**Supporting Materials**

# Biological evaluation of the neocryptolepine derivative MMNC as a potential antitumor agent by PI3K/AKT/mTOR signaling

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**Table S1** The molecular docking scoring of MMNC and proteins

**Figure S1** $^{1}$H NMR spectra of MMNC

**Figure S2** $^{13}$C NMR spectra of MMNC

**Figure S3** Mass spectrometry of MMNC

**Figure S4** Purity test of MMNC by HPLC

**Table S1. The molecular docking scoring of MMNC and proteins**

| Target | PDB ID | Resolution (Å) | Organisms | Docking score |
|---|---|---|---|---|
| CDK1 | 4y72 | 2.3 | *Homo sapiens* | -8.834 |
| MEK | 5eym | 2.7 | *Homo sapiens* | -7.613 |
| PI3K | 6gvf | 2.5 | *Homo sapiens* | -7.543 |
| mTOR | 4jt6 | 3.6 | *Homo sapiens* | -7.45 |
| β-catenin | 3tx7 | 2.76 | *Homo sapiens* | -7.397 |
| JNK | 4y5h | 2.06 | *Homo sapiens* | -7.207 |
| P21 | 5bms | 2.9 | *Homo sapiens* | -7.137 |
| Raf | 5fd2 | 2.89 | *Homo sapiens* | -7.057 |
| Cyclin $E_1$ | 5l2w | 2.8 | *Homo sapiens* | -6.963 |
| Cyclin A | 6gue | 1.99 | *Homo sapiens* | -6.793 |
| AKT | 6hhf | 2.9 | *Homo sapiens* | -6.436 |
| MAPK | 6tca | 3.7 | *Homo sapiens* | -6.113 |
| JAK | 5tq6 | 2.06 | *Homo sapiens* | -5.91 |
| Caspase-3 | 6x8k | 2.17 | *Homo sapiens* | -5.536 |
| E-cadherin | 3l6y | 3 | *Homo sapiens* | -4.314 |
| CDK6 | 1jow | 3.1 | *Homo sapiens* | -4.105 |
| Ras | 7jhp | 2.77 | *Homo sapiens* | -4.048 |
| Bcl-2 | 4b4s | 1.9 | *Homo sapiens* | -3.987 |

