Supplementary Information

Towards Cancer Cell-Specific Phototoxic Organometallic Rhenium(I) Complexes

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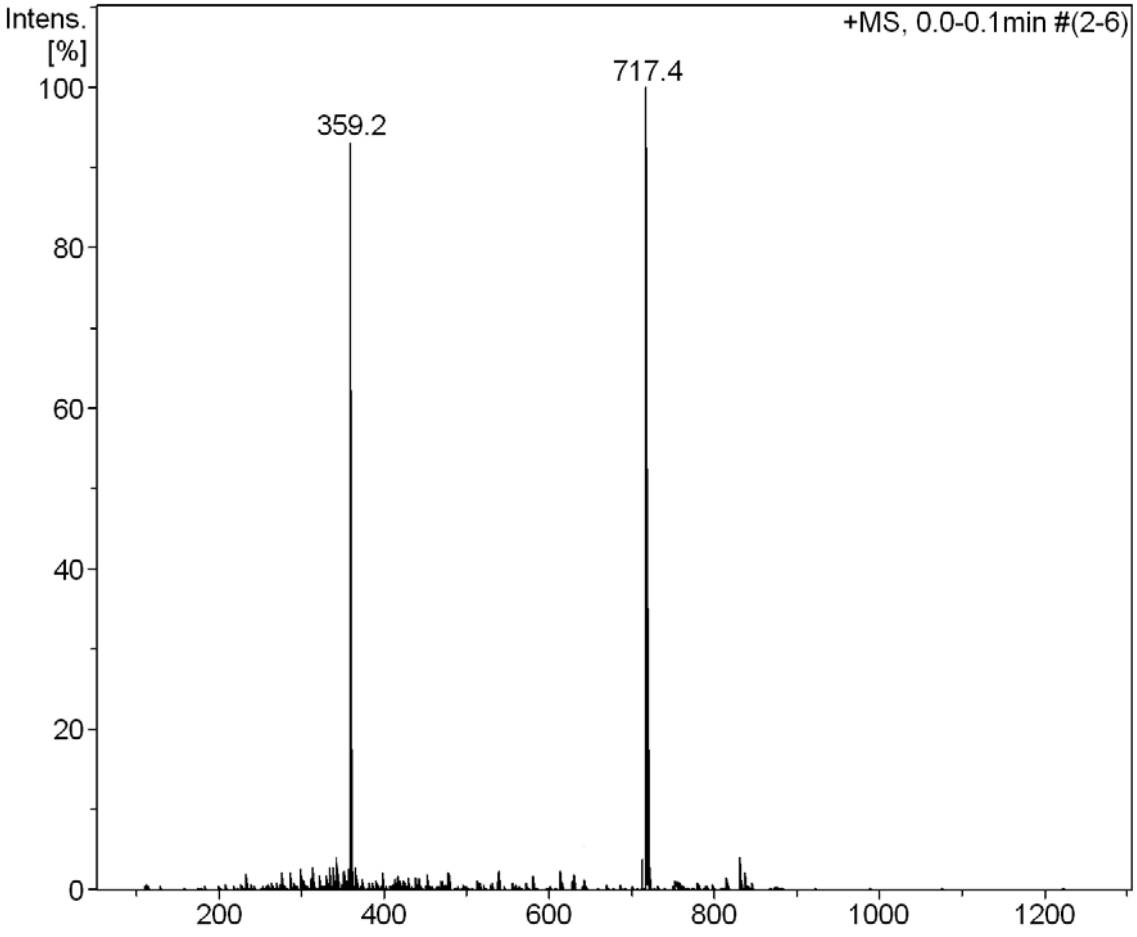


Figure S1. ESI-MS spectrum of NLS.

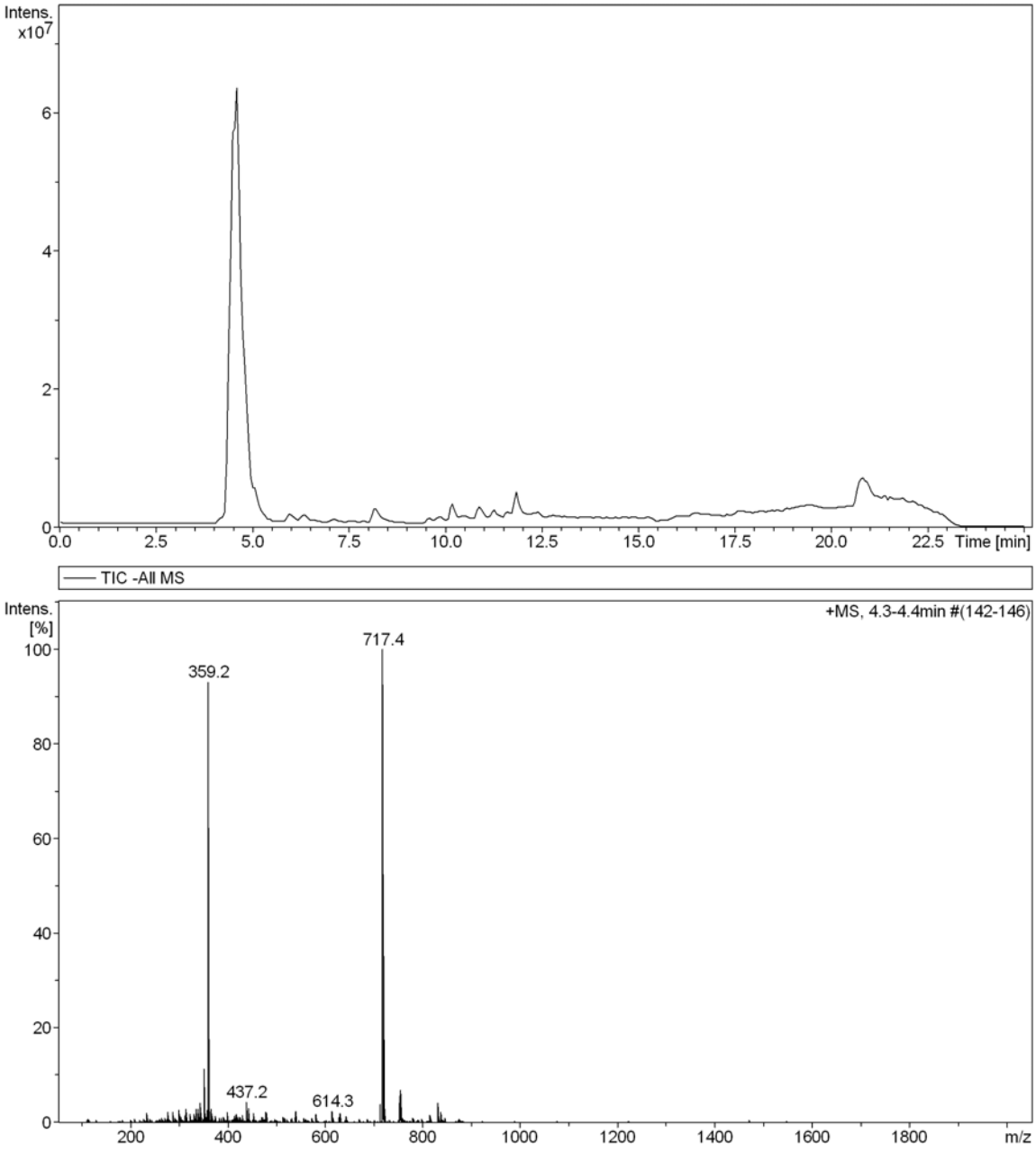


Figure S2. LC-MS spectrum of NLS.

