

Supplementary Materials

for

Novel Chiral Ru(II) Complexes as Potential c-myc G-quadruplex DNA Stabilizers Inducing DNA Damage to Suppress Triple-Negative Breast Cancer Progression

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1801A9999-14 #31-46 RT: 0.05-0.08 AV: 8 NL: 1.60E7
F: TMS + c ESI Full ms [100.0000-1000.0000]

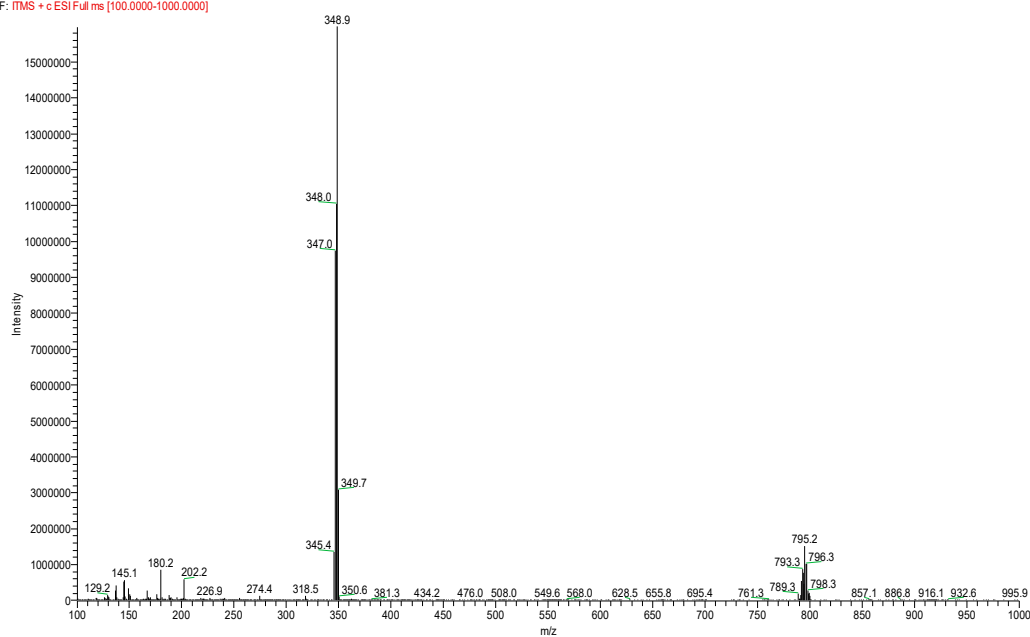


Figure S1. The ESI-MS spectra of Δ -1.

TSQ Quantum Ultra

2018061-08 #10-13 RT: 0.09-0.11 AV: 2 SB: 2 0.00-0.05 0.12 NL: 4.63E7
T: + c ESI QMG [100.000-1000.000]

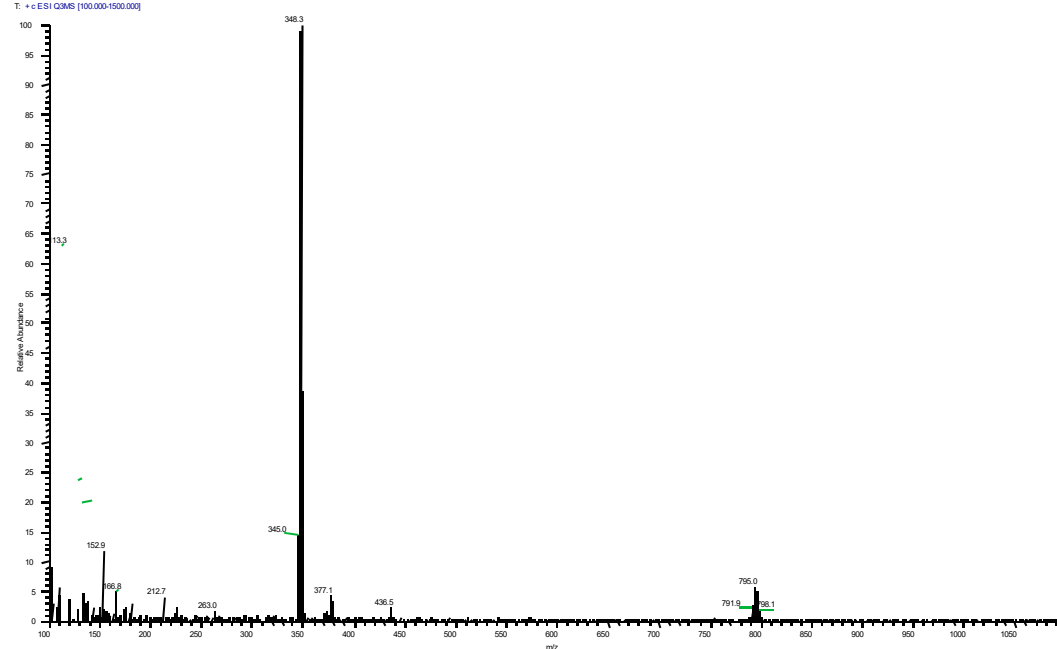


Figure S2. The ESI-MS spectra of Δ -1.

20161211YJHM-09 #15 RT: 0.14 AV: 1 SB: 2 0.01-0.02 NL: 8.13E6
T: + c ESI Q1MS [50.000-1500.000]

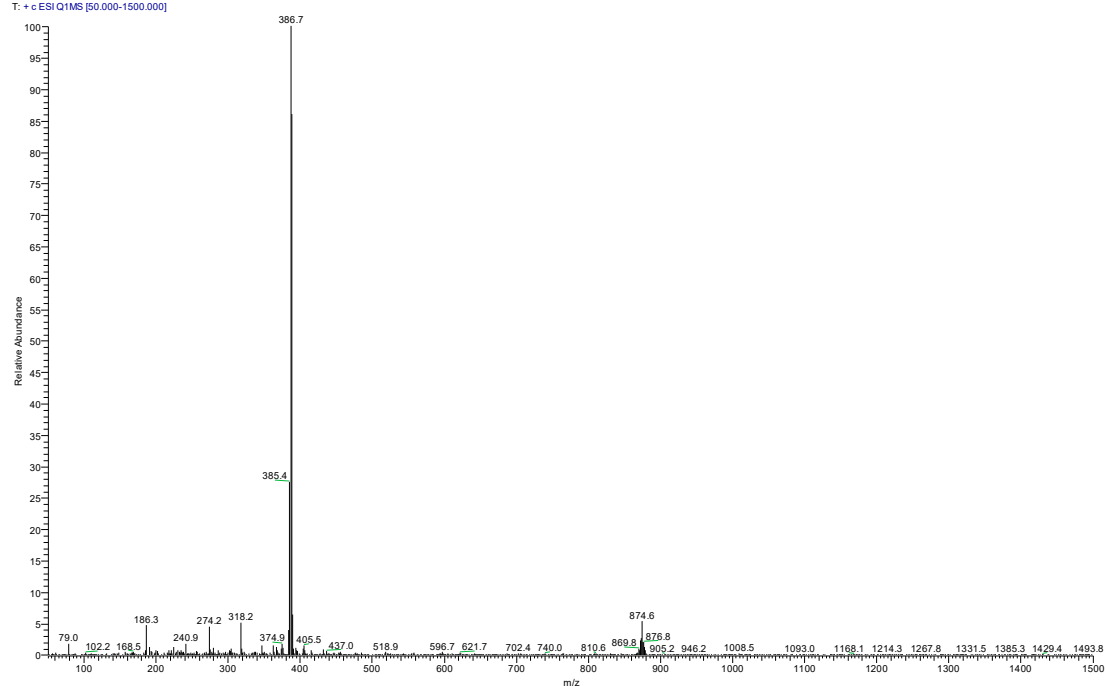


Figure S3. The ESI-MS spectra of Δ -2.

