

Supporting Information

Phenalenyl Based Platinum Anticancer Compounds with Superior Efficacy: Design, Synthesis, Characterization, and Interaction with Nuclear DNA

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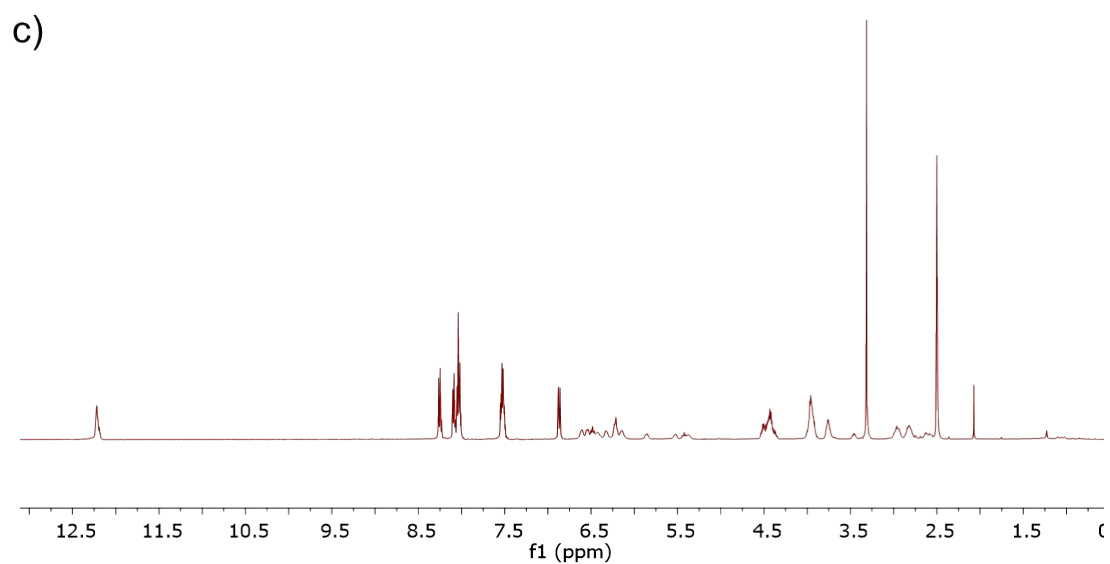
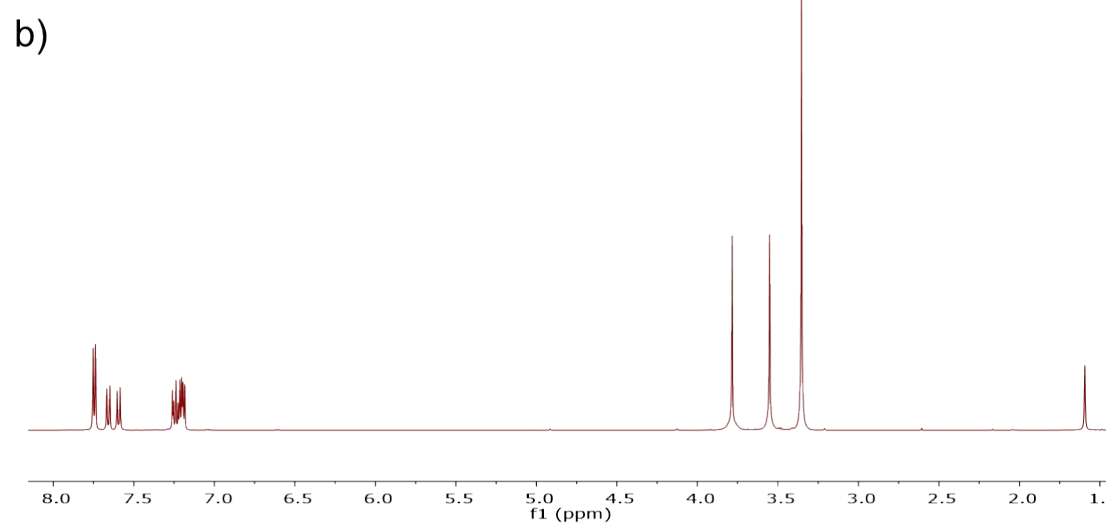
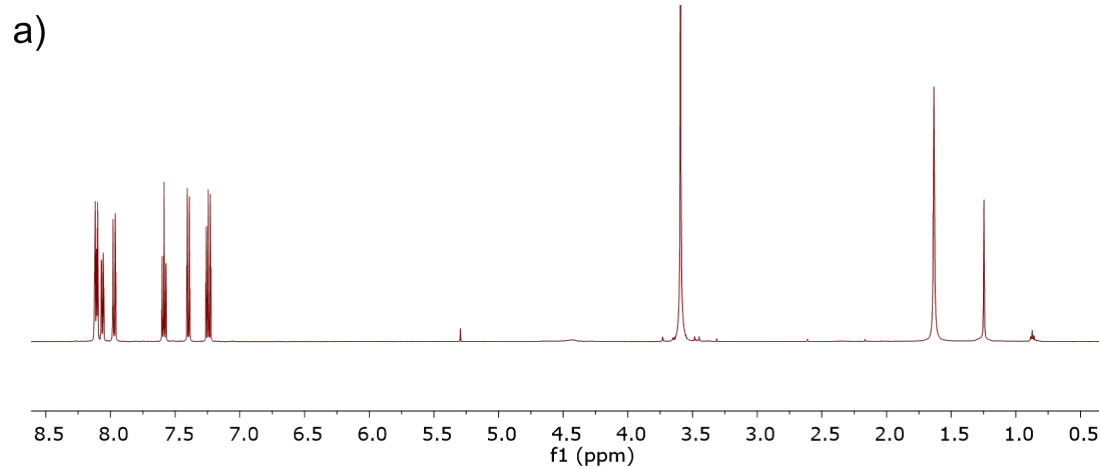
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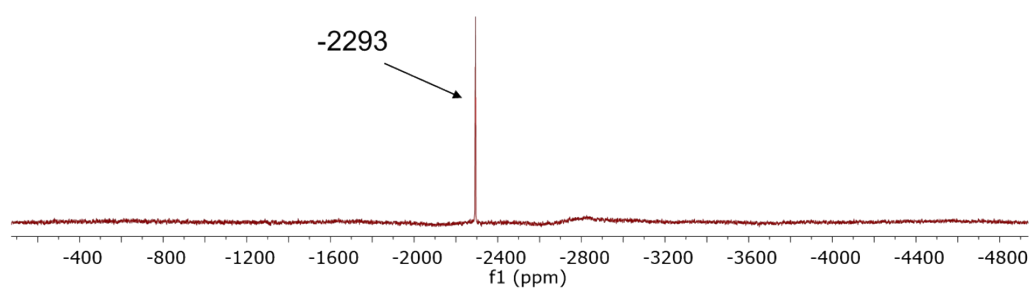
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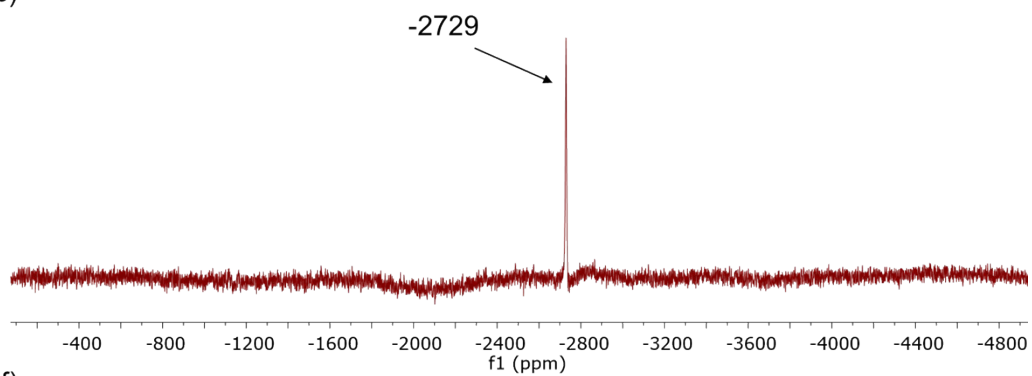
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d)



e)



f)

