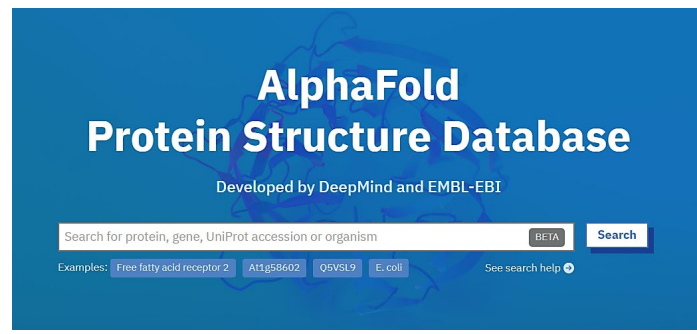
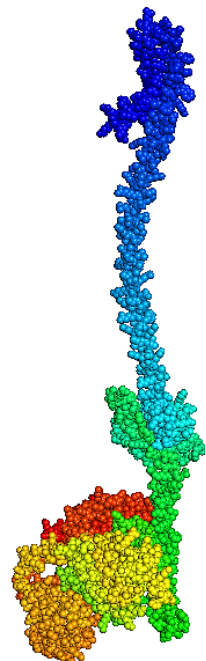


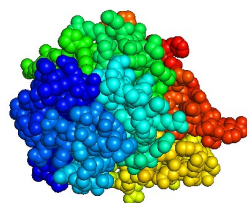
**A** <https://alphafold.ebi.ac.uk/>



Monomeric structures



ArcB



ArcA

ArcB full model docking

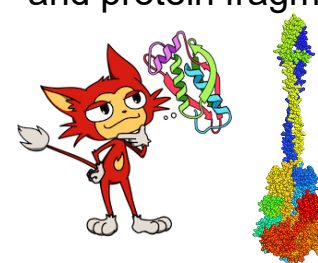
ArcA or ArcB sequence



Sequence analysis, leucine zipper.



**D** AlphaFold2 in collaborative environment  
Generation of multimer models and protein fragments



PAS domain docking

**B** Cavity-detection docking using anaerobic metabolites

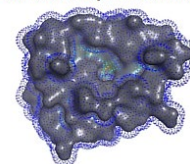
PubChem

<http://clab.labshare.cn/cb-dock/php/blinddock.php>

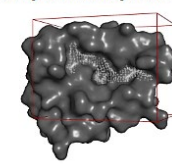
CB-Dock

Cavity-detection guided Blind Docking

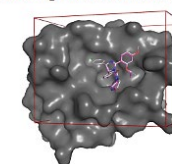
Curvature of protein surface



Cavity detected by clustering



Docking with AutoDock Vina



Anaerobic metabolites  
physiochemical  
characteristics

MolCalc

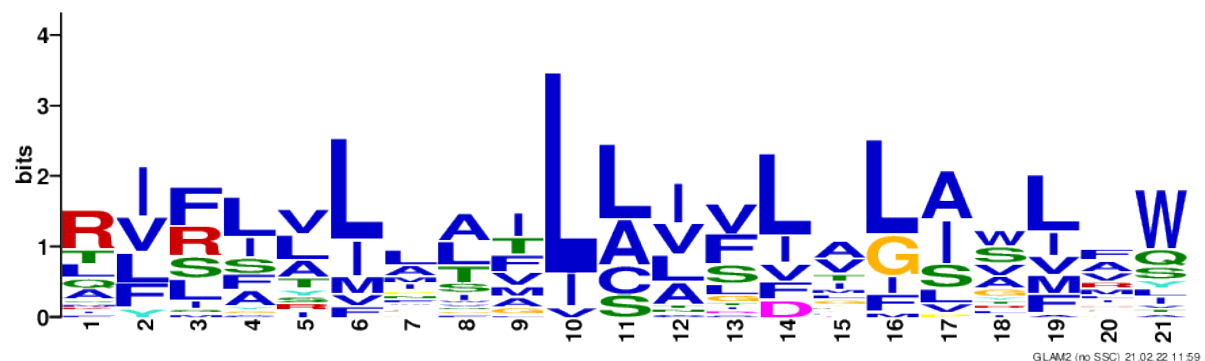
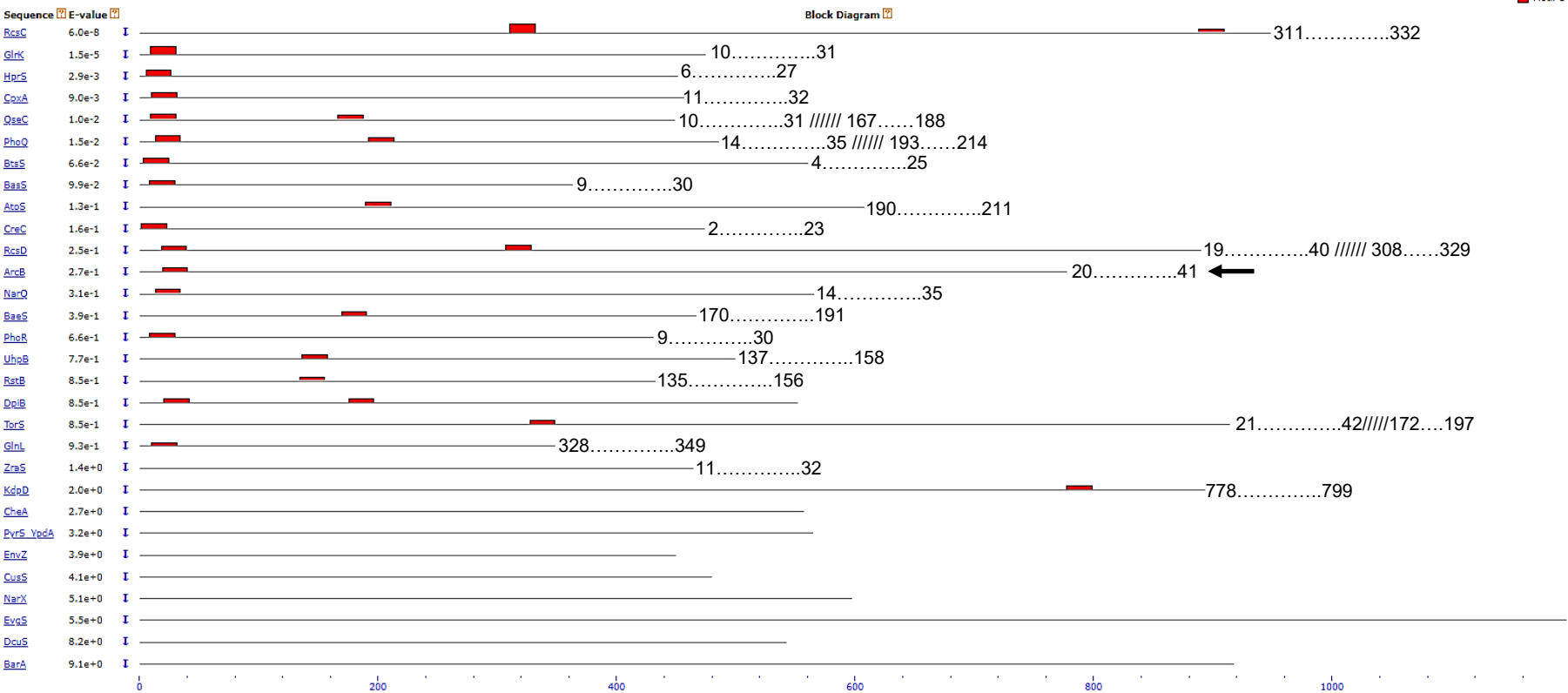
**E** Structural alignment of proteins, protein fragments and protein motif analysis