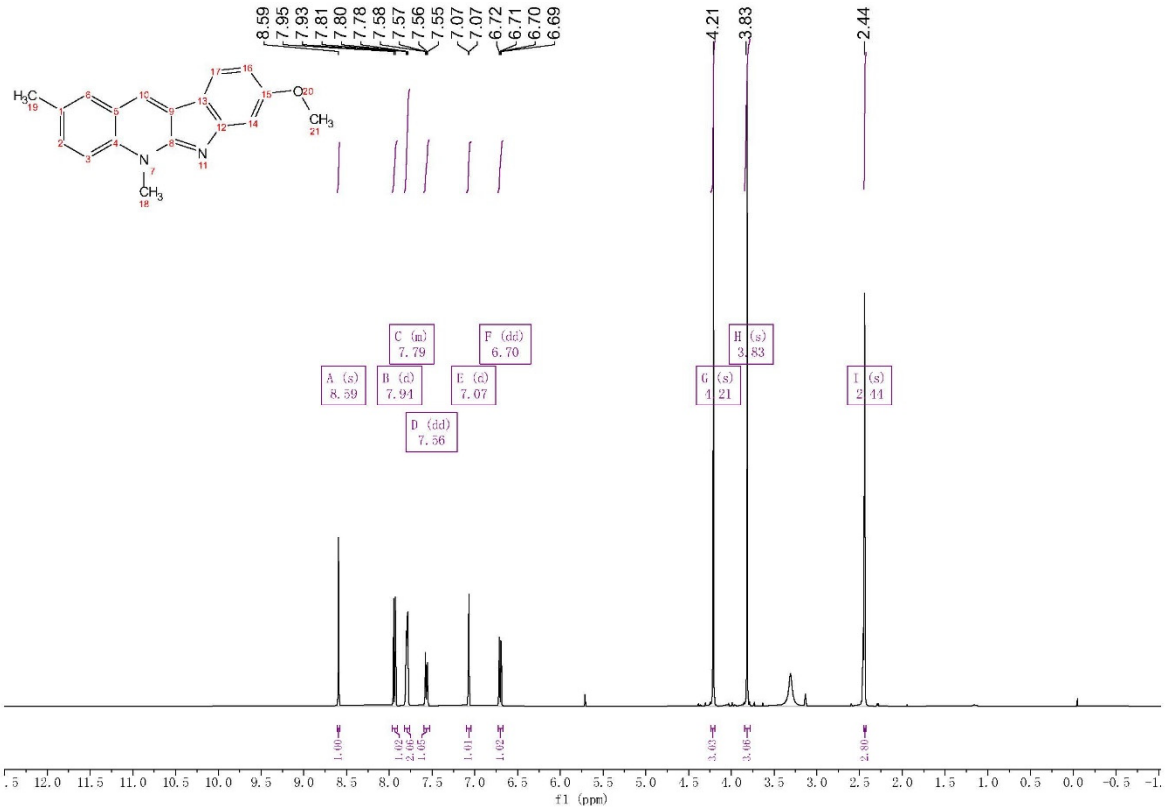


Figure S1 $^{1}$H NMR spectra of MMNC

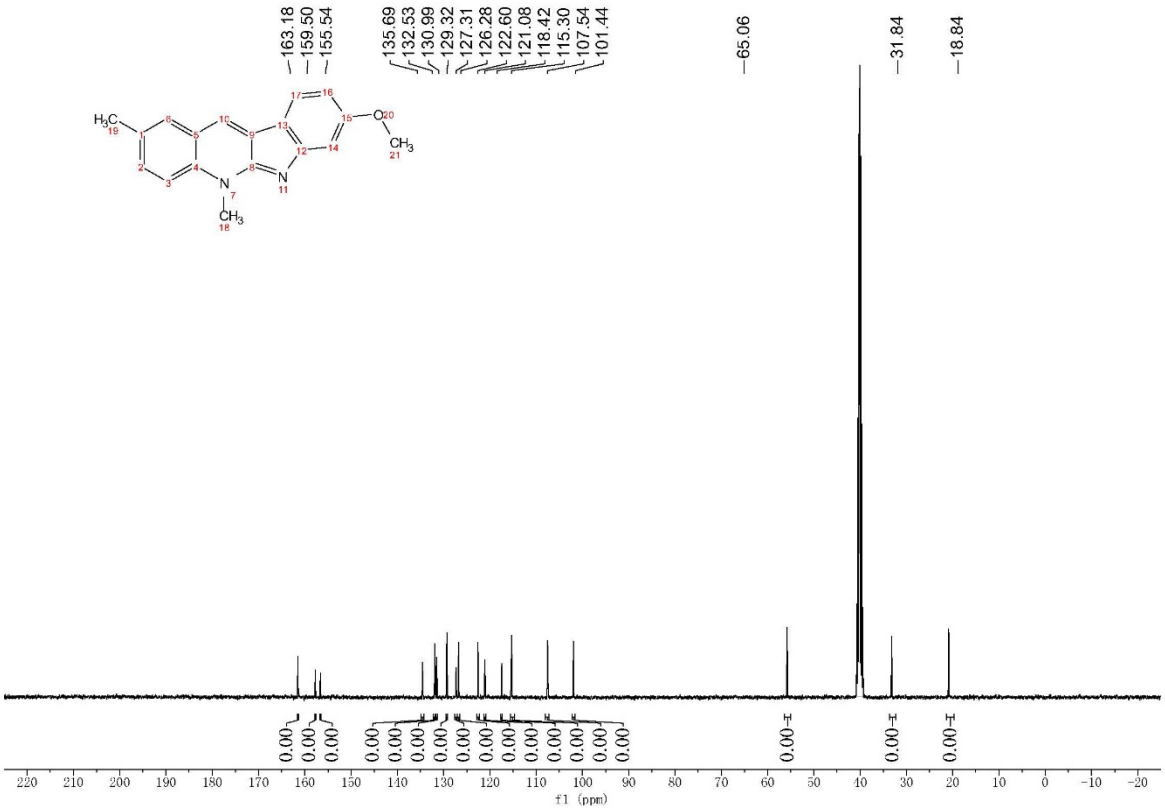


Figure S2 $^{13}$C NMR spectra of MMNC

