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Data Article

Data on docking of phytoconstituents of *Actinidia deliciosa* on dengue viral targets

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ABSTRACT

Major Phytoconstituents of *Actinidia deliciosa* were explored for their anti-viral potential against dengue virus (DENV). The docking of these phytoconstituents was performed on 7 viral targets- 4 DENV non structural protein (NS5-SAM binding domain, NS5 RdRp domain, NS3 helicase & NS2B-NS3 protease) and 3 DENV structural proteins (Envelope protein- β -OD domain, stem domain & Domain III). The analysis was done on the basis of binding affinity, type of interactions (bond type and distance) and interaction with amino acids significant in viral replication. The top 5 phytoconstituents with best docking score have been reported.

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1. Data

The phytoconstituent abundance, folklore usage and reported scientific literature of *Actinidia deliciosa* develops a promising platform for its evaluation as antidengue agent [1,2].

The data includes the outcome of docking of phytoconstituents of *Actinidia deliciosa* against various dengue viral targets. The details of viral targets (Table 1) and list of phytoconstituents (Table 2) are furnished. The top 5 best docked phytoconstituents are listed (Table 3) and image of the topmost phytoconstituent binding to selected viral proteins is provided (Fig. 1). The detail of docking of all phytoconstituents is provided in the supplementary data.

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Specification table

Subject area	Computational and <i>insilico</i> Chemistry
More specific subject area	Docking studies
Type of data	Table, Image, Figure
How data was acquired	Molecular docking(Schrödinger Maestro Release 2016–4) (Schrödinger Release 2016–4: MS Jaguar, Schrödinger, LLC, New York, NY, 2016.), FlexX Lead IT 2.3.2
Data format	Raw & Analyzed
Experimental factors	Docking score and interaction with amino acid residues in the binding pocket
Experimental features	The structures of the 32 phytoconstituents were downloaded from Pubchem and energy minimized using Avogadro software. The minimized structures were docked on selected anti-viral targets using FlexX software.
Data source location	Pharmaceutical Chemistry Laboratory, Dr. D. Y. Patil Institute of Pharmaceutical Sciences & Research, Pimpri, Pune
Data accessibility	Data is with this article

Value of the data

- This is the first article which represents exploration of various phytoconstituents against several dengue virus targets.
- It provides information about the phytoconstituents (belonging to varied classes) and their interaction with the viral targets which will help in investigating and developing other DENV inhibitors.
- The data may be useful for researchers working on discovery and development of anti-dengue agents.
- The promising phytoconstituents identified may serve as potential leads for development of future therapeutics for dengue infection.

Table 1

Dengue viral targets used in docking.

Sr.No.	Protein	PDB ID	Resolution
1.	NS2B– NS3 protease	3UII [3]	2.3 Å
2.	NS3 helicase	2JLV [4]	1.9 Å
3.	NS5 (SAM Binding pocket)	5EHI [5]	1.303 Å
4.	NS5 (RdRp pocket)	5HMZ [6]	1.99 Å
5.	Envelope protein (hydrophobic pocket)	1OKE [7]	2.4 Å
6.	Envelope protein (binding domain 3)	1OKE [7]	2.4 Å
7.	Envelope protein (stem domain)	Model- UniProt B1PNV2 [8], 3j27.1.A	–

Table 2

List of phytoconstituents.

1. Quercetin -3-glucoside	11. Malic acid	22. Ascorbic acid
2. Kaempferol-3-rhamnoside	12. Spermidine	23. 3-Hydroxy-2-butanone
3. Epicatechin	13. Serotonin	24. Phenylethyl alcohol
4. Kaempferol-3-rutinoside	14. p-coumaric acid	25. Ethyl-3-hydroxybutyrate
5. Riboflavine	15. Niacin	26. α -Terpineol
6. Shikimic acid	16. Thiamine	27. 23-Hydroxytormentic acid
7. Caffeic acid	17. Putrescine	28. 3-Methyl-2-butanol
8. Chlorogenic acid	18. Phylloquinone	29. Geraniol
9. Protocatechuic acid	19. Retinol	30. 2-E-hexenal
10. Quinic acid	20. Tocomonoenol	31. α -Tocopherol
	21. δ -Tocopherol	32. 9-cis-neoxanthin

Table 3

Top 5 phytoconstituents and their interactions.

