A computational-based Polyphenol therapy for Non-Small Cell Lung Cancer: Naringin co-amorphous systems for solubility and bioavailability enhancement.

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Figure S1A. Chemical Structure of Ceritinib

Figure S1B. Chemical Structure of Naringin

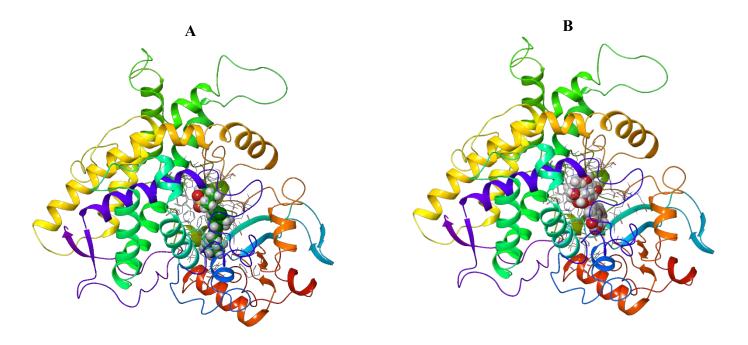


Figure S2. 3D interaction diagram and position of CRT and NRG in the molecular surface of the CYP3A4 protein. (CRT and NRG are highlighted in animated cartoon shapes for better understanding).

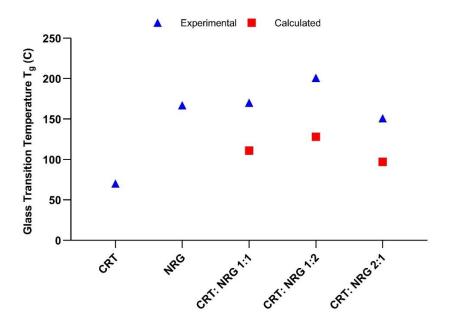


Figure S3. Experimental and Theoretical glass transition temperature (Tg) of Ceritinib (CRT), Naringin (NRG), and co-amorphous systems using Gordon Taylor equation.

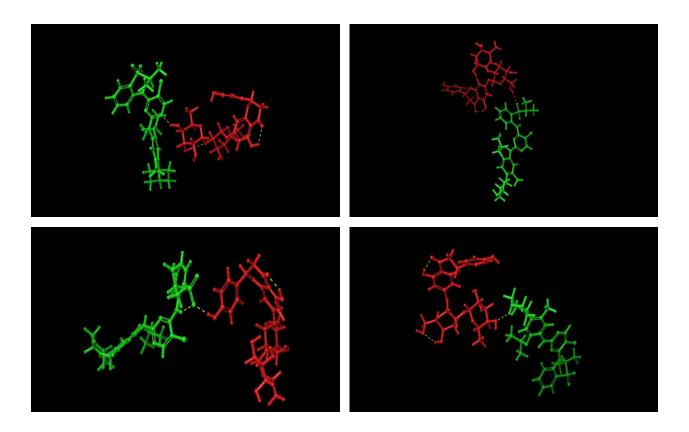


Figure S4. pi-pi interactions between CRT-RTH systems from MD simulation. (Red-CRT, Green- RTH, Blue- pi-pi interactions, Yellow- Hydrogen bonds)

Table S1. NRG and CRT, along with their chemical structure and docking score.

Compound name	Chemical structure	Docking score
		(Kcal/mol)
Naringin	HO,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	-10.970
Ceritinib	HN N N CI	-9.035

Table S2. 2D interaction diagram alongwith binding interaction of NRG and CRT at the binding site of the CYP3A4 protein

Compound	Chemical structure	Binding
name		interactions
Naringin		ARG212,
	THR 308 305 SER 241	THR224,
	304 AE 220	ARG372
	HO BE	(H-bond
	\mathcal{L}	interaction)
	HOOH 195	
	HO CH ARG	
	212 PHE 105 107 PHE 108 107 PHE 108 108 PHE 10	
	213 370 GAY	
	MET NOTE OF THE PARTY OF THE PA	
	HO OH	
	776R 2224	
	GLU 223 75	
	374 PHE 2	

