# A few additional examples.

In **Fig.1**. various kinases are presented, with which the interactions of the active site of the MYC peptide were studied.

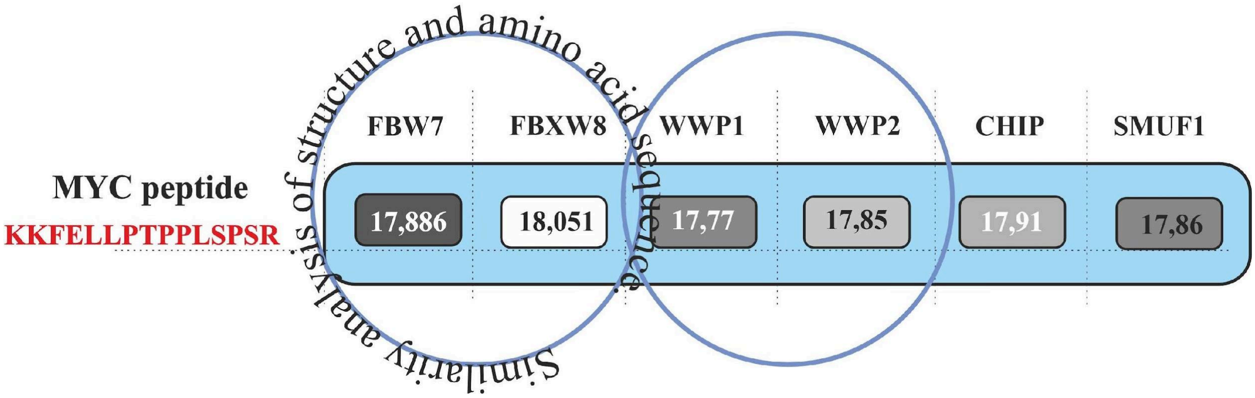


**Figure 1.**

The structures of the ligases **FBW7** and **FBXW8**, **WWP**1 and **WWP2** are somewhat similar, so they are studied in pairs. We are interested in the smallest numerical values obtained.

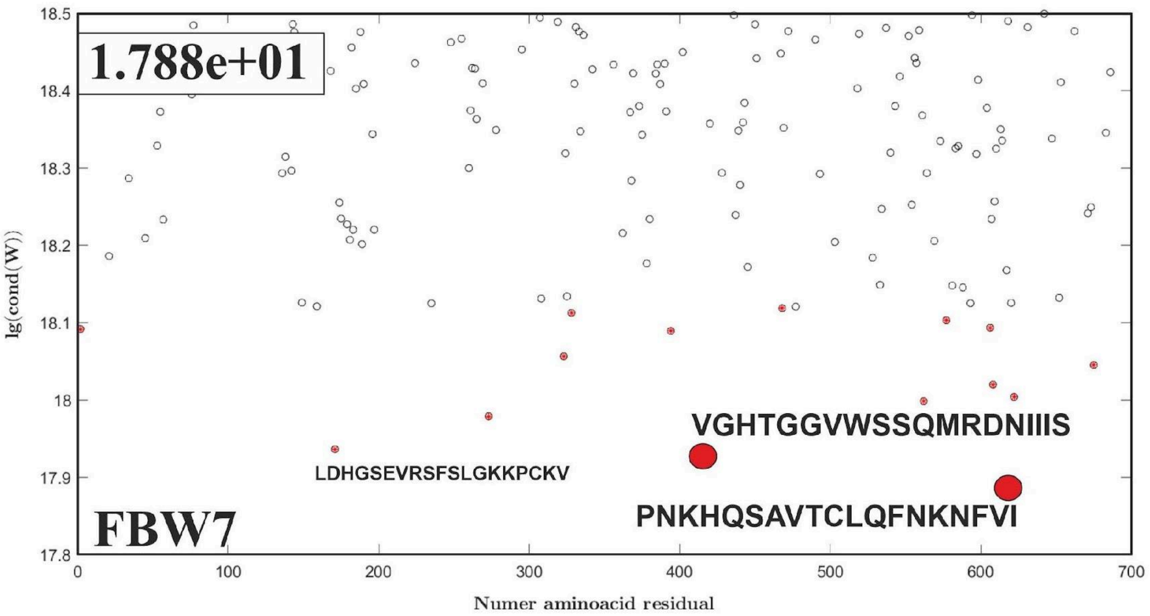
**Figures 2** and **3** contain information about the results of numerical calculations, as well as the structure of **FBW7** and **FBXW8** ligases.

**Figure 4** contains the results of numerical calculations indicating the domains and amino acid sequences that interact with the MYC peptide.

The second part of the **figure 4** contains an overlay of three-dimensional structures of two **FBW7** and **FBXW8** ligases in the region of the "propeller" domains.

**Figures 5** and **6** contain the results of calculations for **WWP1** and **WWP2** molecules when interacting with the MYC peptide.

