

Molecular interaction studies on ellagic acid for its anticancer potential targeting pyruvate dehydrogenase kinase 3

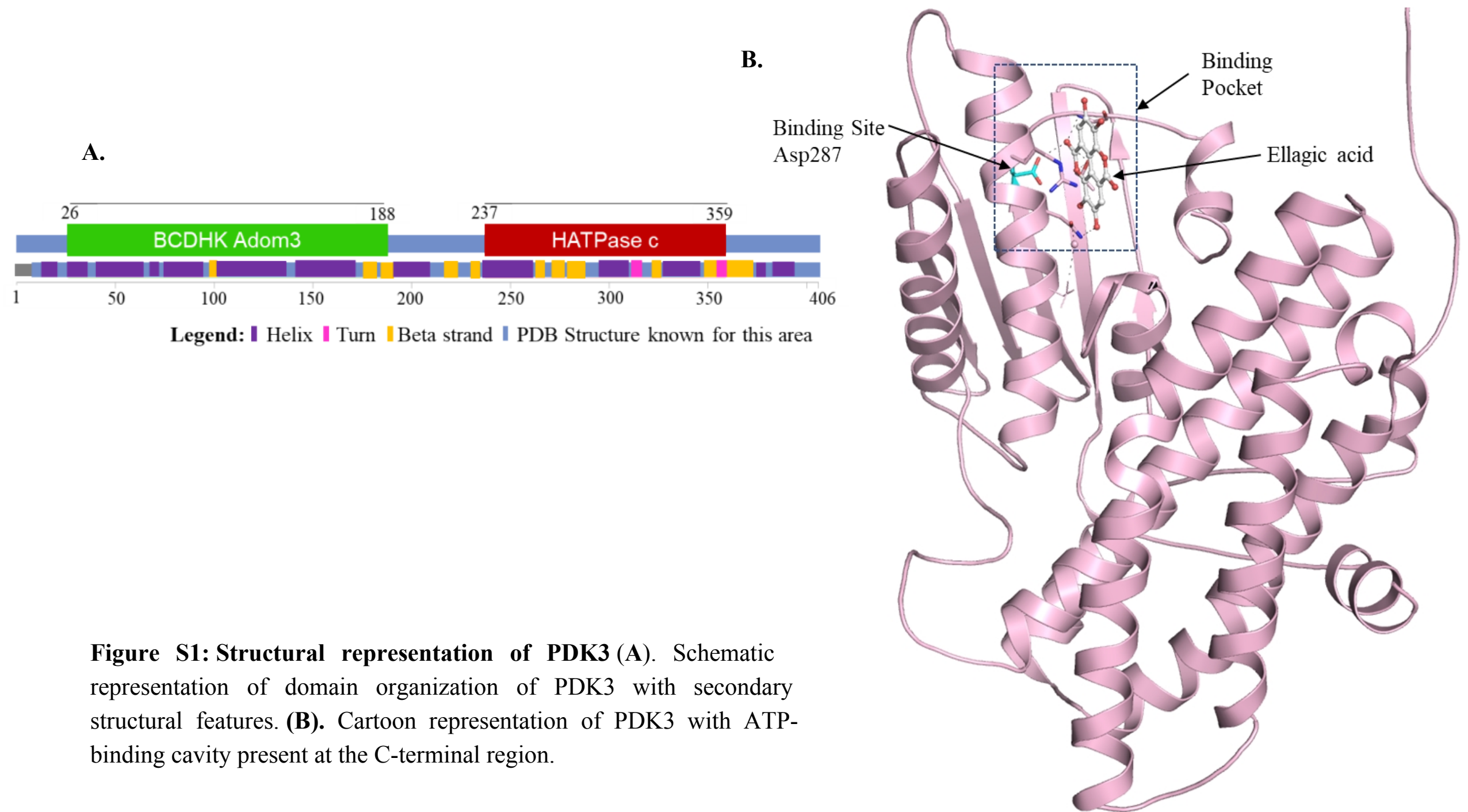
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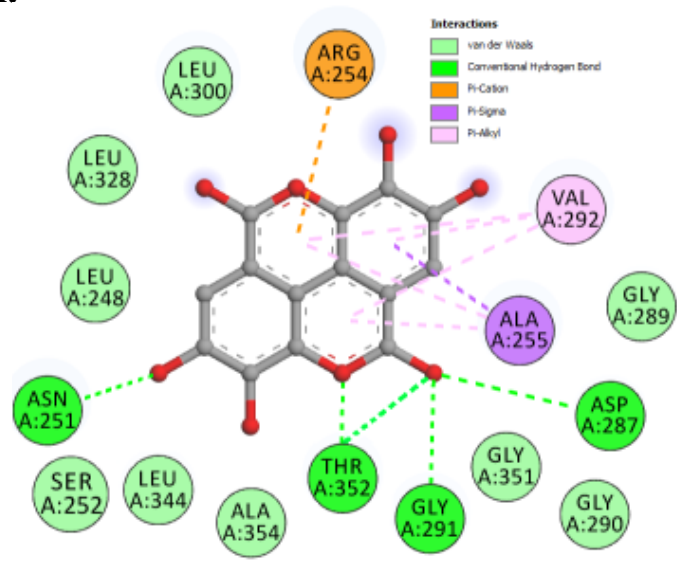