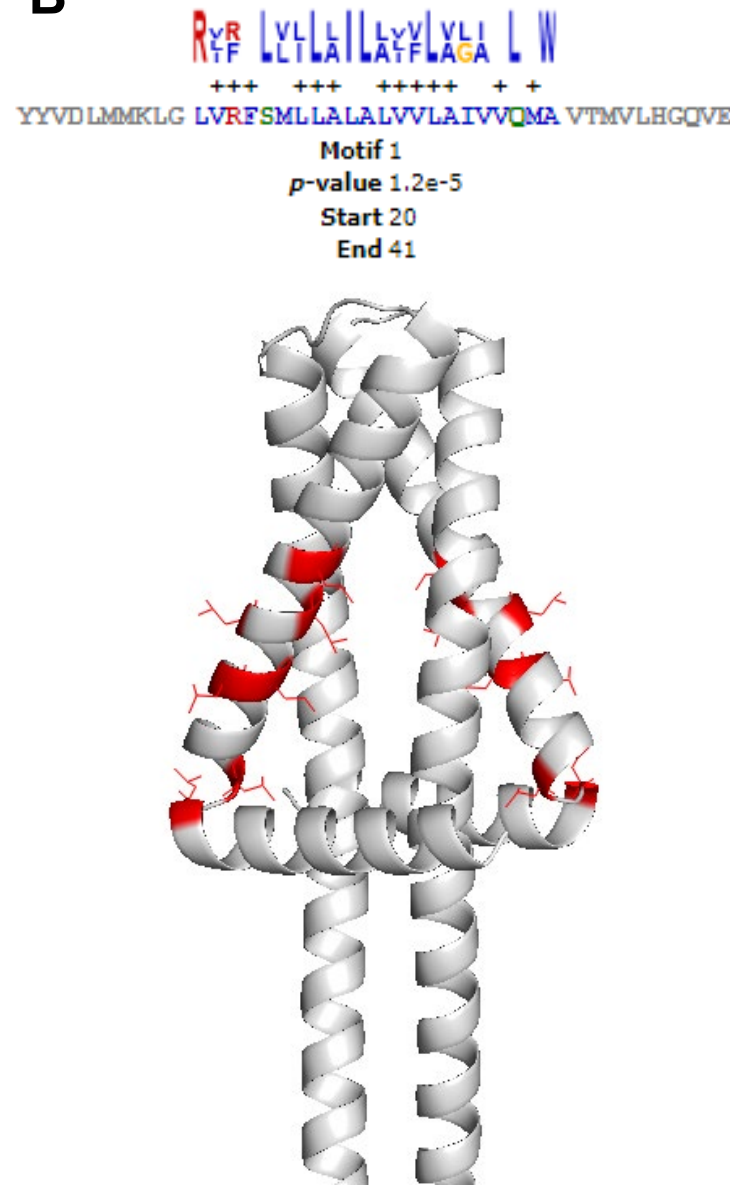
**F** Visualization



A



B

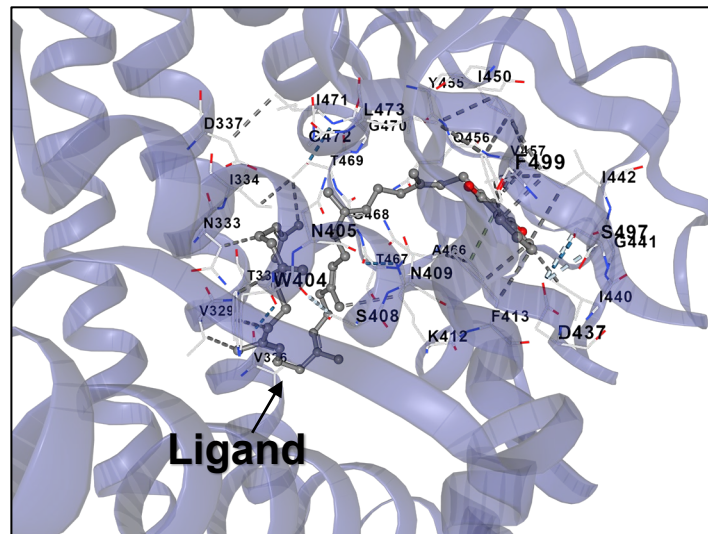


Supplementary Figure 2

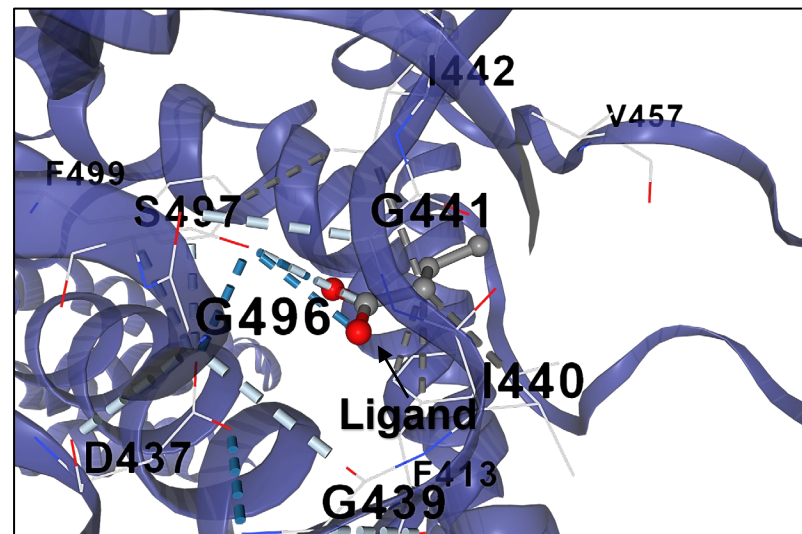
|     |                   |                   |                   |                   |                    |     |
|-----|-------------------|-------------------|-------------------|-------------------|--------------------|-----|
| 1   | MKQIRLLAQY        | YVDLMMKLGL        | VRFSMLLALA        | LVVLAIVVQM        | AVTMVLHGQV         | 50  |
| 51  | ESIDVIRSIF        | FGLLITPWAV        | YFLSVVVEQL        | EESRQRLSRL        | VQKLEEMRER         | 100 |
|     |                   |                   |                   | 1                 | 11                 |     |
| 101 | DLSLVNQLKD        | NIAQLNQEIA        | VREKAEAELO        | ETFGQLKIEI        | <u>KEREETQIQQL</u> | 150 |
|     |                   |                   |                   |                   | 61                 |     |
| 151 | <u>EQQSSFLRSF</u> | <u>LDASPDLVFY</u> | <u>RNEDKEFSGC</u> | <u>NRAMELLTGK</u> | <u>SEKQLVHLKP</u>  | 200 |
|     | 62                |                   |                   |                   | 111                |     |
| 201 | <u>ADVYSPEAAA</u> | <u>KVIETDEKVF</u> | <u>RHNVSLTYEQ</u> | <u>WLDYPDGRKA</u> | <u>CFEIRKVPYY</u>  | 250 |
|     | 112               |                   | 140               |                   |                    |     |
| 251 | <u>DRVGKRHGLM</u> | <u>GFGRDITERK</u> | <u>RYQDALERAS</u> | RDKTTFISTI        | SHELRTPLNG         | 300 |
| 301 | IVGLSRILLD        | TELTAEQEKY        | LKTIHVSAVT        | LGNIFNDIID        | MDKMERRKVQ         | 350 |
| 351 | LDNQPVDFTS        | FLADLENLSA        | LQAQQKGLRF        | NLEPTLPLPH        | QVITDGTRLR         | 400 |
| 401 | QILWNLISNA        | VKFTQQGQVT        | VRVRYDEGDM        | LHFEVEDSGI        | GIPQDELDKI         | 450 |
| 451 | FAMYYQVKDS        | HGGKPATGTG        | IGLAVSRRLA        | KNMGGDITVT        | SEQGKGSTFT         | 500 |
| 501 | LTIHAPSVAE        | EVDDAFDEDD        | MPLPALNVLL        | VEDIELNVIV        | ARSVLEKLGN         | 550 |
| 551 | SVDVAMTGKA        | ALEMFKPGEY        | DLVLLDIQLP        | DMTGLDISRE        | LTKRYPREDL         | 600 |
| 601 | PPLVALTANV        | LKDKQEYLNA        | GMDDVLSKPL        | SVPALTAMIK        | KFWDTQDDEE         | 650 |
| 651 | STVTTEENSK        | SEALDIPML         | EQYLELVGPK        | LITDGLAVFE        | KMMPGYVSVL         | 700 |
| 701 | ESNLTAQDKK        | GIVEEGHKIK        | GAAGSVGLRH        | LQQLGQQIQS        | PDLPAWEDNV         | 750 |
| 751 | GEWIEEMKEE        | WRHDVEVLKA        | WVAKATKK          |                   |                    | 778 |

