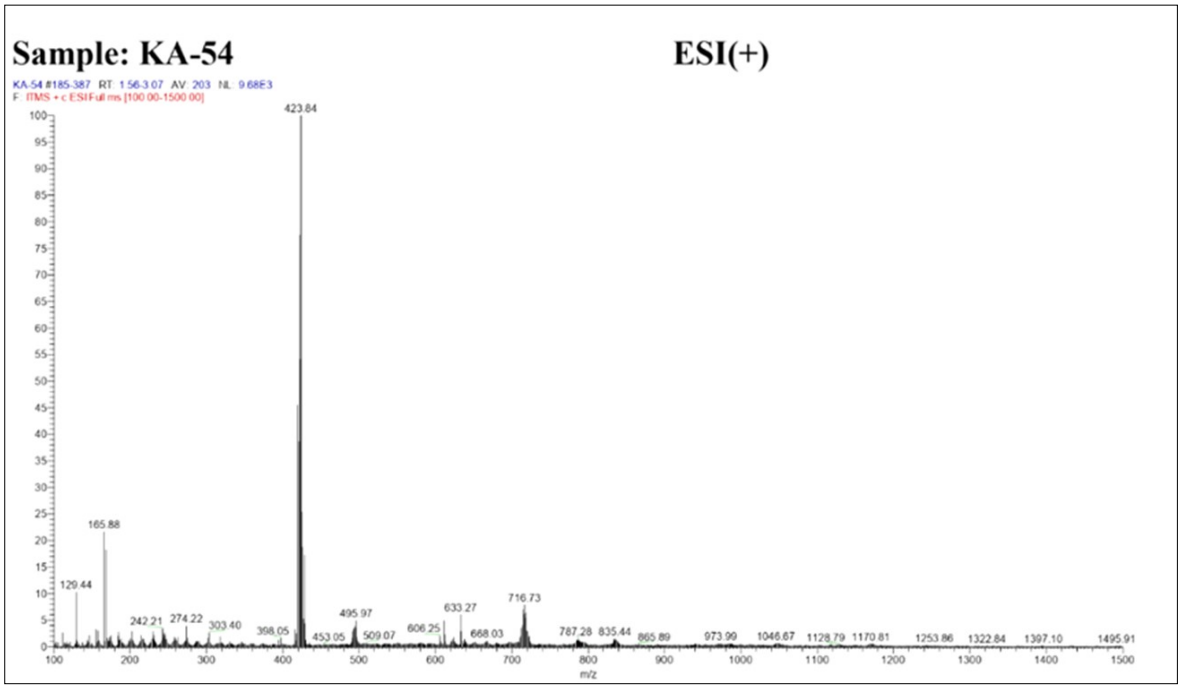


Figure S9. ESI-MS spectrum of **2** recorded in MeOH.