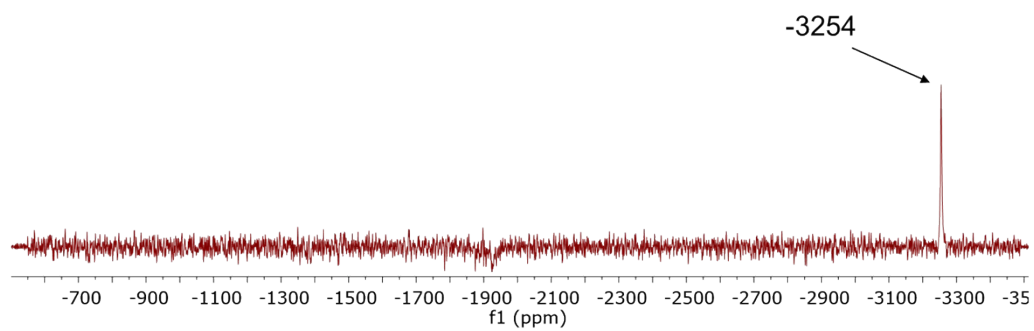


Figure S1. a), b), c) ^1H and d), e), f) ^{195}Pt NMR spectra of compounds **1**, **2** and **3**, respectively.

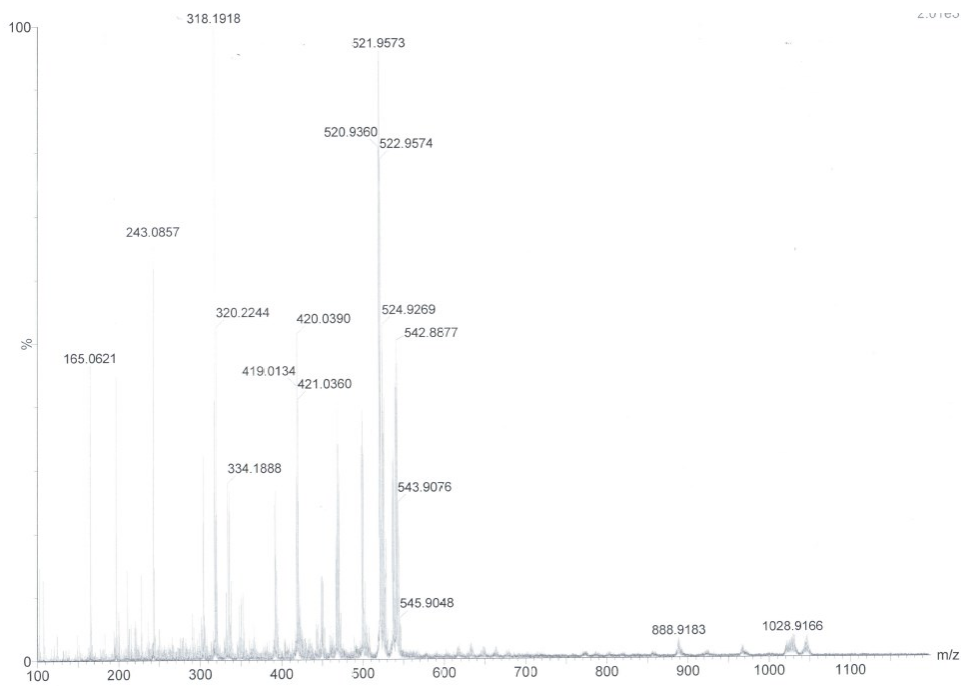


Figure S2. Mass spectrum of compound 1.

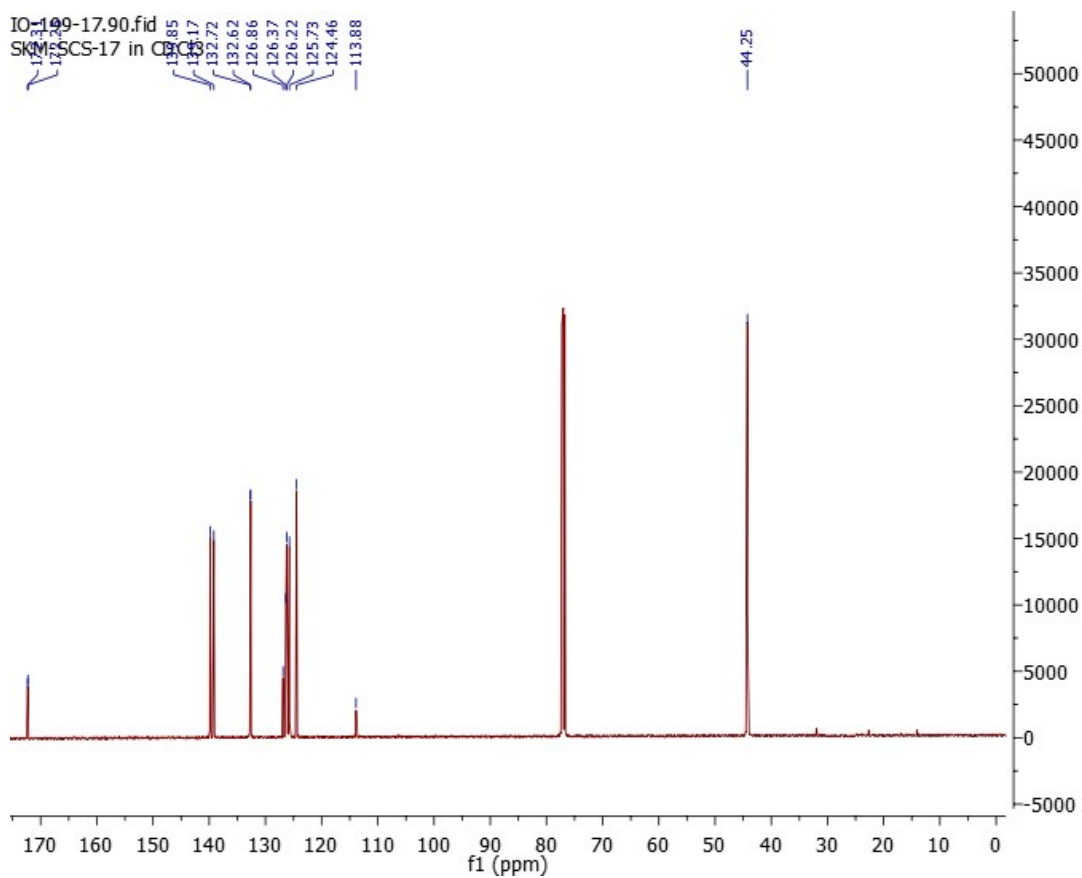


Figure S3. ¹³C NMR spectrum of compound 1.