Supplementary Figure 3

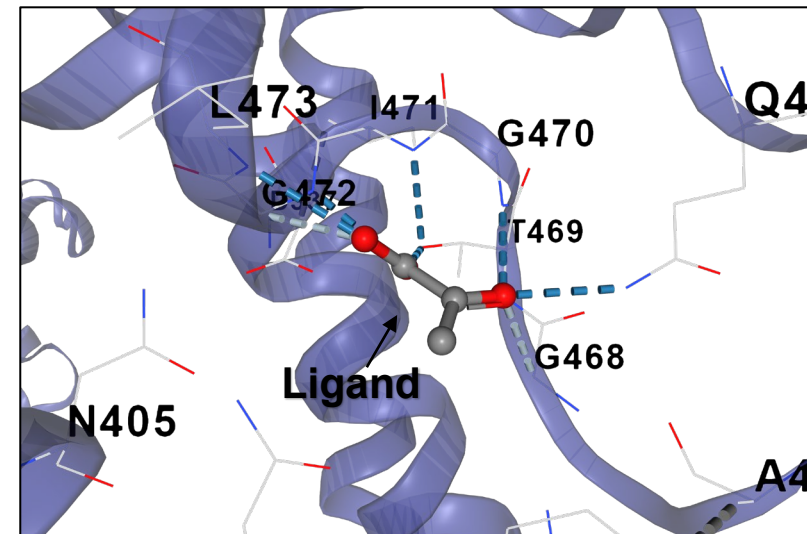
Menaquinone



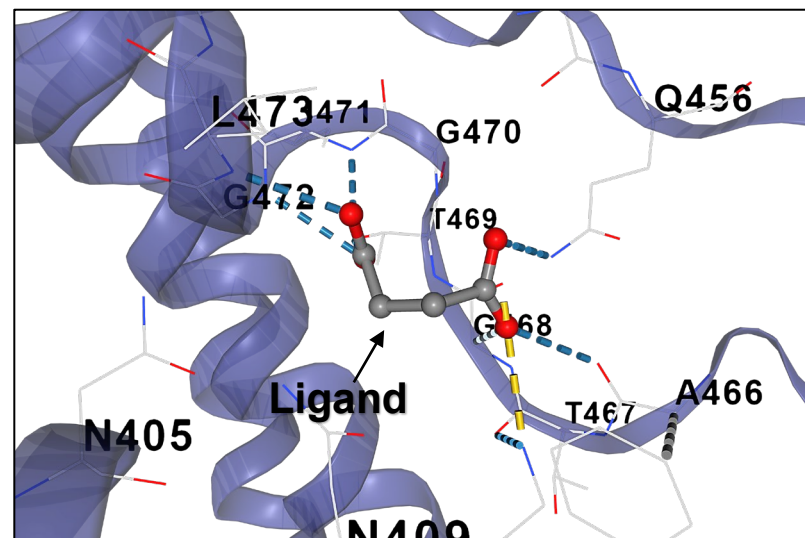
Butyrate



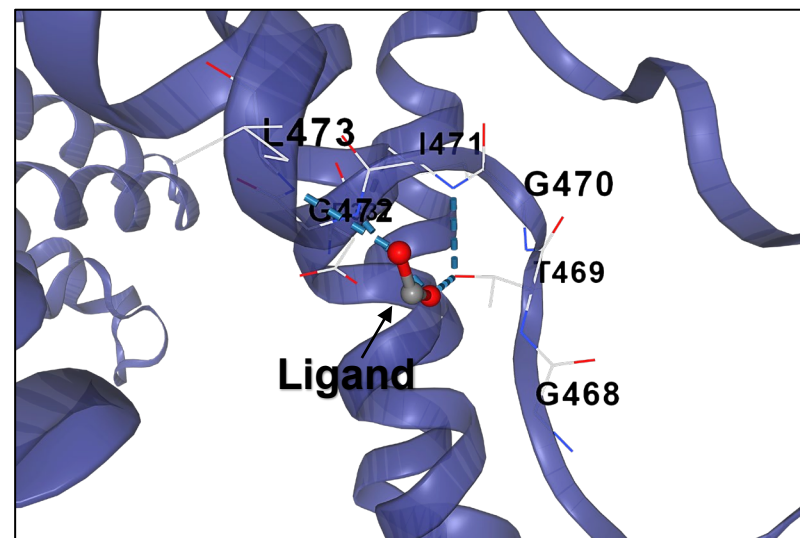
Pyruvate



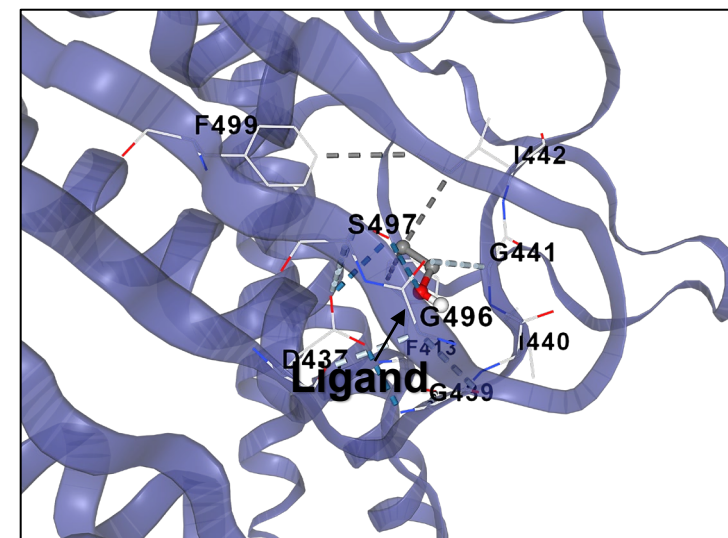
Succinate



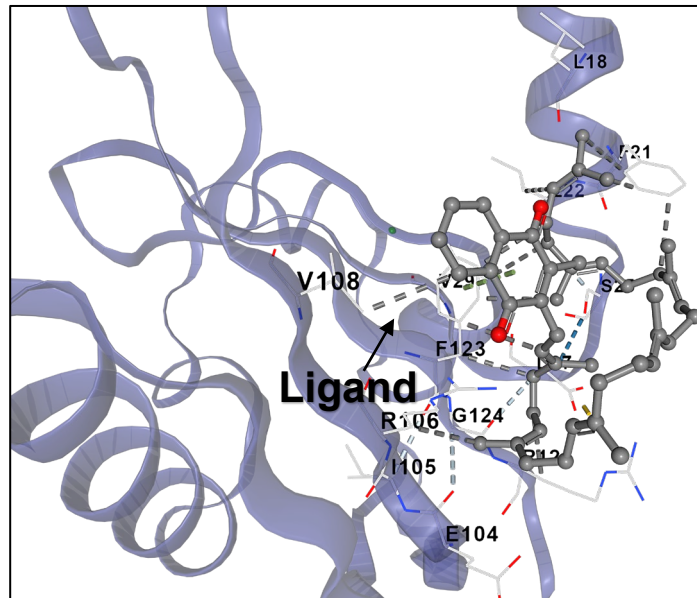
Formate



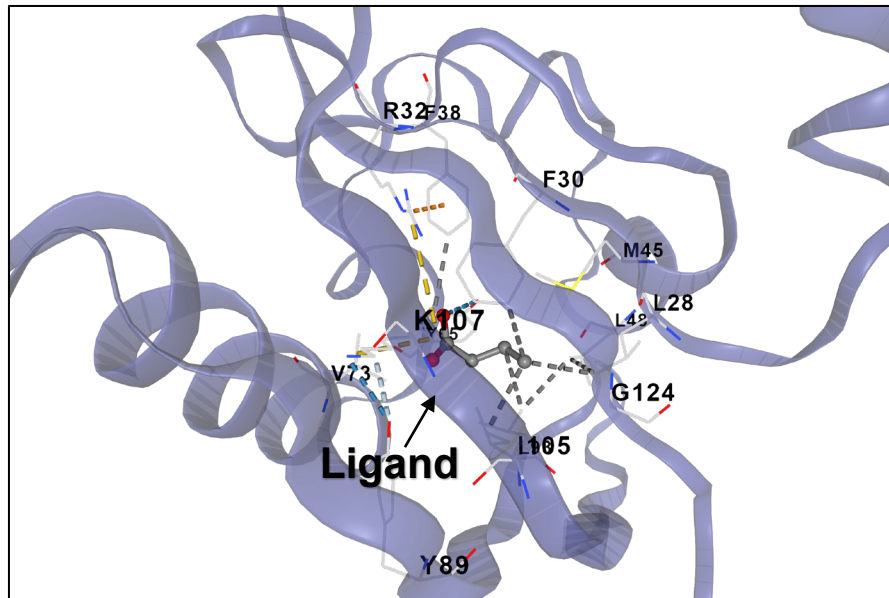
Ethanol



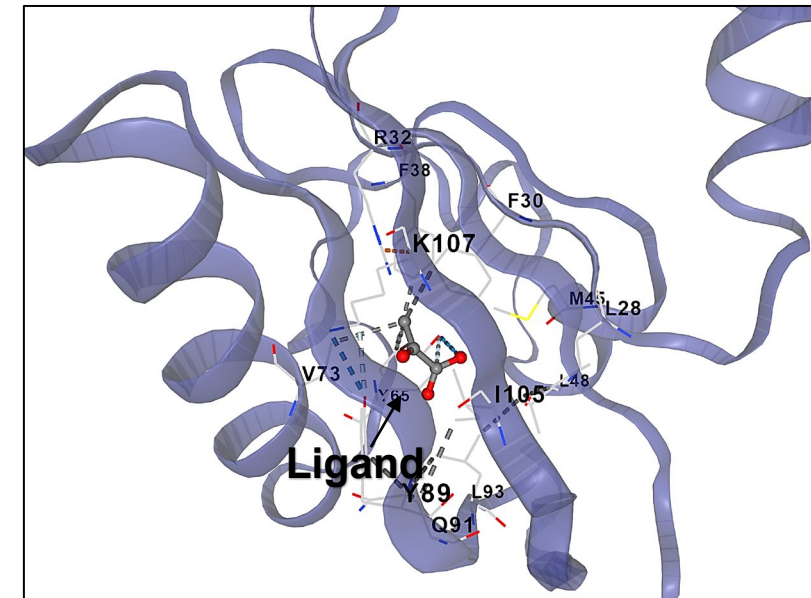
