

Interaction of a new triazole compound with Serum albumins and Proteolytic enzyme Bromelain by Steady state fluorescence and Molecular docking techniques

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Supplementary data

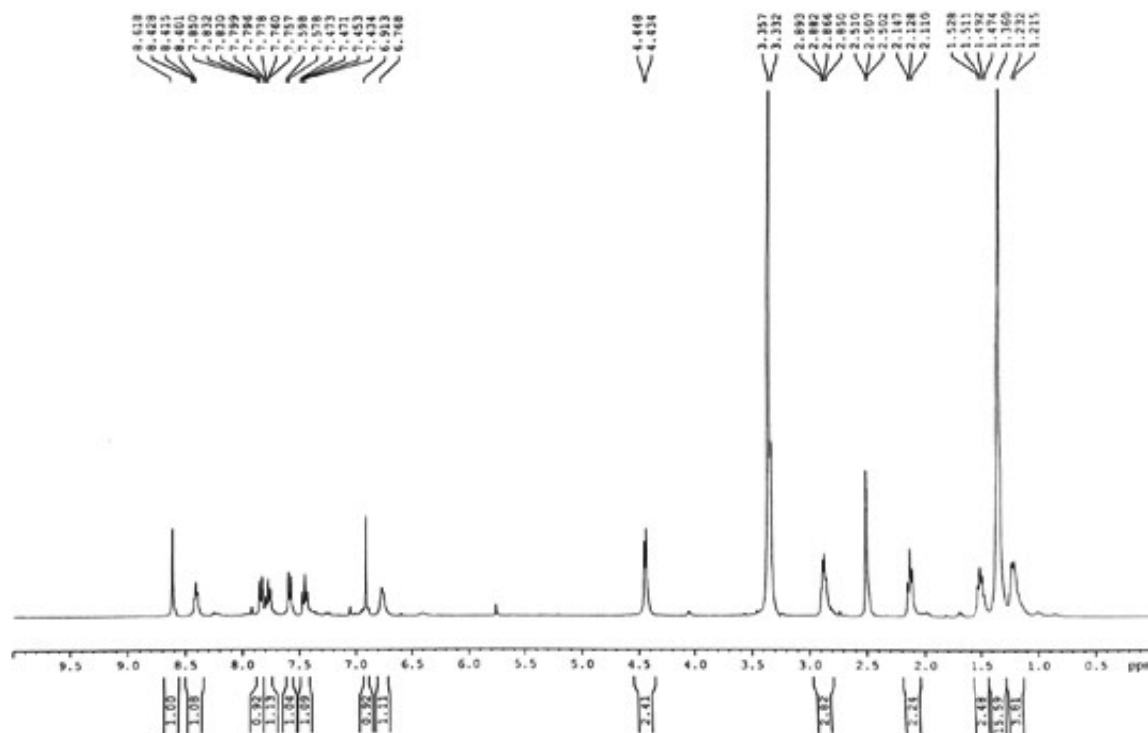


Fig. S1 — ¹H NMR spectra of compound SAM-1

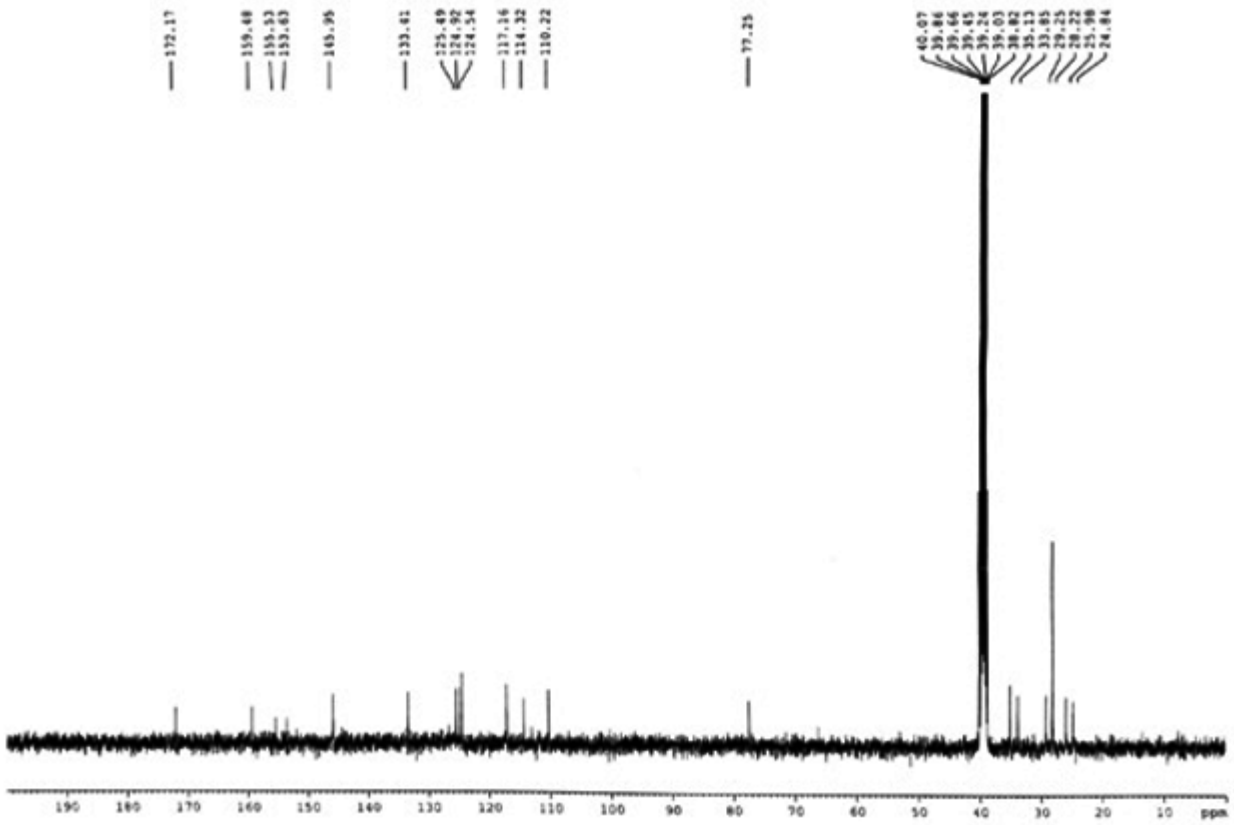
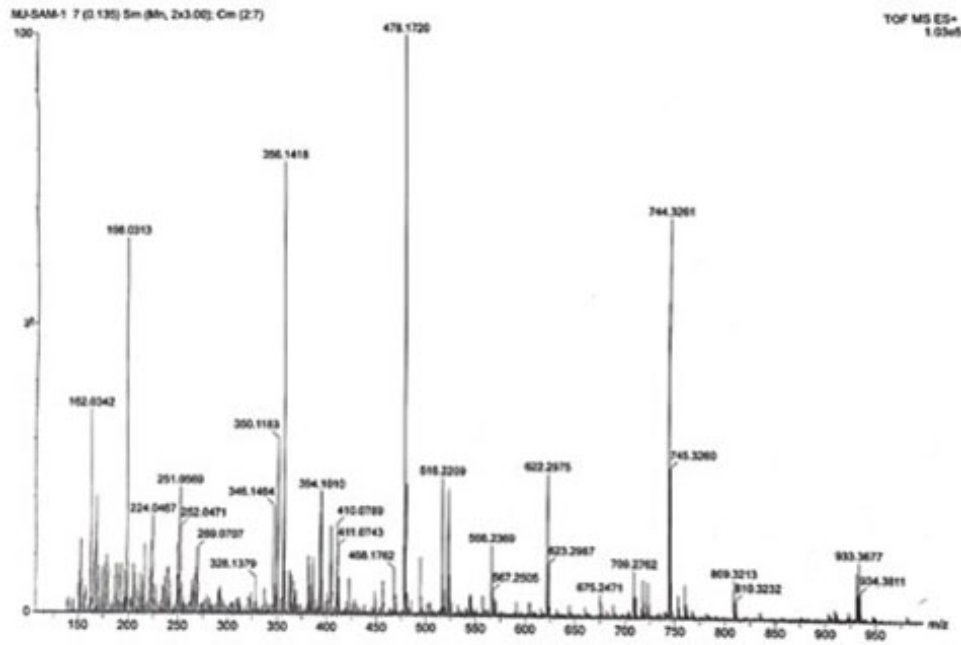
Fig. S2 — ^{13}C NMR spectra of compound SAM-1

