

PNSA, a novel C-terminal inhibitor of HSP90, reverses epithelial-mesenchymal transition and suppresses metastasis of breast cancer cells in vitro

Aotong Zhang¹, Xin Qi¹, Fu Du¹, Guojian Zhang^{1,2}, Dehai Li^{1,2} and Jing Li^{1,2}

¹ Key Laboratory of Marine Drugs, Chinese Ministry of Education, School of Medicine and Pharmacy, Ocean University of China, Qingdao 266003, China

² Open Studio for Druggability Research of Marine Natural Products, Laboratory for Marine Drugs and Bioproducts, Qingdao National Laboratory for Marine Science and Technology, Qingdao 266237, China

* Correspondence: authors: Key Laboratory of Marine Drugs, Chinese Ministry of Education, School of Medicine and Pharmacy, Ocean University of China, Qingdao 266003, China.
lijing_ouc@ouc.edu.cn (Jing.Li); Tel: +81-0532-82031980; Fax: +81-0532-82031980;

Supplemental Information Table of Contents

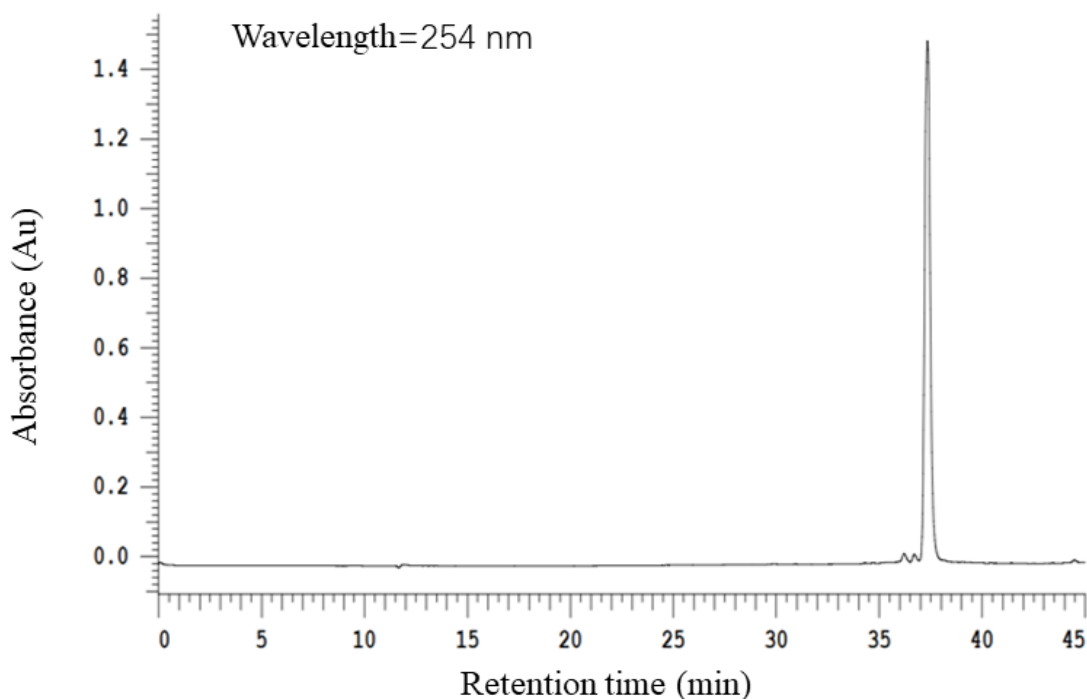
The structure elucidation of PNSA

Figure S1: HPLC-UV analysis of PNSA.

Table S1: Peak purity report of PNSA.

Table S2: HPLC gradient profile for detection of PNSA.

Figure S2: The ¹H NMR (500 MHz) spectrum of PNSA in CD₃OD.



