

Supporting information

For

Enhancement of Cell Uptake and Antitumor Activity of Selenadiazole Derivatives through Interaction and Delivery by Serum Albumin

Results

Table S1

Crystal and experimental data of compound **4c**, **4d** and **4e**.

Compound	4c	4d	4e
Formula weight	262.10	262.10	250.32
Temperature (K)	293	293	293
Wavelength (Å)	1.54184	1.54184	1.54184
Crystal system	Monoclinic	monoclinic	monoclinic
Space group	P2(1)/n	P2(1)/n	P2(1)/n
a/Å	21.9362 (9)	16.3500 (7)	23.715 (3)
b /Å	4.53698 (16)	4.63869 (19)	4.6936 (3)
c /Å	23.8161 (11)	14.6206 (6)	24.378 (3)
α°	90	90	90
β°	112.119 (5)	102.521 (4)	117.245 (14)
γ°	90	90	90
Z	8	4	8
D _c /g cm ⁻³	1.586	1.608	1.559
Absorption coefficient mm ⁻¹	4.501	4.566	4.127
F(000)	1016.0	508.0	1136.0
Goodness-of-fit on F ²	1.083	0.838	1.053
Data / parameters	3471/271	1718/141	3822/291
R ₁ , wR ₂ [I>2σ(I)] ^a	0.0535, 0.1531	0.0353, 0.1066	0.0596, 0.1425
R ₁ , wR ₂ (all data) ^a	0.0652, 0.1373	0.0303, 0.0784	0.0484, 0.1347

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|, wR_2 = [\sum w(|F_o| - |F_c|)^2]^{1/2}, w = [\sigma^2(F_o)^2 + (0.1(\max(0, F_o^2) + 2 F_c^2/3))^2]^{-1}$$

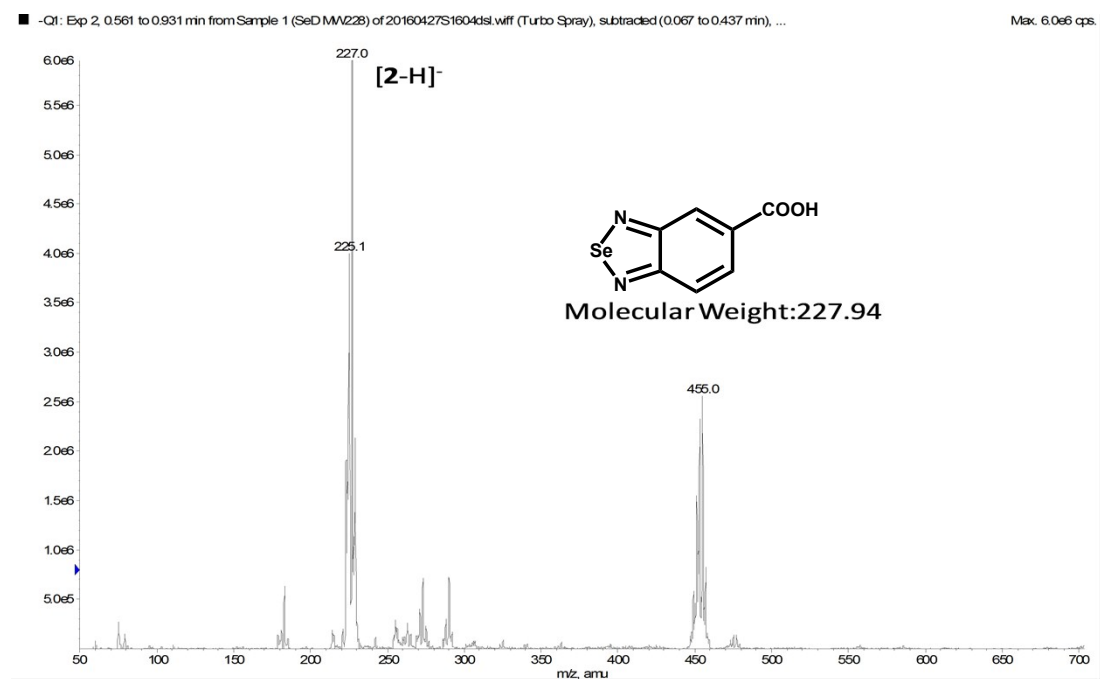


Figure S1. The ESI-MS spectrum of **2**.

