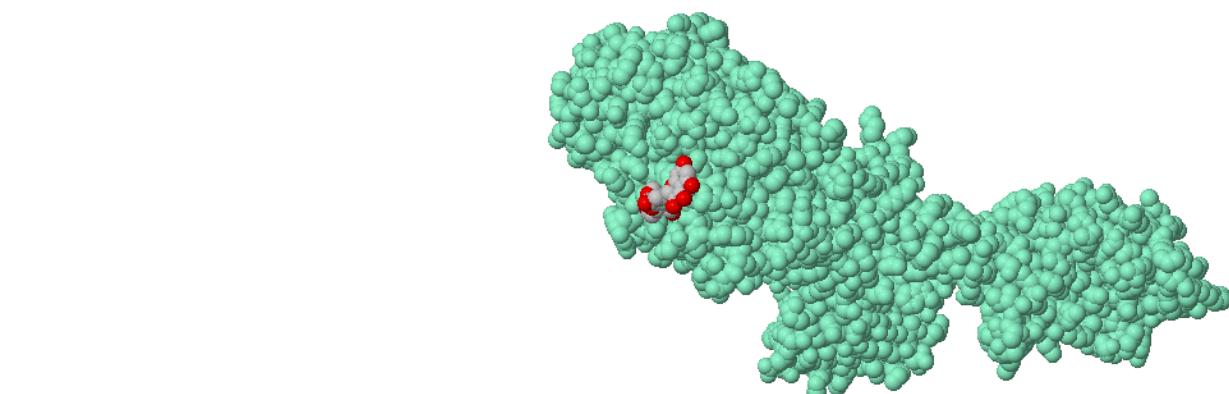


Table S1: Consensus phenolic pharmacophore spatial arrangements

Pharmacophore class	x	y	z	Radius
Hydrogen donor	1.11	2.35	3.27	0.50
Hydrogen acceptor	2.82	1.43	1.10	0.50
Aromatic	5.87	-0.18	-0.23	0.10
Hydrophobic	0.11	0.12	0.98	1.00
Hydrophobic	5.87	-0.18	-0.23	1.00



Pharmacophore Filters Viewer Submit Query

Pharmacophore Class	x	y	z	Radius	Enabled
Aromatic	5.46	45.42	17.02	1.10	<input type="checkbox"/>
Aromatic	5.87	-0.18	-0.23	1.10	<input checked="" type="checkbox"/>
Aromatic	-5.67	-1.45	-0.01	1.10	<input type="checkbox"/>
HydrogenDonor	13.01	45.42	19.92	0.50	<input type="checkbox"/>
HydrogenDonor	1.11	2.35	3.27	0.50	<input checked="" type="checkbox"/>
HydrogenDonor	-3.08	2.94	-0.40	0.50	<input type="checkbox"/>

Results >

Name	RMSD	Mass	RBnds
ZINC16323329	0.687	316	10
ZINC71880298	0.578	343	7
ZINC32929396	0.223	368	13
ZINC90656964	0.598	359	8
ZINC41512164	0.760	382	6
ZINC21150279	0.222	395	8
ZINC91077762	0.573	333	4
ZINC78610139	0.587	358	8
ZINC78929280	0.407	434	8
ZINC80964722	0.542	277	6
ZINC12185911	0.666	382	9
ZINC06503658	0.646	282	6
ZINC32088674	0.229	353	8
ZINC88605626	0.517	332	4
ZINC93858242	0.556	252	8
ZINC15670928	0.219	296	8
ZINC66920762	0.626	395	5
ZINC93797524	0.409	397	6
ZINC72164980	0.639	299	3

<< < 1 2 3 4 5 6 7 8 > >>

1,550 hits
55.633s

Save Results...

Figure S1: Observed 1550 hit compounds

Table S2: Average RMSD, ROG, and SASA of top five phenolics and amoxicillin following 120 ns simulation at the allosteric site of PBP2a of *S. aureus*

Systems	RMSD (Å)	RMSF (Å)	ROG (Å)	SASA (Å)
Unbound PBP2a	6.86 ± 1.18	2.71 ± 1.17	35.37 ± 0.45	26786.05 ± 473.91
PBP2a + Amoxicillin	3.34 ± 0.90	2.56 ± 1.32	37.16 ± 0.27	25452.79 ± 2301.39
PBP2a + Silicristin	3.48 ± 0.80	2.45 ± 1.11	36.93 ± 0.29	25466.88 ± 478.49
PBP2a + propan-2-one	4.17 ± 1.06	2.49 ± 1.14	36.12 ± 0.49	24802.25 ± 453.11
PBP2a + Epigallocatechin 4-benzylthioether	6.45 ± 2.33	3.48 ± 1.84	35.30 ± 0.88	25165.36 ± 509.79
PBP2a + chroman-4-one	3.24 ± 1.17	2.55 ± 1.32	36.89 ± 0.34	25844.78 ± 455.36
PBP2a + Epicatechin gallate	3.69 ± 0.68	2.06 ± 0.95	36.86 ± 0.21	25231.59 ± 459.17