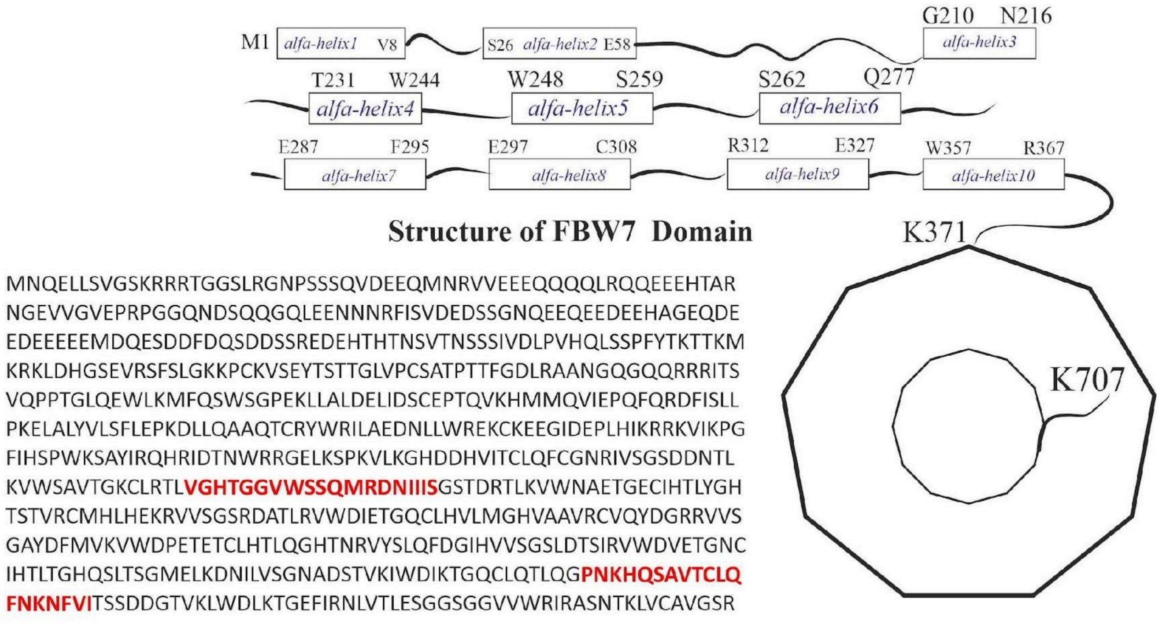
**Figures 7** and **8** contain the results of calculations of the interaction of the MYC peptide with **CHIP** and **SMUF** ligases, indicating the structure of the molecules



Shift plot of the MYC peptide along the amino acid sequence of the FBW7 ligase

| | | | |
|---|---|---|---|
| **619** | **PNKHQSAVTCLQFNKNFVI** | **KKFELLPTPPLSPSRRSGL** | **1.788611e+01** |
| **417** | **VGHTGGVWSSQMRDNIIIS** | **KKFELLPTPPLSPSRRSGL** | **1.793076e+01** |
| **171** | **LDHGSEVRSFSLGKKPCKV** | **KKFELLPTPPLSPSRRSGL** | **1.793632e+01** |
| 273 | PQFQRDFISLLPKELALYV | KKFELLPTPPLSPSRRSGL | 1.797889e+01 |
| 562 | IRVWDVETGNCIHTLTGHQ | KKFELLPTPPLSPSRRSGL | 1.799851e+01 |
| 622 | HQSAVTCLQFNKNFVITSS | KKFELLPTPPLSPSRRSGL | 1.800396e+01 |
| 608 | KTGQCLQTLQGPNKHQSAV | KKFELLPTPPLSPSRRSGL | 1.802002e+01 |
| 675 | RASNTKLVCAVGSRNGTEE | KKFELLPTPPLSPSRRSGL | 1.804516e+01 |

