

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

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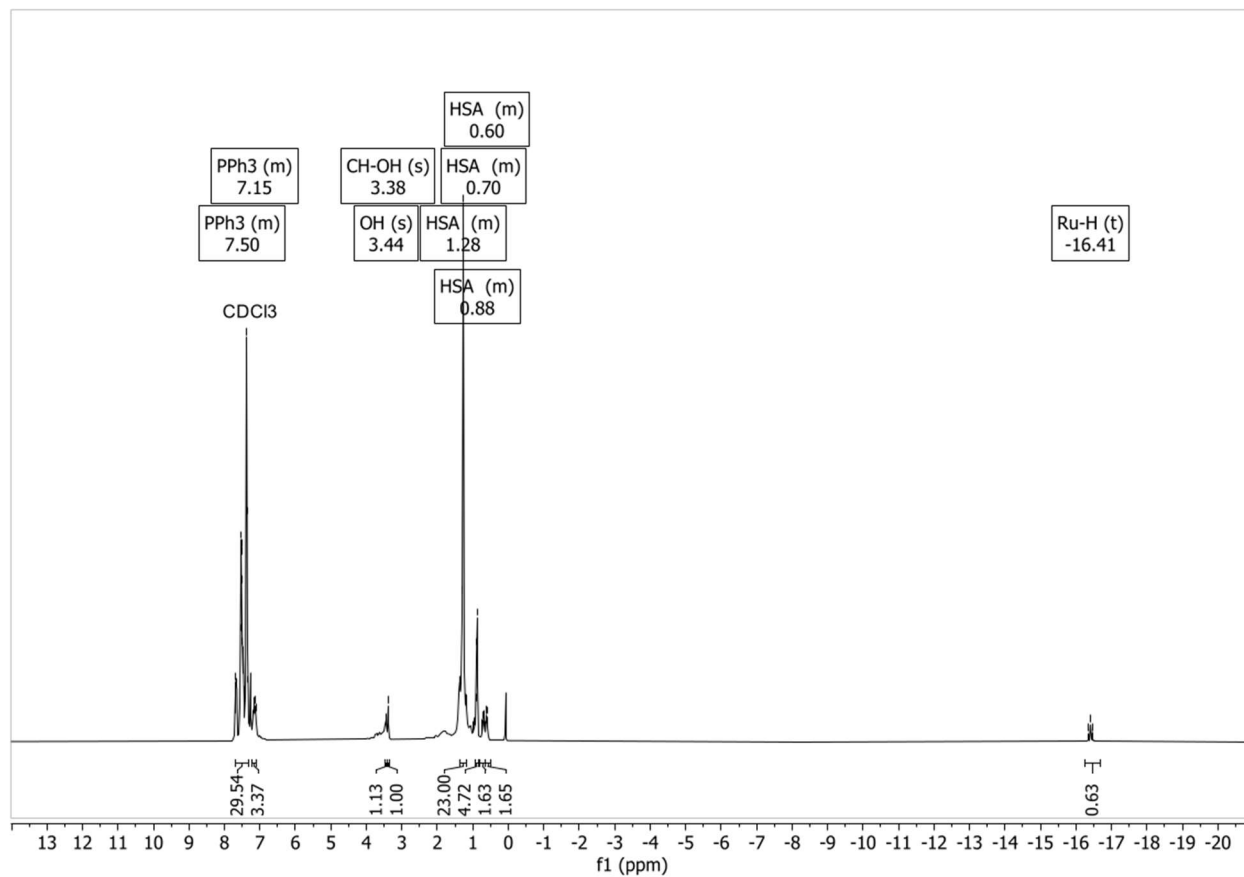
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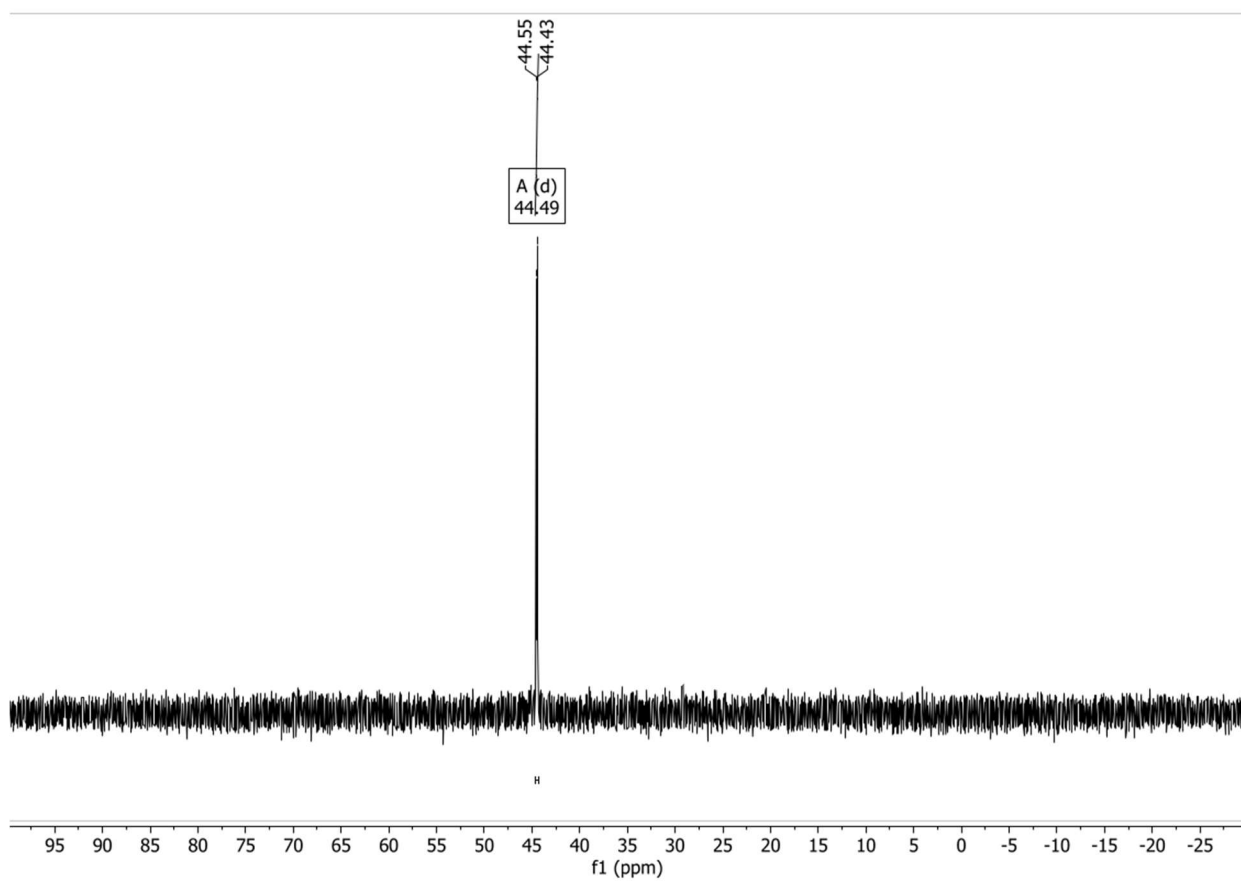
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Characterization of **2** (Ru-7-HSA)

