

**Table S1 – Targets list**

| <b><u>Target<br/>name</u></b> | <b><u>CASP<br/>competition</u></b> | <b><u>Target<br/>name</u></b> | <b><u>CASP<br/>competition</u></b> | <b><u>Target<br/>name</u></b> | <b><u>CASP<br/>competition</u></b> |
|-------------------------------|------------------------------------|-------------------------------|------------------------------------|-------------------------------|------------------------------------|
| T0517                         | 9                                  | T0561                         | 9                                  | T0597                         | 9                                  |
| T0520                         | 9                                  | T0562                         | 9                                  | T0598                         | 9                                  |
| T0521                         | 9                                  | T0564                         | 9                                  | T0599                         | 9                                  |
| T0522                         | 9                                  | T0566                         | 9                                  | T0600*                        | 9                                  |
| T0523                         | 9                                  | T0567                         | 9                                  | T0601                         | 9                                  |
| T0525                         | 9                                  | T0568                         | 9                                  | T0602                         | 9                                  |
| T0528                         | 9                                  | T0569                         | 9                                  | T0603                         | 9                                  |
| T0529                         | 9                                  | T0570                         | 9                                  | T0604                         | 9                                  |
| T0530                         | 9                                  | T0571                         | 9                                  | T0605*                        | 9                                  |
| T0531                         | 9                                  | T0572                         | 9                                  | T0606                         | 9                                  |
| T0533                         | 9                                  | T0573                         | 9                                  | T0607                         | 9                                  |
| T0534                         | 9                                  | T0574                         | 9                                  | T0608                         | 9                                  |
| T0535*                        | 9                                  | T0575                         | 9                                  | T0609                         | 9                                  |
| T0536                         | 9                                  | T0576                         | 9                                  | T0610                         | 9                                  |
| T0537                         | 9                                  | T0577                         | 9                                  | T0611                         | 9                                  |
| T0538                         | 9                                  | T0578                         | 9                                  | T0612                         | 9                                  |
| T0539                         | 9                                  | T0579                         | 9                                  | T0614                         | 9                                  |
| T0540                         | 9                                  | T0580                         | 9                                  | T0615                         | 9                                  |
| T0541                         | 9                                  | T0581                         | 9                                  | T0616                         | 9                                  |
| T0542                         | 9                                  | T0582                         | 9                                  | T0617                         | 9                                  |
| T0545                         | 9                                  | T0584                         | 9                                  | T0618                         | 9                                  |
| T0546*                        | 9                                  | T0585                         | 9                                  | T0619                         | 9                                  |
| T0547                         | 9                                  | T0586                         | 9                                  | T0620                         | 9                                  |
| T0548                         | 9                                  | T0587                         | 9                                  | T0621                         | 9                                  |
| T0549                         | 9                                  | T0588                         | 9                                  | T0622                         | 9                                  |
| T0550                         | 9                                  | T0589                         | 9                                  | T0623                         | 9                                  |
| T0551                         | 9                                  | T0590                         | 9                                  | T0624                         | 9                                  |
| T0555                         | 9                                  | T0592                         | 9                                  | T0625                         | 9                                  |
| T0557                         | 9                                  | T0593                         | 9                                  | T0626                         | 9                                  |
| T0558                         | 9                                  | T0594                         | 9                                  | T0627                         | 9                                  |
| T0560                         | 9                                  | T0596                         | 9                                  | T0628                         | 9                                  |

\* - Targets that are exclude from the training set.