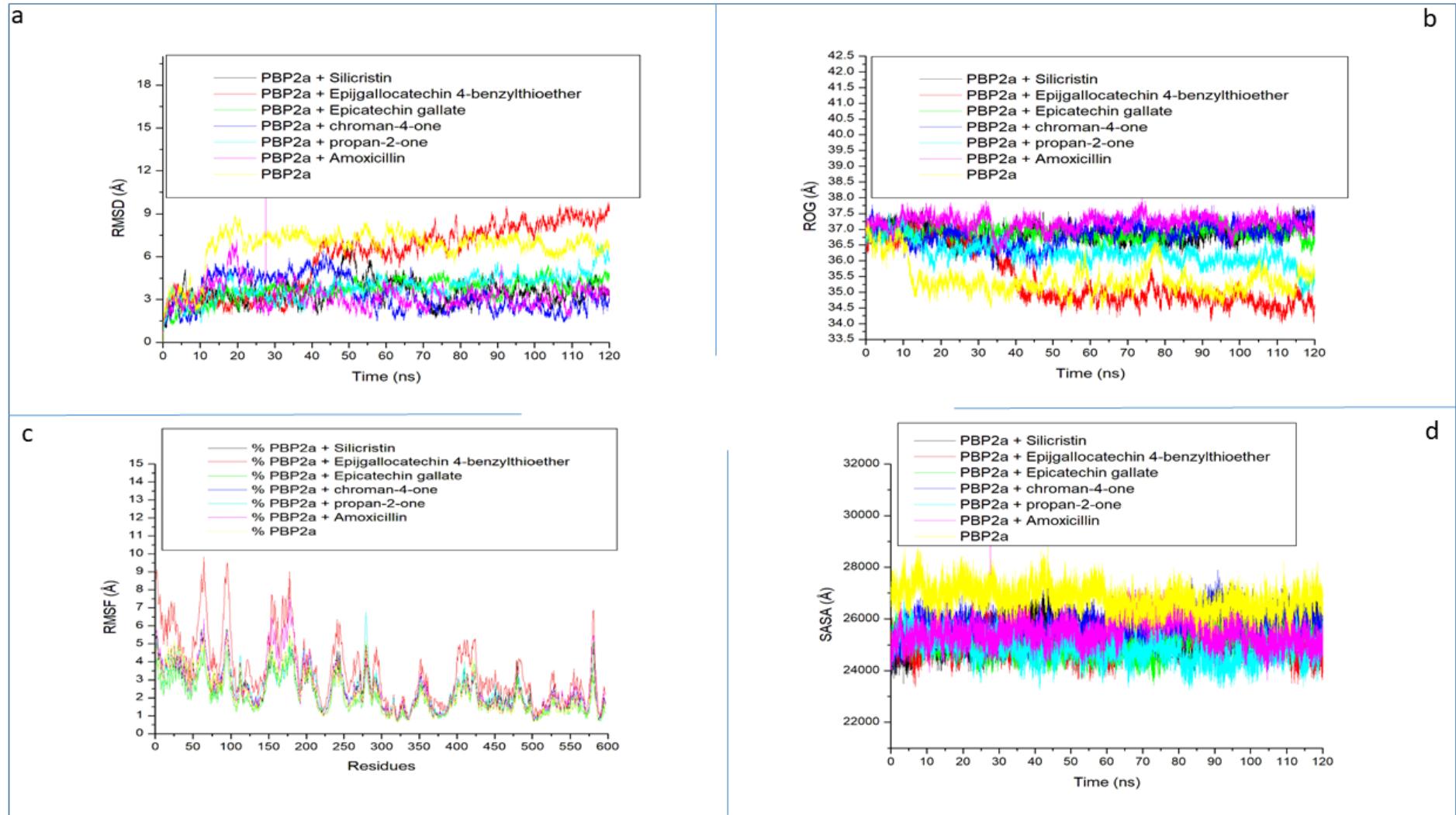


Figure S2: Comparative (a) root mean squared deviation (RMSD), (b) radius of gyration (ROG), (c) root mean squared fluctuation (RMSF), and (d) solvent-accessible surface area (SASA) plots of alpha-carbon, top five phenolics, and amoxicillin against the allosteric site PBP2a of *Staphylococcus aureus* over a 120 ns MD simulation period

Table S3: 2D plot interactions of the top five phenolics at the active and allosteric sites after 120 ns simulation