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**RSC Advances: RA-REV-04-2019-
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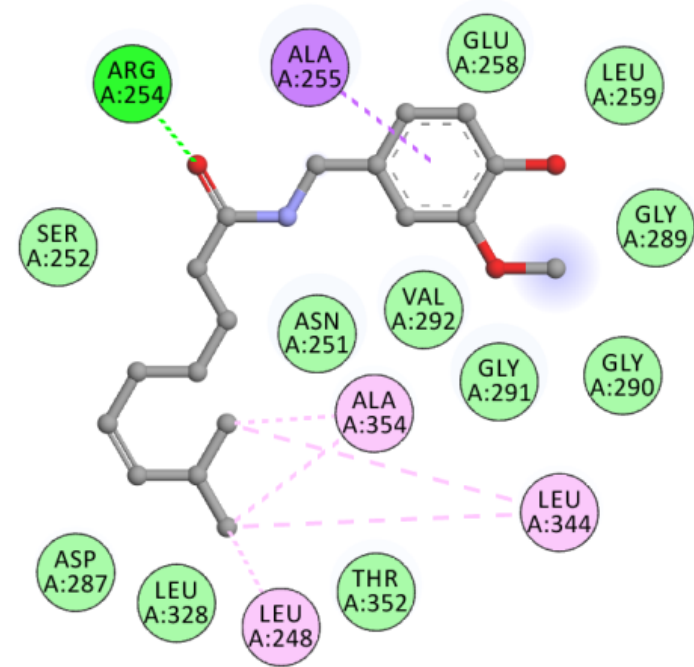
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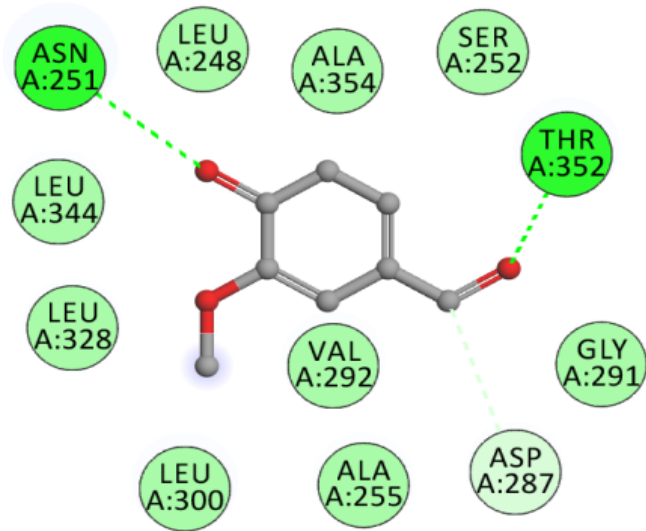
A.



