Synthesis and Antiproliferative Insights of Lipophilic Ru(II)-Hydroxy Stearic Acids Hybrid Species

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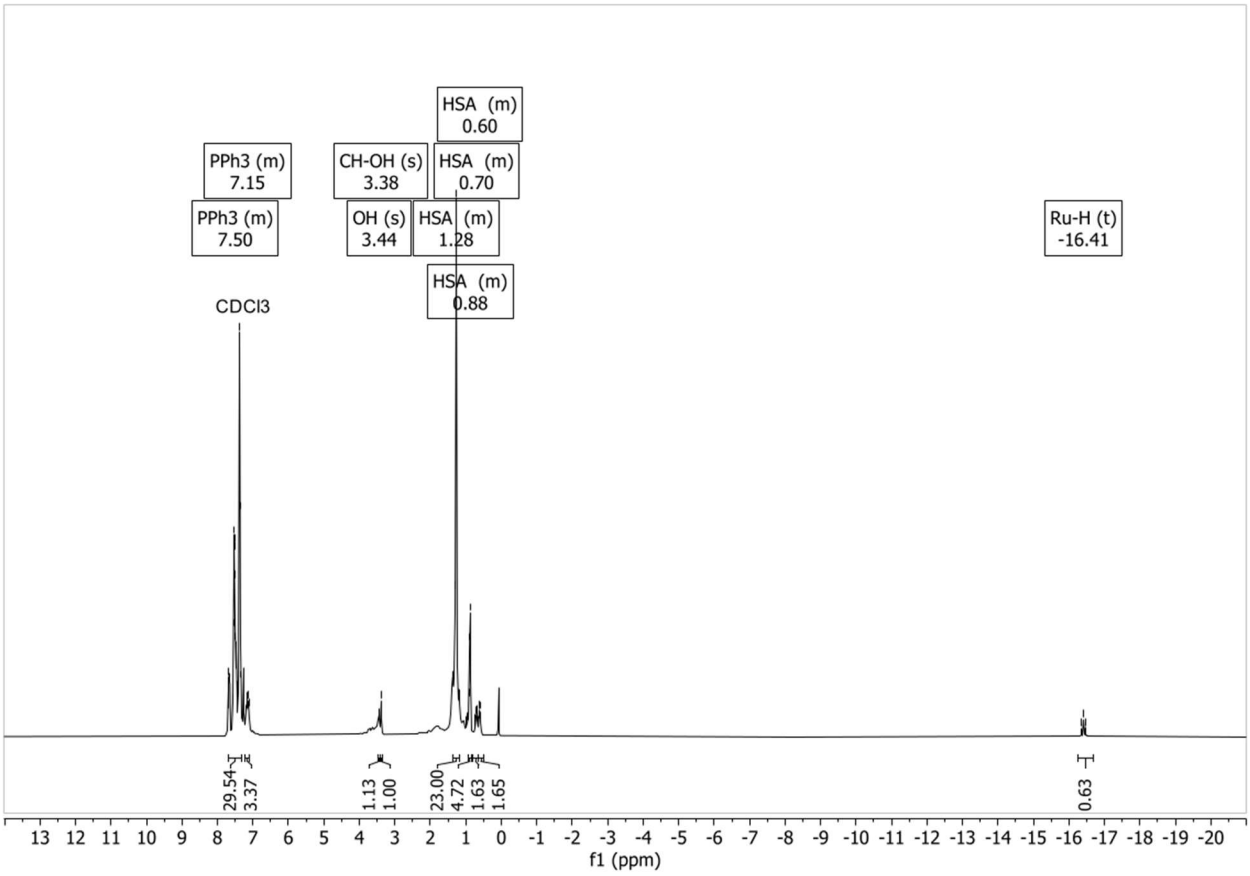
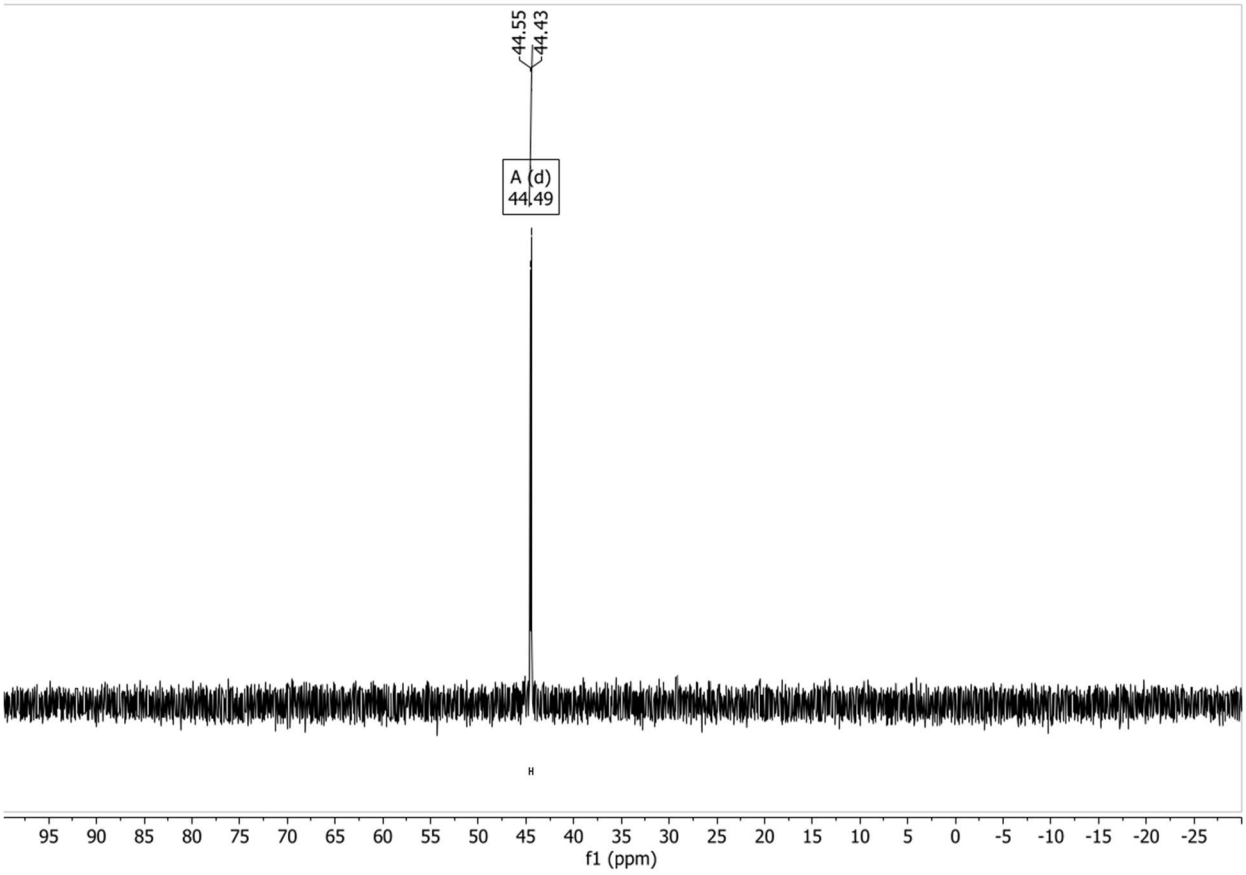
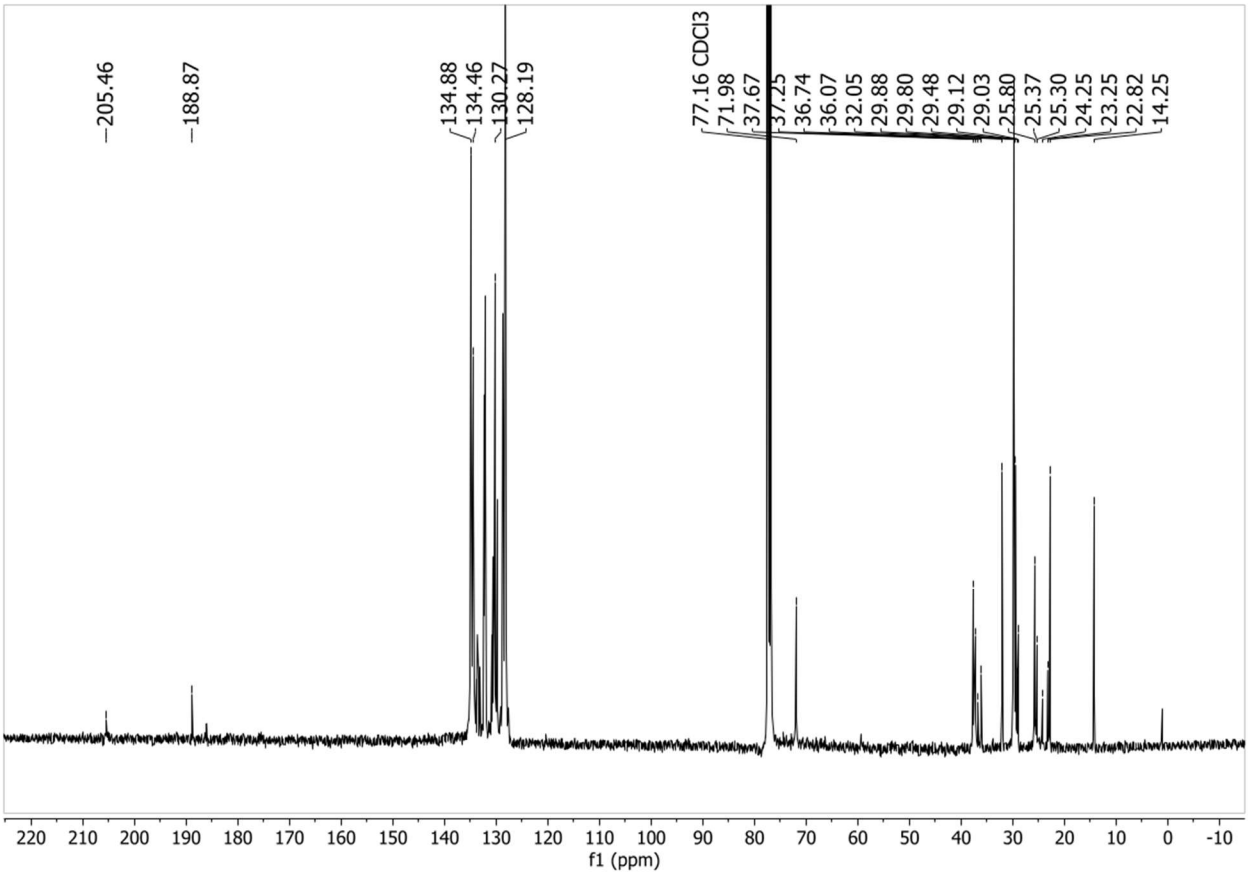