| <u>Target<br/>name</u> | <u>CASP<br/>competition</u> | <u>Target<br/>name</u> | <u>CASP<br/>competition</u> | <u>Target<br/>name</u> | <u>CASP<br/>competition</u> |
|------------------------|-----------------------------|------------------------|-----------------------------|------------------------|-----------------------------|
| T0629                  | 9                           | T0676                  | 10                          | T0720                  | 10                          |
| T0630                  | 9                           | T0678                  | 10                          | T0721                  | 10                          |
| T0632                  | 9                           | T0680                  | 10                          | T0722                  | 10                          |
| T0634                  | 9                           | T0681                  | 10                          | T0723                  | 10                          |
| T0635                  | 9                           | T0682                  | 10                          | T0724                  | 10                          |
| T0637                  | 9                           | T0683                  | 10                          | T0726                  | 10                          |
| T0638                  | 9                           | T0684                  | 10                          | T0727                  | 10                          |
| T0639                  | 9                           | T0685                  | 10                          | T0729                  | 10                          |
| T0641                  | 9                           | T0687                  | 10                          | T0731*                 | 10                          |
| T0643                  | 9                           | T0688                  | 10                          | T0732                  | 10                          |
| T0644                  | 10                          | T0689                  | 10                          | T0733                  | 10                          |
| T0648                  | 10                          | T0691                  | 10                          | T0734                  | 10                          |
| T0649                  | 10                          | T0692                  | 10                          | T0735                  | 10                          |
| T0651                  | 10                          | T0693                  | 10                          | T0736                  | 10                          |
| T0652                  | 10                          | T0694                  | 10                          | T0737                  | 10                          |
| T0654                  | 10                          | T0695                  | 10                          | T0742                  | 10                          |
| T0655                  | 10                          | T0696*                 | 10                          | T0743                  | 10                          |
| T0657                  | 10                          | T0697                  | 10                          | T0744                  | 10                          |
| T0658                  | 10                          | T0698                  | 10                          | T0745                  | 10                          |
| T0659*                 | 10                          | T0700                  | 10                          | T0746                  | 10                          |
| T0661                  | 10                          | T0703                  | 10                          | T0747                  | 10                          |
| T0662*                 | 10                          | T0704                  | 10                          | T0749                  | 10                          |
| T0663                  | 10                          | T0705                  | 10                          | T0750                  | 10                          |
| T0665                  | 10                          | T0706*                 | 10                          | T0751                  | 10                          |
| T0666                  | 10                          | T0708                  | 10                          | T0752                  | 10                          |
| T0667                  | 10                          | T0710                  | 10                          | T0753                  | 10                          |
| T0668                  | 10                          | T0711                  | 10                          | T0754                  | 10                          |
| T0672                  | 10                          | T0712                  | 10                          | T0755                  | 10                          |
| T0673                  | 10                          | T0715                  | 10                          | T0756                  | 10                          |
| T0674                  | 10                          | T0716                  | 10                          | T0757                  | 10                          |
| T0675                  | 10                          | T0717                  | 10                          | T0758                  | 10                          |

\* - Targets that are exclude from the training set.

| <u>Target<br/>name</u> | <u>CASP<br/>competition</u> | <u>Target<br/>name</u> | <u>CASP<br/>competition</u> | <u>Target<br/>name</u> | <u>CASP<br/>competition</u> |
|------------------------|-----------------------------|------------------------|-----------------------------|------------------------|-----------------------------|
| T0759*                 | 11                          | T0794                  | 11                          | T0841                  | 11                          |
| T0760                  | 11                          | T0796                  | 11                          | T0843                  | 11                          |
| T0761                  | 11                          | T0797*                 | 11                          | T0845                  | 11                          |
| T0762                  | 11                          | T0798                  | 11                          | T0846                  | 11                          |
| T0763                  | 11                          | T0799                  | 11                          | T0847                  | 11                          |
| T0764                  | 11                          | T0800                  | 11                          | T0848                  | 11                          |
| T0765                  | 11                          | T0802                  | 11                          | T0849                  | 11                          |
| T0766                  | 11                          | T0803                  | 11                          | T0851                  | 11                          |
| T0767                  | 11                          | T0806                  | 11                          | T0852                  | 11                          |
| T0768                  | 11                          | T0807                  | 11                          | T0853                  | 11                          |
| T0770                  | 11                          | T0808                  | 11                          | T0854                  | 11                          |
| T0771                  | 11                          | T0812                  | 11                          | T0855                  | 11                          |
| T0772                  | 11                          | T0813                  | 11                          | T0856                  | 11                          |
| T0773                  | 11                          | T0814                  | 11                          | T0857                  | 11                          |
| T0774                  | 11                          | T0815                  | 11                          | T0858                  | 11                          |
| T0775                  | 11                          | T0816                  | 11                          | T0860                  | 12                          |
| T0776                  | 11                          | T0817                  | 11                          | T0861                  | 12                          |
| T0777                  | 11                          | T0818                  | 11                          | T0862*                 | 12                          |
| T0780                  | 11                          | T0819                  | 11                          | T0865                  | 12                          |
| T0781                  | 11                          | T0821                  | 11                          | T0866*                 | 12                          |
| T0782                  | 11                          | T0822                  | 11                          | T0868                  | 12                          |
| T0783                  | 11                          | T0826                  | 11                          | T0869                  | 12                          |
| T0784                  | 11                          | T0828                  | 11                          | T0870                  | 12                          |
| T0785                  | 11                          | T0829                  | 11                          | T0872                  | 12                          |
| T0786                  | 11                          | T0830                  | 11                          | T0877                  | 12                          |
| T0787*                 | 11                          | T0831                  | 11                          | T0878                  | 12                          |
| T0788                  | 11                          | T0832                  | 11                          | T0879                  | 12                          |
| T0790                  | 11                          | T0833                  | 11                          | T0882                  | 12                          |
| T0791                  | 11                          | T0834                  | 11                          | T0884                  | 12                          |
| T0792                  | 11                          | T0837                  | 11                          | T0885                  | 12                          |
| T0793                  | 11                          | T0840                  | 11                          | T0889                  | 12                          |