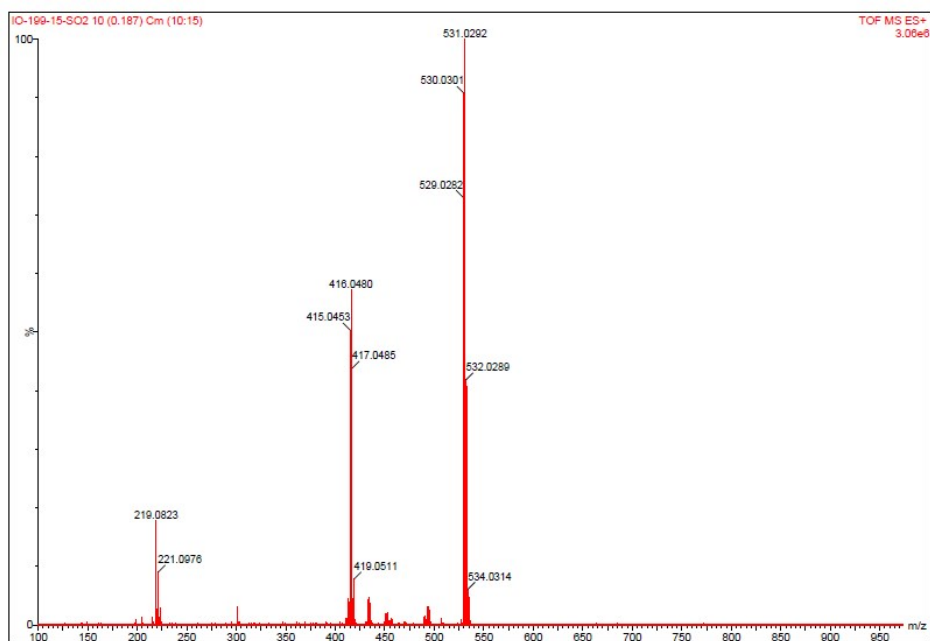


Figure S4. Mass spectrum of compound 2.

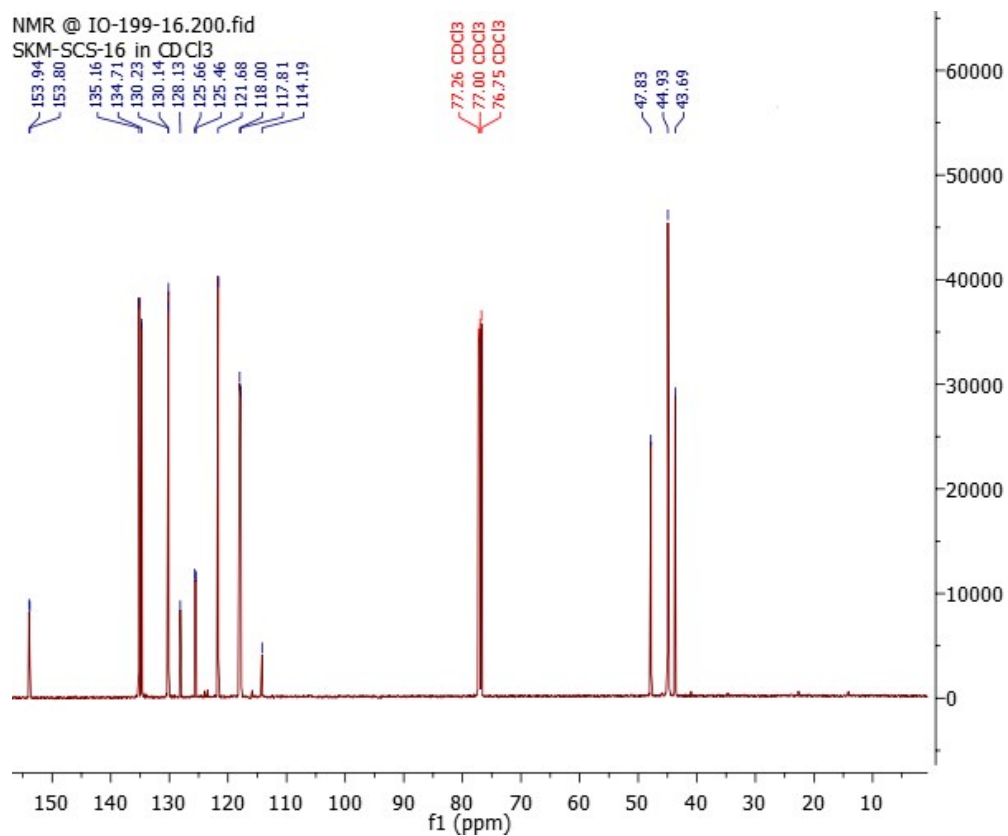


Figure S5. ^{13}C NMR spectrum of compound 2.

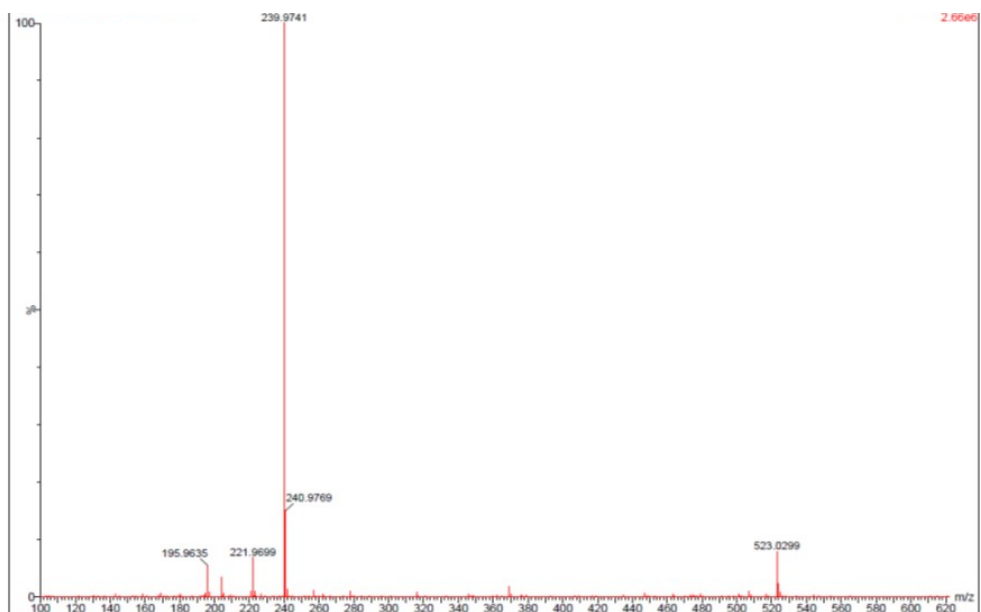


Figure S6. Mass spectrum of compound **3b**.

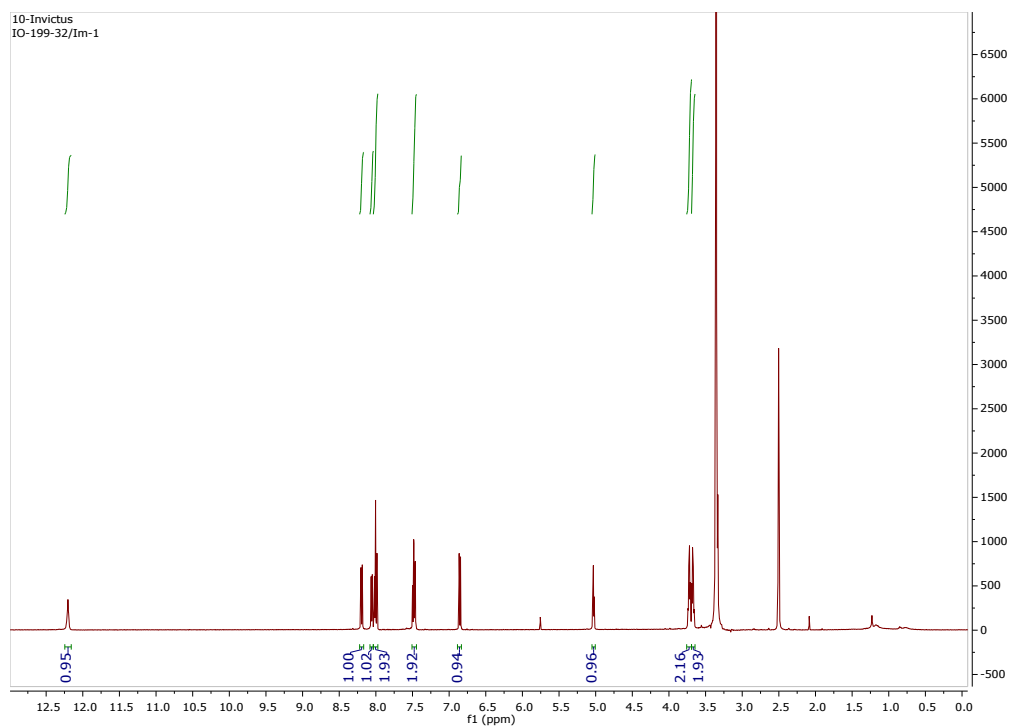


Figure S7. ¹H NMR spectrum of compound **3b**.