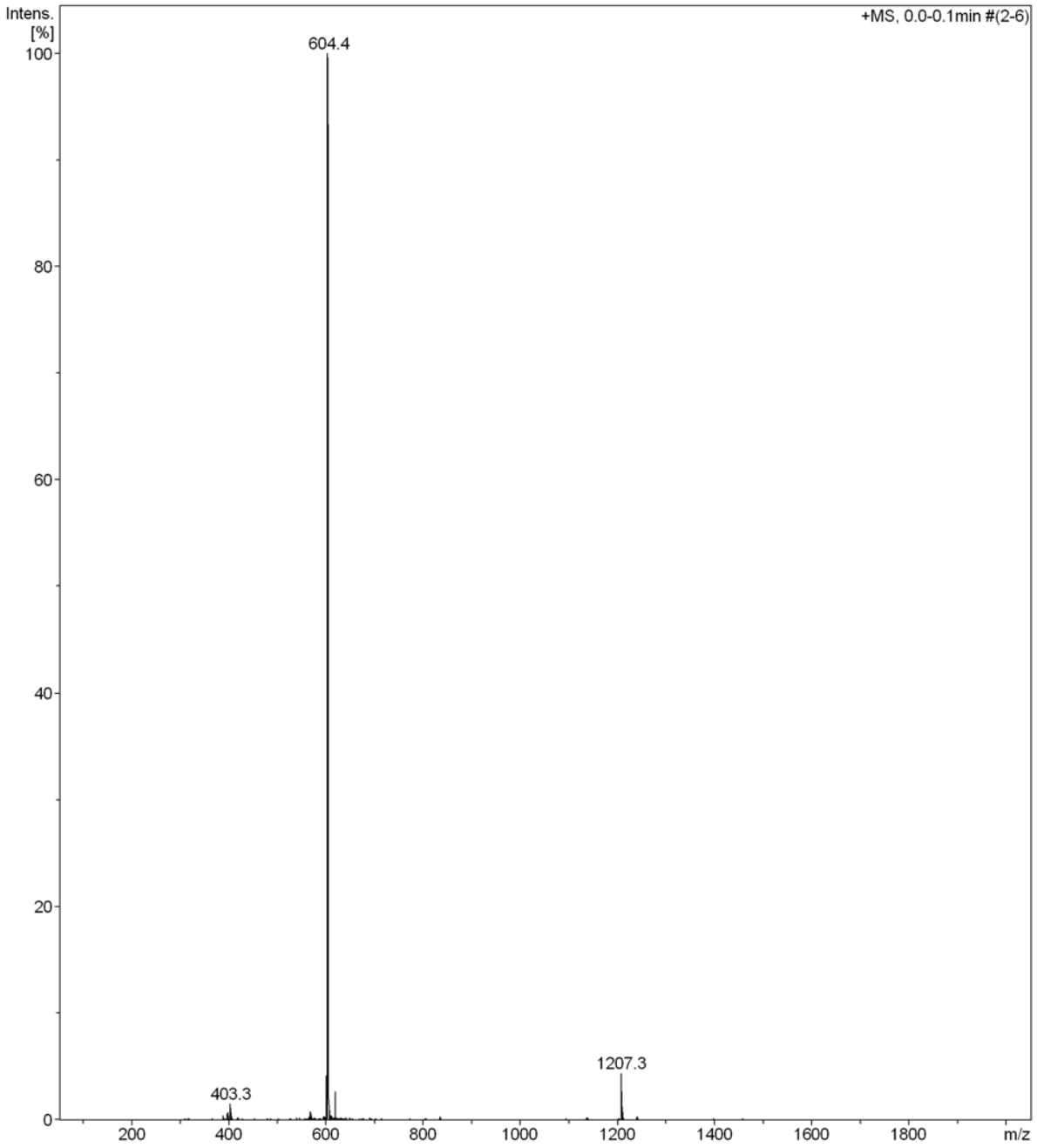


Figure S3. ESI-MS spectrum of Bombesin .

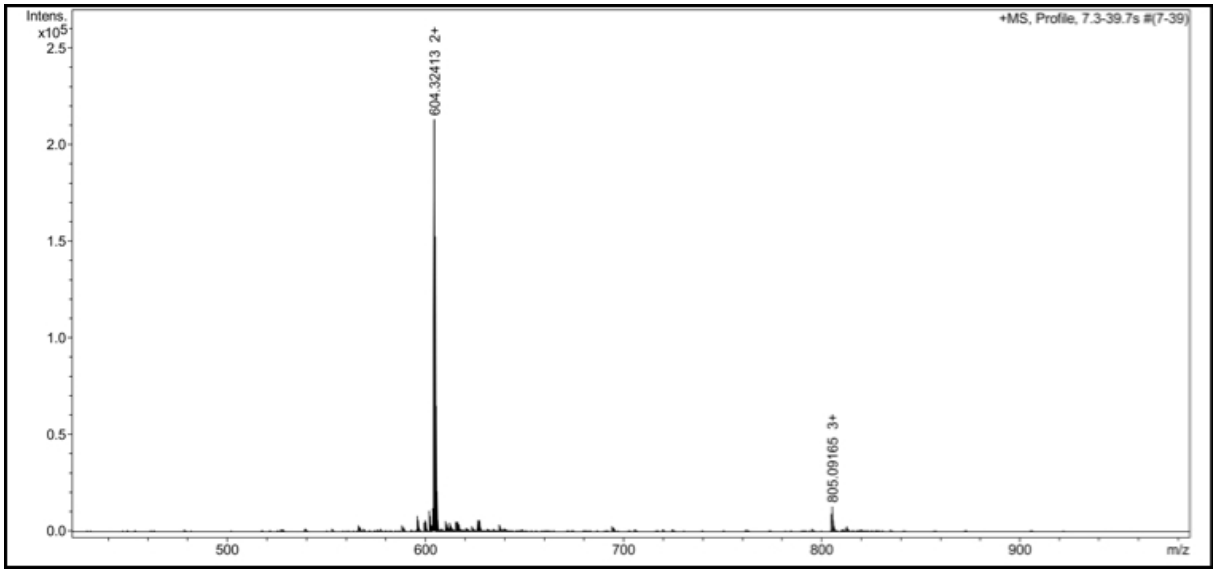


Figure S4. HR ESI-MS spectrum of Bombesin.

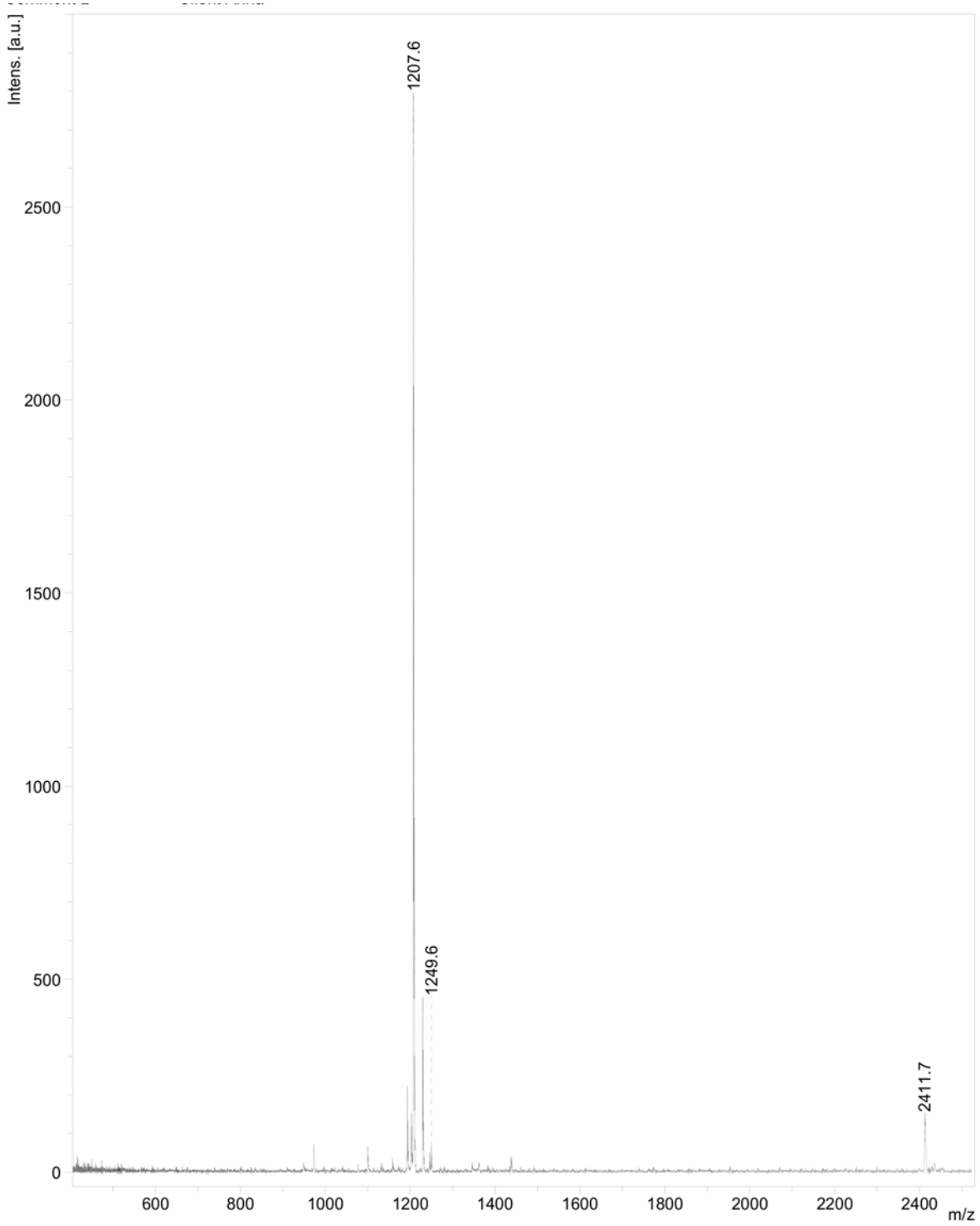


Figure S5. MALDI-TOF spectrum of Bombesin.

