

## **Supporting Information**

### **Identifying Cysteine, *N*-Acetylcysteine, and Glutathione-Conjugates as Novel Metabolites of Aristolochic Acid I: Emergence of a New Detoxification Pathway**

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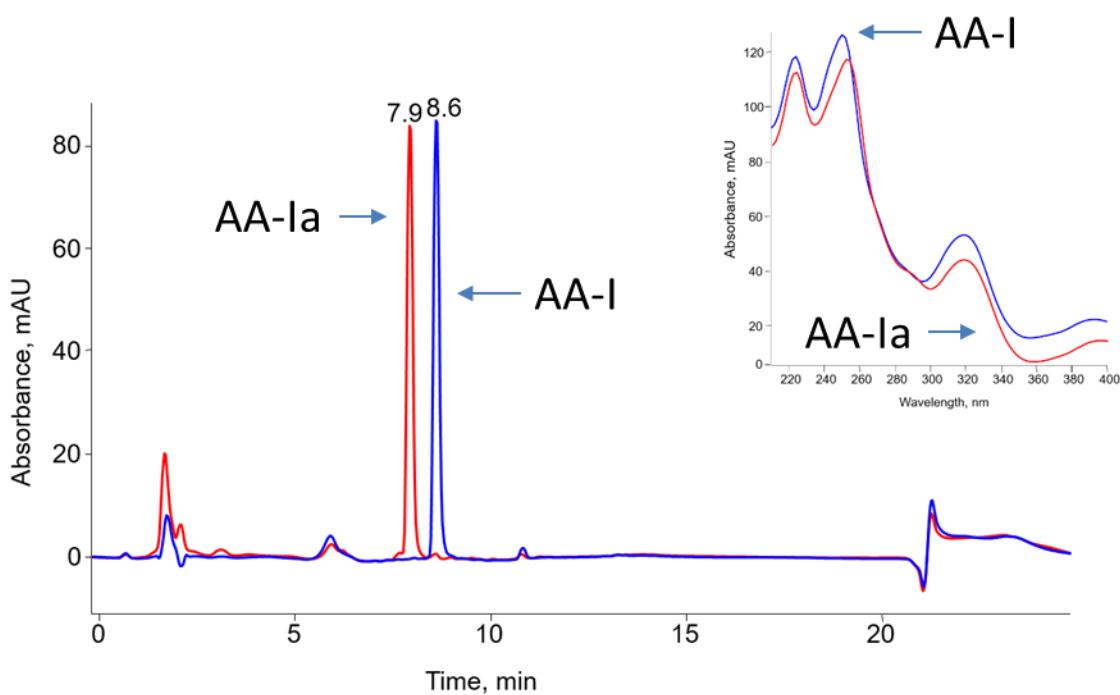
<sup>§</sup> J. Z. and C.-K. C. contributed equally to this work.

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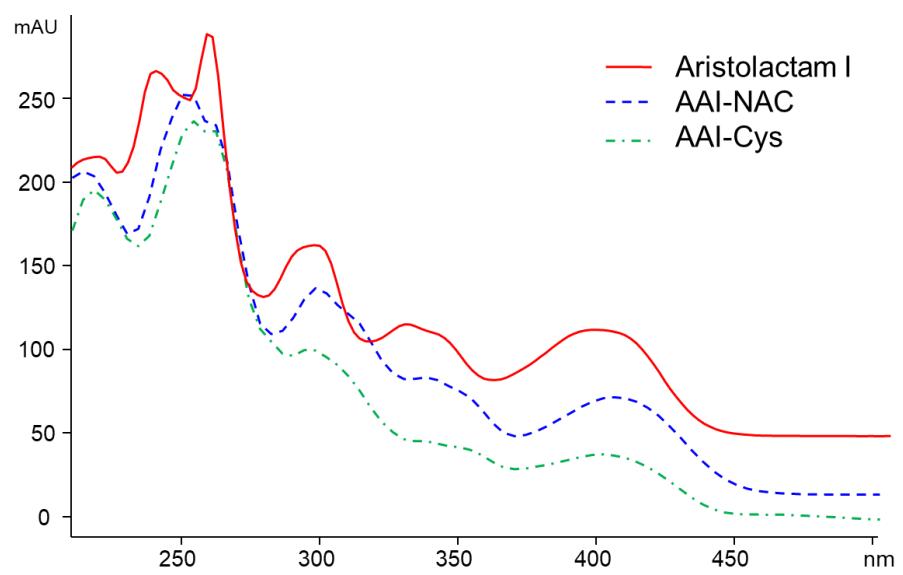
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**Table S1:** Optimized MS and MS<sup>2</sup> parameters used in quantitation of AA-I and its metabolites.