1611B9004-04#11-13 RT: 0.10-0.12 AV: 2 NL: 7.68E6
F: + c ESI Q3MS [50.000-1000.000]

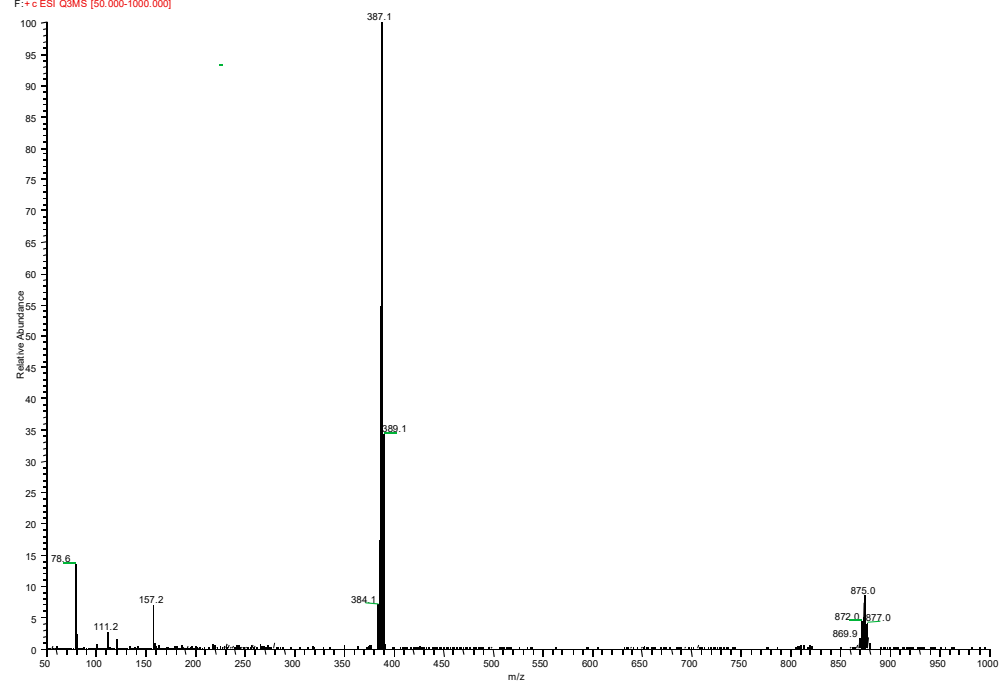


Figure S4. The ESI-MS spectra of Δ -2.

1711c0989-05 #7 RT: 0.06 AV: 1 SB: 2 0.01-0.02, 0.32 NL: 3.94E6
T: + c ESI Q3MS [100.000-1500.000]

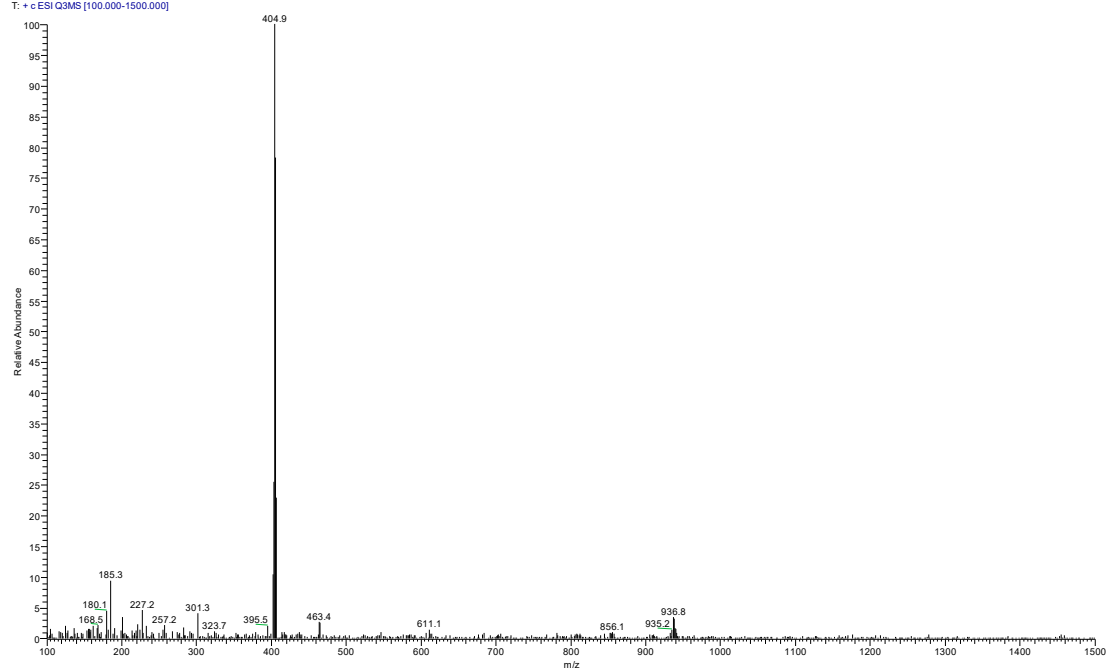


Figure S5. The ESI-MS spectra of Δ -3.

1711D0182-03#16-24 RT: 0.07-0.09 AV: 4 SB: 3 0.01-0.03 NL: 4.35E6
F: ITMS + c ESI Full ms [100.00-1500.00]

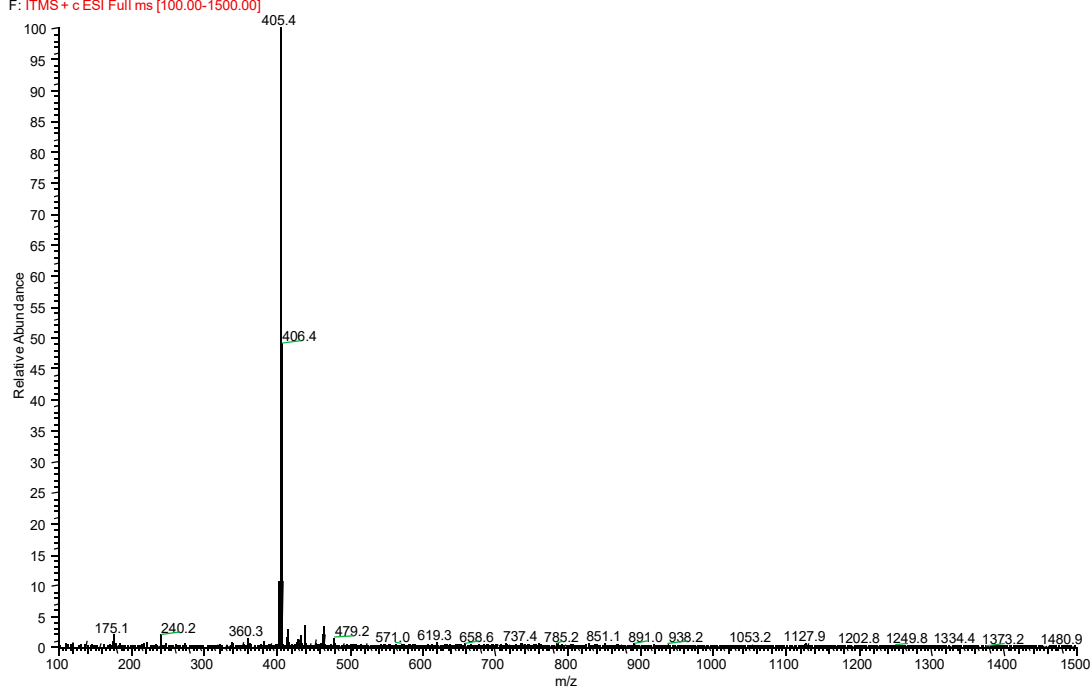


Figure S6. The ESI-MS spectra of Δ -3.

