

Supplementary Materials: Design, Synthesis and In Vitro Evaluation of the Photoactivatable Prodrug of the PARP Inhibitor Talazoparib

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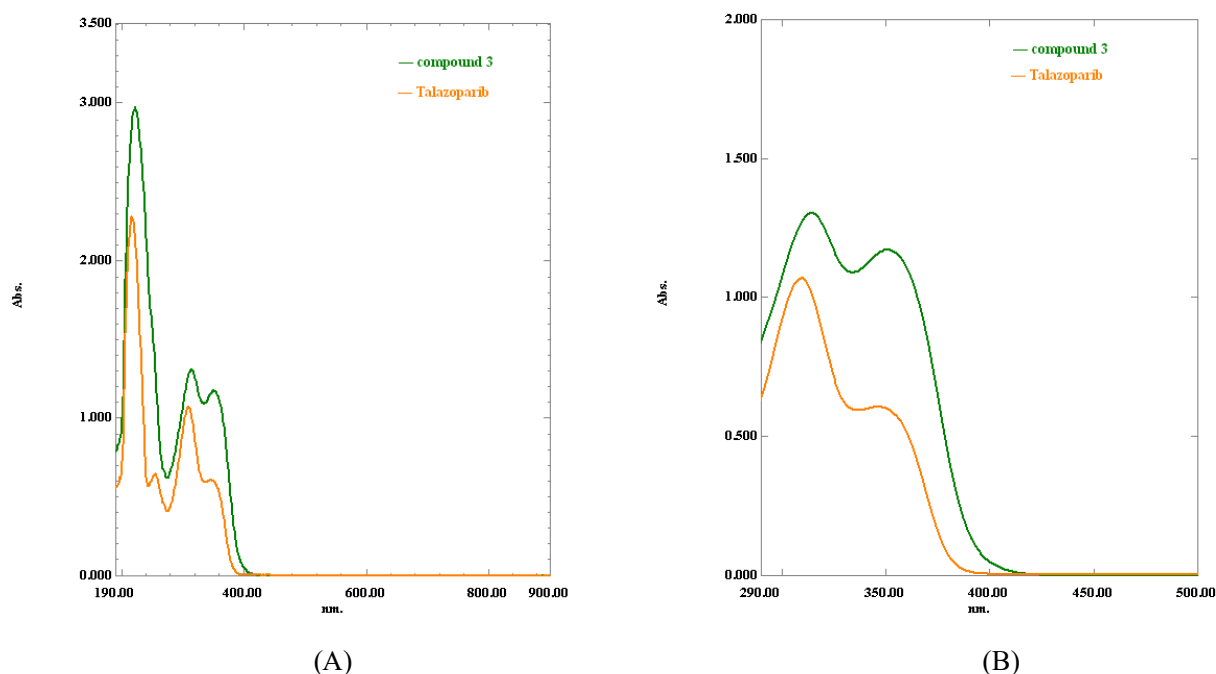


Figure S1. UV/Vis absorption spectra of Compound 3 and Talazoparib in methanol solution. (A) Full wavelength scanning; (B) Local UV/Vis absorption spectra with a wavelength range of 290-500 nm. Compound 3 and Talazoparib were tested at a same concentration of 0.1 mM. Introduction of the PPG into the parent compound's molecular structure leads to increased light absorption around 365 nm. Wavelengths shorter than 300 nm is highly energetic and can easily damage tissues and cells. Therefore, 365 nm was considered as the optimal wavelength for deprotection.

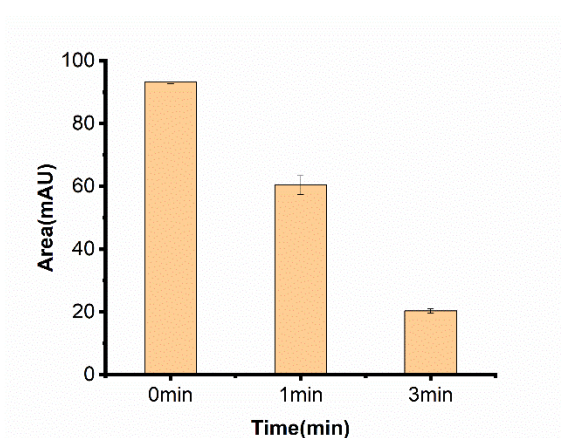


Figure S2. UV-cleavage test on the Compound 3 in culture medium DMEM. Compound 3 were dissolved in DMEM medium containing 0.1 %DMSO and added to 96-well plates at a final concentration of 10 μ M. After being irradiated for 1 min and 3 min at 365 nm respectively, the samples were analyzed by HPLC. The peak area is plotted against the irradiation time.

