Supporting information

ID-Checker technology for the highly selective macroscale delivery of anticancer agents to the cancer cells

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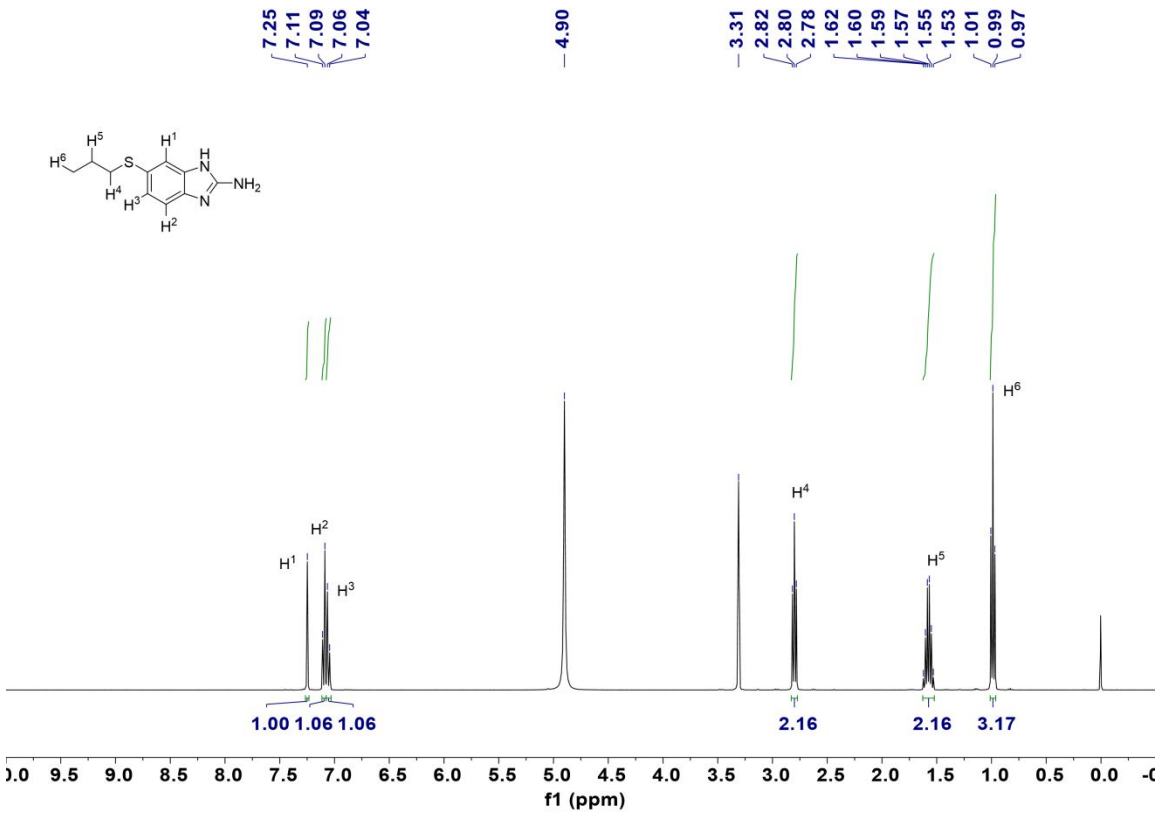


Figure S1. ^{1}H NMR spectrum of **Al-NH$_2$** in CD_3OD.

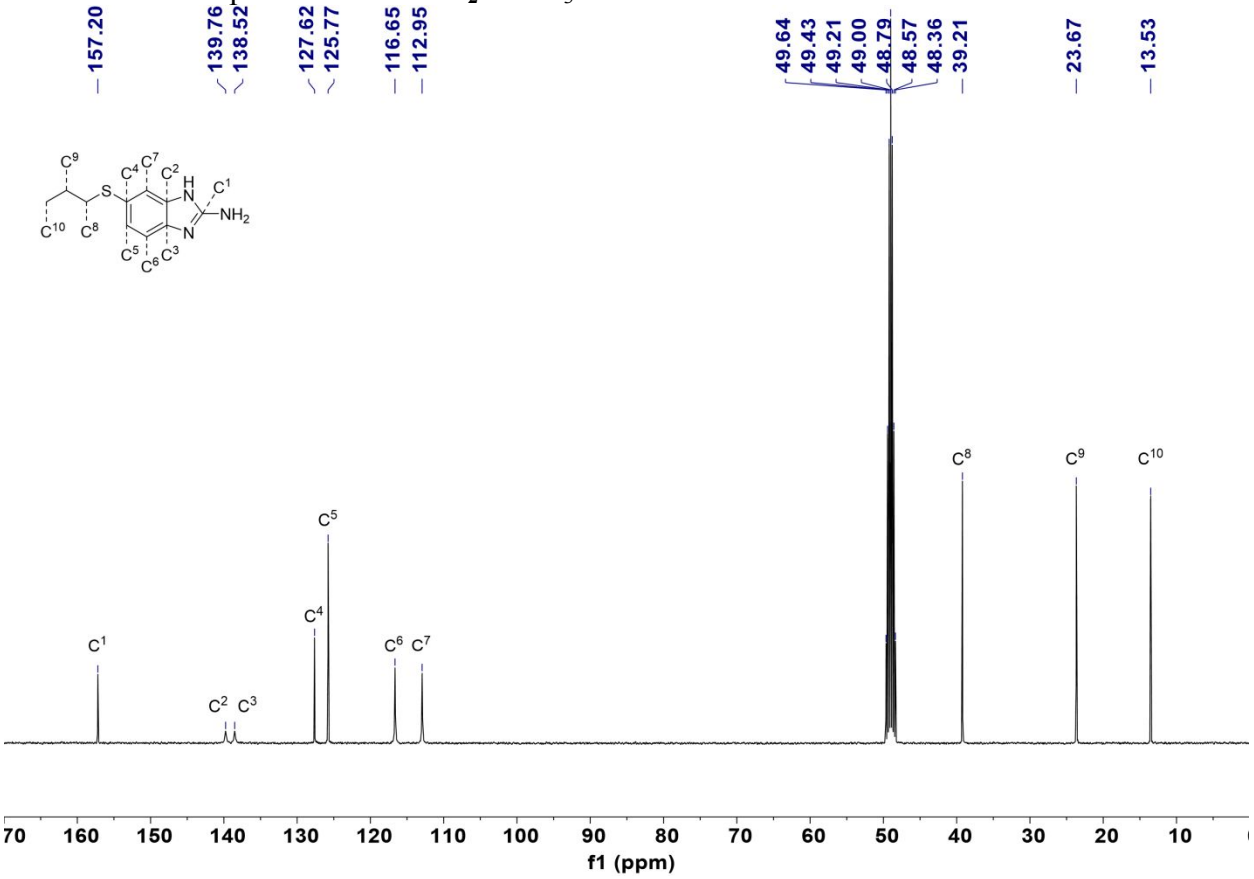


Figure S2. ^{13}C NMR spectrum of **Al-NH$_2$** in CD_3OD.