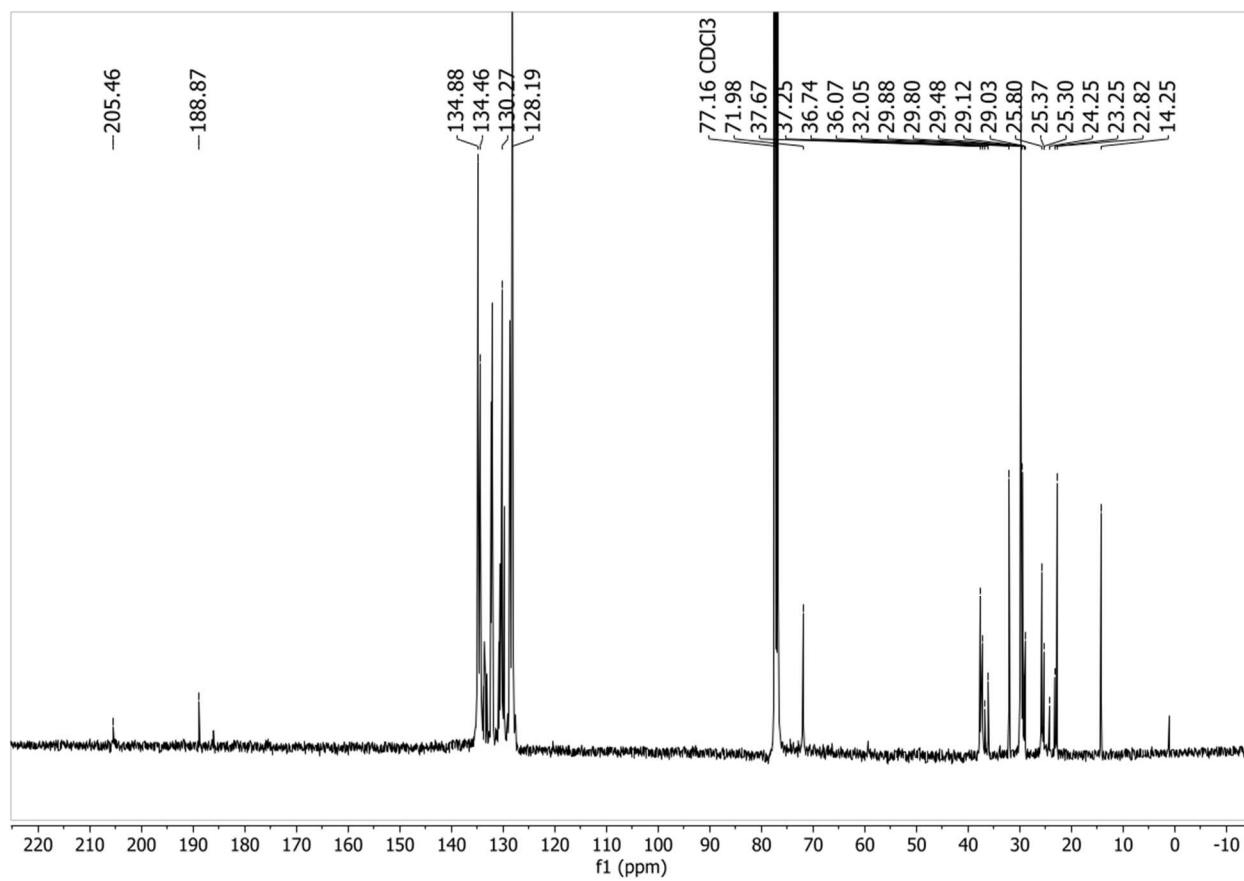
NMR spectra of **2**



S1: ¹H NMR spectrum of **2** in CDCl₃

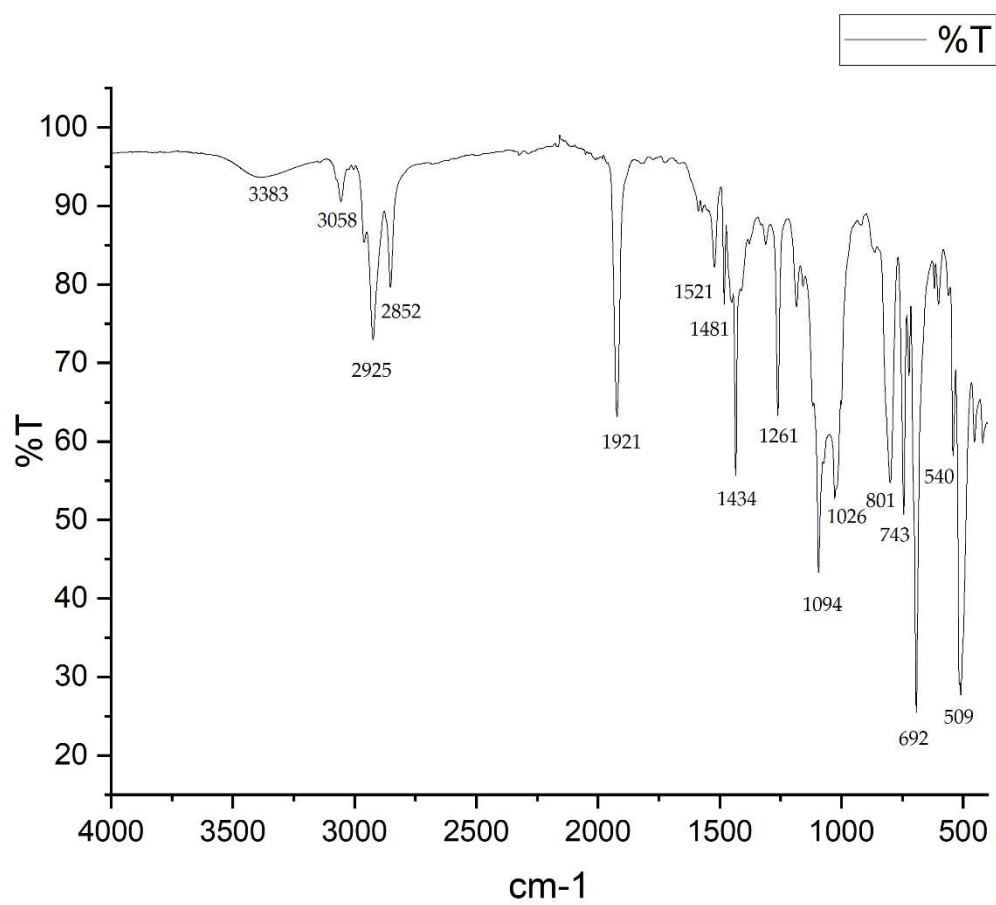


S2: ^{31}P spectrum of 2 in CDCl_3



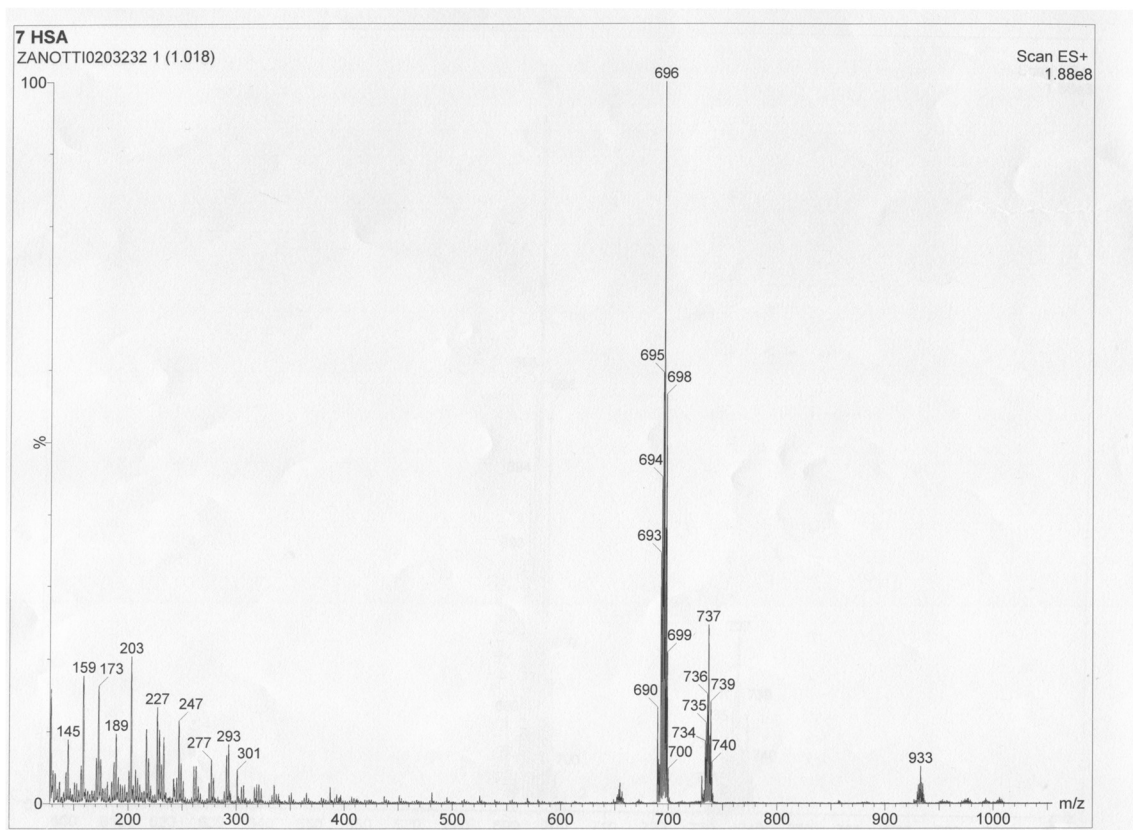
