Yue-Wei Guo, Med chem 2013, 3:4
http://dx.doi.org/10.4172/2161-0444.S1.007

OMICS Group Conferences
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2nd International Conference on
Medicinal Chemistry & Computer Aided Drug Designing
October 15-17, 2013 Hampton Inn Tropicana, Las Vegas, NV, USA

Chemistry, bioactivity, and computational prediction of binding modes for sarsolenane and capnosane diterpenes as PTP1B inhibitors from the hainan soft coral *Sarcophyton trocheliophorum* Marenzeller

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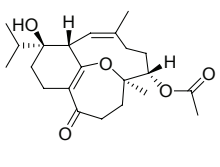
Three new sarsolenane diterpenes, dihydrosarsolenone (2), methyl dihydrosarsolenoneate (3), and secodihydrosarsolenone (4) (exemplified by 2), and two new capnosane diterpenes, sartrochelilides A (6) and B (7) (exemplified by 6), were isolated together with the known analogue sarsolilide A (5), from the Hainan soft coral *Sarcophyton trocheliophorum* marenzeller. Their structures were elucidated by detailed spectroscopic analysis and by comparison with reported data. The absolute configurations of compounds 2 and 6 were determined by TDDFT ECD calculations. In the biotest *in vitro*, compounds 4-6 exhibited different levels of inhibitory activity against protein tyrosine phosphatase 1B (PTP1B), of which 5 showed the strongest inhibitory activity, being similar to that of positive control oleanolic acid. This is the first report of PTP1B inhibitory activity for sarsolenane and capnosane diterpenes. The discovery promotes computational predictions of binding modes for the enzyme and both kinds of metabolites.



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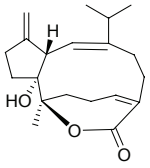

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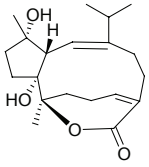

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Biography

Yue-Wei Guo has completed his Ph.D. at the age of 38 years from Naples University and postdoctoral studies from both Istituto di Chimica Biomoleculare-CNR, Italy and Hokaido University, Japan. He is the Professor of Shanghai Institute of Materia Medica-CAS. He has published more than 250 papers in reputed journals and serving as editorial board members of several reputed national/international journals.

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