Supplementary information

Elucidation of Dietary Polyphenolics as Potential Inhibitor of Microtubule Affinity Regulating Kinase 4: In silico and In vitro Studies

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Running Head: MARK4 inhibitors

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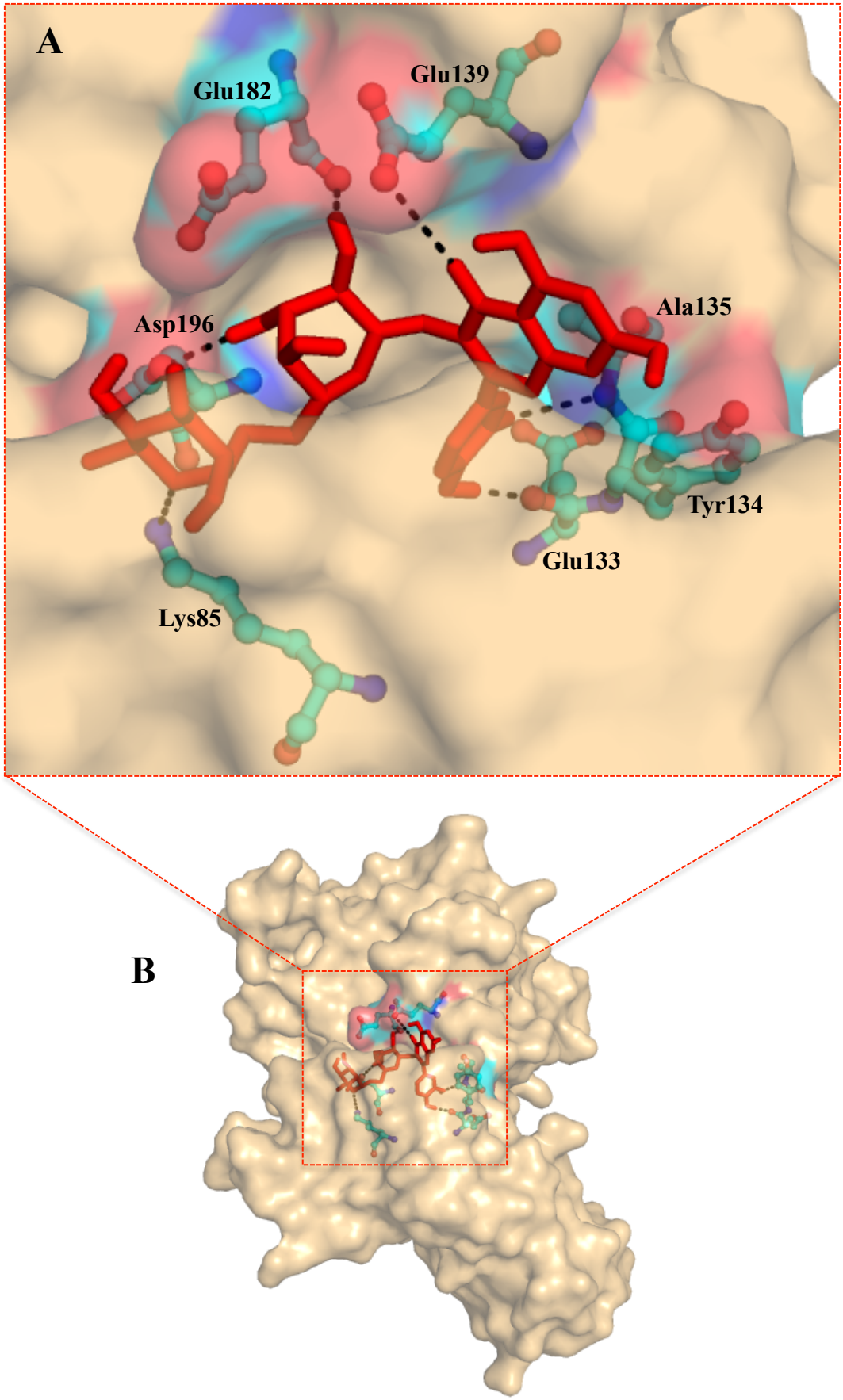

Figure S1: Binding of rutin with MARK4. **(A)** Enlarged surface view showing the binding of rutin with MARK4 **(B)** Surface view of rutin binding to MARK4. Interacting residues of MARK4 (ball and stick model) and rutin (stick model).