Menaquinone



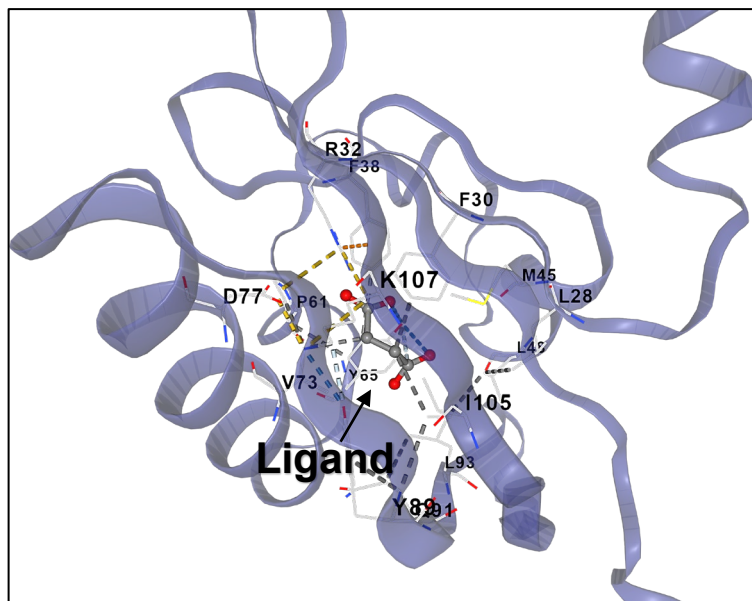
Butyrate



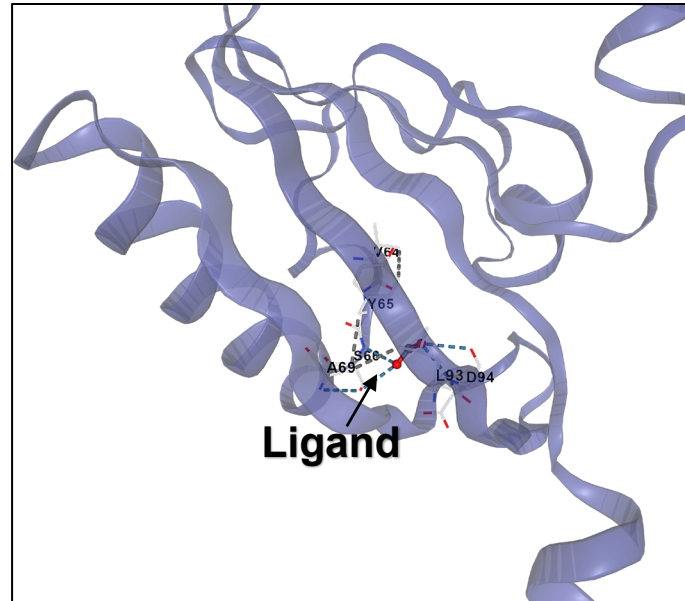
Pyruvate



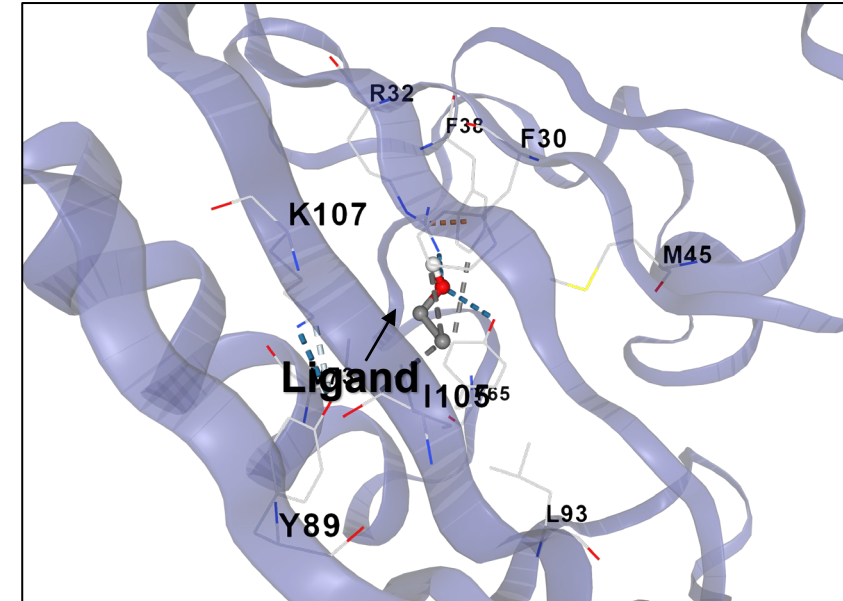
Succinate



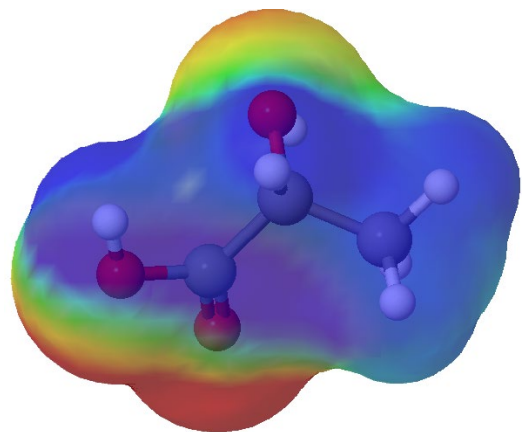
Formate



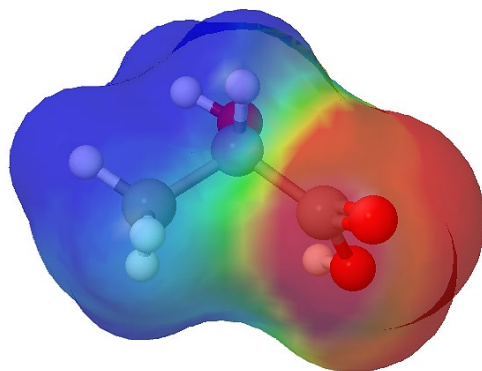
Ethanol



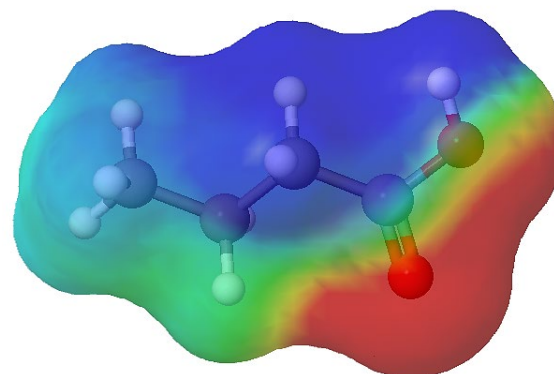
D-lactate



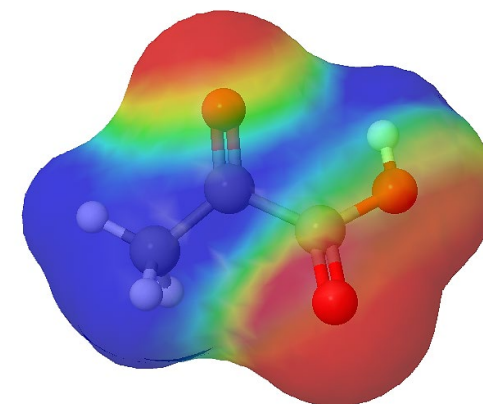
L-lactate