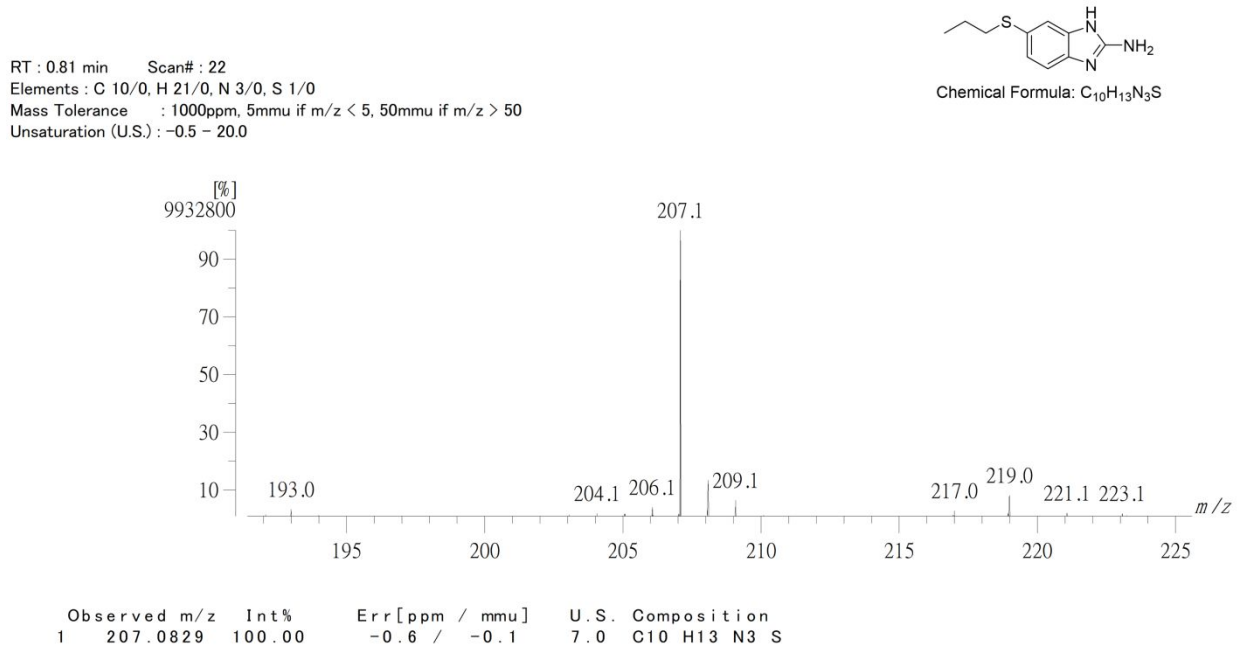


Figure S3. Mass spectrum of **Al-NH_2**.

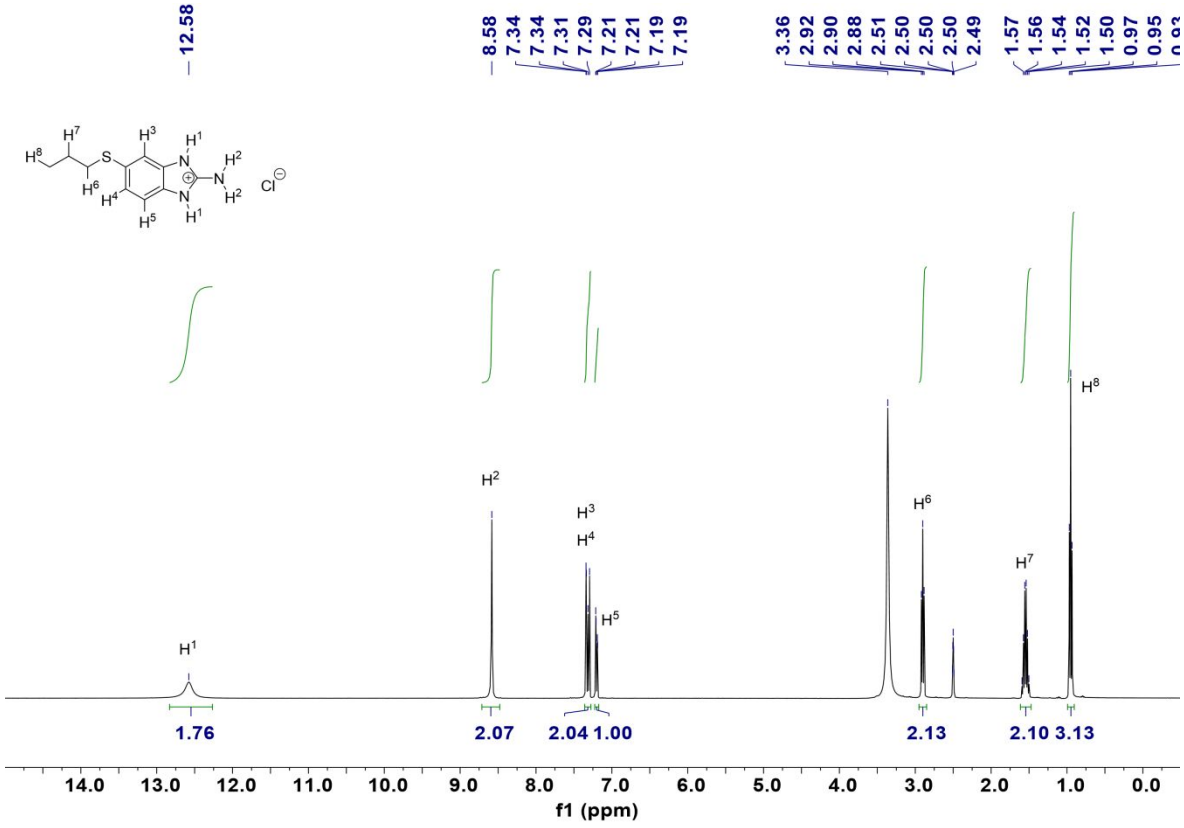


Figure S4. ^{1}H NMR spectrum of **Al-NH_2.HCl** in DMSO-d_6.