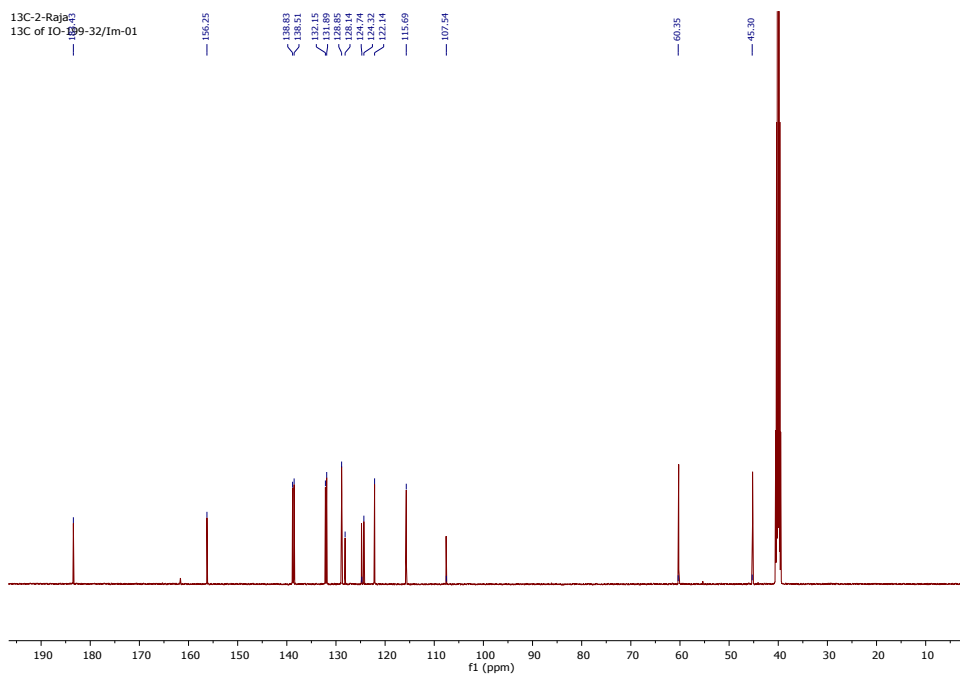


Figure S8. ^{13}C NMR spectrum of compound **3b**.

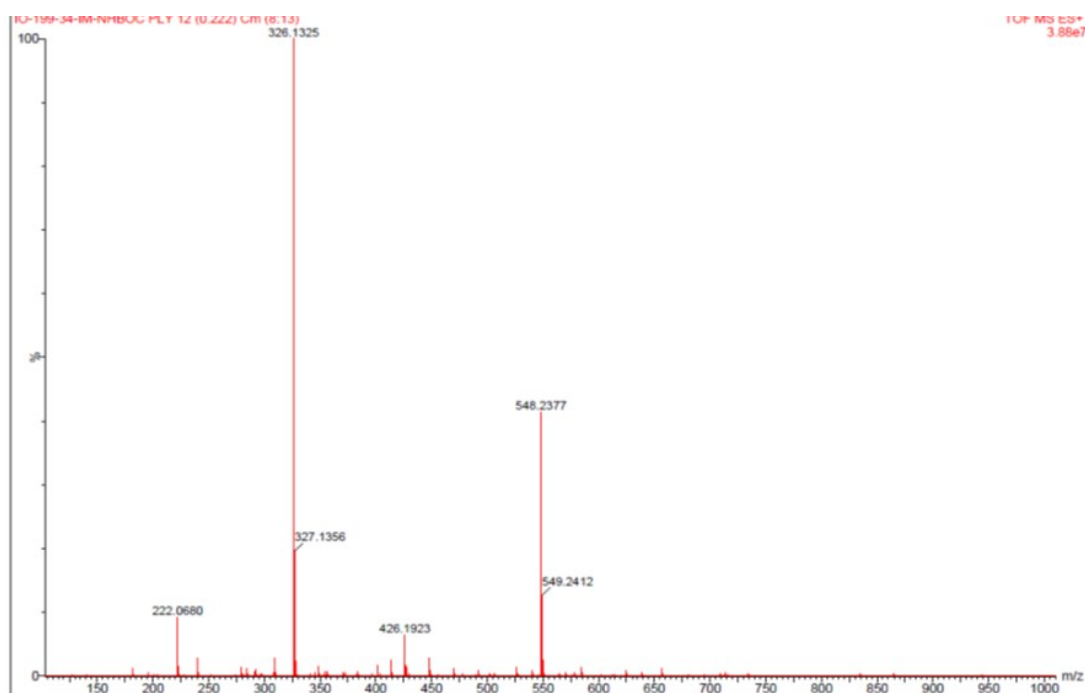


Figure S9. Mass spectrum of compound **3c**.

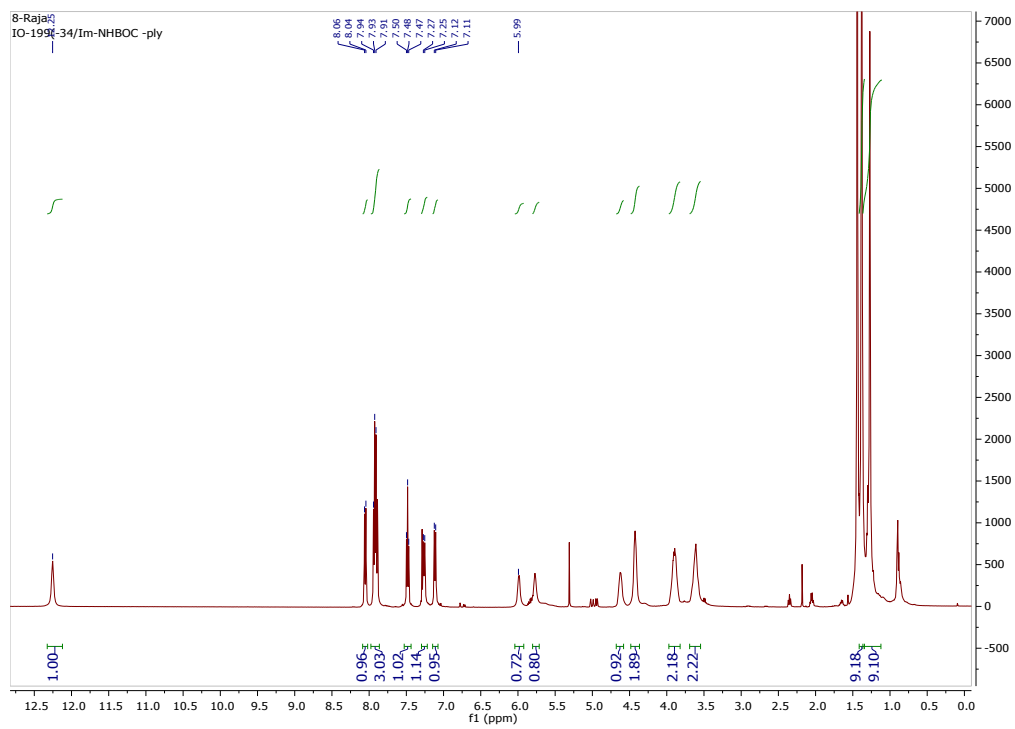


Figure S10. ^1H NMR spectrum of compound **3c**.