Sr. No.	Target	Name of the phytoconstituent	Binding energy (kCal/mol)	Interactions	Type of interaction	Bond distance (Å)	
1.	3UII	Kaempferol 3-rutinoside	-32.2516	Asp A:81	3 H-Bonds	1.811, 1.856, 2.408	
				Asn B:152	H-Bond	2.509	
				Tyr B:161	H-Bond	2.131	
				Gly B:151	H-Bond	1.819	
				Tyr B:150	H-Bond	2.153	
				His B:51	Pi-Pi stacking	4.159	
		Riboflavin	-31.0863	Riboflavin	Val B:36	H-Bond	1.636
					Ser B:135	H-Bond	1.932
					Lys B:131	H-Bond	2.232
					Gly B:153	2 H-Bond	2.057, 2.21
					His B:51	Pi-Pi stacking	4.182
					TyrB:161	H-Bond	2.071
		Kaempferol 3-rhamnoside	-28.4051	Kaempferol 3-rhamnoside	Gly B:151	2 H-Bonds	1.783, 2.222
					His 51	H-Bond	1.837
					Lys 131	H-Bond	1.831
					Gly 151	2 H-Bonds	1.849, 2.178
					Tyr 161	H-Bond	2.32
					Gly 153	H-Bond	2.231
		Quercetin 3-glucoside	-28.1772	Quercetin 3-glucoside	Asn 152	H-Bond	2.251
					His 51	Pi- Pi stacking	4.13
					Arg 54	H-Bond	2.634
					Asn 152	H-Bond	2.149
					Gly 153	H-Bond	1.883
					Tyr 161	H-Bond	1.73
Chlorogenic acid	-25.997	Chlorogenic acid	Gly 151	H-Bond	1.870		
			Lys 131	H-Bond	2.374		
			Tyr 150	H-Bond	2.075		
			Val 36	H-Bond	2.190		
			Thr A:83	H-Bond	1.866		
			Gly B:151	H-Bond	1.904		
2.	2JLV	Malic acid	-50.8132	Phe B:130	H-Bond	2.440	
				Gly B:133	H-Bond	1.727	
				Ser B:135	H-Bond	2.186	
				Gly 198	H-Bond	1.84	
				Lys 199	H-Bond	1.92	
				Arg 463	2 Salt bridges	4.19, 4.31	
		Ascorbic acid	-42.0454	Ascorbic acid	Arg 460	2 H-Bonds	1.90, 2.29
					Gly 196	H-Bond	1.53
					Arg 460	H-Bond	2.04, 2.16
					Thr 200	H-Bond	2.14
					Gln 456	H-Bond	1.75, 1.96
					Gly 196	H-Bond	2.06
Shikimic acid	-40.3817	Shikimic acid	Ala 316	H-Bond	2.18		
			Glu 285	H-Bond	2.12		
			Thr 200	H-Bond	2.23		
			Gly 198	2 H-Bonds	1.69, 2.07		
			Lys 199	2 H-Bonds	1.89, 2.11		
			Lys 199	H-Bond	1.95		
Quinic acid	-37.6124	Quinic acid	Salt bridge		4.85		
			Arg 463	H-Bond	1.82		
			Arg 460	H-Bond	2.39		
			Gly 414	H-Bond	2.19		
			Asn 416	H-Bond	2.00		
			Thr 200	H-Bond	1.47		
				Glu 285	H-Bond	1.79	
				Gly 414	H-Bond	2.27	
				Thr 200	H-Bond	1.70	
				Lys 199	Salt bridge	4.17	

(continued on next page)

Table 3 (continued)