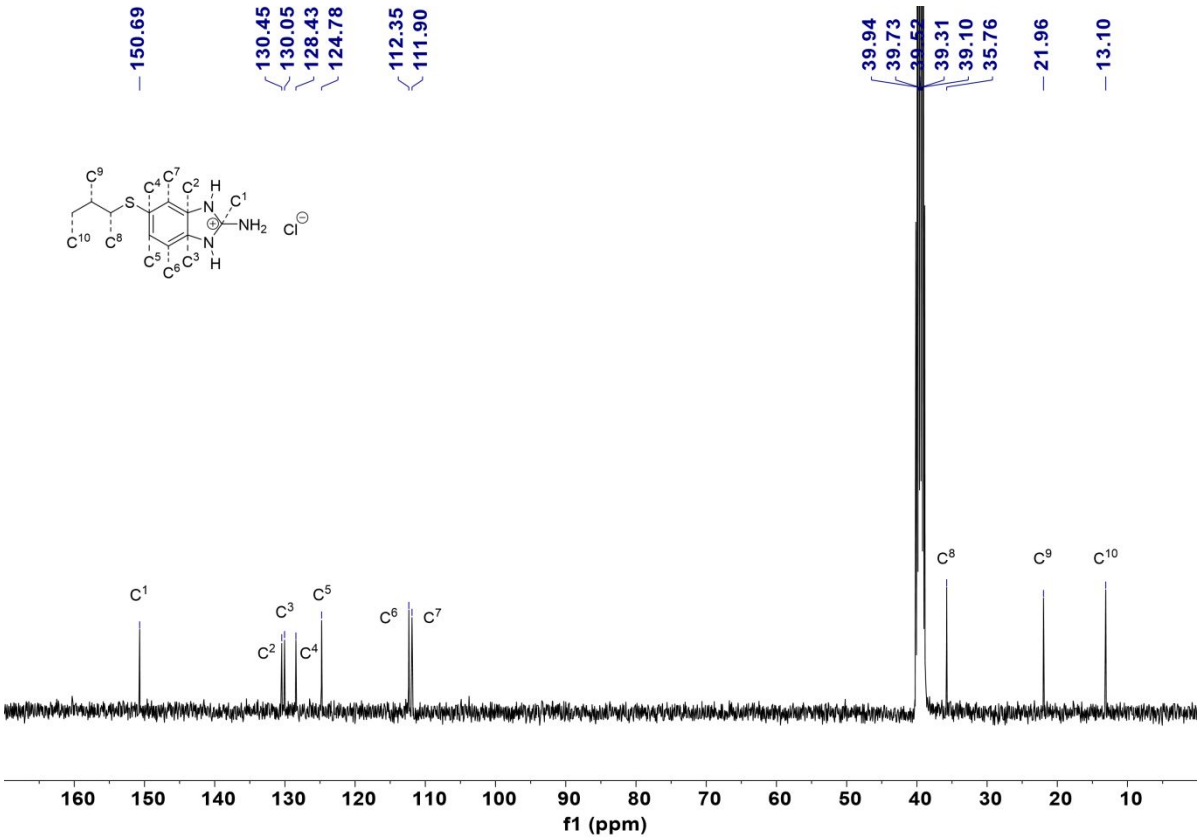


Fig. S5. ^{13}C NMR spectrum of **Al-NH_2.HCl** in DMSO-d_6.

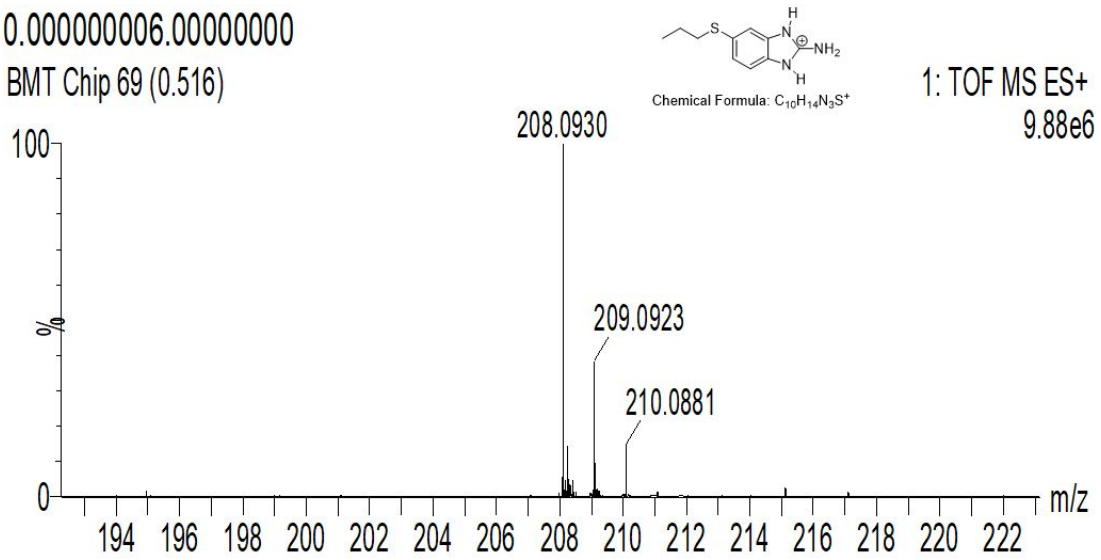


Fig. S6. Mass spectrum of **Al-NH_2.HCl**

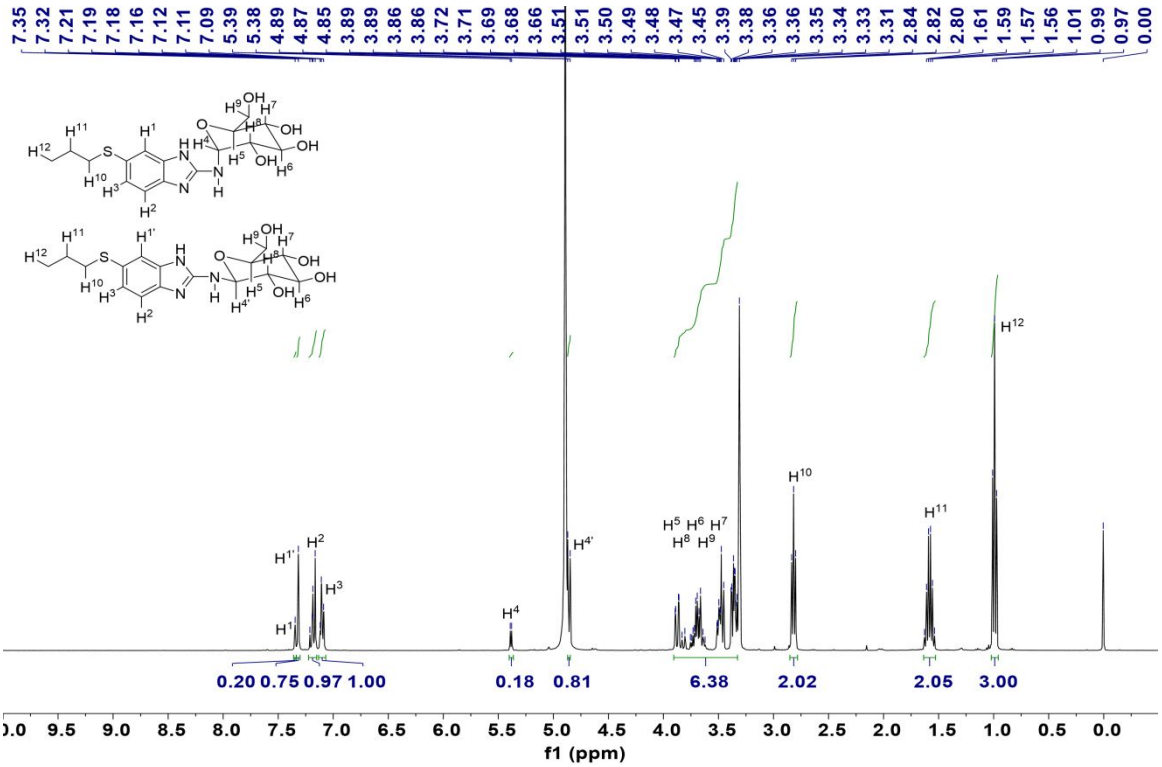


Fig. S7. ^{1}H NMR spectrum of **Al-G** in CD_3OD.