B.



C.



D.

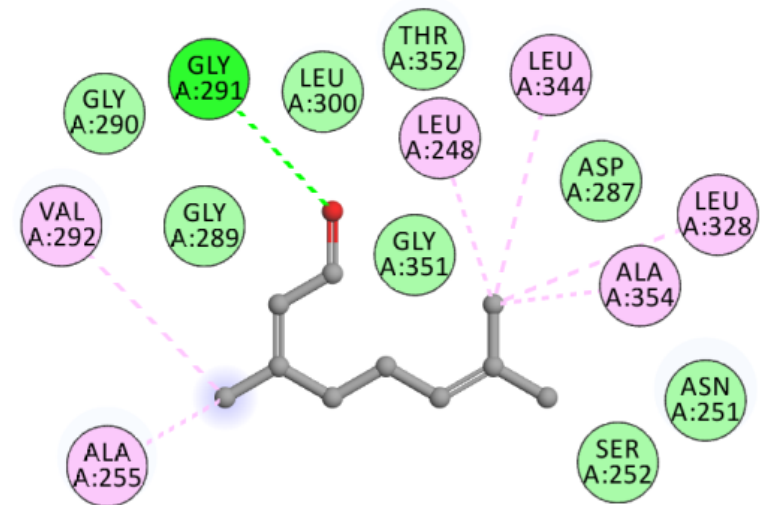
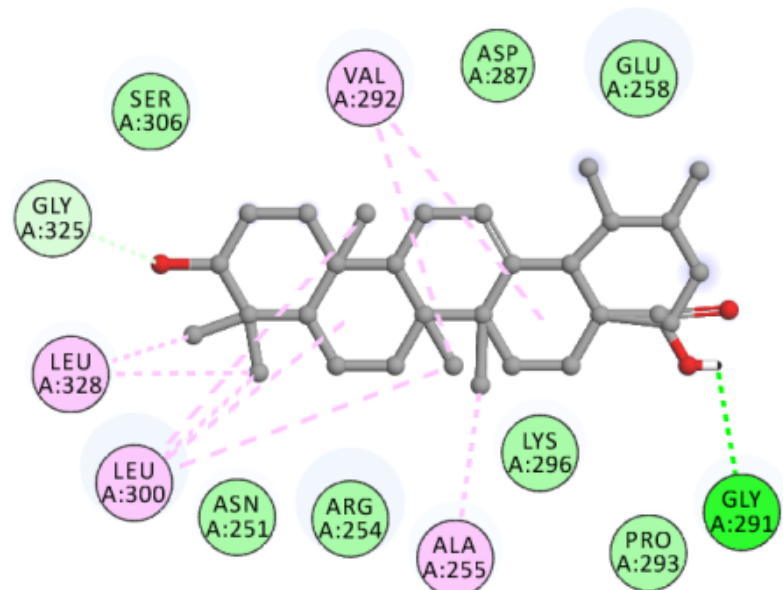
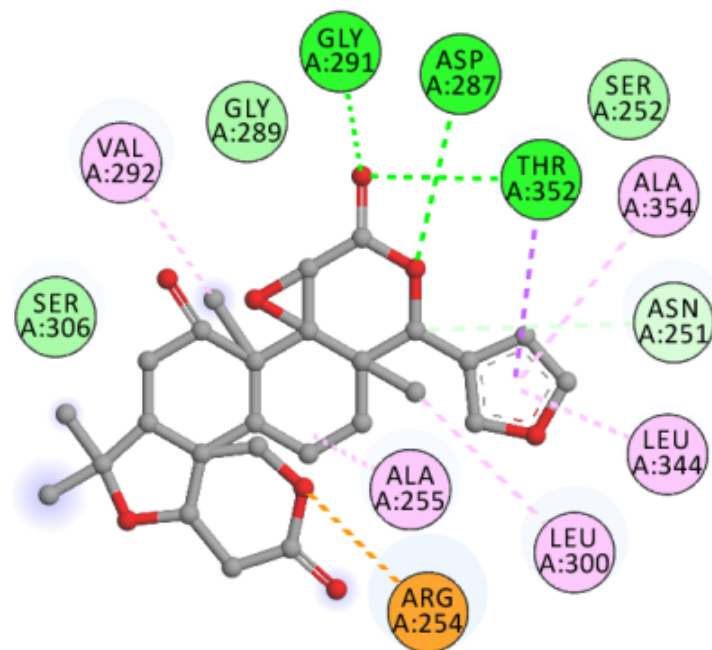