S1: *^{1}H NMR spectrum of **2** in $CDCl_3$*

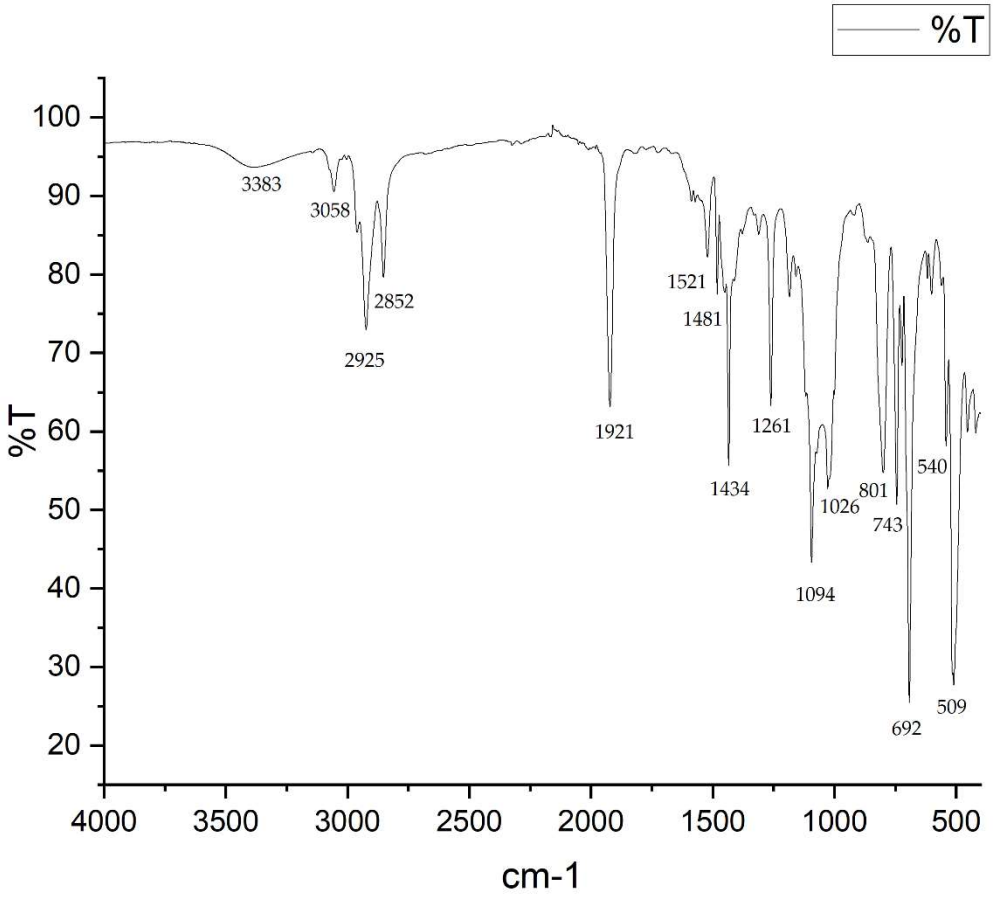


*S2: ^{31}P spectrum of **2** in $CDCl_3$*



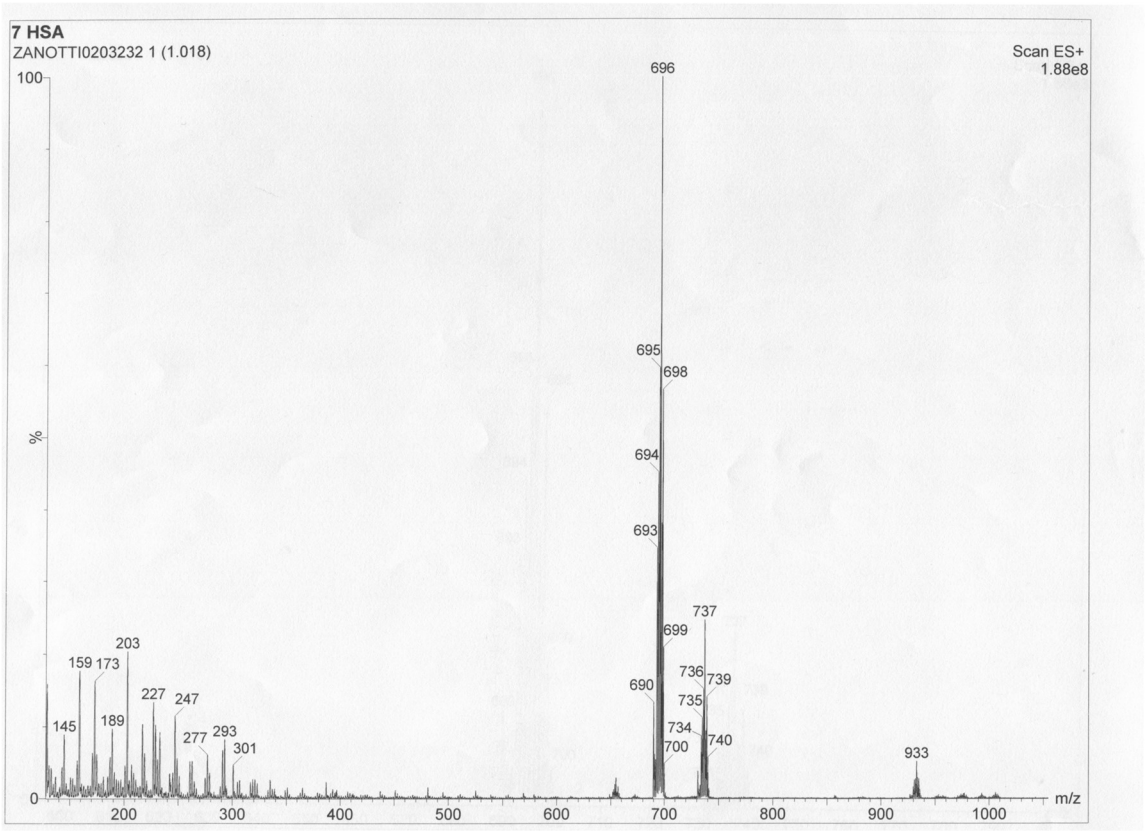
*S3: ^{13}C spectrum of **2** in $CDCl_3$*