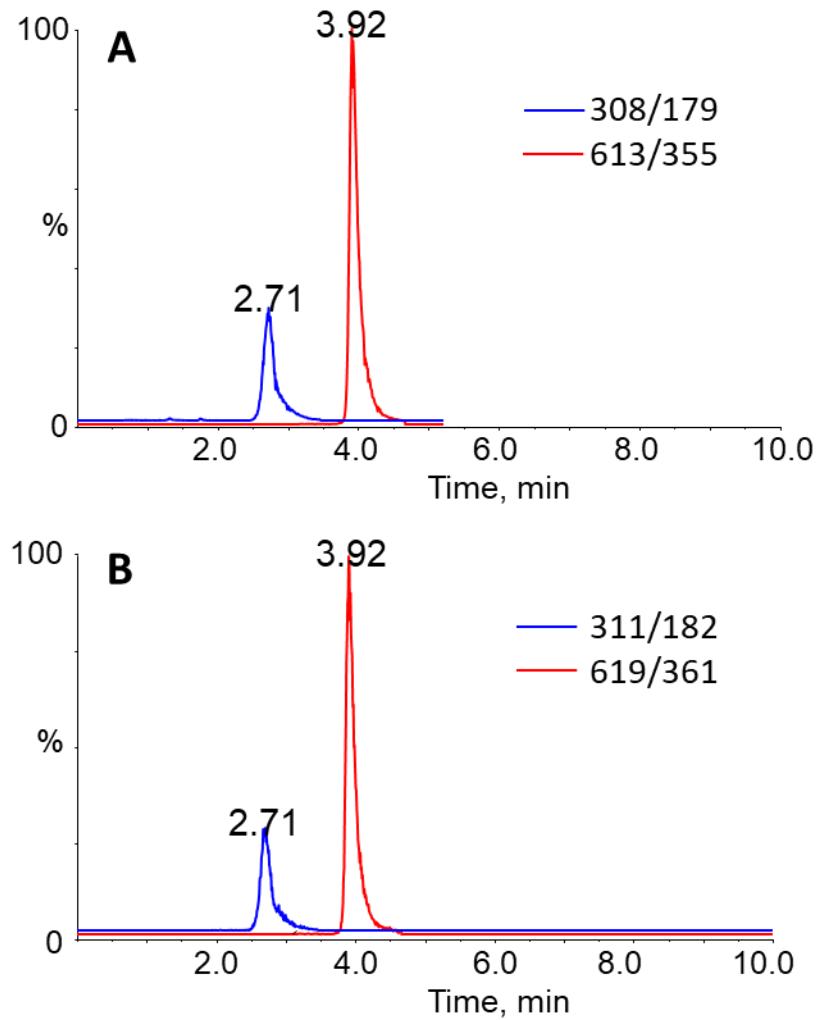
Capillary voltage	1.0 kV			
Source temperature	150 °C			
Desolvation temperature	650 °C			
Cone gas flow	150 L/hr			
Desolvation gas flow	850 L/hr			
Collision gas flow	0.15 mL/min			
Nebulizer gas flow	7.0 bar			
	Precursor ion, <i>m/z</i>	Product ion, <i>m/z</i>	Cone voltage, V	Collision energy, eV
AA-I	359	298	8	8
	359	324	8	12
AA-Ia	345	284	25	10
	345	310	25	8
AL-I	294	279	40	22
	294	251	40	30
AAI-Cys	413	324	25	15
	413	294	25	22
AAI-NAC	455	162	30	15
	455	294	30	12
AAI-GSH	599	177	35	22
	599	294	35	30