S3: ^{13}C spectrum of 2 in CDCl_3

IR spectrum of 2

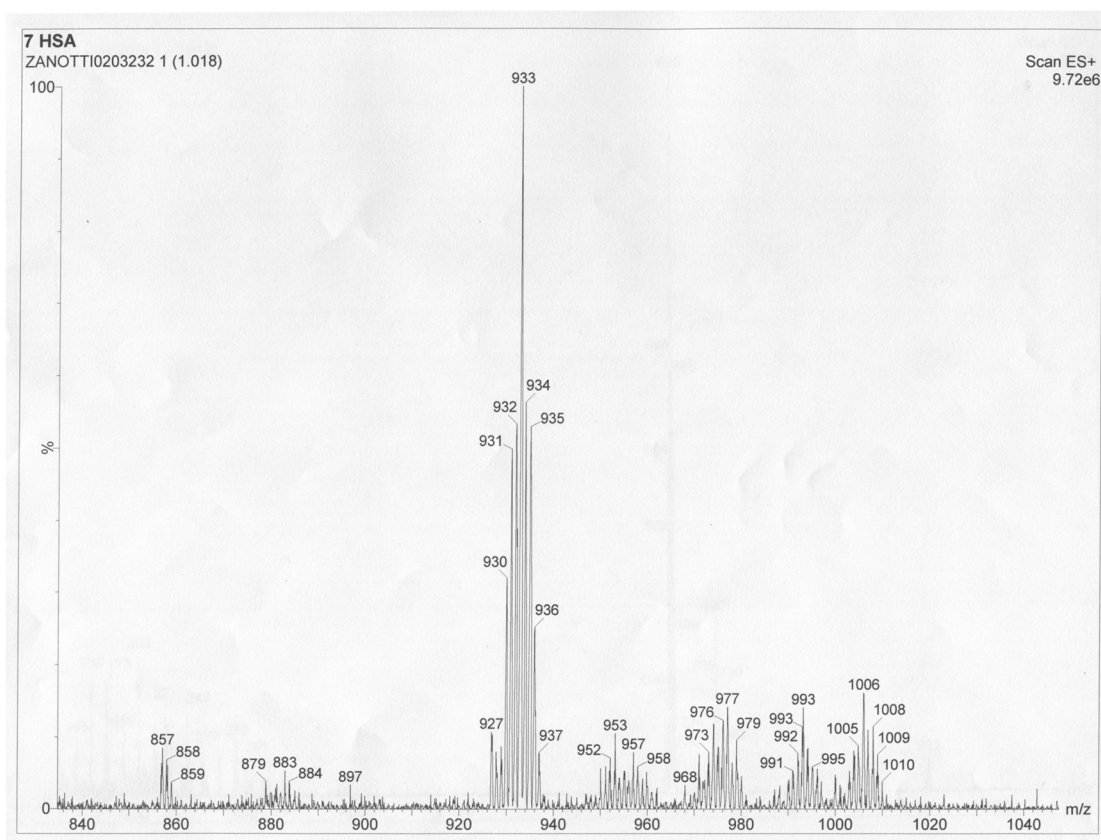


S4: IR spectrum of 2

Mass Spectra of 2

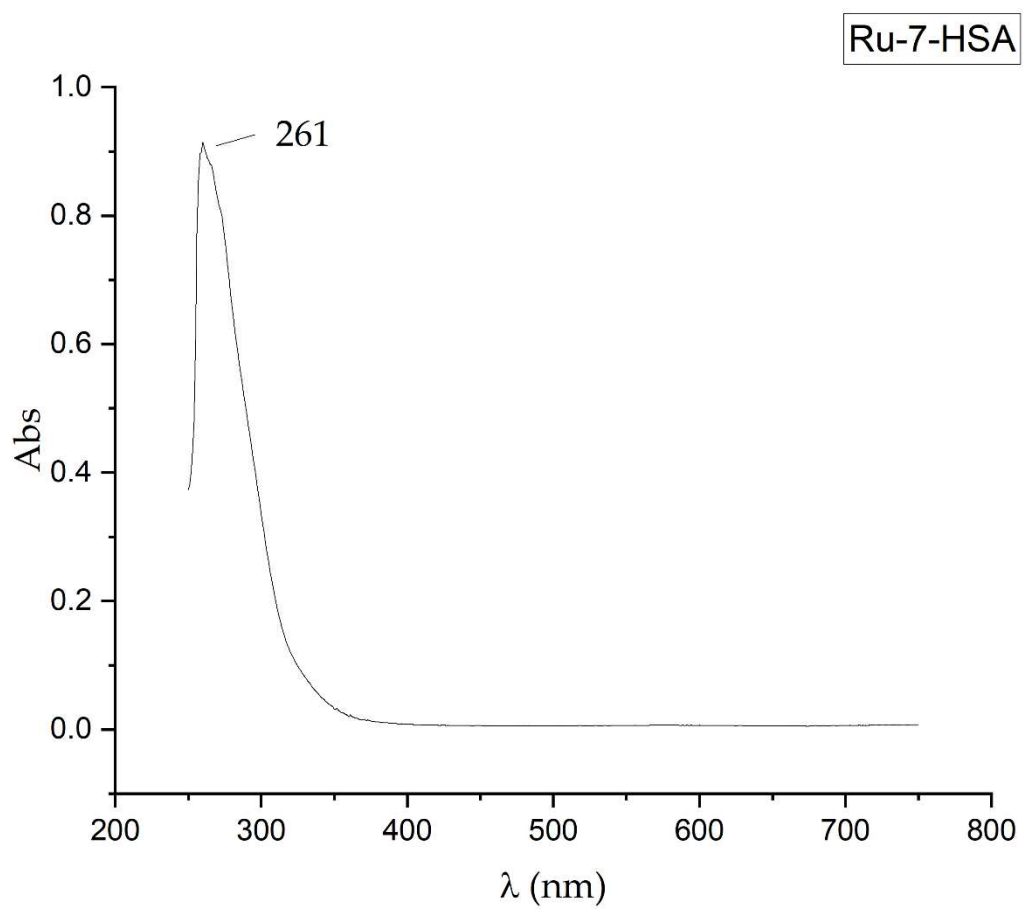


S5: Mass Spectrum of 2 (Positive mode)