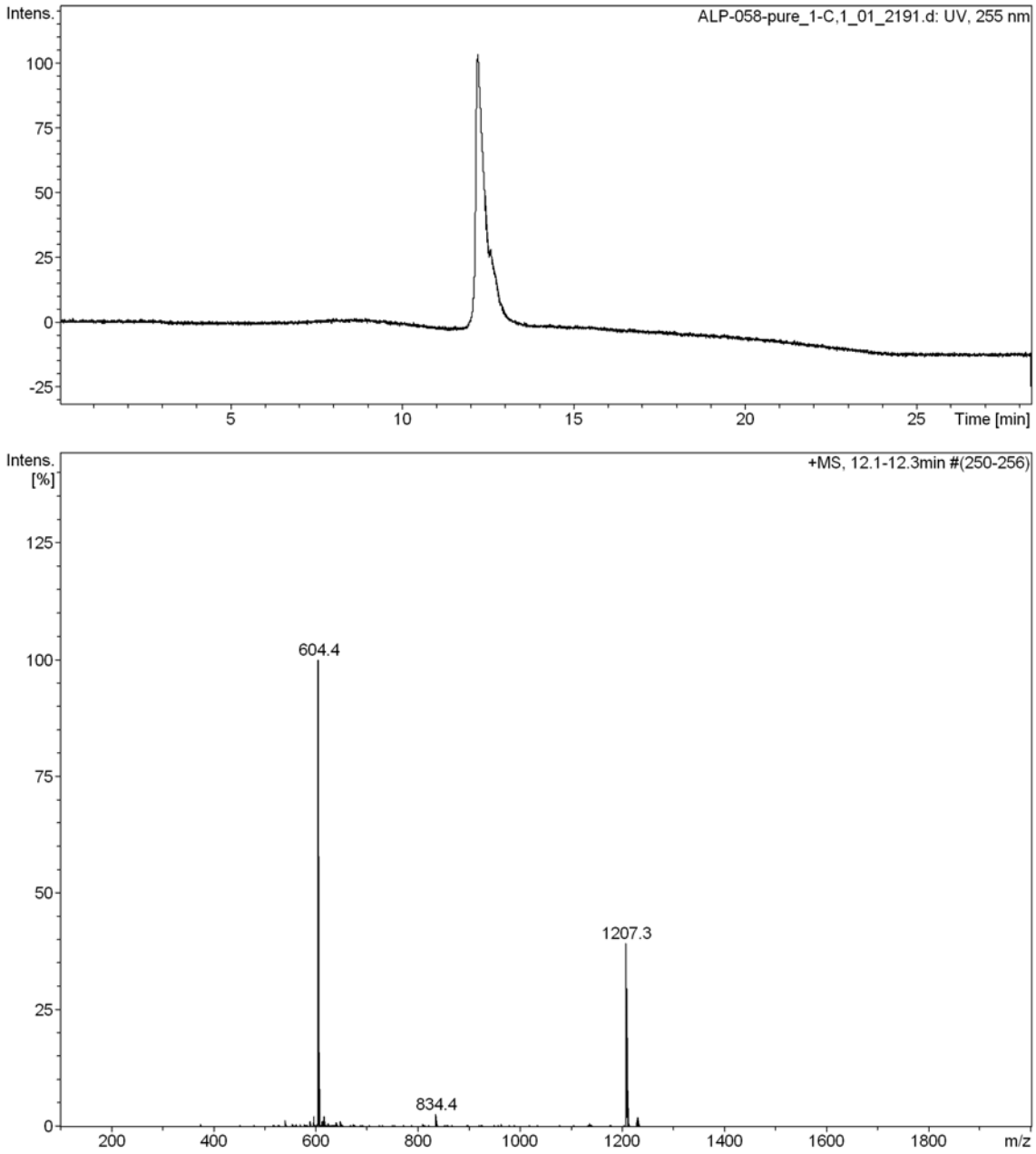


Figure S6. LC-MS spectrum of Bombesin.

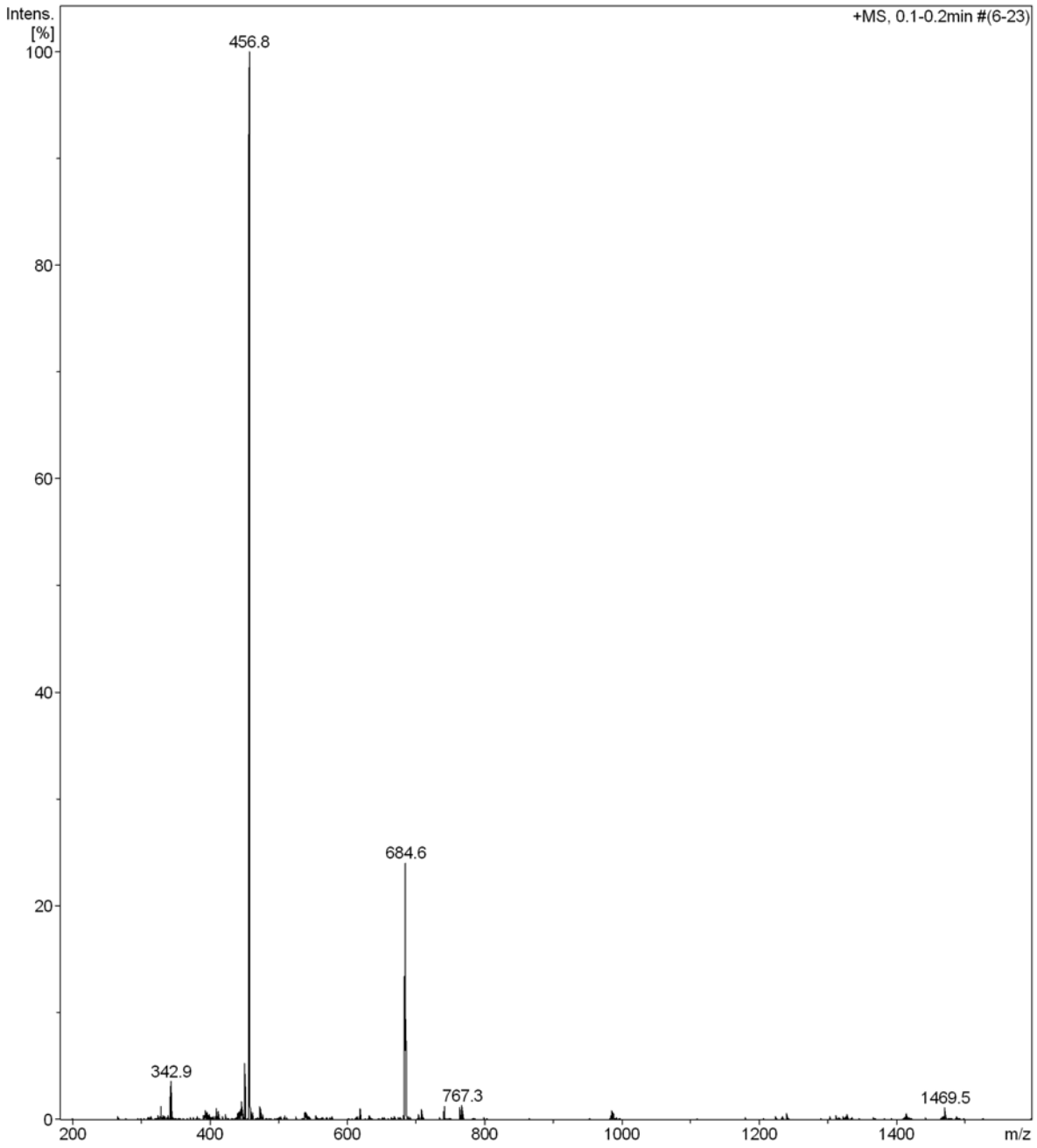


Figure S7. ESI-MS spectrum of **Re-NLS**.

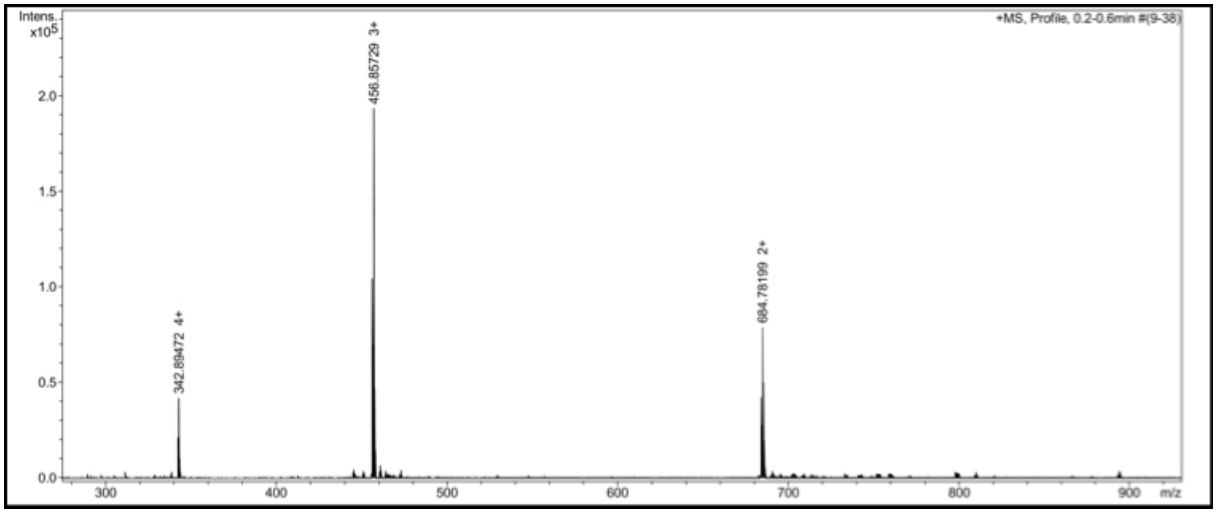


Figure S8. HR ESI-MS spectrum of **Re-NLS**.

