

# Formulation and Characterization of $\beta$ -Cyclodextrins–Nitazoxanide Inclusion Complexes: Enhanced Solubility, In Vitro Drug Release, and Antiviral Activity in Vero Cells

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**Table S1.** UV-Vis spectra of NTX (422 nm) with various concentration of  $\beta$ -CD at pH 7.4.

$\beta$ -CD concentration	Absorbance	$1/[\beta\text{-C}]$	$1/[A-A_0]$
		D]	
0	0.257	0	0
0.002	0.397	500	7.142
0.004	0.586	250	3.039
0.006	0.802	166.66	1.834
0.008	0.983	125	1.377
0.010	1.198	100	1.062
0.012	1.338	83.33	0.925
Binding constant (K) ( $M^{-1}$ )			61.26
Gibbs free energy ( $\Delta G$ ) (Kcal/mol)			-10.36

**Table S2.** UV-Vis spectra of NTX (422 nm) with various concentration of H $\beta$ -CD at pH 7.4.

H $\beta$ -CD concentration	Absorbance	$[1/H\beta\text{-CD}]$	$[1/A-A_0]$
0	0.257	0	0
0.002	0.512	500	3.921
0.004	0.737	250	2.083
0.006	0.932	166.66	1.481
0.008	1.155	125	1.113
0.010	1.406	100	0.870
0.012	1.654	83.33	0.715
Binding constant (K) ( $M^{-1}$ )			94.18
Gibbs free energy ( $\Delta G$ ) (Kcal/mol)			-11.45

**Table S3.** Molecular docking studies using PatchDock and FireDock servers scores for the top 5 docked models of  $\beta$ -CD:NTX inclusion complex.

S. No.	PatchDock server				FireDock server		
	Score	Area (Å <sup>2</sup> )	ACE (kcal/mol)	Global Energy (kcal/mol)	Attractive VdW (kcal/mol)	Repulsive VdW (kcal/mol)	ACE (kcal/mol)
1	3664	441.60	-336.83	-32.16	-12.10	2.63	-11.98
2	3536	420.50	-317.00	-31.21	-12.25	10.43	-13.58
3	3520	463.10	-344.76	-29.47	-10.51	10.28	-13.80
4	3466	419.50	-331.76	-27.73	-12.37	14.18	-13.08
5	3428	410.40	-319.72	-27.73	-11.34	6.10	-10.81

**Table S4.** Molecular docking studies using PatchDock and FireDock servers scores for the top 5 docked models of H $\beta$ -CD:NTX inclusion complex.

S. No.	PatchDock server				FireDock server		
	Score	Area (Å <sup>2</sup> )	ACE (kcal/mol)	Global Energy (kcal/mol)	Attractive VdW (kcal/mol)	Repulsive VdW (kcal/mol)	ACE (kcal/mol)
1	3520	437.60	-342.80	-45.23	-14.22	2.39	-16.40
2	3504	429.60	-282.75	-42.63	-13.56	1.69	-15.20
3	3414	433.10	-337.80	-38.14	-12.21	3.59	-14.30
4	3380	396.40	-317.04	-37.92	-13.55	4.26	-13.83
5	3340	410.30	-317.44	-37.54	-14.62	3.84	-13.18