#### SUPPLEMENTARY MATERIAL

### Velucarpin D, a new pterocarpan from the stems of *Dalbergia velutina* and its cytotoxicity

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### Abstract

A new pterocarpan, named velucarpin D (1), along with nine known pterocarpans (2-10) were isolated from the stems of *Dalbergia velutina*. Their structures were determined by spectroscopic analysis. All isolated compounds were evaluated for their cytotoxicity against five human cancer cell lines (KB, HeLa S-3, MCF-7, Hep G2, and HT-29). Compound 2 showed potent cytotoxicity against all the five human cancer cell lines with IC<sub>50</sub> values in the range of 4.74-8.46  $\mu$ M. In addition, compounds 1, 3, 4, 5 and 9 showed moderate cytotoxicity against both KB and HeLa S-3 cells with IC<sub>50</sub> values in the range of 14.23-29.35  $\mu$ M.

Keywords: Velucarpin D, Dalbergia velutina, Pterocarpans, Cytotoxicity

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	$IC_{50} (\mu M) \pm SD$					
Compounds	KB	HeLa S-3	MCF-7	Hep G2	HT-29	
1	$15.08 \pm 1.36$	$26.41 \pm 1.77$	NT	NT	NT	
2	$6.58\pm0.13$	$4.74\pm0.15$	$4.84\pm0.26$	$8.46 \pm 2.34$	$7.22\pm0.13$	
3	$14.23 \pm 1.25$	$18.15\pm0.43$	NT	NT	NT	
4	$18.77\pm2.15$	$23.25\pm0.71$	NT	NT	NT	
5	$16.62\pm0.38$	$28.69 \pm 6.84$	NT	NT	NT	
6	$74.43 \pm 6.17$	>100	NT	NT	NT	
7	$47.24{\pm}2.94$	$75.62\pm9.81$	NT	NT	NT	
8	$31.99\pm0.97$	$79.09\pm0.71$	NT	NT	NT	
9	$29.35\pm2.51$	$25.21 \pm 3.26$	NT	NT	NT	
10	$86.37 \pm 6.48$	>100	NT	NT	NT	
Doxorubicin	$0.01\pm0.00$	$0.12\pm0.13$	$0.49\pm0.01$	$1.43\pm0.18$	$0.34\pm0.04$	

Table S1 In vitro cytotoxicity of compounds 1-10 against five human cancer cell lines

Note: NT = Not tested

 $(IC_{50} \le 10 \ \mu M = \text{good activity}, 10 \ \mu M < IC_{50} \le 30 \ \mu M = \text{moderate activity}, IC_{50} > 100 \ \mu M = \text{inactive})$ 



Figure S1 Selected HMBC (arrow curves) and COSY (bold lines) correlations in 1



Figure S2 CD spectrum of velucarpin D (1) in MeOH



Figure S3 <sup>1</sup>H NMR spectrum of 1 in CDCl<sub>3</sub>



Figure S4<sup>13</sup>C NMR spectrum of 1 in CDCl<sub>3</sub>



Figure S5 COSY NMR spectrum of 1 in CDCl<sub>3</sub>



Figure S6 HSQC NMR spectrum of 1 in CDCl<sub>3</sub>



Figure S7 HMBC NMR spectrum of 1 in CDCl<sub>3</sub>



Figure S8 HRESIMS spectrum of 1