Supplementary Materials: Chemical Identity of Interaction of Protein with Reactive Metabolite of Diosbulbin B In Vitro and In Vivo

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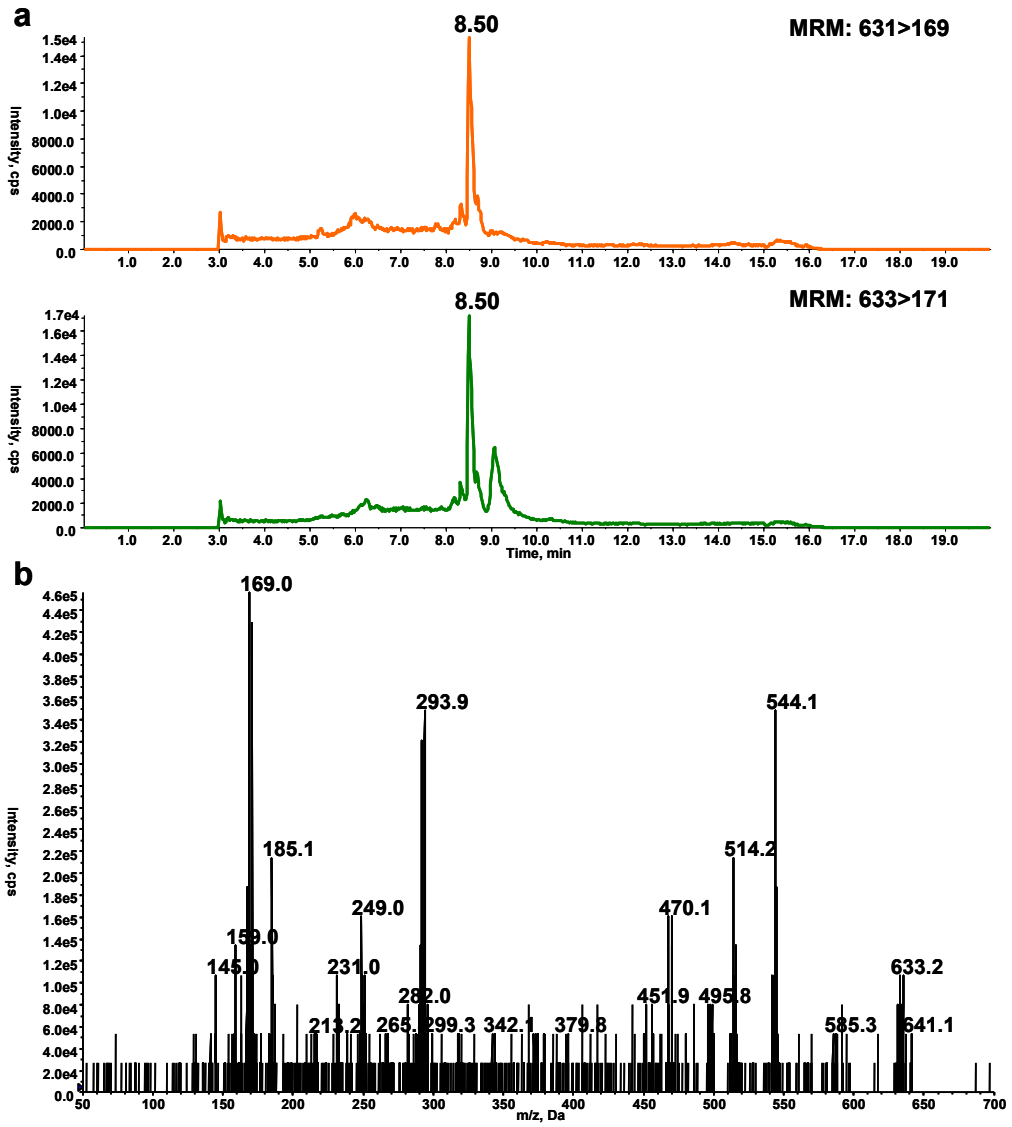