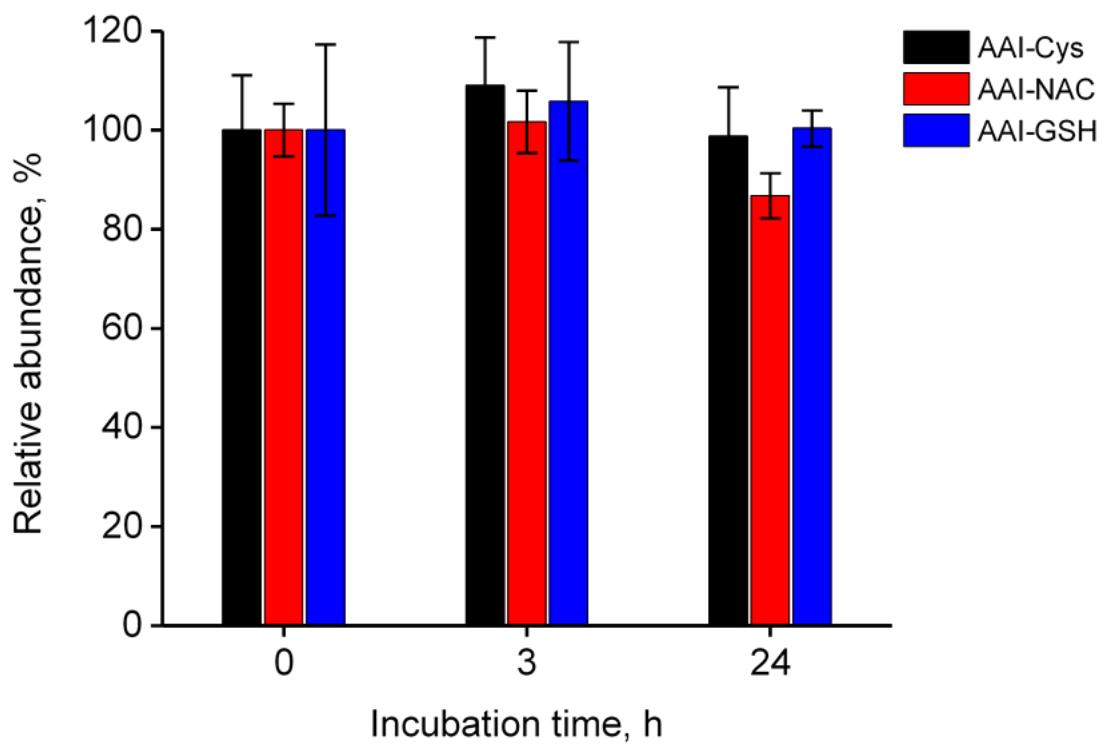
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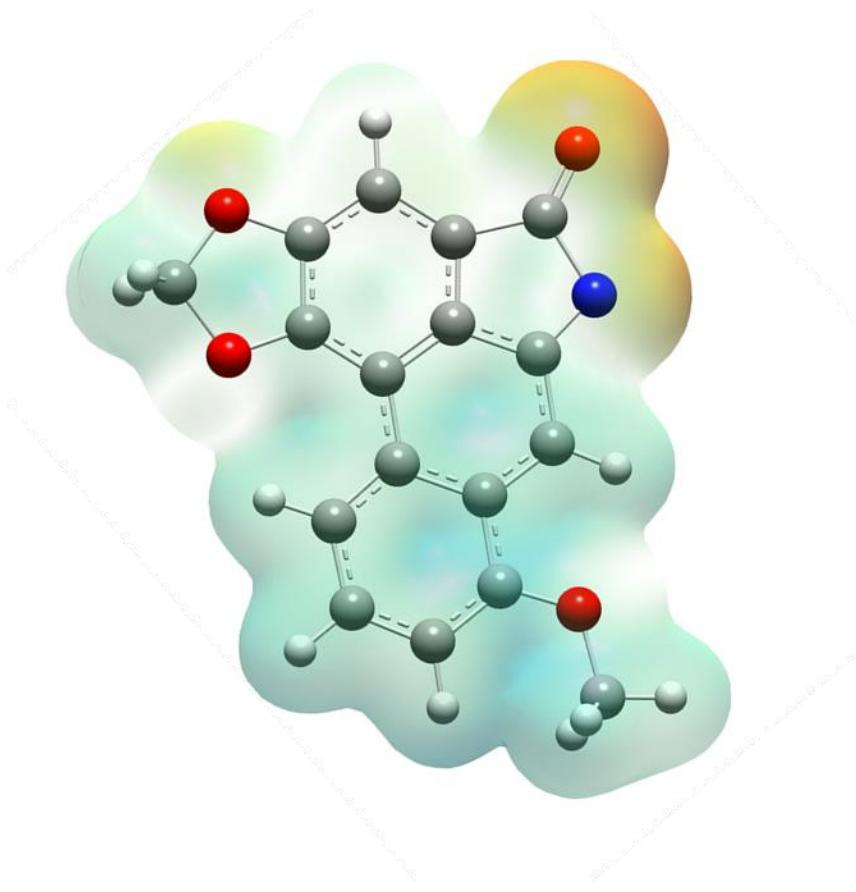
**Fig S2.** UV-absorption spectra of aristolactam I, the cysteine- and *N*-acetylcysteine conjugated metabolites of aristolactam I.