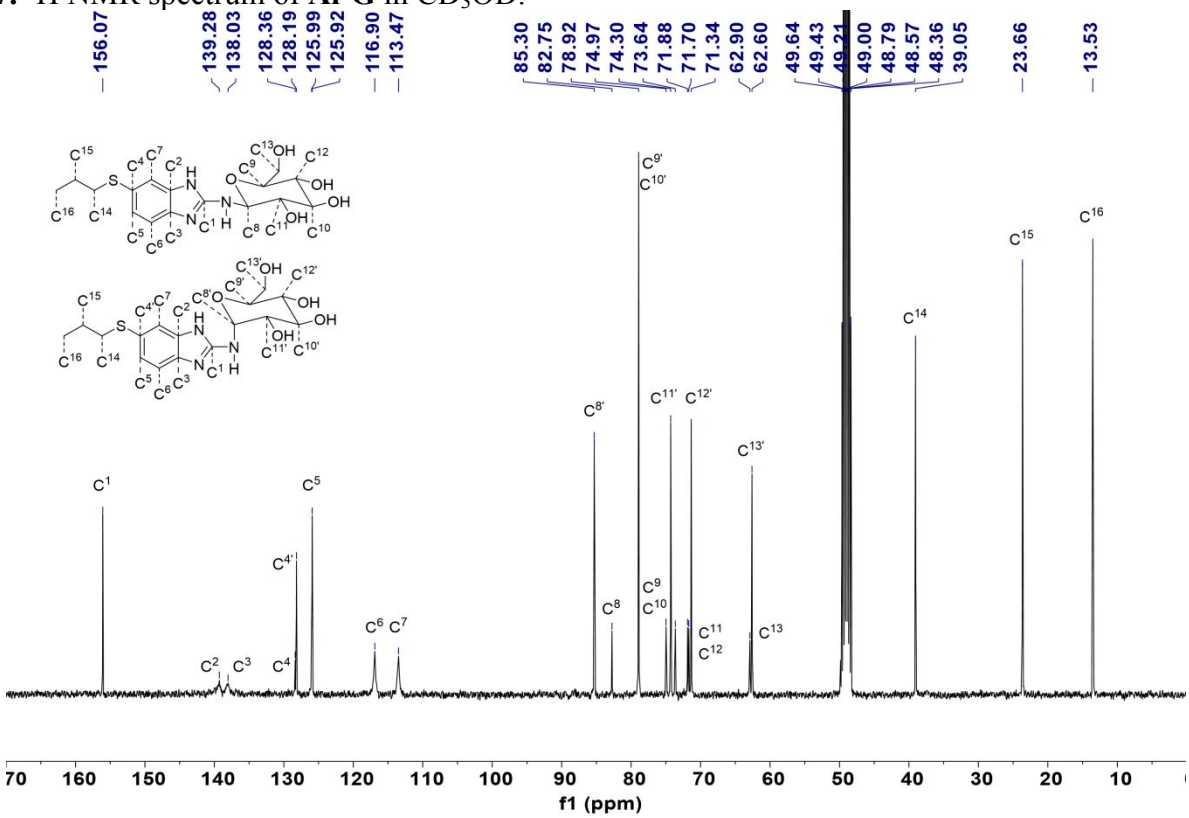


Fig. S8. ^{13}C NMR spectrum of **Al-G** in CD_3OD.

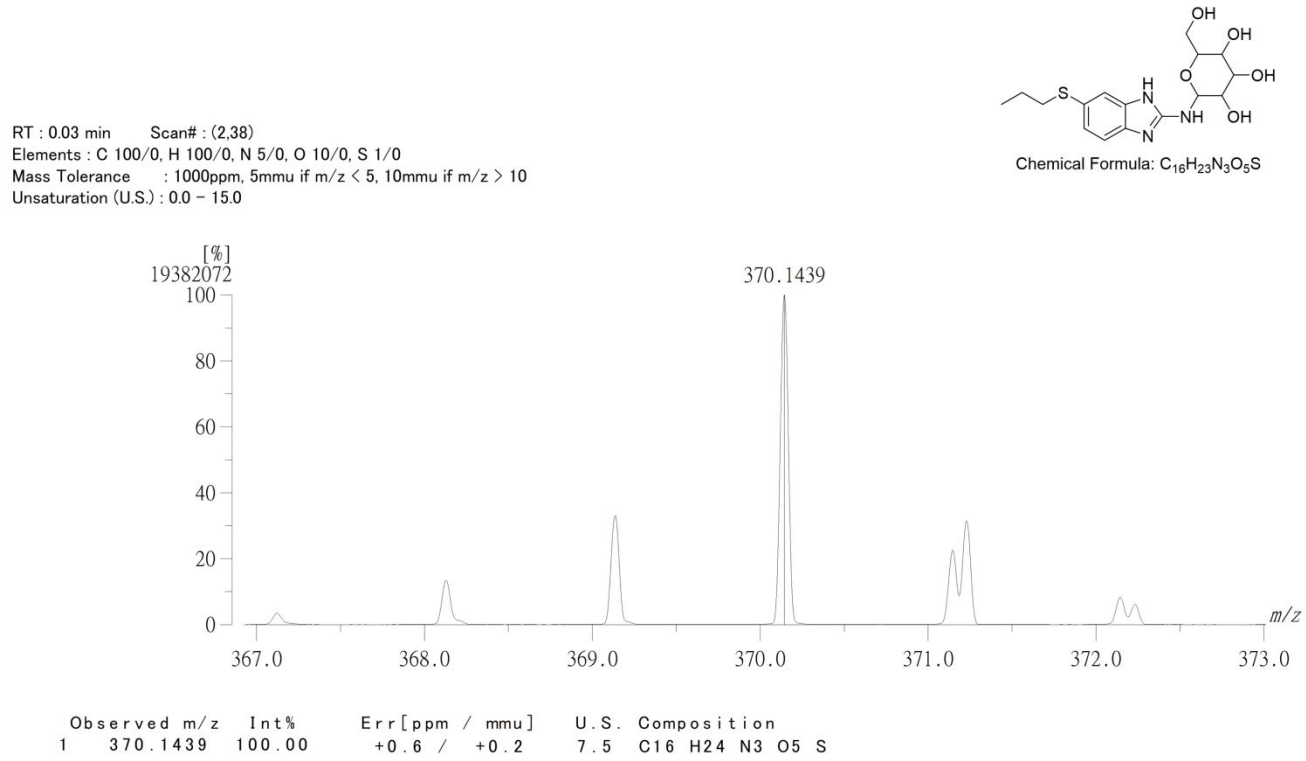
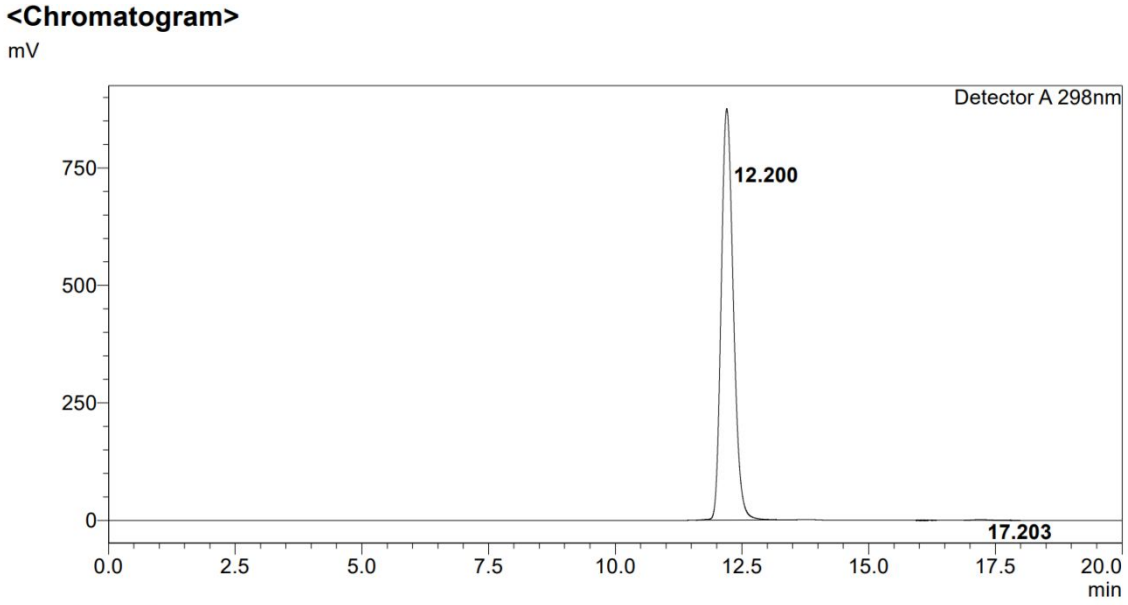


