

Table S3. Toxicity score of designed compounds

Compound	Hepatotoxicity		Carcinogenicity		Immunotoxicity		Mutagenicity		Cytotoxicity	
	Toxicity	Prob	Toxicity	Prob	Toxicity	Prob	Toxicity	Prob	Toxicity	Prob
8a	Ina-	0.54	Ina-	0.56	Ina-	0.86	Ina-	0.60	Ina-	0.78
8b	Ina-	0.55	Ina-	0.55	Ina-	0.84	Ina-	0.59	Ina-	0.79

Ina- : Inactive