ABSTRACT

DETERMINATION STUDIES OF FLAVONOID ANTIOXIDANT ACTIVITY AND SUBSTITUTED KAEMPFEROL WITH WITHDRAWING AND DONOR ELECTRON GROUP BASED ON AUSTIN MODEL 1 (AM1) AS SEMI-EMPIRICAL METHOD

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Measurement of flavonoid activity from antioxidant has been studied, it is based on average of the bond dissociation enthalphy (BDE), single electron transfer-proton transfer (SET-PT), proton affinity (PA), and electron transfer enthalphy (ETE). These study used AM1 semi-empiric methods. The result showed that the antioxidant activity of flavonoid could be determine by simple and double linear of regression equation such as

$y = 41{,}897 + 0{,}002\ BDE_{rt} + 0{,}355\ SET\text{-}PT_{rt} - 0{,}338\ PA_{rt}$

$y = 41{,}077 + 0{,}018\ SET\text{-}PT_{rt} + 0{,}340\ ETE_{rt}$

$y = 41{,}301 + 0{,}342\ ETE_{rt}$

the value of R^2 are 0,923; 0,923; and 0,916. Respectivety these equation are used to determine the antioxidant activity of kaempferol which are substituted with withdrawing electron group (Cl, F, CN, NO and NO_2) and donor electron group ($NHCH_3$, $N(CH_3)_2$, and OCH_3) on C5' and C6'. Substituted group for those withdrawing and donor electron on C5' increased the antioxidant activity, except for CH_3, NH_2, $NHCH_3$, $N(CH_3)_2$, and OCH_3, decreased the antioxidant activity. Meanwhile antioxidant activity is increased by adding withdrawing electron and donor electron group C6', and decreased by present of Cl, F, NH_2, and $N(CH_3)_2$ group of C6'

Keywords: Flavonoid, Kaempferol, Semi-empirical AM1, QSAR