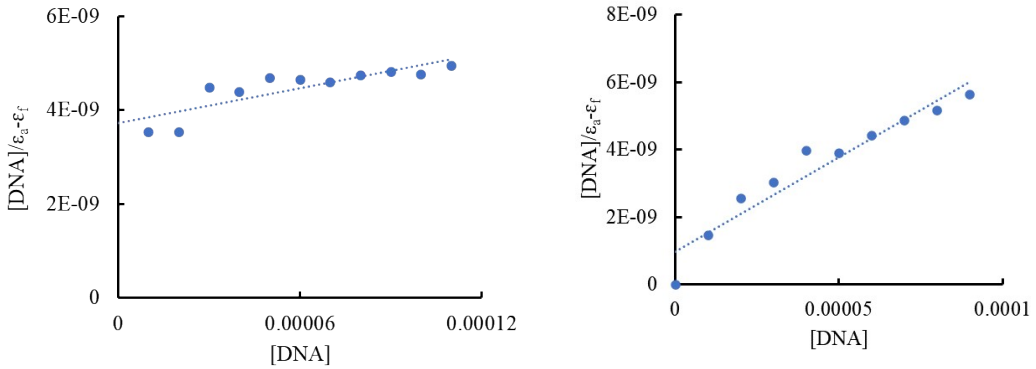
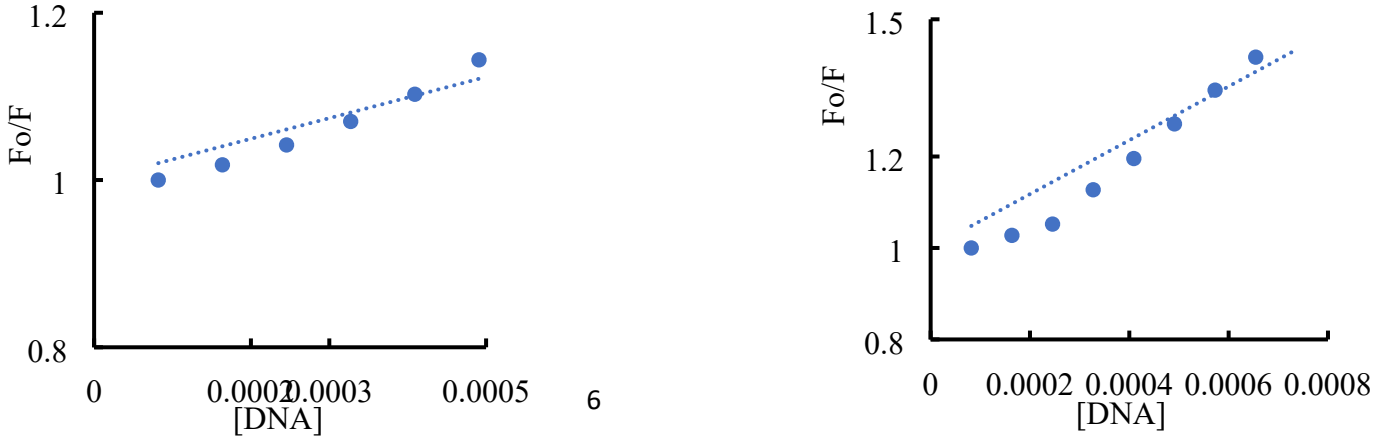


Figure S10. Plot for calculating intrinsic binding constant (a) **1** and (b) **2**.