Supplementary Figure S1. HPLC-UV analysis of PNSA. The PNSA was analyzed by HPLC made by the HITACHI company equipped with a 5430 diode array detector and a

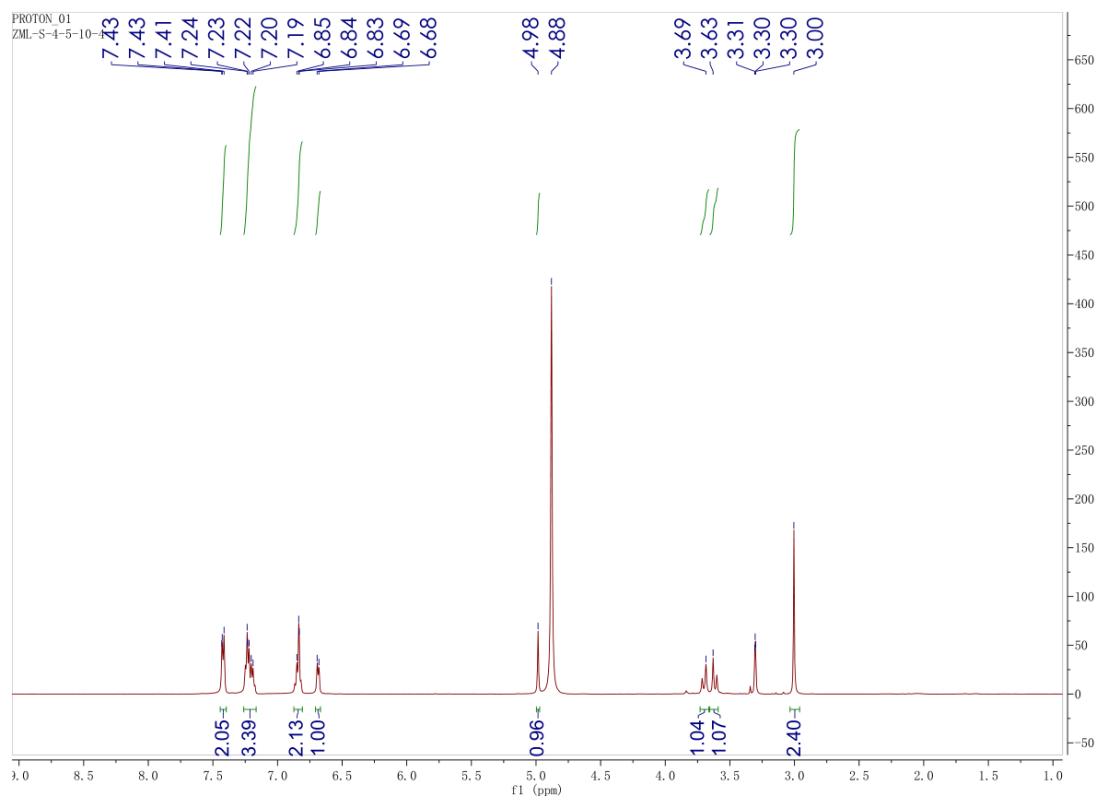
C18 column (YMC-Pack ODS-A, 4.6 × 250 mm, 5 μm, 1 mL/min) by using stepwise gradient elution with 5–100% MeOH–H₂O (0-5 min: 5%; 5-35 min: 5%-100%; 35-40 min: 100%; 40.1-45 min 5%).

Supplementary Table S1. Peak purity report of PNSA.

| No. | RT | Area | Concentration |
|-----|--------|----------|---------------|
| 1 | 36.200 | 148084 | 1.127 |
| 2 | 37.333 | 12988293 | 98.873 |
| | | 13136377 | 100.00 |

Supplementary Table S2. HPLC gradient profile for detection of PNSA (A: Methanol B: Water).

| Time (min) | Solvent A (%) | Solvent B (%) | Flow (mL/min) |
|------------|---------------|---------------|---------------|
| 0.0 | 5.0 | 95.0 | 1.000 |
| 5.0 | 5.0 | 95.0 | 1.000 |
| 35.0 | 100.0 | 0.0 | 1.000 |
| 40.0 | 100.0 | 0.0 | 1.000 |
| 40.1 | 5.0 | 95.0 | 1.000 |
| 45.0 | 5.0 | 95.0 | 1.000 |



Supplementary Figure S2. The ¹H NMR (500 MHz) spectrum of PNSA in CD₃OD.