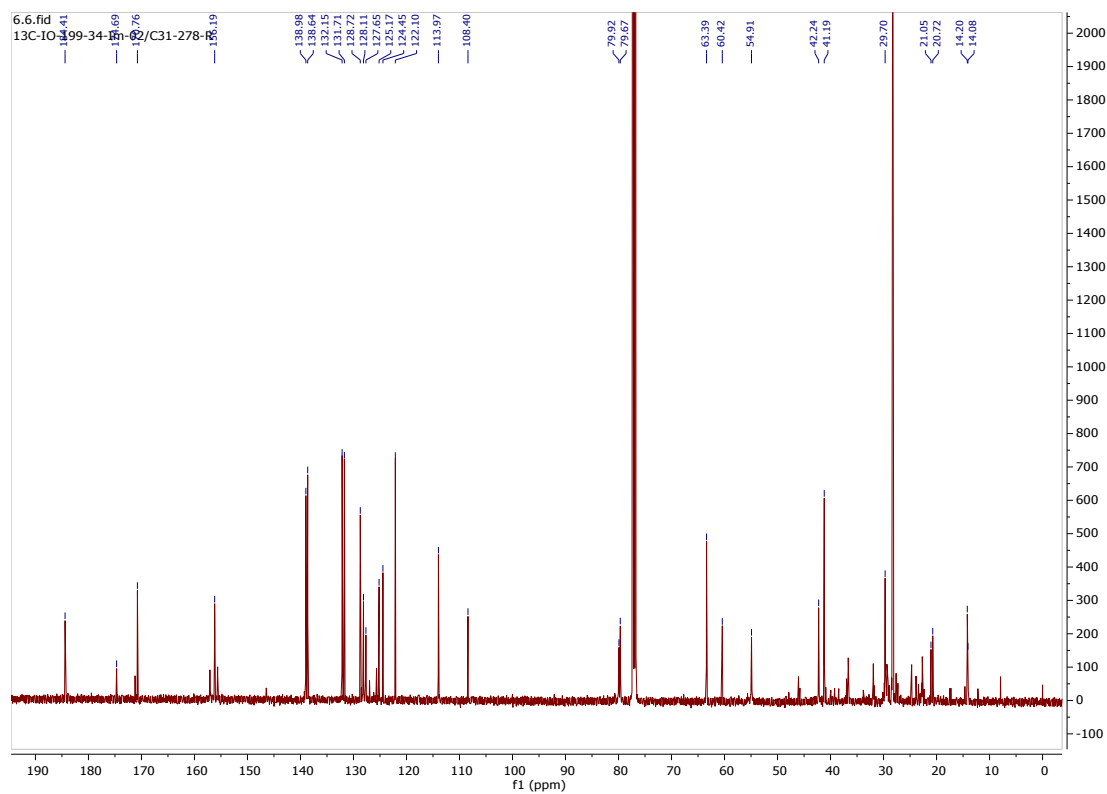


Figure S11. ^{13}C NMR spectrum of compound **3c**.

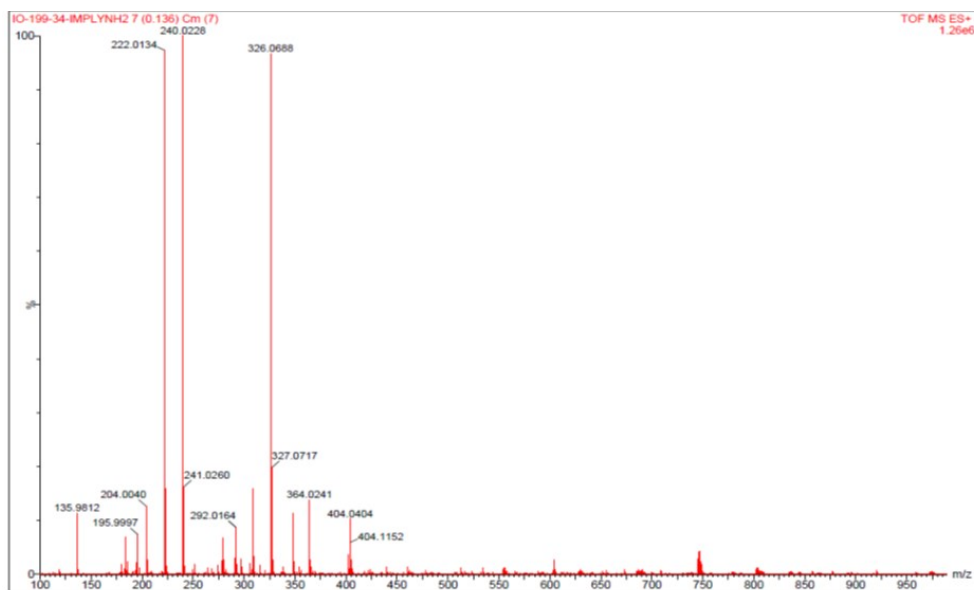


Figure S12. Mass spectrum of compound 3c.

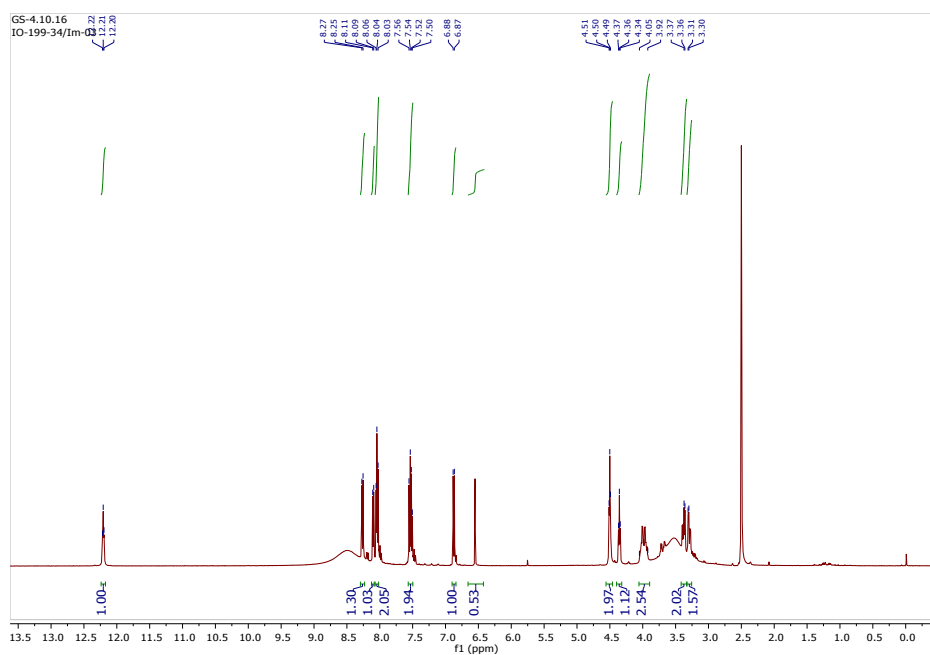


Figure S13. ¹H NMR spectrum of compound 3c.