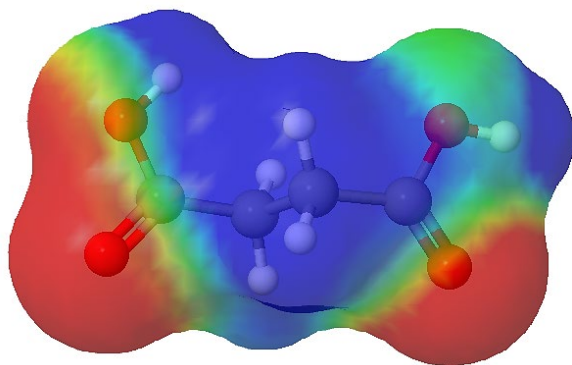
Butyrate



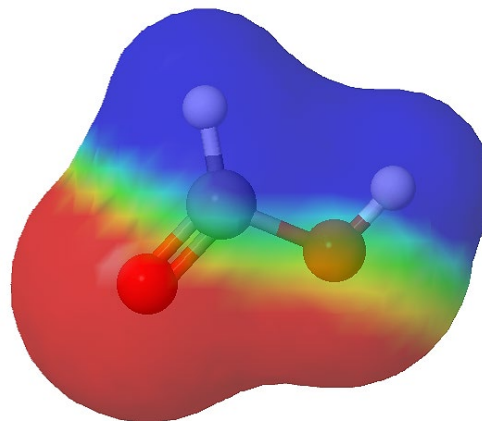
Pyruvate



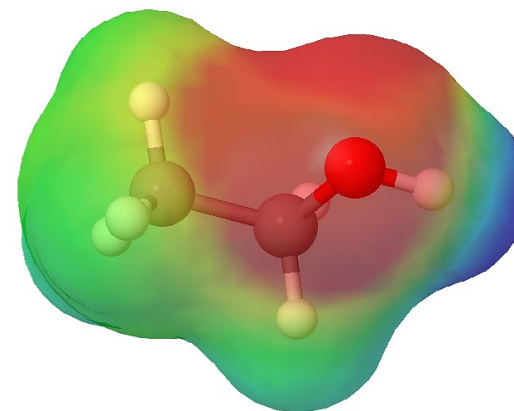
Succinate

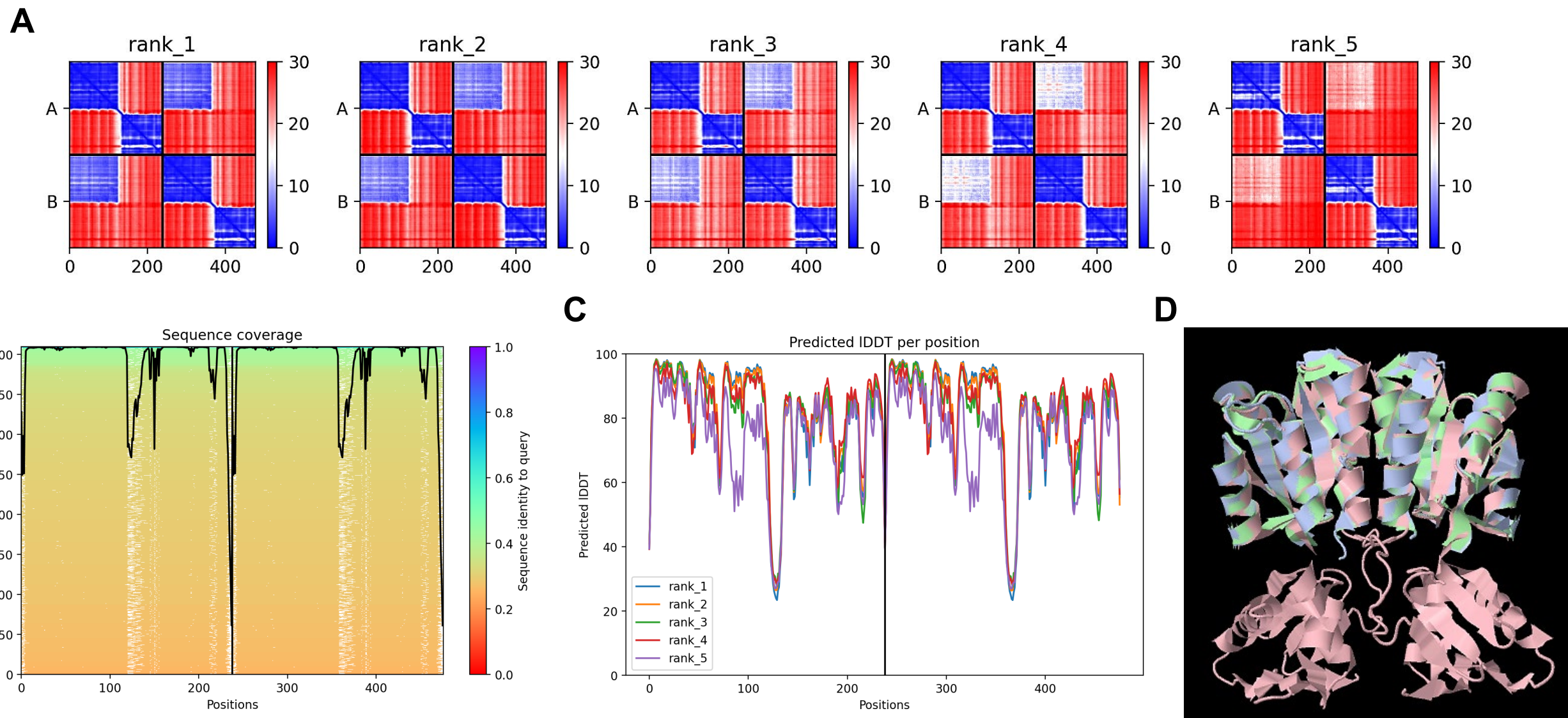


Formate

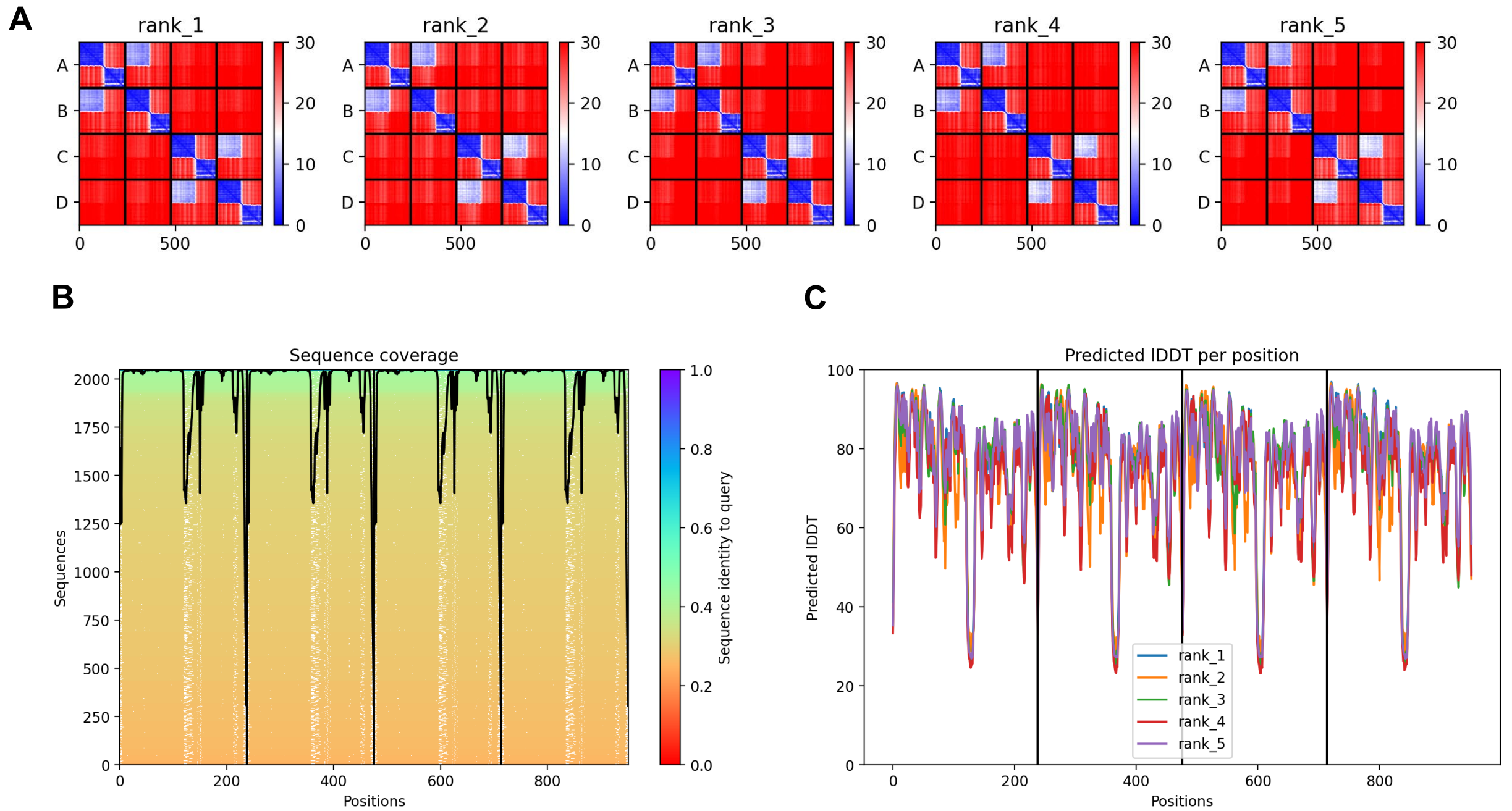


Ethanol

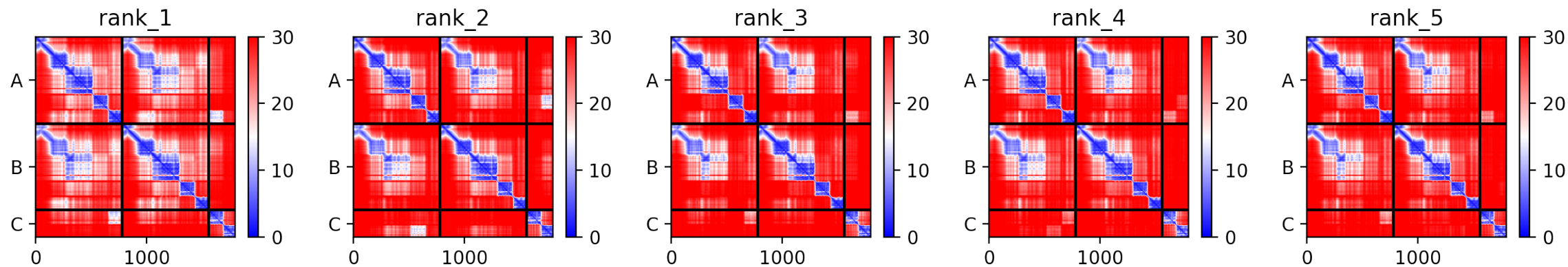
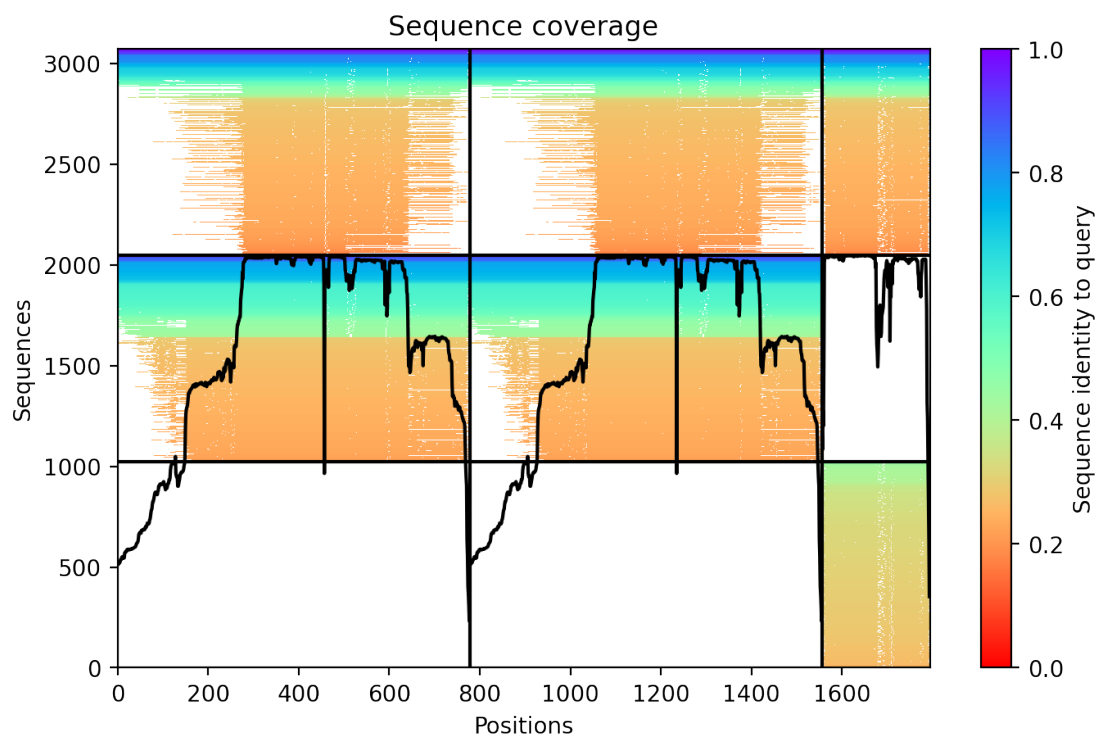
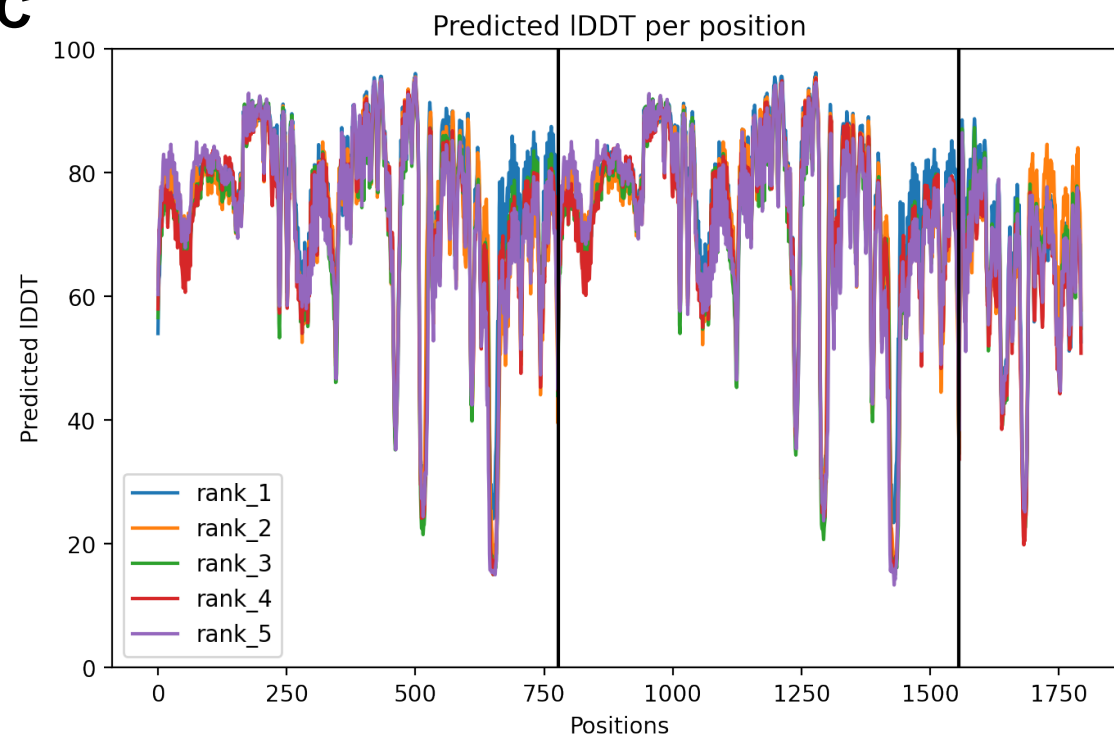