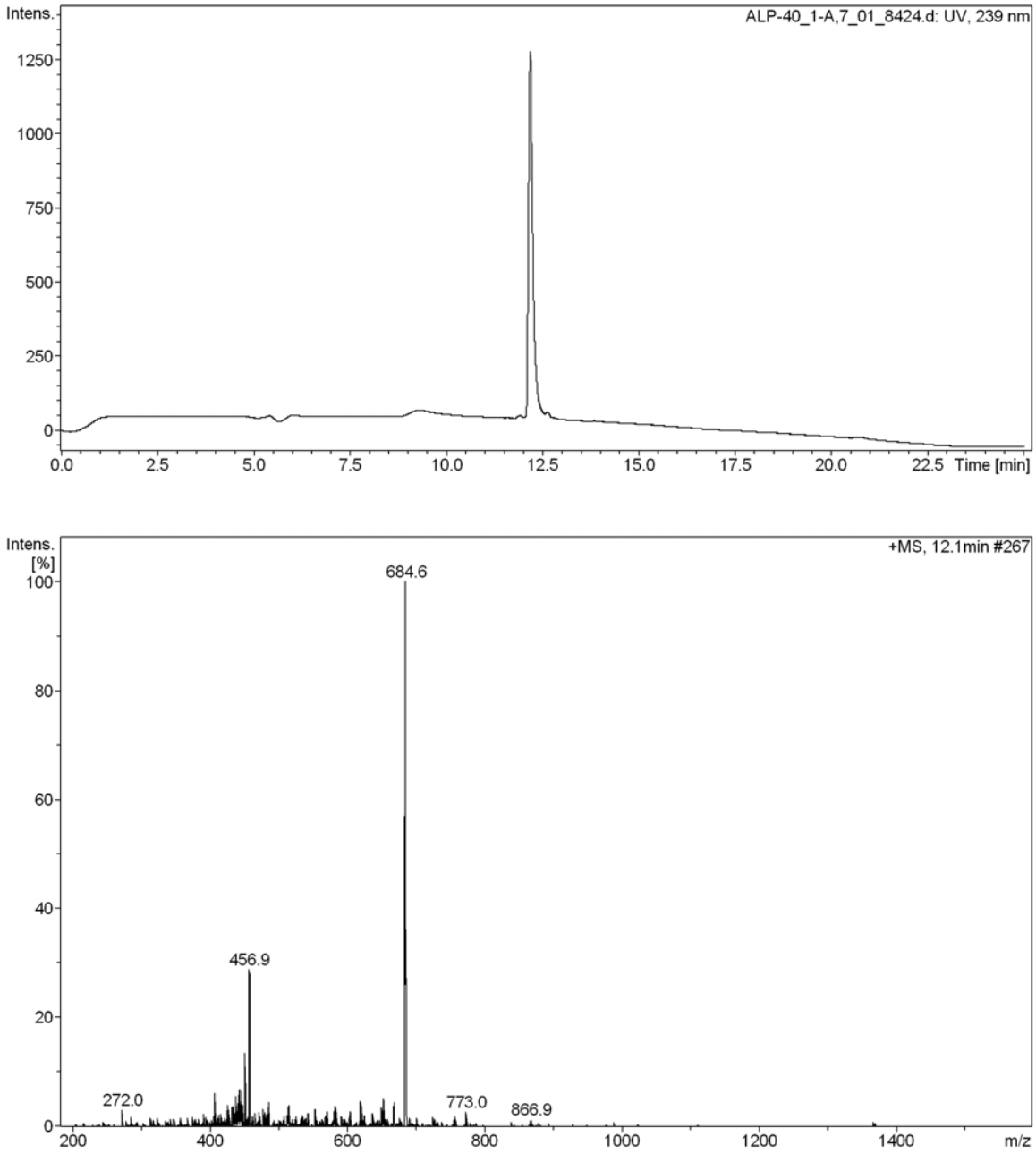


Figure S9. LC-MS spectra of **Re-NLS**.

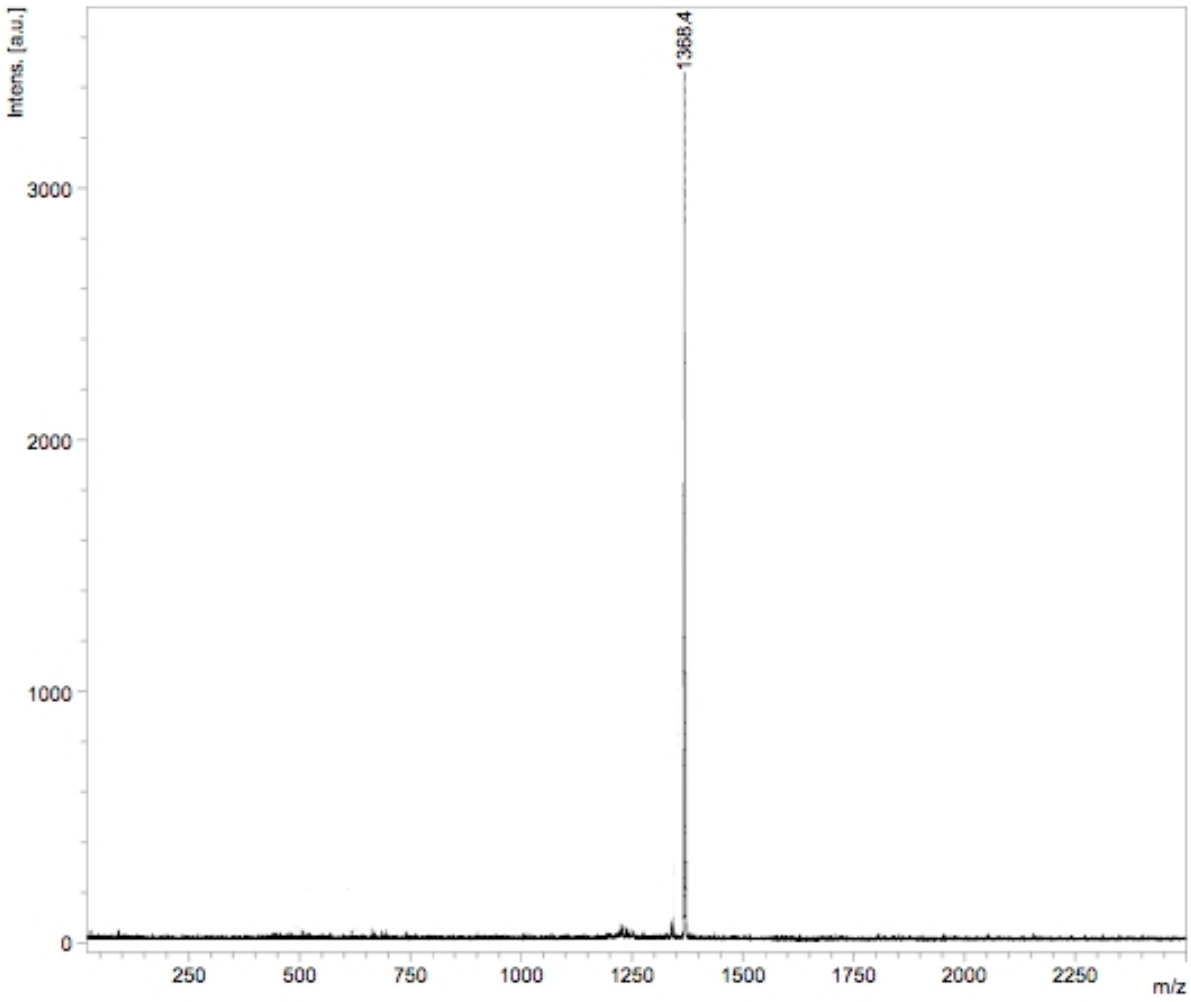


Figure S10. MALDI-TOF spectrum of **Re-NLS**.