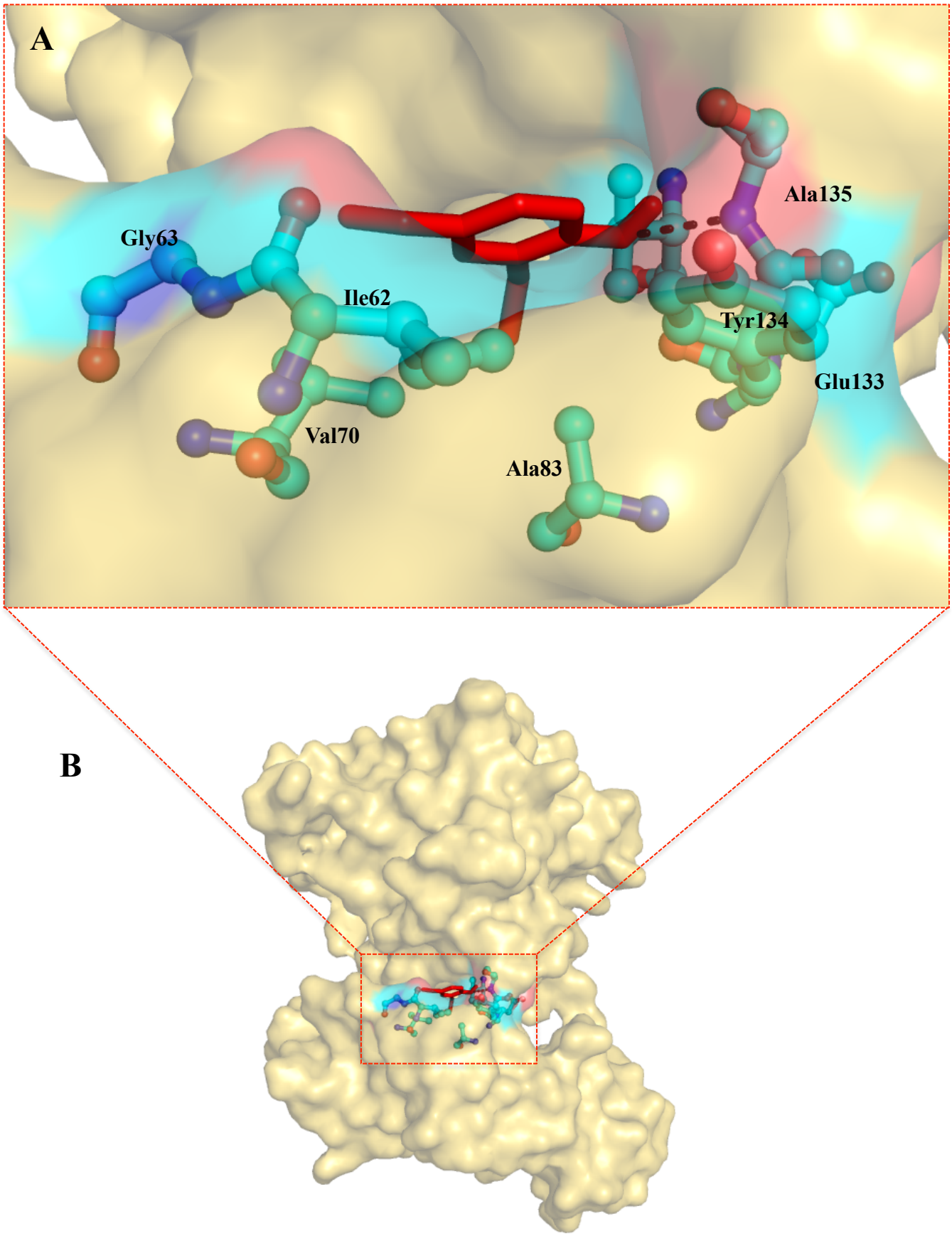

Figure S2: Binding of vanillin with MARK4. **(A)** Enlarged surface view showing the binding of vanillin with MARK4 **(B)** Surface view of vanillin binding to MARK4. Interacting residues of MARK4 (ball and stick model) and rutin (stick model).