Figure S1. DIOB was oxidized by DMDO, and the resulting mixture was reacted with Cys and then with BBA, followed by LC-MS/MS analysis. **a**: Extracted ion chromatograms of MRM scans of *m*/*z* 631→169 (orange) and 633→171 (green). **b**: MS/MS spectrum of synthetic pyrrole **6.**

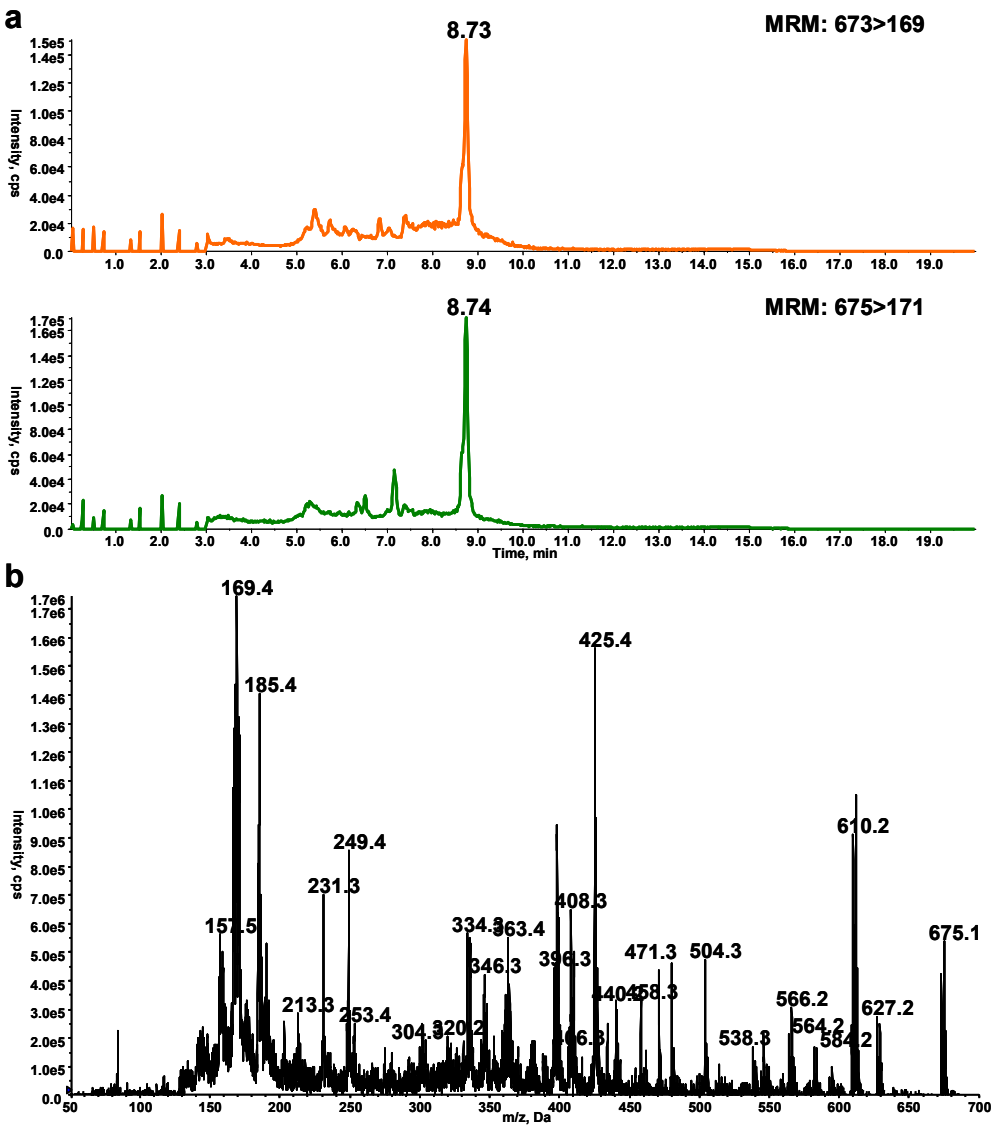

Figure S2. DIOB was oxidized by DMDO, and the resulting mixture was reacted with Lys and then with BBM, followed by LC-MS/MS analysis. **a**: Extracted ion chromatograms of MRM scans of *m*/*z* 673→169 (orange) and 675→171 (green). **b**: MS/MS spectrum of synthetic pyrrole **10.**

