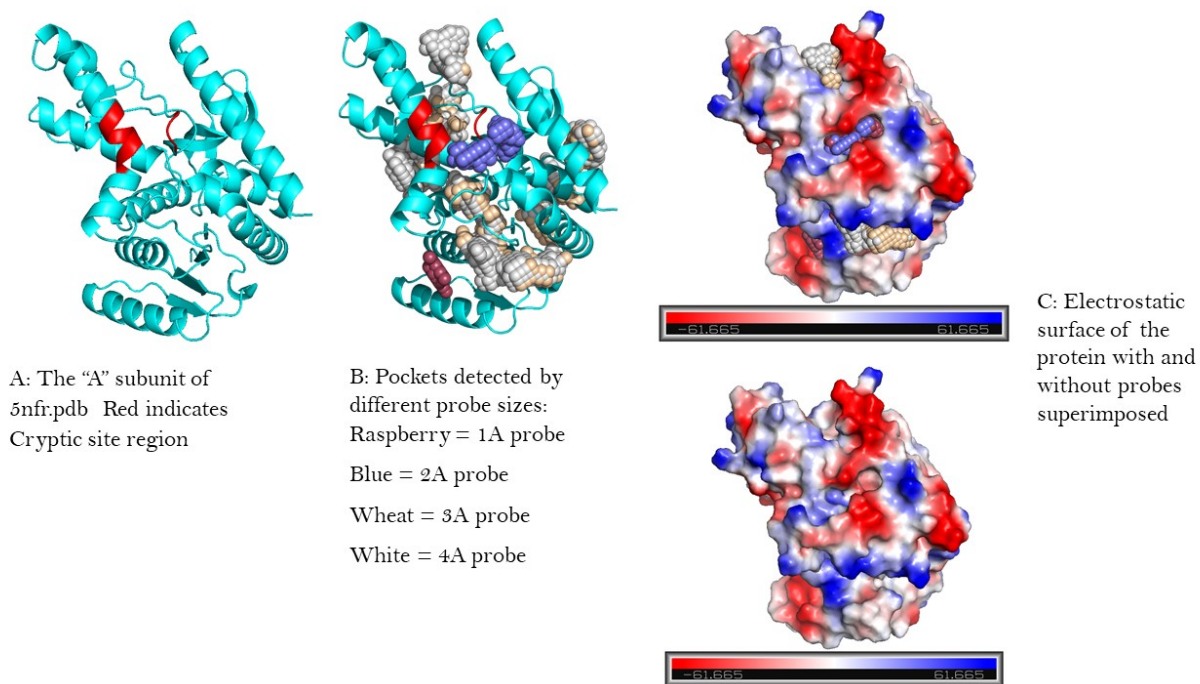


Using POCASA to Detect Pockets on Plasmodium falciparum Malate Dehydrogenase

POCASA (<http://g6altair.sci.hokudai.ac.jp/g6/service/pocasa/>) uses probes of defined size to “roll” over the surface of a protein to detect cavities. To detect pockets on the surface of Plasmodium falciparum MDH we used the “A” subunit of 5nfr.pdb with varying probes sizes from 1Å to 4Å. The remaining parameters used were SPF = 16 (to remove noise points), PDF = 18 (which recovers useful pocket points deleted by SPF with a Top N limit of 5. A grid size of 1Å which determines the size of the unit grid in the 3D grid system used to map the protein surface.



Supporting Output from POCASA (see below) indicates that the cryptic site region has two subsites with a total volume of 343Å^3 with subsite 1 contributing 95Å^3 and subsite 2 contributing 248Å^3 . The cryptic site is not detected by 3Å or 4Å probes indicating that it is relatively shallow, but as shown by the electrostatic surface has distinctive charge properties.

Probe Radius : 1
Grid Size : 1.0
Single Point Flag : 16
Protein Depth Flag : 18

5nfr_subunit_A.pdb:

Pocket 88's volume is 181, VD value is 1119, the average VD is 6.18416

Pocket 336's volume is 45, VD value is 158, the average VD is 3.51852

Pocket 436's volume is 35, VD value is 85, the average VD is 2.42857

Pocket 30's volume is 33, VD value is 77, the average VD is 2.34343

Pocket 219's volume is 31, VD value is 75, the average VD is 2.43011

The rank order

For pockets:

Rank 1 is Pocket 88, the volume is 181, VD value is 1119

Rank 2 is Pocket 336, the volume is 45, VD value is 158

Rank 3 is Pocket 436, the volume is 35, VD value is 85

Rank 4 is Pocket 30, the volume is 33, VD value is 77

Rank 5 is Pocket 219, the volume is 31, VD value is 75

POCASA 1.1 – Result

You can access this result for the next one week with URL:

<http://g6altair.sci.hokudai.ac.jp/g6/service/pocasa/show.cgi?q=457486bef4451f826402121d711cdd27f169be2f>

Date: 2021/04/18 03:11:23
 Processing time: 0.471 sec
 Filename: 5nfr_subunit_A
 Probe radius: 1 Å
 SPF: 16
 PDF: 18
 Top N: 5
 Grid size: 1.0 Å

Output files

- [5nfr_subunit_A.pdb](#)
- [5nfr_subunit_A_Parameters.txt](#)
- [5nfr_subunit_A_Pocket_DepthCenters.pdb](#)
- [5nfr_subunit_A_TopN_pockets.pdb](#)
- [5nfr_subunit_A_simple.pdb](#)

Program's output

```
commandline arguments: 5nfr_subunit_A.pdb
1 1.0 16 18 5 NULL protein
```

```
----- POCASA Version 1.1 -----
```

```
The simple PDB file is
5nfr_subunit_A_simple.pdb !
```

```
The first chain in the input file will be
used for searching!
The first chain is CHAIN A
Find TER mark
```

```
Begin to search pockets and cavities :
```

```
Roll the probe sphere !
```

```
Finish rolling the probe sphere !
```

```
First Clust loop
```

```
There are 5 3D pockets(cavities) found !
```

Rank order

For pockets:

```
Rank 1 is Pocket 88, the volume is 181, VD
value is 1119
Rank 2 is Pocket 336, the volume is 45, VD
value is 158
Rank 3 is Pocket 436, the volume is 35, VD
value is 85
Rank 4 is Pocket 30, the volume is 33, VD
value is 77
Rank 5 is Pocket 219, the volume is 31, VD
value is 75
```

Check the result immediately with Jmol

Protein view: Wireframe Cartoon
 van der Waals Surface

Pockets and cavities:

No. 88
 No. 336
 No. 436
 No. 30
 No. 219

Select All

Deselect All

Jmol: an open-source Java viewer for chemical
 structures in 3D. <http://www.jmol.org/>

The TopN pocket file is
5nfr_subunit_A_TopN_pockets.pdb

The TopN pocket depth center PDB file is
5nfr_subunit_A_Pocket_DepthCenters.pdb

For Top N pockets(cavities):

Pocket 88's volume is 181, VD value is
1119, the average VD is 6.18416

Pocket 336's volume is 45, VD value is 158,
the average VD is 3.51852

Pocket 436's volume is 35, VD value is 85,
the average VD is 2.42857

Pocket 30's volume is 33, VD value is 77,
the average VD is 2.34343

Pocket 219's volume is 31, VD value is 75,
the average VD is 2.43011

Search process is completed and Thank you
for using it !

[\[Back\]](#) [\[Manual\]](#) [\[Laboratory of X-ray structural biology\]](#)

Probe Radius : 2
Grid Size : 1.0
Single Point Flag : 16
Protein Depth Flag : 18

5nfr_subunit_A.pdb:

Pocket 98's volume is 292, VD value is 1439, the average VD is 4.93037

Pocket 199's volume is 217, VD value is 531, the average VD is 2.45008

Pocket 363's volume is 50, VD value is 217, the average VD is 4.34

Pocket 476's volume is 49, VD value is 118, the average VD is 2.41497

Pocket 222's volume is 46, VD value is 119, the average VD is 2.5942

The rank order

For pockets:

Rank 1 is Pocket 98, the volume is 292, VD value is 1439

Rank 2 is Pocket 199, the volume is 217, VD value is 531

Rank 3 is Pocket 363, the volume is 50, VD value is 217

Rank 4 is Pocket 222, the volume is 46, VD value is 119

Rank 5 is Pocket 476, the volume is 49, VD value is 118

POCASA 1.1 – Result

You can access this result for the next one week with URL:

<http://g6altair.sci.hokudai.ac.jp/g6/service/pocasa/show.cgi?q=1da86e9e7de3a37e824fc0b1c29d5df7c571a9a2>

Date: 2021/04/18 03:13:59
 Processing time: 0.628 sec
 Filename: 5nfr_subunit_A
 Probe radius: 2 Å
 SPF: 16
 PDF: 18
 Top N: 5
 Grid size: 1.0 Å

Output files

- [5nfr_subunit_A.pdb](#)
- [5nfr_subunit_A.Parameters.txt](#)
- [5nfr_subunit_A_Pocket_DepthCenters.pdb](#)
- [5nfr_subunit_A_TopN_pockets.pdb](#)
- [5nfr_subunit_A_simple.pdb](#)