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

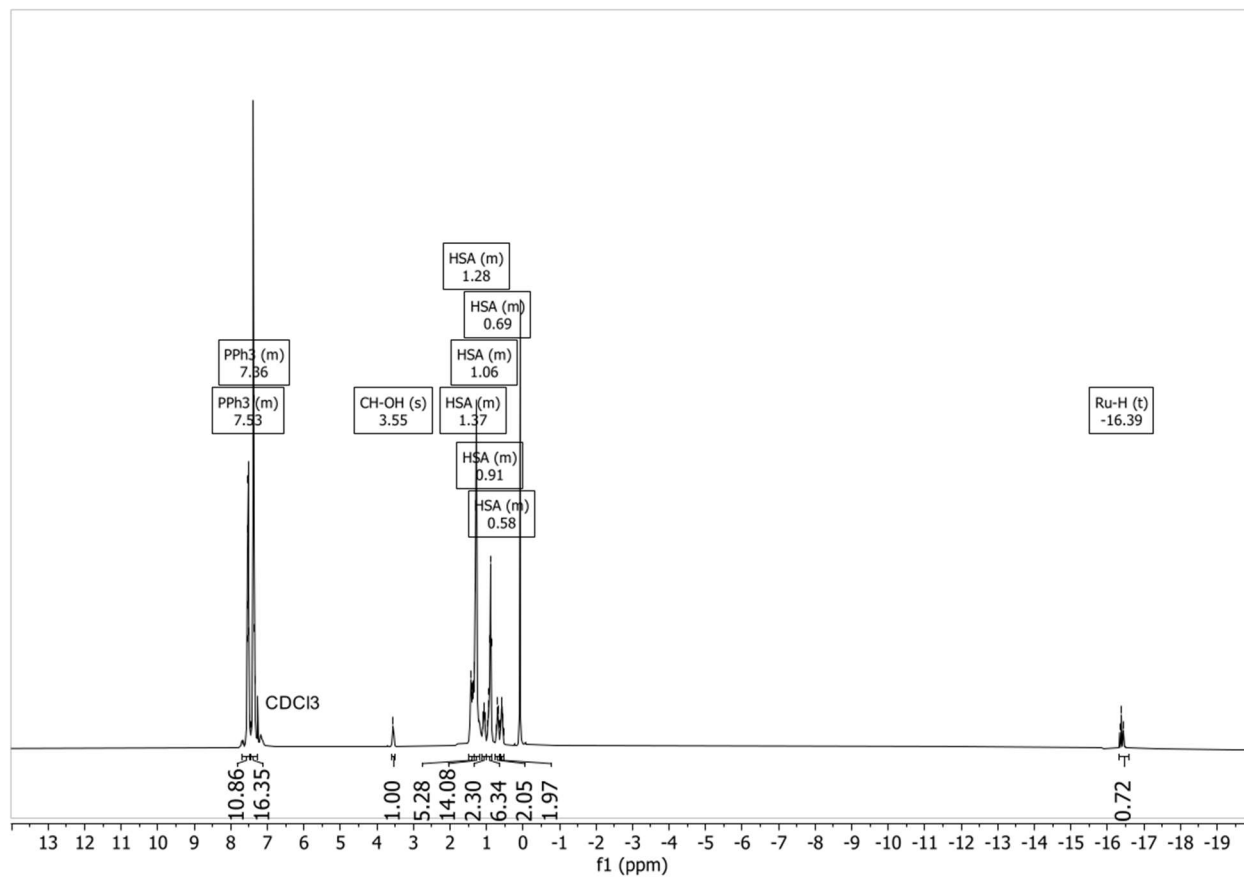
UV-vis spectrum of **2**



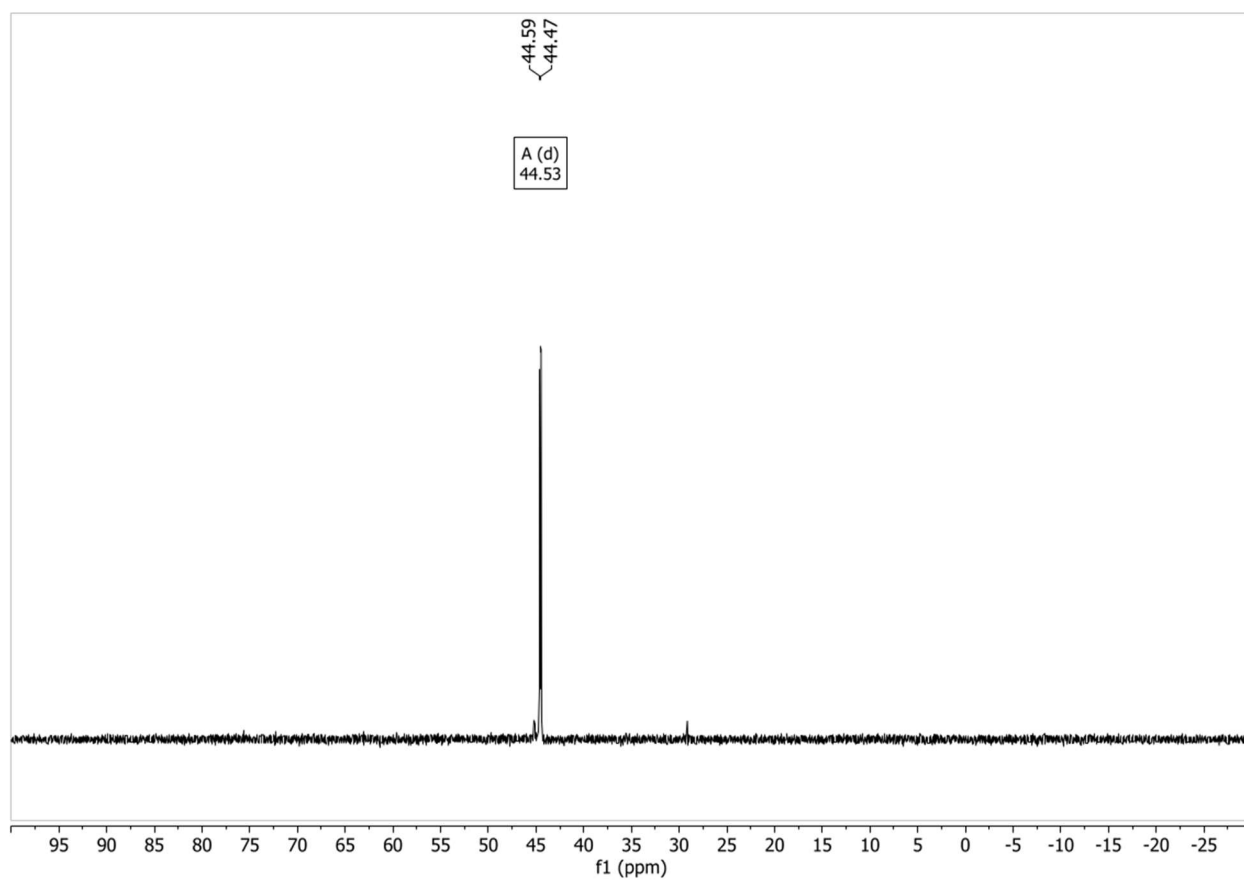
S7: UV-vis spectrum of **2** in DMSO

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

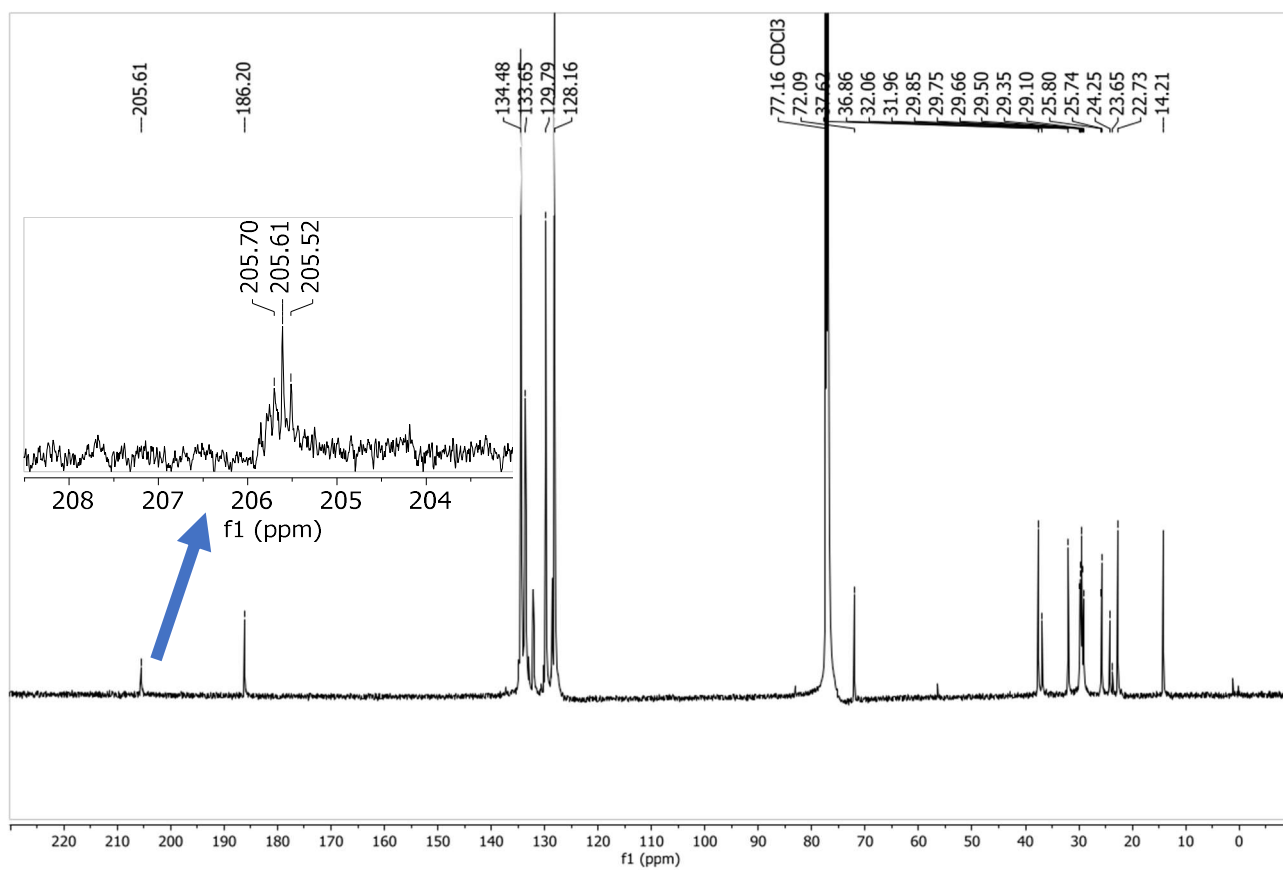
NMR spectra of **3**



S8: ¹H NMR spectrum of **3** in CDCl₃