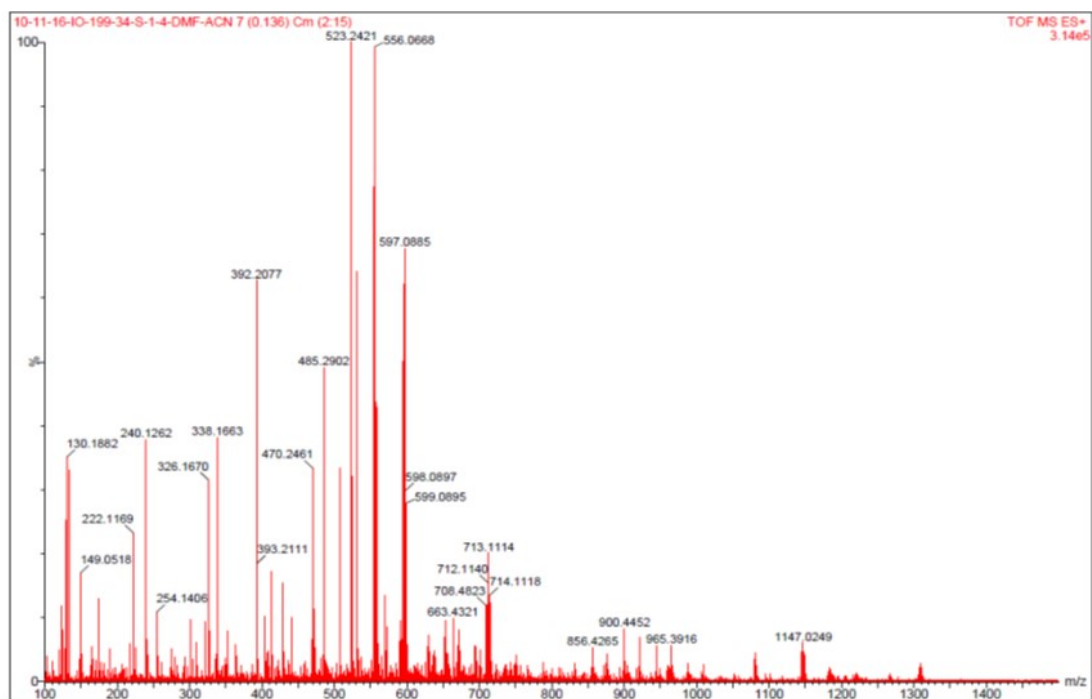


Figure S14. Mass spectrum of compound 3.

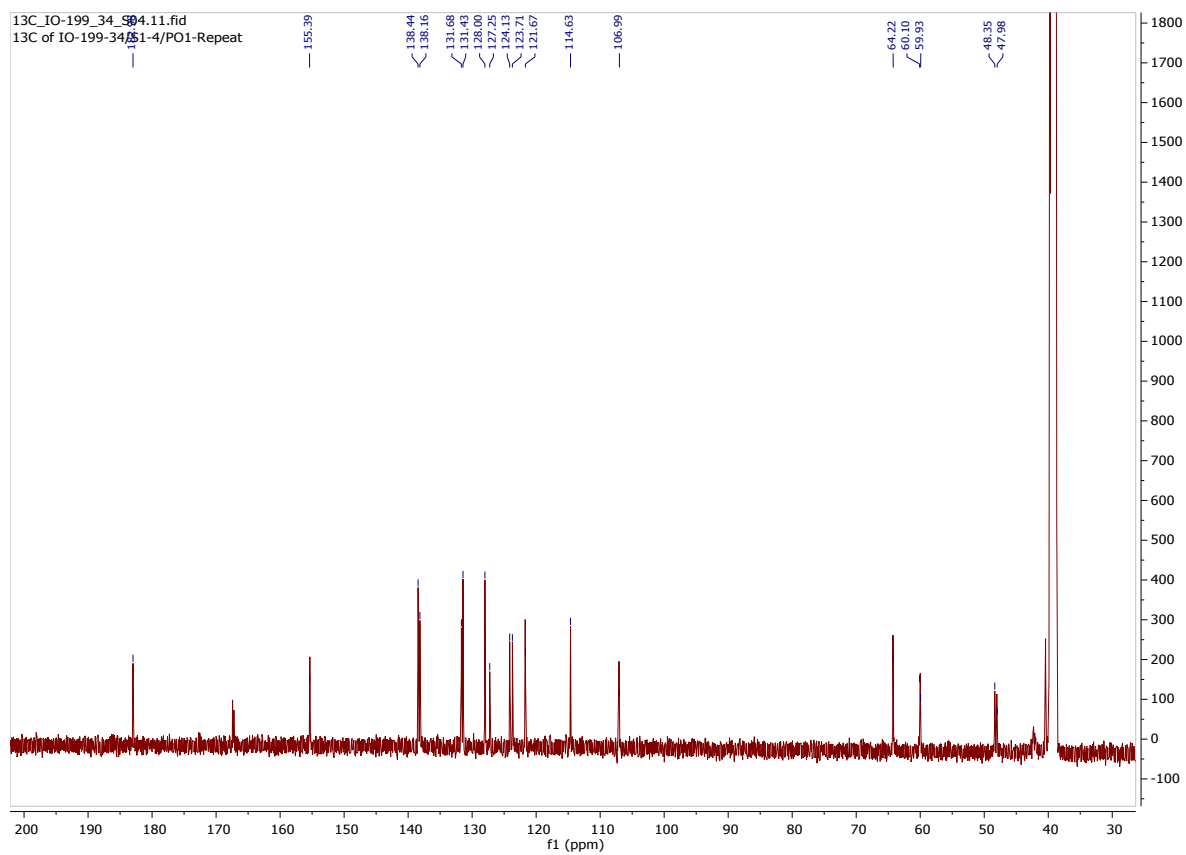
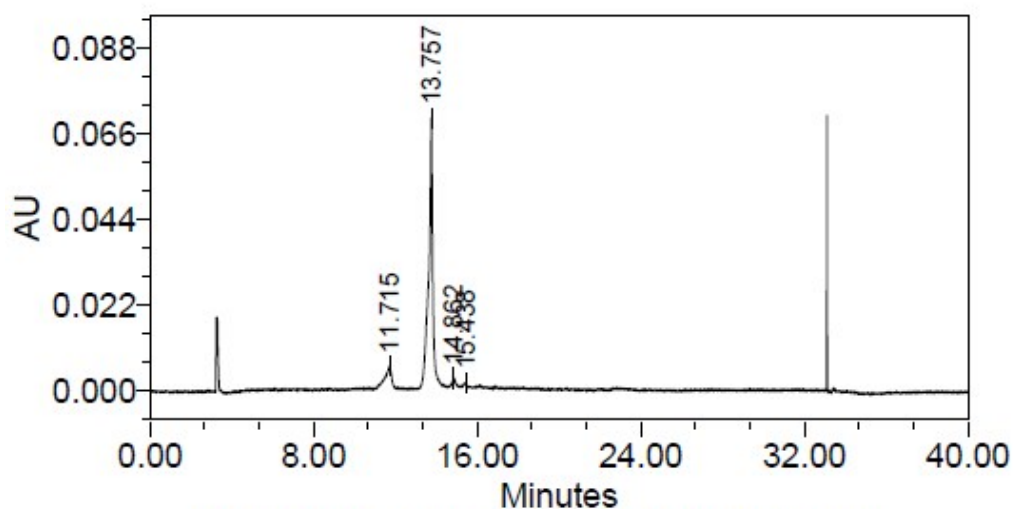


Figure S15. ¹³C NMR spectrum of compound 3.



— Channel Description 2998 Ch2 440nm@1.2nm

Peak Results

	RT	Area	Height	% Area	Total Area
1	11.715	113818	5430	10.68	1065849
2	13.757	927475	68705	87.02	1065849
3	14.862	17330	2067	1.63	1065849
4	15.438	7225	1037	0.68	1065849

Figure S16. HPLC profile of compound **3**.