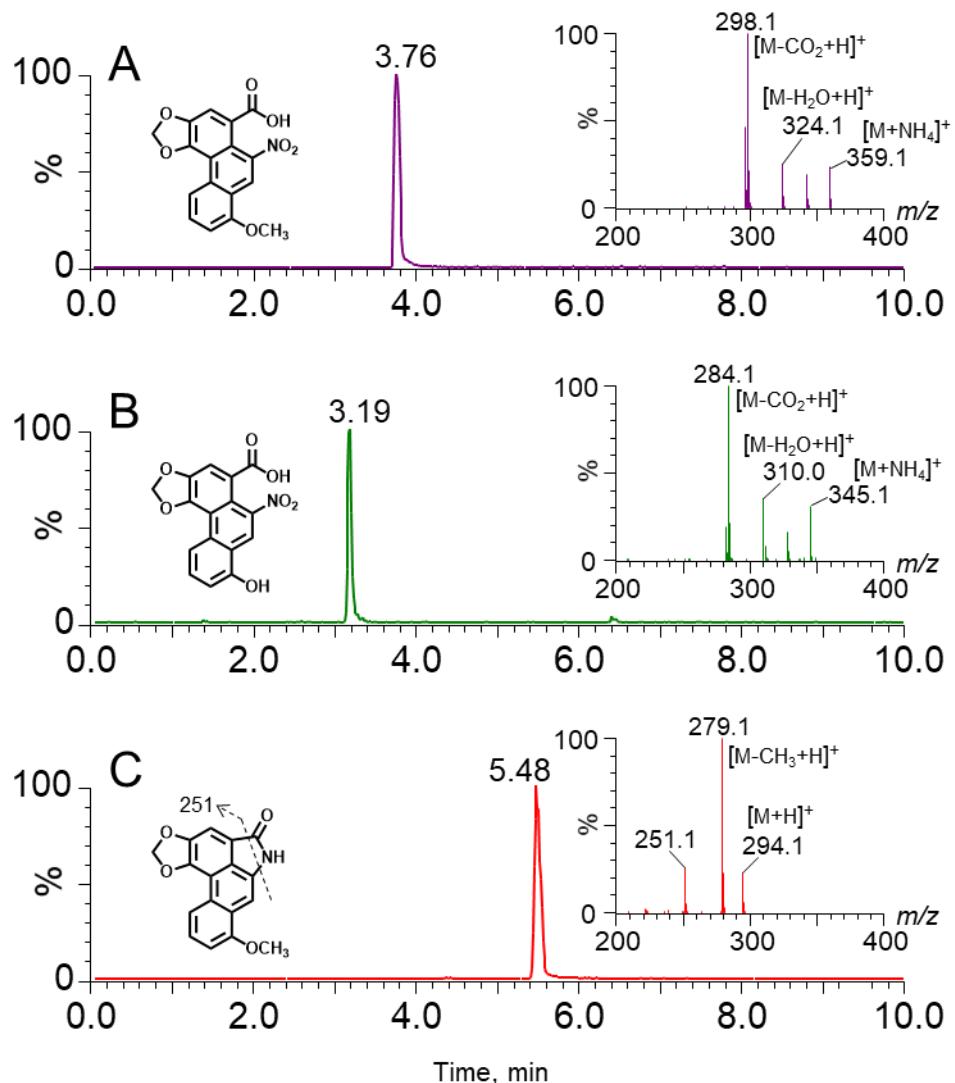
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**Fig S6.** Representative chromatograms from LC-MS/MS analysis of (A) AA-I, (B) AA-Ia, and (C) aristolactam I. Shown in the insets are the MS/MS spectrum of the corresponding  $[M+NH_4]^+$  (for AA-I and AA-Ia)  $[M+H]^+$  (for aristolactam I) ions.

## REFERENCES

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, revision D.01; Gaussian, Inc.: Wallingford, CT, 2009.