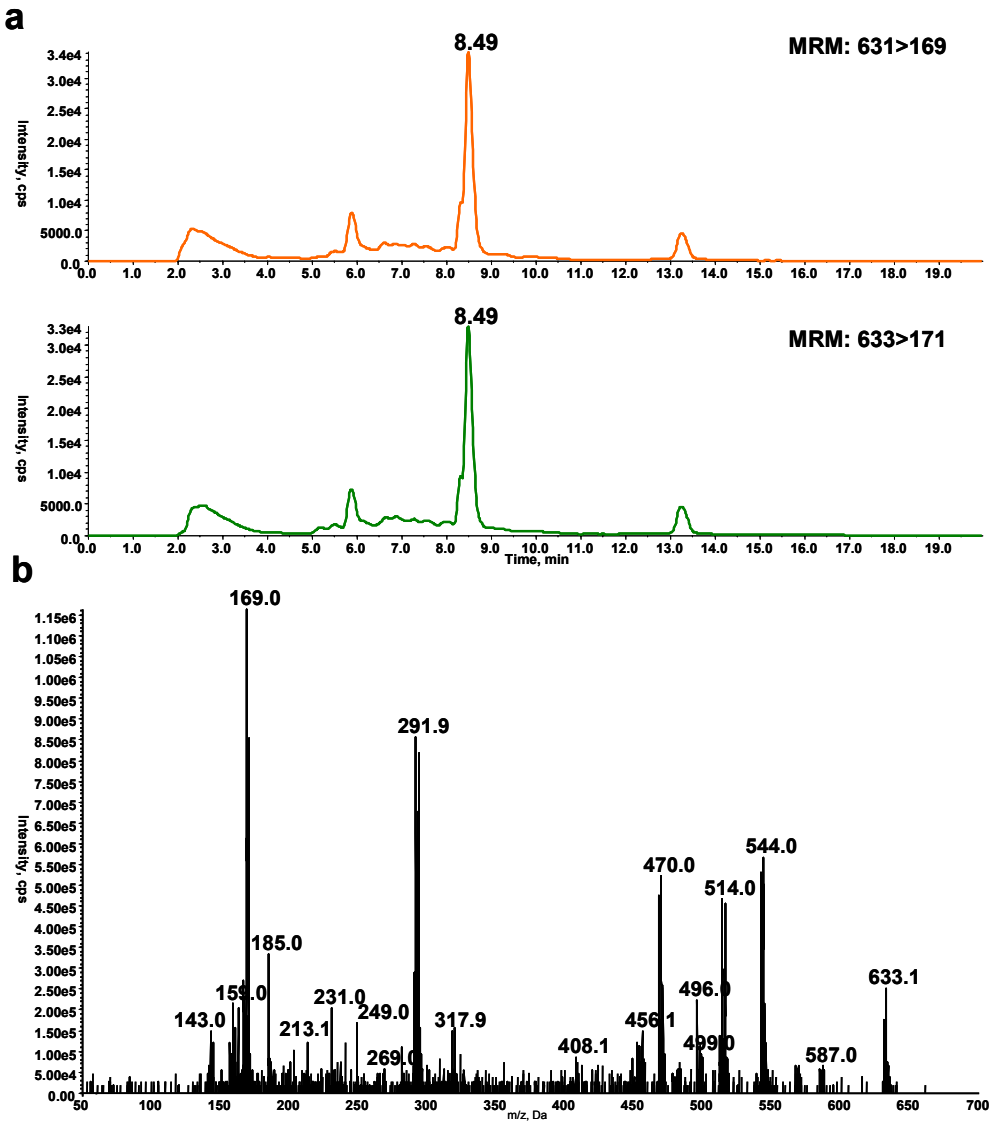

Figure S3. DIOB was oxidized by DMDO, and the resulting mixture was reacted with microsomal protein and then with BBA, followed by complete proteolytic digestion and LC-MS/MS analysis. **a**: Extracted ion chromatograms of MRM scans of *m*/*z* 631→169 (orange) and 633→171 (green). **b**: MS/MS spectrum of synthetic pyrrole **6.**

