***In silico* analysis of RNA-dependent RNA polymerase of the SARS-CoV-2 and potentiality of the pre-existing drugs**

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**Supplementary table 1a: list of residues participating in hydrogen bonding.** In the following table the alphabet just after the residue number denotes the chain ID of that specific residue. Alphabet “A” indicates the residue is belonging to nsp12 and other alphabet indicates that the residue is from nsp7-8 hexadecameric structure.

|  |  |  |
| --- | --- | --- |
| **Name of the interaction** | **Hydrogen bonds** | |
| **Residue** | **Amino acid** |
| Nsp12 to RNA | 39A | Asn |
| 41A | Lys |
| 78A | Ser |
| 725A | His |
| 729A | Glu |
| 733A | Arg |
| 733A | Arg |
| 734A | Asn |
| Nsp12 to drug | 817A | Thr |
| 817A | Thr |
| 817A | Thr |
| 819A | Leu |
| 831A | Tyr |
| 872A | His |
| 877A | Tyr |
| (Nsp12 to Nsp7-8) to RNA | 21B | Arg |
| 21B | Arg |
| 21L | Arg |
| 27D | Lys |
| 75F | Arg |
| 80F | Arg |

**Supplementary table 1b: list of residues participating in hydrogen bonding.** In the following table the alphabet just after the residue number denotes the chain ID of that specific residue. Alphabet “A” indicates the residue is belonging to nsp12 and other alphabet indicates that the residue is from nsp7-8 hexadecameric structure.

|  |  |  |
| --- | --- | --- |
| **((Nsp12 to drug) to Nsp7-8) to RNA** | | |
| **Name of the interaction** | **Hydrogen bonds** | |
| **Residue** | **Amino acid** |
| IDX\_184 | 21J | Arg |
| 23B | Glu |
| 26D | Ser |
| 29B | Trp |
| 69G | Gln |
| 75F | Arg |
| Remdisivir | 31I | Gln |
| 54I | Ser |
| 57I | Ser |
| 61E | Lys |
| 65G | Gln |
| 406A | Ala |
| 408A | Gln |
| Rivabirin | 19D | Gln |
| 21C | Arg |
| 21D | Arg |
| 23D | Glu |
| 27J | Lys |
| 34A | Gln |
| 37A | Asn |
| 65F | Gln |
| 73G | Gln |
| 76G | Ser |
| 77G | Glu |
| 80G | Arg |
| 80G | Arg |
| 164G | Ser |
| 164G | Ser |
| Galidesevir | 27B | Lys |
| 61E | Lys |
| 65E | Gln |
| 65G | Gln |
| 127F | Lys |
| Setrobuvir | 21J | Arg |
| 24I | Ser |
| 26D | Ser |
| 37I | Asn |
| 73G | Gln |
| 73G | Gln |
| 75F | Arg |
| Sofosbuvir | 499A | Asp |
| 521A | Tyr |
| 814A | Ser |
| 903A | Tyr |
| Tenofovir | 19D | Gln |
| 21C | Arg |
| 23C | Glu |
| 23C | Glu |
| 30B | Ala |
| 37A | Asn |
| 80G | Arg |
| YAK | 21C | Arg |
| 21C | Arg |
| 21D | Arg |
| 21D | Arg |
| 23A | Glu |
| 27J | Lys |
| 34A | Gln |
| 37A | Asn |
| 65F | Gln |
| 73G | Gln |
| 76G | Ser |
| 80G | Arg |
| 80G | Arg |
| 164G | Ser |
| 164G | Ser |

**Supplementary table 1c: list of residues participating in hydrogen bonding.** In the following table the alphabet just after the residue number denotes the chain ID of that specific residue. Alphabet “A” indicates the residue is belonging to nsp12 and other alphabet indicates that the residue is from nsp7-8 hexadecameric structure.

|  |  |  |
| --- | --- | --- |
| **((Nsp12 to Nsp7-8) to drug) to RNA** | | |
| **Name of the interaction** | **Hydrogen bonds** | |
| **Residue** | **Amino acid** |
| IDX\_184 | 21J | Arg |
| 26D | Ser |
| 73G | Gln |
| 75F | Arg |
| 80G | Arg |
| Remdisivir | 21J | Arg |
| 26D | Ser |
| 73G | Gln |
| 75F | Arg |
| 80G | Arg |
| Rivabirin | 21J | Arg |
| 26D | Ser |
| 73G | Gln |
| 75F | Arg |
| 80G | Arg |
| Galidesevir | 21J | Arg |
| 26D | Ser |
| 73G | Gln |
| 75F | Arg |
| 80G | Arg |
| Setrobuvir | 21J | Arg |
| 26D | Ser |
| 73G | Gln |
| 75F | Arg |
| 80G | Arg |
| Sofosbuvir | 21J | Arg |
| 26D | Ser |
| 29B | Trp |
| 73G | Gln |
| 75F | Arg |
| 80G | Arg |
| Tenofovir | 21J | Arg |
| 26D | Ser |
| 73G | Gln |
| 75F | Arg |
| 80G | Arg |
| YAK | 21J | Arg |
| 26D | Ser |
| 73G | Gln |
| 75F | Arg |
| 80G | Arg |