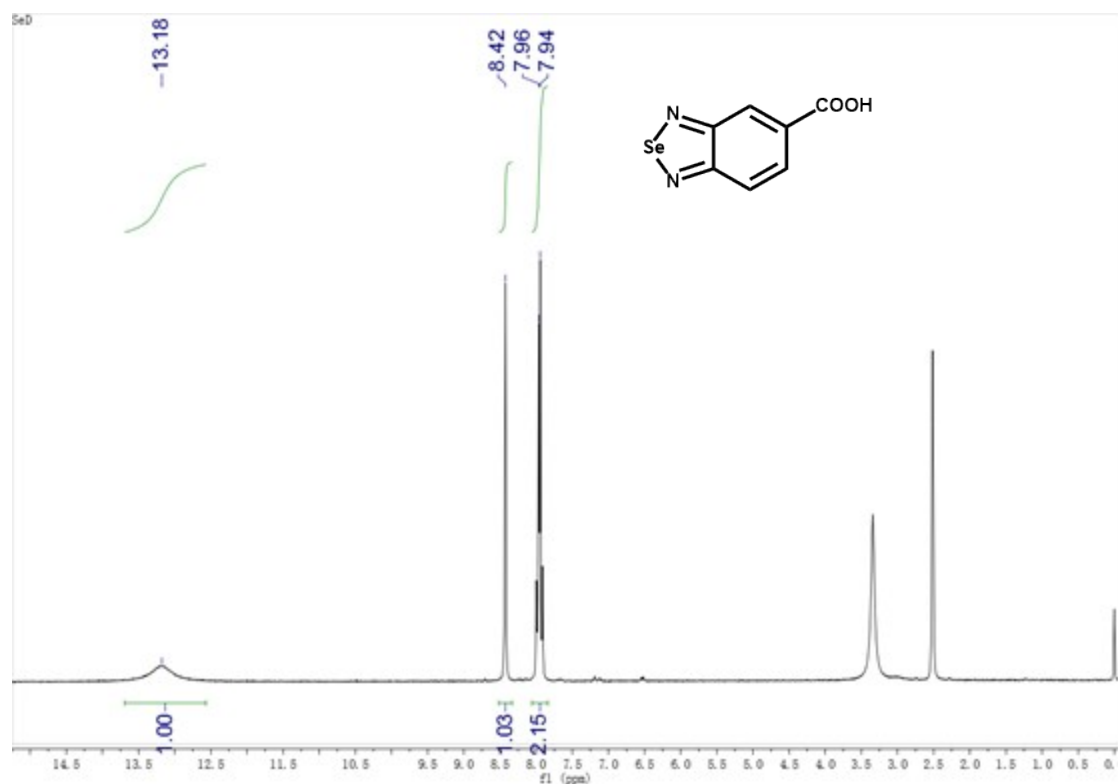


Figure S2. The ¹H NMR spectra of **2**.

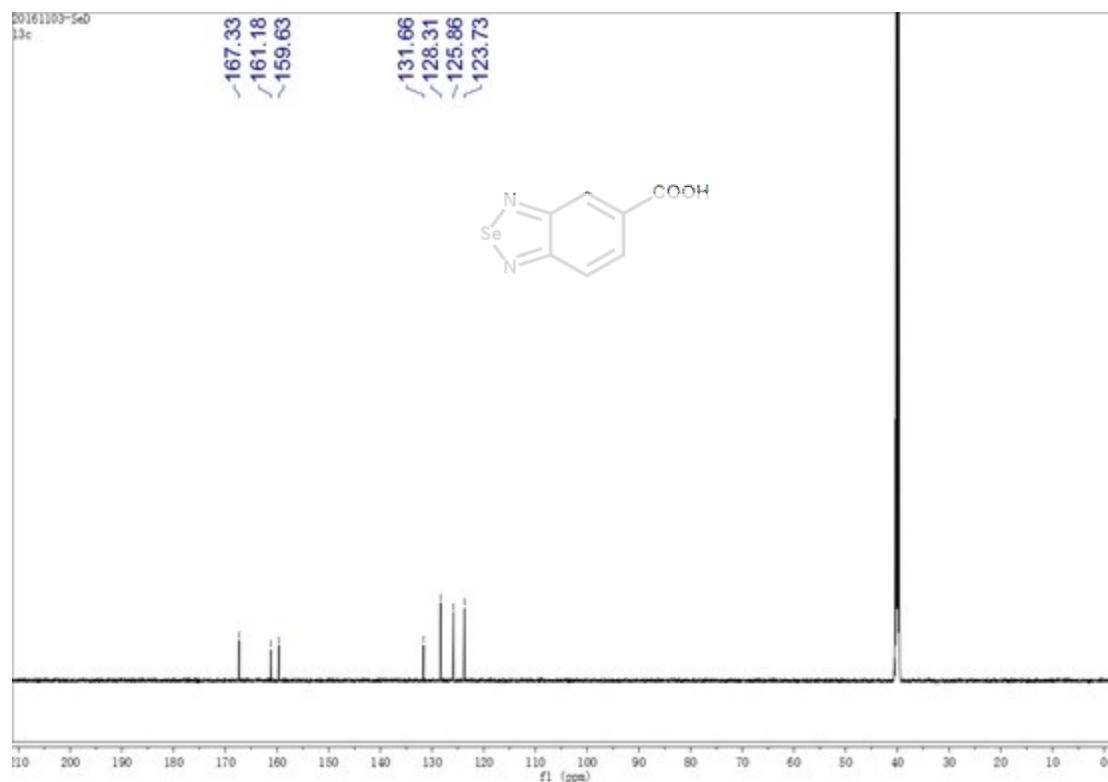


Figure S3. The ^{13}C NMR spectra of **2**.