Fig. S3 — Mass spectra of compound SAM-1

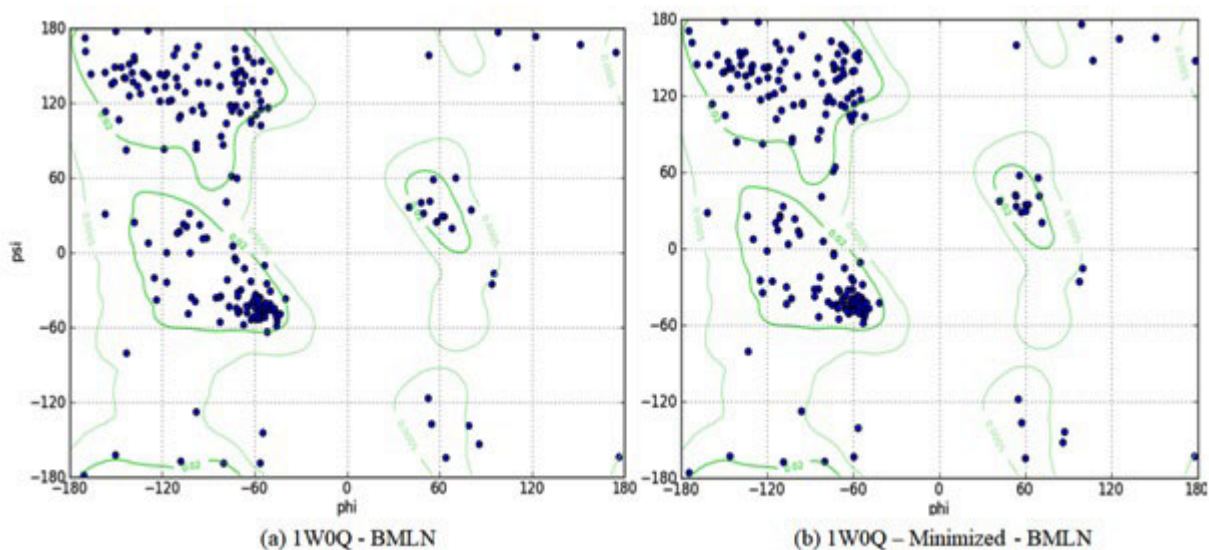


Fig. S4 — Ramachandran Plot of Bromelain protein

Table S1 — ADMET Prediction from pKCSM

Property	Model Name	Predicted Value	Unit
Absorption	Water solubility	-4.574	Numeric (log mol/L)
Absorption	Caco2 permeability	0.245	Numeric (log Papp in 10 ⁻⁶ cm/s)
Absorption	Intestinal absorption (human)	78.654	Numeric (% Absorbed)
Absorption	Skin Permeability	-2.845	Numeric (log Kp)
Absorption	P-glycoprotein substrate	Yes	Categorical (Yes/No)
Absorption	P-glycoprotein I inhibitor	Yes	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	Yes	Categorical (Yes/No)
Distribution	VDss (human)	-0.317	Numeric (log L/kg)
Distribution	Fraction unbound (human)	0.155	Numeric (Fu)
Distribution	BBB permeability	-1.48	Numeric (log BB)
Distribution	CNS permeability	-3.092	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	Yes	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitor	Yes	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitor	Yes	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitor	Yes	Categorical (Yes/No)
Excretion	Total Clearance	0.987	Numeric (log ml/min/kg)
Excretion	Renal OCT2 substrate	No	Categorical (Yes/No)
Toxicity	AMES toxicity	No	Categorical (Yes/No)
Toxicity	Max. tolerated dose (human)	-0.589	Numeric (log mg/kg/day)
Toxicity	hERG I inhibitor	No	Categorical (Yes/No)
Toxicity	hERG II inhibitor	Yes	Categorical (Yes/No)
Toxicity	Oral Rat Acute Toxicity (LD50)	2.446	Numeric (mol/kg)
Toxicity	Oral Rat Chronic Toxicity (LOAEL)	0.808	Numeric (log mg/kg_bw/day)
Toxicity	Hepatotoxicity	Yes	Categorical (Yes/No)
Toxicity	Skin Sensitisation	No	Categorical (Yes/No)
Toxicity	<i>T. Pyriformis</i> toxicity	0.366	Numeric (log ug/L)
Toxicity	Minnow toxicity	1.212	Numeric (log mM)