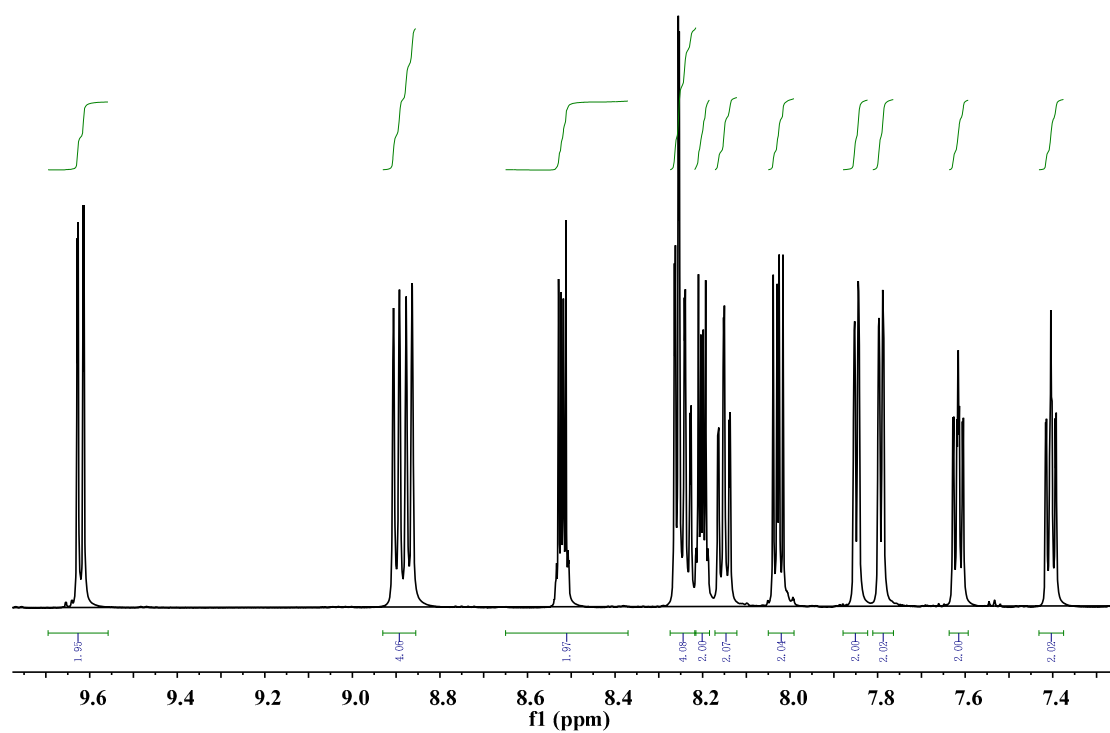


Figure S7. The ^1H NMR spectra of Δ -1.

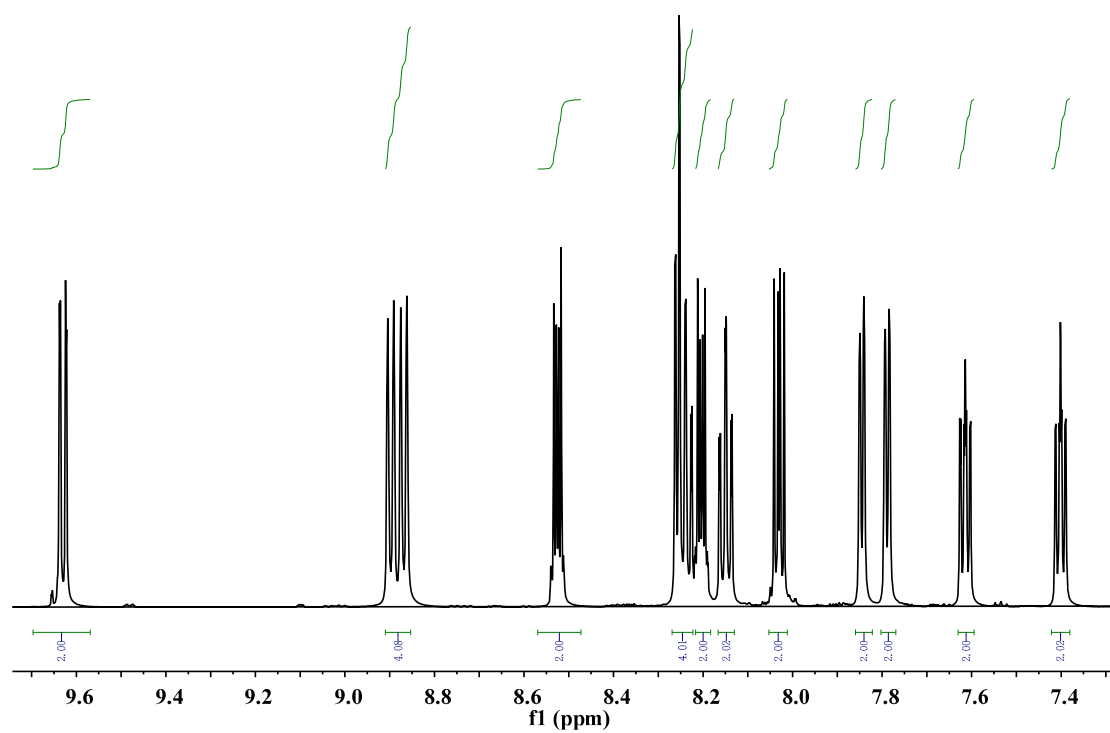


Figure S8. The ^1H NMR spectra of Δ -1.