IR spectrum of **2**

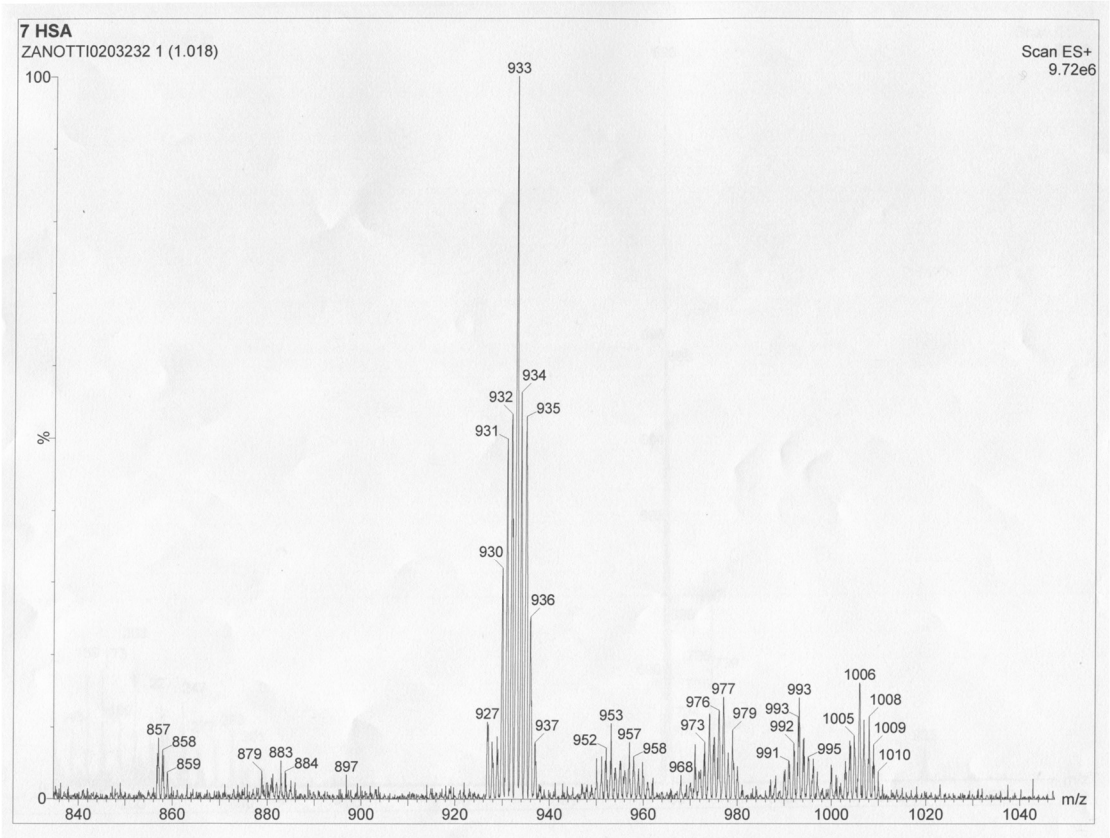


*S4: IR spectrum of **2***

Mass Spectra of **2**

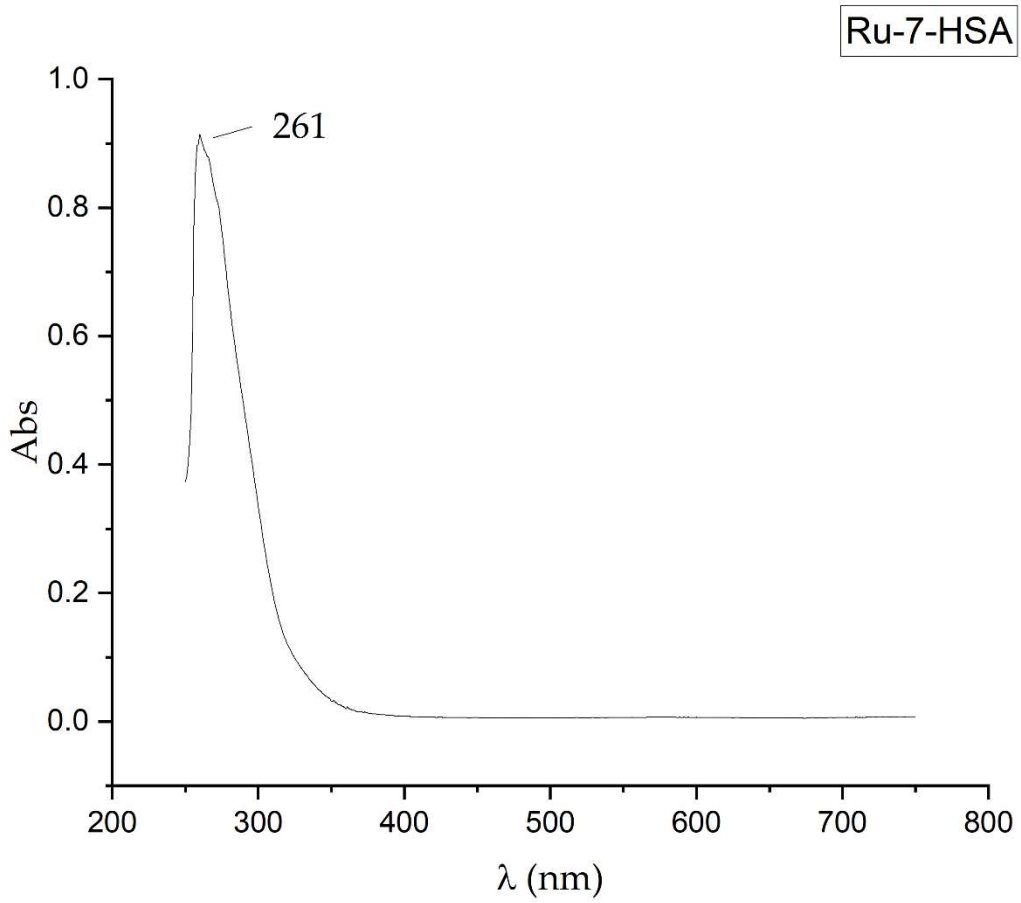


***S5**: Mass Spectrum of **2** (Positive mode)*



***S6**: Mass spectrum of **2** (Positive mode, m/z: 840 - 1040)*

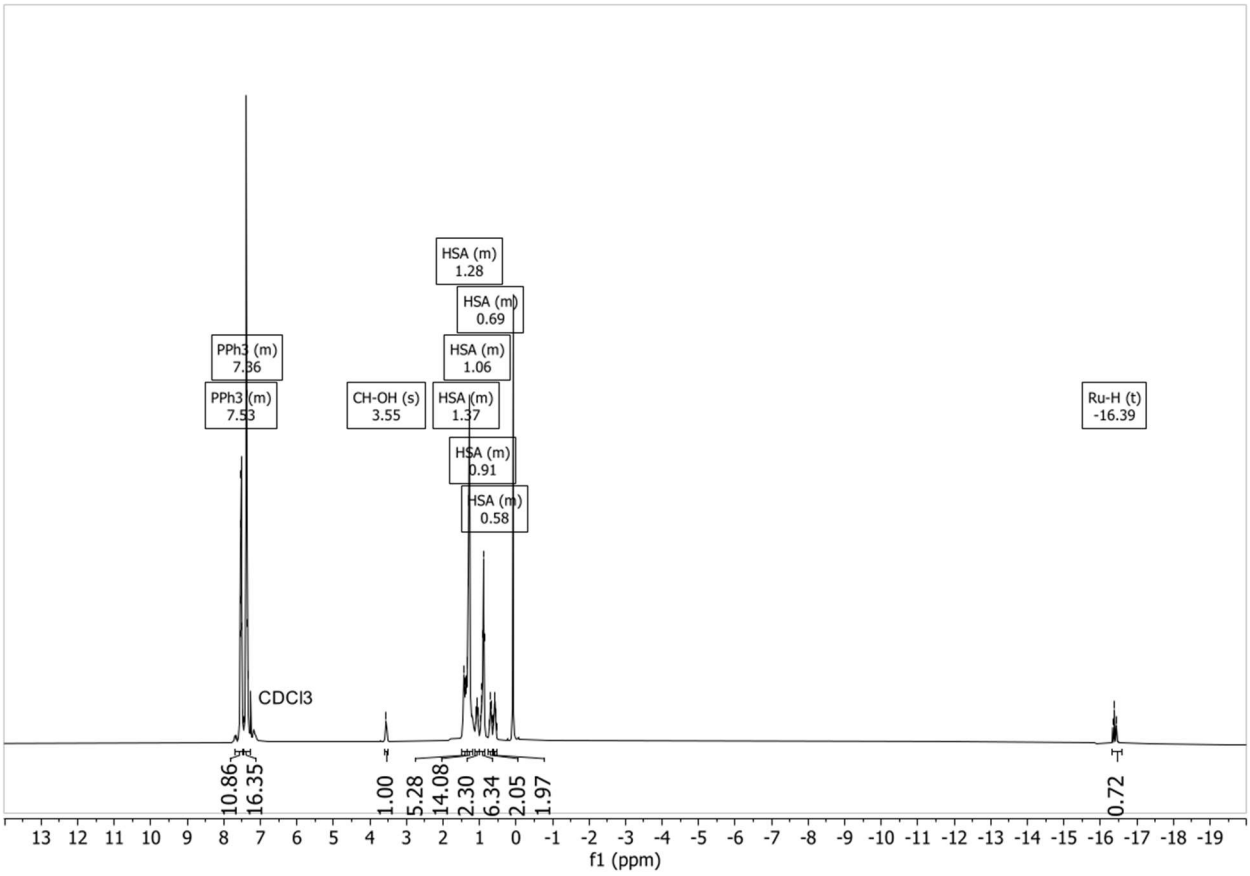
UV-vis spectrum of **2**



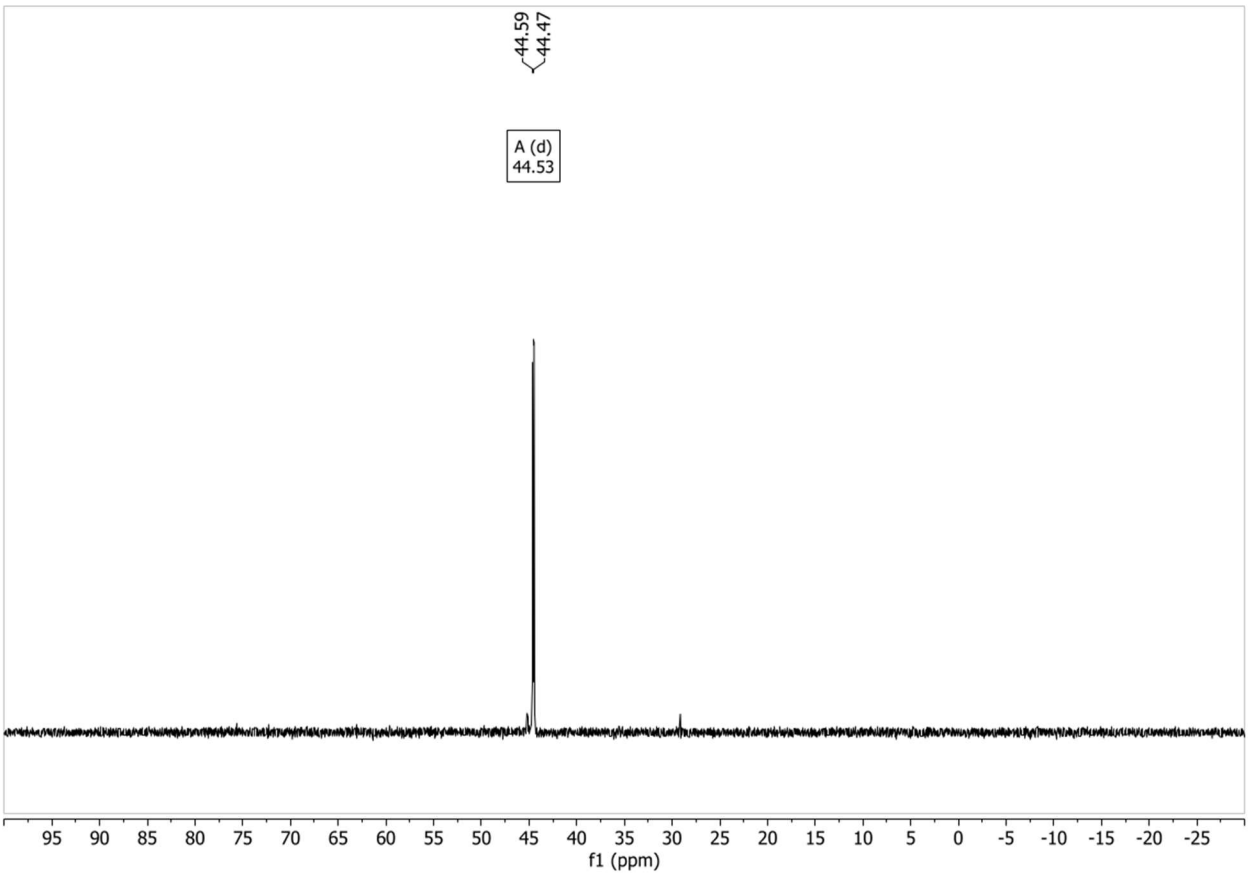
***S7**: UV-vis spectrum of **2** in DMSO*

