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-empirical methods. The result showed that the antioxidant
activity of flavonoid could be determine by simple and double linear of regression
equation such as

\[ y = 41.897 + 0.002 \text{BDE}_\text{n} + 0.355 \text{SET-PT}_\text{n} - 0.338 \text{PA}_\text{n} \]
\[ y = 41.077 + 0.018 \text{SET-PT}_\text{n} + 0.340 \text{ETE}_\text{n} \]
\[ y = 41.301 + 0.342 \text{ETE}_\text{n} \]

the value of \( R^2 \) are 0.923; 0.923; and 0.916. Respectively these equation are
used to determine the antioxidant activity of kaempferol which are substituted with
withdrawing electron group (Cl, F, CN, NO and NO₂) and donor electron group
(NHCH₃, N(CH₃)₂, and OCH₃) on C5’ and C6’. Substituted group for those
withdrawing and donor electron on C5’ increased the antioxidant activity, except for
CH₃, NH₂, NHCH₃, N(CH₃)₂, and OCH₃, 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, NH₂, and N(CH₃)₂ group of C6’

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