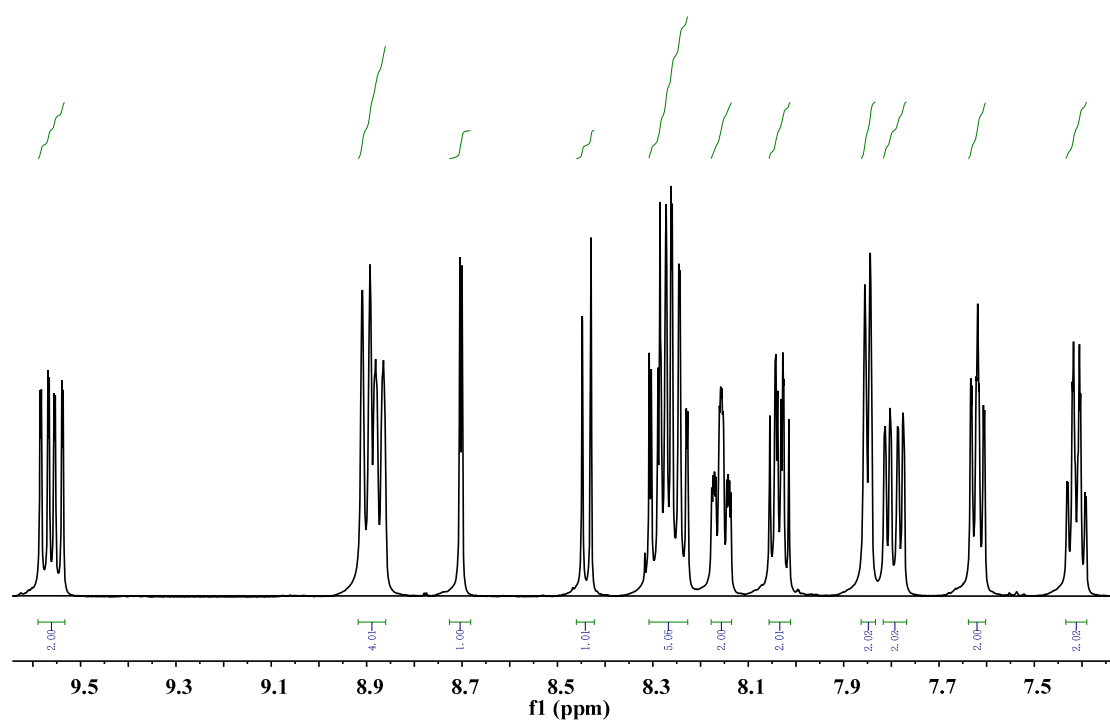


Figure S9. The ^1H NMR spectra of Δ -2.

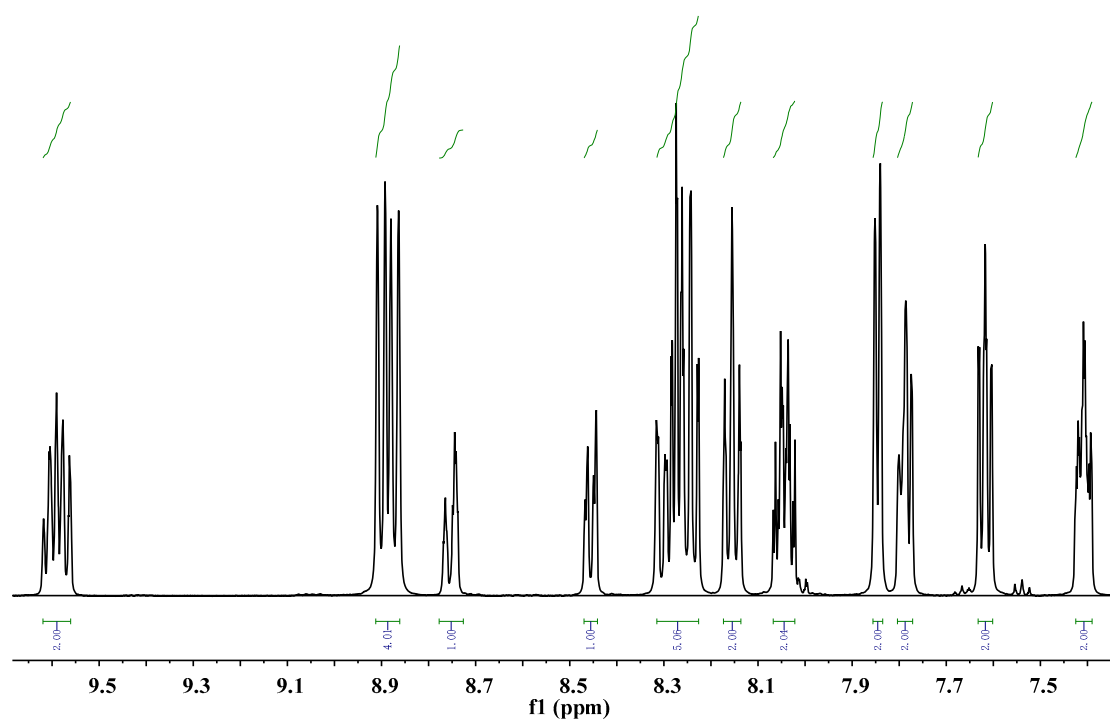


Figure S10. The ^1H NMR spectra of Δ -2.

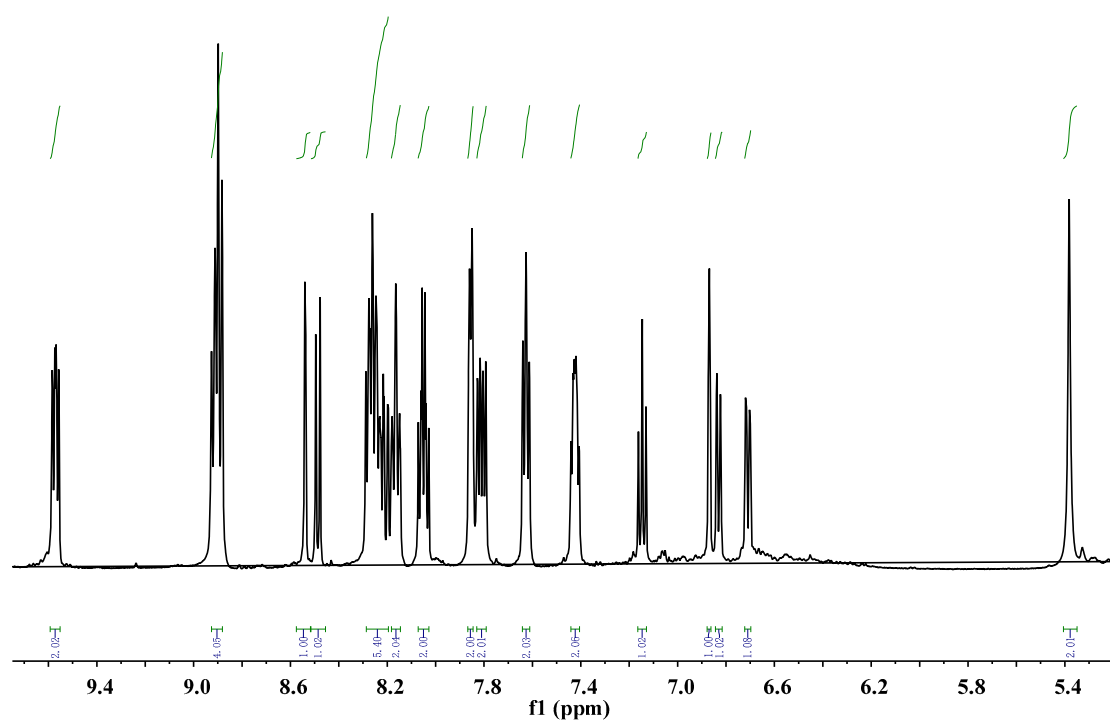


Figure S11. The ^1H NMR spectra of Δ -3.