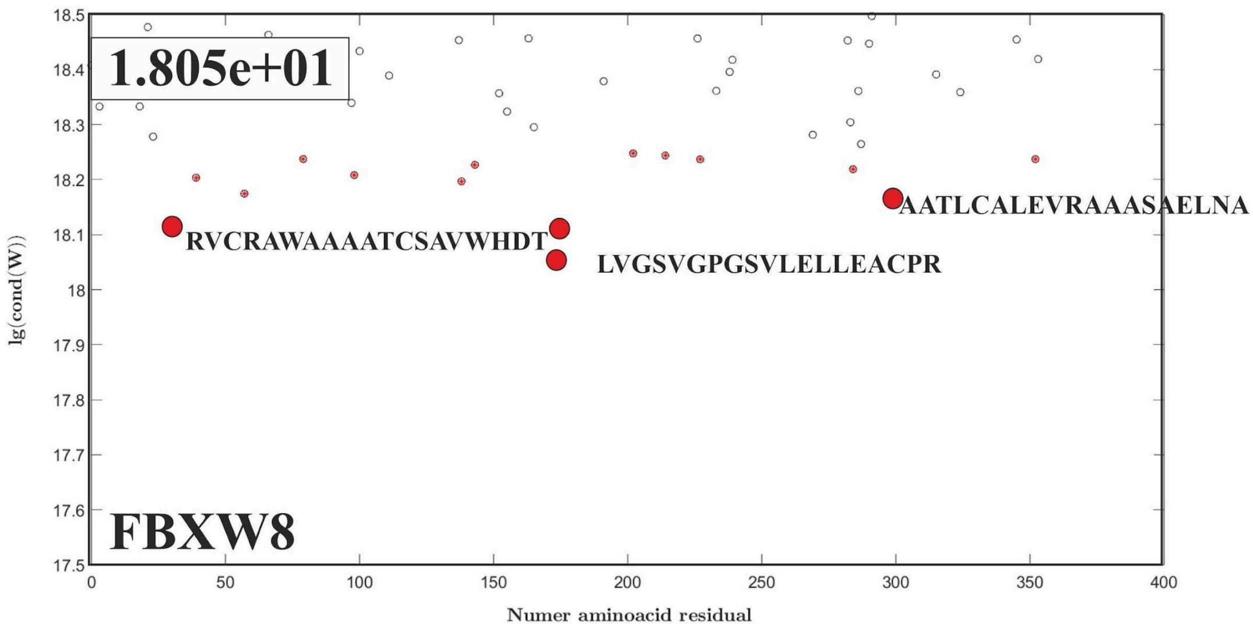
Sampling of the obtained results



Structure of FBW7 Domain

MNQELLSVGSKRRRTGGSLRGNPSSSQVDEEQMNRVVEEEQQQQLRQQEEEHTAR
NGEVVGVEPRPGGQNDSQQGQLEENNNRFISVDEDSSGNQEEQEEDEEHAGEQDE
EDEEEEEMDQESDDFDQSDDSSREDEHTHTNSVTNSSSIVDLPVHQLSSPFYTKTTKM
KRKLDHGSEVRSFSLGKKPCKVSEYTSTTGLVPCSATPTTFGDLRAANGQGQQRRRITS
VQPPTGLQEWLKMFQSWSGPEKLLALDELIDSCEPTQVKHMMQVIEPQFQRDFISLL
PKELALYVLSFLEPKDLLQAAQTCRYWRILAEDNLLWREKCKEEGIDEPLHIKRRKVIKPG
FIHSPWKSAYIRQHRIDTNWRRGELKSPKVLKGHDDHVITCLQFCGNRIVSGSDDNTL
KVWSAVTGKCLRTL**VGHTGGVWSSQMRDNIIIS**GSTDRTLKVWNAETGECIHTLYGH
TSTVRCMHLHEKRVVSGSRDATLRVWDIETGQCLHVLMGHVAAVRCVQYDGRRVVS
GAYDFMVKVWDPETETCLHTLQGHTNRVYSLQFDGIHVVSGSLDTSIRVWDVETGNC
IHTLTGHQSLTSGMELKDNILVSGNADSTVKIWDIKTGQCLQTLQG**PNKHQSAVTCLQ**
**FNKNFVI**TSSDDGTVKLWDLKTGEFIRNLVTLESGGSGGVVWRIRASNTKLVCAVGSR

**Figure 2.** The results of numerical analysis of the interaction of the MYC peptide with the **FBW7** ligase, indicating the amino acid sequences, as well as the structure of the " propeller" domain.



**Shift plot of the MYC peptide along the amino acid sequence of the FBXW8 ligase**

| | | | |
|---|---|---|---|
| **173** | **LVGSVGPGSVLELLEACPR** | **KKFELLPTPPLSPSRRSGL** | **1.805165e+01** |
| **174** | **VGSVGPGSVLELLEACPRL** | **KKFELLPTPPLSPSRRSGL** | **1.811519e+01** |
| **29** | **RVCRAWAAAATCSAVWHDT** | **KKFELLPTPPLSPSRRSGL** | **1.811570e+01** |
| **299** | **AATLCALEVRAAASAELNA** | **KKFELLPTPPLSPSRRSGL** | **1.817078e+01** |
| 57 | GMLPPYLSACLDHIHNLRL | KKFELLPTPPLSPSRRSGL | 1.817457e+01 |
| 138 | HLDLRRLSFTLDDALVLQA | KKFELLPTPPLSPSRRSGL | 1.819692e+01 |
| 39 | TCSAVWHDTKISCECELEG | KKFELLPTPPLSPSRRSGL | 1.820355e+01 |
| 98 | RAPGLRGLRLECRGEKPLF | KKFELLPTPPLSPSRRSGL | 1.820815e+01 |
| 284 | SGDTVGPVRFAAHHYAATL | KKFELLPTPPLSPSRRSGL | 1.821891e+01 |
| 143 | RLSFTLDDALVLQAARSCP | KKFELLPTPPLSPSRRSGL | 1.822686e+01 |
| 227 | CPEDARASPLPNEAWVALR | KKFELLPTPPLSPSRRSGL | 1.823675e+01 |
| 352 | RLRTYTLKLTREPHPWRPT | KKFELLPTPPLSPSRRSGL | 1.823720e+01 |
| 79 | PSRKPSRRAAIELLMVLAG | KKFELLPTPPLSPSRRSGL | 1.823744e+01 |
| 214 | DRAPFALLALRCACPEDAR | KKFELLPTPPLSPSRRSGL | 1.824370e+01 |
| 202 | LSHAILEALAAPDRAPFAL | KKFELLPTPPLSPSRRSGL | 1.824752e+01 |

**Sampling of the obtained results**

**Figure 3.** The results of numerical analysis of the interaction of the MYC peptide with the **FBXW8** ligase, indicating the amino acid sequences.