Figure S2: 2D representation of PDK3 residues interacting to (A) Ellagic Acid (B) Capsaicin (C) Vanillin (D) Citral

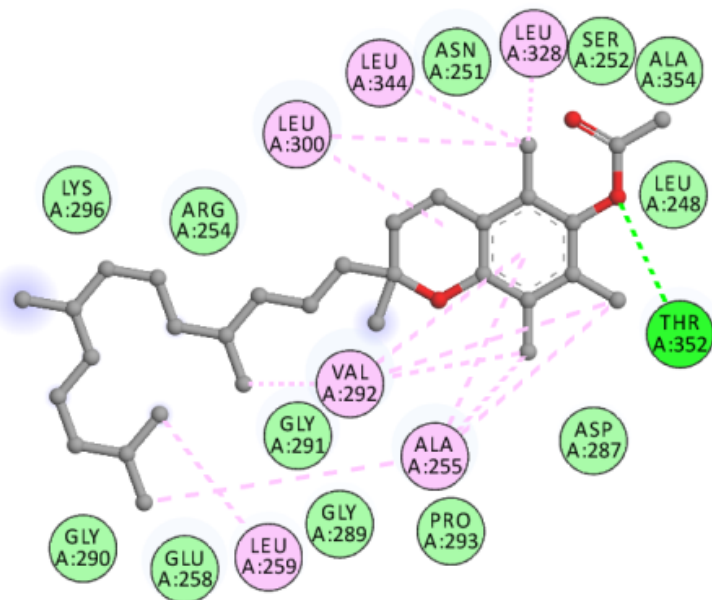
A.



B.



C.



D.

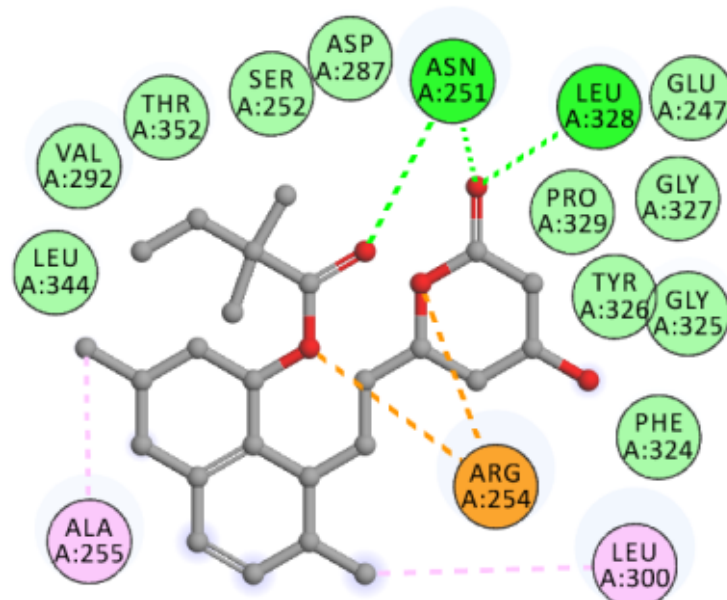


Figure S3: 2D representation of PDK3 residues interacting to (A) Ursolic Acid (B) Limonin (C) DL- α tocopherol acetate (D) Simvastatin.