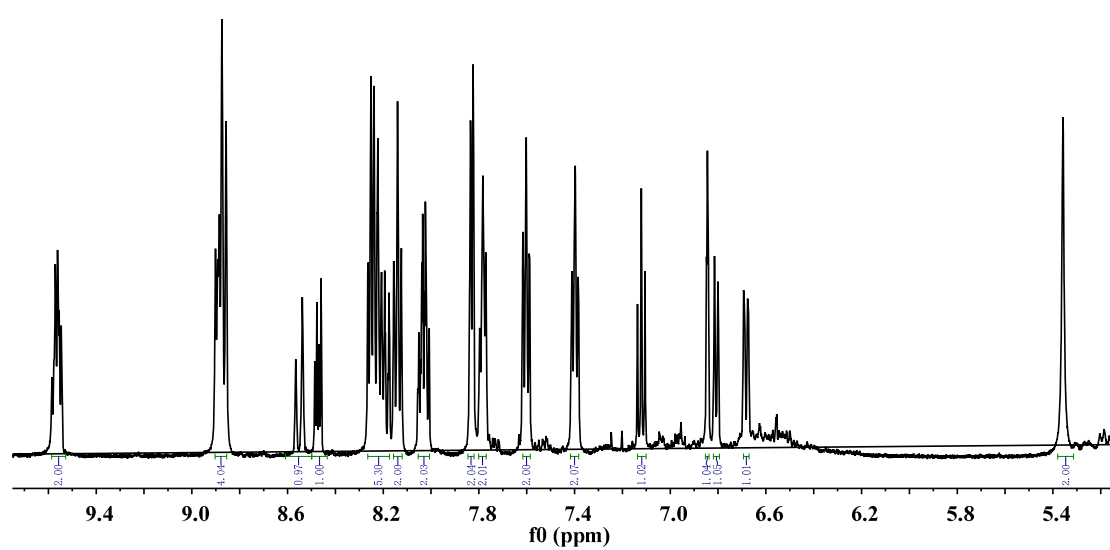


Figure S12. The ^1H NMR spectra of Δ -3.

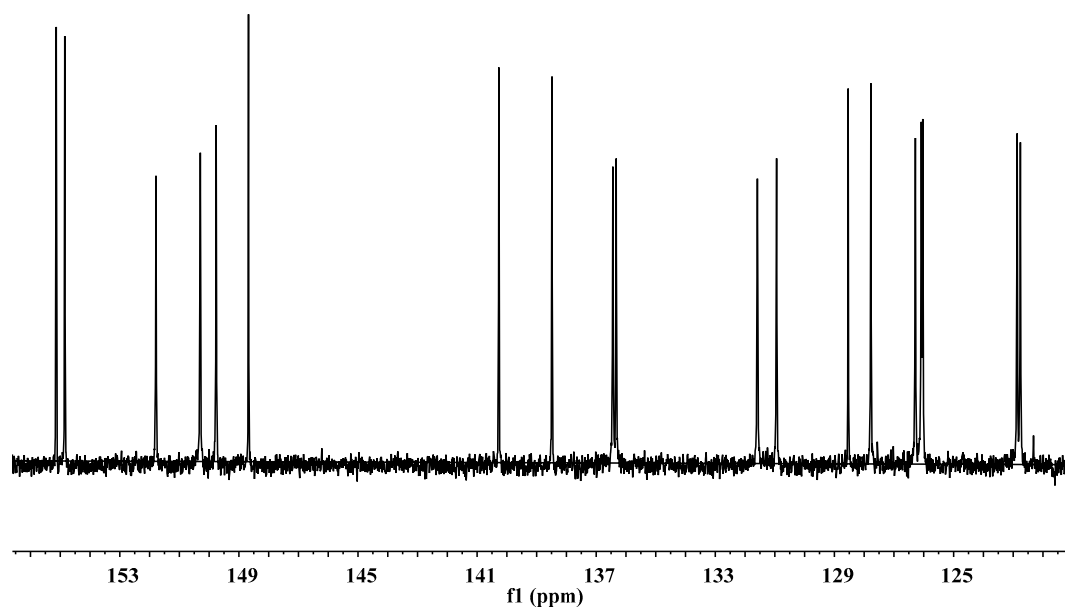


Figure S13. The ^{13}C NMR spectra of Δ -1.

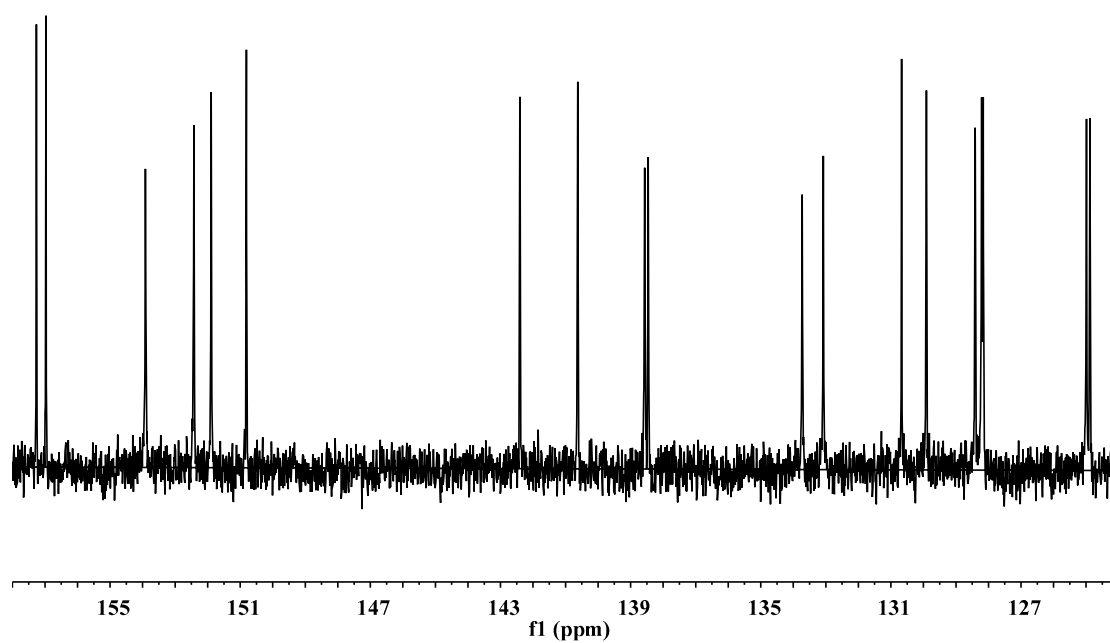


Figure S14. The ^{13}C NMR spectra of Δ -1.

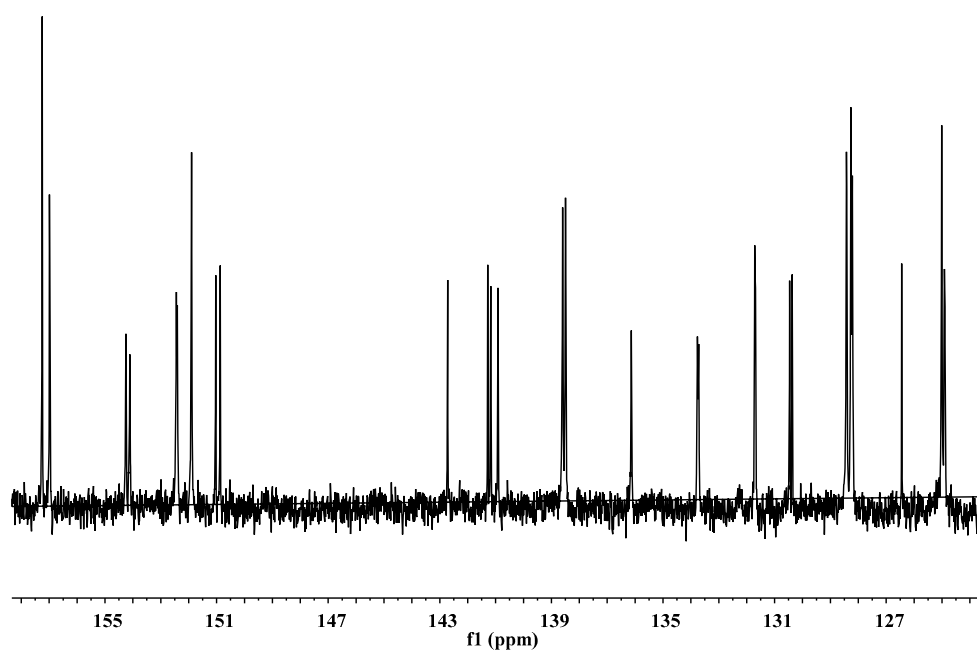


Figure S15. The ^{13}C NMR spectra of Δ -2.