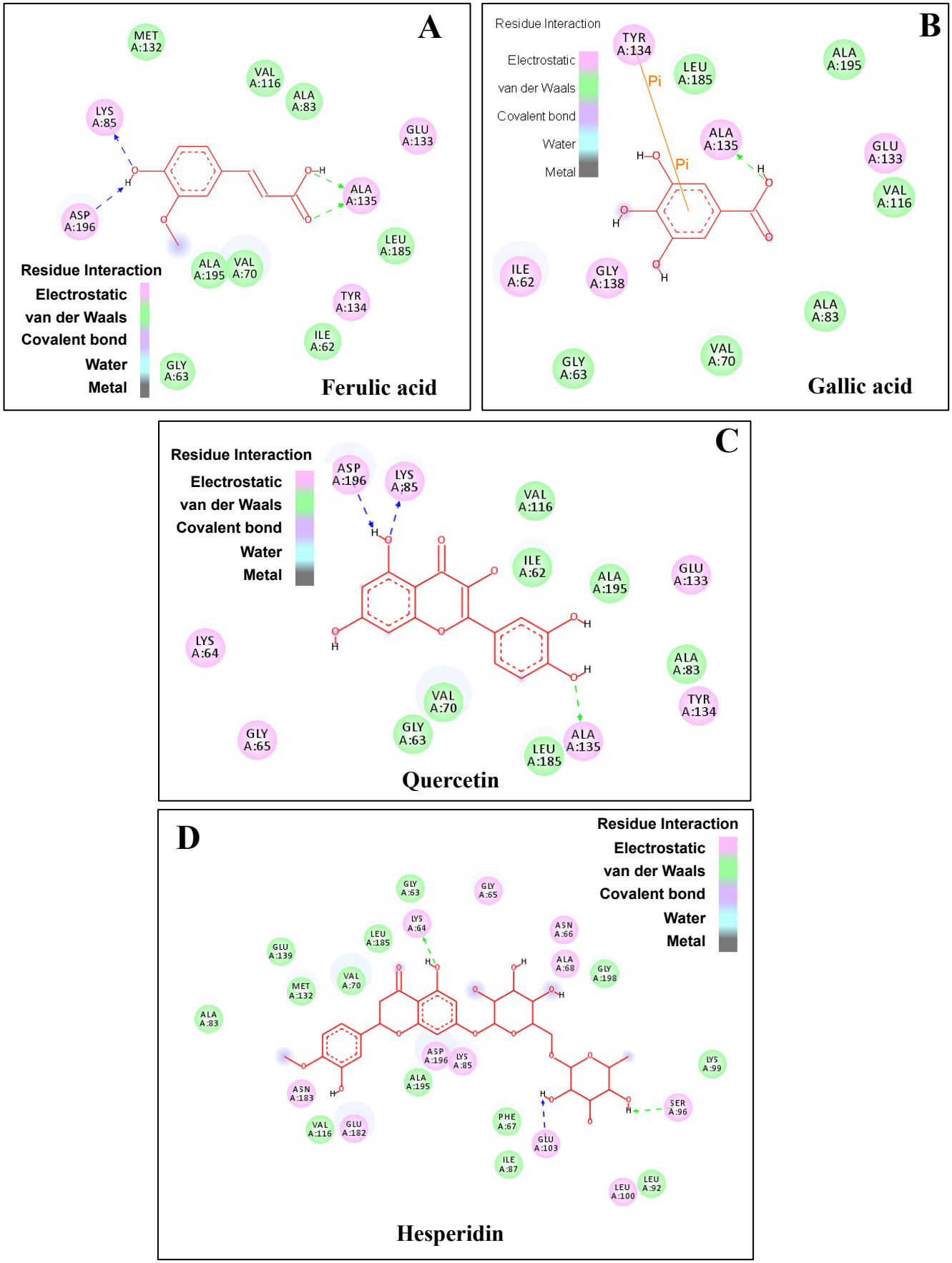

Figure S3: 2D schematic diagram of docking model of ferulic acid, gallic acid, quercetin and hesperidin with MARK4. Residues involved in hydrogen bonding, charge or polar interactions, Van der Waals interactions are represented by respective colour indicated in inset of figure.