Characterization of **3 (Ru-9-HSA)**

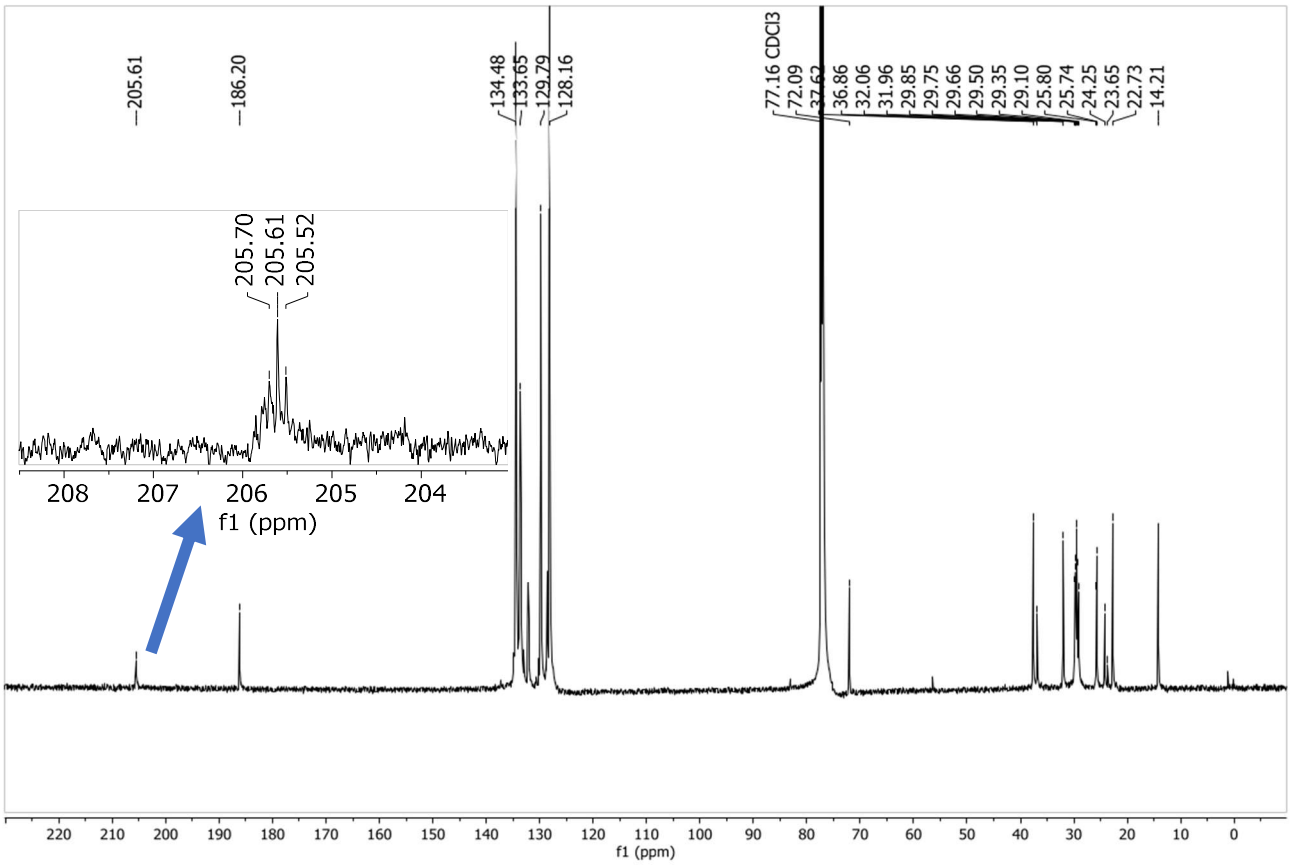
NMR spectra of **3**



*S8: ^{1}H NMR spectrum of **3** in $CDCl_3$*

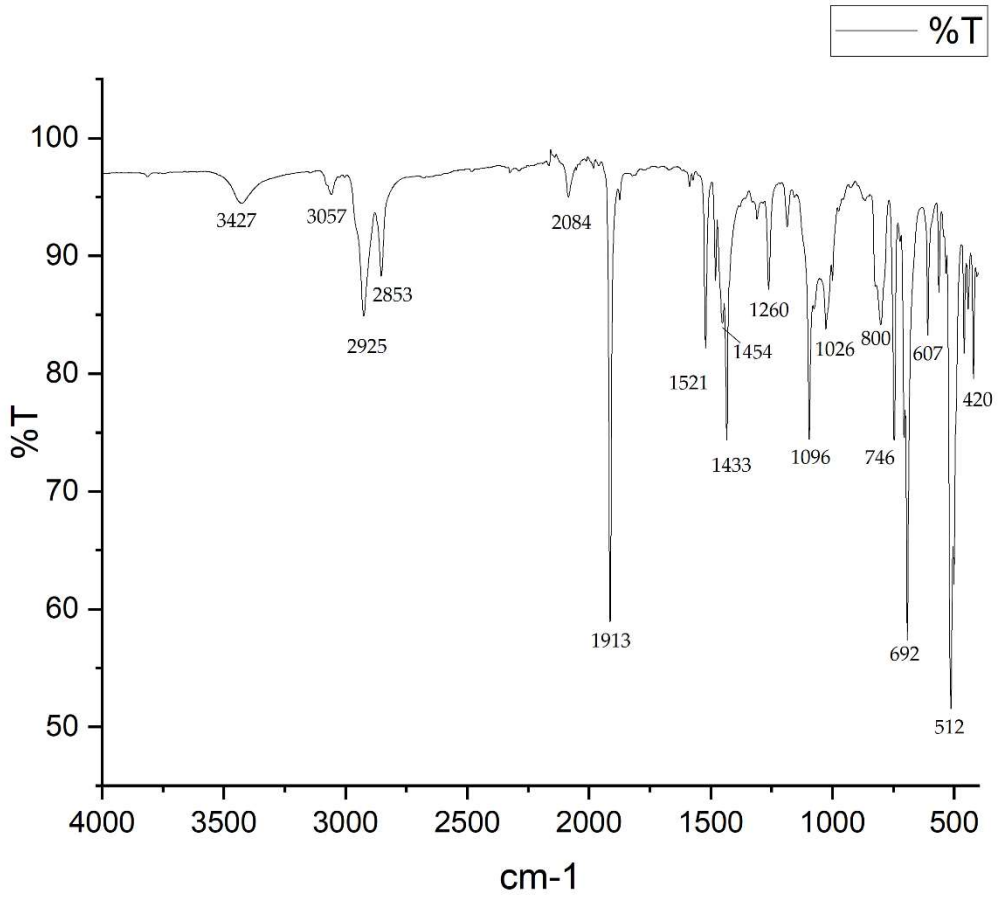


***S9**: [31]P NMR spectrum of **3** in $CDCl_3$*



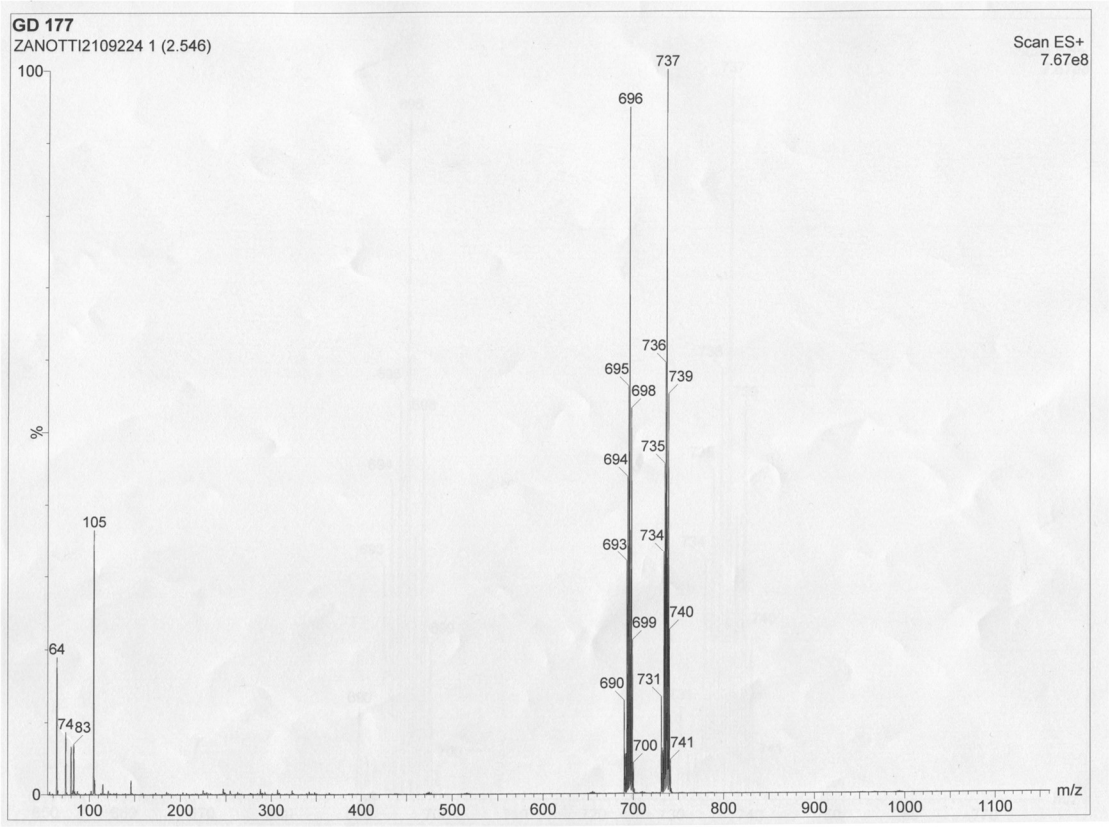
***S10**: ^{13}C spectrum of **3** in $CDCl_3$*