Qualitative Analysis Report

Data Filename	5519.d	Sample Name	LIG-0308
Instrument Name	TOF G6230A	Acquired Time	2019-08-23
Acq Method	YCL.M	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

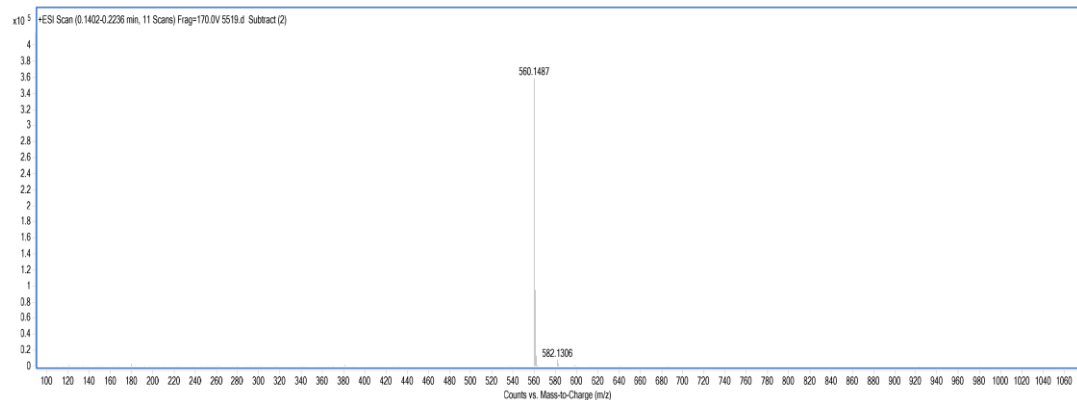


Figure S5. Mass spectrometry of compound 3.

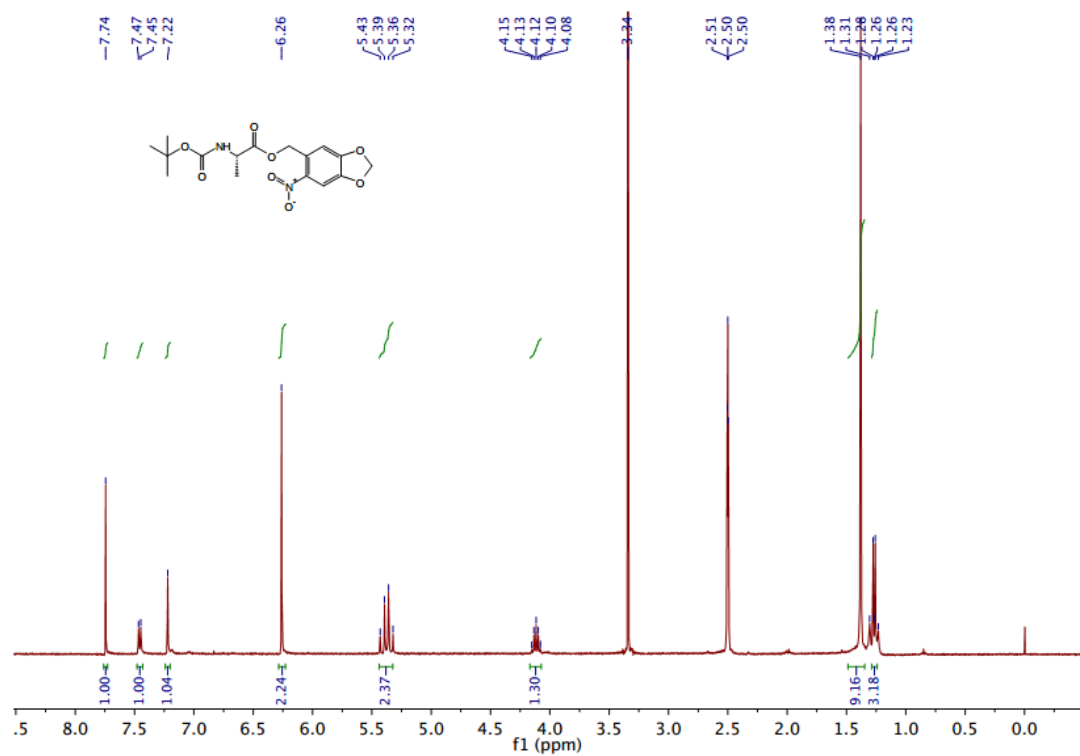


Figure S6. ¹H-NMR spectrometry of compound 6.

Qualitative Analysis Report

Data Filename	5520.d	Sample Name	LIG-0307
Instrument Name	TOF G6230A	Acquired Time	2019-08-23
Acq Method	YCL.M	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

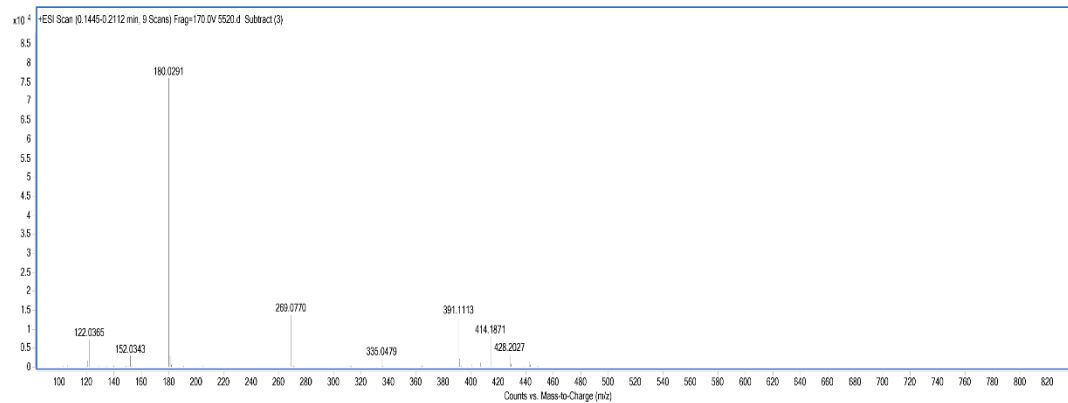


Figure S7. Mass spectrometry of compound 6.