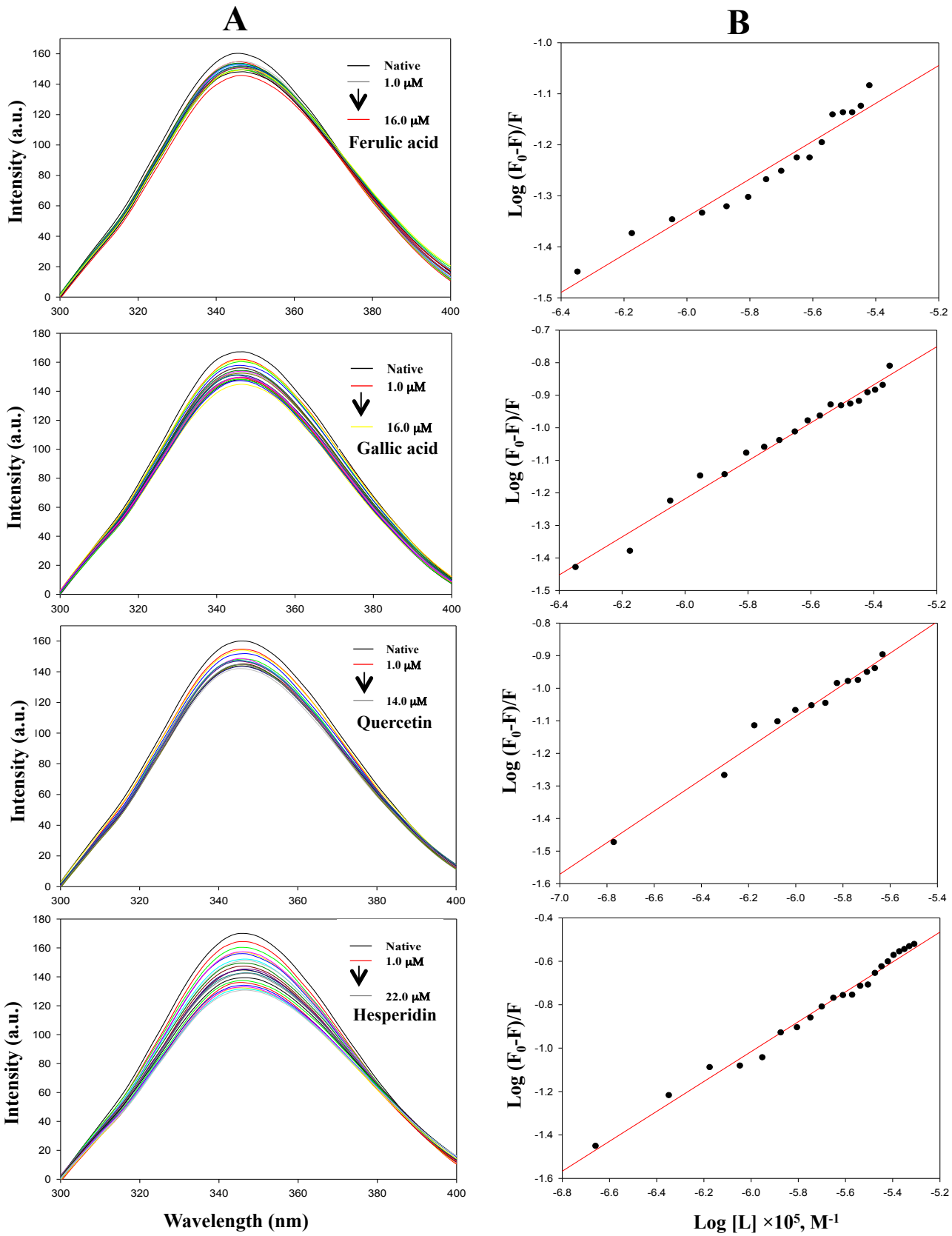

Figure S4. Binding pattern of ferulic acid, gallic acid, quercetin and hesperidin, respectively observed using fluorescence spectroscopy. **(A)** Fluorescence spectra of MARK4 (4µM) with increasing concentration of each compound (0-100µM). Excitation wavelength was fixed to 280nm and emission was recorded in the range 300-400 nm. **(B)** Modified Stern-Volmer plot showing quenching of MARK4 by each mentioned compound.

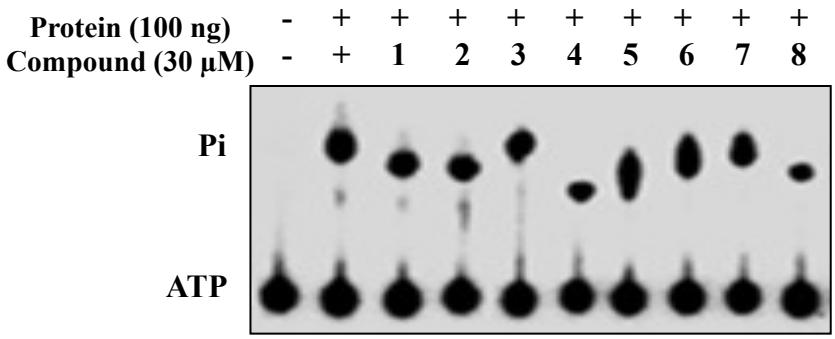

Figure S5: ATPase enzyme assay of MARK4. Shows the hydrolysis of Pi from ATP, position of Pi and ATP spots are indicated on left side. Lane 1, negative control (without protein); lane 2, 100 nM MARK4 (positive control); number 1&2= gallic acid, 3= quercetin, 4=rutin, 5= ferulic acid, 6&7= hesperidin and 8 represent the vanillin, respectively.