Program's output

```
commandline arguments: 5nfr_subunit_A.pdb
2 1.0 16 18 5 NULL protein
```

```
----- POCASA Version 1.1 -----
```

```
The simple PDB file is
5nfr_subunit_A_simple.pdb !
```

```
The first chain in the input file will be
used for searching!
The first chain is CHAIN A
Find TER mark
```

```
Begin to search pockets and cavities :
```

```
Roll the probe sphere !
```

```
Finish rolling the probe sphere !
```

```
First Clust loop
```

```
There are 10 3D pockets(cavities) found !
```

Rank order

For pockets:

```
Rank 1 is Pocket 98, the volume is 292, VD
value is 1439
Rank 2 is Pocket 199, the volume is 217, VD
value is 531
Rank 3 is Pocket 363, the volume is 50, VD
value is 217
Rank 4 is Pocket 222, the volume is 46, VD
value is 119
Rank 5 is Pocket 476, the volume is 49, VD
value is 118
```

Check the result immediately with Jmol

Protein view: Wireframe Cartoon
 van der Waals Surface

Pockets and cavities:

Jmol: an open-source Java viewer for chemical structures in 3D. <http://www.jmol.org/>

The TopN pocket file is
5nfr_subunit_A_TopN_pockets.pdb

The TopN pocket depth center PDB file is
5nfr_subunit_A_Pocket_DepthCenters.pdb

For Top N pockets(cavities):

Pocket 98's volume is 292, VD value is
1439, the average VD is 4.93037

Pocket 199's volume is 217, VD value is
531, the average VD is 2.45008

Pocket 363's volume is 50, VD value is 217,
the average VD is 4.34

Pocket 476's volume is 49, VD value is 118,
the average VD is 2.41497

Pocket 222's volume is 46, VD value is 119,
the average VD is 2.5942

Search process is completed and Thank you
for using it !

[\[Back\]](#) [\[Manual\]](#) [\[Laboratory of X-ray structural biology.\]](#)

Probe Radius : 3
Grid Size : 1.0
Single Point Flag : 16
Protein Depth Flag : 18

5nfr_subunit_A.pdb:

Pocket 135's volume is 419, VD value is 1178, the average VD is 2.81305
Pocket 112's volume is 386, VD value is 1737, the average VD is 4.50173
Pocket 358's volume is 128, VD value is 304, the average VD is 2.3776
Pocket 375's volume is 103, VD value is 247, the average VD is 2.39806
Pocket 511's volume is 91, VD value is 233, the average VD is 2.5641

The rank order

For pockets:

Rank 1 is Pocket 112, the volume is 386, VD value is 1737
Rank 2 is Pocket 135, the volume is 419, VD value is 1178
Rank 3 is Pocket 358, the volume is 128, VD value is 304
Rank 4 is Pocket 375, the volume is 103, VD value is 247
Rank 5 is Pocket 511, the volume is 91, VD value is 233

POCASA 1.1 – Result

You can access this result for the next one week with URL:

<http://g6altair.sci.hokudai.ac.jp/g6/service/pocasa/show.cgi?q=eb70ef8b9e70f0adee6bda92d1c11edb80c8696d>

Date: 2021/04/18 23:37:26
 Processing time: 0.853 sec
 Filename: 5nfr_subunit_A
 Probe radius: 3 Å
 SPF: 16
 PDF: 18
 Top N: 5
 Grid size: 1.0 Å

Output files

- [5nfr_subunit_A.pdb](#)
- [5nfr_subunit_A_Parameters.txt](#)
- [5nfr_subunit_A_Pocket_DepthCenters.pdb](#)
- [5nfr_subunit_A_TopN_pockets.pdb](#)
- [5nfr_subunit_A_simple.pdb](#)

Program's output

```
commandline arguments: 5nfr_subunit_A.pdb
3 1.0 16 18 5 NULL all
```

```
----- POCASA Version 1.1 -----
```

```
The simple PDB file is
5nfr_subunit_A_simple.pdb !
```

```
The first chain in the input file will be
used for searching!
The first chain is CHAIN A
Find TER mark
```

```
Begin to search pockets and cavities :
```

```
Roll the probe sphere !
```

```
Finish rolling the probe sphere !
```

```
First Clust loop
```

```
There are 16 3D pockets(cavities) found !
```

Rank order

For pockets:

```
Rank 1 is Pocket 112, the volume is 386, VD
value is 1737
Rank 2 is Pocket 135, the volume is 419, VD
value is 1178
Rank 3 is Pocket 358, the volume is 128, VD
value is 304
Rank 4 is Pocket 375, the volume is 103, VD
value is 247
Rank 5 is Pocket 511, the volume is 91, VD
value is 233
```

Check the result immediately with Jmol

Protein view: Wireframe Cartoon
 van der Waals Surface

Pockets and cavities:

No. 135 ▲
 No. 112
 No. 358
 No. 375
 No. 511

Select All

Deselect All

Jmol: an open-source Java viewer for chemical
 structures in 3D. <http://www.jmol.org/>

The TopN pocket file is
5nfr_subunit_A_TopN_pockets.pdb

The TopN pocket depth center PDB file is
5nfr_subunit_A_Pocket_DepthCenters.pdb

For Top N pockets(cavities):

Pocket 135's volume is 419, VD value is
1178, the average VD is 2.81305

Pocket 112's volume is 386, VD value is
1737, the average VD is 4.50173

Pocket 358's volume is 128, VD value is
304, the average VD is 2.3776

Pocket 375's volume is 103, VD value is
247, the average VD is 2.39806

Pocket 511's volume is 91, VD value is 233,
the average VD is 2.5641

Search process is completed and Thank you
for using it !

[\[Back\]](#) [\[Manual\]](#) [\[Laboratory of X-ray structural biology\]](#)

Probe Radius : 4
Grid Size : 1.0
Single Point Flag : 16
Protein Depth Flag : 18

5nfr_subunit_A.pdb:

Pocket 122's volume is 574, VD value is 1585, the average VD is 2.76249
Pocket 95's volume is 394, VD value is 1792, the average VD is 4.54992
Pocket 391's volume is 158, VD value is 398, the average VD is 2.51899
Pocket 395's volume is 105, VD value is 253, the average VD is 2.4127
Pocket 540's volume is 95, VD value is 243, the average VD is 2.5614

The rank order

For pockets:

Rank 1 is Pocket 95, the volume is 394, VD value is 1792
Rank 2 is Pocket 122, the volume is 574, VD value is 1585
Rank 3 is Pocket 391, the volume is 158, VD value is 398
Rank 4 is Pocket 395, the volume is 105, VD value is 253
Rank 5 is Pocket 540, the volume is 95, VD value is 243

POCASA 1.1 – Result

You can access this result for the next one week with URL:

<http://g6altair.sci.hokudai.ac.jp/g6/service/pocasa/show.cgi?q=92bbe730dc23a267f73702ec79c33e2ef208ae35>

Date: 2021/04/18 03:15:56
 Processing time: 1.328 sec
 Filename: 5nfr_subunit_A
 Probe radius: 4 Å
 SPF: 16
 PDF: 18
 Top N: 5
 Grid size: 1.0 Å

Output files

- [5nfr_subunit_A.pdb](#)
- [5nfr_subunit_A_Parameters.txt](#)
- [5nfr_subunit_A_Pocket_DepthCenters.pdb](#)
- [5nfr_subunit_A_TopN_pockets.pdb](#)
- [5nfr_subunit_A_simple.pdb](#)

Program's output

commandline arguments: 5nfr_subunit_A.pdb
 4 1.0 16 18 5 NULL protein

----- POCASA Version 1.1 -----

The simple PDB file is
 5nfr_subunit_A_simple.pdb !

The first chain in the input file will be
 used for searching!
 The first chain is CHAIN A
 Find TER mark

Begin to search pockets and cavities :

Roll the probe sphere !

Finish rolling the probe sphere !

First Clust loop

There are 19 3D pockets(cavities) found !

Rank order

For pockets:

Rank 1 is Pocket 95, the volume is 394, VD
 value is 1792
 Rank 2 is Pocket 122, the volume is 574, VD
 value is 1585
 Rank 3 is Pocket 391, the volume is 158, VD
 value is 398
 Rank 4 is Pocket 395, the volume is 105, VD
 value is 253
 Rank 5 is Pocket 540, the volume is 95, VD
 value is 243

Check the result immediately with Jmol

Protein view: Wireframe Cartoon
 van der Waals Surface

Pockets and cavities:

No. 122 ▲
 No. 95
 No. 391
 No. 395
 No. 540

Select All

Deselect All

Jmol: an open-source Java viewer for chemical
 structures in 3D. <http://www.jmol.org/>

Second Clust loop

There are 11 3D pockets(cavities) found !

The TopN pocket file is
5nfr_subunit_A_TopN_pockets.pdb

The TopN pocket depth center PDB file is
5nfr_subunit_A_Pocket_DepthCenters.pdb

For Top N pockets(cavities):

Pocket 122's volume is 574, VD value is 1585, the average VD is 2.76249

Pocket 95's volume is 394, VD value is 1792, the average VD is 4.54992

Pocket 391's volume is 158, VD value is 398, the average VD is 2.51899

Pocket 395's volume is 105, VD value is 253, the average VD is 2.4127

Pocket 540's volume is 95, VD value is 243, the average VD is 2.5614

Search process is completed and Thank you for using it !

[\[Back\]](#) [\[Manual\]](#) [\[Laboratory of X-ray structural biology\]](#)