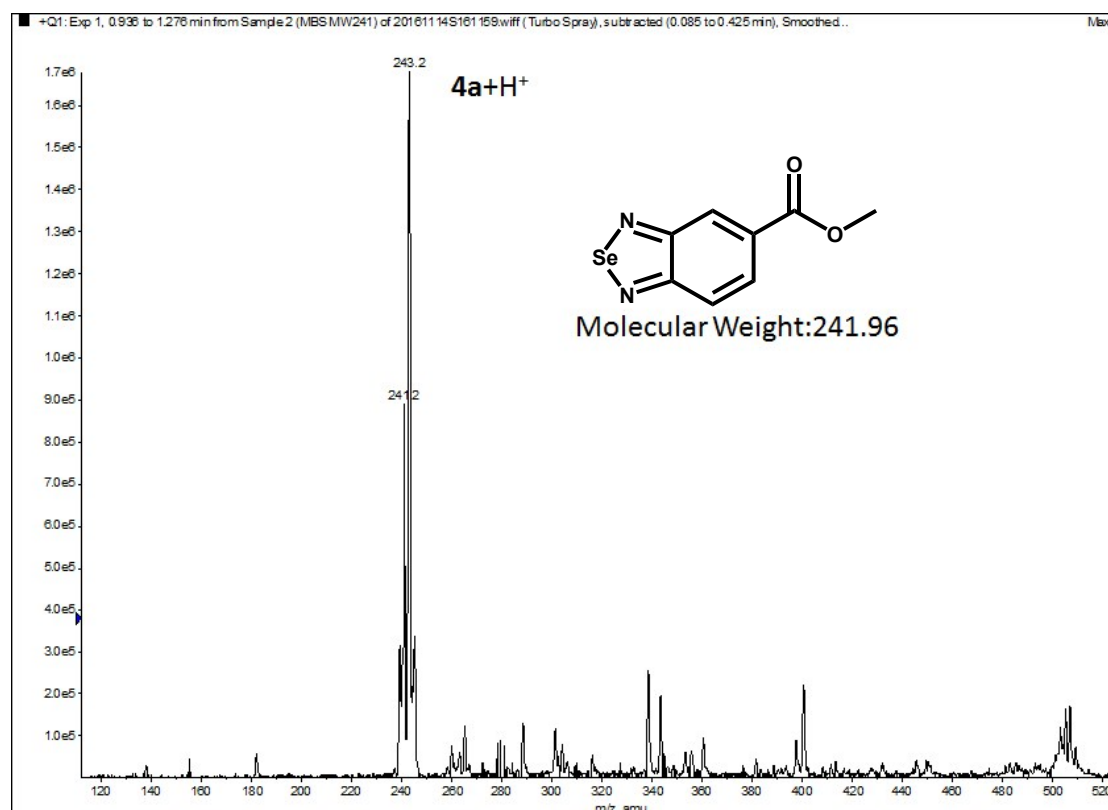


Figure S4. The ESI-MS spectrum of **4a**.

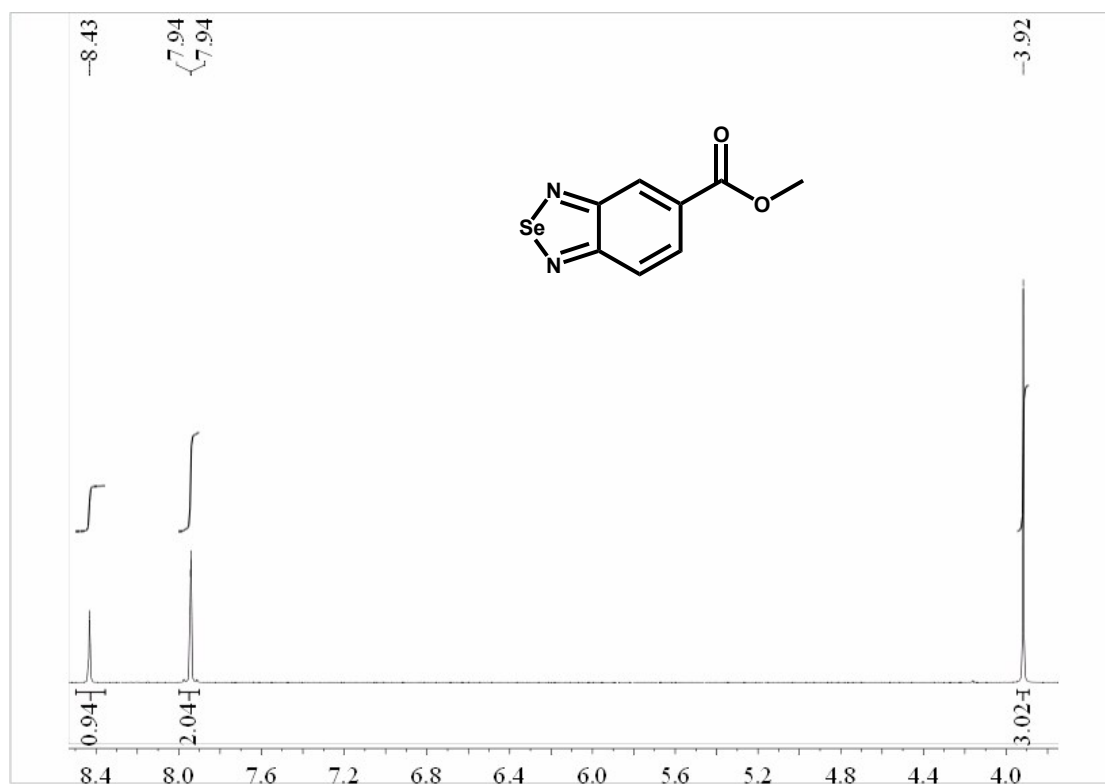


Figure S5. The ^1H NMR spectra of 4a.

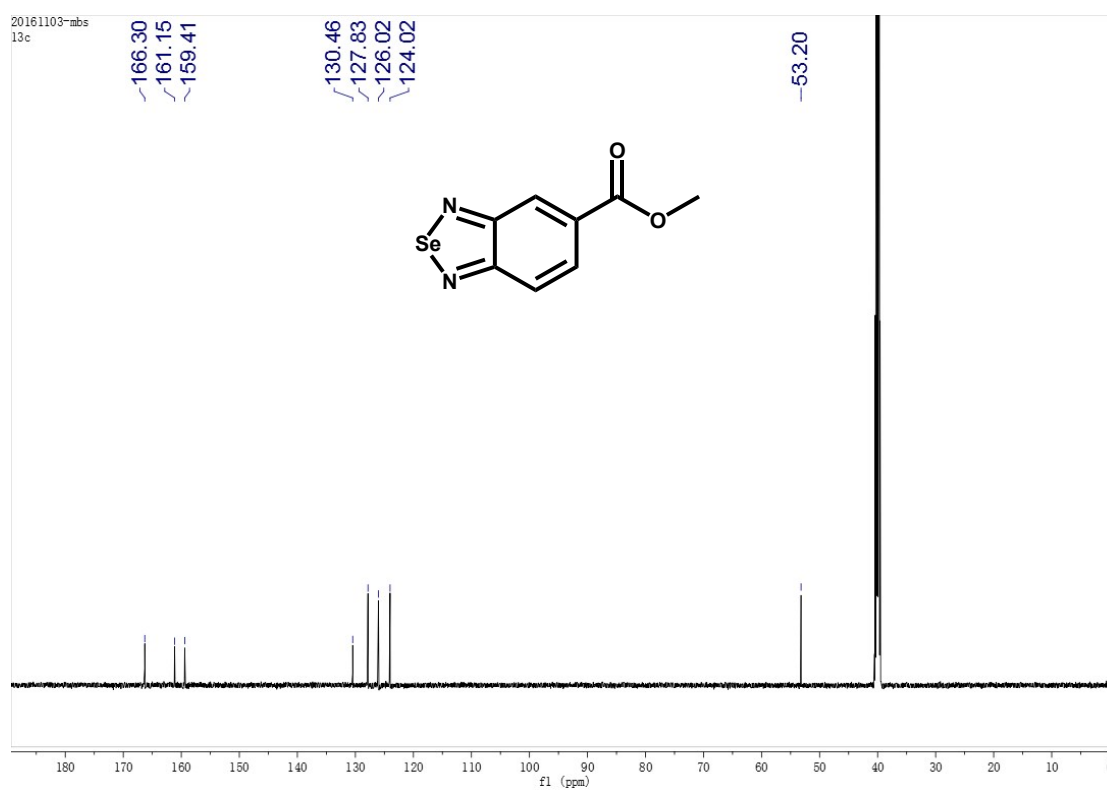


Figure S6. The ^{13}C NMR spectra of 4a.

