docking result tell the affinity of two protein and binning sites and protein -protein docking by Z dock

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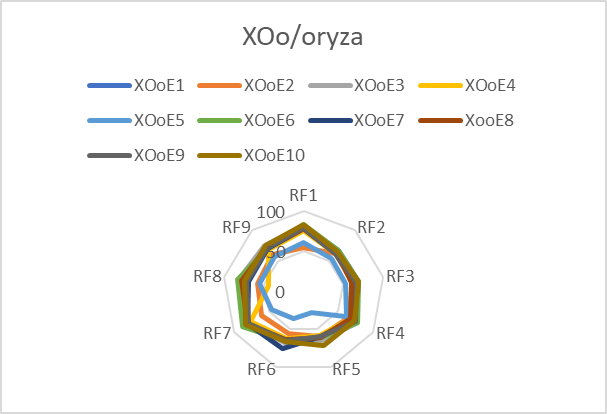
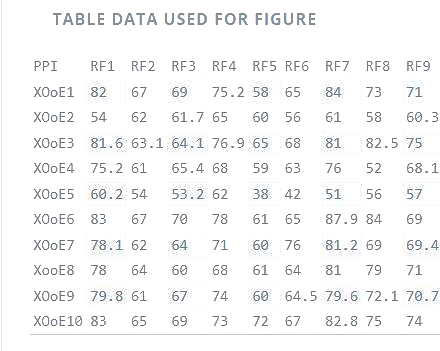
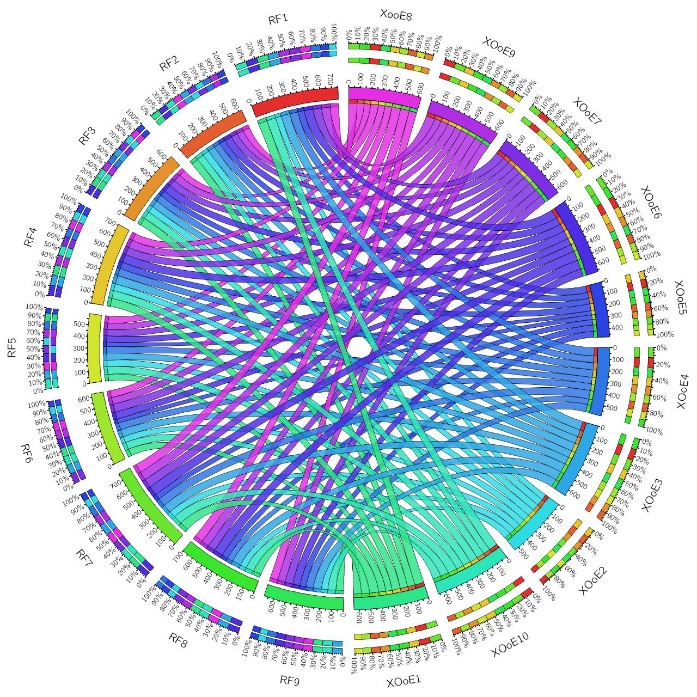