Sr. No.	Target	Name of the phytoconstituent	Binding energy (kCal/mol)	Interactions	Type of interaction	Bond distance (Å)
3.	5EHI	Protocatechuic acid	-37.3468	Gly 198	H-Bond	1.90
				Gly 196	H-Bond	1.98
				Asp 284	H-Bond	1.47
				Glu 285	H-Bond	2.27
				Ala 316	H-Bond	2.06
				Lys 199	H-Bond	1.74
					Pi- cation	3.06
					Salt bridge	4.16
				Gly 196	H-Bond	1.99
				Arg 463	H-Bond	1.71
					H-Bond	1.71
				Arg 460	H-Bond	2.22
		Gly 148	H-Bond	1.99		
		Glu 111	H-Bond	2.28		
		Asp 131	H-Bond	1.58		
		Gly 81	H-Bond	2.2		
		Lys 105	Pi-cation	6.13		
			H-Bond	1.61		
		Lys 130	H-Bond	1.73		
		Thr 104	H-Bond	2.23		
		Gly 148	H-Bond	1.78		
		Thr 104	H-Bond	1.87		
		Lys 105	H-Bond	2.13		
		Lys 130	H-Bond	2.11		
		Asp 131	H-Bond	1.51		
		Lys 130	H-Bond	1.78		
		Val 132	2 H-Bonds	1.70, 2.33		
		Asp 131	H-Bond	2.29		
		Gly 148	H-Bond	1.81		
		Asp 146	H-Bond	2.21		
		Gly 81	H-Bond	1.81		
		Asp 146	2 H-Bonds	1.84, 1.91		
Ser 56	H-Bond	2.23				
Gly 85	H-Bond	2.35				
Gly 86	H-Bond	1.83				
Trp 87	H-Bond	2.27				
Glu 111	H-Bond	1.73				
Thr 104	H-Bond	2.20				
Lys 130	H-Bond	2.13				
Lys 105	H-Bond	2.09				
	Pi cation	6.35				
4.	5HMZ	Caffeic acid	-24.8427	His 798	H-Bond	2.07
				Ser 796	H-Bond	2.3
				Arg 729	Salt bridge	3.74
		Epicatechin	-24.3502	His 798	H-Bond	2.33
				Thr 794	H-Bond	2.08
				Ser 710	H-Bond	1.95
		Chlorogenic acid	-23.9068	Leu 511	H-Bond	2.43
				Arg 729	3 H-Bonds	1.97, 1.99, 2.73
				Ser 710	H-Bond	2.18
		Quinic acid	-22.7297	Arg 729	2 H-Bonds	1.85, 2.01
				Trp 795	H-Bond	2.13
		Kaempferol 3-rhamnoside	-22.0444	Thr 794	H-Bond	1.74
				Tyr 766	H-Bond	2.37
				Thr 793	H-Bond	1.97
				Ser 710	H-Bond	2.29
				Arg 729	Pi cation	5.71
5.	10KE	Chlorogenic acid	-21.3989	Lys 128	2 H-Bonds	1.73, 2.08
				Thr 280	H-Bond	1.8
				Gln 200	H-Bond	1.85

Table 3 (continued)

