

Supporting Information

Synthesis and Biological Evaluation of Novel Olean-28,13 β -lactams as Potential Anti-prostate Cancer Agents

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HPLC assessment of compound purity.

All tested compounds (**10a-i**) with a purity of > 95% were used for subsequent biological assays. We provided the spectra of HPLC assays as below.

Column: Inertex C18 (150 mm × 4.6 mm × 5 μm);

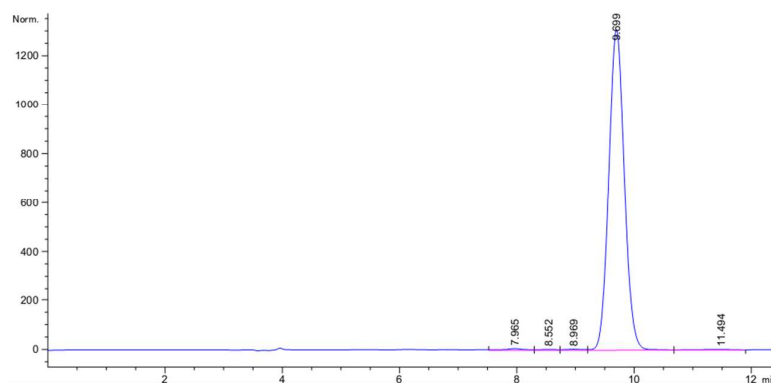
Mobile phase: Methanol-Water (85:15 to 90:10, v/v);

Wavelength: 244 nm;

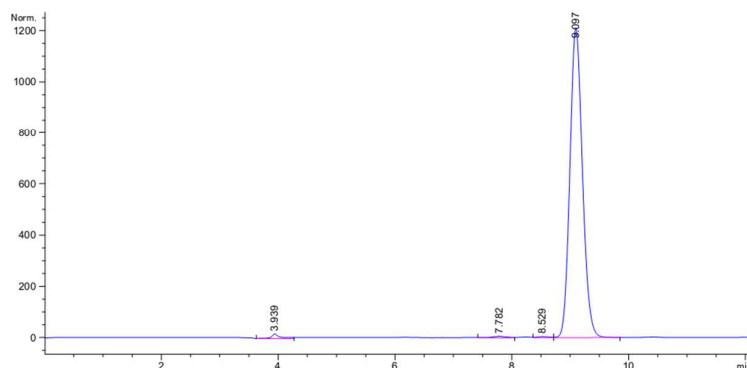
Rate: 0.8 mL/min;

Temperature: 25 °C;