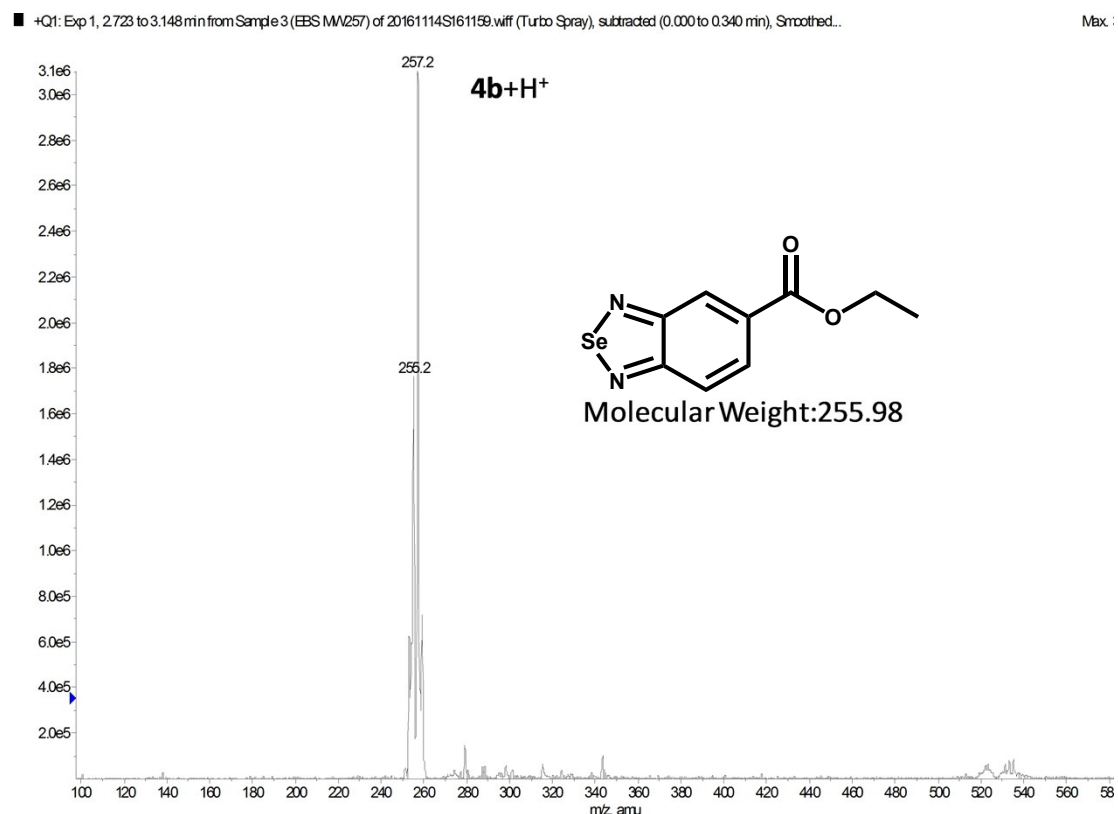


Figure S7. The ESI-MS spectrum of **4b**.

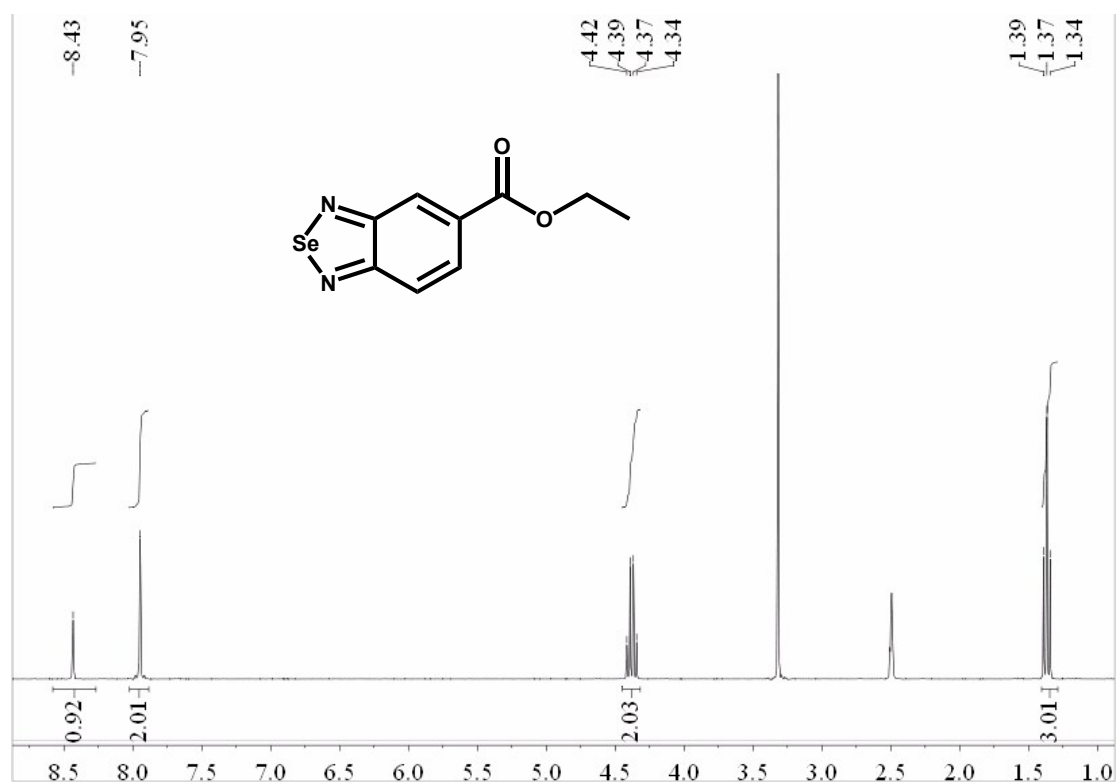


Figure S8. The ¹H NMR spectra of **4b**.