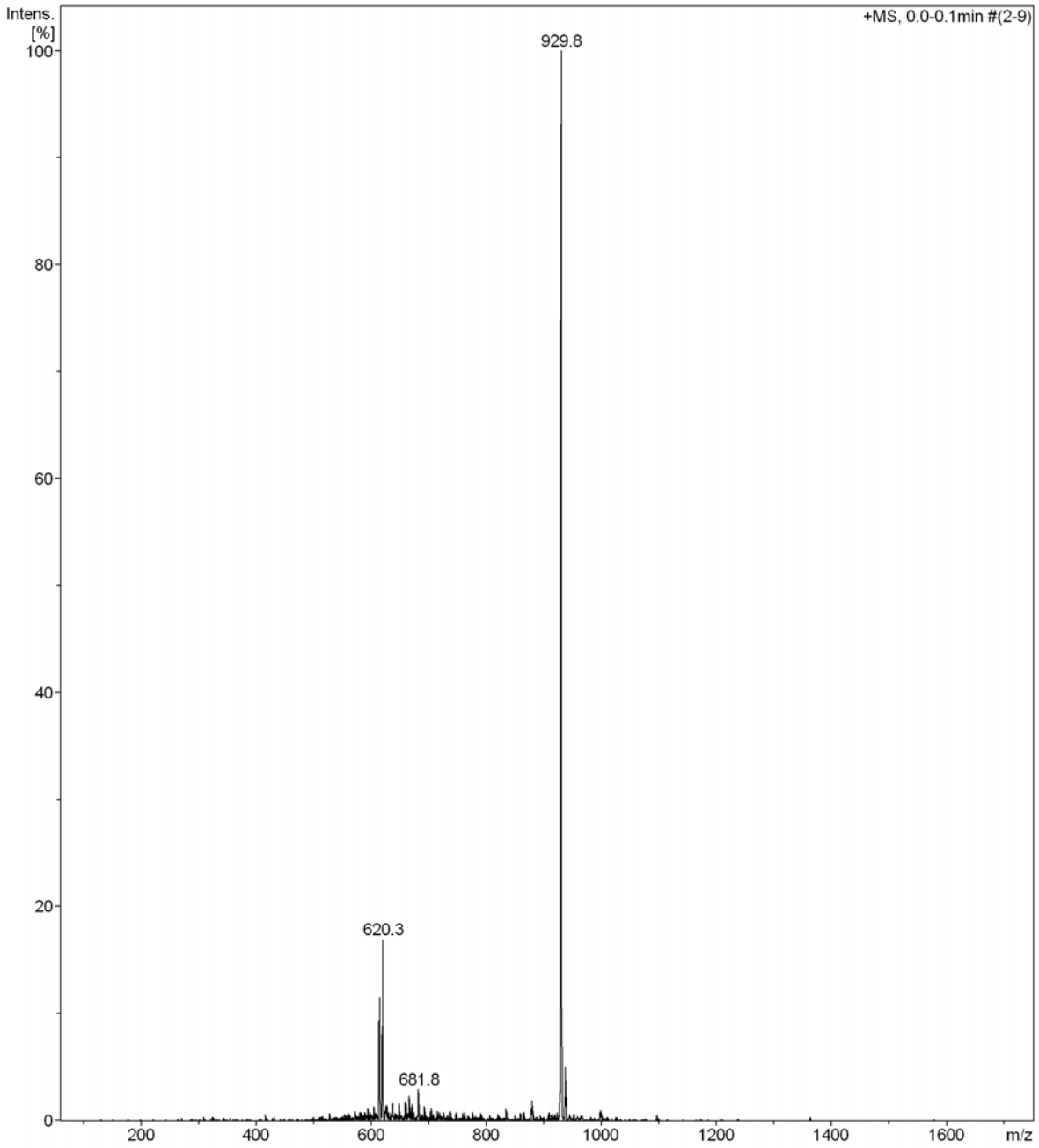


Figure S11. ESI-MS spectrum of **Re-Bombesin**.

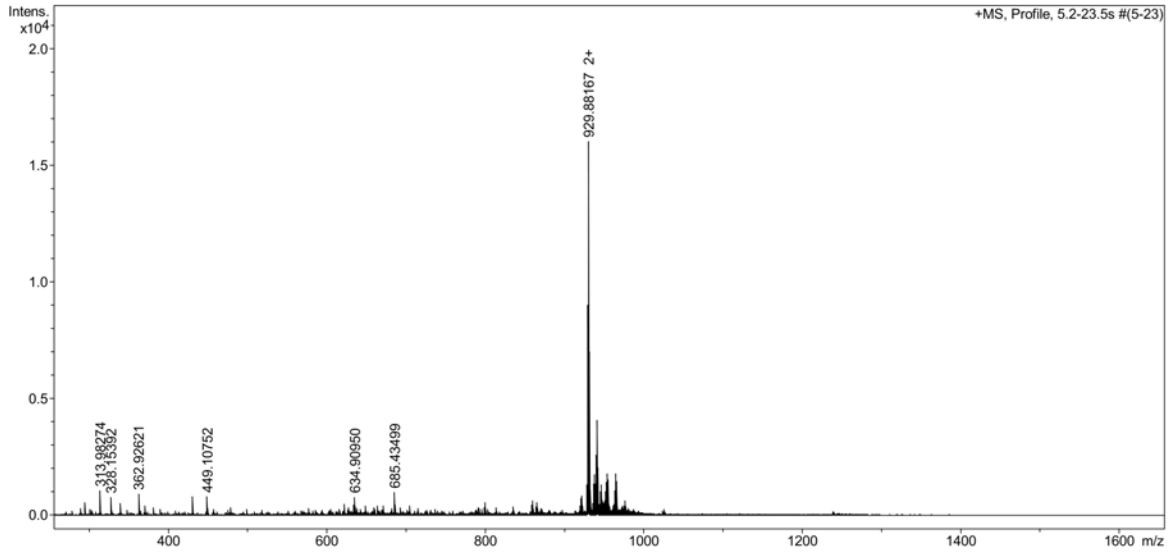


Figure S12. HR ESI-MS spectrum of **Re-Bombesin**.

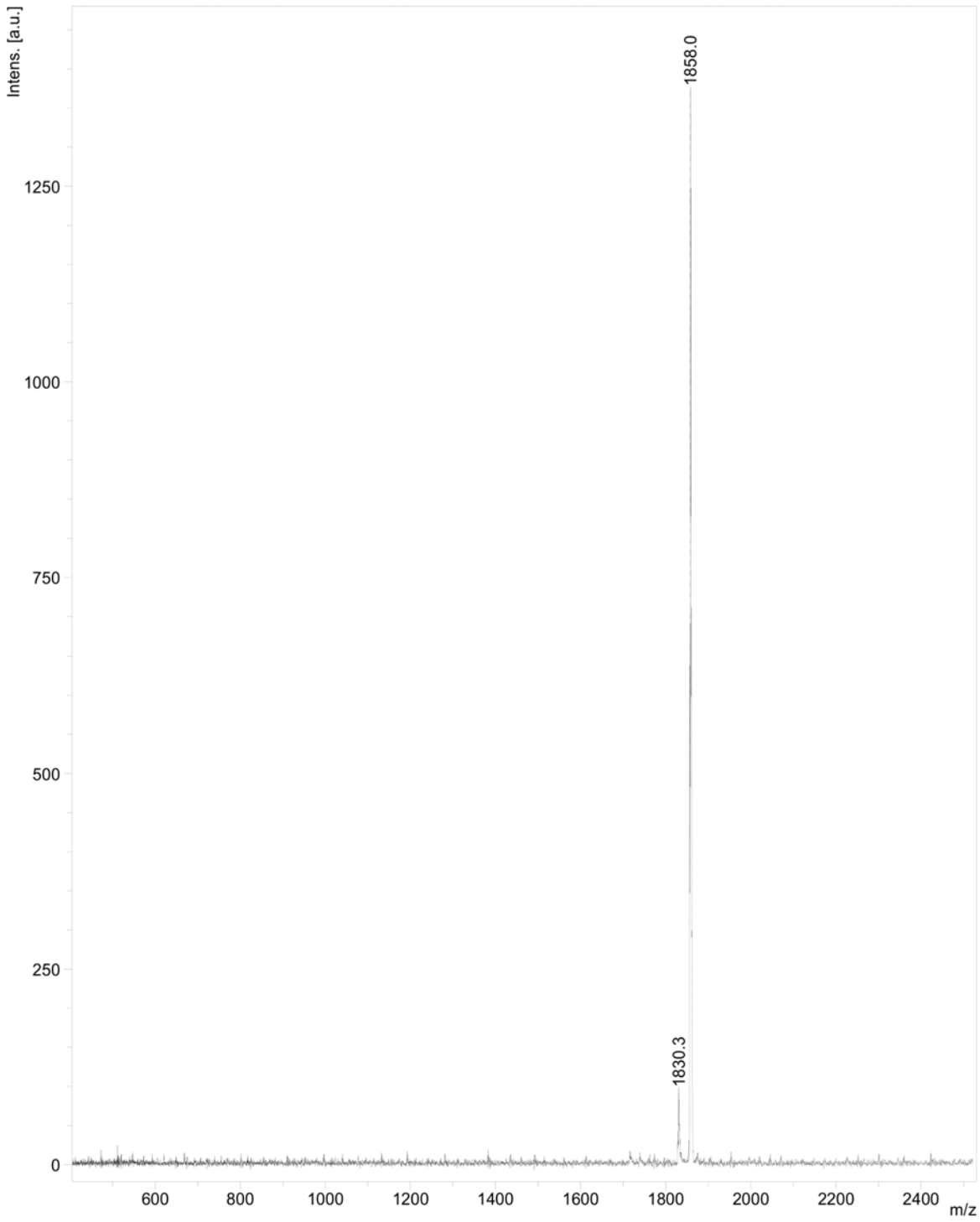


Figure S13. MALDI-TOF spectrum of **Re-Bombesin**.