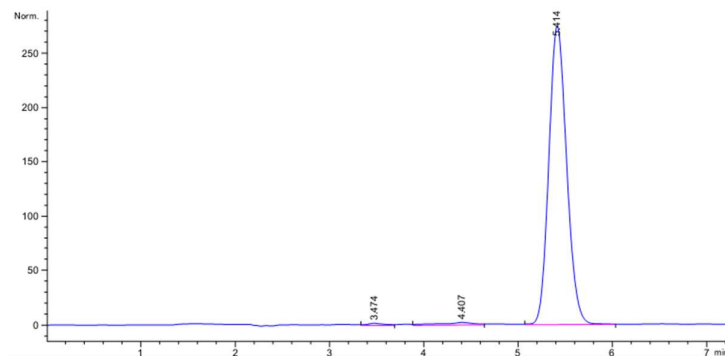
10a, 98.2%



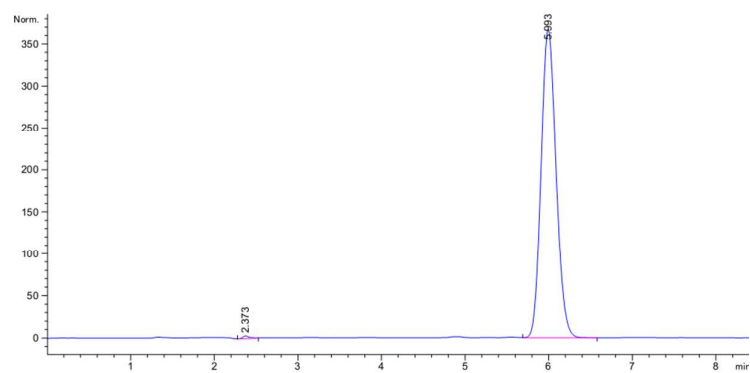
10b, 98.0%



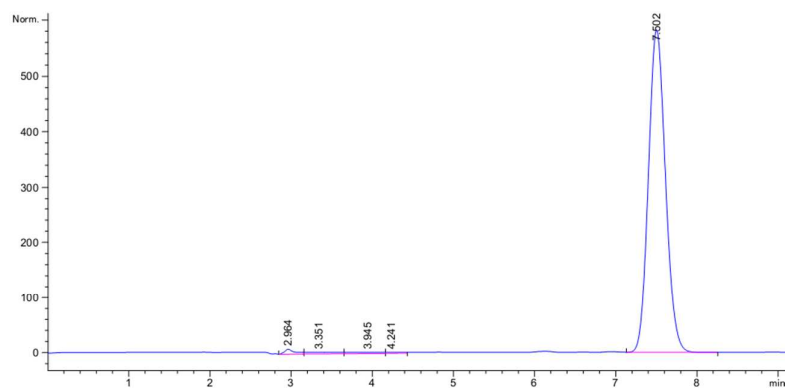
10c, 97.6%



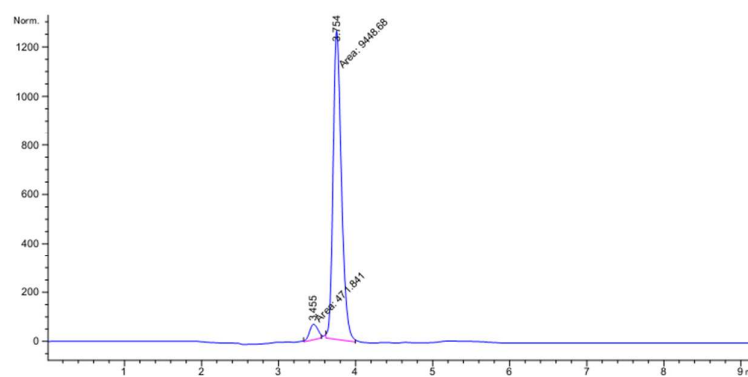
10d, 99.6%



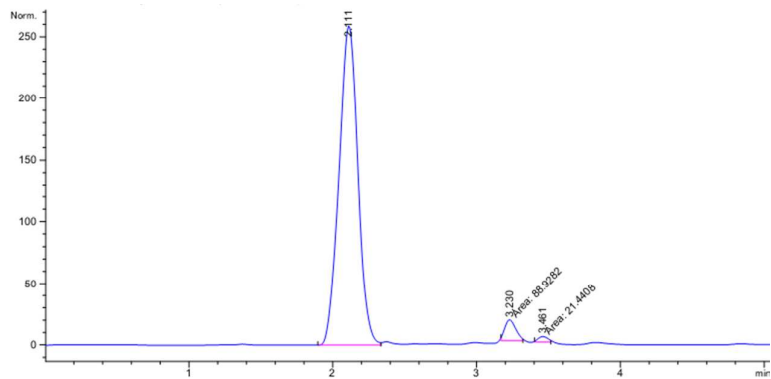
10e, 97%



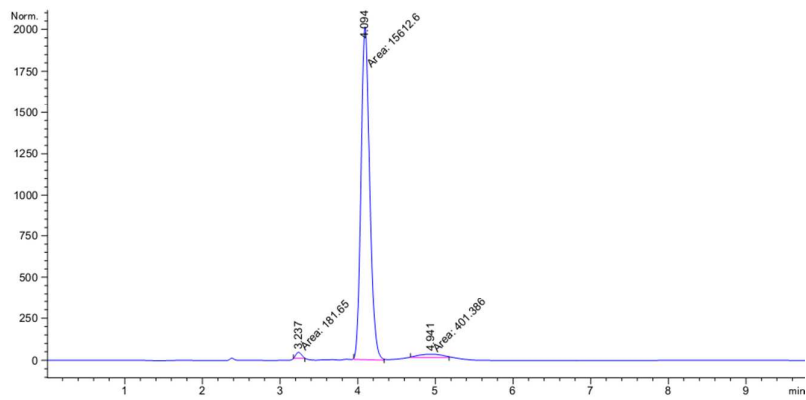
10f, 95.2%



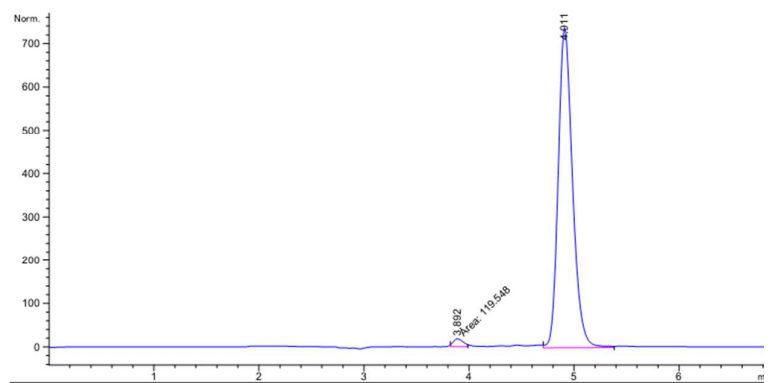
10g, 95.5%



10h, 96.4%



10i, 98.3%



11h, 100%

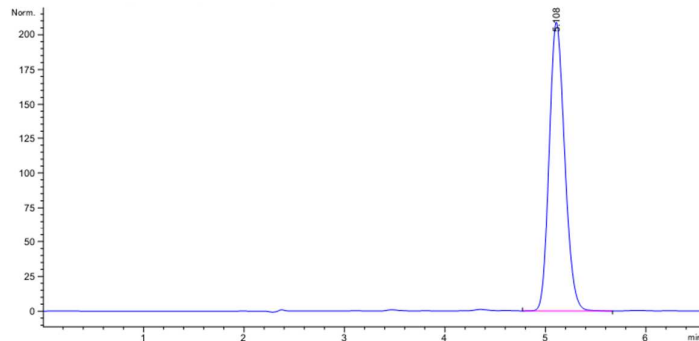
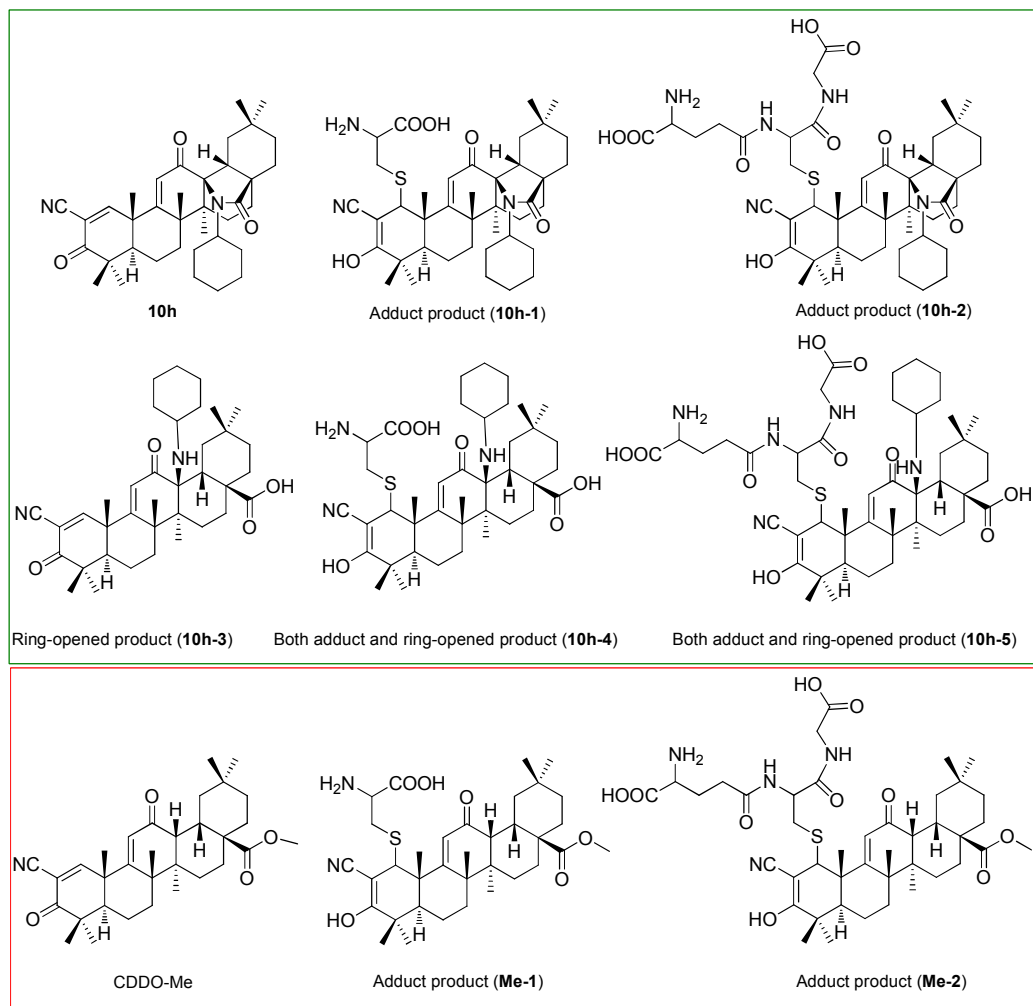


Table S1. The Log *P* of selective compounds

Compd	Log <i>P</i>	Compd	Log <i>P</i>
10a	5.4 ± 0.9	10e	7.2 ± 0.1
10b	5.8 ± 0.9	10f	6.3 ± 0.5
10c	6.1 ± 0.7	10g	4.5 ± 0.5
10d	6.5 ± 0.4	10i	6.8 ± 0.3
CDDO-Im	5.7 ± 0.3		

^aLog *P* values were calculated using the methods reported previously. Data are expressed as the means ± SD from three different programs.

Table S2. Possible metabolic products of **10h** and CDDO-Me.^a



Possible metabolic products	Compd	Cys	GSH	Rat plasma	HLM
Adduct products	10h	yes	yes	yes	yes
	CDDO-Me	yes	yes	yes	yes
Ring-opened products	10h	no	no	no	no
Both adduct and ring-opened products	10h	no	no	no	no

^aTest compound (2 μ M) was incubated in 0.2 mg/mL of cysteine (Cys), glutathione (GSH), rat plasma, or human liver microsomes (HLM) in 0.1 M phosphate buffer at 37°C for 1h.