

OR-36**Two New Compounds from Bark of *Litsea Costalis*: A Comparison of DFT Studies**

Masoumeh Hosseinzadeh^{1,*}, A. Hamid A. Hadi¹, Jamaludin Mohamad², Mohammad A Khalilzadeh³ and Mohammad Reza Zardoost³

¹Department of Chemistry, Faculty of Science, University of Malaya, 50603 Kuala Lumpur Malaysia; ²Institute of Biological Sciences, Faculty of Science, University of Malaya, 50603 Kuala Lumpur, Malaysia; ³Department of Chemistry, Qaemshahr Branch, Islamic Azad University, Qaemshahr, Iran; E-mail: m.hosseinzadeh@siswa.edu.um.my

Two new neolignans, namely biseugenol A-B (**1-2**) were isolated from the bark *Litsea costalis*. The structures of new compounds were on the basis of extensive spectroscopic data analysis. The IR and NMR techniques were combined with quantum chemical calculations in the DFT approach using the hybrid B3LYP exchange-correlation function to confirm the structure of the two new compounds. Compounds showed excellent anticancer activity against cell lines and antioxidant (DPPH).

Keywords: *Litsea costalis*, Lauraceae, Biseugenol A-B, DFT, Anticancer, Antioxidant.