Fig. S9. Mass spectrum of **Al-G**.



<Peak Table>

Detector A 298nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	12.200	874500	99.838	14570874	99.770
2	17.203	1418	0.162	33606	0.230
Total		875918	100.000	14604480	100.000

Fig. S10. HPLC trace for 1mM **Al-NH$_2$** in MeOH (Eluent, 100% MeOH; Pressure, 10 bar; Injection volume, 10 μL; Oven temp., 40 °C).

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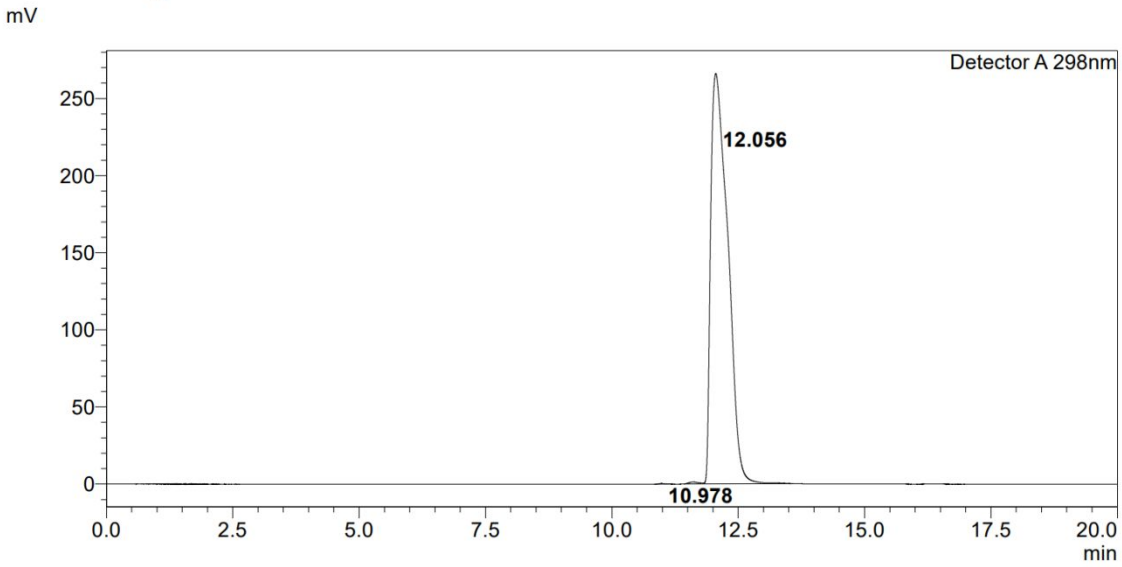


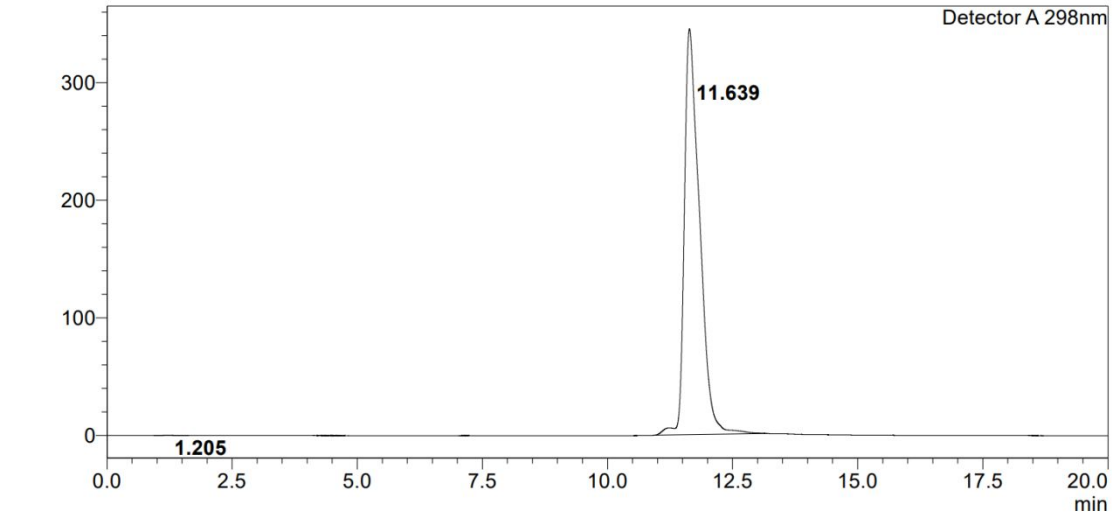
<Peak Table>

Detector A 298nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	10.978	394	0.148	2776	0.044
2	12.056	266026	99.852	6274852	99.956
Total		266420	100.000	6277628	100.000

Fig. S11. HPLC traces for **Al-NH_2.HCl** (Eluent, 100% MeOH; Pressure, 10 bar; Injection volume, 10 μL; Oven temp., 40 °C).