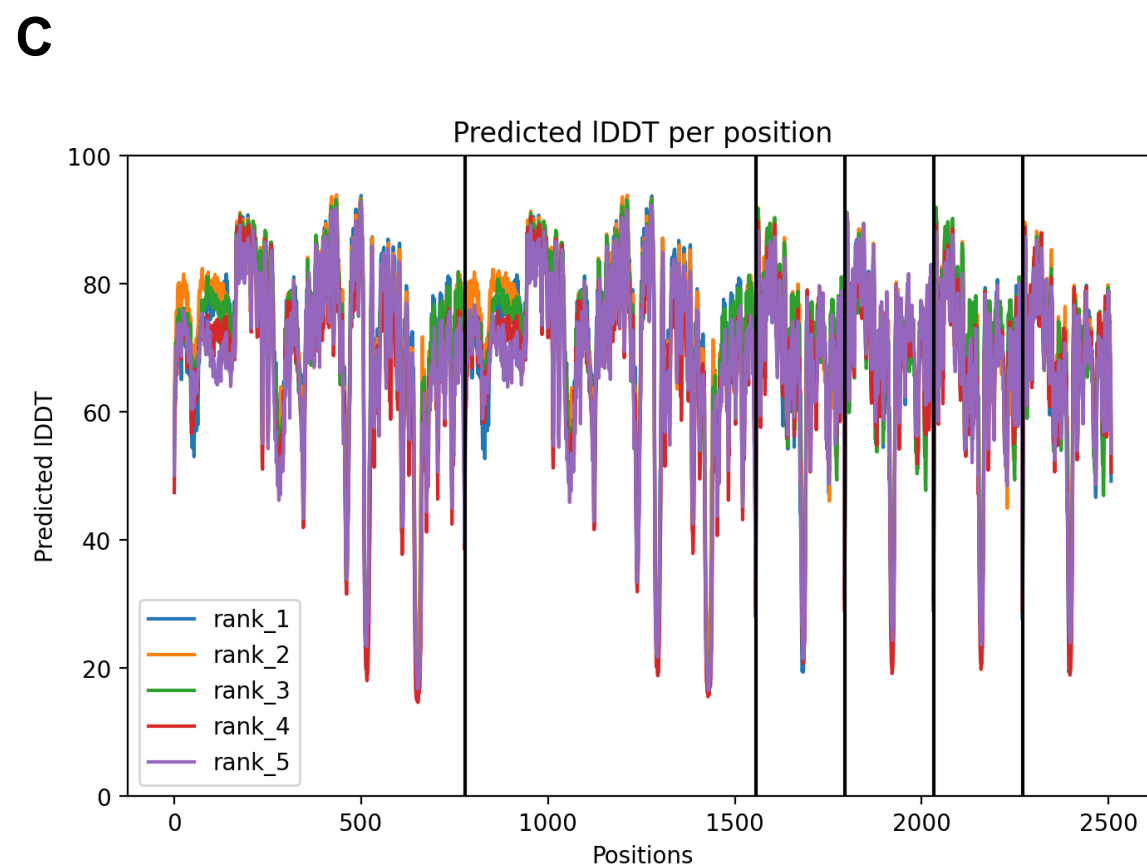
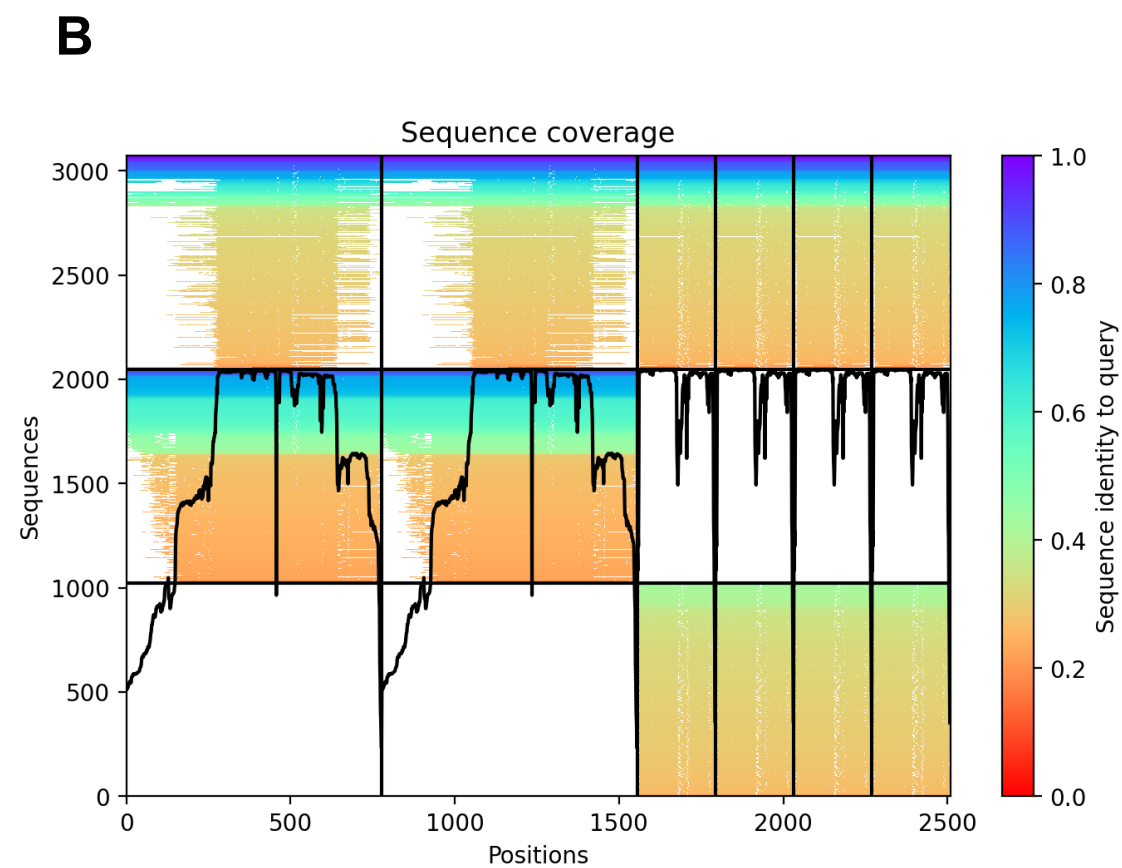
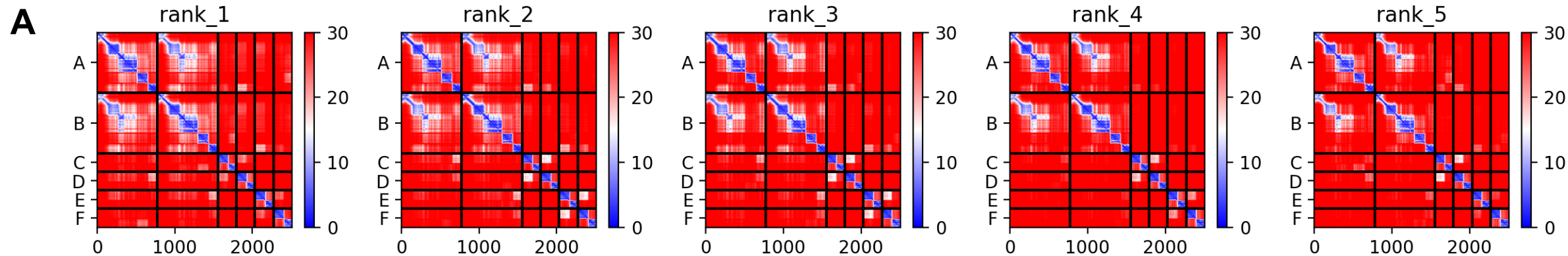