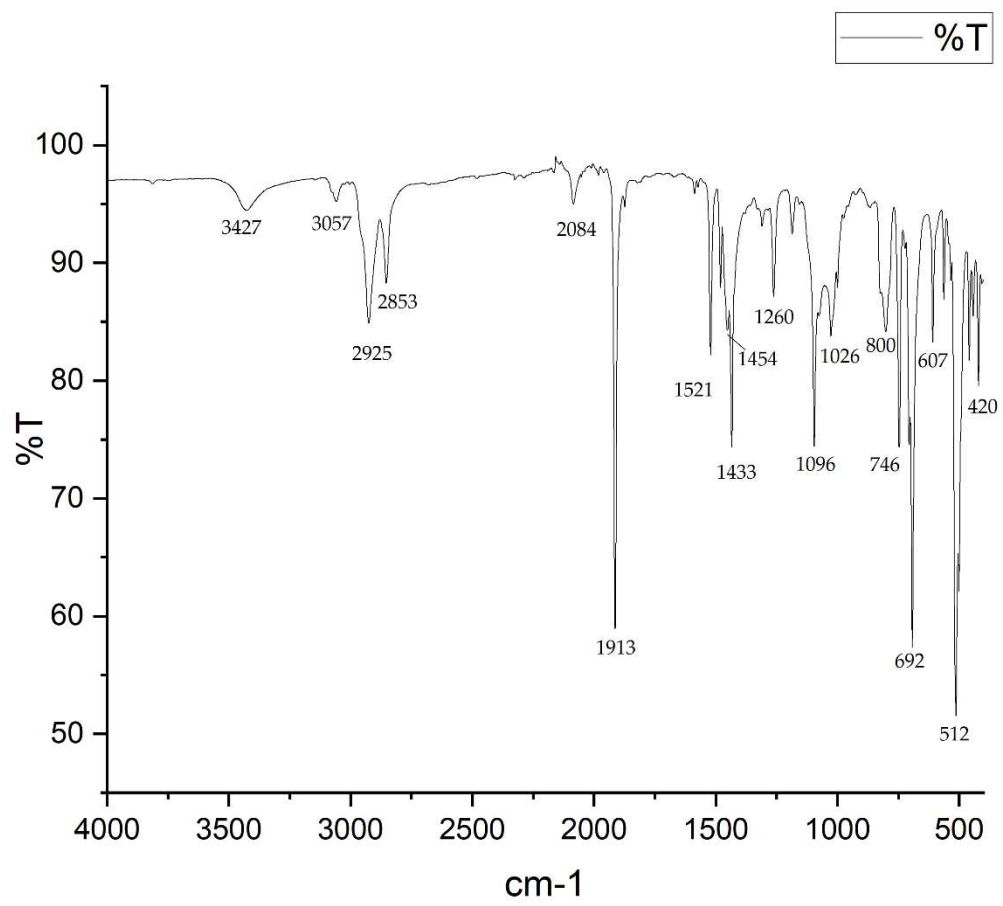


S9: ^{31}P NMR spectrum of **3** in CDCl_3



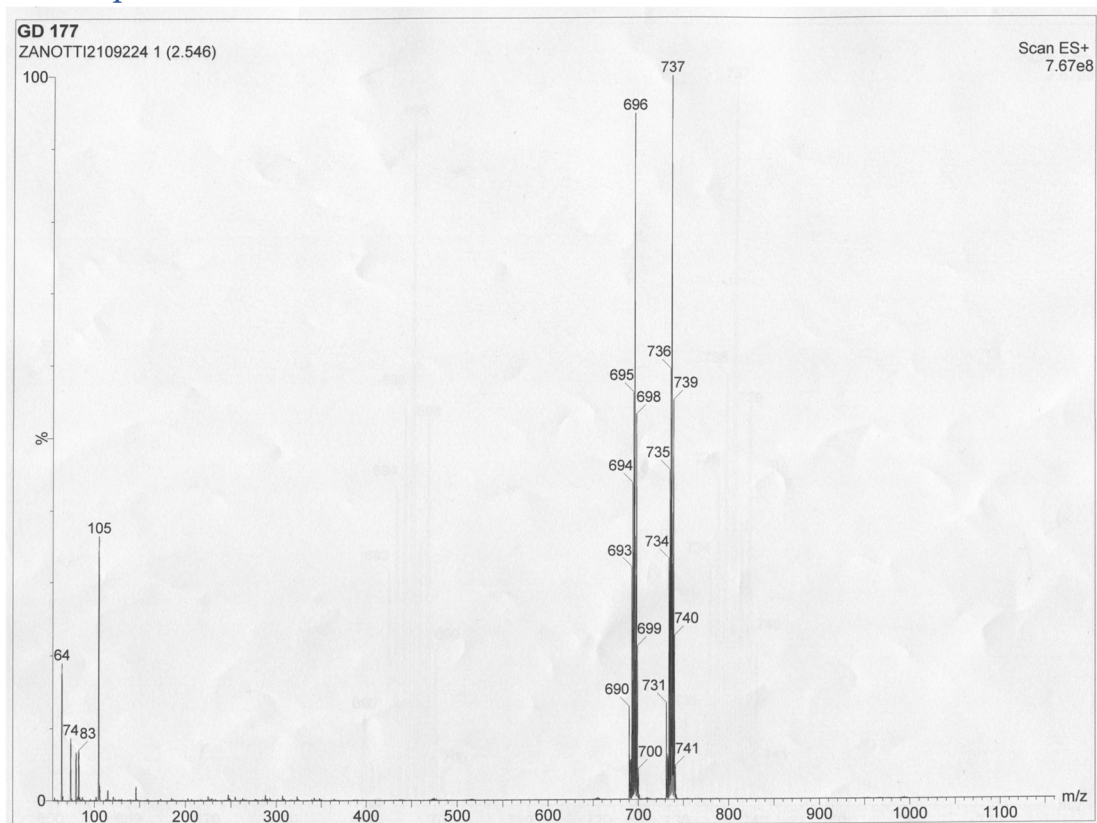
S10: ¹³C spectrum of **3** in CDCl₃

IR spectrum of **3**

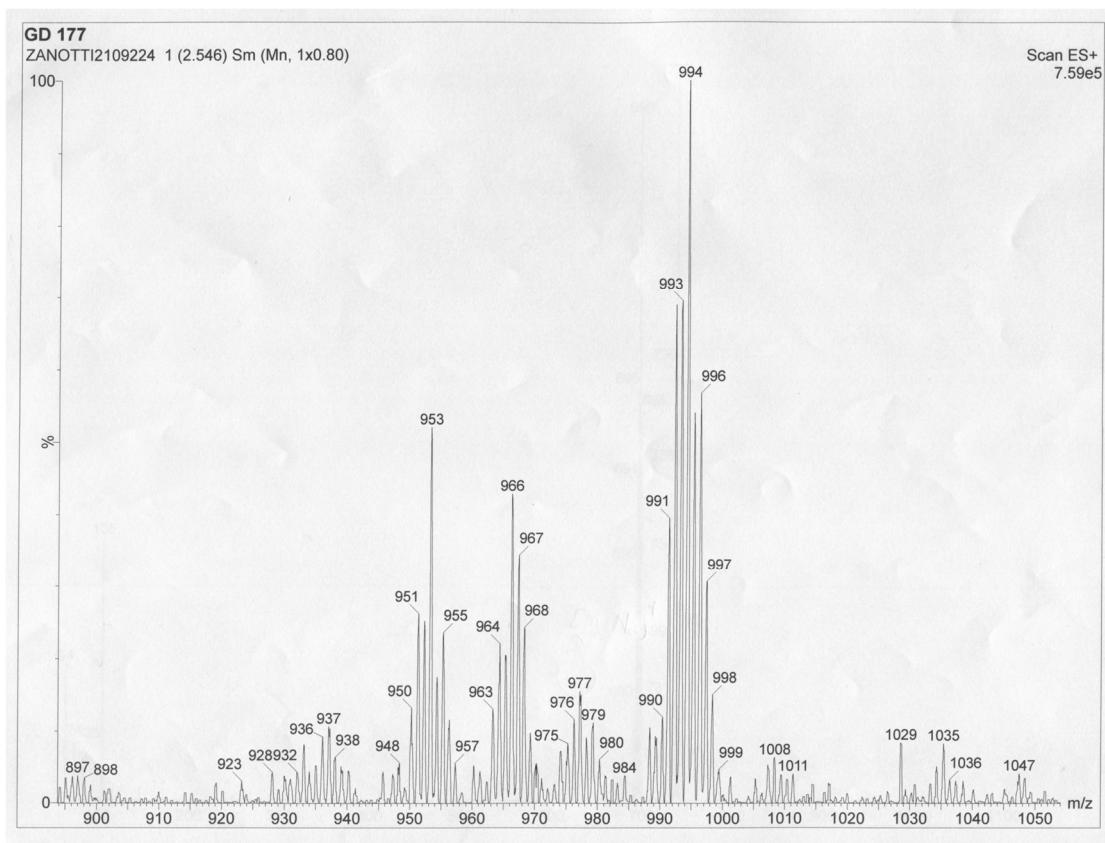


S11: IR spectrum of 3

Mass Spectra of 3

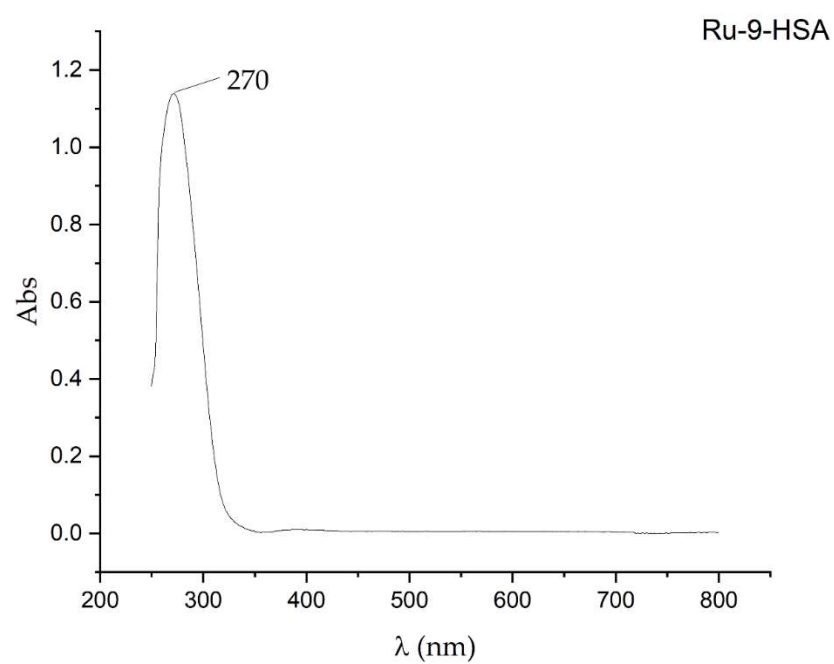


S12: Mass spectrum of 3 (positive mode)