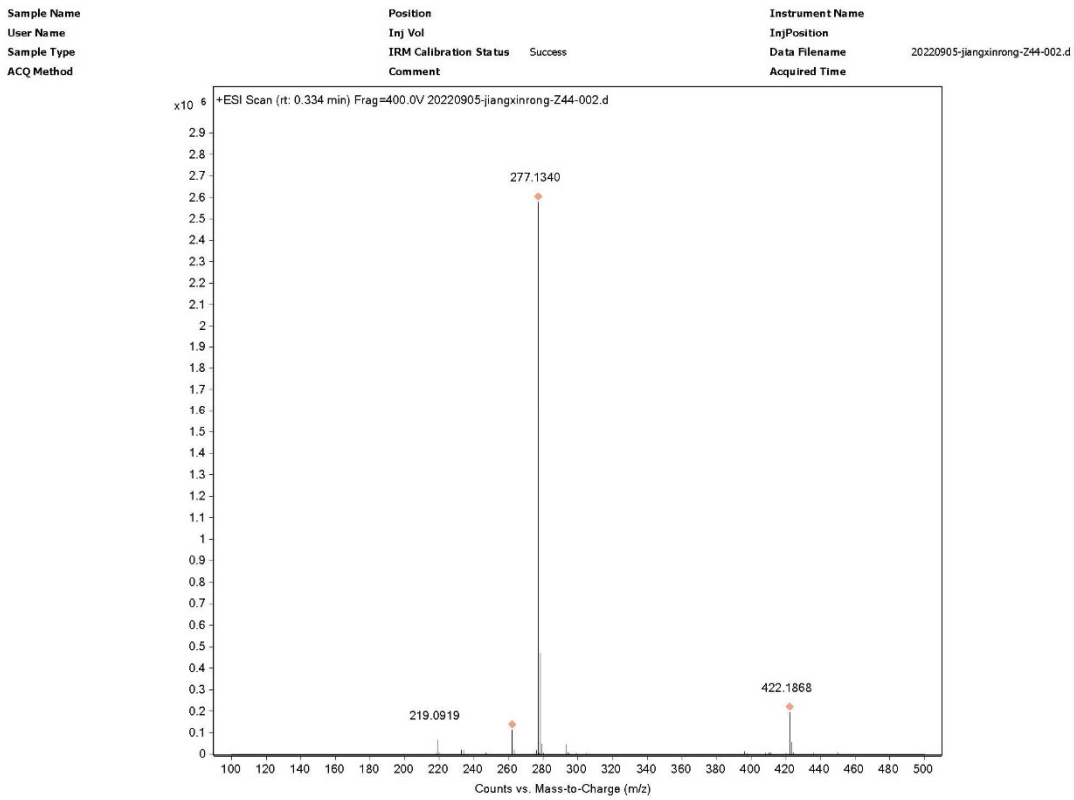


Figure S3 Mass spectrometry of MMNC

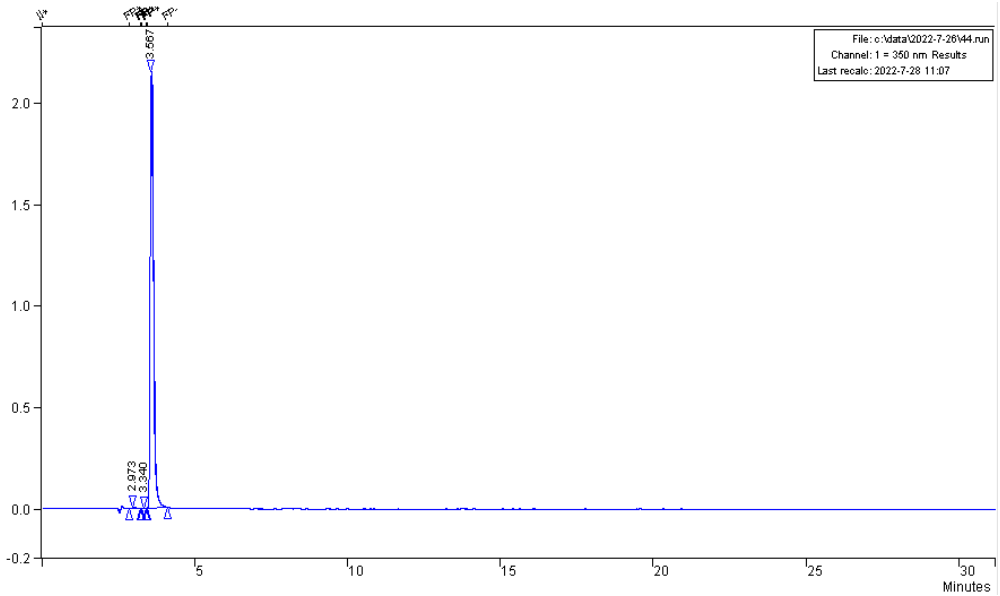


Figure S4 Purity test of MMNC by HPLC