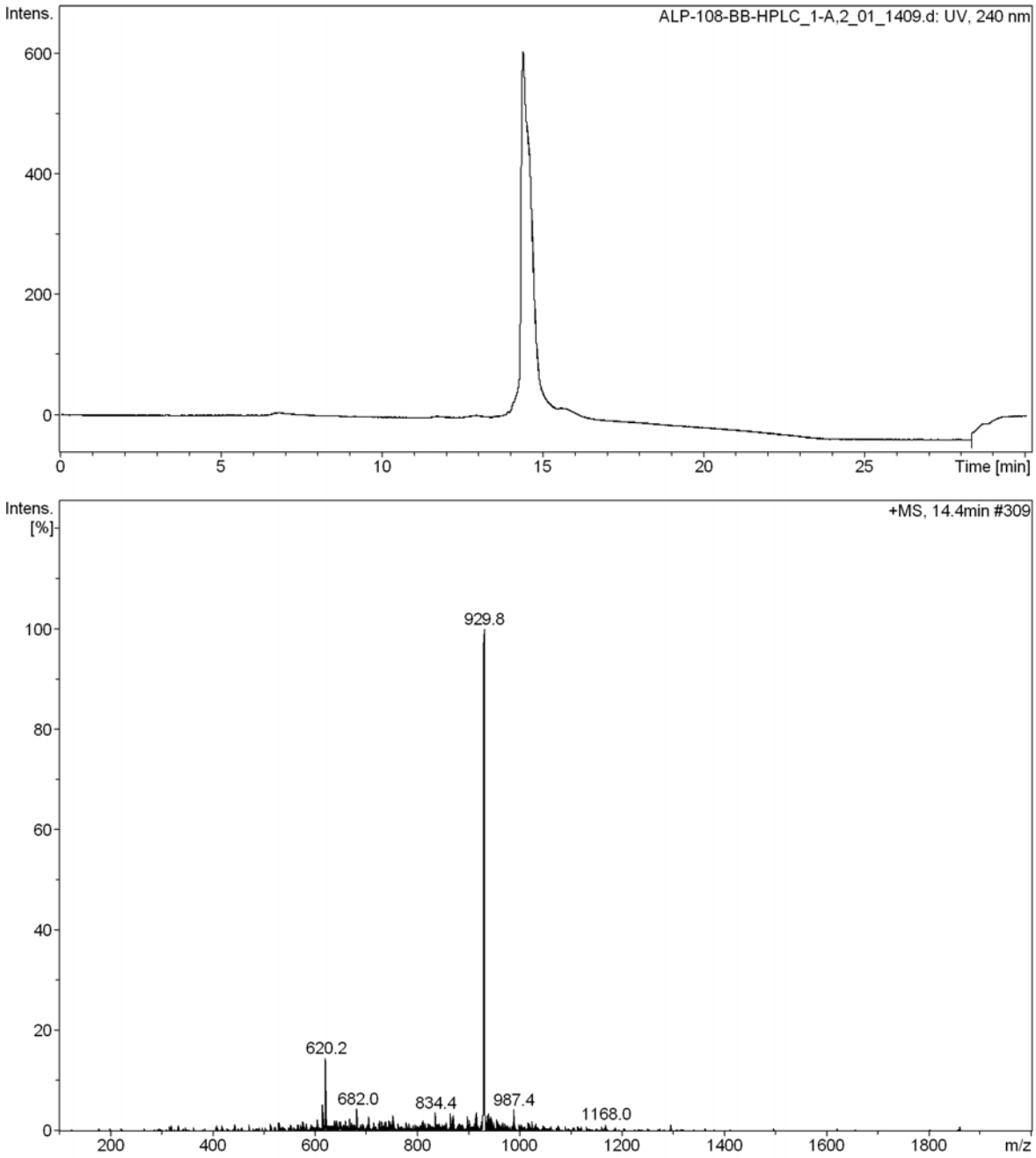
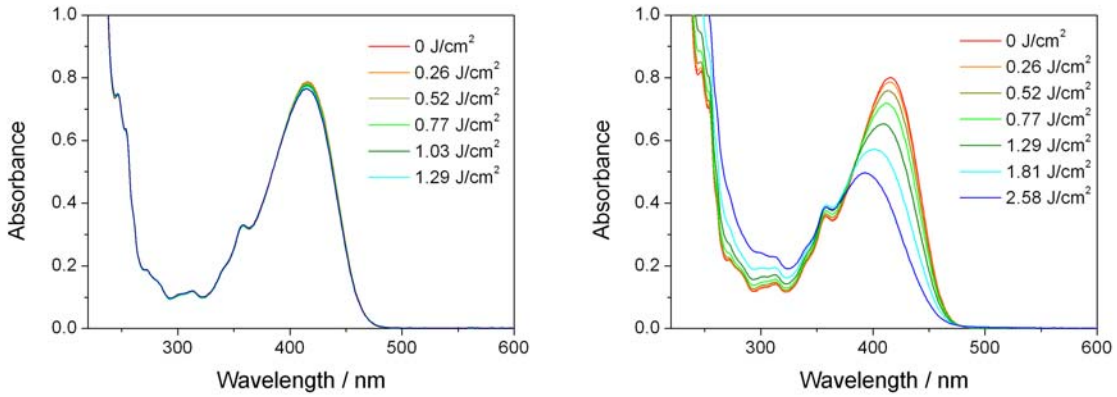
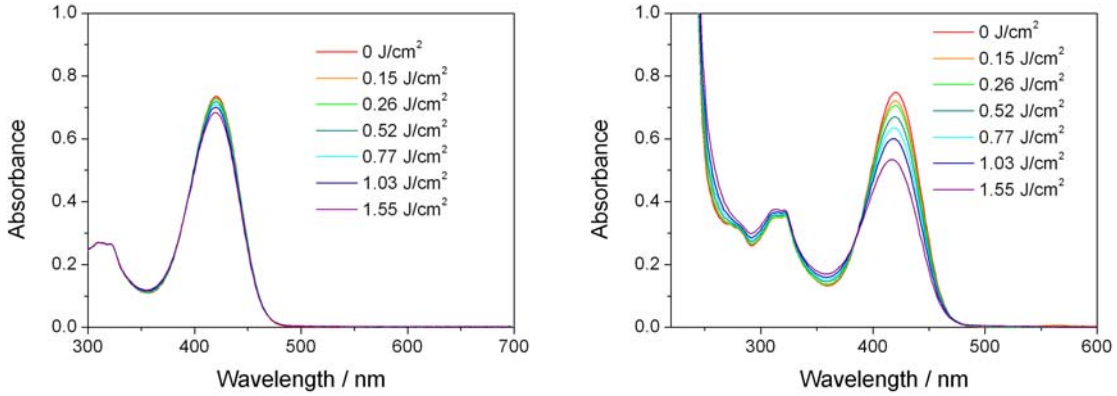


Figure S14. LC-MS spectrum of **Re-Bombesin**.

A



B



C

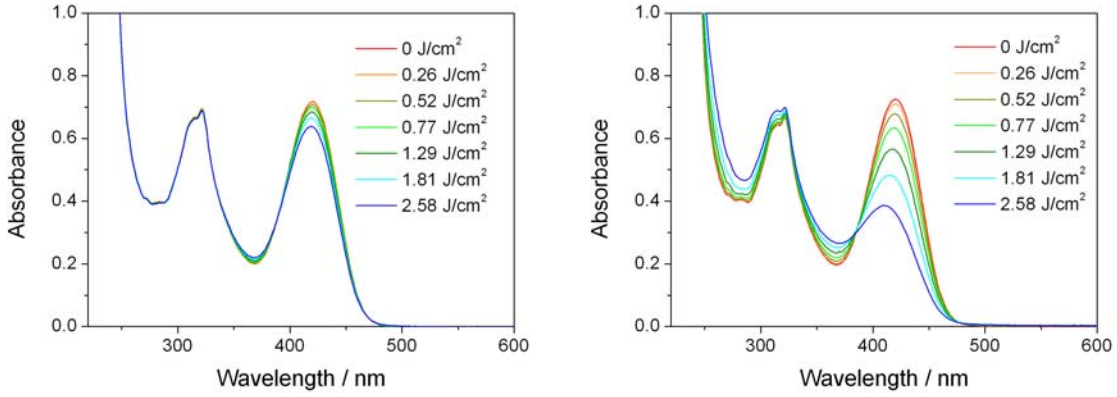
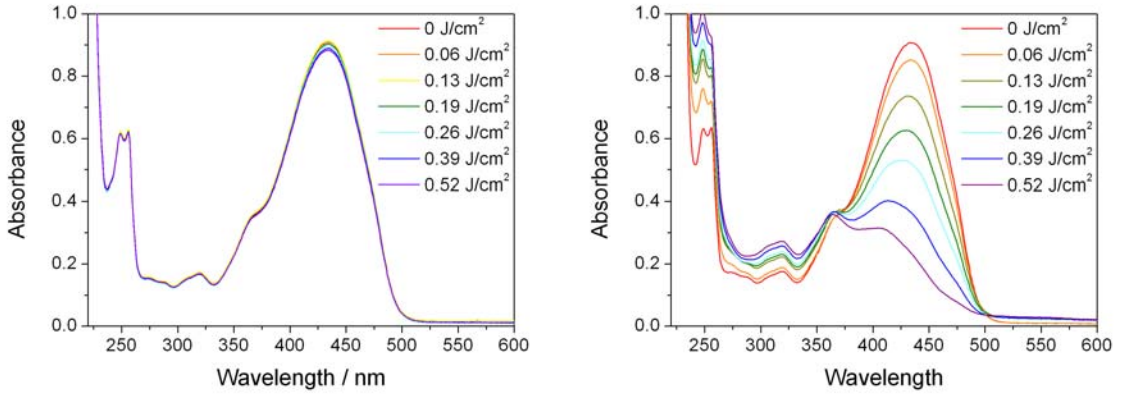
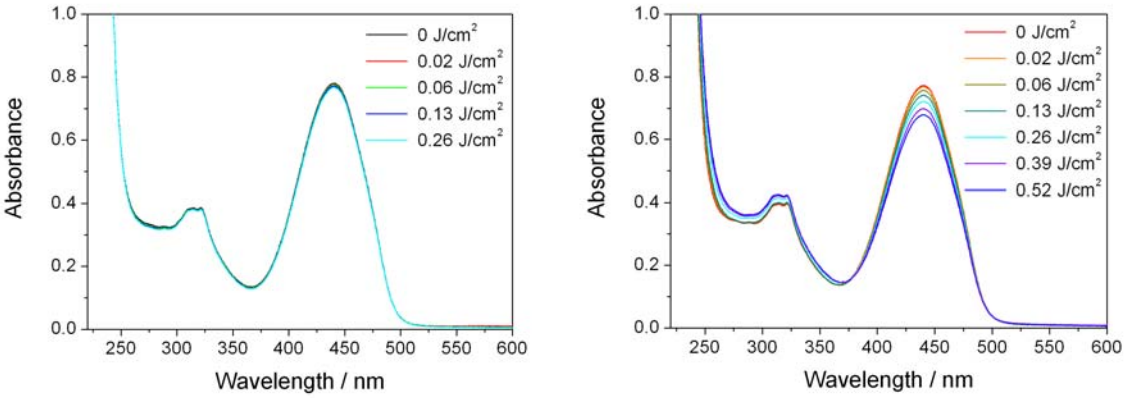


