Supplemental data

Drug Metabolism and Disposition

Metabolism of Diosbulbin B *in vitro* and *in vivo* in Rats: Formation of Reactive Metabolites and Human Enzymes Involved

Baohua Yang, Wei Liu, Kaixian Chen, Zhengtao Wang, Changhong Wang

The MOE Key Laboratory for Standardization of Chinese Medicines and The SATCM Key Laboratory for New Resources and Quality Evaluation of Chinese Medicines; Institute of Chinese Materia Medica, Shanghai University of Traditional Chinese Medicine, 1200 Cailun Road, Shanghai 201210, China. (BY, WL, KC, ZW and CW)

Shanghai R&D Centre for Standardization of Chinese Medicines, 199 Guoshoujing Road, Shanghai 201210, China. (KC, ZW and CW)

Running Title:

Reactive Metabolites of Diosbulbin B and Human Enzymes Involved

Corresponding authors:

Changhong Wang, E-mail address: wchcxm@hotmail.com; Zhengtao Wang, Email address: wangzht@hotmail.com; Phone: + 86 21 51322511; Fax: + 86 21 51322519

NMR analysis for M31a and M31b

Chemical synthesized M31 (about 11mg) was dissolved in 0.5 mL of DMSO-*d*6 for NMR spectra to be recorded on a Bruker 600 MHz spectrometer. Signals similar to those of diosbulbin B in ^{13}C-NMR spectrum were all doubled, which indicates that M31 is composed of two isomers. HMBC correlations help to distinguish the signals belonging to each one (Figure1 and 2) and NOESY correlations contribute to determine the configuration of C12 (Figure 3).