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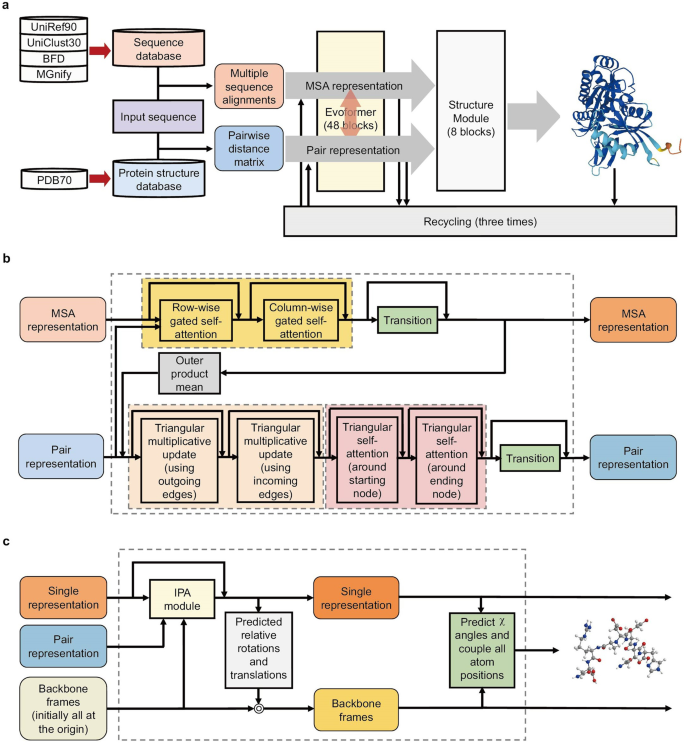
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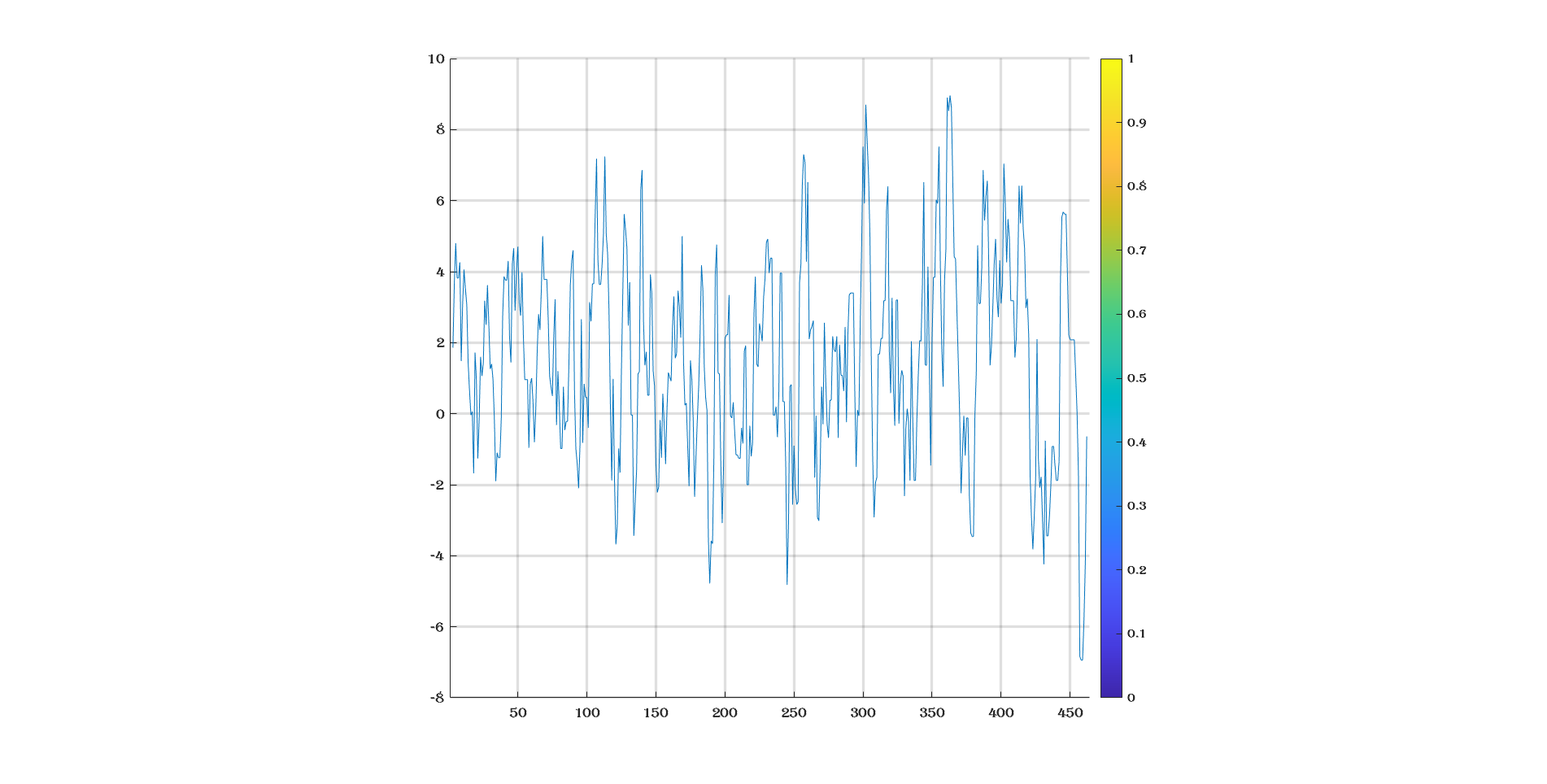
Neural network tell the interaction of two different protein and its rate