Figure S15. Singlet oxygen detection in acetonitrile by indirect method: negative control on the left; A) phenalenone; B) **Re-NH$_2$**; C) **Re-COOH**.

A



B



C

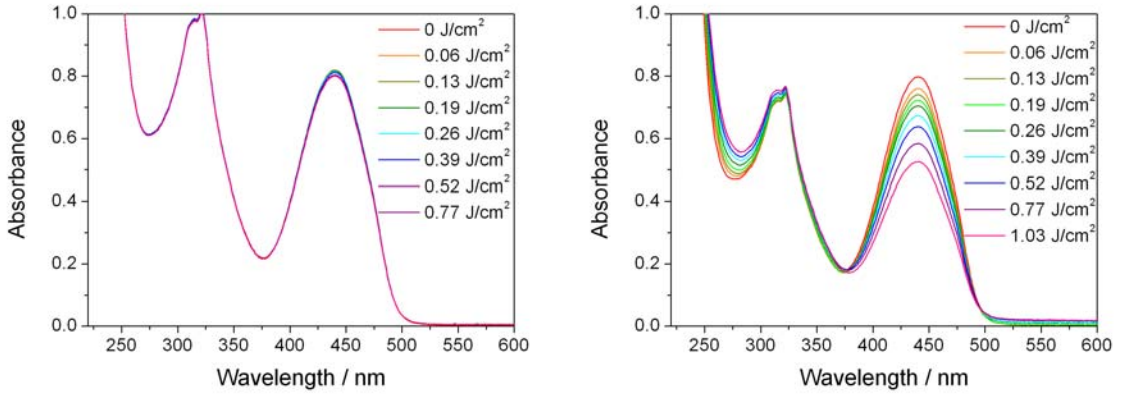


Figure S16. Singlet oxygen detection in PBS buffer by indirect method: negative control on the left; A) phenalenone; B) **Re-NH$_2$**; C) **Re-COOH**.

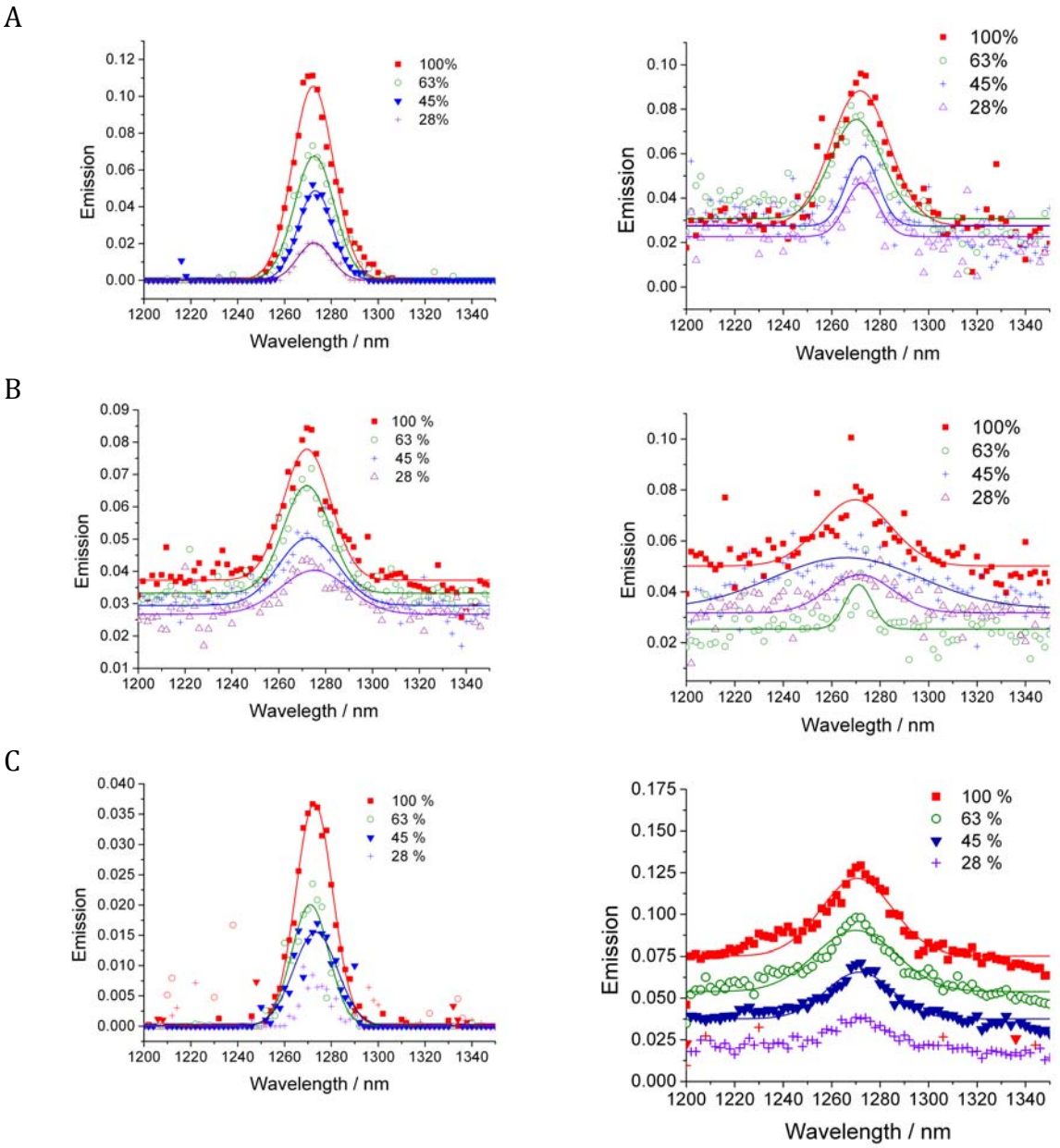


Figure S17. Singlet oxygen near-IR luminescence in acetonitrile (on the left) and D_2O (on the right): A) phenalenone; B) **Re-NH$_2$**; C) **Re-COOH**.

