

Supplementary Materials

MARK4 Inhibited by AChE Inhibitors, Donepezil and Rivastigmine Tartrate: Insights into Alzheimer's Disease Therapy

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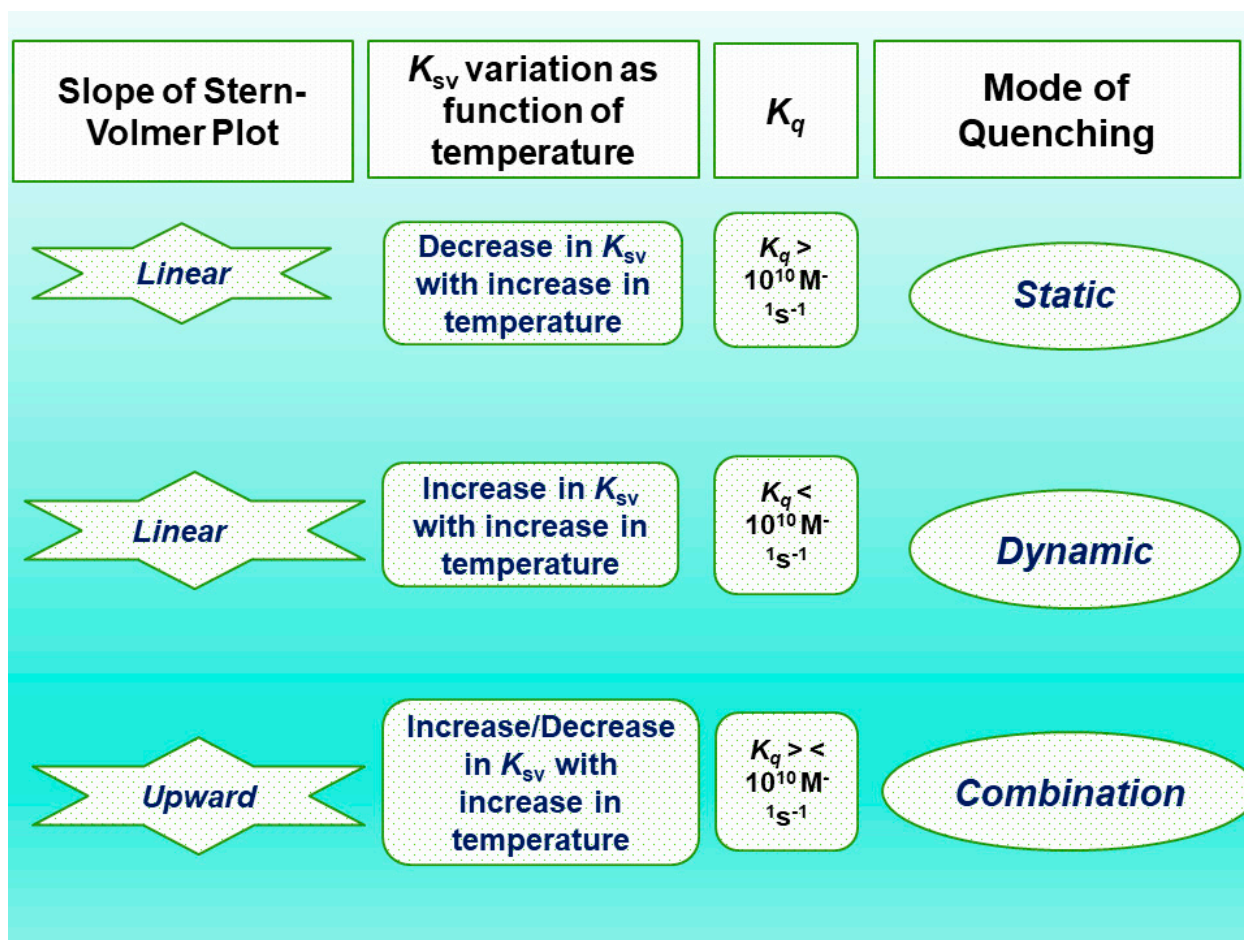


Figure S1. Graphical representation of the operative mode of quenching for specific protein-ligand interaction.

Table S1. Thermodynamic parameters obtained from ITC measurements.

MARK4-DP		
K_a (association constant), M^{-1}	ΔH (enthalpy change), cal/mol	ΔS (cal/mol/deg)
$K_{a1} = 6.79 \times 10^5 \pm 2.4 \times 10^5$	$\Delta H_1 = 8444 \pm 1.82 \times 10^3$	$\Delta S_1 = 51.2$
$K_{a2} = 1. \times 10^5 \pm 1.9 \times 10^3$	$\Delta H_2 = -6.88 \times 10^4 \pm 5.48 \times 10^3$	$\Delta S_2 = -207$
$K_{a3} = 9.37 \times 10^4 \pm 3.0 \times 10^3$	$\Delta H_3 = 1.01 \times 10^5 \pm 7.49 \times 10^3$	$\Delta S_3 = 368$
$K_{a3} = -1.044 \times 10^5 \pm 4.68 \times 10^3 M$	$\Delta H_4 = -4.91 \times 10^6 \pm 5.6 \times 10^6$	$\Delta S_4 = -327$
MARK4-RT		
K_a (association constant), M^{-1}	ΔH (enthalpy change), cal/mol	ΔS (cal/mol/deg)
$K_{a1} = 1.02 \times 10^5 \pm 2.8 \times 10^5$	$\Delta H_1 = 1329 \pm 3.05 \times 10^3$	$\Delta S_1 = 31.1$
$K_{a2} = 1.17 \times 10^5 \pm 7.3 \times 10^4$	$\Delta H_2 = -2.15 \times 10^5 \pm 9.07 \times 10^4$	$\Delta S_2 = -700$
$K_{a3} = 2.00 \times 10^5 \pm 1.6 \times 10^5$	$\Delta H_3 = 7.86 \times 10^5 \pm 2.26 \times 10^5$	$\Delta S_3 = 2.66 \times 10^3$
$K_{a3} = 5.44 \times 10^4 \pm 2.54 \times 10$	$\Delta H_4 = 2.23 \times 10^6 \pm 4.8 \times 10^5$	$\Delta S_4 = -7.47 \times 10^3$