Generated by cirsos software

Table data fig: use to tell the data taken for developing this network



table based on working of alpha fold protein and MSA and all the structural prediction algorithms and binding of two protein and by EBI library



Stability of protein by matlab

pH level 7.4

the value and graph generated tell the stability of protein in 7 ph

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **PPI** | **V1** | **V2** | **V3** | **V4** | **V5** | **V6** | **V7** | **V8** | **V9** |
| XOoE1 | 82 | 67 | 69 | 75.2 | 58 | 65 | 84 | 73 | 71 |
| XOoE2 | 54 | 62 | 61.7 | 65 | 60 | 56 | 61 | 58 | 60.3 |
| XOoE3 | 81.6 | 63.1 | 64.1 | 76.9 | 65 | 68 | 81 | 82.5 | 75 |
| XOoE4 | 75.2 | 61 | 65.4 | 68 | 59 | 63 | 76 | 52 | 68.1 |
| XOoE5 | 60.2 | 54 | 53.2 | 62 | 38 | 42 | 51 | 56 | 57 |
| XOoE6 | 83 | 67 | 70 | 78 | 61 | 65 | 87.9 | 84 | 69 |
| XOoE7 | 78.1 | 62 | 64 | 71 | 60 | 76 | 81.2 | 69 | 69.4 |
| XooE8 | 78 | 64 | 60 | 68 | 61 | 64 | 81 | 79 | 71 |
| XOoE9 | 79.8 | 61 | 67 | 74 | 60 | 64.5 | 79.6 | 72.1 | 70.7 |
| XOoE10 | 83 | 65 | 69 | 73 | 72 | 67 | 82.8 | 75 | 74 |
|  |  |  |  |  |  |  |  |  |  |

**PPI interaction of data by AI generated (alphafold2) by deep mind (google)**

Interaction of one effector and one receptor at one time and by per-residue confidence score (pLDDT) between 0 and 100 The structural module of AF2 also creates the model confidence predictions, reported as the predicted local distance difference test (pLDDT) scores. The pLDDT scores are in the range of [0, 100]. High pLDDT scores (e.g., > 80) indicate high confidence of the residue structure, and low pLDDT scores (e.g., < 50)

Result I got:

|  |  |  |
| --- | --- | --- |
| ONE RECEPTOR – ONE EFFECTOR | P1-V1, P1-V7, P3-V1, P3-V7, P3-V8, P6-V1, P6-V7, P6-V8, P7-V7, P8-V8, P10-V1, P10-V7 | BASED ON COVERAGE  HIGHT-6  MEDIUM-6 |
| ONE RECEPTOR – MANY EFFECTOR | HIGH-P10, P1, P3, P6, P7, P9 | Least p5 |
| MANY EFFECTOR – ONE RECEPTOR | V1, V7, V8, V4, V9 | Least v5 |

|  |  |  |
| --- | --- | --- |
| 81-90 |  | Highest coverage value |
| 75-81 |  | Mid highest coverage |
| 65-75 |  | Average coverage value |
| 55-65 |  | MID lower coverage value |
| 30-55 |  | Lowest coverage value |

Xoo(EP)

Rice(RP)

RP1

RP2

RP3

RP4

RP5

RP6

RP7

RP8

RP9

RP10

EP1

**XOo(Xanthomonas Oryza) (p)**

* bidirectional sugar transporter SWEET2b
* xopx
* xopq
* xopl
* avrbs1
* ABC transporter ATP-binding protein [Xanthomonas oryzae]
* nucleoside hydrolase [Xanthomonas oryzae]
* IS3 family transposase [Xanthomonas oryzae]
* **MFS transporter [Xanthomonas oryzae]**
* **AdeC/AdeK/OprM family multidrug efflux complex outer membrane factor [Xanthomonas oryzae]**

|  |
| --- |
| **Rice (Oryza sativa) (v)**   * **receptor like kinase, partial [Oryza sativa Indica Group]** * **ethylene receptor 3 isoform 2 precursor [Oryza sativa Japonica Group]** * **wall-associated receptor kinase-like 3 [Oryza sativa Japonica Group]** * **putative receptor protein kinase ZmPK1 [Oryza sativa Japonica Group]** * **TPA\_inf: WRKY transcription factor 30 [Oryza sativa Japonica Group]** * **RecName: Full=Calcium-binding protein CBP; Short=OsCBP** * **subtilisin-like protease Pr1B, partial [Metarhizium anisopliae]** * **type-1 proteins geranylgeranyltransferase subunit beta [Pyricularia oryzae Y34** |