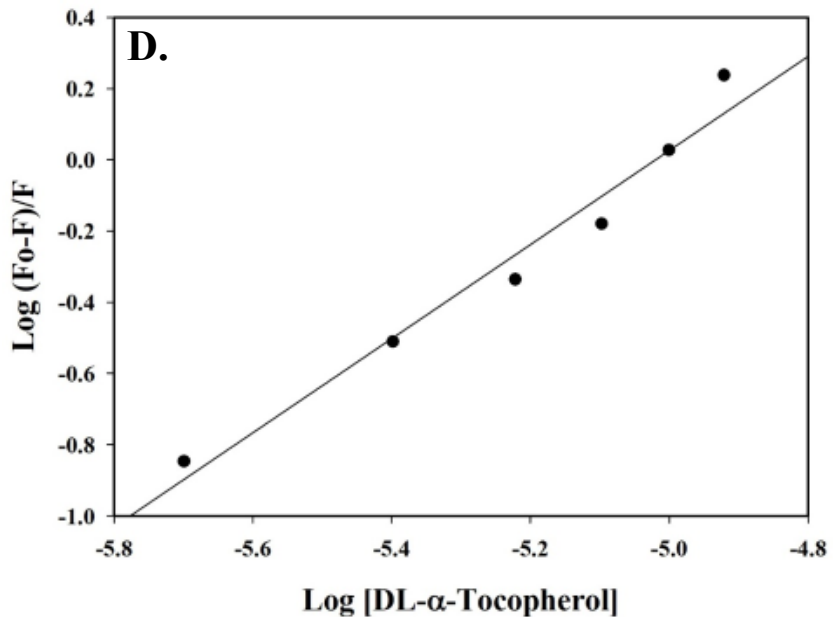
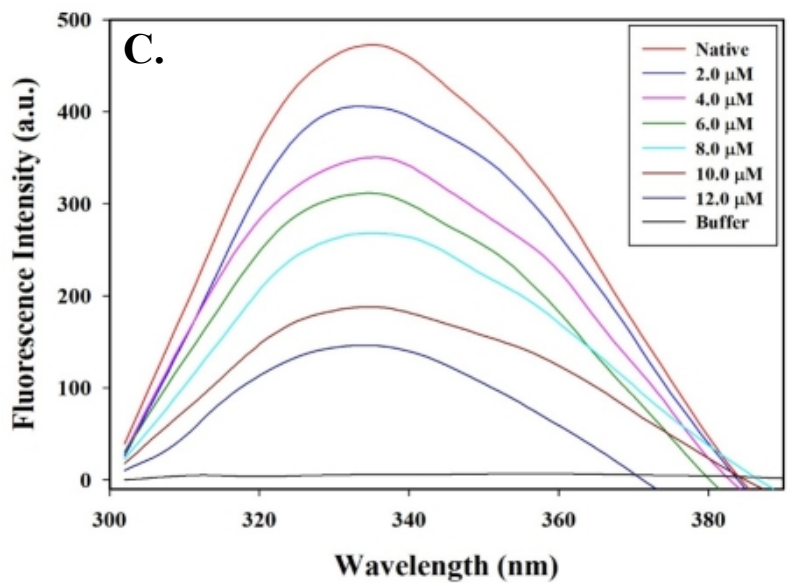