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

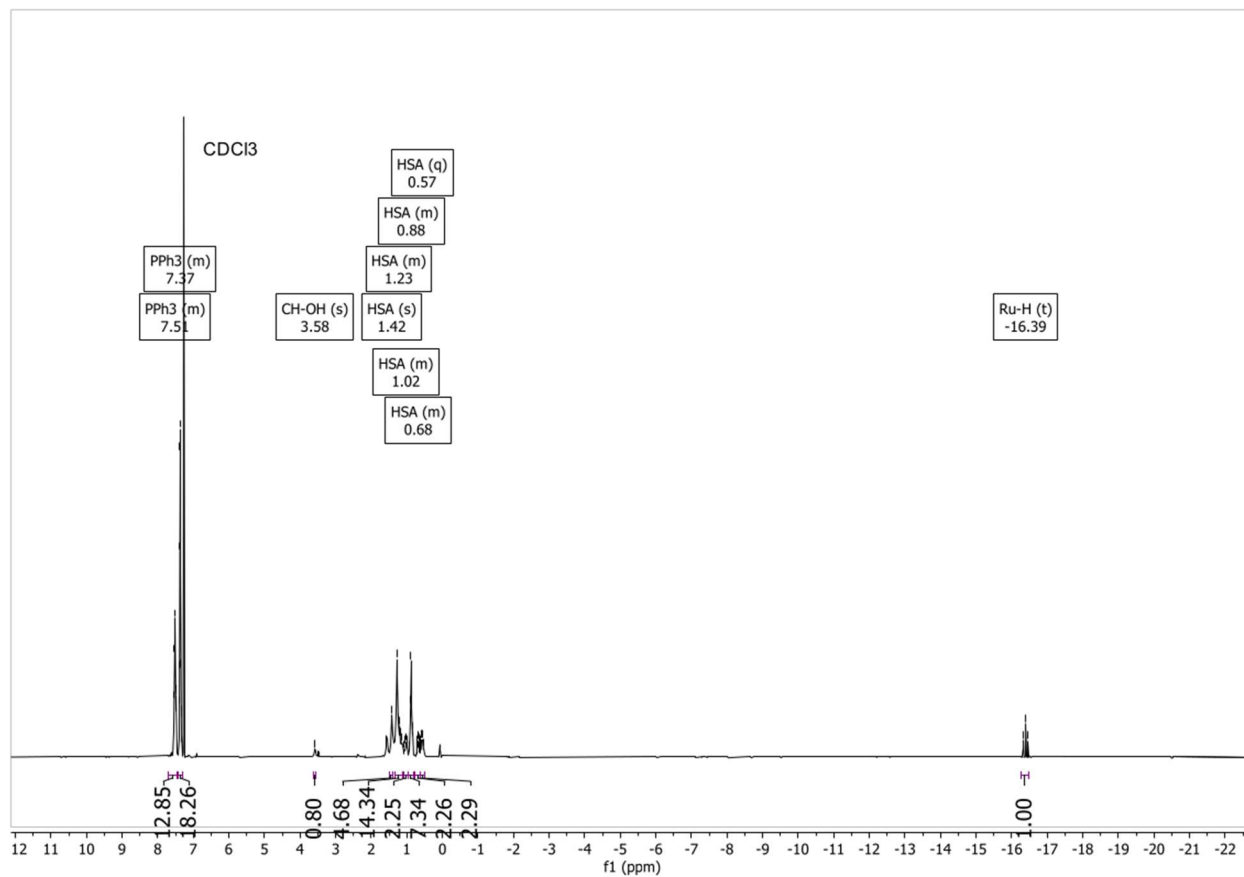
UV-vis spectrum of **3**



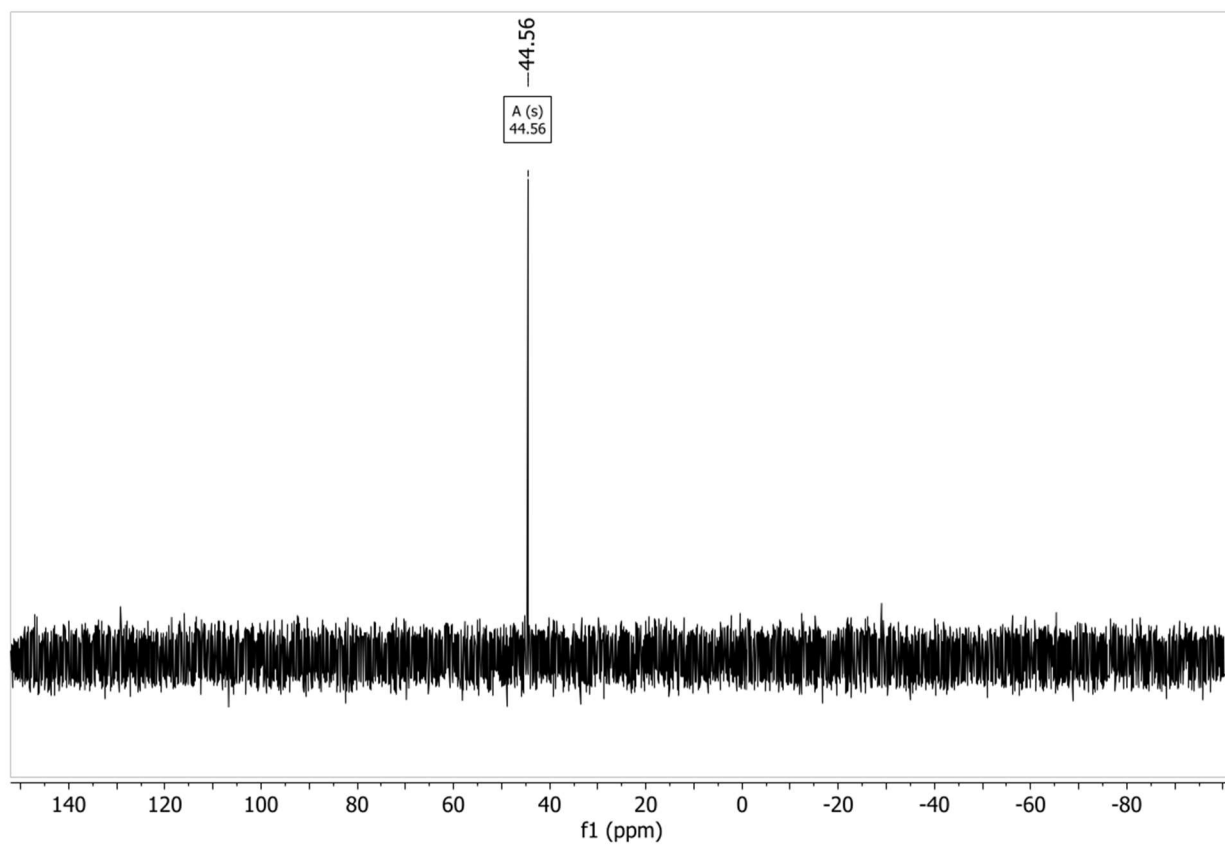
*S14: UV-vis spectrum of **3** in DMSO*

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

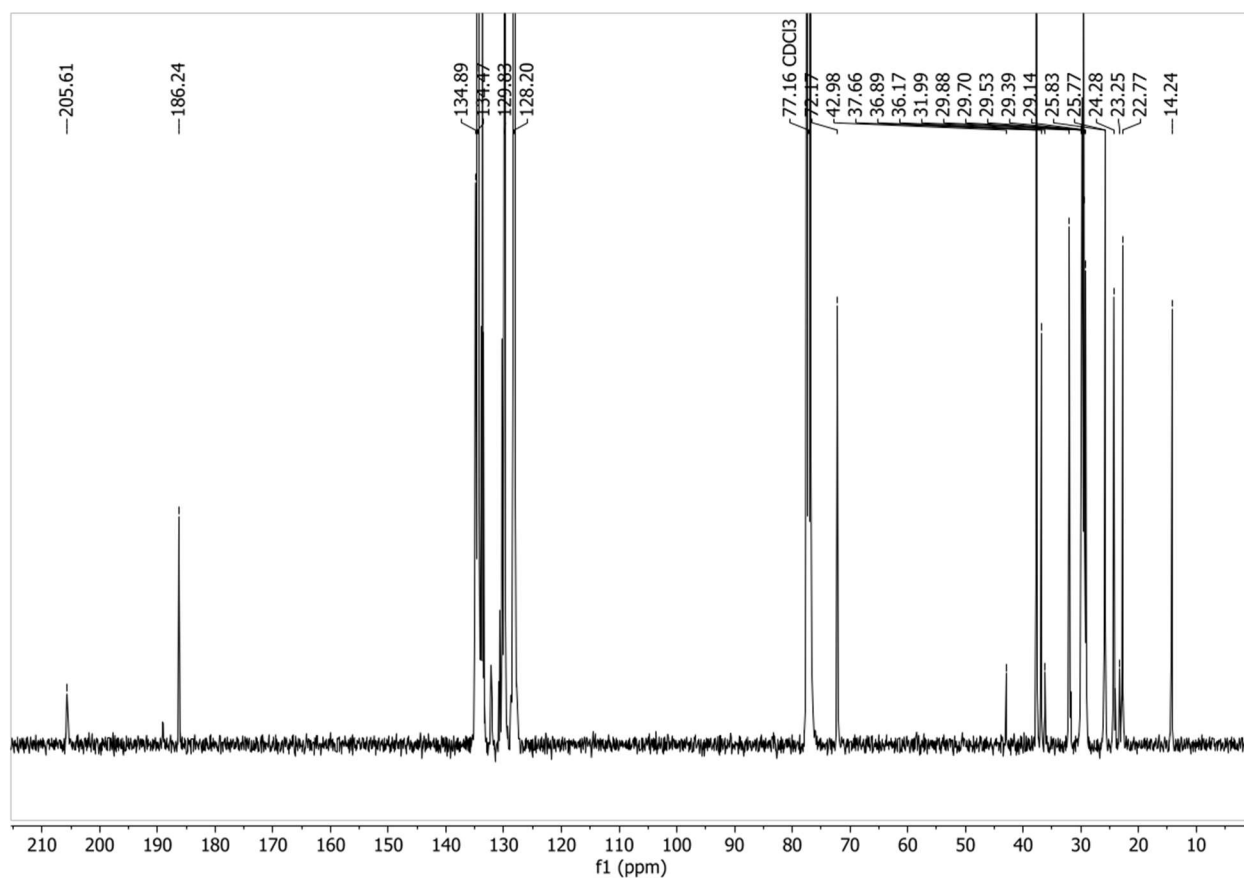
NMR spectra of **4**



S15: ¹H NMR spectrum of **4** in CDCl₃