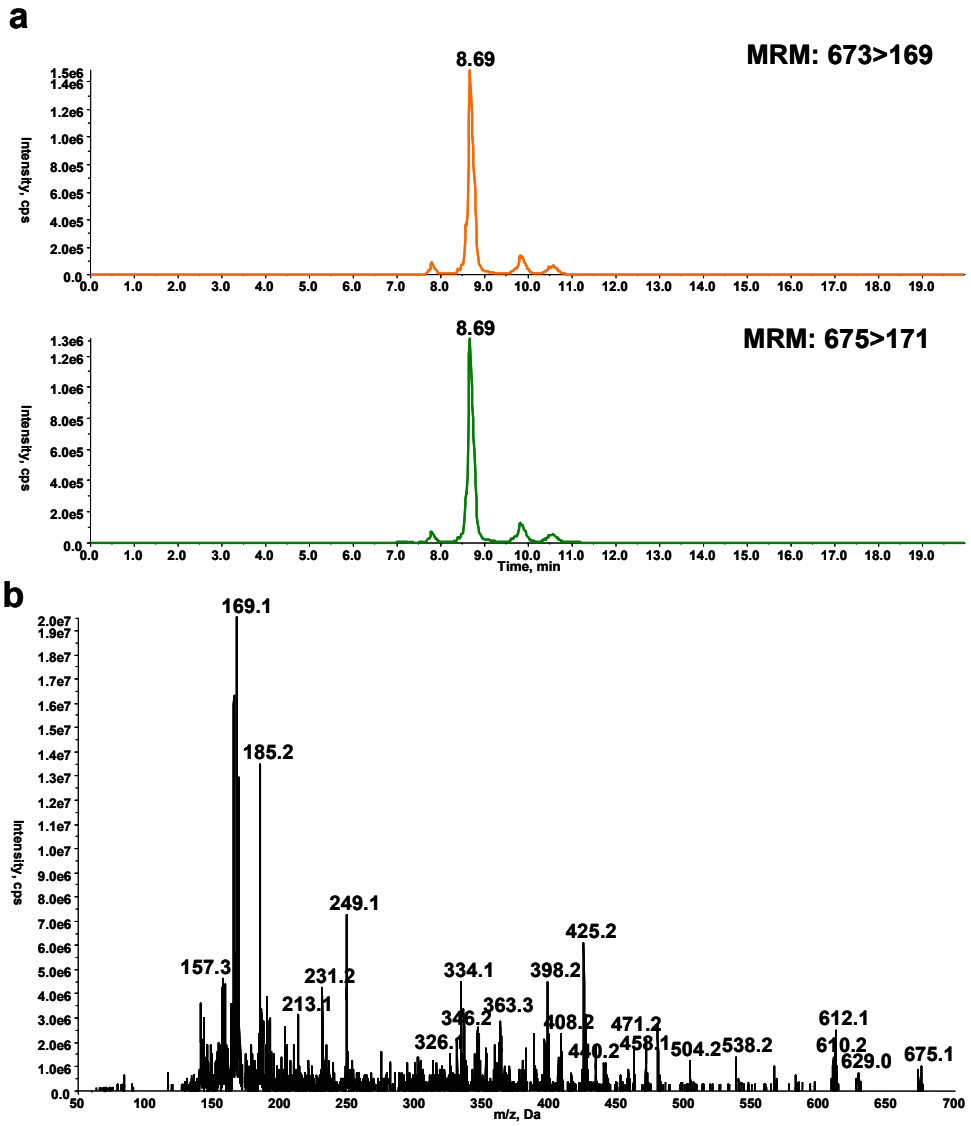

Figure S4. DIOB was oxidized by DMDO, and the resulting mixture was reacted with microsomal protein and then with BBM, followed by complete proteolytic digestion and LC-MS/MS analysis. **a**: Extracted ion chromatograms of MRM scans of *m*/*z* 673→169 (orange) and 675→171 (green). **b**: MS/MS spectrum of synthetic pyrrole **10.**