**Supplementary Figure 7**

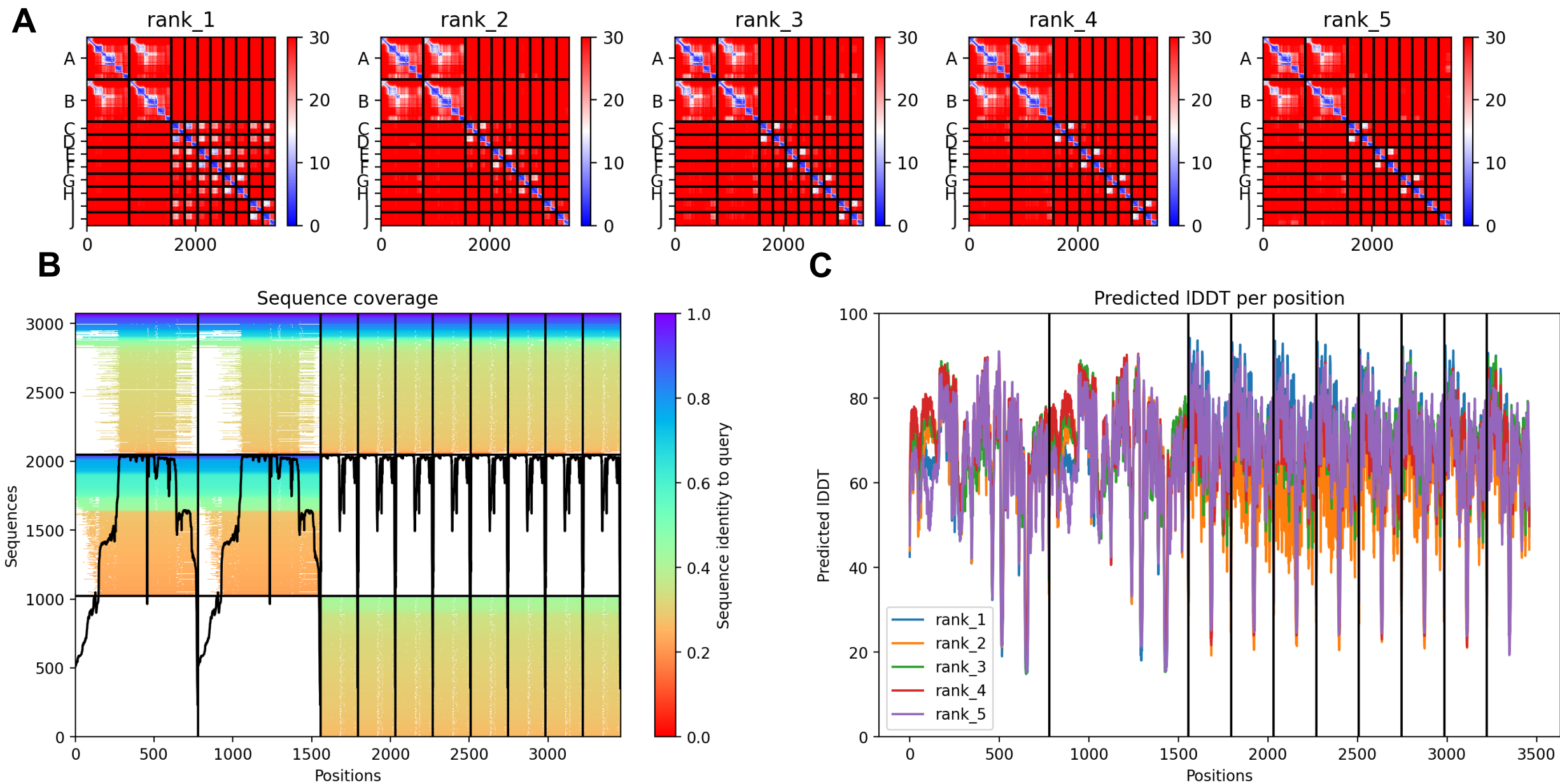


**Supplementary Figure 8**

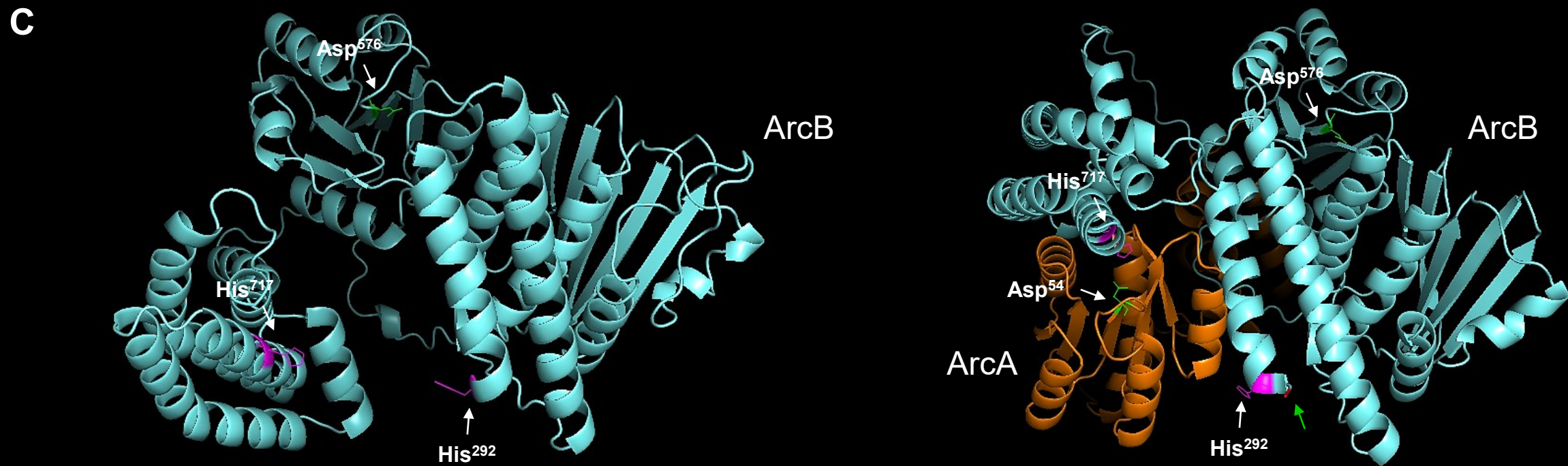
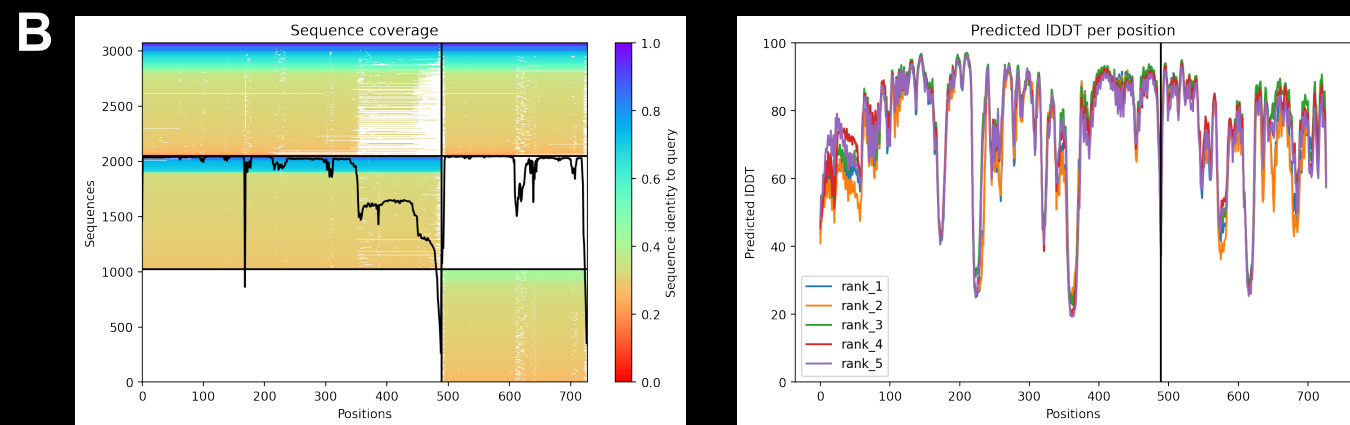
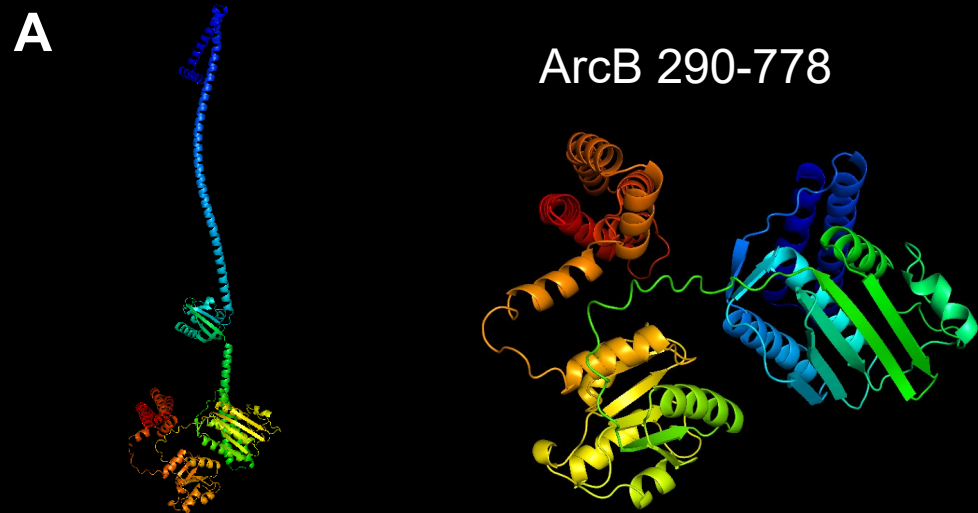
**A****B****C****Supplementary Figure 9**