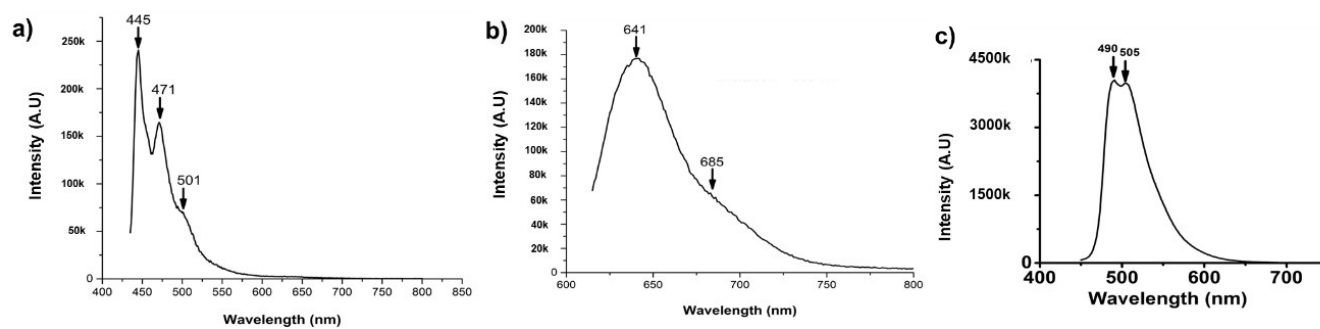


Figure S17. Emission spectra of a) compound **1**, b) compound **2** and c) compound **3** in their respective γ_{\max} of excitation wavelengths 420 nm (for **1**), 600 nm (for **2**) and 440 nm (for **3**).

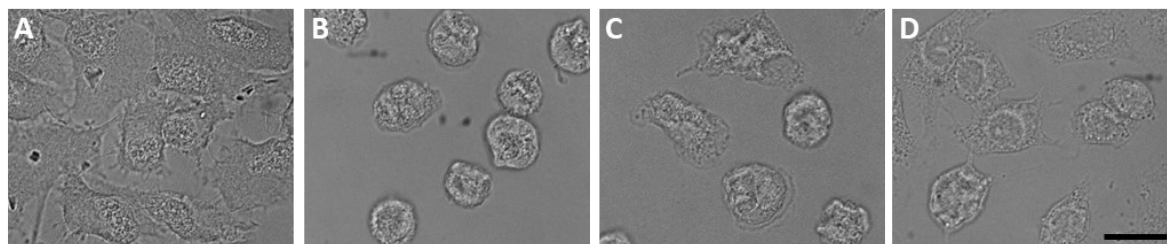


Figure S18. Morphology of A549 cells following treatment with compounds for 24 hours. (A) untreated, (B) compound **1**, (C) compound **2**, (D) compound **3**. Scale bar 20 μm .

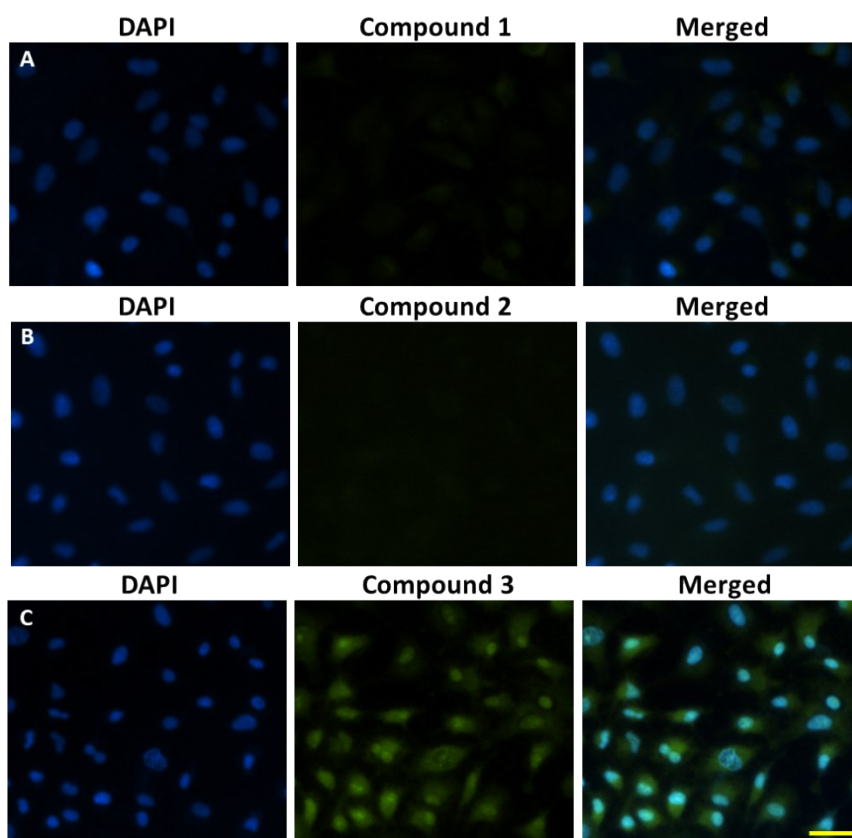


Figure S19. Fluorescence intensity in A549 cells post treatment with compounds. (A) compound 1; (B) compound 2; (C) compound 3. Scale bar 20 μm .

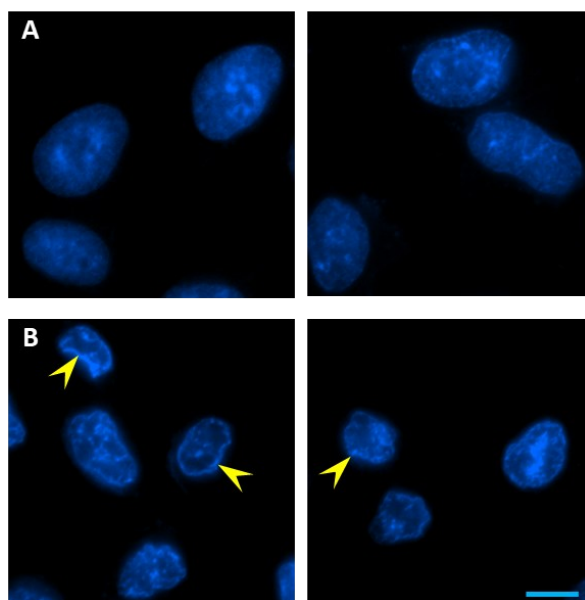


Figure S20. Representative images showing morphological changes of A549 nuclei. (A) untreated cells, showing normal nuclei; (B) cells treated with compound 1 show ring or necklace nuclear condensation (arrowhead). Scale bar 10 μm .