<Chromatogram>



<Peak Table>

Detector A 298nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	1.205	192	0.055	3592	0.049
2	11.639	345059	99.945	7345757	99.951
Total		345251	100.000	7349348	100.000

Fig. S12. HPLC traces for **Al-G** Eluent, 100% MeOH; Pressure, 10 bar; Injection volume, 10 μL; Oven temp., 40 °C).

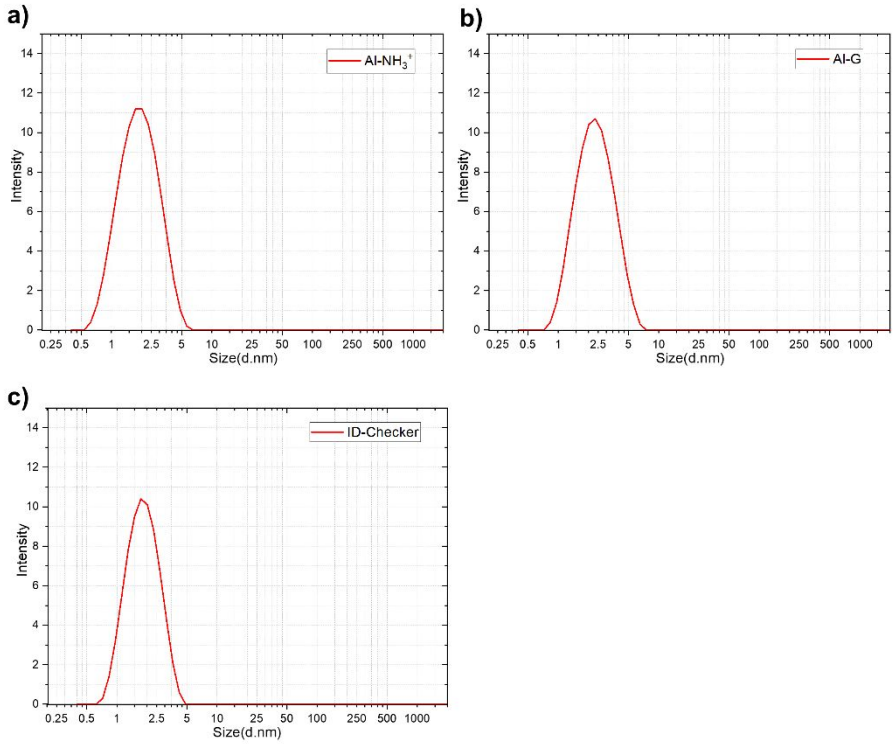


Figure S13. DLS data representing the particle size of a) **Al-NH_3^+** aggregate, b) **Al-G aggregate**, and c) **ID-Checker**

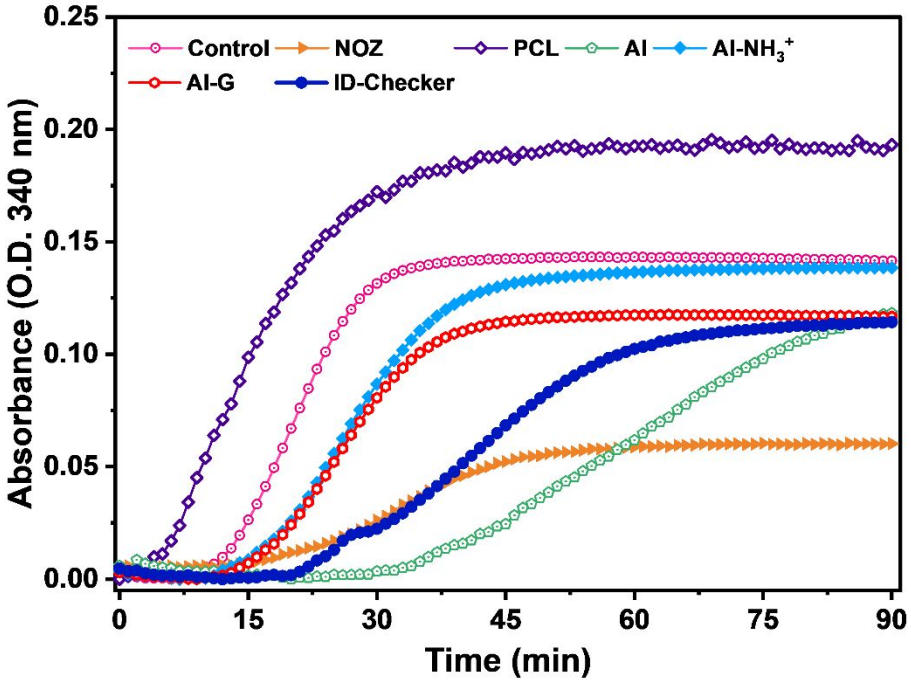


Fig. S14. Effects of NOZ, PCL, **Al**, **Al-NH_3^+** aggregate, **Al-G** aggregate, and **ID-Checker** on tubulin polymerization. Effect of **ID-Checker** on tubulin polymerization. Polymerization of purified tubulin into microtubules was measured using spectrometer over 90 min at 1 min interval by incubating it at 37 °C in the absence (control) or presence of 0.20 μM **ID-Checker**, 20 μM NOZ, 20 μM PCL, 20 μM **Al**, 20 μM **Al-NH_3^+** aggregate, and 20 μM **Al-G** aggregate.