**Color indicates the identified amino acid sequences that are involved in binding to the MYC peptide.**

MNQELLSVGSKRRRTGGSLRGNPSSSQVDEEQMNRVVEEEQQQQLRQQEEEHTARNGEVVGVEPRPGGQNDSQQGQLEENNNRFISVDEDS
SGNQEEQEEDEEHAGEQDEEDEEEEEMDQESDDFDQSDDSSREDEHTHTNSVTNSSSIVDLPVHQLSSPFYTKTTKMKRKLDHGSEVRSFSLGKK
PCKVSEYTSTTGLVPCSATPTTFGDLRAANGQGQQRRRITSVQPPTGLQEWLKMFQSWSGPEKLLALDELIDSCEPTQVKHMMQVIEPQFQRDFI
SLLPKELALYVLSFLEPKDLLQAAQTCRYWRILAEDNLLWREKCKEEGIDEPLHIKRRKVIKPGFIHSPWKSAYIRQHRIDTNWRRGELKSPKVLKGHD
DHVITCLQFCGNRIVSGSDDNTLKVWSAVTGKCLRTLVGHTGGVWSSQMRDNIIISGSTDRTLKVWNAETGECIHTLYGHTSTVRCMHLHEKRVV
SGSRDATLRVWDIETGQCLHVLMGHVAAVRCVQYDGRRVVSGAYDFMVKVWDPETETCLHTLQGHTNRVYSLQFDGIHVVSGSLDTSIRVWDV
ETGNCIHTLTGHQSLTSGMELKDNILVSGNADSTVKIWDIKTGQCLQTLQGPNKHQSAVTCLQFNKNFVITSSDDGTVKLWDLKTGEFIRNLVTLES
GGSGGVVWRIRASNTKLVCAVGSRNGTEETKLLVLDFDVDMK

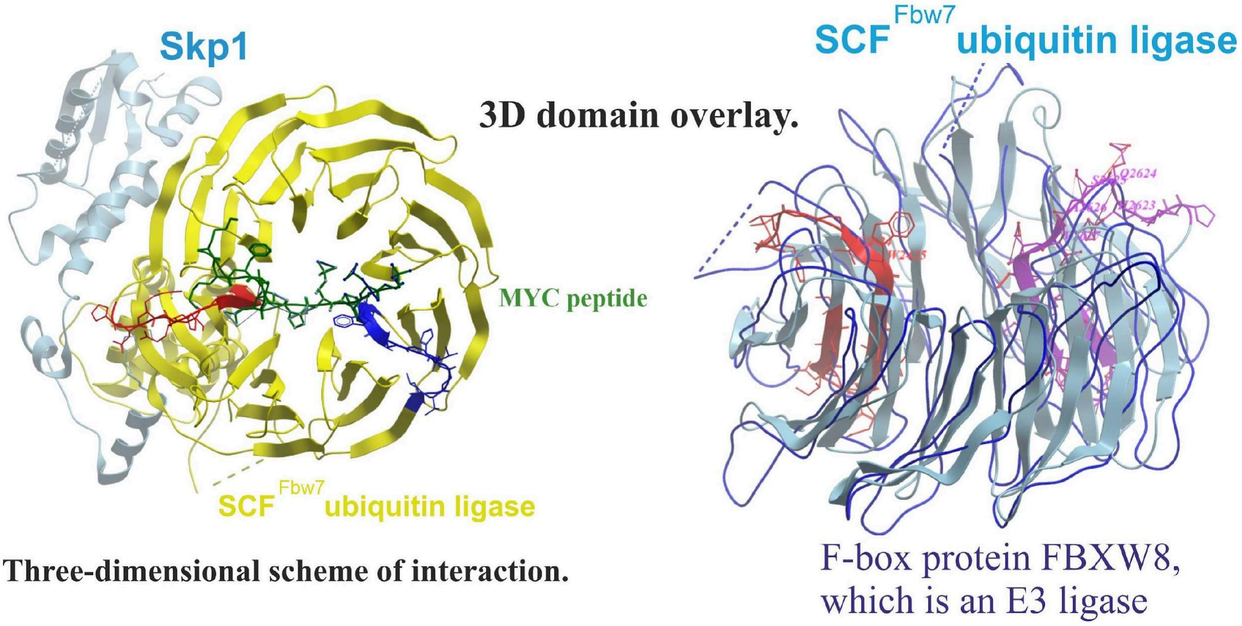
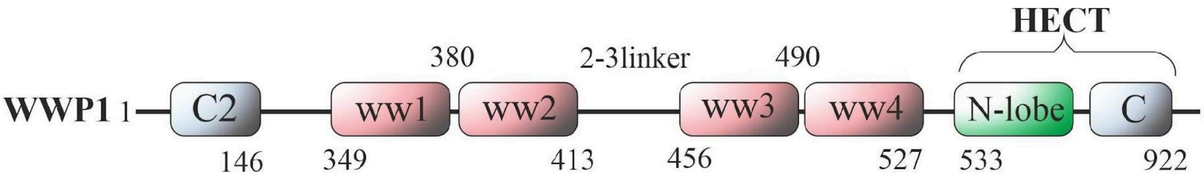
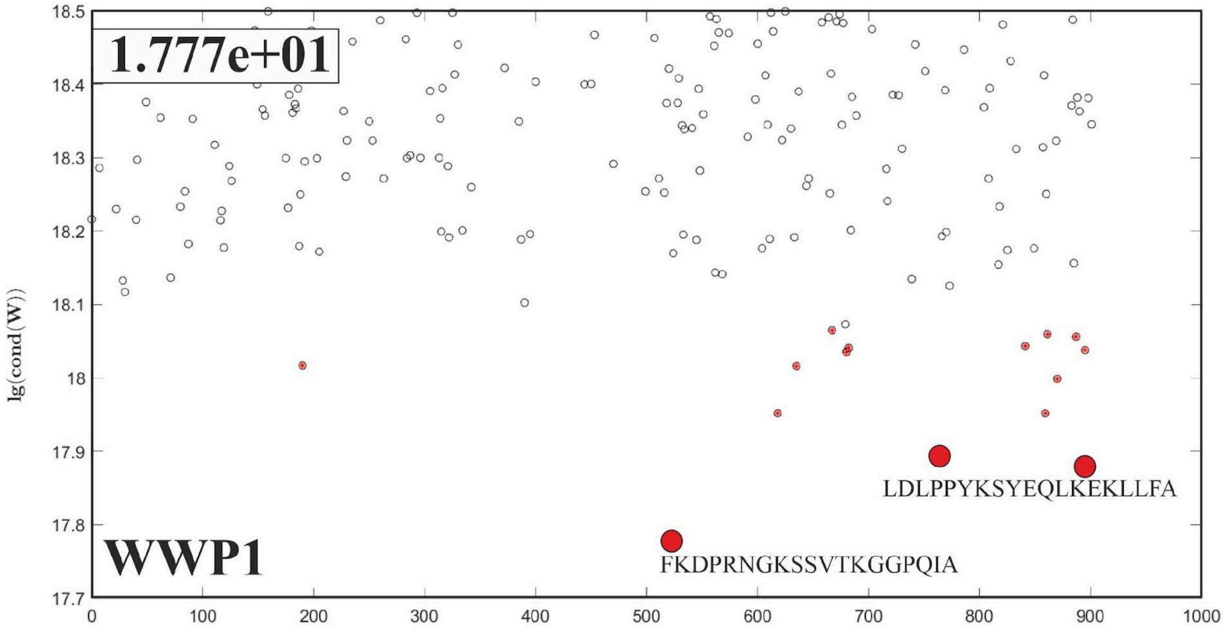