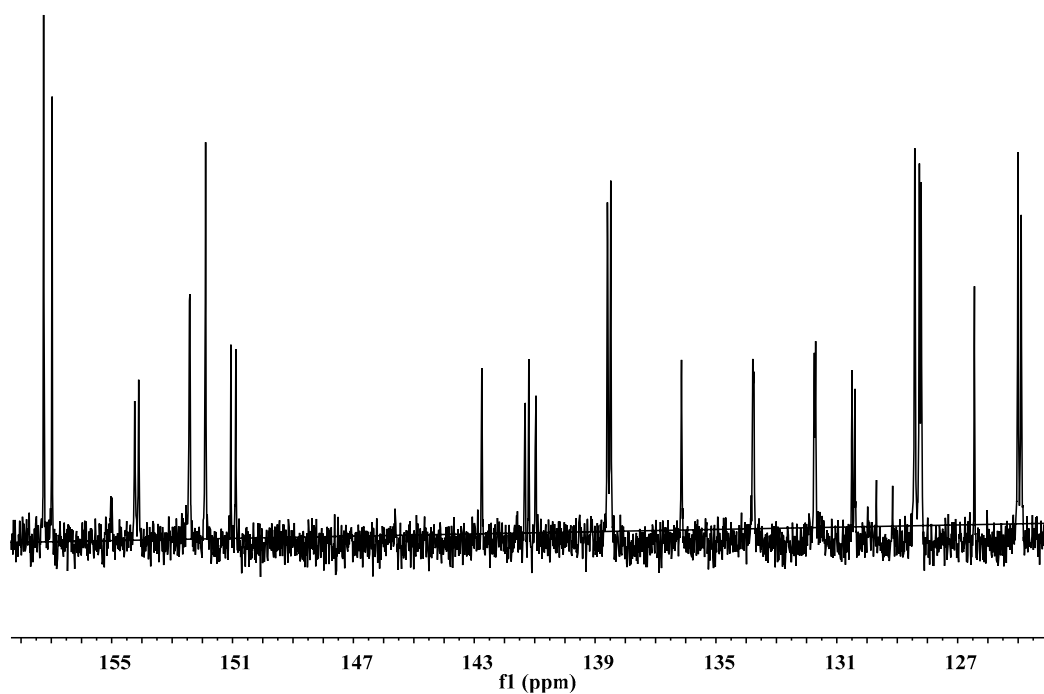


Figure S16. The ^{13}C NMR spectra of Δ -2.

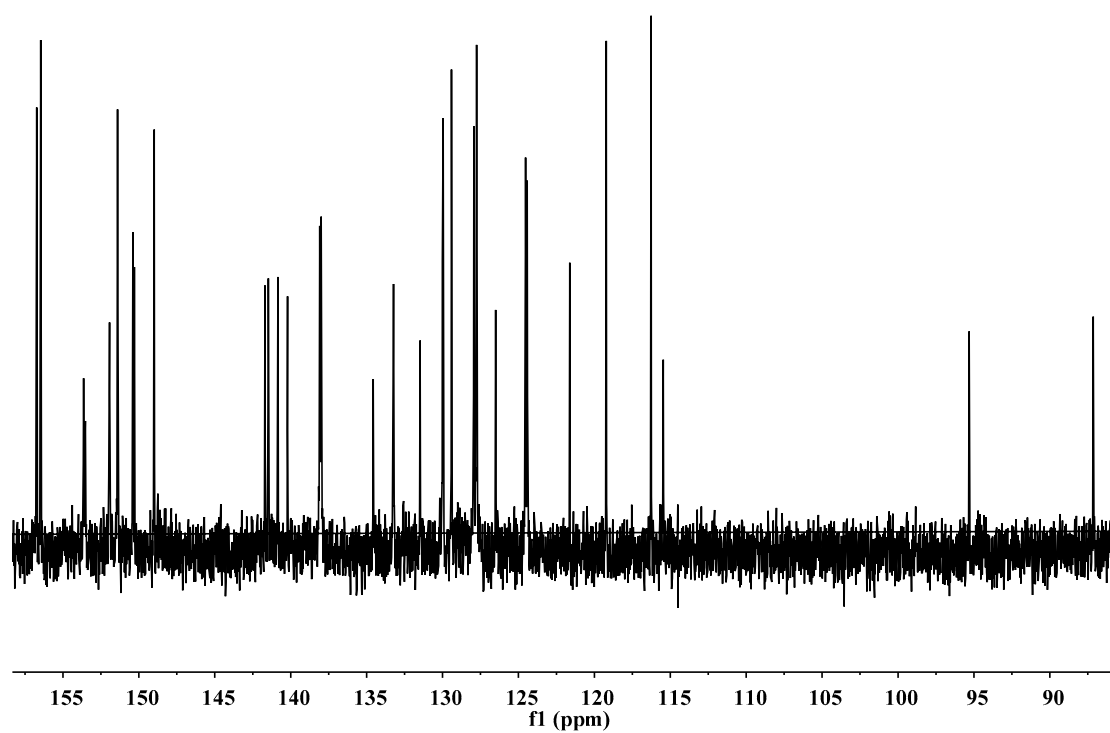


Figure S17. The ^{13}C NMR spectra of $\Delta\text{-3}$.

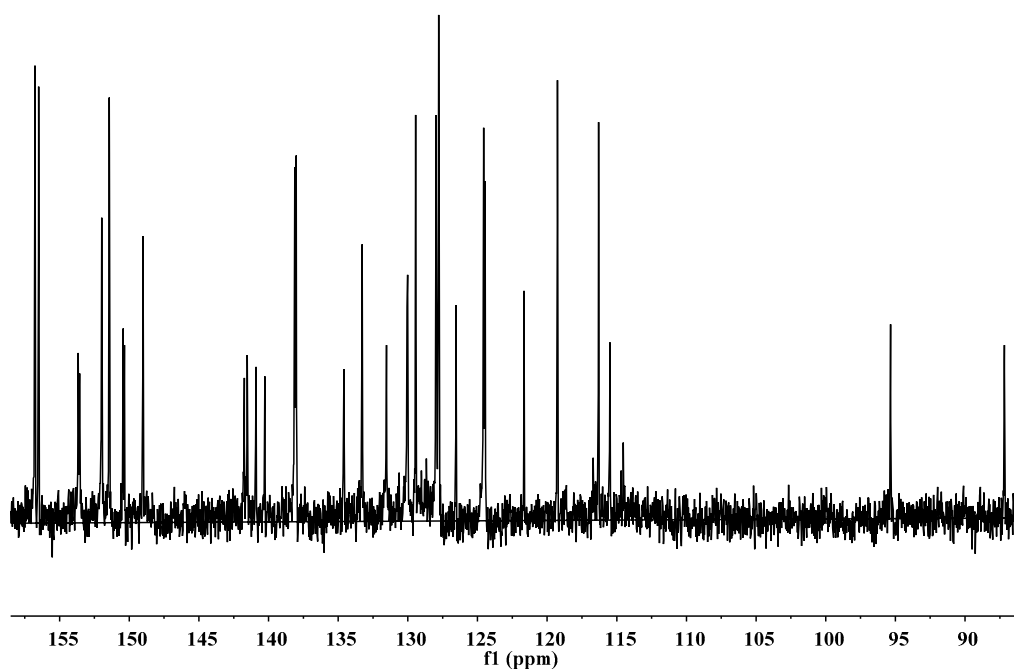


Figure S18. The ^{13}C NMR spectra of $\Delta\text{-3}$.