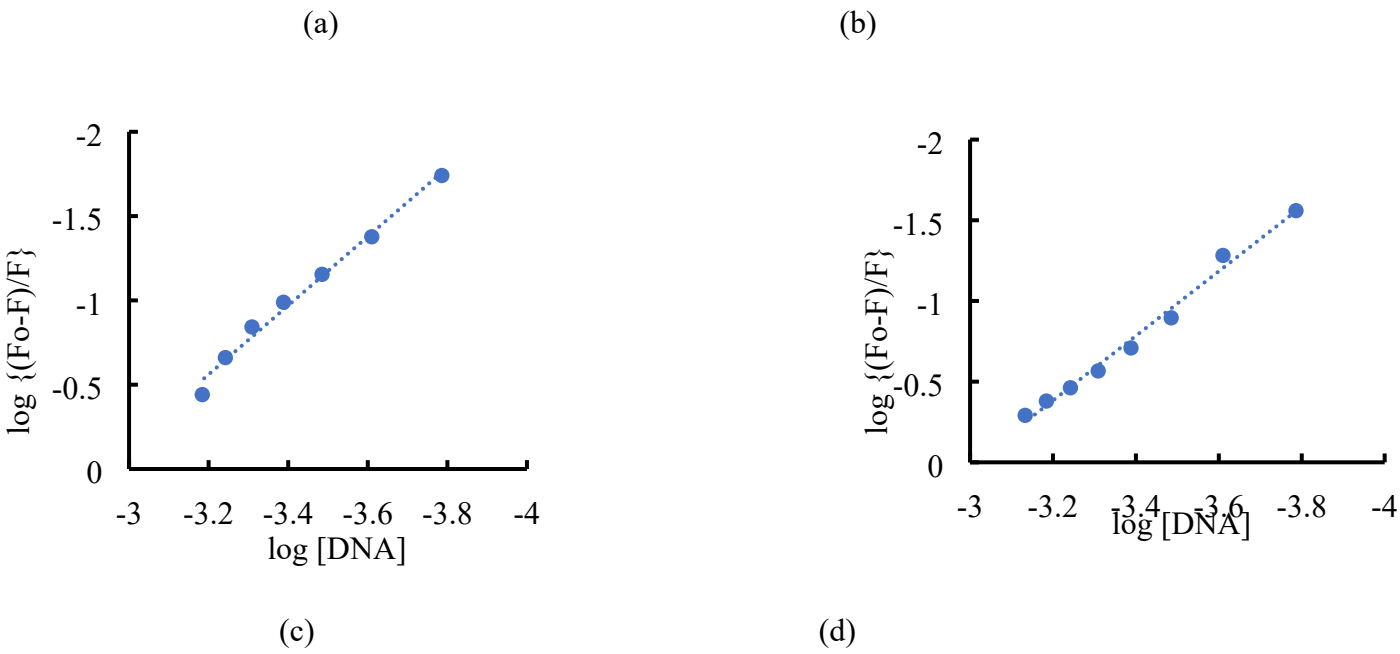


Figure S11. Stern-Volmer plots of (a) **1** and (b) **2** and the Van`t Hoff plot of (c) **1** and (d) **2**, respectively.

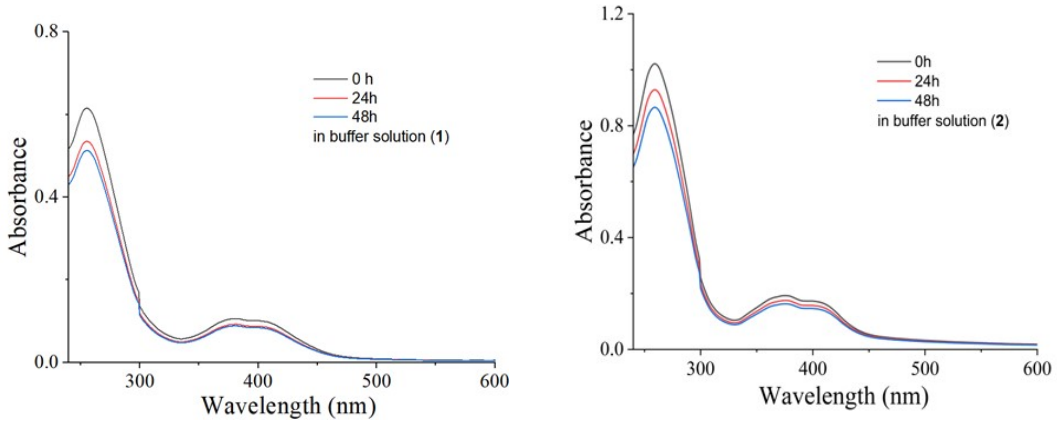


Figure S12. Absorption spectra at 0, 24 and 48h of the complexes **1** and **2** in buffer solution.

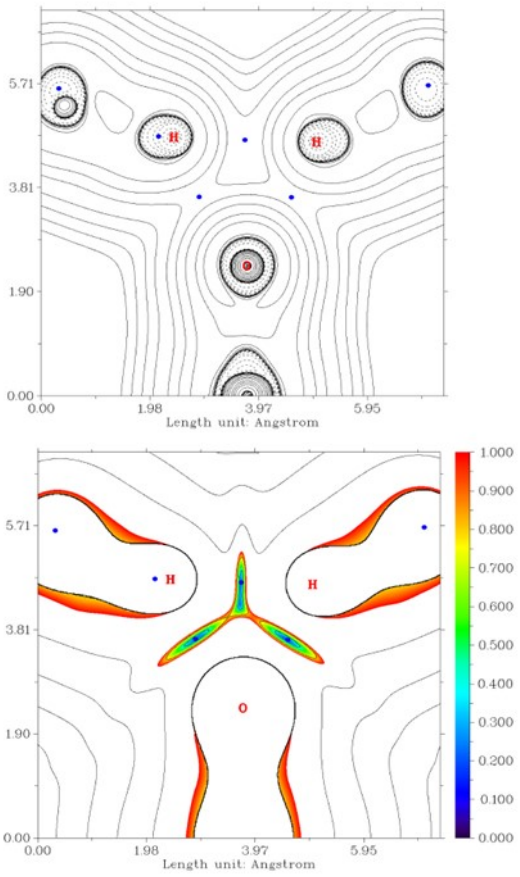


Figure S13. 2D plots of the Laplacian of the electron density, $\Delta^2\rho(r)$ (top), and RDG function for the same projection (bottom), showing the non-covalent contacts between aromatic H atoms of phenyl groups and uncoordinated O atom in **2**.