EP2

EP3

EP4

EP5

EP6

EP7

EP8

EP9

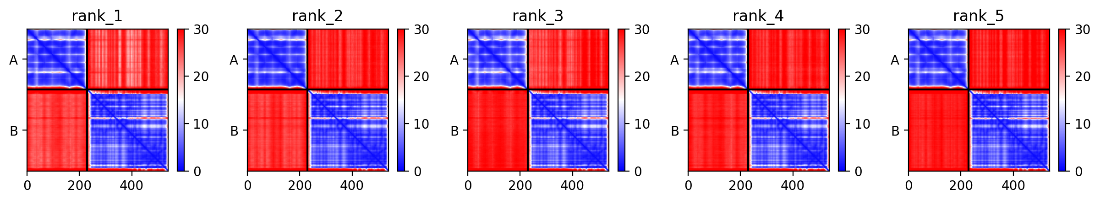
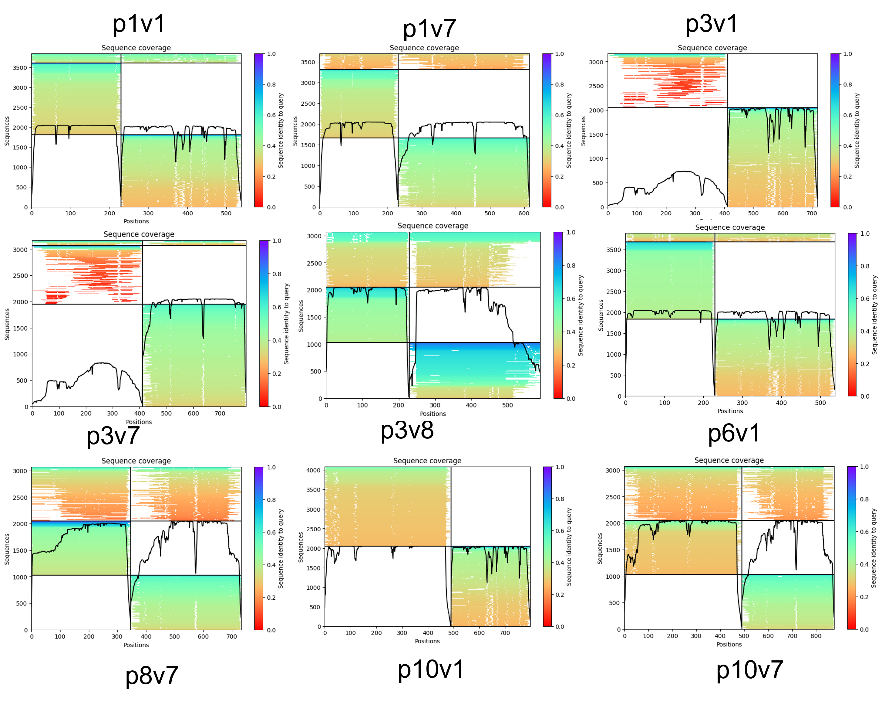
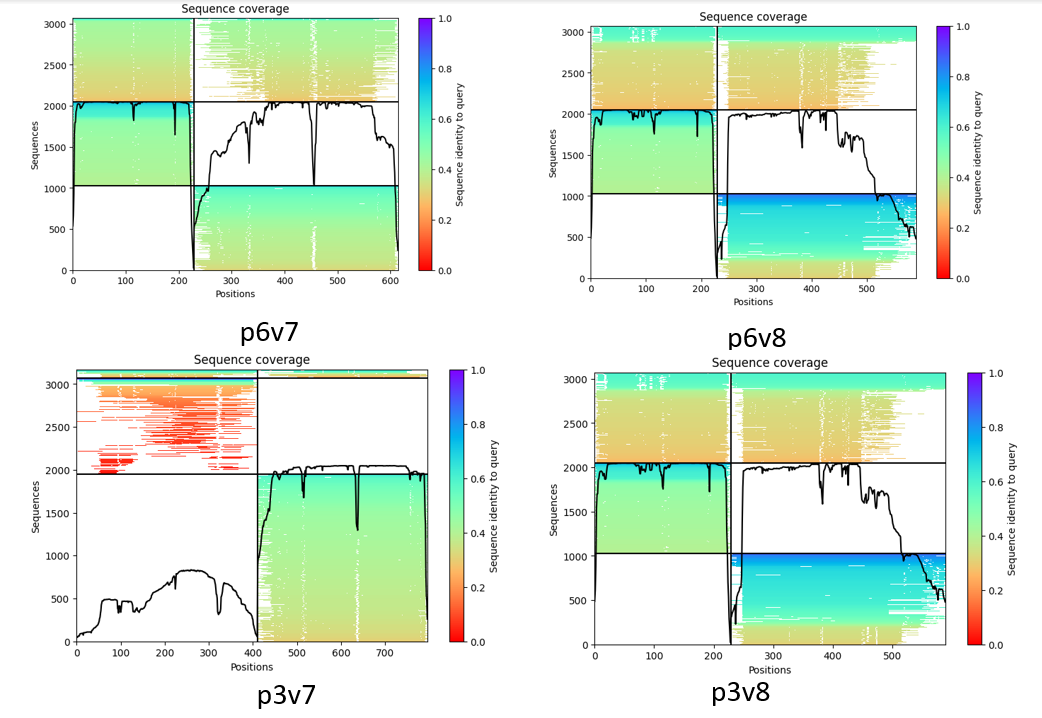
EP10