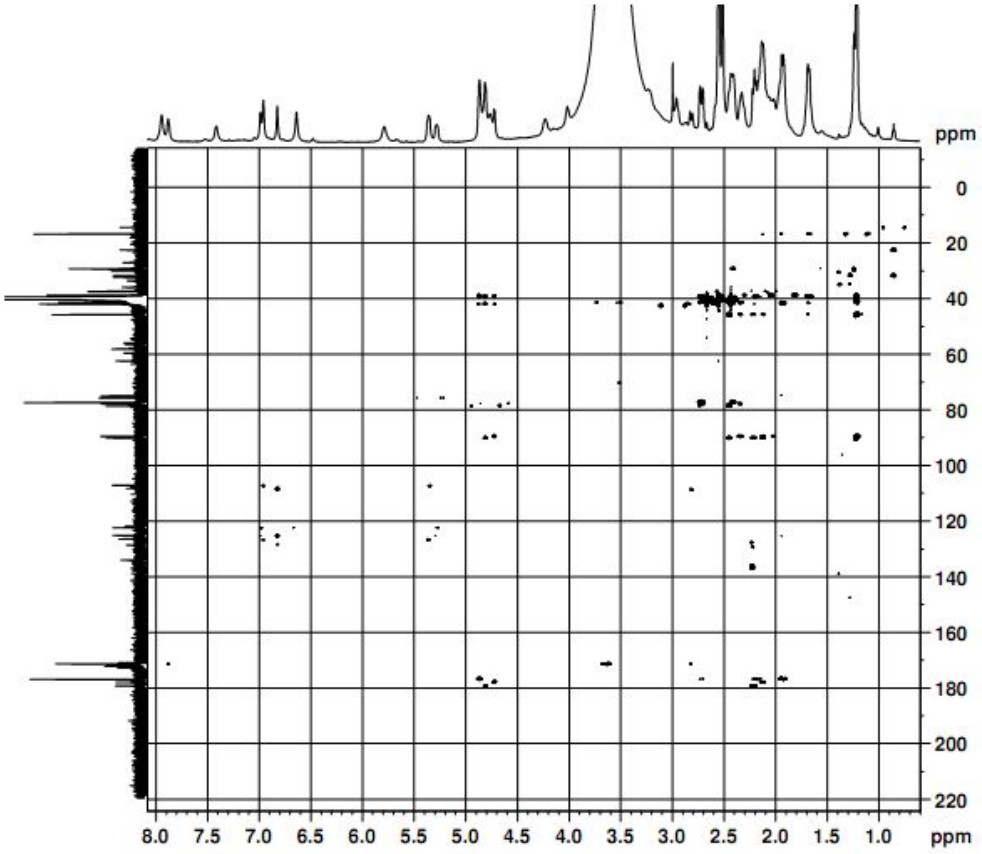

Figure 1 HMBC for M31a and M31b

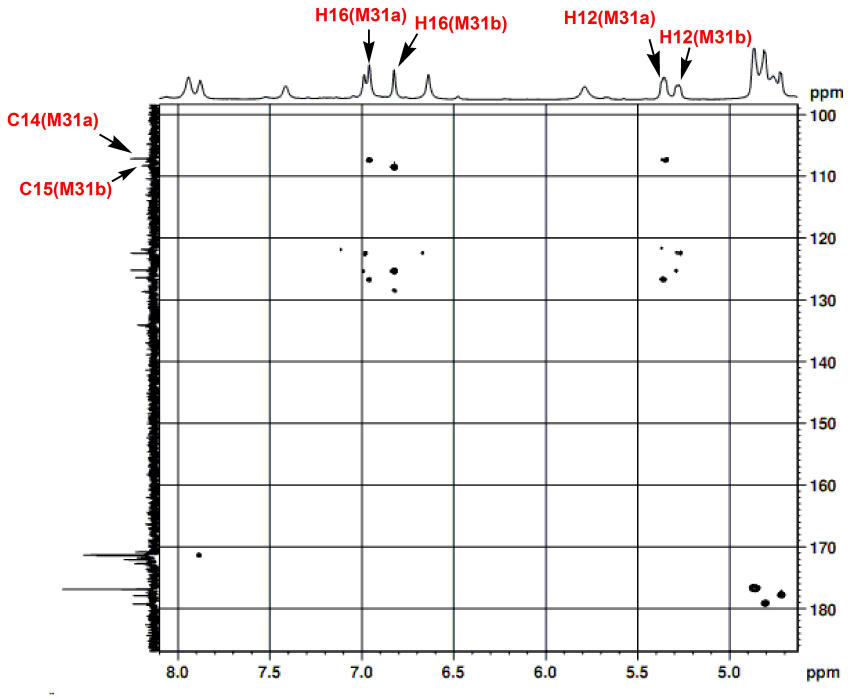

Figure 2 Gradient HMBC for M31a and M31b

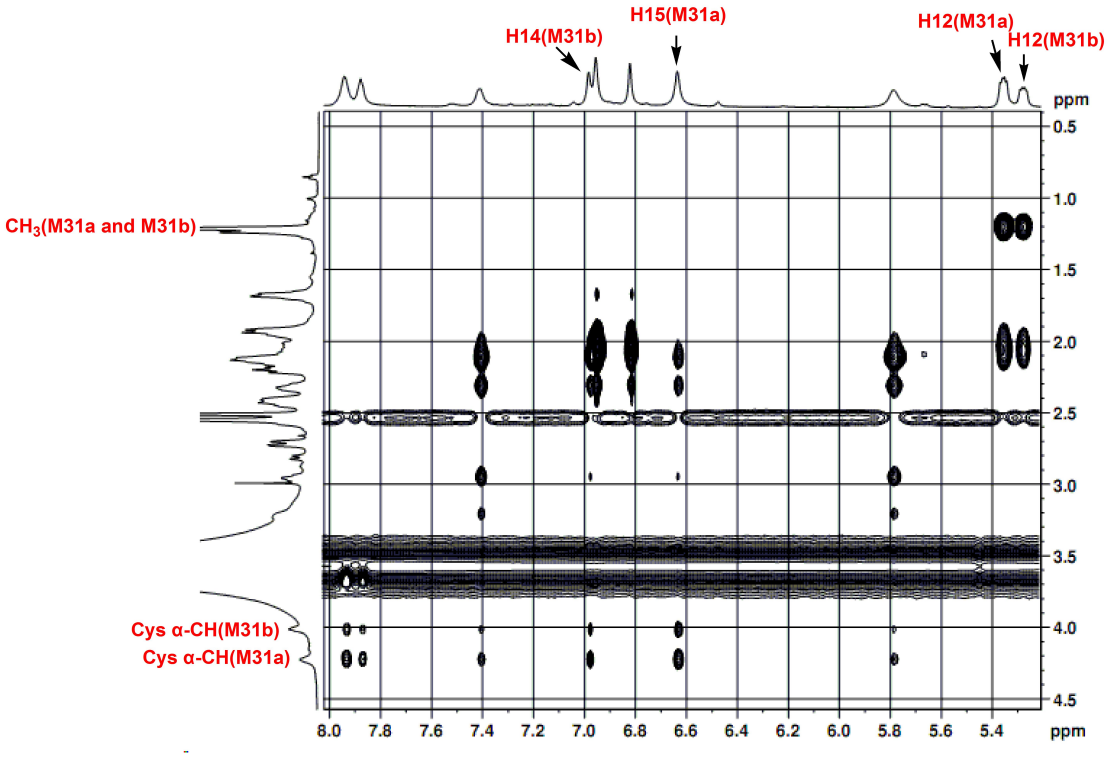

Figure 3 Gradient NOESY for M31a and M31b