pharmaceuticals

Supplementary Material

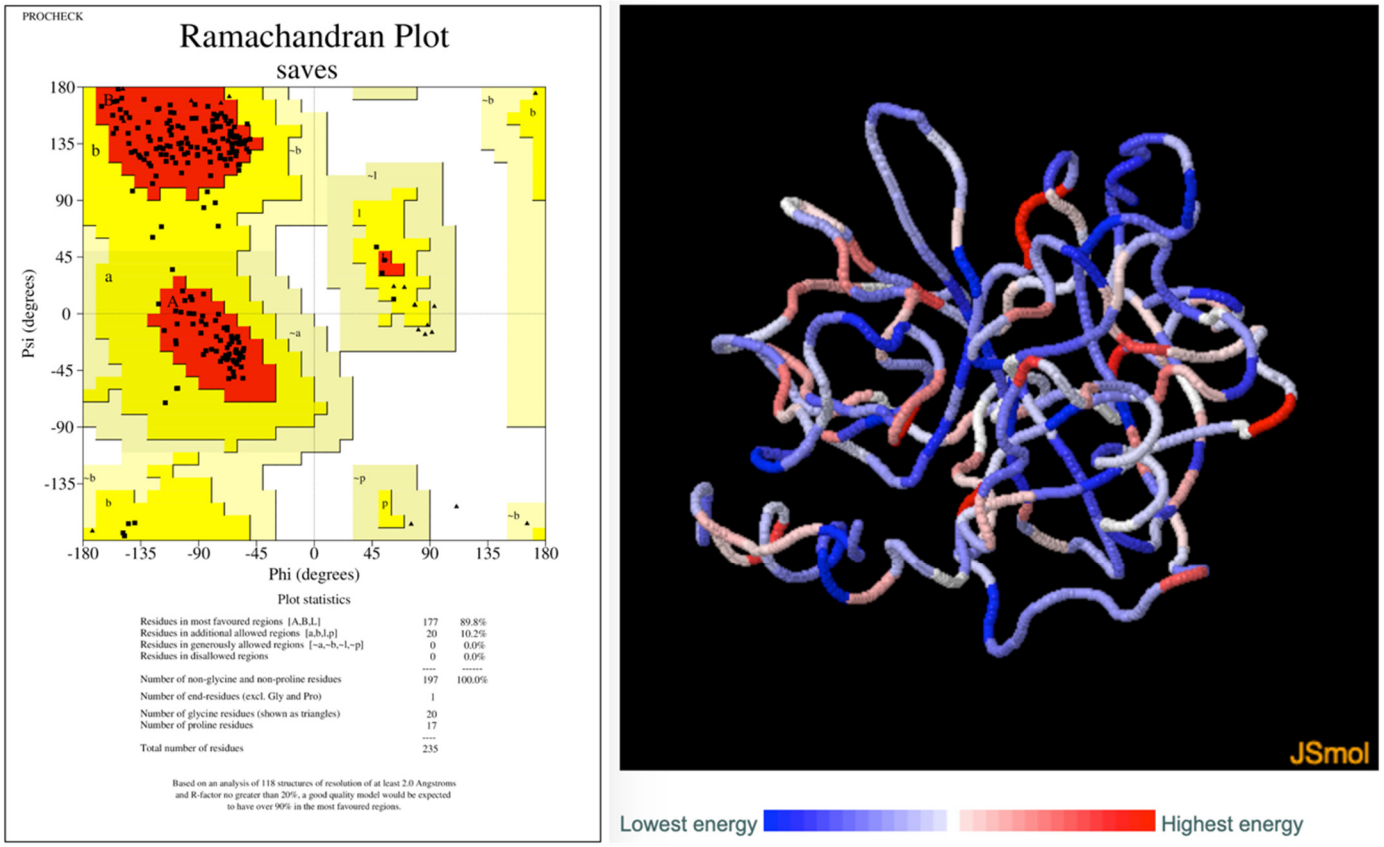


Figure S1. Stereochemical quality of the modeled serine proteinase using PROCHECK. **https://www.ebi.ac.uk/thornton-srv/software/PROCHECK/manual/parameters/manopt_01.html**