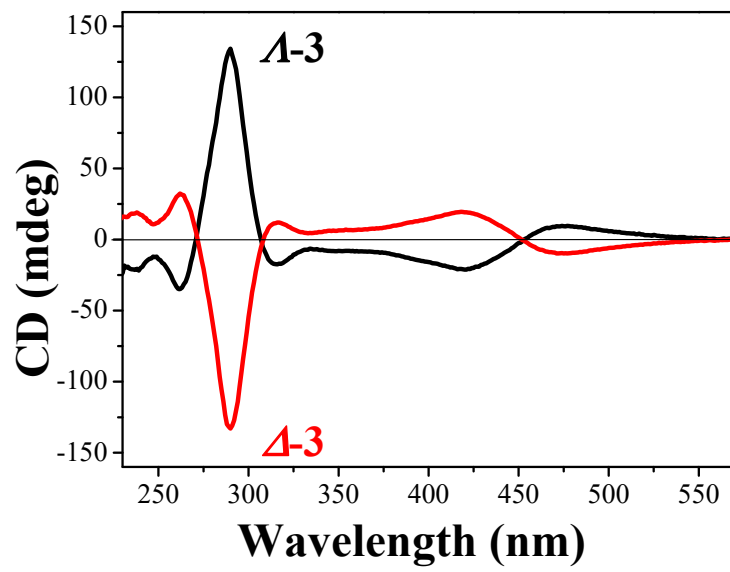


Figure S19. The CD spectra of Λ -3 and Δ -3.

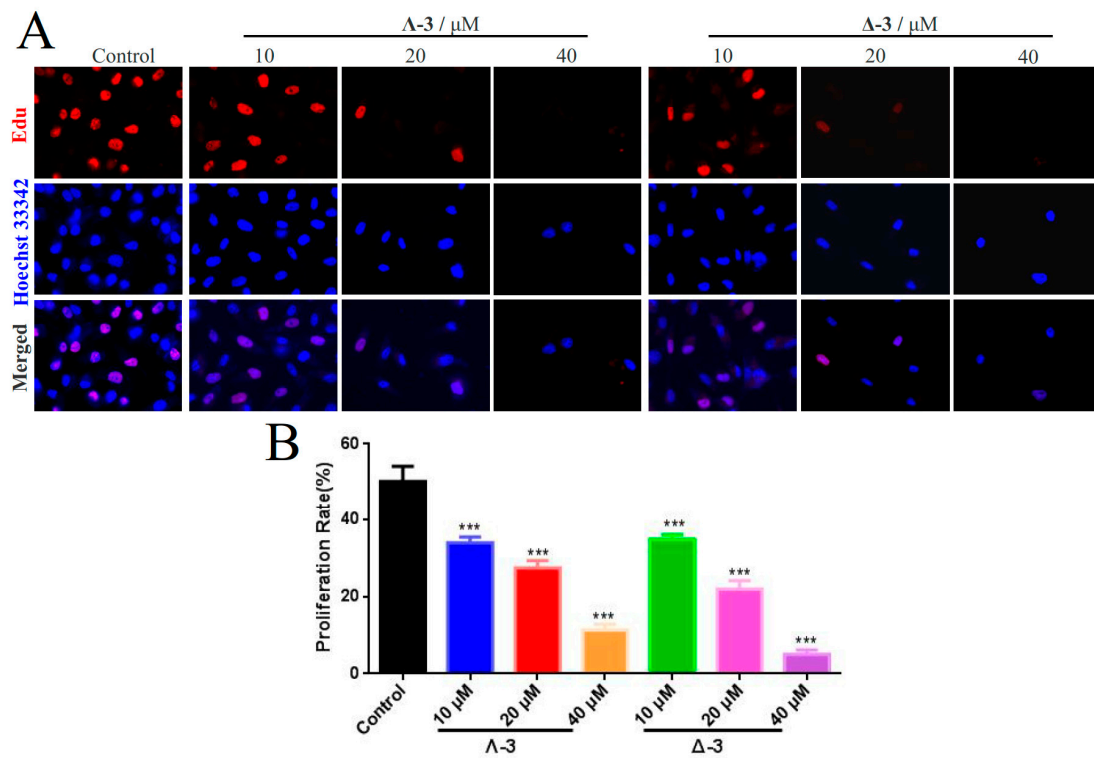


Figure S20. (A) EdU proliferation assay analysis and (B) proliferation rate of the effect of Λ -3 and Δ -3 on the growth of MDA-MB-231 cells.

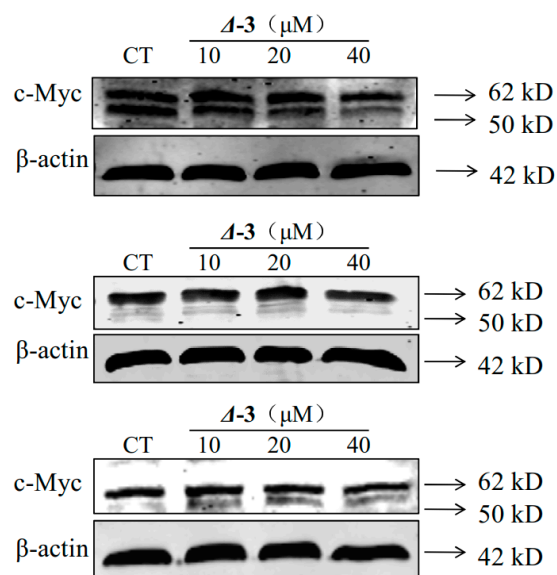


Figure S21. The expression of c-myc protein changed after dealt with Δ -3 (0, 10, 20 and 40 μ M) in MDA-MB 231 cells for 72 h (three repeat measurement).

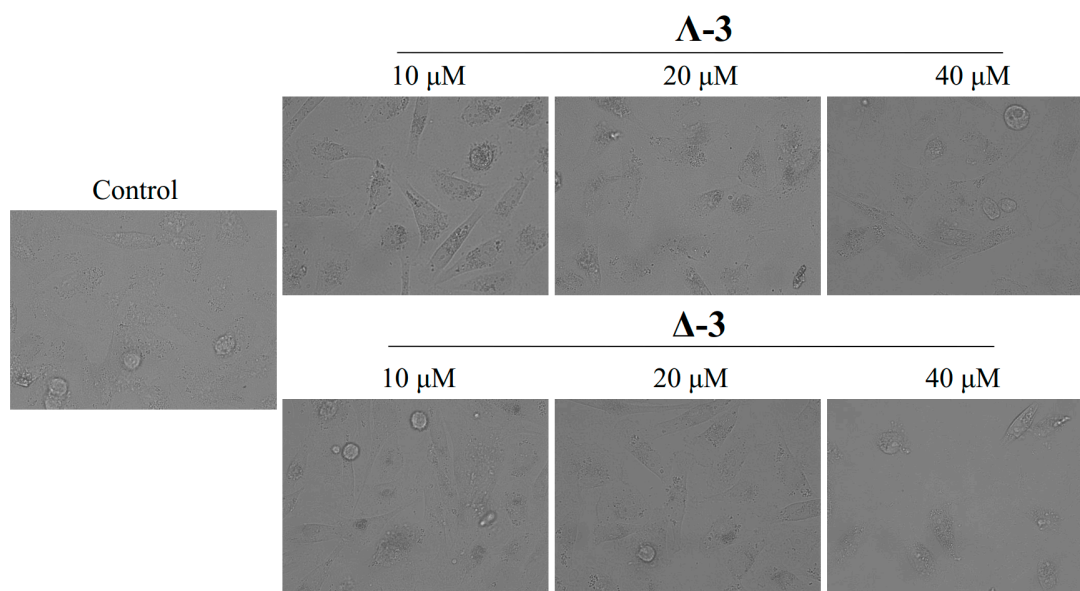


Figure S22. The morphological change of MDA-MB-231 cells in the absence and presence of Δ -3 and Δ -3 (0,10, 20 and 40 μ M) for 72 h.