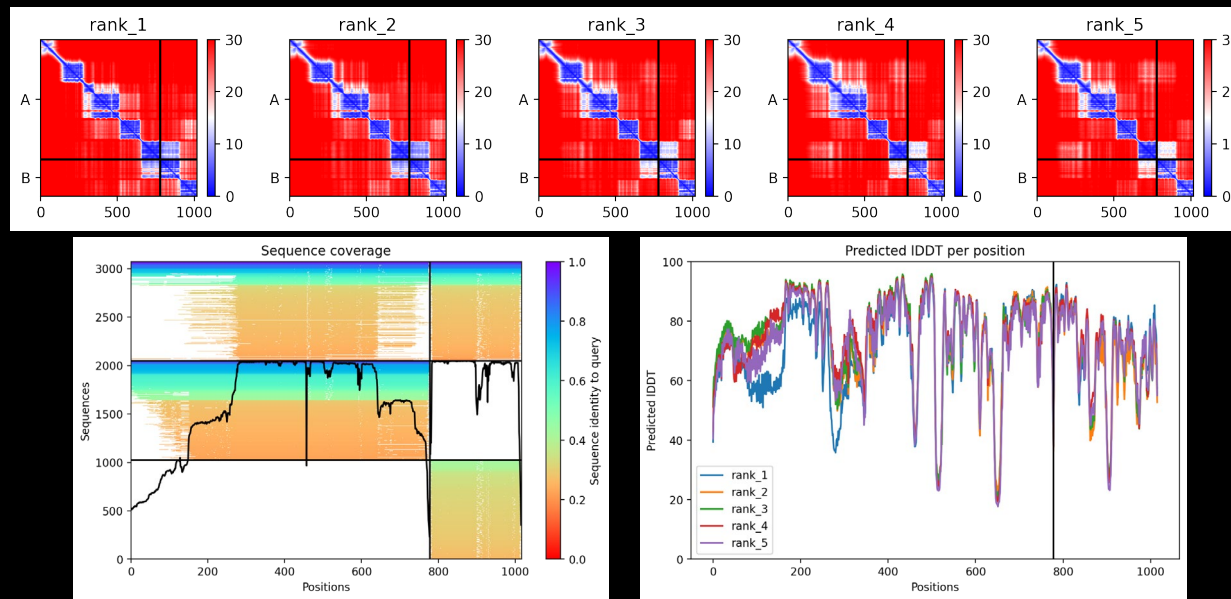
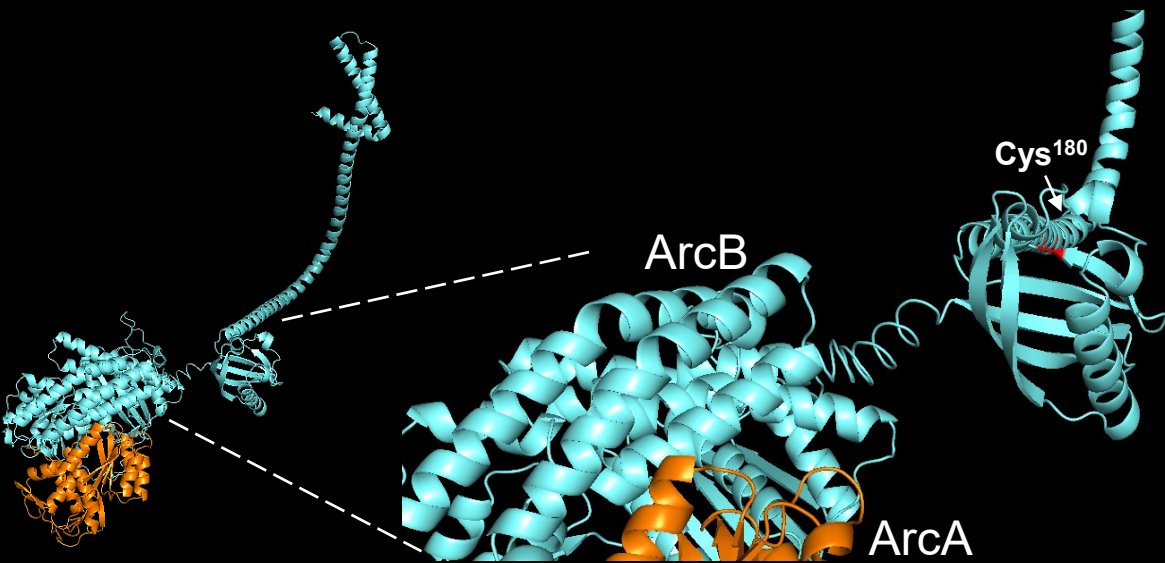
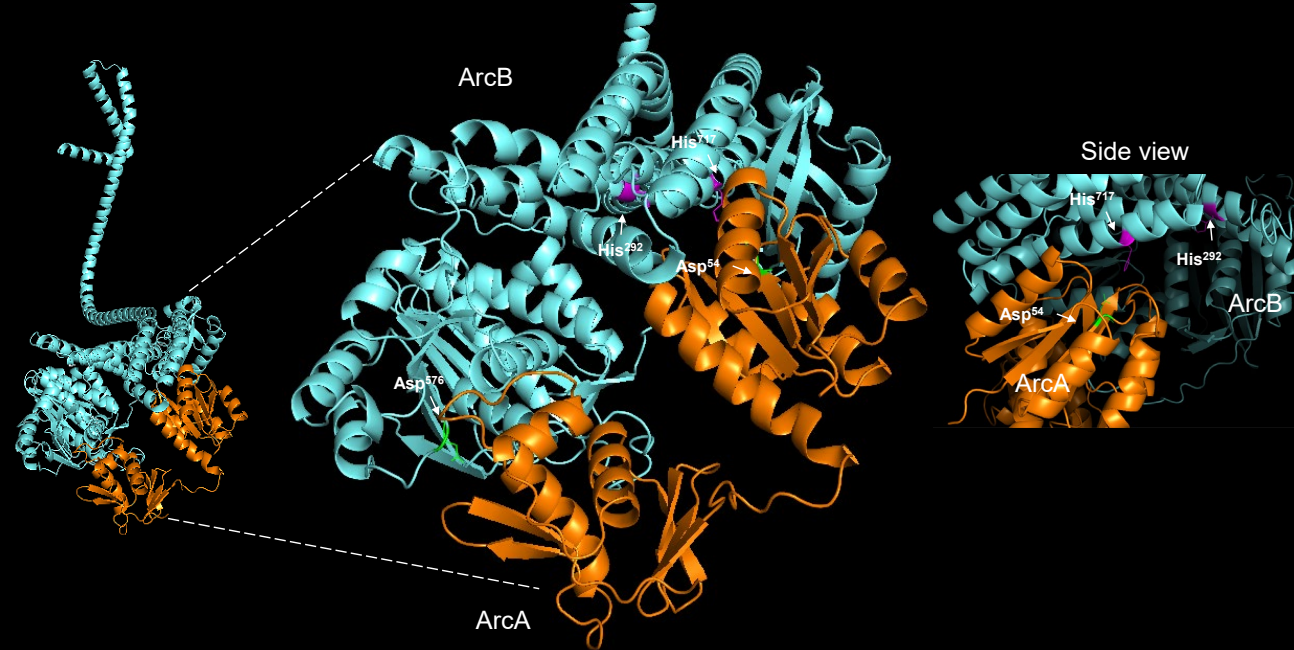
**Supplementary Figure 10**



**Supplementary Figure 11**



Supplementary Figure 12

**A****B****C**

**Supplementary Figure 13**