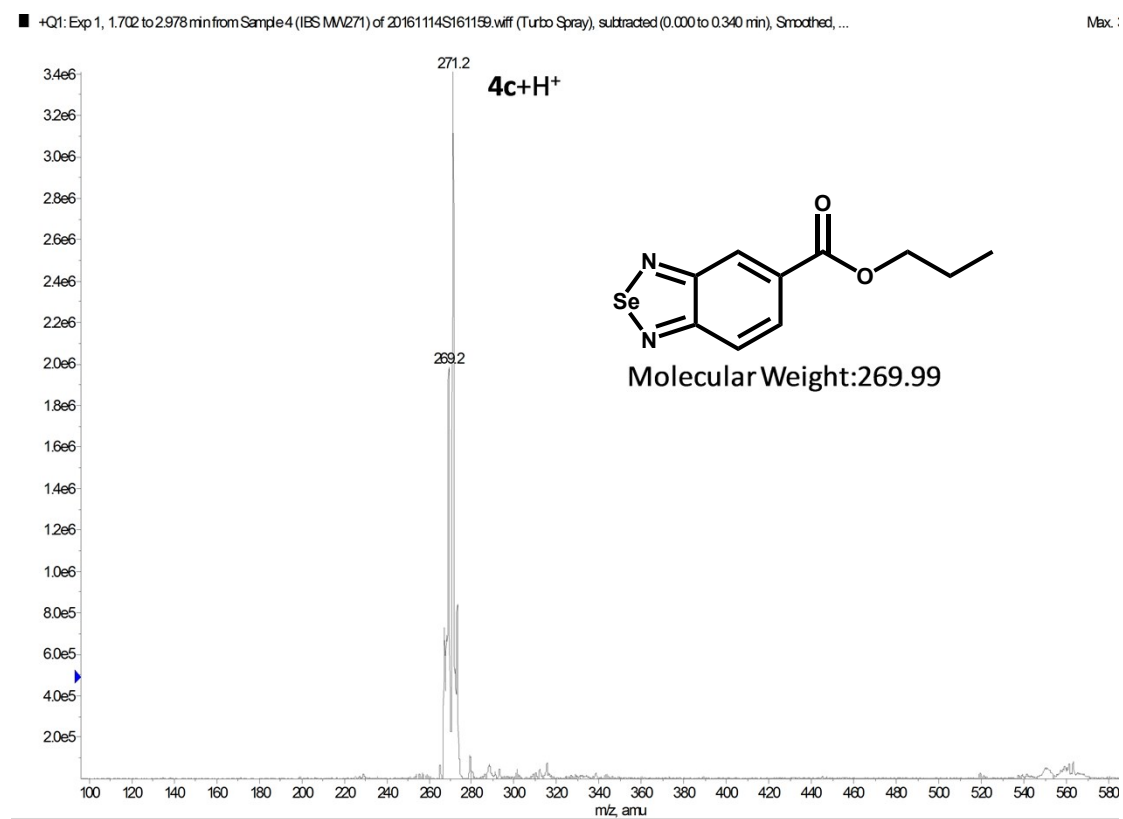


Figure S10. The ESI-MS spectrum of **4c**.

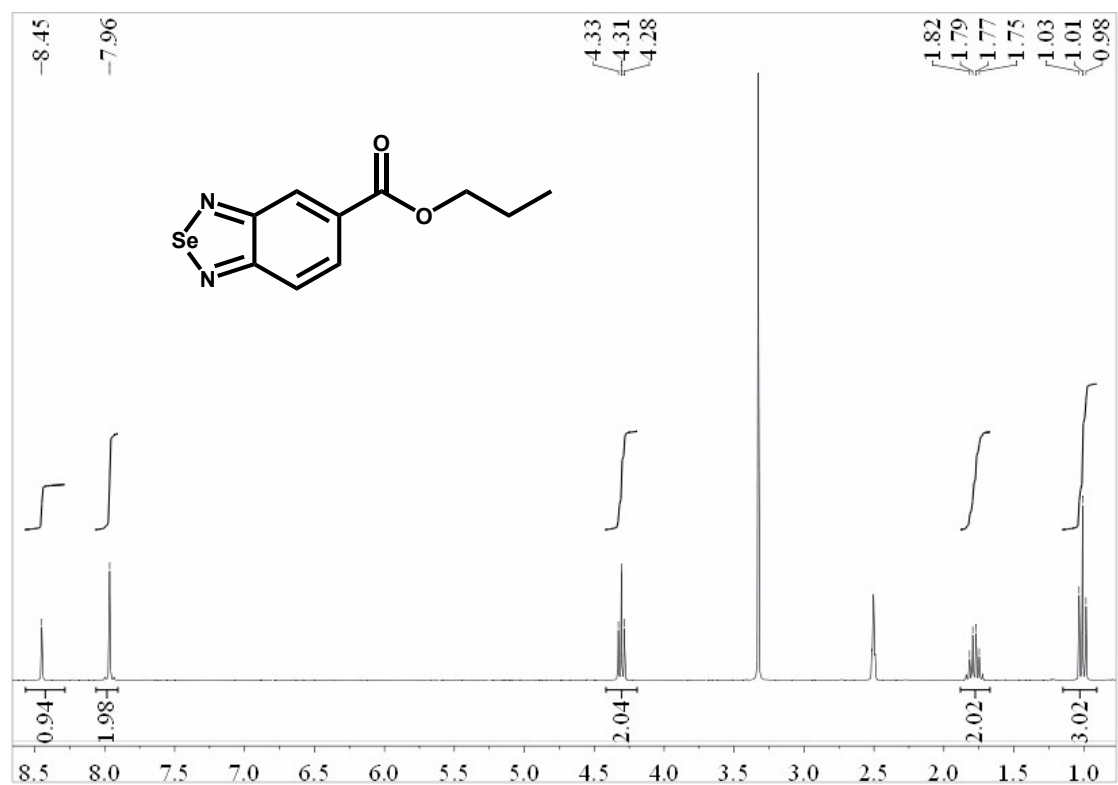


Figure S11. The ^1H NMR spectra of **4c**.