IR spectrum of **3**

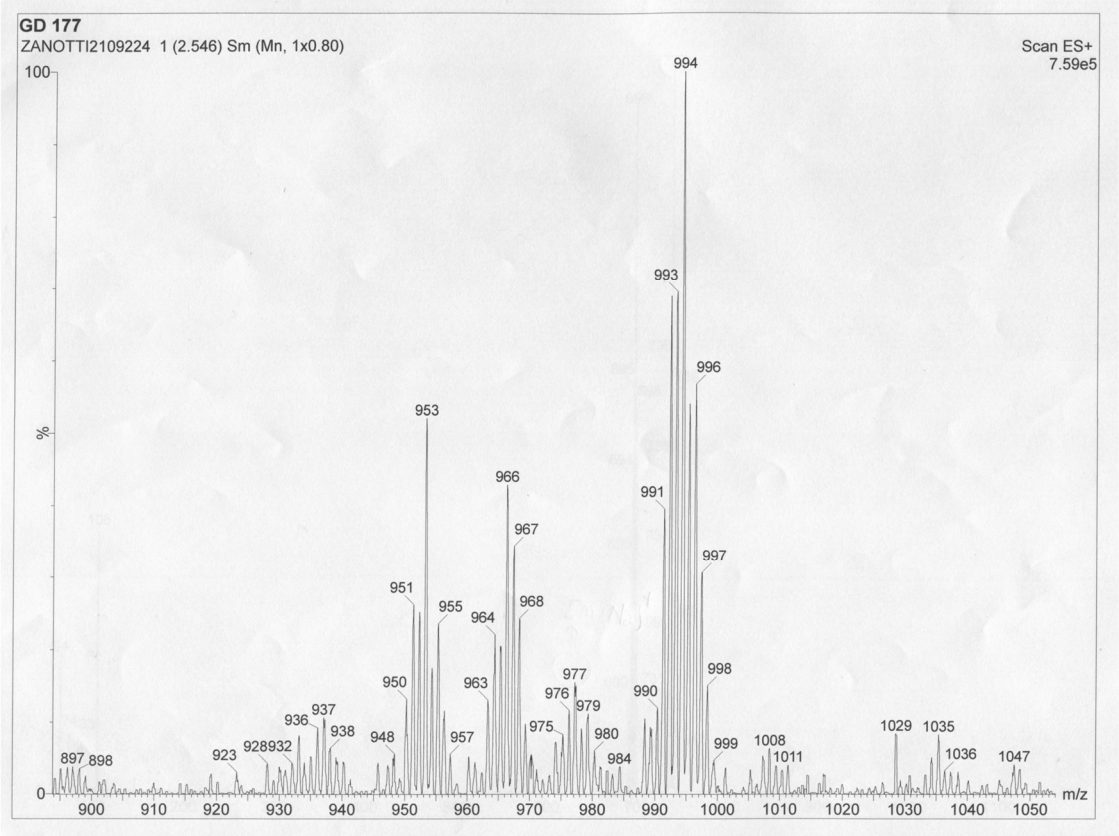


S11: IR spectrum of **3**

Mass Spectra of **3**

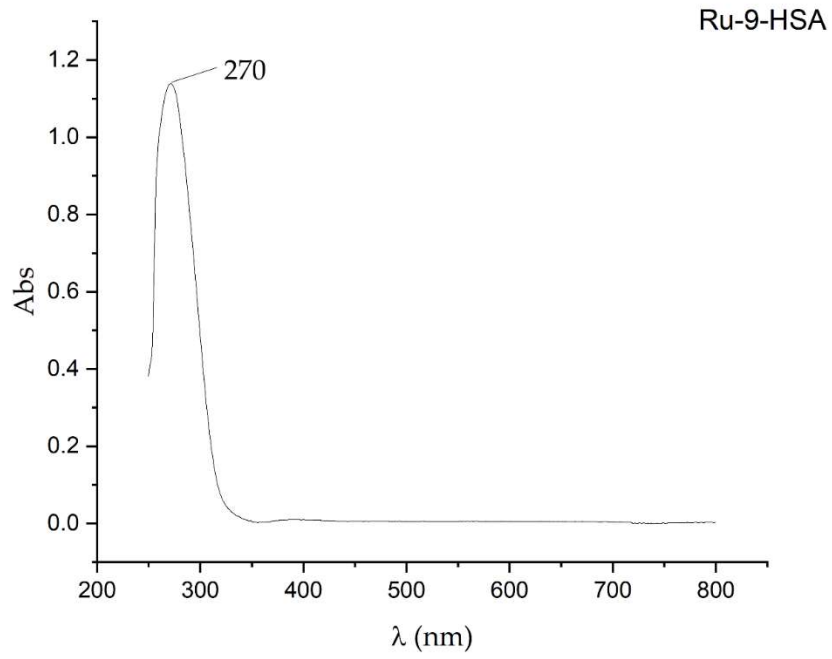


***S12**: Mass spectrum of **3** (positive mode)*



***S13**: Mass spectrum of **3** (positive mode, m/z: 900 - 1050)*

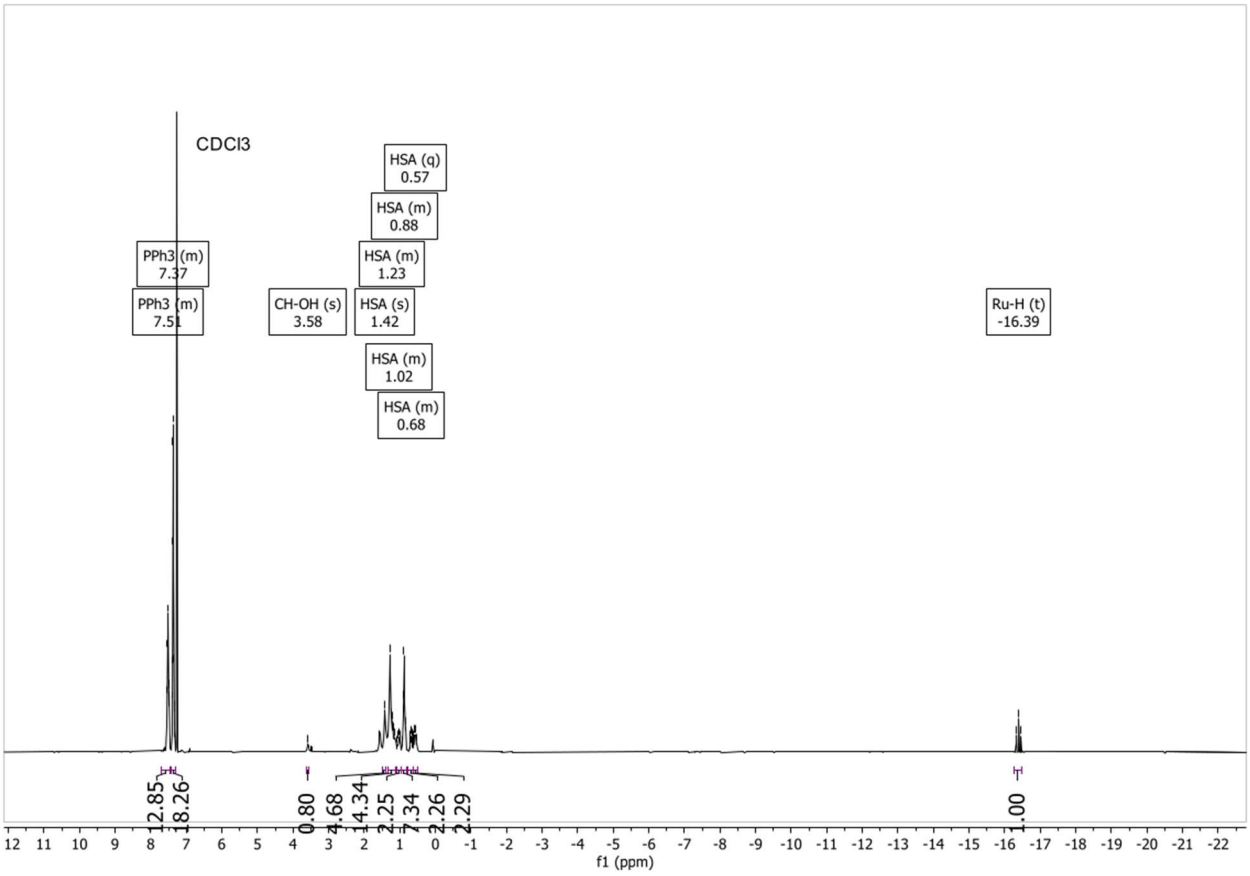
UV-vis spectrum of **3**



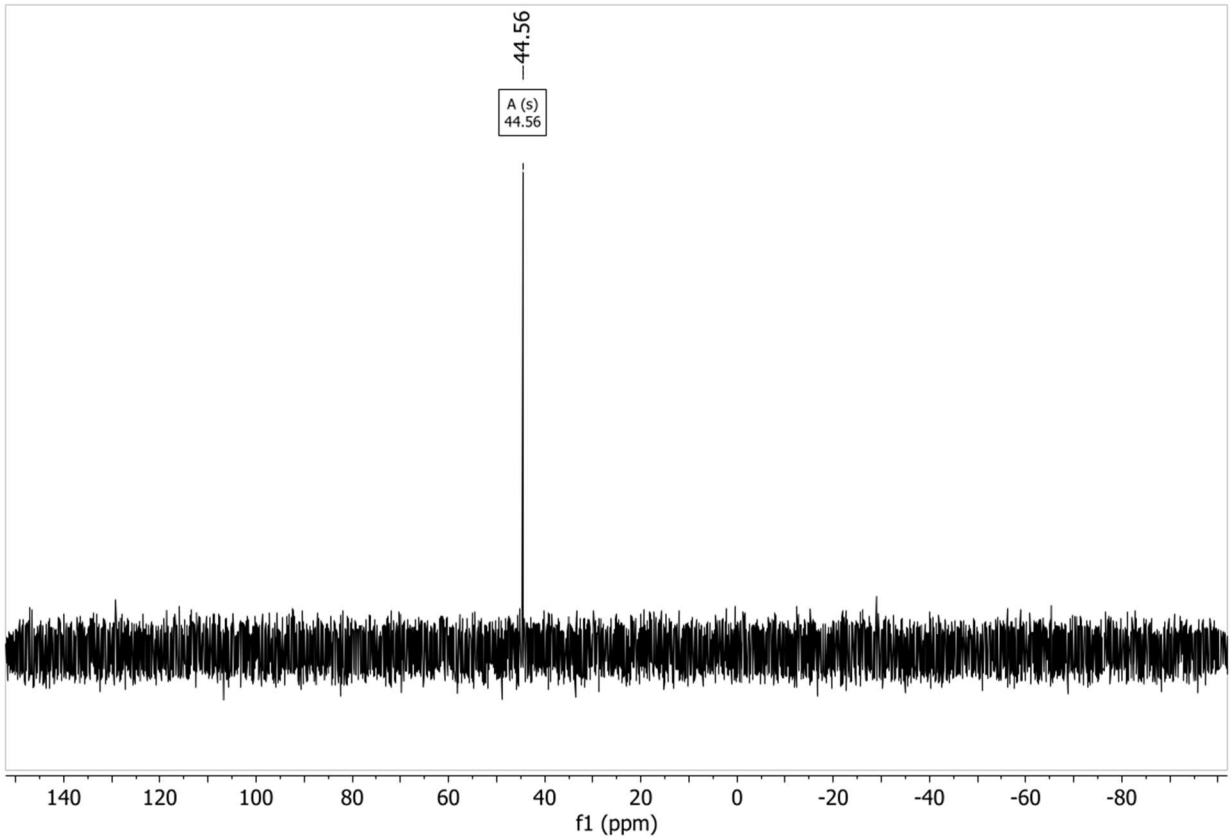
***S14**: UV-vis spectrum of **3** in DMSO*