Sr. No.	Target	Name of the phytoconstituent	Binding energy (kCal/mol)	Interactions	Type of interaction	Bond distance (Å)
				Ala 50	H-Bond	2.36
				Glu 49	H-Bond	2.26
		Serotonin	-20.906	Thr 48	H-Bond	1.63
				Thr 280	H-Bond	1.62
		Epicatechin	-19.2868	Thr 48	H-Bond	1.99
				Phe 279	H-Bond	2.21
				Thr 280	H-Bond	2.06
		Quercetin 3-glucoside	-19.1458	Gln 271	H-Bond	2.43
				Thr 48	H-Bond	2.04
				Glu 49	H-Bond	1.82
		Caffeic acid	-18.9577	Ala 50	H-Bond	1.48
				Thr 48	2 H-Bonds	1.83, 1.92
				Ala 50	H-Bond	1.94
				Lys 128	Salt bridge	2.69
6.	1OKE- Domain III	Epicatechin	-20.691	Ile 335	2 H-Bonds	1.73, 1.78
				Phe 337	H-Bond	2.20
		Kaempferol 3-rhamnoside	-14.6036	Leu 351	H-Bond	1.89
				Phe 337	H-Bond	2.08
		Protocatechuic acid	-14.4177	Gly 381	H-Bond	1.90
				Phe 337	H-Bond	1.93
				Pro 356	H-Bond	1.93
				Asn 355	H-Bond	1.88
		Serotonin	-14.2435	Glu 338	Salt bridge	3.77
				Ile 335	H-Bond	1.54
				Asn 355	H-Bond	2.17
		Shikimic acid	-13.6214	Asn 355	2 H-Bonds	2.06, 2.08
				Phe 337	H-Bond	2.01
7.	Model- Uniprot B1PNV2, 3j27.1.A	Protocatechuic acid	-19.4906	Arg 691	2 H-Bonds	1.65, 1.89
					Salt bridge	2.61
				Phe 702	H-Bond	1.80
		Shikimic acid	-18.5522	Arg 691	H-Bond	1.81
					Salt bridge	2.88
				Phe 702	H-Bond	2.12
		p-coumaric acid	-18.4392	Arg 691	2 H-Bonds	1.52, 2.03
		Caffeic acid	-17.9774	Arg 691	H-Bond	1.74
					Salt bridge	2.85
				Trp 700	H-Bond	1.79
		Malic acid	-17.3804	Arg 691	2 H-Bonds	1.94, 1.98
					Salt bridge	4.08

2. Experimental design, materials, and methods

2.1. Selection & retrieval of target structures

The selection of targets was done on the basis of literature survey. The docking was carried out on 4 non structural (NS2B-NS3, NS3 helicase, NS5 methyltransferase, NS5 RdRp domain) proteins and 3 possible target sites in envelope protein of the dengue virus.

The crystal structures of the selected dengue non structural proteins and envelope protein were retrieved from protein data bank. (PDB database, www.rcsb.org). The downloaded protein structure was prepared prior to docking using Schrödinger Maestro release 2016–4. Briefly the protein preparation was done by preprocessing the structures for assignment of bonds and bond orders, addition of hydrogens, filling in missing loops or side chains, capping uncapped termini, adjusting bonds and formal charges for metals, and correcting mislabeled elements, removing water