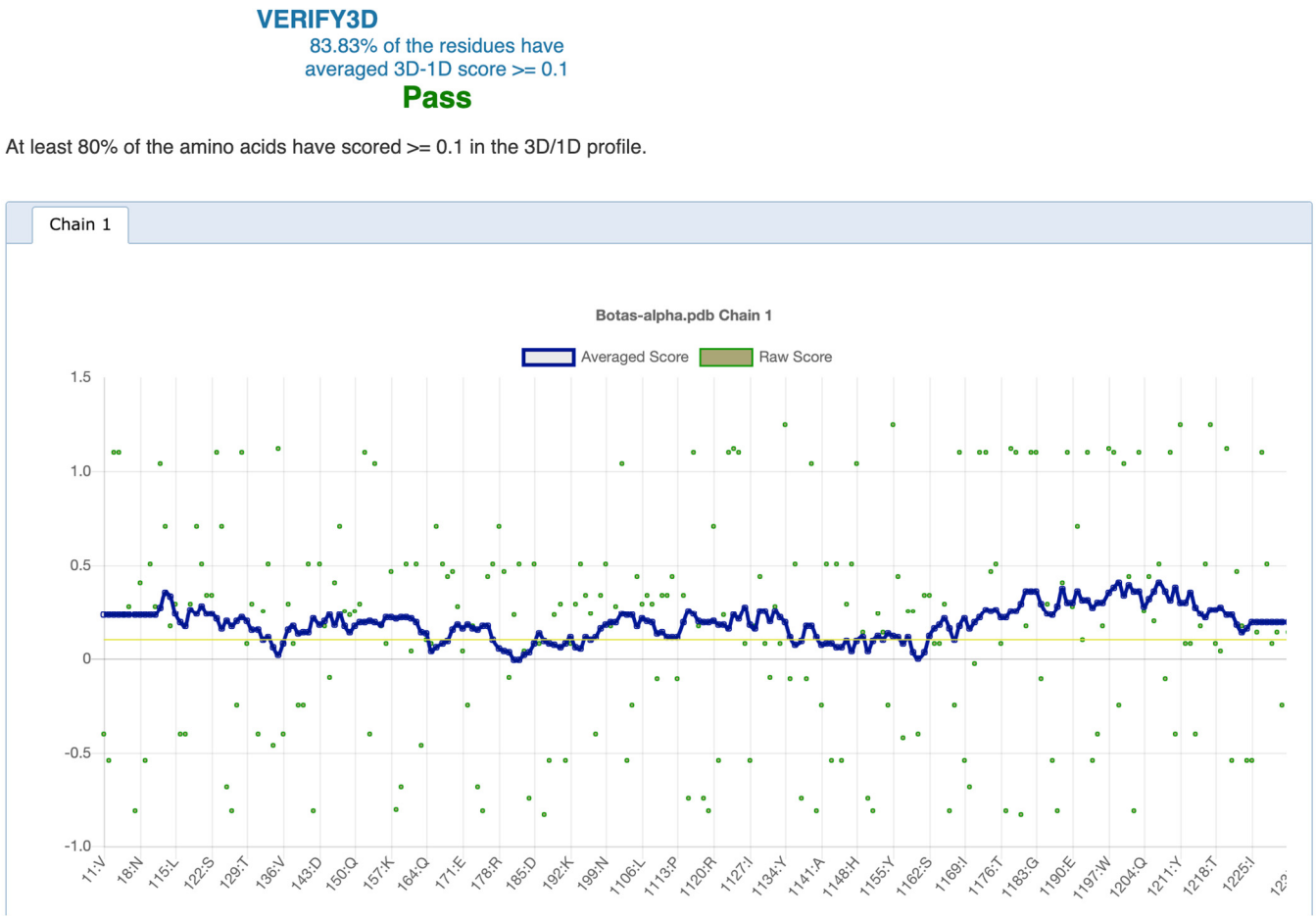


Figure S2. Compatibility of an atomic model (3D) with its amino acid sequence (1D).