Characterization of **4 (Ru-12-HSA)**

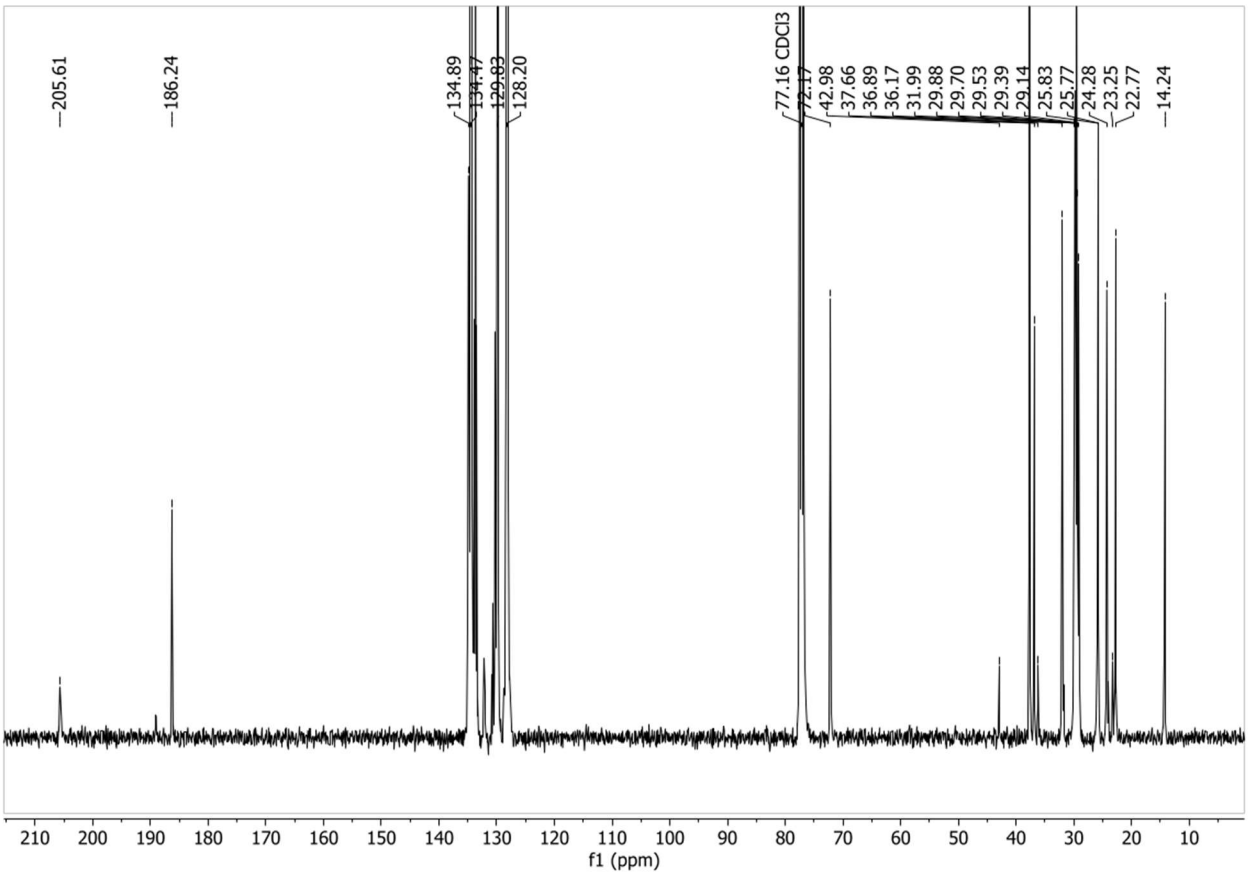
NMR spectra of **4**



***S15**: [1]H NMR spectrum of **4** in $CDCl_3$*

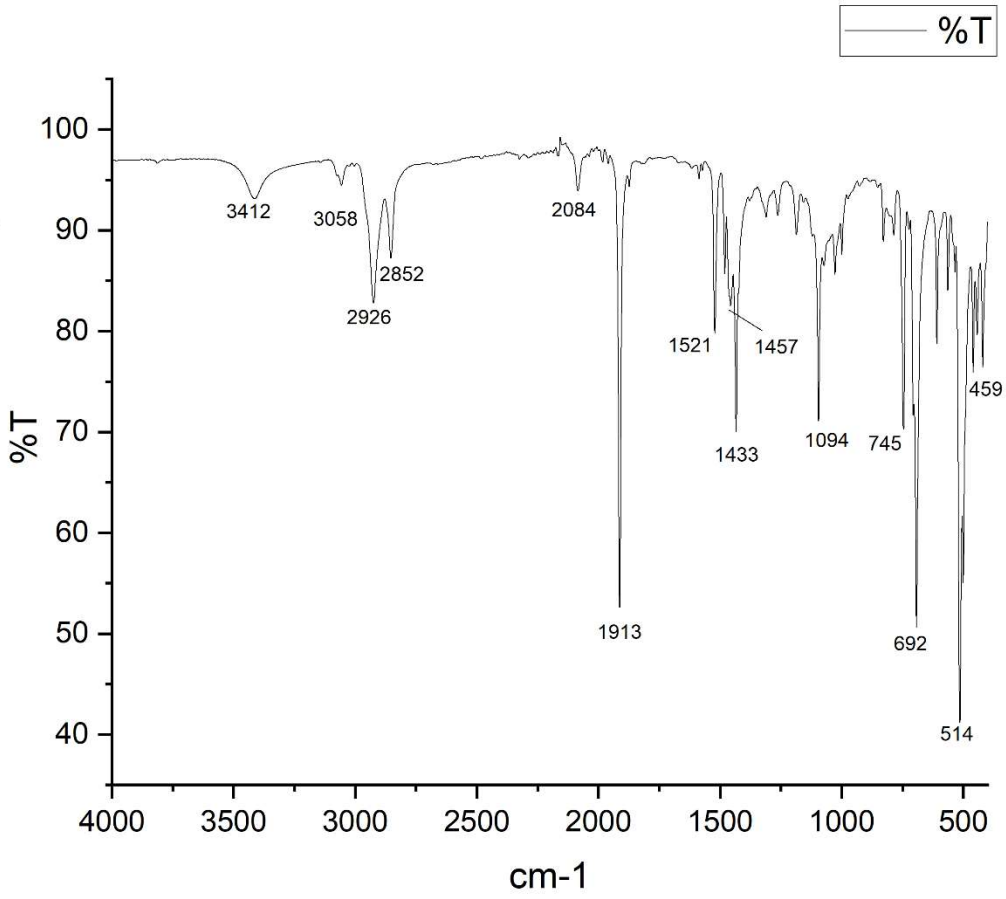


***S16**: ^{31}P NMR spectrum of **4** in $CDCl_3$*



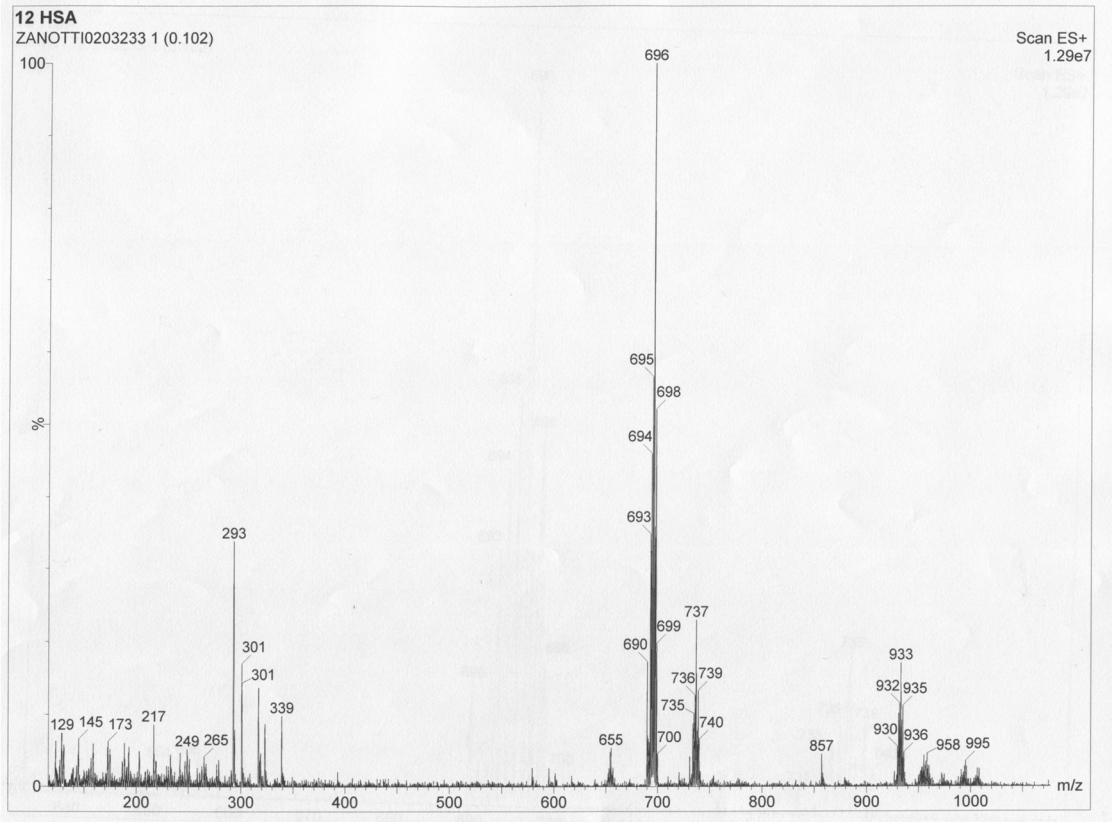
***S17**: [13]C NMR spectrum of **4** in $CDCl_3$*