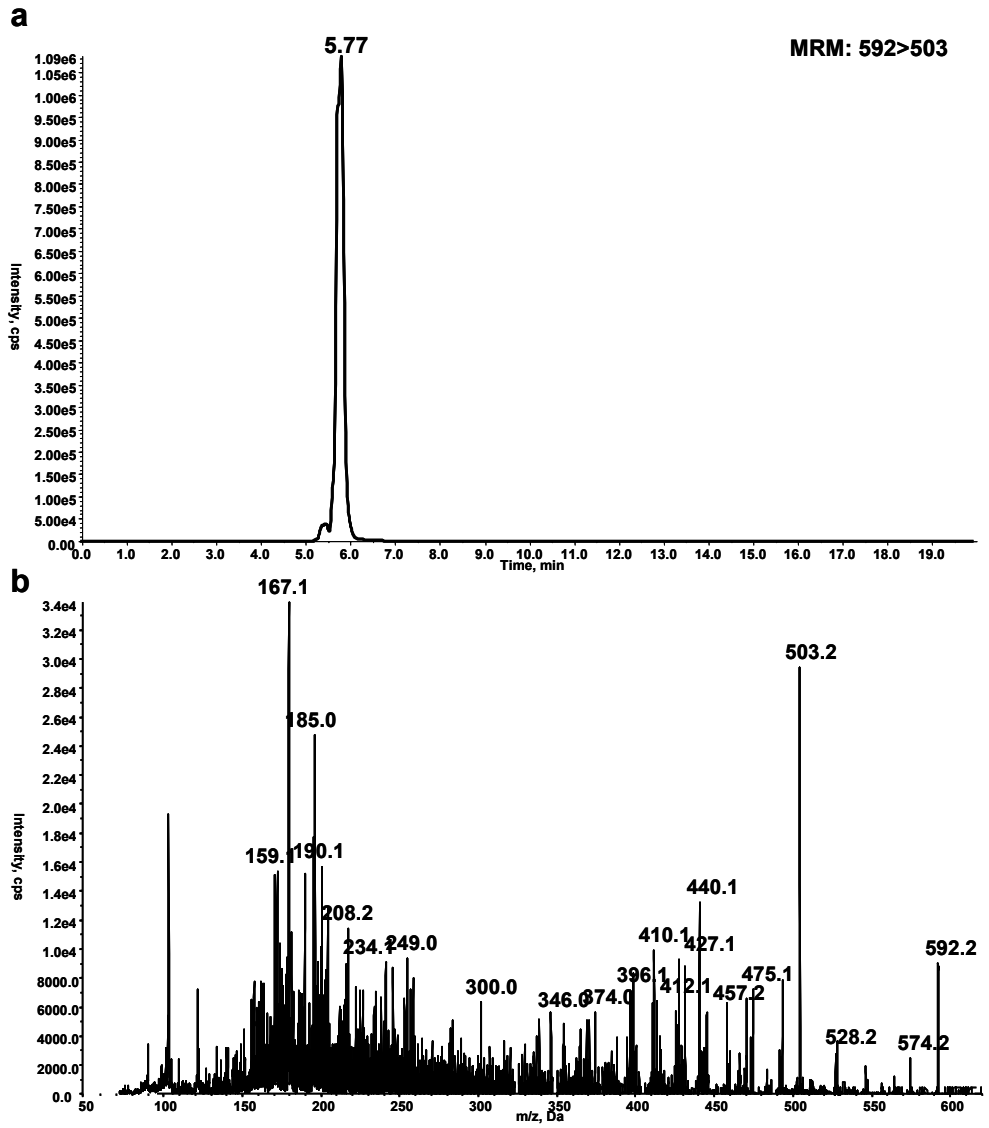

Figure S5. DIOB was oxidized by DMDO, and the resulting mixture was reacted with Cys and Lys, followed by LC-MS/MS analysis. **a**: Extracted ion chromatogram of MRM scan of *m*/*z* 592→503. **b:** MS/MS spectrum of synthetic pyrrole **12.**