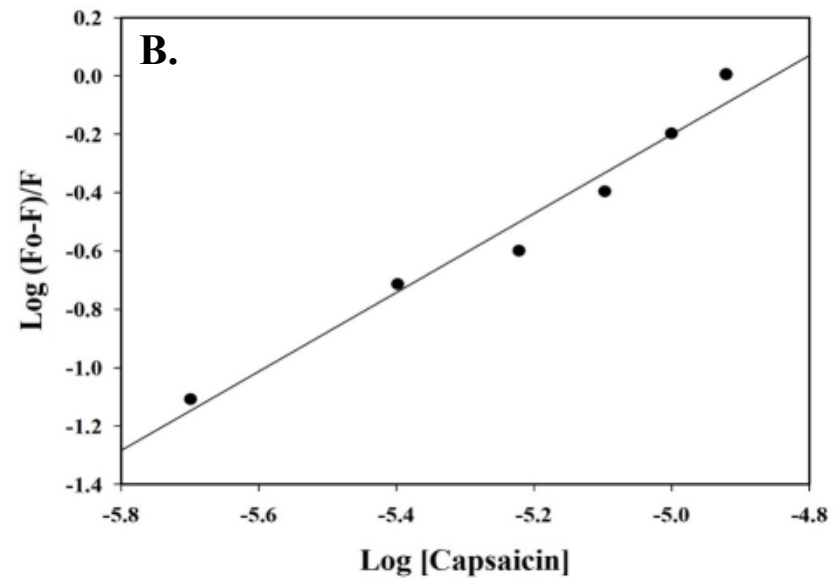
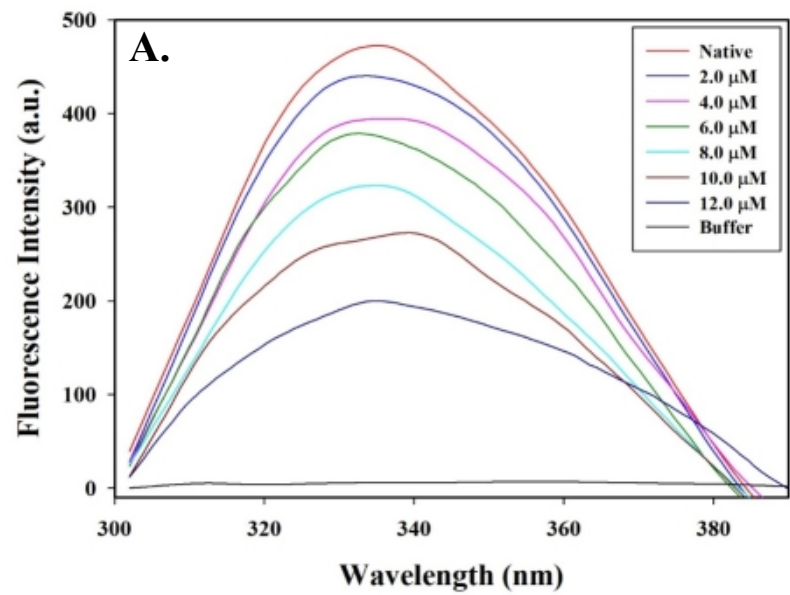


