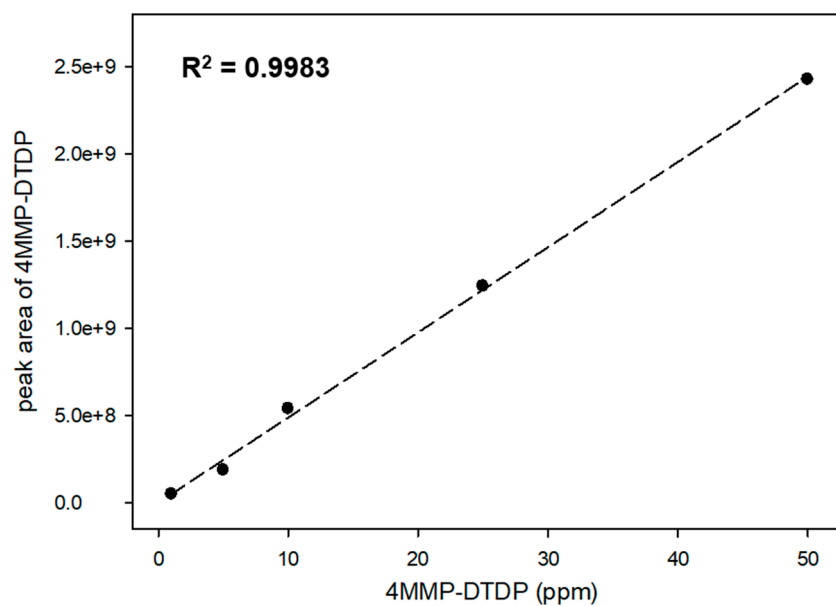


Supplementary Table S1. Comparison of different purification methods for cys-4MMP production.

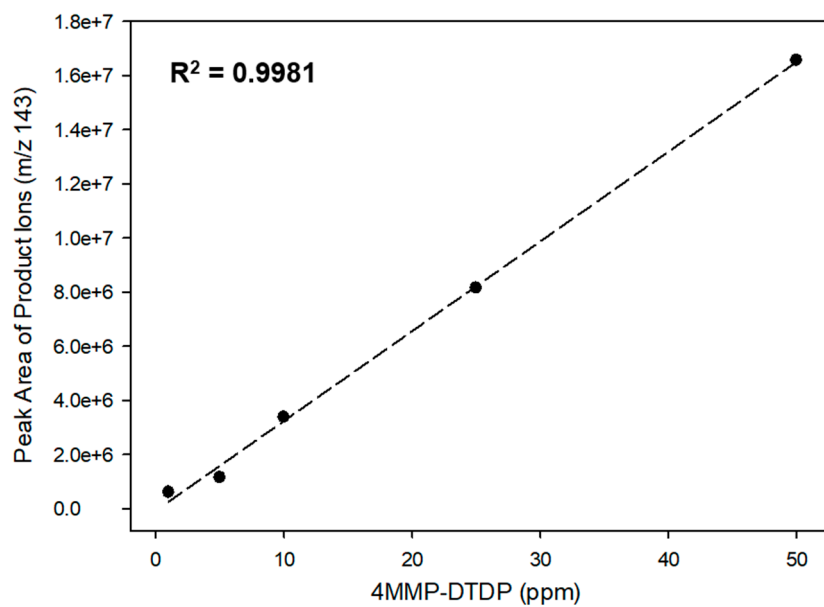
Starting Material	End Product	Purification	Purity	Yield	Toxic Chemical Used	Ref
Cys·HCl·H ₂ O	Cys-4MMP	Silica column C ₁₈	NA	NA	None	[8]
Cysteine	Cys-4MMP	<ul style="list-style-type: none">• Extraction• Filtration and crystallization	Approx. 33%	22%	None	[21]
Cysteine	deuterated Cys-4MMP	Extraction	Approx. 41%	NA	Yes	[22]
Cys·HCl·H ₂ O	Cys-4MMP	<ul style="list-style-type: none">• Extraction• Silica gel column• Recrystallization	NMR grade	29.7–35%	None	This study

NA, not applicable.

A



B



Supplementary Figure S1. Standard calibration curves of 4MMP-DTDP in the concentration range of 1 ppm to 50 ppm were based on the extracted ion chromatogram of (A) precursor ion signal of 4MMP-DTDP at m/z 242.0, and (B) product ion signal of 4MMP-DTDP at m/z 144.0.