**Supplementary table 1d: list of residues participating in hydrogen bonding.** In the following table the alphabet just after the residue number denotes the chain ID of that specific residue. Alphabet “A” indicates the residue is belonging to nsp12 and other alphabet indicates that the residue is from nsp7-8 hexadecameric structure.

|  |  |  |
| --- | --- | --- |
| **Nsp12 to drug** | | |
| **Name of the interaction** | **Hydrogen bonds** | |
| **Residue** | **Amino acid** |
| IDX\_184 | 817A | THR |
| 817A | THR |
| 817A | THR |
| 819A | LEU |
| 831A | TYR |
| 872A | HIS |
| 877A | TYR |
| Galdisevir | 52A | ASN |
| 52A | ASN |
| 52A | ASN |
| 52A | ASN |
| 116A | ARG |
| 121A | LYS |
| 217A | TYR |
| 218A | ASP |
| 218A | ASP |
| Remdisivir | 50A | LYS |
| 52A | ASN |
| 54A | CYS |
| 116A | ARG |
| 116A | ARG |
| 218A | ASP |
| 218A | ASP |
| Rivabirin | 343A | SER |
| 356A | ASN |
| 360A | ASN |
| 360A | ASN |
| 370A | GLU |
| 373A | VAL |
| 374A | TYR |
| 377A | ASP |
| 530A | TYR |
| Setrobuvir | 835A | SER |
| 877A | TYR |
| Tenofovir | 120A | THR |
| 123A | THR |
| 208A | ASP |
| YAK\_CID | 34A | ALA |
| Sofosbuvir | 911A | ASN |
| 914A | ARG |
| 914A | ARG |
| 915A | TYR |
| 919A | GLU |

**Supplementary table 1e: list of residues participating in hydrogen bonding.** In the following table the alphabet just after the residue number denotes the chain ID of that specific residue. Alphabet “A” indicates the residue is belonging to nsp12 and other alphabet indicates that the residue is from nsp7-8 hexadecameric structure.

|  |  |  |
| --- | --- | --- |
| **(Nsp12 to drug) to RNA** | | |
| **Name of the interaction** | **Hydrogen bonds** | |
|  | **Residue** | **Amino acid** |
| IDX\_184 | 499A | Asp |
| 521A | Tyr |
| 814A | Ser |
| 861A | Ser |
| 903A | Tyr |
| Remdisivir | 499A | Asp |
| 521A | Tyr |
| 814A | Ser |
| 861A | Ser |
| 903A | Tyr |
| Galidesevir | 499A | Asp |
| 521A | Tyr |
| 814A | Ser |
| 861A | Ser |
| 903A | Tyr |
| Rivabirin | 492A | Gln |
| 499A | Asp |
| 521A | Tyr |
| 814A | Ser |
| 861A | Ser |
| 903A | Tyr |
| Setrobuvir | 38A | Tyr |
| 40A | Asp |
| 78A | Ser |
| 79A | Asn |
| 220A | Gly |
| 722A | Asn |
| 722A | Asn |
| 734A | Asn |
| Sofosbuvir | 499A | Asp |
| 521A | Tyr |
| 814A | Ser |
| 903A | Tyr |
| Tenofovir | 499A | Asp |
| 521A | Tyr |
| 814A | Ser |
| 861A | Ser |
| 903A | Tyr |
| YAK | 499A | Asp |
| 521A | Tyr |
| 814A | Ser |
| 861A | Ser |
| 903A | Tyr |

**Supplementary table 1f: list of residues participating in hydrogen bonding.** In the following table the alphabet just after the residue number denotes the chain ID of that specific residue. Alphabet “A” indicates the residue is belonging to nsp12 and other alphabet indicates that the residue is from nsp7-8 hexadecameric structure.

|  |  |  |
| --- | --- | --- |
| **(Nsp12 to Nsp7-8) to drug** | | |
| **Name of the interaction** | **Hydrogen bonds** |  |
|  | **Residue** | **Amino acid** |
| IDX\_184 | 19B | GLN |
| 21B | ARG |
| 21B | ARG |
| 37C | ASN |
| 80F | ARG |
| Remdisivir | 140G | ASN |
| 408A | GLN |
| 507A | ASN |
| 507A | ASN |
| Rivabirin | 343A | SER |
| 343A | SER |
| 356A | ASN |
| 360A | ASN |
| 360A | ASN |
| 370A | GLU |
| 373A | VAL |
| 374A | TYR |
| 377A | ASP |
| 530A | TYR |
| Galidesevir | 33A | ARG |
| 50A | LYS |
| 50A | LYS |
| 52A | ASN |
| 121A | LYS |
| 123A | THR |
| 123A | THR |
| 209A | ASN |
| 217A | TYR |
| 218A | ASP |
| 218A | ASP |
| Setrobuvir | 15B | SER |
| 15C | SER |
| 19C | GLN |
| 36B | HIS |
| 37B | ASN |
| Sofosbuvir | 18B | GLN |
| 18C | GLN |
| 18C | GLN |
| 21C | ARG |
| 23C | GLU |
| 24C | SER |
| Tenofovir | 343A | SER |
| 356A | ASN |
| 377A | ASP |
| 377A | ASP |
| 530A | TYR |
| YAK | 15B | SER |