Figure S12. The ^{13}C NMR spectra of **4c**.

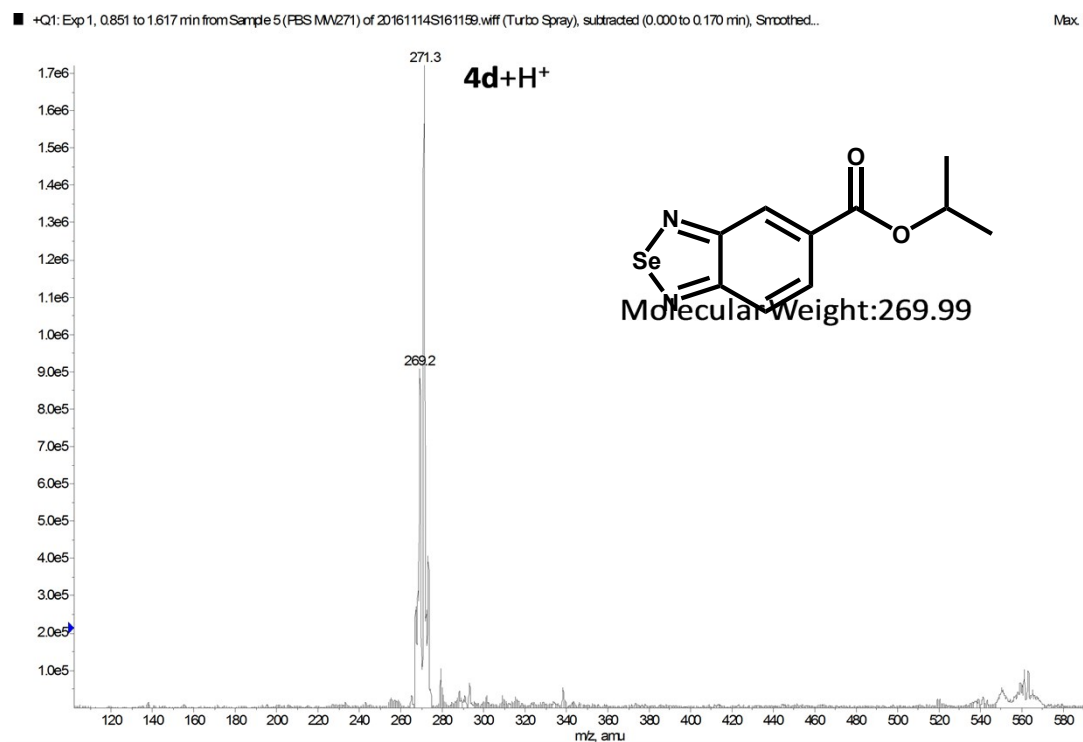


Figure S13. The ESI-MS spectrum of **4d**.

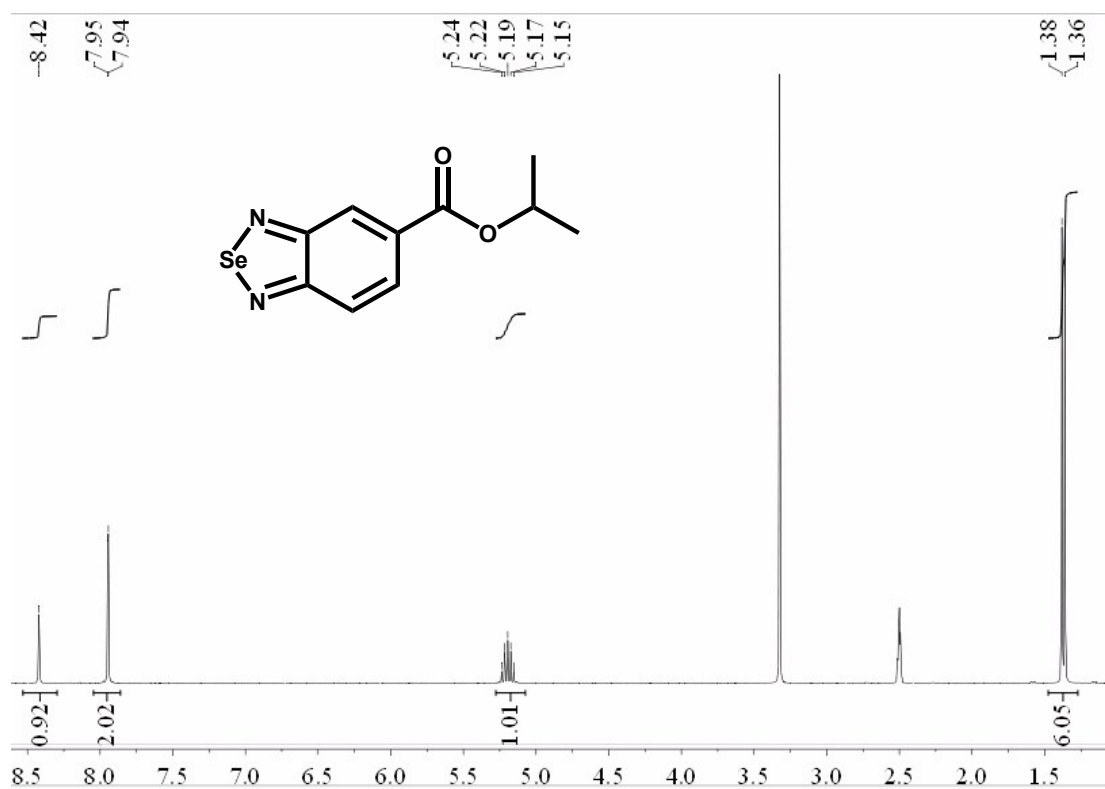


Figure S14. The ¹H NMR spectra of **4d**.



