

Supplementary Materials

Computational analysis of *Allium sativum* compounds to identify thermolabile hemolysin inhibitors against *Vibrio alginolyticus* in shrimp

Authors

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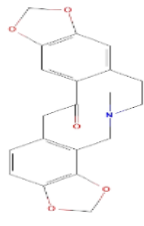
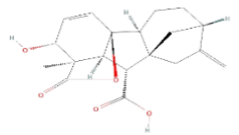
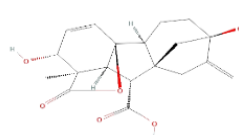
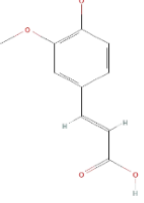
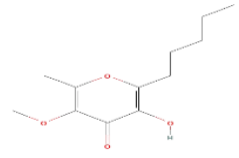
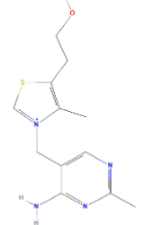
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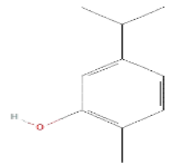
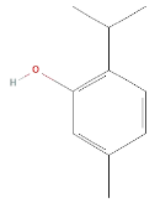
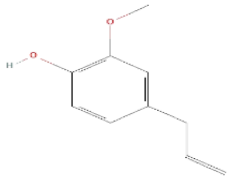
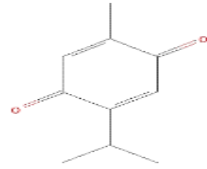
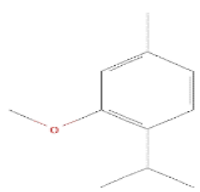
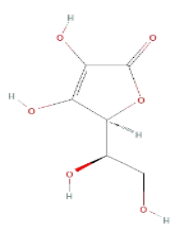
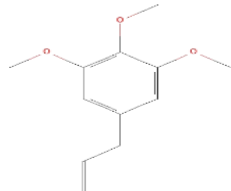
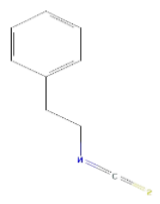
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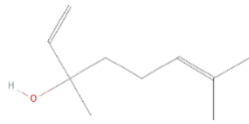
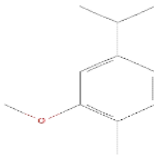
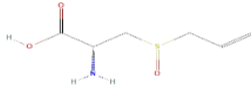

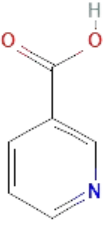
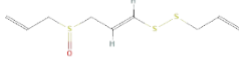
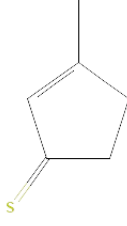
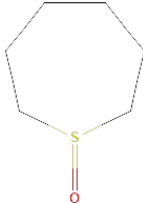
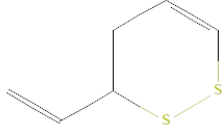
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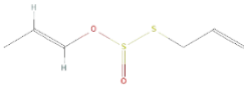
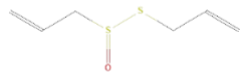

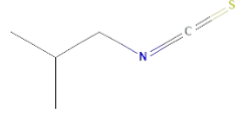



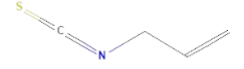




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Supplementary Table 1. List of 35 compounds of *Allium sativum* with their identity, chemical name, molecular weight, chemical formula, two-dimensional (2D) structure, and molecular docking scores.

Si. No.	PubChem ID	Chemical Name	Molecular Weight (g/mol)	Chemical Formula	Chemical Structure (2D)	Docking Score (Kcal/mol)
1.	4970	Protopine	353.37	C ₂₀ H ₁₉ NO ₅		9.4
2.	92782	Gibberellin A7	330.37	C ₁₉ H ₂₂ O ₅		8.0
3.	6466	Gibberellic acid	346.37	C ₁₉ H ₂₂ O ₆		7.4
4.	445858	Ferulic acid	194.18	C ₁₀ H ₁₀ O ₄		7.1
5.	86374	Allixin	226.27	C ₁₂ H ₁₈ O ₄		6.8
6.	1130	Thiamine	265.35	C ₁₂ H ₁₇ N ₄ OS +		6.5

7.	10364	Carvacrol	150.22	C ₁₀ H ₁₄ O		6.4
8.	6989	Thymol	150.22	C ₁₀ H ₁₄ O		6.2
9.	3314	Eugenol	164.20	C ₁₀ H ₁₂ O ₂		6.2
10.	10281	Thymoquinone	164.20	C ₁₀ H ₁₂ O ₂		6.2
11.	14104	2-Isopropyl-5-methyl anisole	164.24	C ₁₁ H ₁₆ O		6.0
12.	54670067	Ascorbic acid	176.12	C ₆ H ₈ O ₆		5.9
13.	10248	Elemicin	208.25	C ₁₂ H ₁₆ O ₃		5.8
14.	16741	Phenethyl isothiocyanate	163.24	C ₉ H ₉ NS		5.5

15.	6549	Linalool	154.25	C ₁₀ H ₁₈ O		5.5
16.	80790	Carvacrol methyl ether	164.24	C ₁₁ H ₁₆ O		5.4
17.	87310	3-(Allylsulphinyl)-L-alanine	177.22	C ₆ H ₁₁ NO ₃ S		5.3
18.	8158	Nonanoic acid	158.24	C ₉ H ₁₈ O ₂		5.3
19.	938	Nicotinic acid	123.11	C ₆ H ₅ NO ₂		5.3
20.	5386591	Ajoene	234.40	C ₉ H ₁₄ S ₃		4.9
21.	14252428	3-Methyl-2-cyclopentene-1-thione	112.19	C ₆ H ₈ S		4.8
22.	535250	Hexamethylene sulfoxide	132.22	C ₆ H ₁₂ OS		4.6
23.	10219489	3-Vinyl-1,2-dithiin	142.24	C ₆ H ₆ S ₂		4.4

24.	129704166	1-Propenyl allyl thiosulfinate	178.27	C ₆ H ₁₀ O ₂ S ₂		4.4
25.	65036	Allicin	162.27	C ₆ H ₁₀ OS ₂		4.0
26.	16591	Allyl propyl disulfide	148.29	C ₆ H ₁₂ S ₂		4.0
27.	68960	Isobutyl isothiocyanate	115.20	C ₅ H ₉ NS		3.9
28.	16315	Diallyl trisulfide	178.34	C ₆ H ₁₀ S ₃		3.9
29.	16590	Diallyl disulfide	146.27	C ₆ H ₁₀ S ₂		3.9
30.	11617	Diallyl sulfide	114.21	C ₆ H ₁₀ S		3.6
31.	5971	Allyl isothiocyanate	99.15	C ₄ H ₅ S		3.5
32.	61926	Allyl methyl trisulfide	152.30	C ₄ H ₈ S ₃		3.4
33.	7858	Allyl alcohol	58.08	C ₃ H ₆ O		3.4
34.	62434	Allyl methyl disulfide	120.24	C ₄ H ₈ S ₂		3.1
35.	19310	Dimethyl trisulfide	126.26	C ₂ H ₆ S ₃		2.5