Figure S4: Fluorescence emission spectrum of (A) Capsaicin and (C) DL- α -Tocopherol. Stern Volmer plot of (B) Capsaicin and (D) DL-Tocopherol binding to the PDK3.

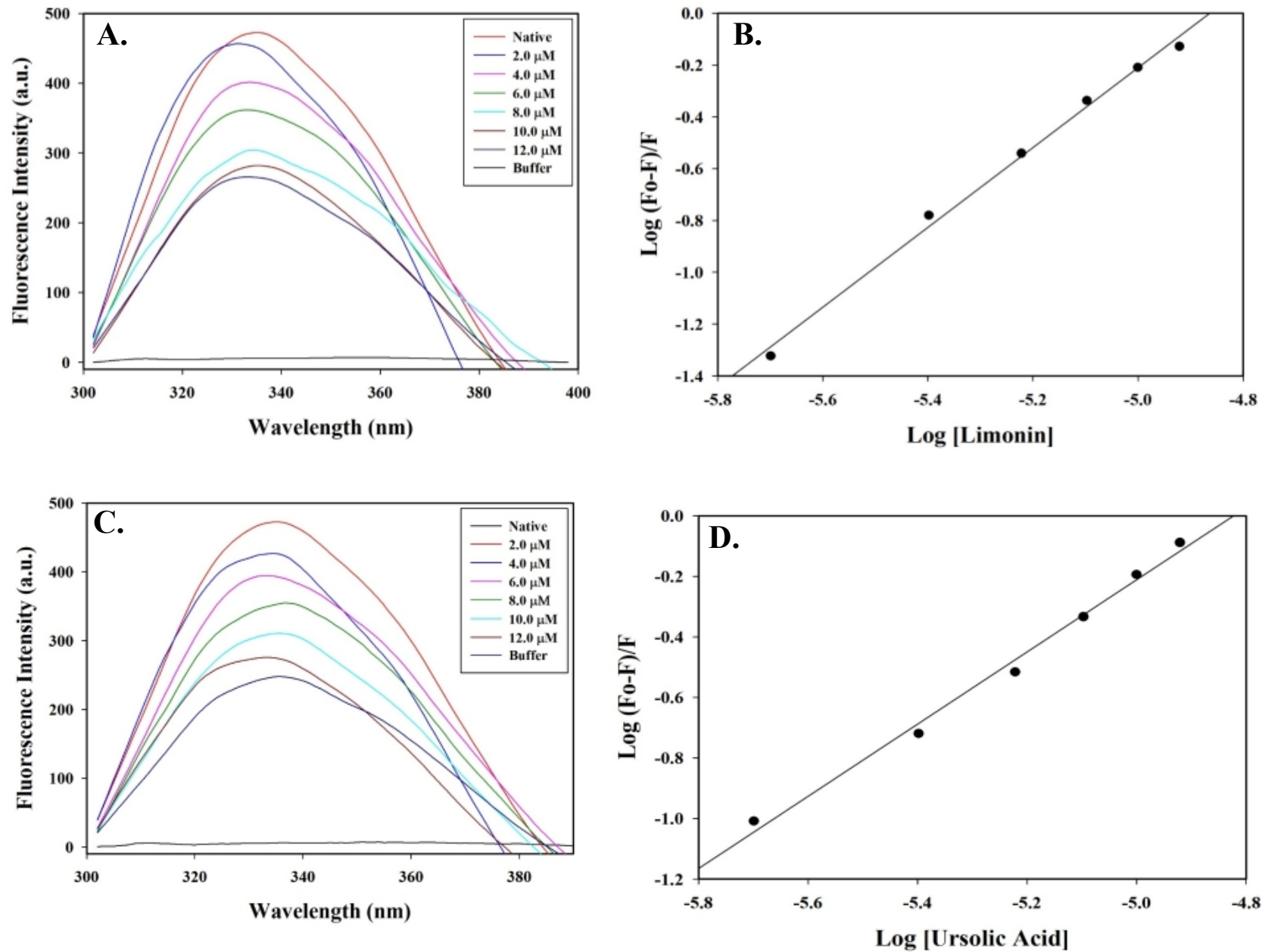


Figure S5: Fluorescence emission spectrum of (A) Limonin and (C) Ursolic acid. Stern Volmer plot of (B) Limonin and (D) Ursolic acid binding to the PDK3.