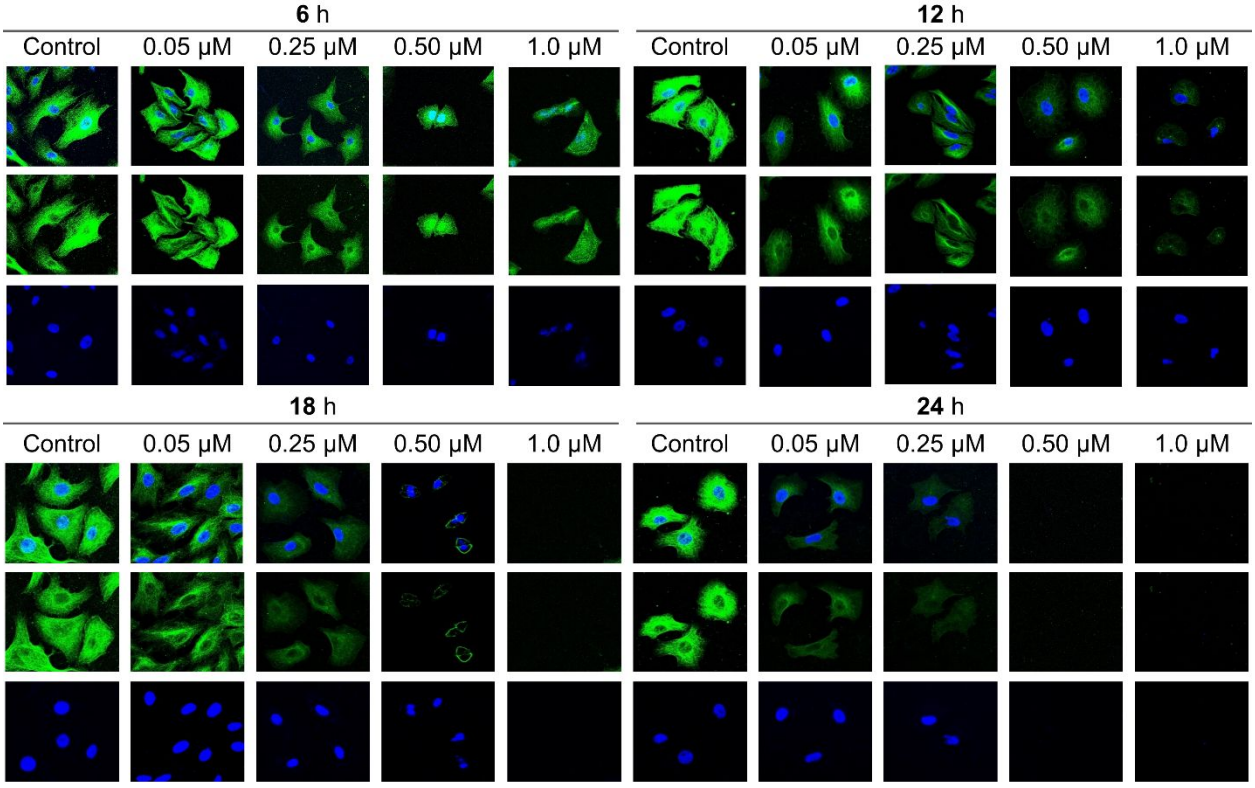


Fig. S15. Immunofluorescence staining of microtubules in A549 cells. Cells were treated with vehicle (0.9% saline), 0.05, 0.25, 0.50, and 1.0 μM **ID-Checker** for 6, 12, 18, and 24 h. Cells were incubated with anti-α-tubulin antibody followed by anti-mouse IgG/FITC antibody (green fluorescence) to stain the microtubules, and nuclei were stained by subsequent incubation of cells with (DAPI, blue fluorescence). Bottom, DAPI; middle, microtubule network; top, merged images observed by confocal microscopy.

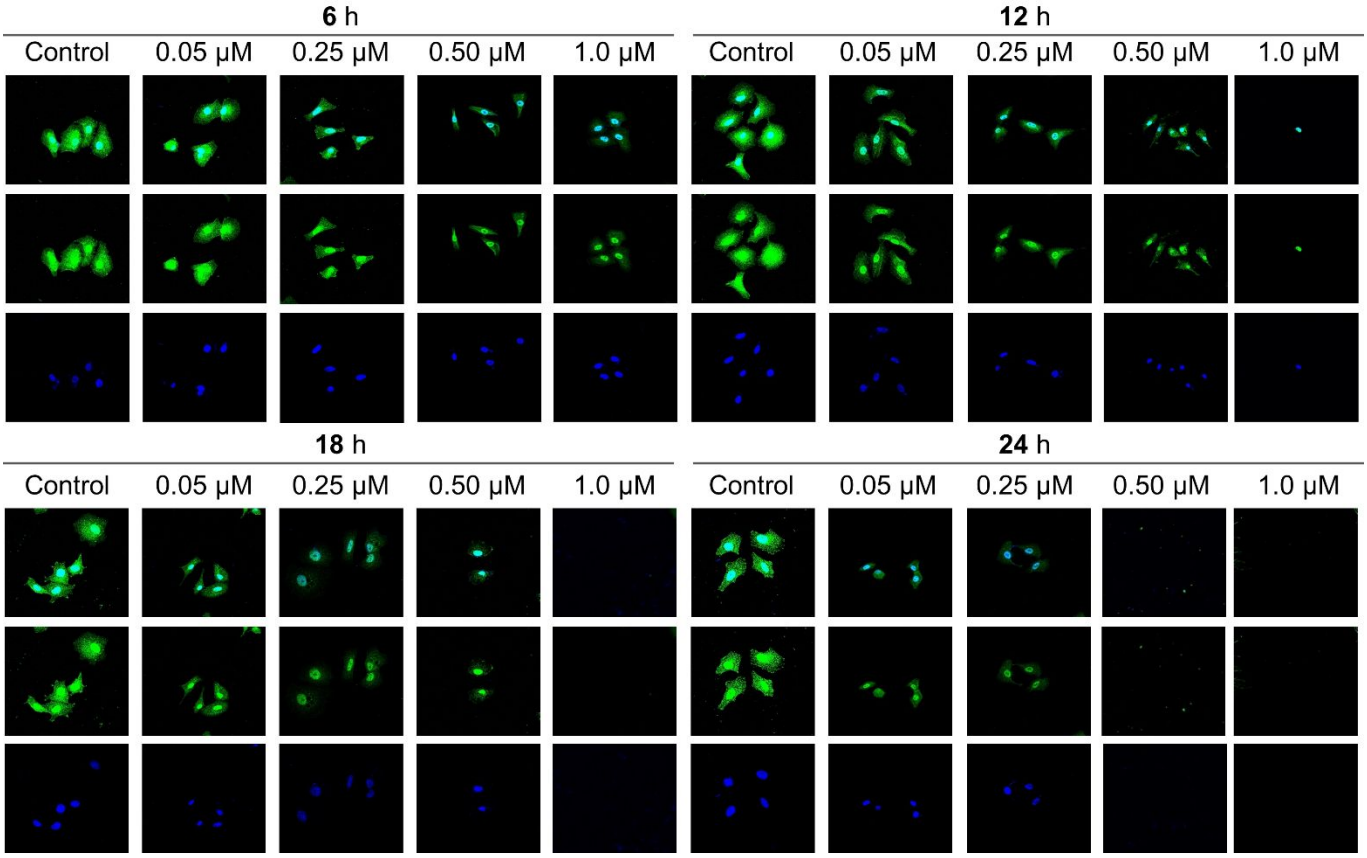


Fig. S16. Immunofluorescence staining of GLUT1 channels in A549 cells. Cells were treated with vehicle (0.9% saline), 0.05, 0.25, 0.50 and 1.0 μM **ID-Checker** for 6, 12, 18, and 24 h. Cells were incubated with rabbit anti-GLUT1 antibody followed by donkey anti-rabbit IgG/ALEXA488 antibody (green fluorescence) to stain the GLUT channels and nuclei were stained by subsequent incubation of cells with DAPI (blue fluorescence). Bottom, DAPI; middle, GLUT channels; top, merged images observed by confocal microscopy.