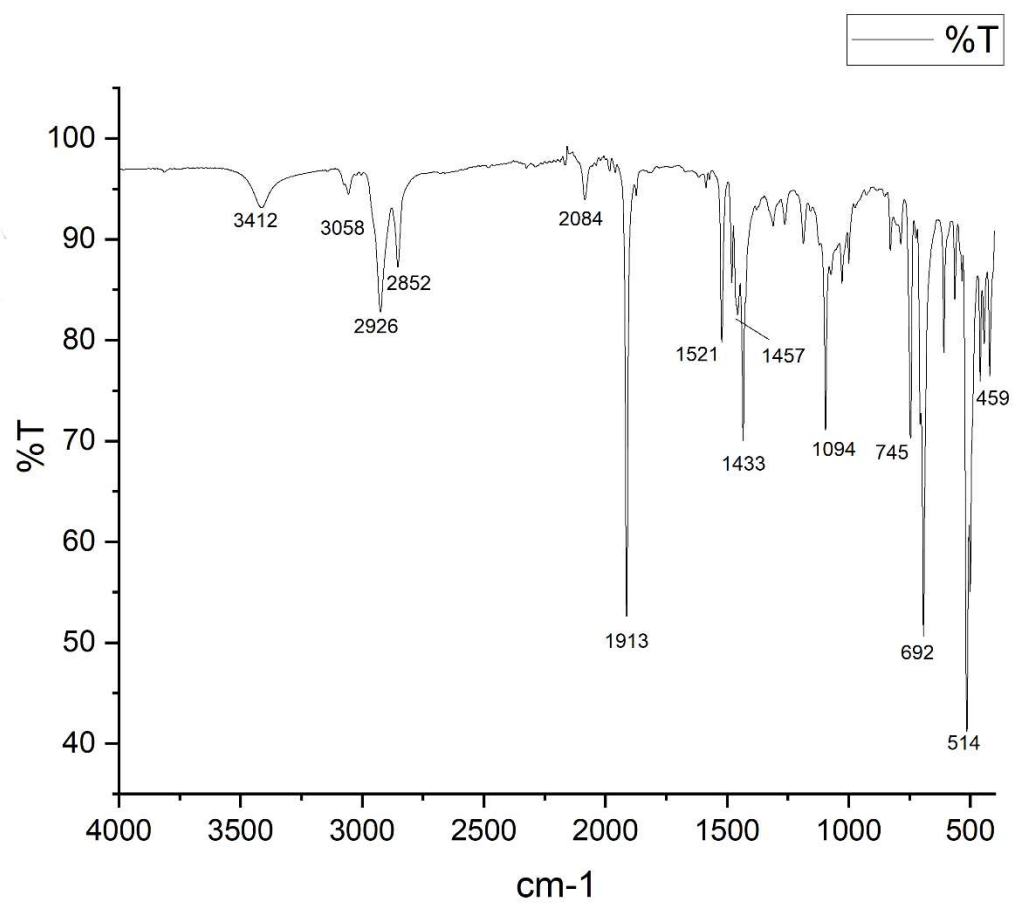


S16: ^{31}P NMR spectrum of **4** in CDCl_3



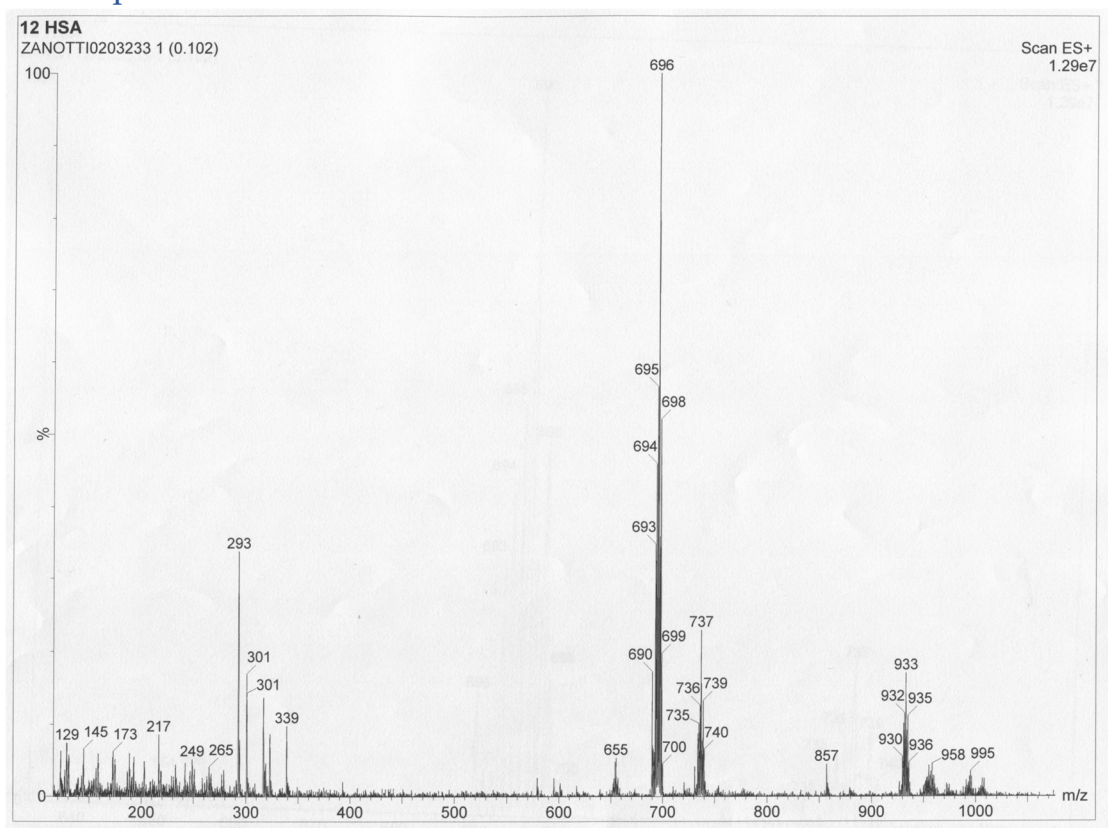
S17: ¹³C NMR spectrum of **4** in CDCl₃

IR Spectrum of **4**

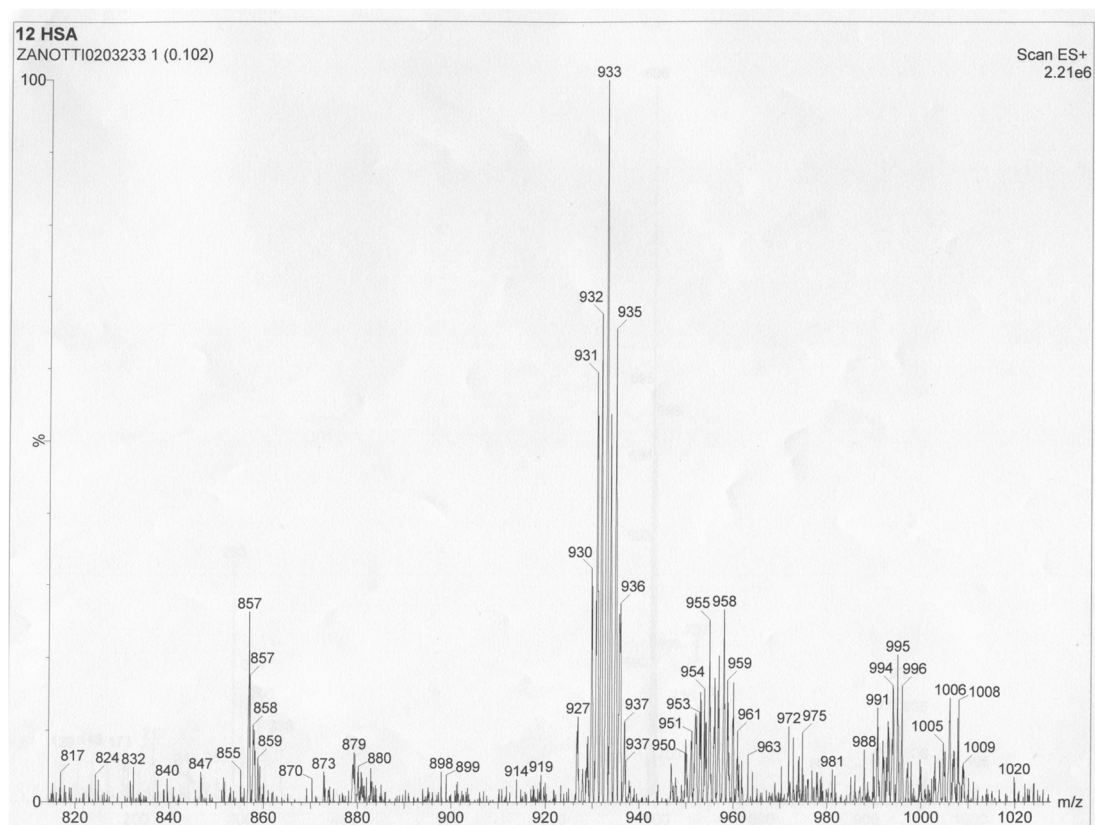


S18: IR spectrum of 4

Mass Spectra of 4

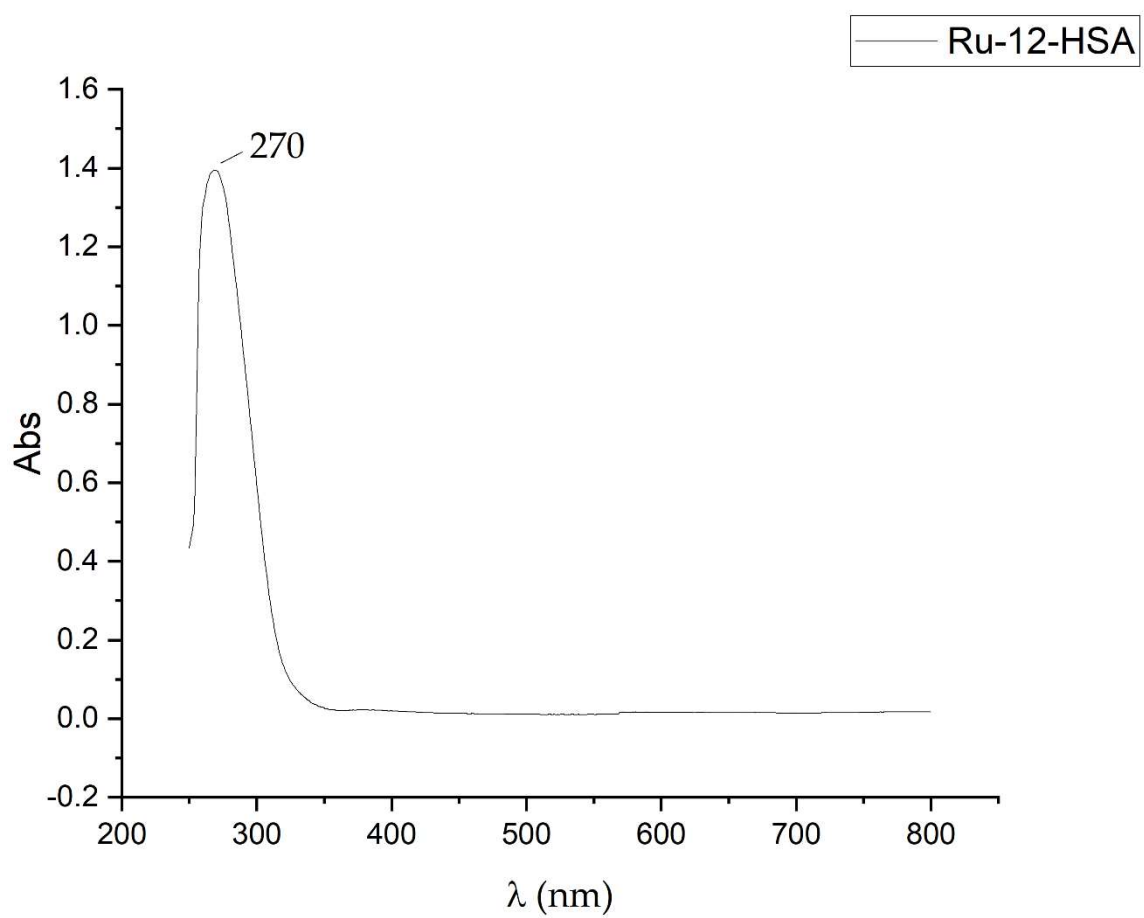


S19: Mass spectrum of 4 (positive mode)



