



Apoptosis Inducing Factor (AIF) Stabilizes Menadione-Conjugate Product in Programmed Cell Death

Hesti L. Wiraswati^{1,3}, Muhamad A. Martoprawiro^{1,2},
Akhmaloka¹, Fida M. Warganegara^{1*}

¹Department of Chemistry, Institut Teknologi Bandung, Jl. Ganeca 10, Bandung 40132, Indonesia

²Department of Computational Sciences, Institut Teknologi Bandung, Jl. Ganeca 10, Bandung 40132, Indonesia

³Université Paris Sud, Paris-Cedex, France

Abstract: Understanding the role of AIF modulate menadione cytotoxicity may lead Apoptosis Inducing Factor (AIF) contribution as potential target of cancer drugs. Previous studies reported the impact of mitochondrial AIF to cytotoxicity of menadione (2-methyl-1,4-naphthoquinone). Specifically, recent study revealed that AIF depletion reduced the level of thiodione (arylation product of menadione and reduced glutathione, GSH) and increased endogenous GSH. However, how AIF modulate menadione-GSH arylation, has not been elaborated yet. This study investigated the involvement of AIF to arylation capacity of menadione using in silico approach. Molecular interaction between residues on AIF and functional groups of menadione were investigated using *AutoDockVina* software. The result confirmed that AIF is involved in the conjugation of menadione and GSH to form thiodione. AIF also tends to stabilize thiodione formation rather than interact with menadione or GSH directly. Moreover, AIF doesn't show transferase catalytic site which reinforce the notion that AIF stabilizes conjugate product-thiodione.

Keywords : AIF, menadione, apoptosis, docking.

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