\* - Targets that are exclude from the training set.

| <u>Target<br/>name</u> | <u>CASP<br/>competition</u> | <u>Target<br/>name</u> | <u>CASP<br/>competition</u> | <u>Target<br/>name</u> | <u>CASP<br/>competition</u> |
|------------------------|-----------------------------|------------------------|-----------------------------|------------------------|-----------------------------|
| T0891                  | 12                          | T0957s2                | 13                          | T1021s2                | 13                          |
| T0893                  | 12                          | T0958                  | 13                          | T1021s3                | 13                          |
| T0894                  | 12                          | T0960                  | 13                          | T1022s1                | 13                          |
| T0895                  | 12                          | T0961                  | 13                          | T1022s2                | 13                          |
| T0900                  | 12                          | T0963                  | 13                          |                        |                             |
| T0902                  | 12                          | T0965                  | 13                          |                        |                             |
| T0903                  | 12                          | T0966                  | 13                          |                        |                             |
| T0904                  | 12                          | T0967                  | 13                          |                        |                             |
| T0909                  | 12                          | T0968s1                | 13                          |                        |                             |
| T0912                  | 12                          | T0968s2                | 13                          |                        |                             |
| T0918                  | 12                          | T0969                  | 13                          |                        |                             |
| T0920                  | 12                          | T0970                  | 13                          |                        |                             |
| T0921                  | 12                          | T0971                  | 13                          |                        |                             |
| T0922*                 | 12                          | T0976                  | 13                          |                        |                             |
| T0928                  | 12                          | T0980s1                | 13                          |                        |                             |
| T0929                  | 12                          | T0980s2                | 13                          |                        |                             |
| T0930*                 | 12                          | T0984                  | 13                          |                        |                             |
| T0932                  | 12                          | T0986s1                | 13                          |                        |                             |
| T0933                  | 12                          | T0986s2                | 13                          |                        |                             |
| T0942*                 | 12                          | T0990                  | 13                          |                        |                             |
| T0943                  | 12                          | T1000                  | 13                          |                        |                             |
| T0944                  | 12                          | T1003                  | 13                          |                        |                             |
| T0945                  | 12                          | T1005                  | 13                          |                        |                             |
| T0948                  | 12                          | T1006                  | 13                          |                        |                             |
| T0950                  | 13                          | T1008                  | 13                          |                        |                             |
| T0951                  | 13                          | T1009                  | 13                          |                        |                             |
| T0953s1                | 13                          | T1011                  | 13                          |                        |                             |
| T0953s2                | 13                          | T1014                  | 13                          |                        |                             |
| T0954                  | 13                          | T1016                  | 13                          |                        |                             |
| T0955*                 | 13                          | T1018                  | 13                          |                        |                             |
| T0957s1                | 13                          | T1021s1                | 13                          |                        |                             |

\* - Targets that are exclude from the training set.