Supplementary information for

VIPERdb v3.0: a structure-based data analytics platform for viral capsids

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Table S1. List of tools accessible from the Data menu

Tool	**Description of the functionality**	**Location**
Family Index	Shows a list of structures available in a specific virus family	Menu Data-> Family index
Genus Index	Shows a list of structures available in a specific virus genus	Menu Data-> Genus index
T-number Index	Shows a list of structures with specific icosahedral organization (e.g., T=1, T=3 etc.,)	Menu Data-> T-number index
X-Ray Structures	Shows a list of structures that are determined by X-Ray crystallography	Menu Data-> X-Ray index
Cryo-EM Structures	Shows a list of structures that are determined by Cryo-electron microscopy (cryo-EM).	Menu Data-> Cryo-EM index
Model Structures	Shows a list of structures that are built using homology modelling methods.	Menu Data-> Model index
Helical Structures	Shows a list of helical virus structures.	Menu Data-> Helical structures
Other Structures (non-icosahedral)	Shows a list of non-icosahedral virus structures (e.g., Geminiviruses)	Menu Data-> Other structures
Crystal Information	Provides the details of crystallization conditions, space groups and inter-particle contacts for a limited number of crystal structures of viruses	Menu Data-> Crystal information

Table S2. List of web-based tools accessible from the Utilities menu

Tool	Description of the functionality	Location
Oligomer Generator	Allows to build coat protein oligomers of choice (e.g., dimers, pentamers, half-virus particle)	Menu Utilities-> Oligomer generator
Submit to Viper	Allows the users to submit their coordinates for structural analysis and generate VIPERdb style web-pages. This tool requires manual intervention by the VIPERdb curators.	Menu Utilities-> Submit to Viper
Web API	Provides a list of APIs available and the necessary syntax for using the API services.	Menu Utilities-> Web API
Reposition a capsid at the center of a box	Repositions a capsid at the center of a box	Menu Utilities-> Reposition a capsid at the center of a box
Icosahedral Server	Provides the details and images of various T-numbered lattices, corresponding h, k indices, paper templates of the hexagonal net and instructions on how to fold them into specific T-numbered icosahedral capsids.	Menu Utilities-> Icosahedral server
Gallery Maker	Gallery Maker Generates montage of various graphical representations of viral capsids and coat protein subunits available in the database, grouped according to their genus/family	Menu Utilities-> Gallery Maker
Contact Finder	Lists the occurrences of a specific residue pair (e.g., Asp-Arg) and its associated properties present at subunit interfaces in all or a chosen group of viruses.	Menu Utilities-> Contact Finder
Icosahedral Matrices	Provides with a list of 60 icosahedral rotation matrices in VIPER standard orientation.	Menu Utilities-> Icosahedral Matrices
Amino Acid Info	Provides the annotation of each amino acid in the capsid in terms of its properties and contributions (e.g., residue type, contacts, association energies, location).	Menu Utilities-> Amino acid info
Secondary Structure Info	Maps the predicted secondary structure information onto the amino acid sequence of the selected CP subunit(s).	Menu Utilities-> Secondary structure info
Multiple structure sequence alignment (MSSA)	Aligns multiple structures and derives the structure-based sequence alignment and annotates the aligned residues with their respective structural roles.	Menu Utilities-> Multiple structure sequence alignment (MSSA)
Anomaly detection tool	Identifies the capsid outliers within a virus family based on the structural descriptors.	Menu Utilities-> Anomaly detection tool
Capsid Map Tool	Display 2D and 3D representation of the CPs in IAU for various structural interrogations.	Menu Utilities-> Capsid maps tool
PDB to VIPER	Utility that transforms the PDB coordinates into VIPER convention based on BIOMT matrices stored in the PDB files.	Menu Utilities-> PDB to VIPER

Table S3. Information accessed from the info_page

Tool	**Information provided**	**Location**
Info_page	Detailed description of each virus in terms of virus taxonomy, capsid dimensions, architecture, pictorial representations and structure-derived annotations.	Can be accessed by specifying PDB-ID or virus name in the search window or via hyperlinks provided.
Illustrations	Various kinds of pictorial representations generated using UCSF Chimera, TexMol and Molscript.	Illustrations tab
Fold-a-Virus	An illustration of flattened capsid (icosahedron) that can be downloaded printed and folded into a paper model of a capsid. These illustrations were generated by UCSF Chimera program (1) using the script file courtesy of Drs. Tom Goddard of UCSF and Padmaja Natarajan of TSRI.	Fold-a-Virus tab
JsMol	A JSmol utility to interact with the atomic models in the icosahedral asymmetric unit (I.A.U).	JsMol tab
Capsid Maps	A Google Maps based utility that maps (projects) various structure-derived annotations onto the space of icosahedral asymmetric unit and enables one to compare the interfaces of different capsids. See Carrillo-Tripp et al (2,3) for further description.	Capsid Maps tab
Related viruses	Provides a list of virus structures that belong to the same family or genus that are available in VIPERdb.	Related viruses tab
Accessible surface profiles	Identifies the surface exposed residues in each (unique) subunit. Mouse of over the graph, pointing at the data points, to identify residues that are highly surface exposed (i.e., peaks). Click on the link "how are these calculated" (at the top) for more information.	Accessed through Annotations tab.
Contact Tables	Shows a table of residue pairs that are in contact at various subunit interfaces.	Accessed through Annotations tab.
Association Energies	A table of unique subunit-subunit interfaces and their estimated association energies and buried surface areas sorted in the decreasing order of the strength of their binding energies. Association energies are calculated based on the buried surface areas and atomic solvation parameters as described in references cited at the bottom of the table. It also identifies the symmetry operation associated with generating the corresponding interface.	Accessed through Annotations tab.
Q-Scores	Provides correspondence between (unique) pairs of interfaces, estimated based on the equivalent pairs of contacting residues and measured in terms of Q-scores (See Damodaran et al (4)). The Q-scores vary between 0 and 1. The higher the Q-score (closer to 1) the greater the correspondence/similarity between the pairs of interfaces.	Accessed through Annotations tab.
Construct oligomer of the virus	Provides a direct link to the oligomer generator utility.	Accessed through Annotations tab.
Secondary Structure	Provides a direct link to the secondary structure prediction utility.	Accessed through Annotations tab.

References

1. Pettersen, E.F., Goddard, T.D., Huang, C.C., Couch, G.S., Greenblatt, D.M., Meng, E.C. and Ferrin, T.E. (2004) UCSF Chimera--a visualization system for exploratory research and analysis. *J Comput Chem*, **25**, 1605-1612.
2. Carrillo-Tripp, M., Brooks, C.L., 3rd and Reddy, V.S. (2008) A novel method to map and compare protein-protein interactions in spherical viral capsids. *Proteins*, **73**, 644-655.
3. Carrillo-Tripp, M., Montiel-Garcia, D.J., Brooks, C.L., 3rd and Reddy, V.S. (2015) CapsidMaps: protein-protein interaction pattern discovery platform for the structural analysis of virus capsids using Google Maps. *J Struct Biol*, **190**, 47-55.
4. Damodaran, K.V., Reddy, V.S., Johnson, J.E. and Brooks, C.L., III. (2002) A general method to quantify quasi-equivalence in icosahedral viruses. **324**, 723-737.