IR Spectrum of **4**

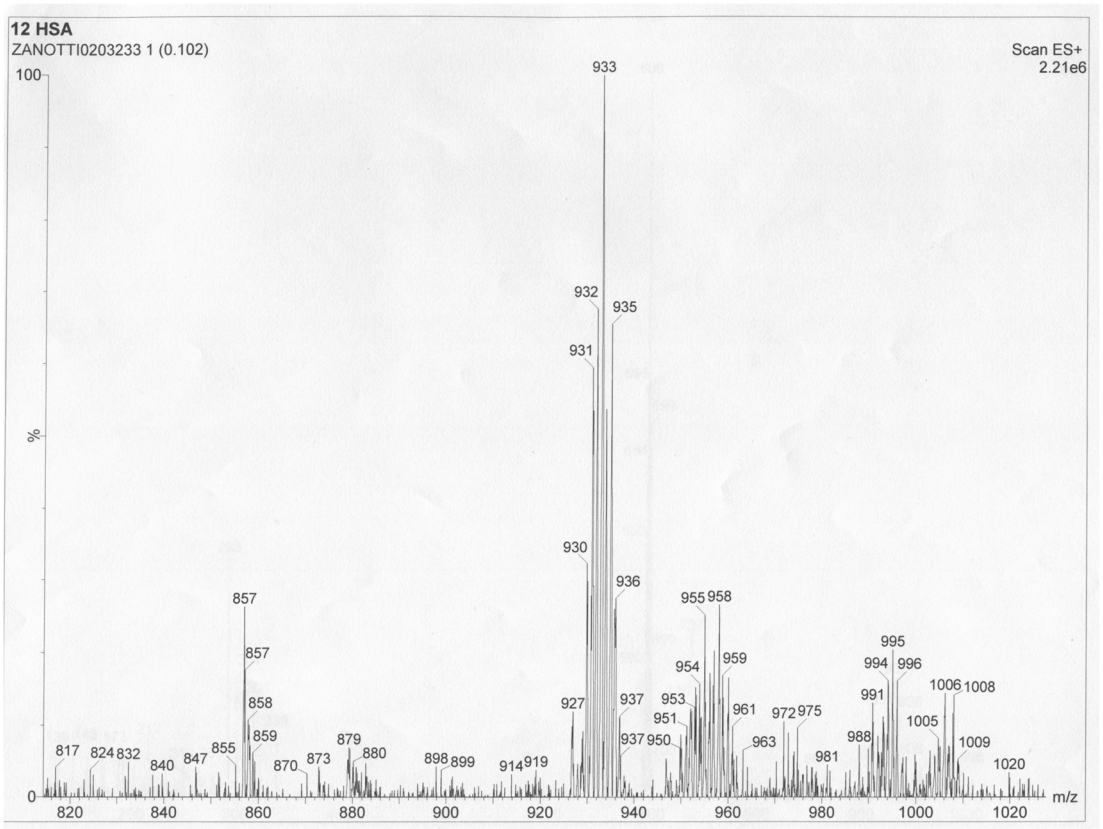


S18**: IR spectrum of **4

Mass Spectra of **4**

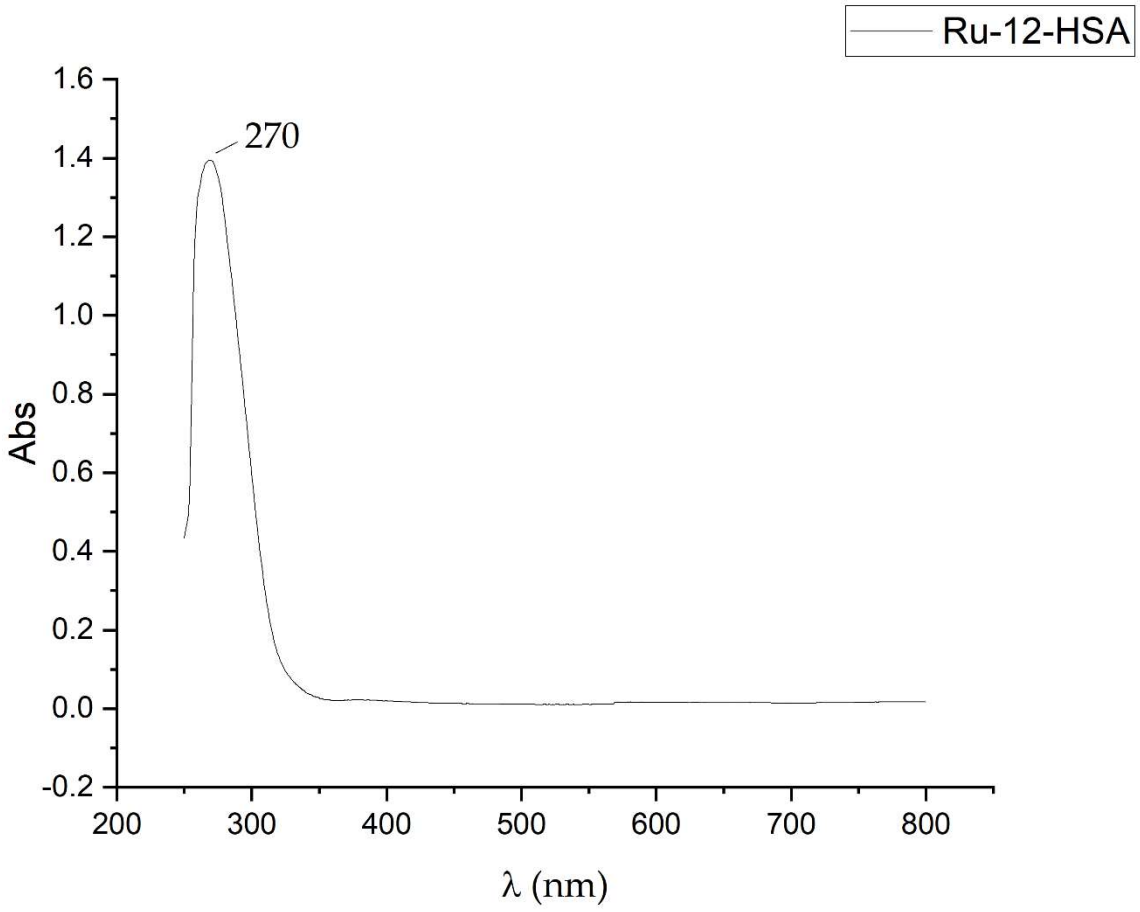


***S19**: Mass spectrum of **4** (positive mode)*



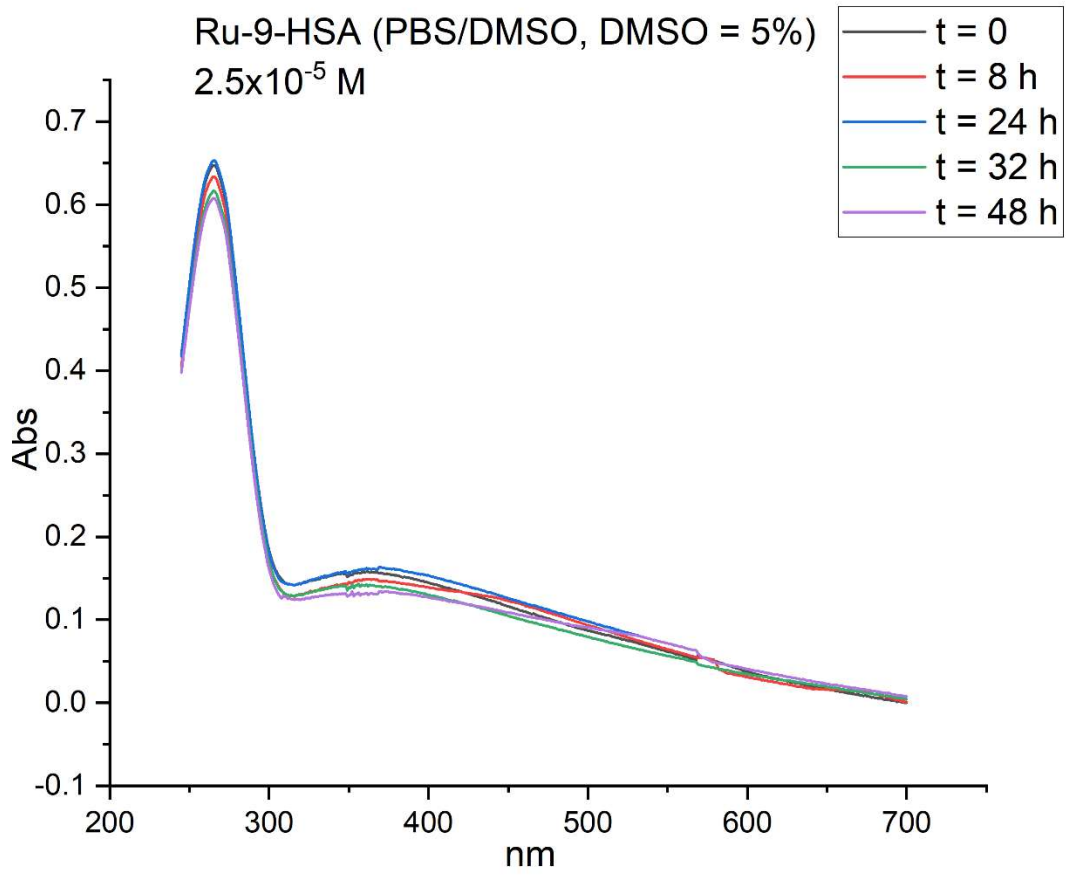
***S20**: Mass spectrum of **4** (positive mode, m/z: 820 - 1020)*

UV-vis spectrum of **4**

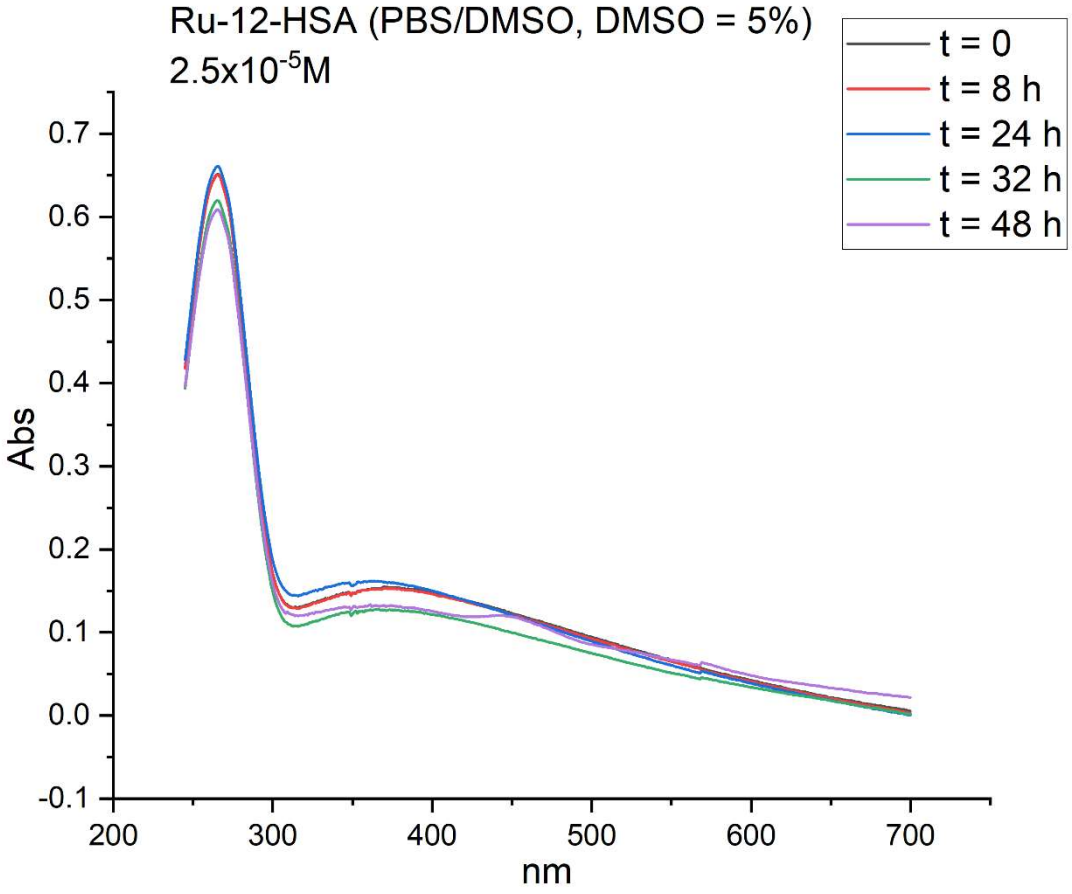


***S21**: UV-vis spectrum of **4** in DMSO*

Stability studies of complexes **3** and **4** in solution

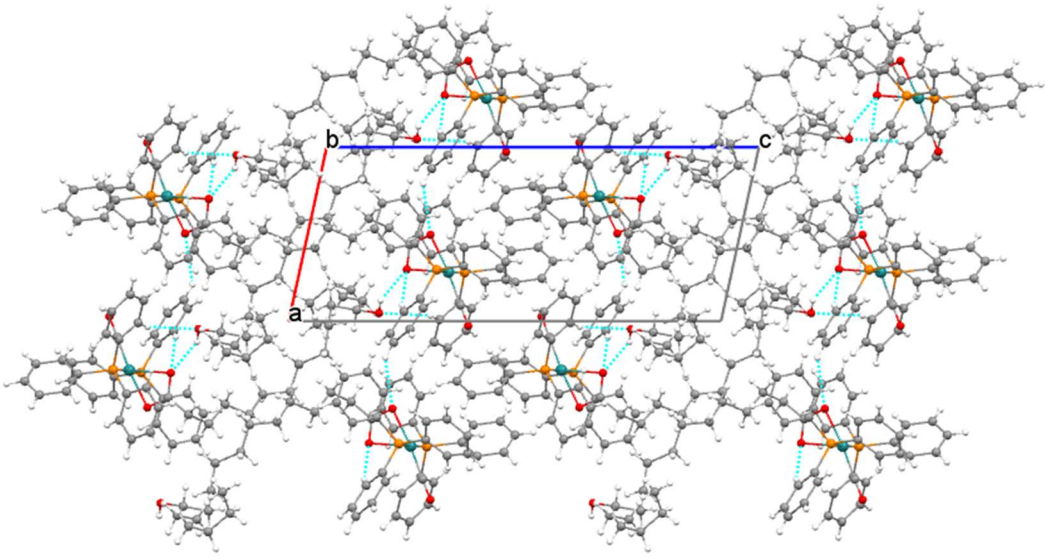


***S22**: Stability of **3** in PBS/DMSO (DMSO = 5%) at 37°C over 48 h; time-resolved UV-vis spectrum.*



*S23: Stability of **4** in PBS/DMSO (DMSO = 5%) at 37°C over 48 h; time-resolved UV-vis spectrum*

X-ray Crystallography



***S24**: View down the b axis of the crystal packing of 4*

Table S1**. Crystal data and experimental details for **4

Compound	**4**
Formula	$C_{55}H_{65}O_4P_2Ru$
Fw	953.08
T, K	100(2)
λ, Å	1.54178
Crystal symmetry	Triclinic