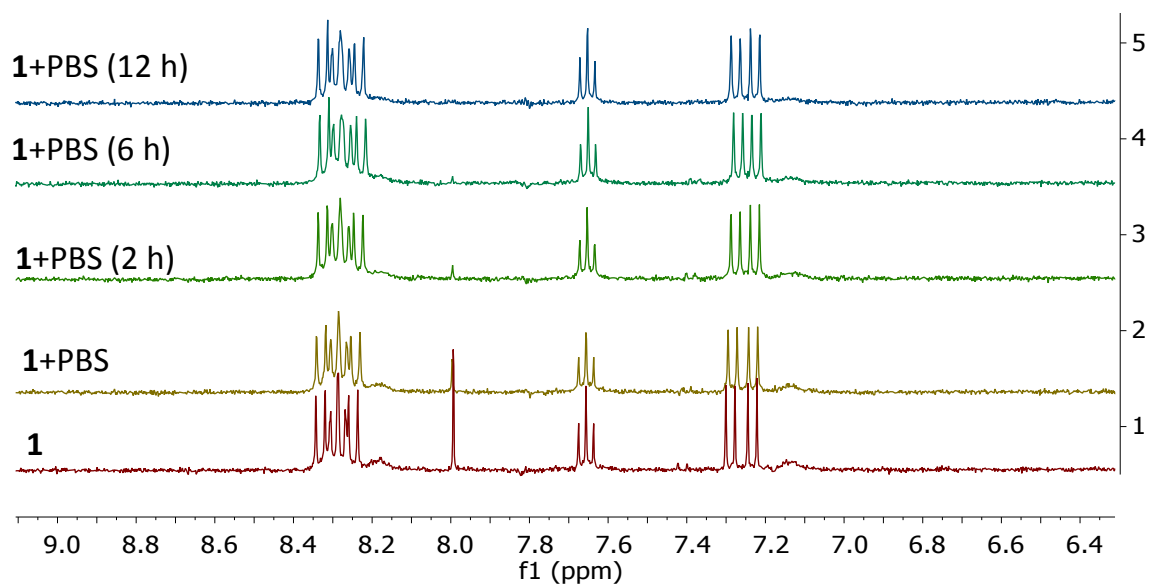


Figure S21. ^1H NMR monitoring of compound **1** in presence of PBS.

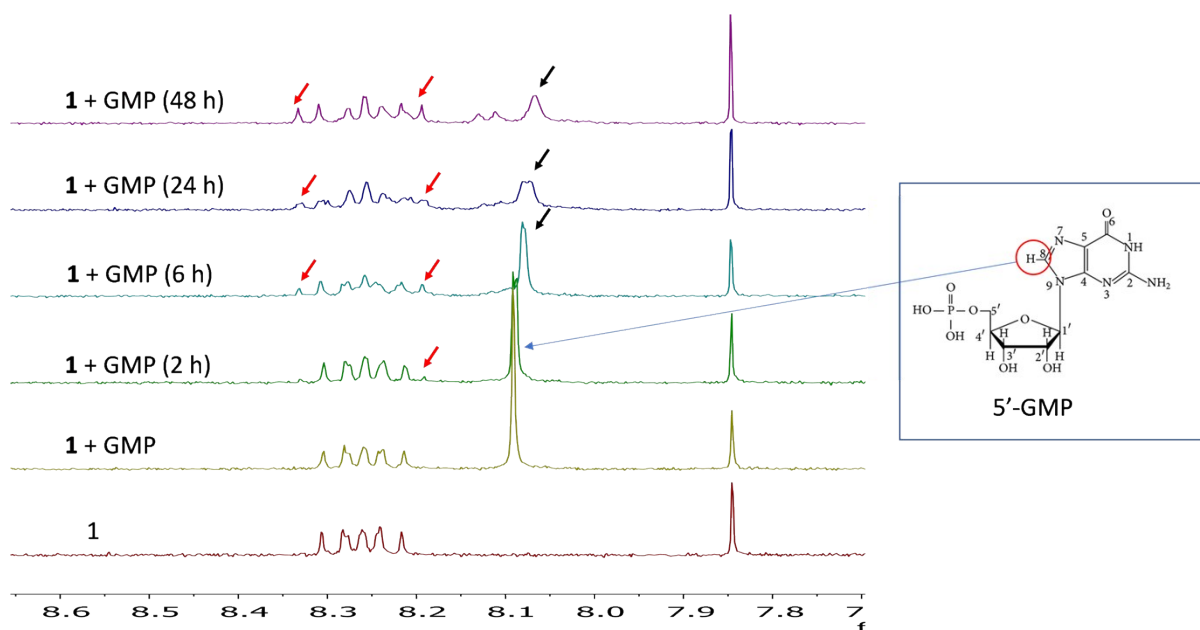


Figure S22. ^1H NMR monitoring of compound **1** in presence of 5'-GMP. (Black arrow indicates the change in H8 of 5'-GMP and Red arrows indicate the appearance of new peak after 2 h of 5'-GMP addition).

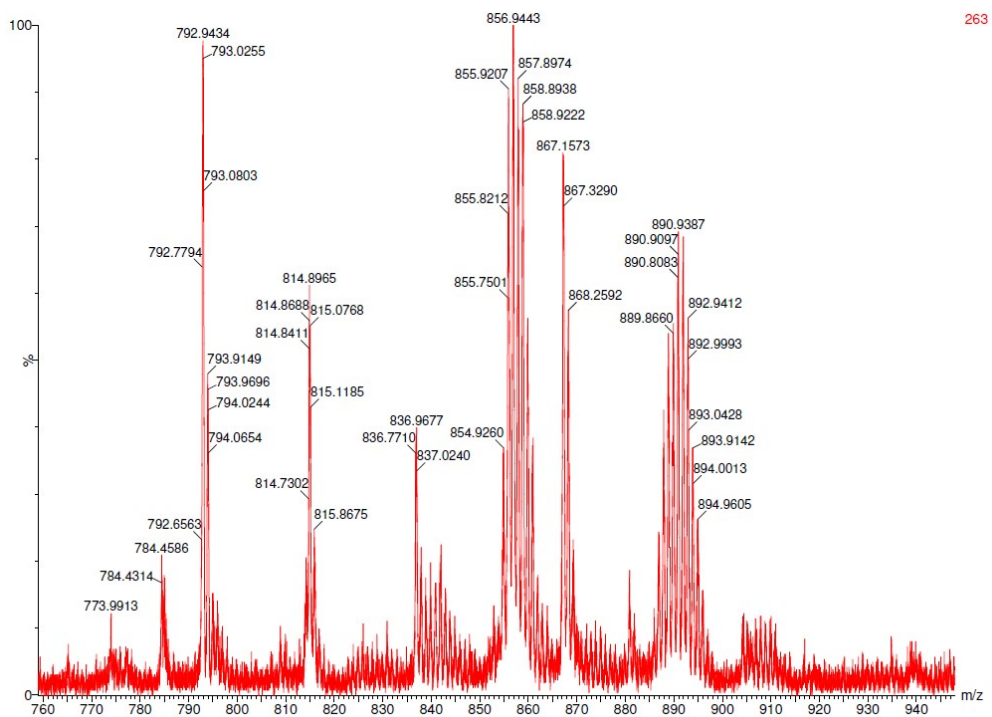


Figure S23. Mass spectrum of the reaction mixture of compound **1** and 5'-GMP

Table S1. Crystal data and structure refinement for complex **1**.

Empirical formula	C ₃₁ H ₂₇ Cl ₅ O ₆ Pt ₂ S ₂
Formula weight	1127.08
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	13.4285(7)
b/Å	15.7599(9)
c/Å	16.4621(9)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å ³	3483.9(3)
Z	4
ρ _{calc} /g/cm ³	2.149
μ/mm ⁻¹	8.568
F(000)	2136.0
Crystal size/mm ³	0.6 × 0.4 × 0.2
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.7 to 52.74
Index ranges	-15 ≤ h ≤ 16, -19 ≤ k ≤ 19, -20 ≤ l ≤ 19
Reflections collected	22167
Independent reflections	7112 [R _{int} = 0.0536, R _{sigma} = 0.0612]
Data/restraints/parameters	7112/0/419
Goodness-of-fit on F ²	1.069
Final R indexes [>=2σ (I)]	R ₁ = 0.0408, wR ₂ = 0.0799
Final R indexes [all data]	R ₁ = 0.0690, wR ₂ = 0.0897
Largest diff. peak/hole / e Å ⁻³	0.64/-1.40
Flack parameter	-0.007(5)