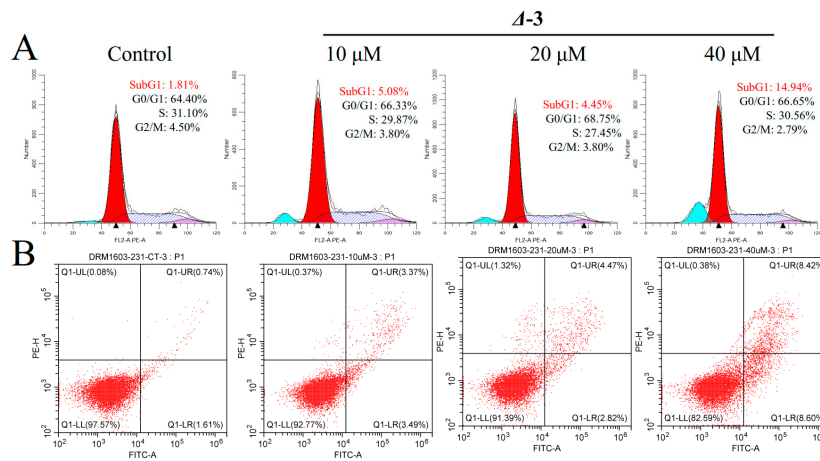
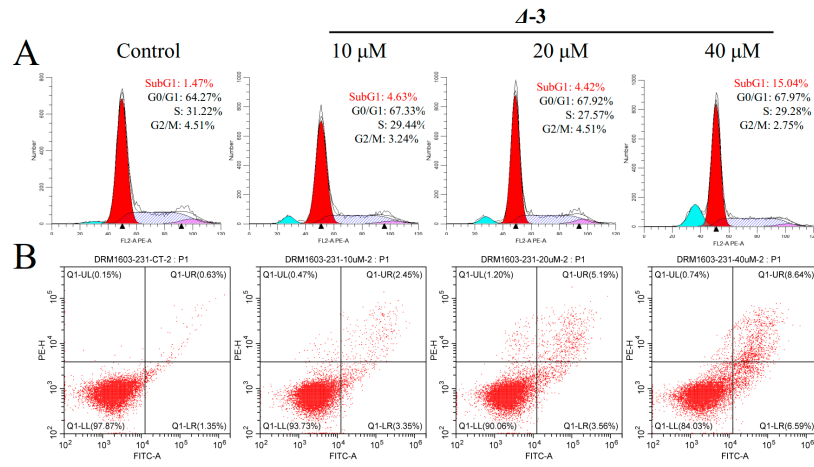
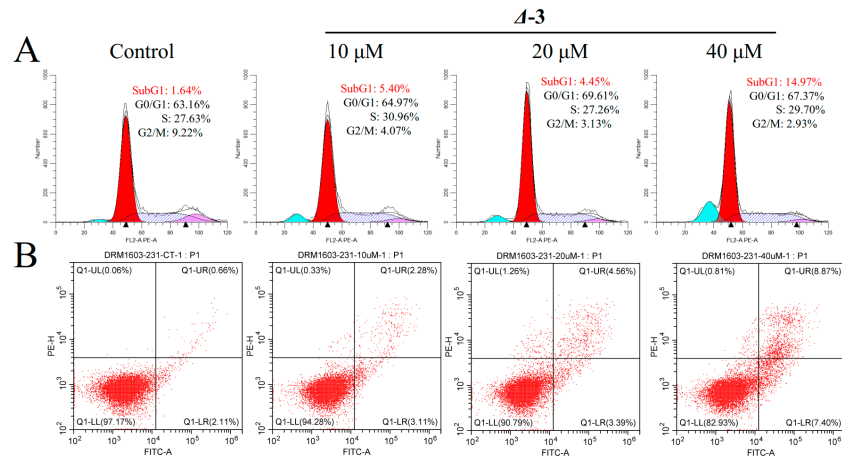


Figure S23. Cell cycle distribution (A) and apoptosis (B) of MDA-MB-231 cells incubated with **4-3** (0, 10, 20 and 40 μ M) for 72 h tested by flow cytometric analysis (three biological repetition).

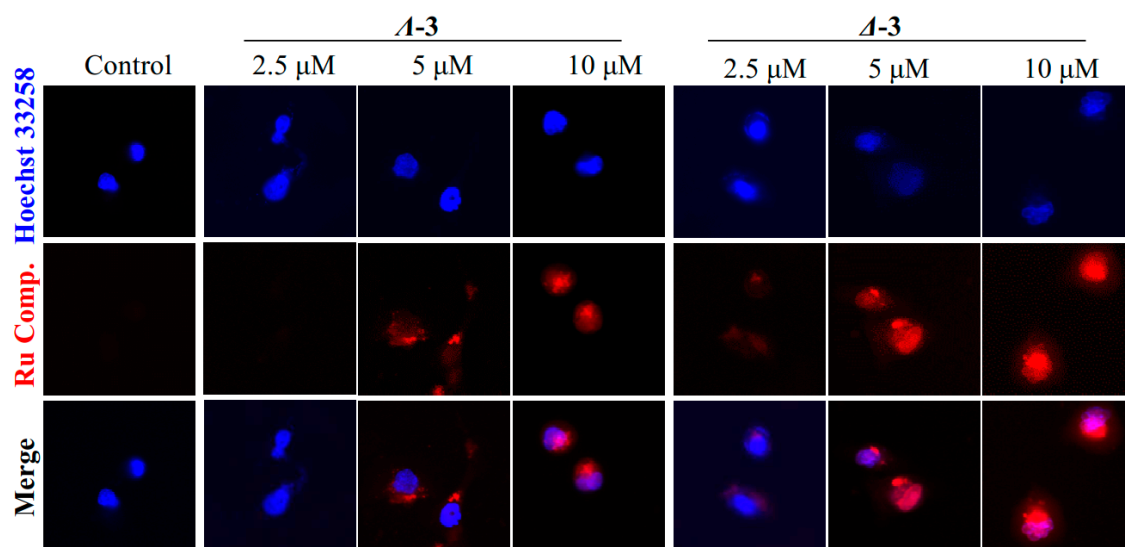


Figure S24. The cellular localization of ***Λ -3*** and ***Δ -3*** in MDA-MB-231 cells.

MDA-MB-231 cells treated with ***Λ -3*** and ***Δ -3*** (2.5, 5 and 10 μ M) for 24 h. Red:

Ru(II) complex, blue: Hoechst33258.