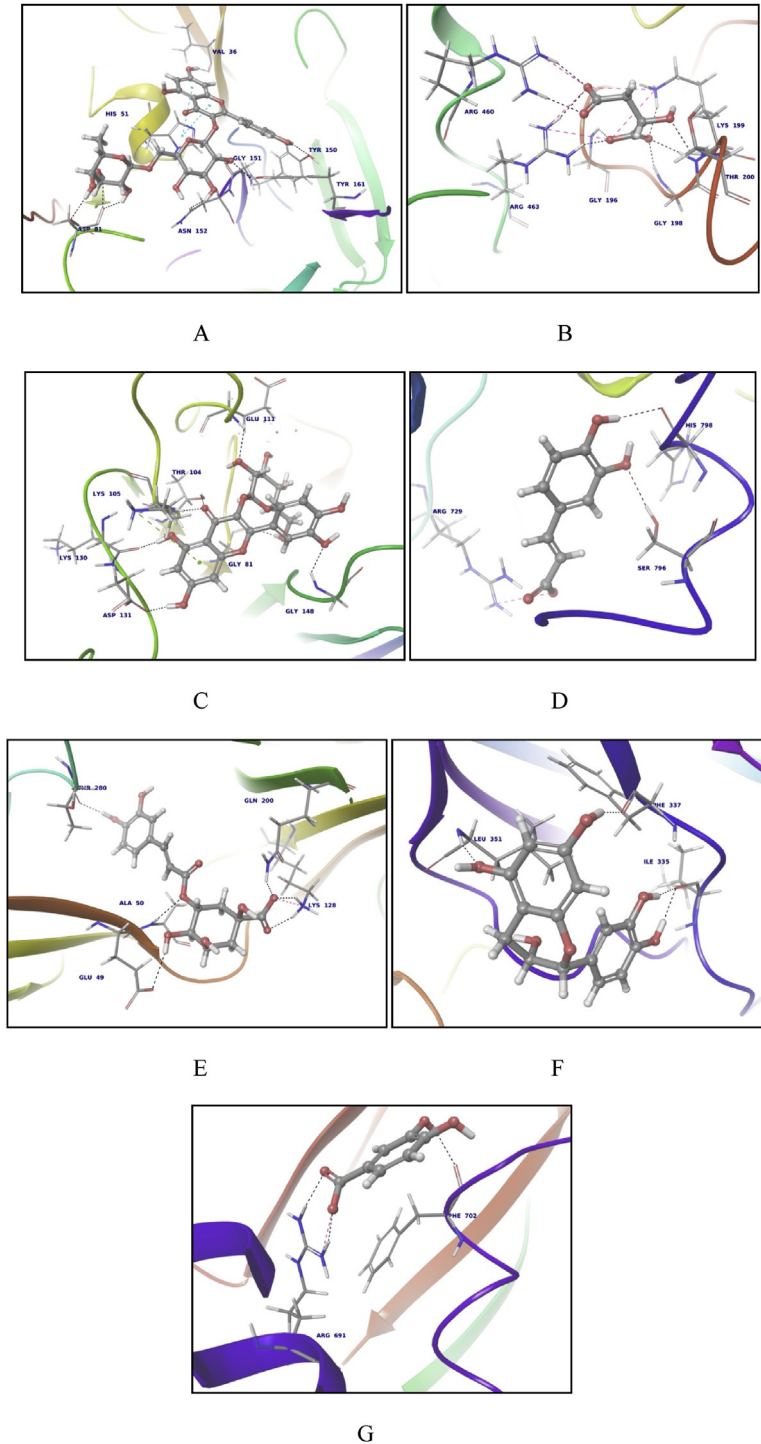


Fig. 1. (All targets are shown as ribbon diagrams and phytoconstituents as ball and stick representation) A. 3UII – Kaempferol-3-rutinoside, B. 2JLV- Malic acid, C. 5EHI-Quercetin-3-glucoside, D. 5HMZ-Caffeic acid, E. IOKE-Chlorogenic acid, F. IOKE domain 3-Epicatechin, G. Stem Domain- Protocatechuic acid.

molecules, removing unwanted chains and optimization of hydrogen bonded structures followed by refinement.

The Table 1 gives details of X-ray crystallographic models of targets used for docking.

No suitable protein structure was available in protein data bank for stem domain of the envelope protein. A model was created using dengue full length dengue envelope protein (UniProt ID-B1PNV2_9FLAV) with SWISS-MODEL [9].

The receptor preparation was done using Schrodinger Maestro Protein preparation wizard.

2.2. Ligand preparation and molecular docking

The structures of the selected 32 phytoconstituents of *Actinidia deliciosa* were downloaded from Pubchem (<https://pubchem.ncbi.nlm.nih.gov/>). The energy minimisation was done using Avogadro software and structures were saved in sdf format. The minimized structures were docked on the prepared protein targets after converting to 3d structures and refinement, using FlexX Lead IT 2.3.2 software.

The best phytoconstituent was identified on the basis of binding energy and interaction with amino acid residues important for viral replication. Table 3 gives the top 5 phytoconstituents based on binding energy and Fig. 1 gives the best docked phytoconstituent per dengue viral target.

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Transparency document

Transparency document associated with this article can be found in the online version at <https://doi.org/10.1016/j.dib.2019.103996>.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.dib.2019.103996>.

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