Figure S15. The ^{13}C NMR spectra of **4d**.

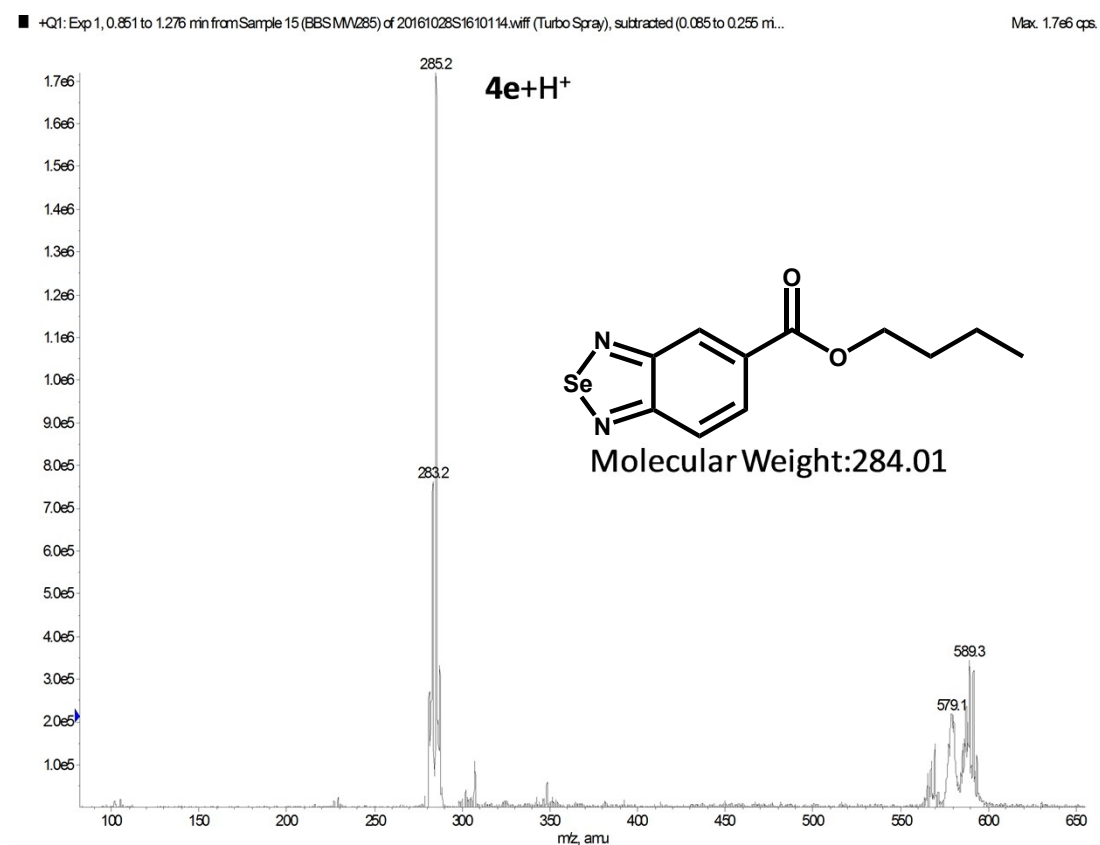


Figure S16. The ESI-MS spectrum of **4e**.

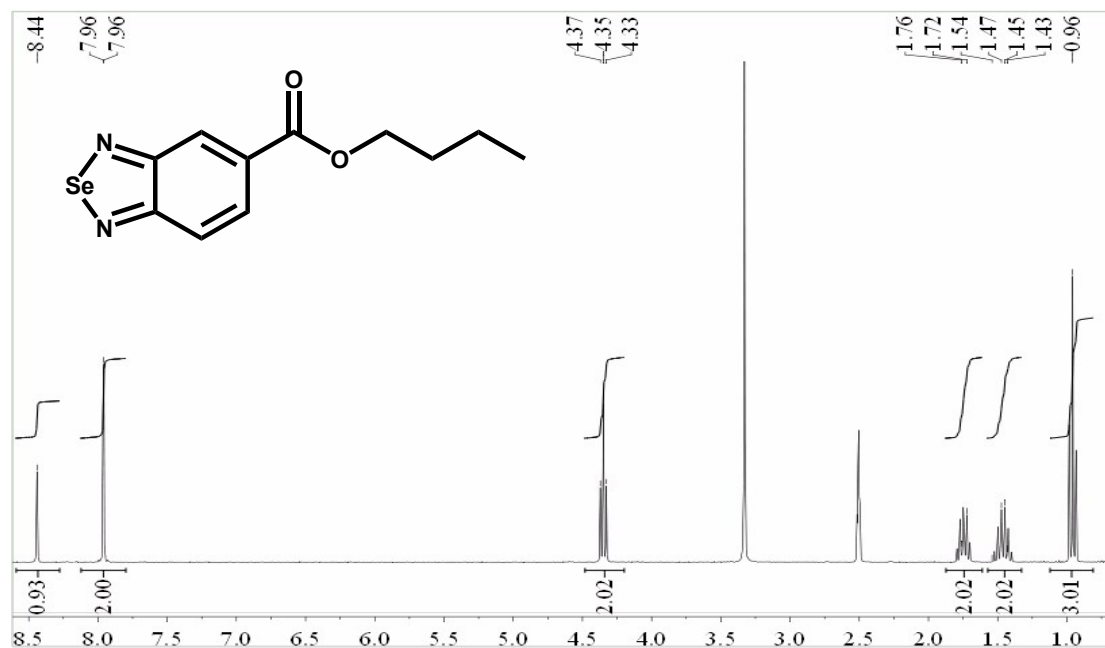


Figure S17. The ¹H NMR spectra of **4e**.