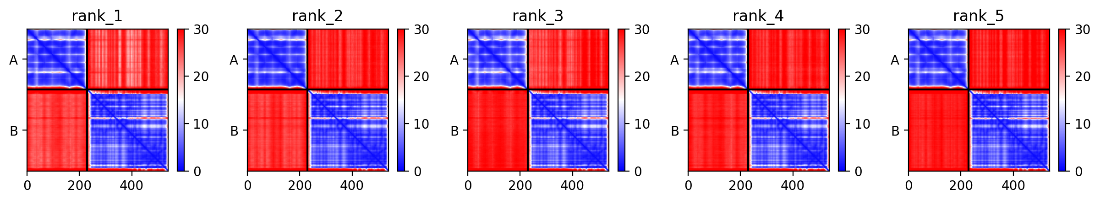
Neural network of p(effector) interaction by v (receptor protein)

Different colour tells the different protein interaction

1p\*10v= 10PV

9p\*10v = 90 interaction result





**All the graph of one effector and one receptor-based model**

* Plddt graph show the error rate value the blue colour show the amount of accuracy in PPI structure also the site of protein binding
* Generated by google colab pro
* Alpha fold algorithms to predict the interaction and binding sites

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **PPI** | **RP1** | **RP2** | **RP3** | **RP4** | **RP5** | **RP6** | **RP7** | **RP8** | **RP9** | **RP10** |
| EP1 | 80 | 67 | 69 | 76 | 63 | 65 | 75 | 71 | 68 | 78 |
| EP2 | 54 | 62 | 61.7 | 65 | 60 | 56 | 61 | 58 | 60.3 | 59 |
| EP3 | 81.6 | 63.1 | 64.1 | 76.9 | 65 | 68 | 81 | 82.5 | 75 | 79 |
| EP4 | 75.2 | 61 | 65.4 | 68 | 59 | 63 | 76 | 52 | 68.1 | 50 |
| EP5 | 60.2 | 54 | 53.2 | 62 | 38 | 42 | 51 | 56 | 57 | 84 |
| EP6 | 83 | 67 | 70 | 78 | 61 | 65 | 87.9 | 84 | 69 | 54 |
| EP7 | 78.1 | 62 | 64 | 71 | 60 | 76 | 81.2 | 69 | 69.4 | 64 |
| EP8 | 78 | 64 | 60 | 68 | 61 | 64 | 81 | 79 | 71 | 78 |
| EP9 | 79.8 | 61 | 67 | 74 | 60 | 64.5 | 79.6 | 72.1 | 70.7 | 79 |
| EP10 | 83 | 62 | 74 | 73 | 52 | 84 | 82.8 | 75 | 74 | 50 |