Table S1. Crystallographic data and structure refinement details for **1**.

	1		
Empirical formula	$C_{27}H_{23}NO_2Sn$	Z	4
Formula weight	512.15	ρ_{calc} (g/cm^3)	1.512
Crystal system	monoclinic	F000	1032
Space group	$P2_1/c$	μ (mm^{-1})	1.159
a (Å)	18.047(3)	Rfl. measured	25689
b (Å)	10.1048(14)	Obs/Unique rfl.	4521 / 3001
c (Å)	12.5842(18)	Nº parameters	280
α (º)	90	Rint	0.1547
β (º)	101.298(5)	R(F) (I >=2σ(I))	0.0974

γ (º)	90	wR (F^2) (all data)	0.2719
V (Å^3)	2250.4(6)	GOF (F^2)	1.018

Table S2. Cartesian coordinates of the structure 1 optimized at the B3LYP/ZORA-def2-TZVP(SARC-ZORA-TZVP) level in water (C-PCM model).

C -4.71183107579443 4.47900925554081 -0.16180354291365

C -5.46183710424509 5.67035557657268 -0.39321811590198

C -4.95877575322328 6.67773614803773 -1.26058424334500

C -3.71577949748333 6.48546119808563 -1.87954064296901

C -2.99137421930400 5.33631169209569 -1.65647494137367

C -6.71807918523248 5.86508371382099 0.24388420254655

C -7.46564015576585 7.05181247305169 0.00801998453381

C -6.93018736831223 8.04039051084257 -0.87533634843934

C -5.72979347155122 7.86025406435148 -1.48137255208137

C -5.26234998135099 3.50754954704272 0.73798724587614

C -6.46049204089076 3.69723956657178 1.34503856184785

C -7.23467826985931 4.87647951380069 1.12200302065406

C -8.47151812258959 5.08497402960204 1.74110997315778

C -9.19532128950984 6.24590836052011 1.50278932729843

C -8.69981227132154 7.21985170270828 0.64627920615526

C -2.66531105877944 3.11336807343076 -0.64061384745475

N -1.45279544234698 3.02423236926029 -1.04211053869452

C -0.78065049211448 1.80483615201486 -0.93199359120857

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C 1.26653090871457 0.63317376476974 -0.40645528217338

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C -0.65605509231515 -0.59582412600459 -1.17467161009123

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C 1.41652664601867 -1.87099025014816 -0.63874644498123

O 0.93197821269502 -2.93967177199539 -1.01326656019328

O 2.61842894965615 -1.78586788908080 -0.12789990579303

Sn 3.63734599375775 -3.61077423536360 -0.01149031341644

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H -7.50593512544450 8.94170372150981 -1.04957931896220

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H 4.06423875628901 -3.34671075271233 -2.66274081210865

H 3.03793486181441 -4.77761399459344 -2.38860996975421

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H 6.13012552106508 -3.62723346953555 1.06238112287262

H 5.15689259902222 -2.37518773983111 1.86762033729529

Table S3. Cartesian coordinates of the structure 2 optimized at the B3LYP/ZORA-def2-TZVP(SARC-ZORA-TZVP) level in water (C-PCM model).

C -4.68871445172990 4.48756145064826 -0.15170860365883

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C -3.41080353395171 6.74217633191165 -1.27226170876288

C -2.73079114152193 5.55443543431775 -1.13203895101993

C -6.74900361440568 5.82887495802625 0.11576803645897

C -7.44736824163964 7.05936334469940 -0.02955316085990

C -6.76330865549083 8.17794101561092 -0.59885503627154

C -5.47032343226019 8.07762879028592 -0.99716691826468

C -5.39863057065161 3.37832942783471 0.41595718355457

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