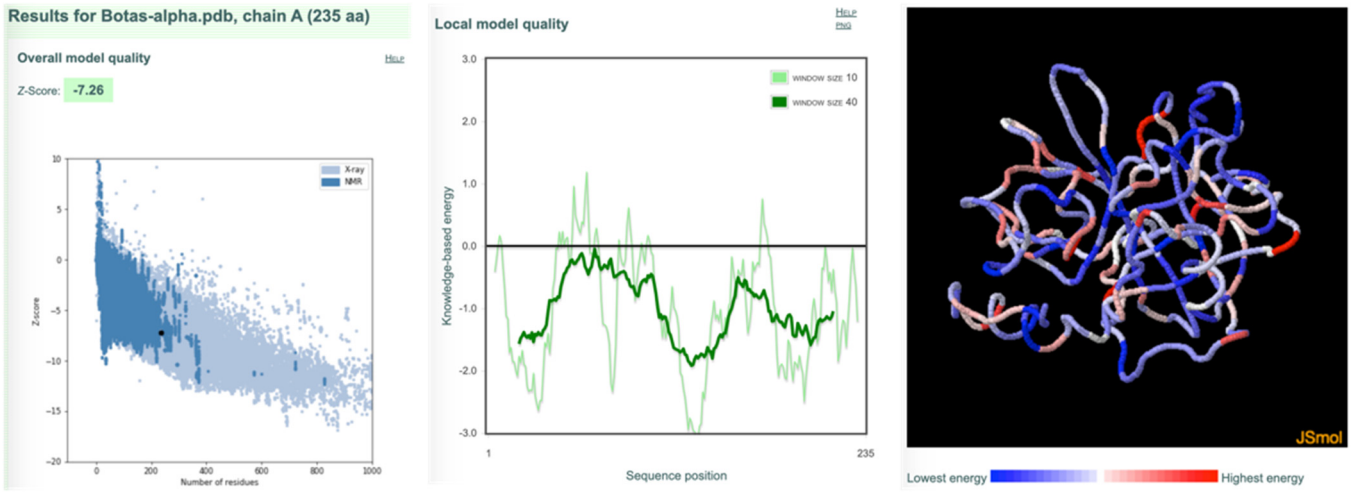


Figure S3. Energetic architecture of the modeled serine proteinase using the ProSA program.

Table S1. Mean effect size (Cohen's d), means, *p*-value, and 95% confidence intervals for the inhibitory activity of caffeine, caffeic, and chlorogenic acid on the pro-coagulant activity of *B. asper* venom

Caffeic acid	Chlorogenic acid	Caffeine	Positive control	
$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	*p* value
64.7 (13.6)	241 (22)	31 (1.46)	23.6 (0.81)	0.001

				Confidence Intervals (95%)	
		p value (Bonferroni)	Cohen's d-effect	Lower	Upper
Positive control	Caffeic acid	0.042	0.774	0.206	1.343
	Caffeine	1.00	0.139	−0.418	0.696
	Chlorogenic acid	<0.001	4.091	3.271	4.912

Table S2. Mean effect size (Cohen's d), means, *p*-value, and 95% confidence intervals for the inhibitory activity of caffeine, caffeic, and chlorogenic acid on the amidolytic activity of *B. asper* venom

Caffeic acid	Chlorogenic acid	Caffeine	Positive control	
$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	*p* value
0.61 (0.03)	0.66 (0.02)	0.57 (0.02)	0.76 (0.001)	0.001

				Confidence Intervals (95%)	
		p value (Bonferroni)	Cohen's d-effect	Lower	Upper
Positive control	**Caffeic acid**	0.001	−1.669	−2567	−0.772
	Caffeine	<0.001	−2.132	−3.073	−1.190
	Chlorogenic acid	0.063	−1.092	−1.948	−0.237

