Supplementary Materials: The Investigation on Quantitative Structure-Activity Relationship of the Anti-Inflammatory Activity for Diterpenoid Alkaloids

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Table S1. The weights for the descriptors and the responders for the three components in the loading plot of PLS-weight in the PLS model.

Variable	Component 1	Component 2	Component3
SAA	0.08536	−0.3313	−0.04633
SAG	0.06451	−0.2963	0.2549
VOL	0.04399	−0.29608	0.2690
HE	−0.2246	0.07921	0.1940
LogP	−0.05427	−0.4194	−0.8050
REF	−0.5720	−0.6755	−0.6162
POL	−0.5076	−0.1768	0.1534
MASS	−0.4082	0.03622	0.2199
BE	0.1623	−0.3474	0.05742
HF	0.3942	−0.1200	−0.1673
$logEC_{50}$	0.5034	0.2134	0.1530

Table S2. The predicted anti-inflammatory activities by PLS-QSAR model and the experiment anti-inflammatory activities and for 3 diterpenoid alkaloids.

Compound Name	Predicted Value (EC_{50})	Experiment Value
songorine	e3.8805	exhibiting inhibitory effect
fuziling	e4.0517	exhibiting no inhibitory effect
delsoline	e0.3014	exhibiting no inhibitory effect

Greater value of EC_{50} indicates lower activity of the compound. The values of EC_{50} $e^{3.8805}$ and $e^{4.0517}$ do not indicate activities for fuziline and delsoline.