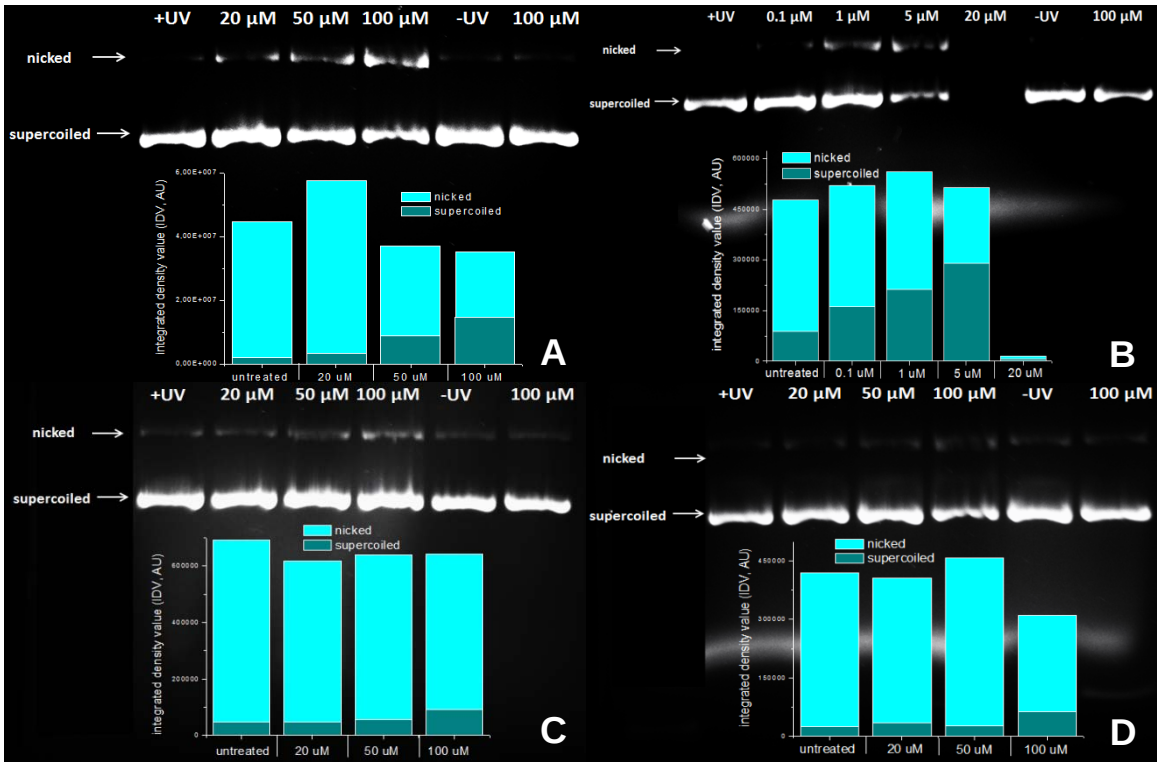


Figure S18. DNA cleavage of pcDNA3 treated with **Re-NH$_2$** (A), **Re-NLS** (B), **Re-COOH** (C) and **Re-Bombesin** (D) at increasing concentrations, not irradiated (left) and irradiated for 10 min. (right); +UV = DNA untreated irradiated; -UV = DNA untreated not irradiated.

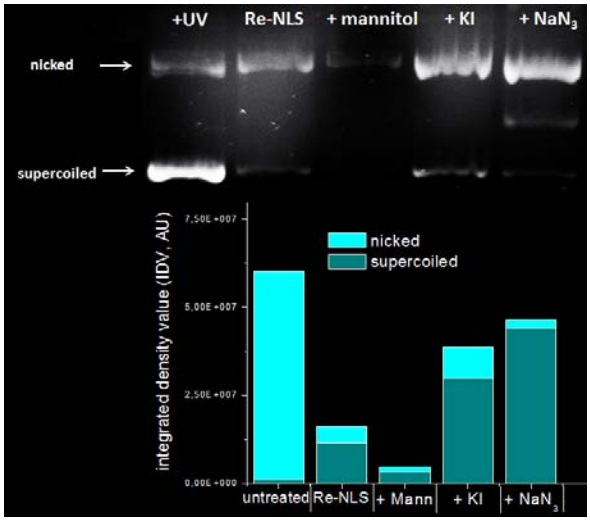


Figure S19. Electrophoresis experiment of DNA photo-cleavage of pcDNA3 plasmid treated with complex **Re-NLS**, complex **Re-NLS** + mannitol (lane 3), complex **Re-NLS** + sodium azide (NaN_3, lane 4) and complex **Re-NLS** + potassium iodide (KI, lane 5); irradiated for 10 minutes; +UV = DNA not treated; cisplatin = DNA treated with cisplatin.

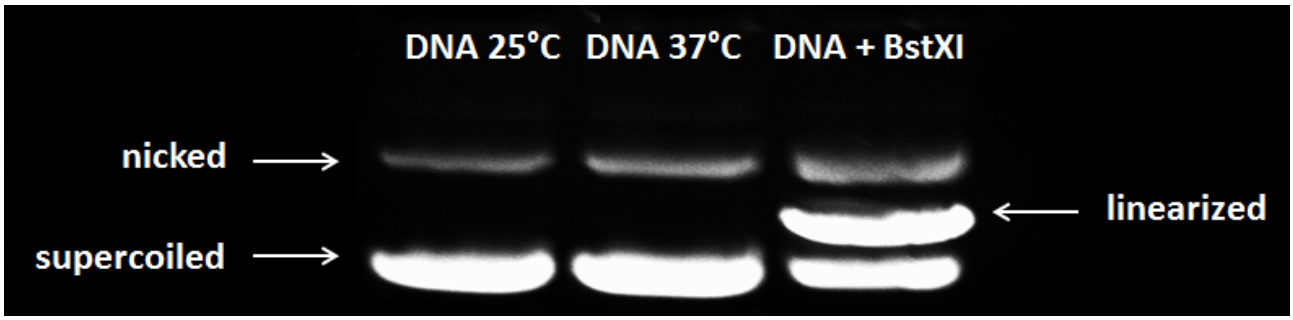


Figure S20. Electrophoresis experiment of DNA cleavage of pcDNA3 plasmid incubated at different temperature (25 °C, lane 1; 37 °C, lane 2) and treated with the restriction enzyme BstXI (lane 4).

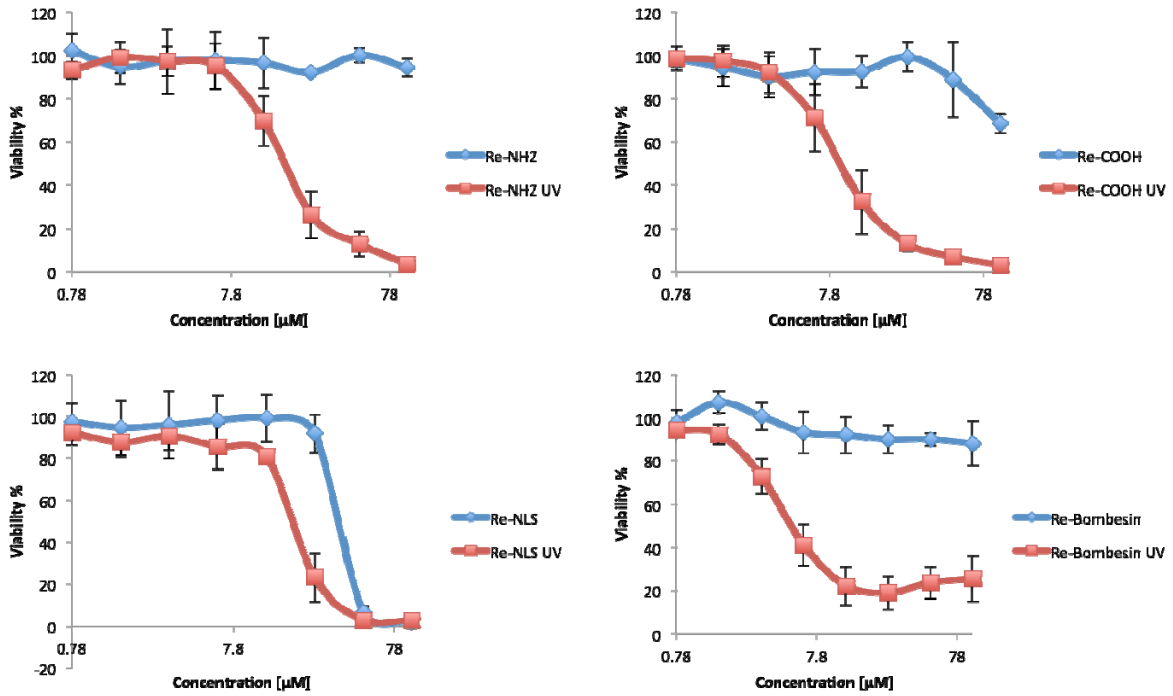


Figure S21. Cytotoxicity of **Re-NH$_2$**, **Re-COOH**, **Re-NLS**, **Re-Bombesin**, on HeLa cells treated for 4h with the complexes, then kept in the dark (blue) or exposed to 10 min UV (red) and measured by the resazurin assay.

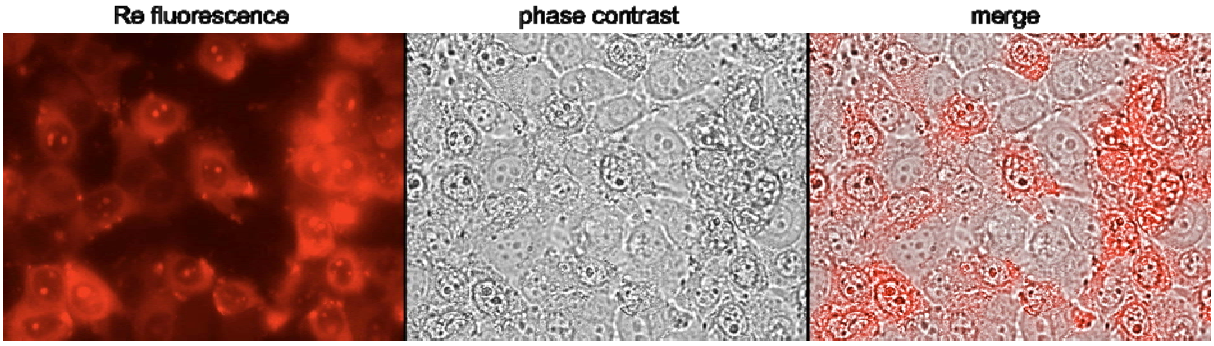


Figure S22. Fluorescence microscopy images showing the distribution of **Re-NLS** after 1h treatment at 100 µM in living HeLa cells.