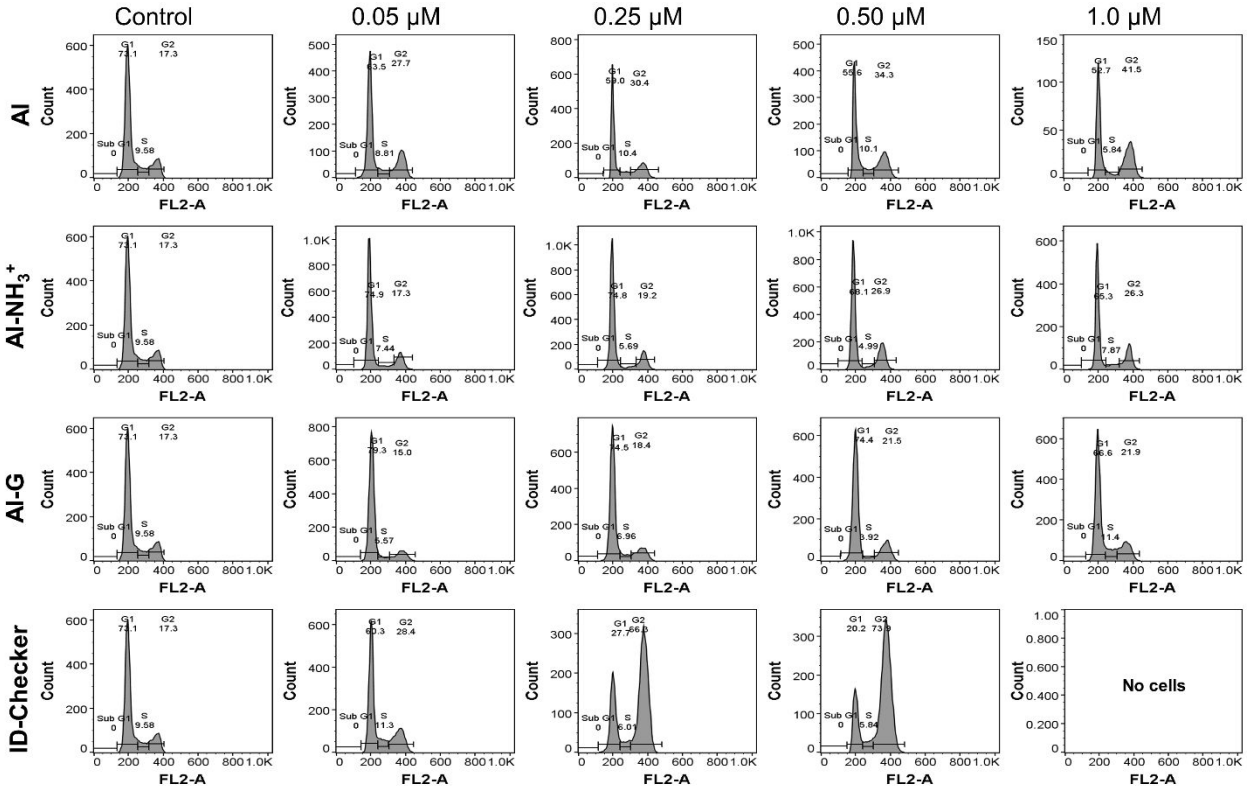


Fig. S17. Effects on the cell cycle distribution of MCF-7 cells upon treatment with **Al**, **AL-NH_3^+**, **Al-G**, and **ID-Checker** at various concentrations (0, 0.05, 0.25, 0.50, and 1.0 μM) 24 h followed by staining with PI to determine the proportion of DNA by flow cytometry.

Table S1. Body weight of experimental animals (g)

Day	G1	G2	G3	G4
0	19.10 ± 0.16	19.00 ± 0.16	19.00 ± 0.16	19.00 ± 0.28
11	19.35 ± 0.20	19.15 ± 0.20	18.85 ± 0.18	19.00 ± 0.13

Table S2. Docking scores for **Al**, **Al-NH_3^+**, and **Al-G** for binding with tubulin in the colchicine and nocodazole binding sites.

Compound	CBS		NBS	
	Glide Score (kcal mol^{-1})	Glide Energy (kcal mol^{-1})	Glide Score (kcal mol^{-1})	Glide Energy (kcal mol^{-1})
Al	-6.64	-49.0	-7.31	-46.9
Al-NH_3^+	-6.44	-33.3	-7.14	-30.7
Al-G	-6.20	-30.9	-6.61	-34.5

CBS, colchicine binding site; NBS, nocodazole binding site

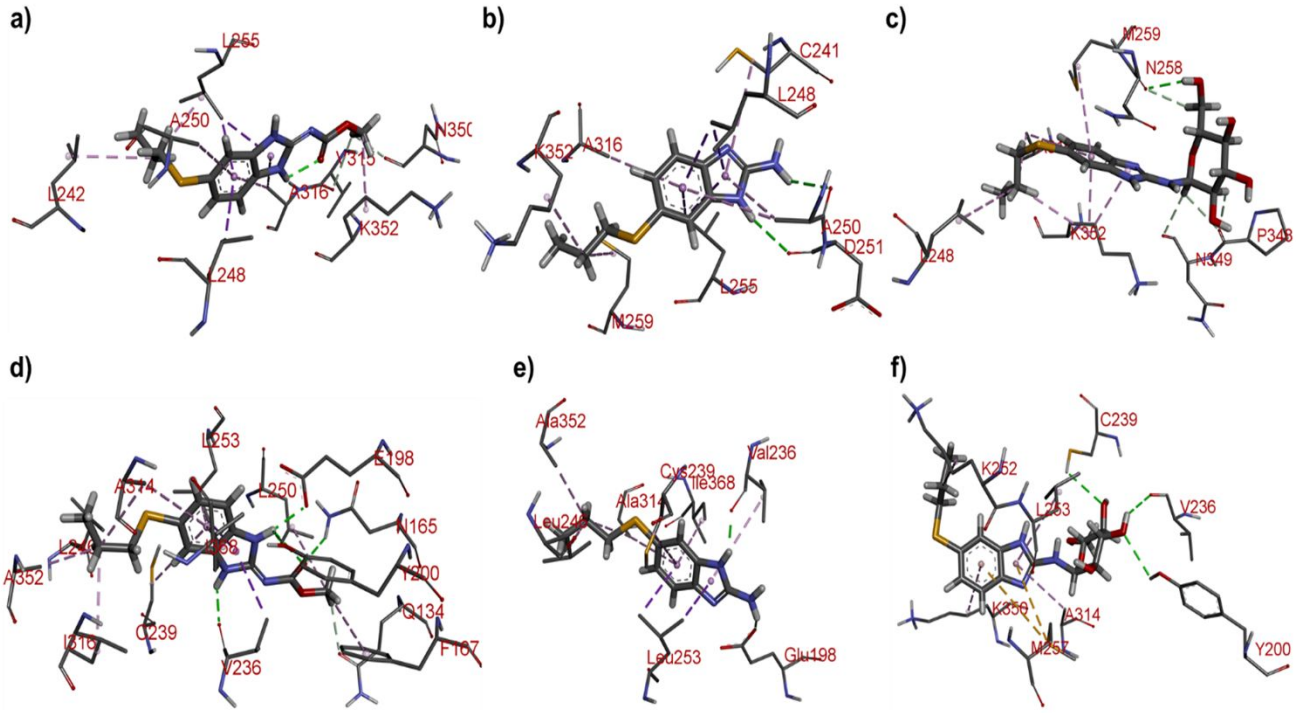


Fig. S18. The docking poses of a) **Al**, b) **AL-NH_3^+**, c) **Al-G**, in colchicine binding site (PDB ID: 4O2B) and d) **Al**, e) **Al-NH_3^+**, f) **Al-G** in the nocodazole binding site of tubulin (PDB ID: 5CA1).