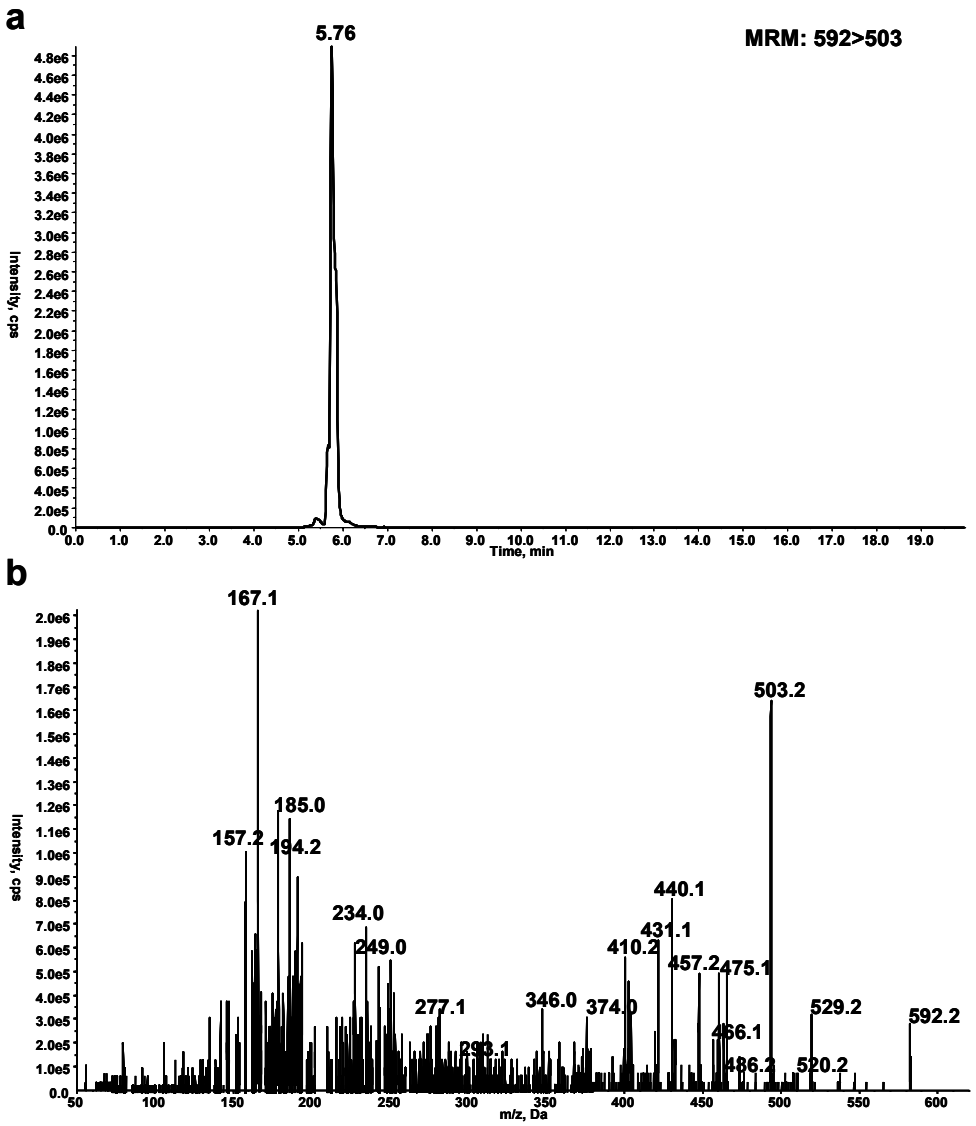

Figure S6. DIOB was oxidized by DMDO, and the resulting mixture was reacted with microsomal protein, followed by complete proteolytic digestion and LC-MS/MS analysis. **a**: Extracted ion chromatogram of MRM scan of *m*/*z* 592→503. **b**: MS/MS spectrum of synthetic pyrrole **12.**