Table S3. Mean effect size (Cohen's d), means, *p*-value, and 95% confidence intervals for the inhibitory activity of caffeine, caffeic, and chlorogenic acid on the phospholipase A_2 activity of *B. asper* venom

Caffeic acid	Chlorogenic acid	Caffeine	Positive control	
$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	*p* value
0.09 (0.004)	0.09 (0.004)	0.101 (0.005)	0.107 (0.004)	0.002

				Confidence Intervals (95%)	
		p value (Bonferroni)	Cohen's d-effect	Lower	Upper
Positive control	**Caffeic acid**	0.004	−1.035	−16.353	−0.4341
	Caffeine	1.000	−0.372	−0.9503	0.2072
	Chlorogenic acid	0.012	−0.927	−15.232	−0.3317

Table S4. Mean effect size (Cohen's d), means, *p*-value, and 95% confidence intervals for the inhibitory activity of caffeine, caffeic, and chlorogenic acid on the proteolytic activity of *B. asper* venom

Caffeic acid	Chlorogenic acid	Caffeine	Positive control	
$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	*p* value
0.377 (0.005)	0.363 (0.003)	0.364 (0.006)	0.353 (0.001)	0.002

				Confidence Intervals (95%)	
		p value (Bonferroni)	Cohen's d-effect	Lower	Upper
Positive control	Caffeic acid	<0.001	12.384	0.6273	1.850
	Caffeine	0.327	0.5644	−0.0186	1.147
	Chlorogenic acid	0.447	0.5223	−0.0597	1.104

Table S5. Mean effect size (Cohen's d), means, *p*-value, and 95% confidence intervals for the inhibitory activity of green and roasted coffee extracts on the pro-coagulant activity of *B. asper* venom

Green Coffee	Roasted Coffee	Positive control	
$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	*p* value
36.5 (1.98)	**33.6 (2.98)**	**31.3 (0.29)**	**<0.001**

				Confidence Intervals (95%)	
		p value (Bonferroni)	Cohen's d-effect	Lower	Upper
Positive control	Green Coffee	< 0.001	−5.4898	−7.33	−3.649
	Roasted Coffee	<0.001	−5.1761	−6.975	−3.377

Table S6. Mean effect size (Cohen's d), means, *p*-value, and 95% confidence intervals for the inhibitory activity of green and roasted coffee extracts on the amidolytic activity of *B. asper* venom

Green Coffee	Roasted Coffee	Positive control	
$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	*p* value
0.465 (0.04)	0.481 (0.04)	0.756 (0.00)	<0.001

				Confidence Intervals (95%)	
		p value (Bonferroni)	Cohen´s d-effect	Lower	Upper
Positive control	Green Coffee	<0.001	−6.419	−8.11	−4.726
	Roasted Coffee	<0.001	6.064	4.45	7.681

Table S7. Mean effect size (Cohen's d), means, *p*-value, and 95% confidence intervals for the inhibitory activity of green and roasted coffee extracts on the phospholipase A_2 activity of *B. asper* venom

Green Coffee	Roasted Coffee	Positive control			
$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	*p* value		
0.069 (0.008)	0.128 (0.019)	0.117 (0.004)	0.002		
				Confidence Intervals (95%)	
		p value (Bonferroni)	Cohen's d-effect	Lower	Upper
Positive control	Green Coffee	0.016	−1.102	−1.870	−0.333
	Roasted Coffee	1.000	−0.234	−0.998	0.530

Table S8. Mean effect size (Cohen's d), means, *p*-value, and 95% confidence intervals for the inhibitory activity of green and roasted coffee extracts on the proteolytic activity of *B. asper* venom

Green Coffee	Roasted Coffee	Positive control			
$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	$\bar{x}$ (SEM)	*p* value		
0.394 (0.008)	0.345 (0.018)	0.510 (0.003)	<0.001		
				Confidence Intervals (95%)	
		p value (Bonferroni)	Cohen's d-effect	Lower	Upper
Positive control	Green Coffee	<0.001	−2.38	−3.251	−1.50
	Roasted Coffee	<0.001	3.39	2.381	4.41