**Figure 4.** The assembled three-dimensional model involving Fbw7 ligase and MYC peptide, the amino acid sequence is shown with indication of the found sequences.

A three-dimensional comparison of the "propeller" domains of two ligases FBXW8 and **FBW7** is given.



**Structure of WW Domain Containing E3 Ubiquitin Protein Ligase 1**

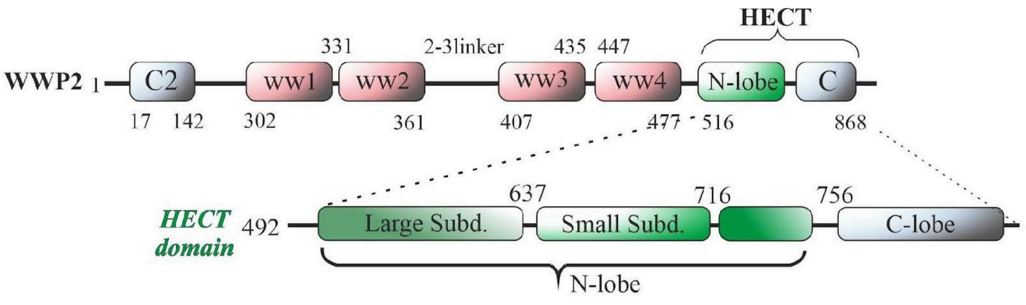


**Shift plot of the MYC peptide along the amino acid sequence of the WWP1 ligase**

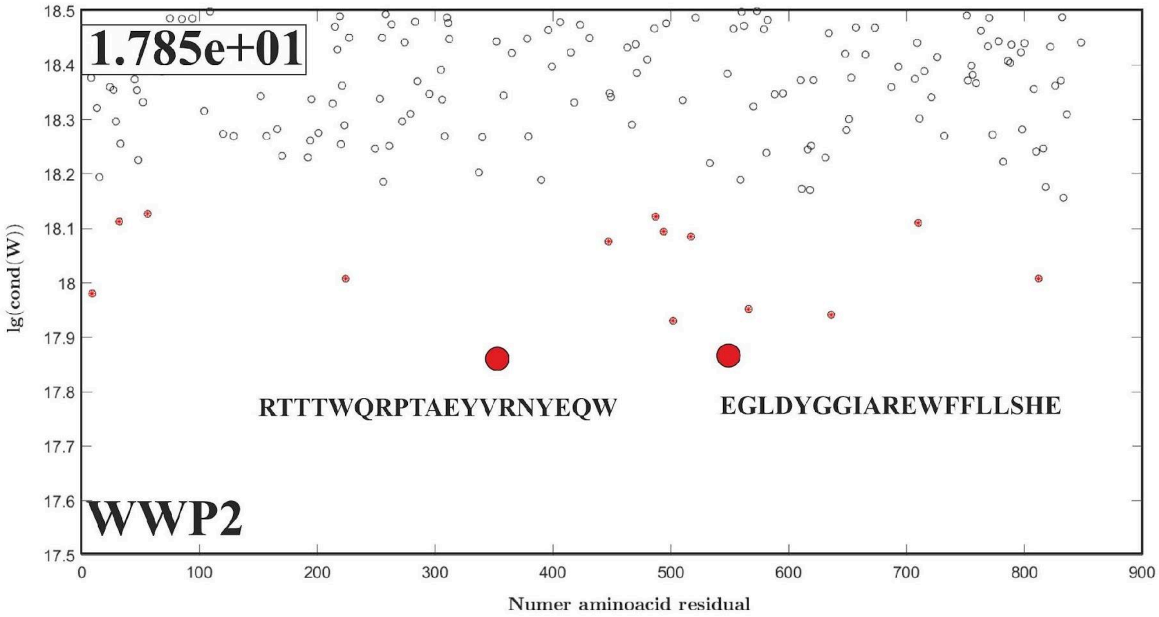
| | | |
|---|---|---|
| **523** | **FKDPRNGKSSVTKGGPQIA** | **KKFELLPTPPLSPSRRSGL 1.777744e+01** |
| **893** | **LDLPPYKSYEQLKEKLLFA** | **KKFELLPTPPLSPSRRSGL 1.787564e+01** |
| 762 | WRFSRGVQEQTKAFLDGFN | KKFELLPTPPLSPSRRSGL 1.789587e+01 |
| 859 | GFAELMGSNGPQKFCIEKV | KKFELLPTPPLSPSRRSGL 1.795186e+01 |
| 618 | LSHEVLNPMYCLFEYAGKN | KKFELLPTPPLSPSRRSGL 1.795195e+01 |
| 870 | QKFCIEKVGKDTWLPRSHT | KKFELLPTPPLSPSRRSGL 1.799886e+01 |
| 635 | KNNYCLQINPASTINPDHL | KKFELLPTPPLSPSRRSGL 1.801605e+01 |
| 190 | NHVPTSTLVQNSCCSYVVN | KKFELLPTPPLSPSRRSGL 1.801677e+01 |
| 680 | PFYKRMLSKKLTIKDLESI | KKFELLPTPPLSPSRRSGL 1.803545e+01 |
| 895 | LPPYKSYEQLKEKLLFAIE | KKFELLPTPPLSPSRRSGL 1.803773e+01 |
| 682 | YKRMLSKKLTIKDLESIDT | KKFELLPTPPLSPSRRSGL 1.804081e+01 |
| 841 | VRMRLLQFVTGTCRLPLGG | KKFELLPTPPLSPSRRSGL 1.804322e+01 |
| 887 | HTCFNRLDLPPYKSYEQLK | KKFELLPTPPLSPSRRSGL 1.805628e+01 |

**Sampling of the obtained results**

**Figure 5.** The results of numerical analysis of the interaction of the MYC peptide with the **WWP1** ligase, indicating the amino acid sequences, as well as the structure of the domain.