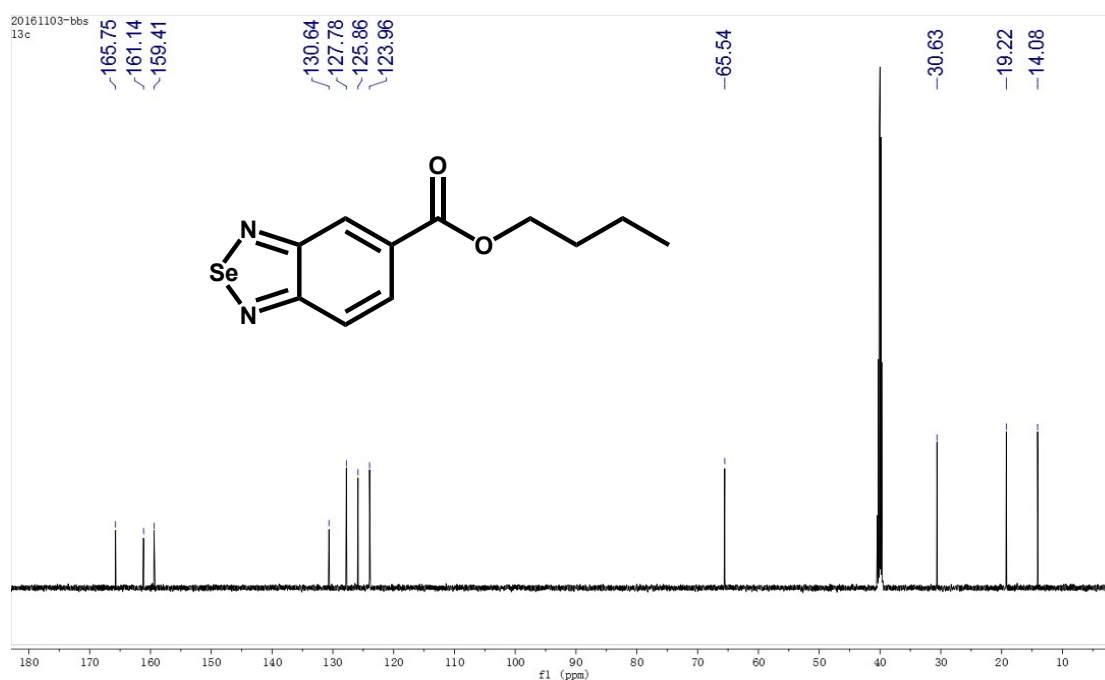


Figure S18. The ¹³C NMR spectra of **4e**.

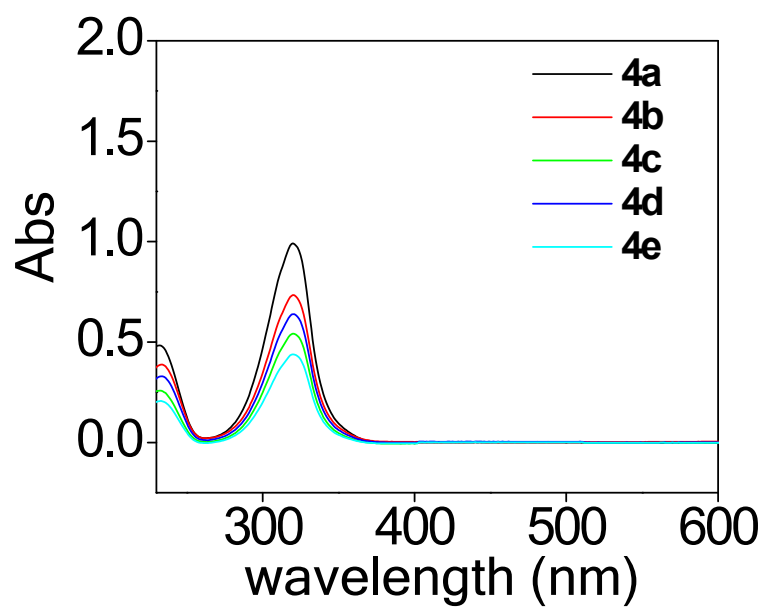


Figure S19. The absorption spectra of **4a**, **4b**, **4c**, **4d** and **4e**.

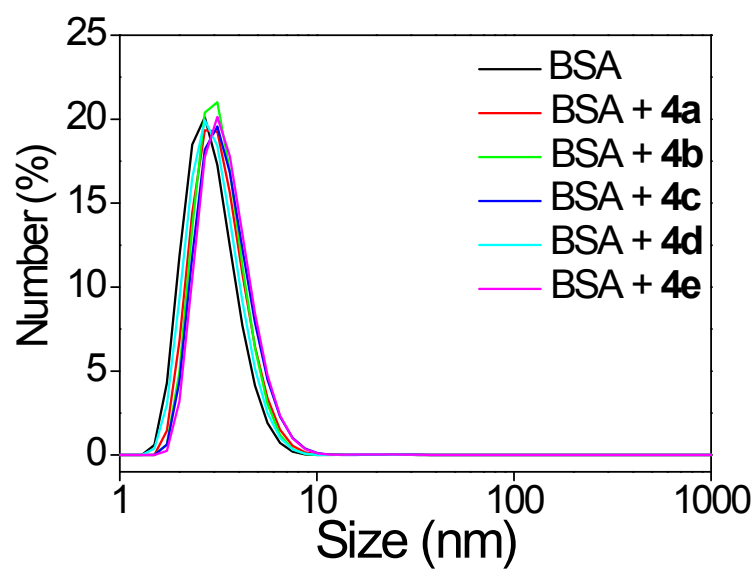


Figure S20. The size distribution of serum albumin (50 μ M) after incubation in DMEM for 72 h.