Space group	P-1
a, Å	9.9781(13)
b, Å	12.0328(15)
c, Å	22.364(3)
α	93.268(7)
β	99.999(7)
γ	113.041(6)
Cell volume, Å^3	2410.1(5)
Z	2
D_c, Mg m^{-3}	1.313
μ(Mo-K$_\alpha$), mm^{-1}	3.607

F(000)	1002
Crystal size/ mm	0.10 x 0.04 x 0.04
θ limits, °	2.025 to 58.925
Reflections collected	31303
Unique obs. Reflections [$F_o > 4\sigma(F_o)$]	6848 [R(int) = 0.1227]
Goodness-of-fit-on F^2	1.041
R_1 (F)[a], wR_2 (F^2) [$I > 2\sigma(I)$][b]	0.1067, 0.2651
Largest diff. peak and hole, e. Å^{-3}	1.592 and -0.783

[a)] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$ where $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where $P = (F_o^2 + F_c^2)/3$.

Table S2. *Intermolecular hydrogen bonds for **4** [Å and °].*

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O3-H3…O1#1	0.84	2.10	2.74(2)	133(1)
C31-H31…O3#1	0.95	2.69	3.39(2)	131.2(8)
C47-H47…O2#2	0.95	2.71	3.43(2)	133

Symmetry transformations used to generate equivalent atoms:

#1 2-x, 1-y, -z; #2 x+1, z