Structure of WW Domain Containing E3 Ubiquitin Protein Ligase 2

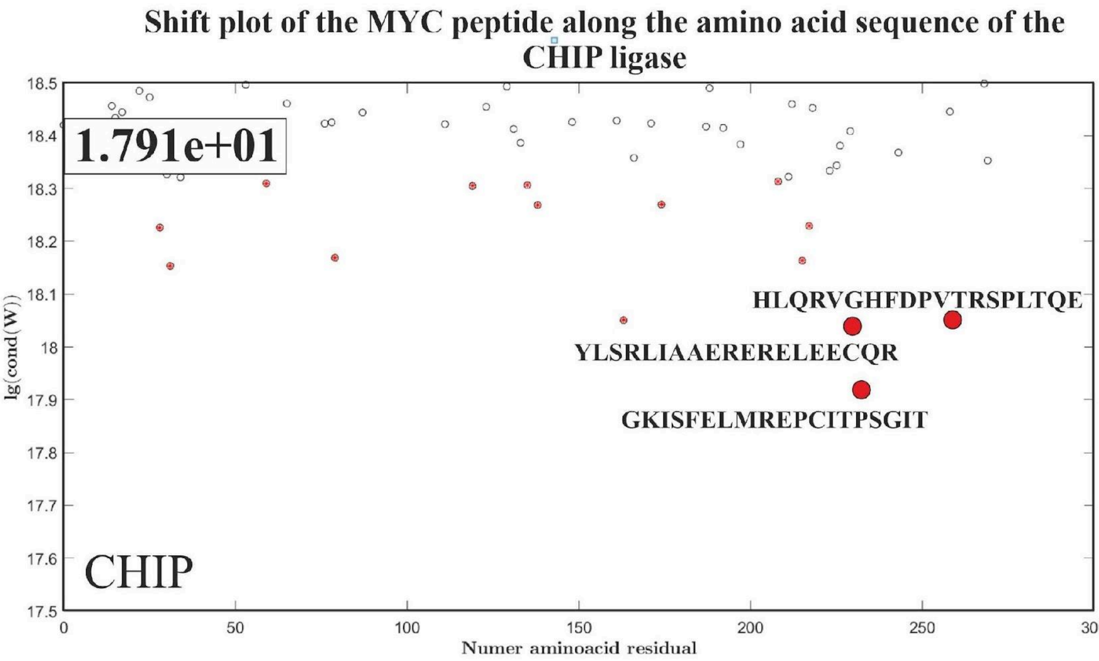


Shift plot of the MYC peptide along the amino acid sequence of the WWP2 ligase

| | | | |
|---|---|---|---|
| **353** | **RTTTWQRPTAEYVRNYEQW** | **KKFELLPTPPLSPSRRSGL** | **1.785669e+01** |
| **551** | **EGLDYGGIAREWFFLLSHE** | **KKFELLPTPPLSPSRRSGL** | **1.786919e+01** |
| 502 | RFLCHSNALPSHVKISVSR | KKFELLPTPPLSPSRRSGL | 1.793021e+01 |
| 636 | KRPTLKDLESIDPEFYNSI | KKFELLPTPPLSPSRRSGL | 1.794161e+01 |
| 566 | LSHEVLNPMYCLFEYAGKN | KKFELLPTPPLSPSRRSGL | 1.795195e+01 |
| 9 | GVALPFEKSQLTLKVVSAK | KKFELLPTPPLSPSRRSGL | 1.798044e+01 |
| 224 | SGHSGLANGTVNDEPTTAT | KKFELLPTPPLSPSRRSGL | 1.800744e+01 |
| 812 | IGSNGPQKFCIDKVGKETW | KKFELLPTPPLSPSRRSGL | 1.800780e+01 |
| 447 | PGWEMKYTSEGVRYFVDHN | KKFELLPTPPLSPSRRSGL | 1.807607e+01 |
| 517 | SVSRQTLFEDSFQQIMNMK | KKFELLPTPPLSPSRRSGL | 1.808469e+01 |
| 494 | FRWKYHQFRFLCHSNALPS | KKFELLPTPPLSPSRRSGL | 1.809416e+01 |
| 710 | WRFTRGVEEQTKAFLDGFN | KKFELLPTPPLSPSRRSGL | 1.811028e+01 |

Sampling of the obtained results

**Figure 6.** The results of numerical analysis of the interaction of the MYC peptide with the **WWP2** ligase, indicating the amino acid sequences, as well as the structure of the domain.



| | | | |
|---|---|---|---|
| **232** | **GKISFELMREPCITPSGIT** | **KKFELLPTPPLSPSRRSGL** | **1.791670e+01** |
| **230** | **LCGKISFELMREPCITPSG** | **KKFELLPTPPLSPSRRSGL** | **1.803913e+01** |
| **259** | **HLQRVGHFDPVTRSPLTQE** | **KKFELLPTPPLSPSRRSGL** | **1.804961e+01** |
| 163 | YLSRLIAAERERELEECQR | KKFELLPTPPLSPSRRSGL | 1.805057e+01 |
| 31 | QGNRLFVGRKYPEAAACYG | KKFELLPTPPLSPSRRSGL | 1.815352e+01 |
| 215 | SQVDEKRKKRDIPDYLCGK | KKFELLPTPPLSPSRRSGL | 1.816347e+01 |
| 79 | LADCRRALELDGQSVKAHF | KKFELLPTPPLSPSRRSGL | 1.816884e+01 |
| 28 | LKEQGNRLFVGRKYPEAAA | KKFELLPTPPLSPSRRSGL | 1.822608e+01 |