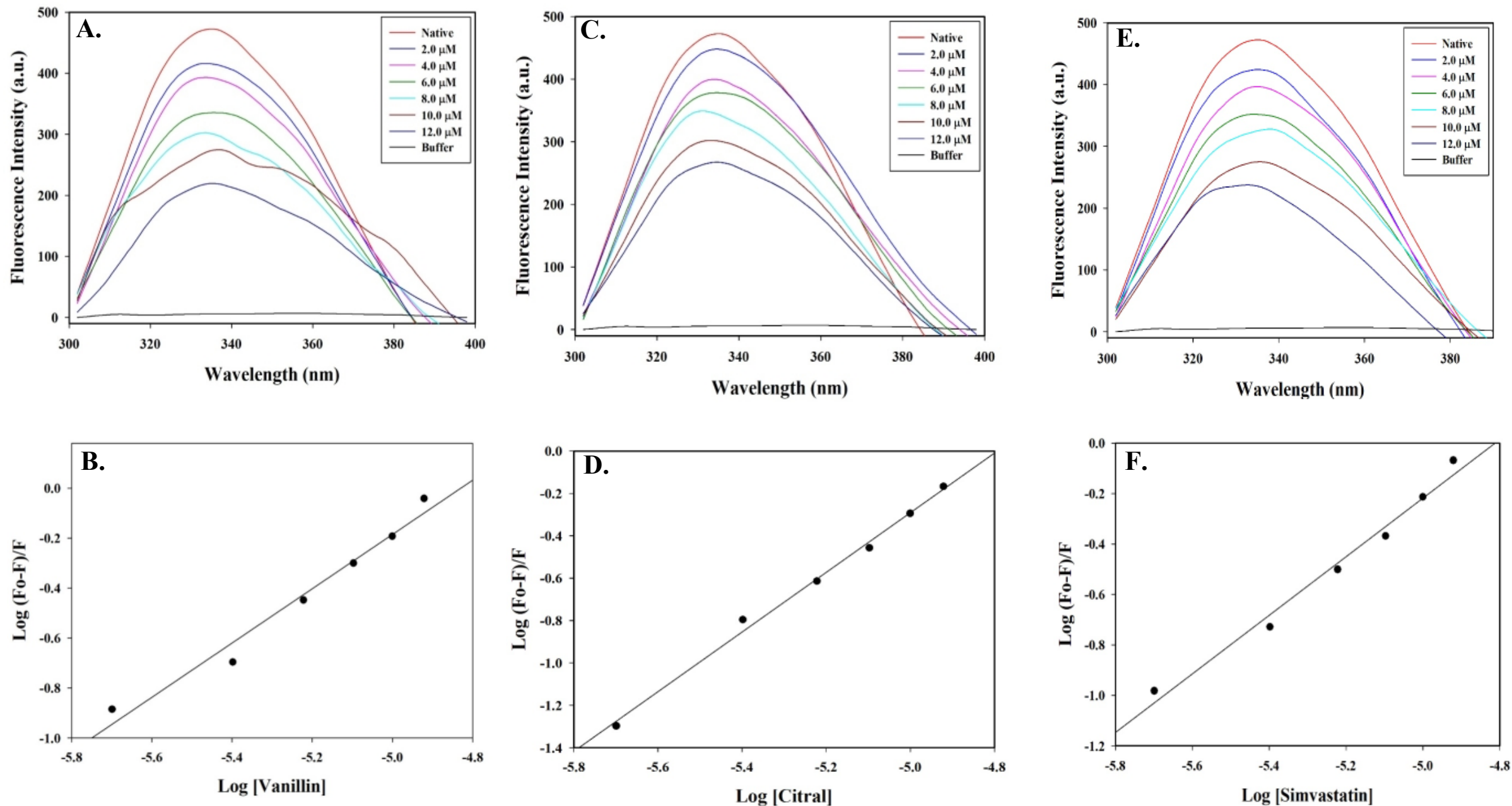


Figure S6: Fluorescence emission spectrum of (A) Vanillin and (C) Citral and (E) Simvastatin. Stern Volmer plot of (B) Vanillin (D) Citral and (F) Simvastatin binding to the PDK3.

Table S1: Percentage of residues participated in average structure formation.

*Structure = α -helix + β -sheet + β -bridge + Turn

Complexes	Percentage of protein secondary structure (SS %)						
	Structure*	Coil	β -sheet	β -bridge	Bend	Turn	α -helix
PDK3	73	18	13	2	9	7	51
PDK3-Ellagic acid	71	19	13	1	10	7	50