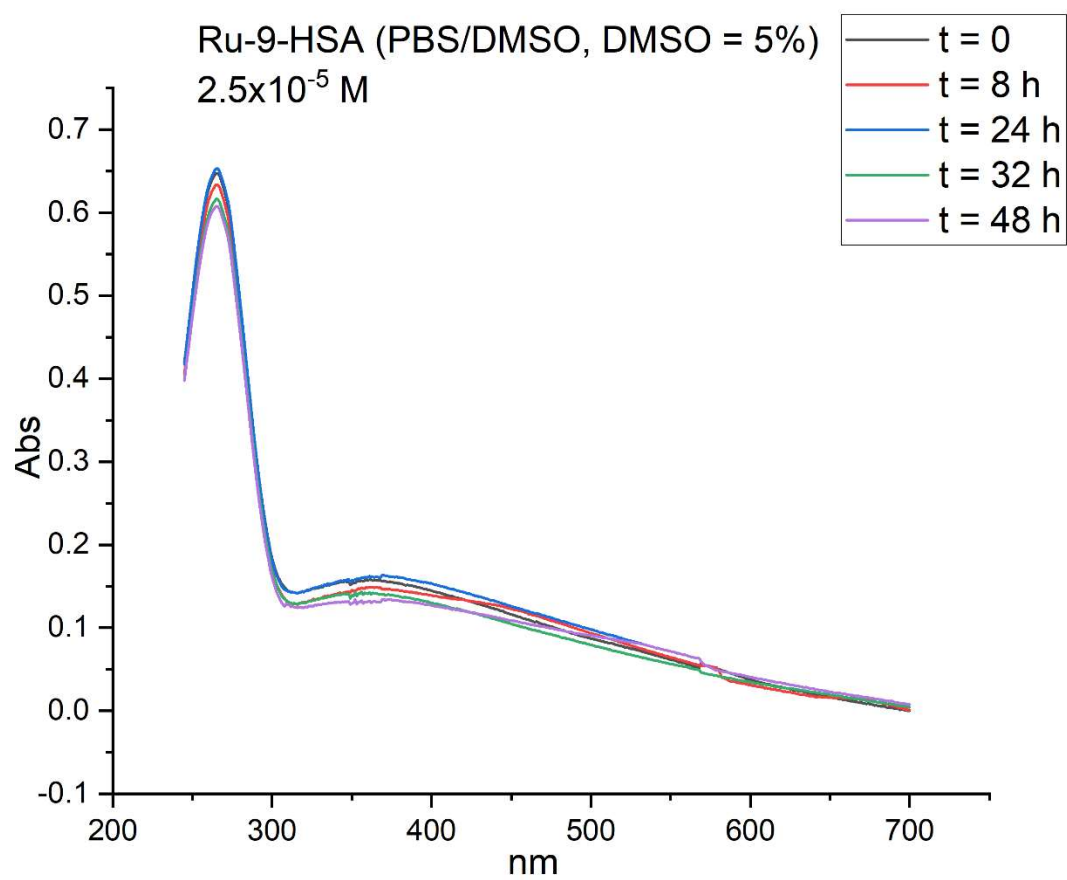
S20: Mass spectrum of 4 (positive mode, m/z: 820 - 1020)

UV-vis spectrum of **4**

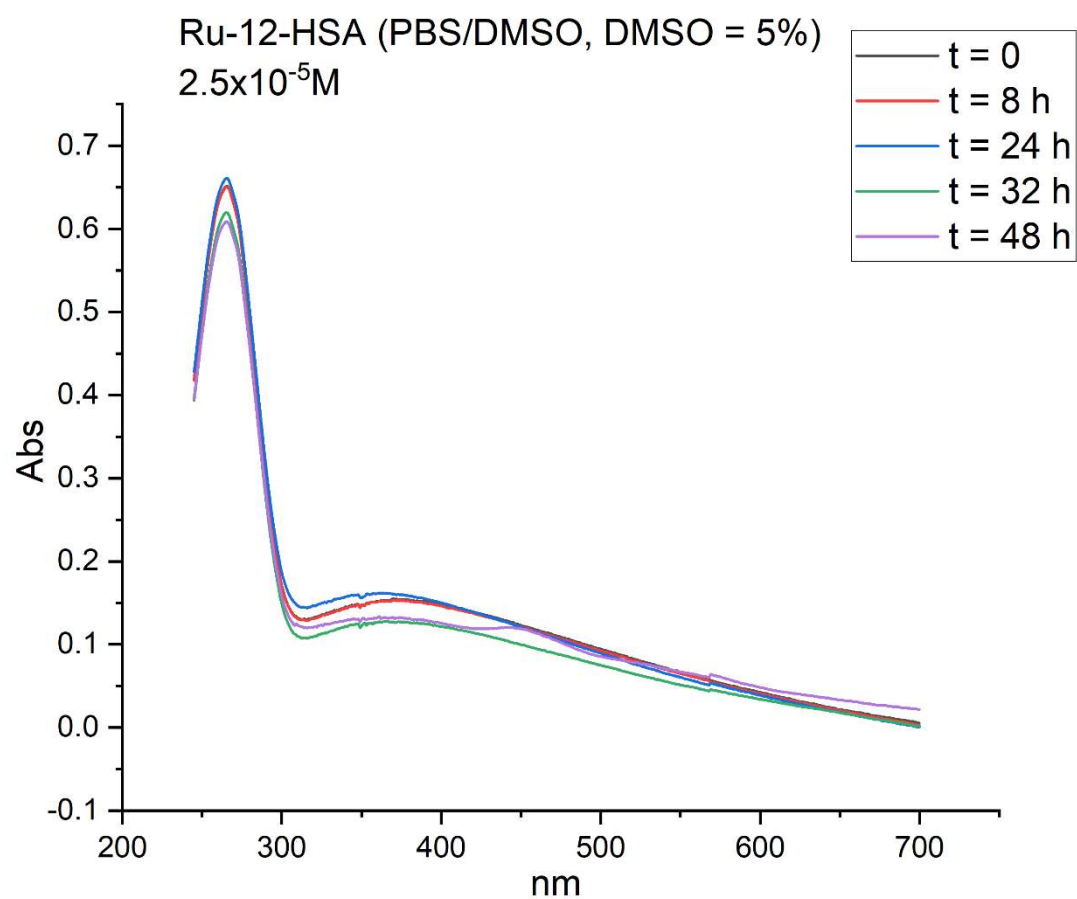


S21: UV-vis spectrum of **4** in DMSO

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

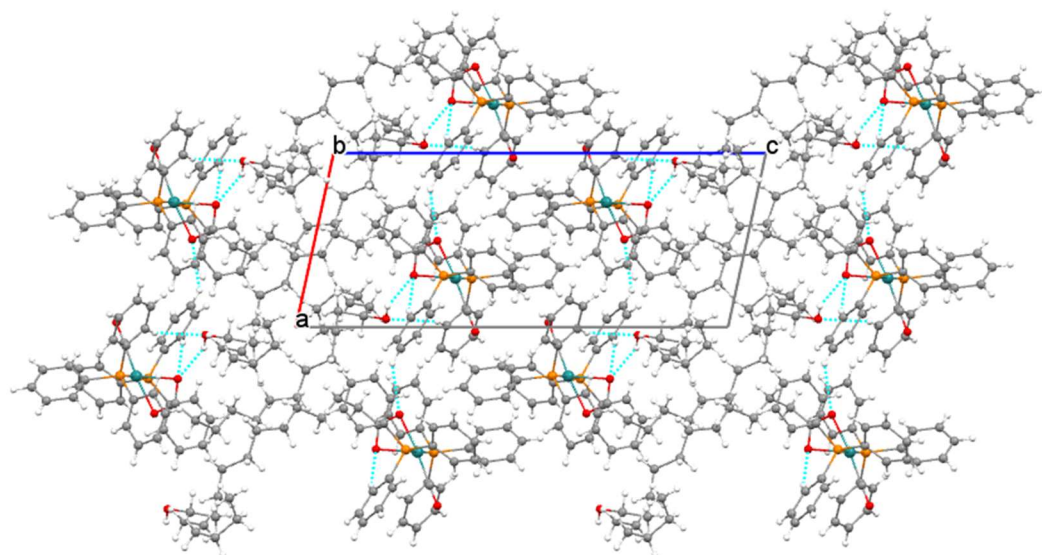


S22: Stability of **3** in PBS/DMSO (DMSO = 5%) at 37°C over 48 h; time-resolved UV-vis spectrum.



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 ₄ P ₂ Ru
Fw	953.08
T, K	100(2)
λ , Å	1.54178
Crystal symmetry	Triclinic
Space group	P-1
<i>a</i> , Å	9.9781(13)
<i>b</i> , Å	12.0328(15)
<i>c</i> , Å	22.364(3)
α	93.268(7)
β	99.999(7)
γ	113.041(6)
Cell volume, Å ³	2410.1(5)
<i>Z</i>	2
<i>D</i> _c , Mg m ⁻³	1.313
μ (Mo-K α), 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. \AA^{-3}	1.592 and -0.783

^a) $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$. ^b) $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$ 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** [\AA 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