**Sampling of the obtained results**

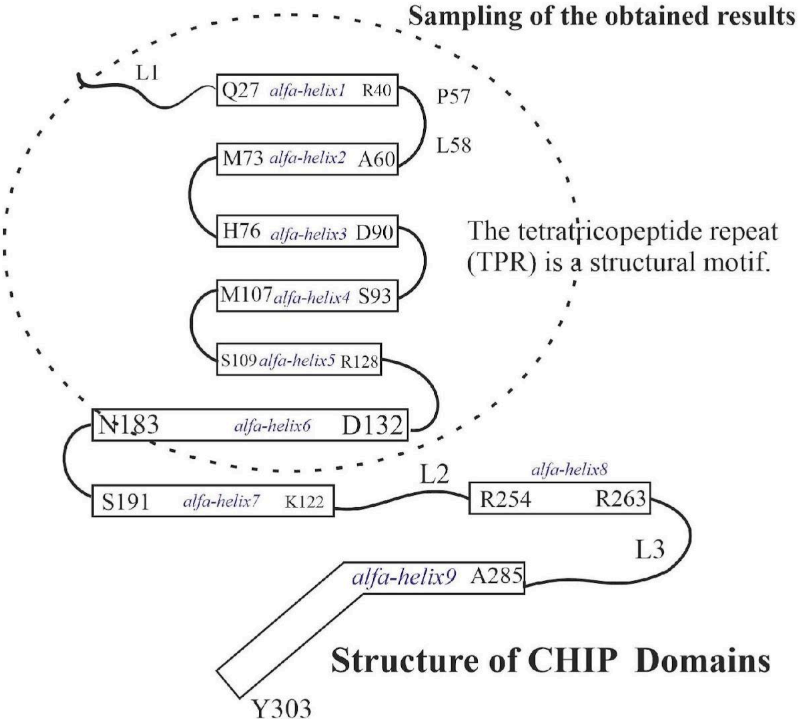
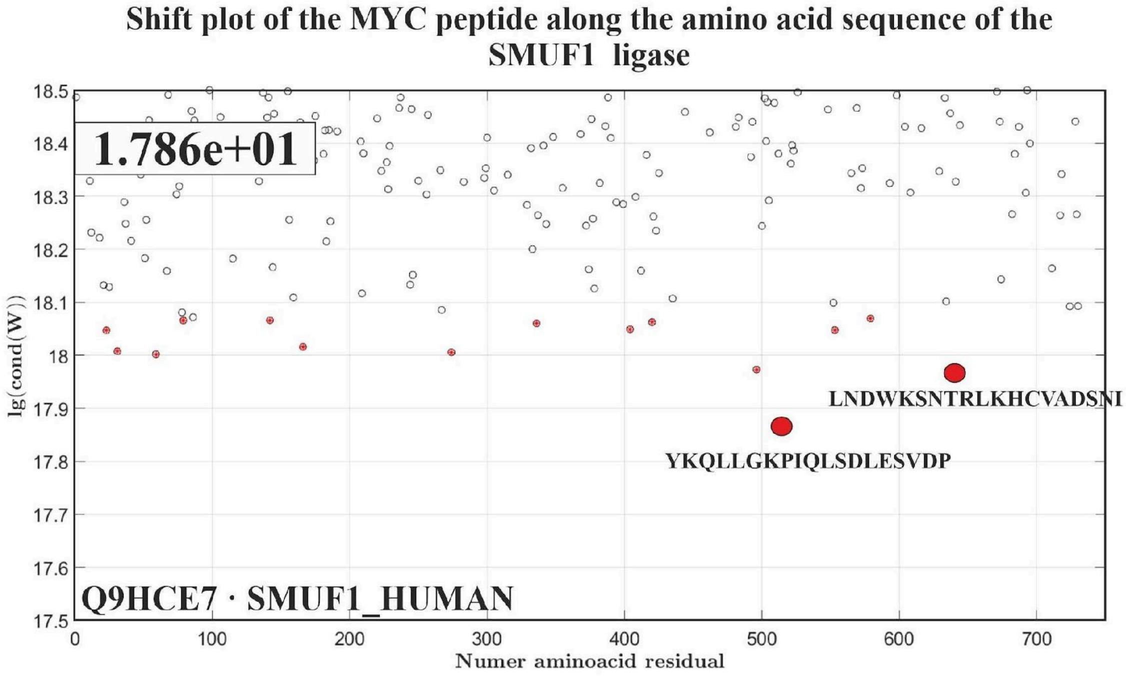


**Figure 7.** The results of numerical analysis of the interaction of the MYC peptide with the **CHIP** ligase, indicating the amino acid sequences, as well as the structure of the domain.



| | | | |
|---|---|---|---|
| **514** | **YKQLLGKPIQLSDLESVDP** | **KKFELLPTPPLSPSRRSGL** | **1.786918e+01** |
| **639** | **LNDWKSNTRLKHCVADSNI** | **KKFELLPTPPLSPSRRSGL** | **1.796568e+01** |
| **496** | **GLAVFHGHYINGGFTVPFY** | **KKFELLPTPPLSPSRRSGL** | **1.797297e+01** |
| 59 | PKWNQHYDLYVGKTDSITI | KKFELLPTPPLSPSRRSGL | 1.800196e+01 |
| 274 | PGGDAAFLYEFLLQGHTSE | KKFELLPTPPLSPSRRSGL | 1.800562e+01 |
| 31 | RLPDPFAKIVVDGSGQCHS | KKFELLPTPPLSPSRRSGL | 1.800731e+01 |
| 166 | GPGRPLSCFMEEPAPYTDS | KKFELLPTPPLSPSRRSGL | 1.801576e+01 |
| 23 | NLAKKDFFRLPDPFAKIVV | KKFELLPTPPLSPSRRSGL | 1.804675e+01 |
| 553 | TFCVEHNAFGRILQHELKP | KKFELLPTPPLSPSRRSGL | 1.804738e+01 |

## Sampling of the obtained results

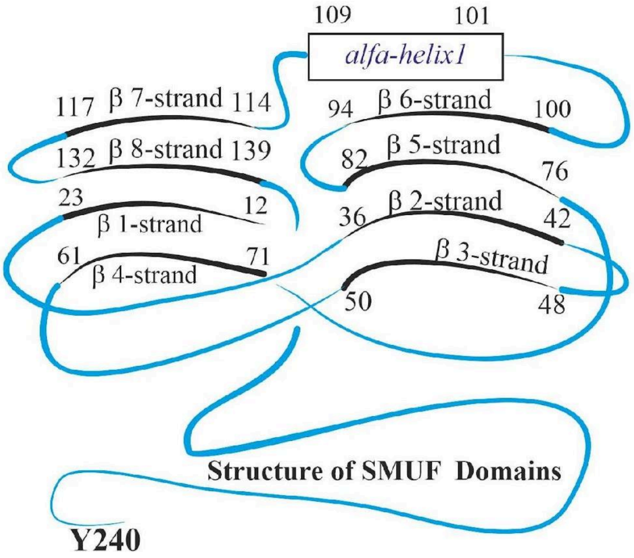


**Figure 8.** The results of numerical analysis of the interaction of the MYC peptide with the **SMUF1** ligase, indicating the amino acid sequences, as well as the structure of the domain.