**Table 1:** Summary some of the most promising drug candidates

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Drug Candidate [structure] | Identified through | Target Protein | Mechanism of Action | Potential Use | Current Status | Reference |
| Remdesivir | Molecular docking | RNA Polymerase | Inhibits viral replication | Antiviral | Approved for emergency use in several countries | Elfiky, A.A., 2020. |
| Favipiravir | Molecular docking | RNA Polymerase | Inhibits viral replication | Antiviral | Approved for emergency use in some countries | Rafi, M.O., Bhattacharje, G., Al-Khafaji, K., et al., 2022. |
| Ribavirin | Molecular docking | RNA Polymerase | Inhibits viral replication | Antiviral | Investigational | Elfiky, A.A., 2020. |
| Ivermectin | Molecular docking | RNA Polymerase, Importin alpha/beta1 | Inhibits viral replication | Antiviral | Investigational | Eweas, A.F., Alhossary, A.A. and Abdel-Moneim, A.S., 2021. |
| Lopinavir/Ritonavir | Molecular docking | Main Protease | Inhibits viral replication | Antiviral | Not recommended by WHO | Shaikh, V.S., Shaikh, Y.I. and Ahmed, K., 2020. |
| Darunavir/Cobicistat | Molecular docking | Main Protease | Inhibits viral replication | Antiviral | Investigational | Marin, R.C., Behl, T., Negrut, N. and Bungau, S., 2021 |
| Nelfinavir | Molecular docking | Main Protease | Inhibits viral replication | Antiviral | Investigational | Xu, Z., Peng, C., Shi, Y., et al., 2020. |
| Camostat mesylate | Molecular docking | TMPRSS2 | Inhibits viral entry | Antiviral | Investigational | Sonawane, K.D., Barale, S.S., Dhanavade, M.J., et al., 2021. |
| Ebselen | Molecular docking and Molecular dynamics simulations | Main Protease, Spike Protein | Inhibits viral replication, prevents cell entry | Antiviral | Investigational | Amporndanai, K., Meng, X., Shang, W., et al., 2021 |
| Quercetin | Molecular docking | Spike Protein | Inhibits viral entry | Antiviral | Investigational | Munafò, F., Donati, E., Brindani, N., et al., 2022. |
| Niclosamide | Molecular docking | TMPRSS2 | Inhibits viral entry | Antiviral | Investigational | Al-Kuraishy, H.M., Al-Gareeb, A.I., Alzahrani, K.J., et al., 2021. |
| Chloroquine/Hydroxychloroquine | Molecular docking | Spike Protein, ACE2 receptor | Inhibits viral entry | Antiviral | Not recommended by WHO | Nimgampalle, M., Devanathan, V. and Saxena, A., 2021 |
| Baricitinib | Molecular docking | AP2-associated protein kinase 1 | Inhibits viral entry | Anti-inflammatory | Approved for emergency use in some countries | Bui, T.Q., Hai, N.T.T., My, T.T.A., et al., 2022. |
| Flavonoids | Molecular docking | RNA Polymerase | Inhibits viral replication | Antiviral | Investigational | Schultz, J.V., Tonel, M.Z., Martins, M.O. and Fagan, S.B., 2023. |
| Curcumin | Molecular docking | Main Protease | Inhibits viral replication | Antiviral | Investigational | Nidom, C.A., Ansori, A.N., et al., 2023. |
| Emodin | Molecular dynamics | RNA Polymerase | Inhibits viral replication | Antiviral | Investigational | Ibeh, R.C., Ikechukwu, G.C., Ukweni, C.J., et al., 2023. |
| Gallic Acid | Molecular docking | Spike Protein, ACE2 receptor | Inhibits viral entry | Antiviral | Investigational | Gu, Y., Liu, M., Staker, B.L., et al., 2023. |
| Theaflavin | Molecular docking | Spike Protein, ACE2 receptor | Inhibits viral entry | Antiviral | Investigational | Putra, W.E., Hidayatullah, A., Heikal, M.F., et al., 2023. |
| Catechins | Molecular docking | Spike Protein, ACE2 receptor | Inhibits viral entry | Antiviral | Investigational | Hossain, A., Rahman, M.E., Rahman, M.S., et al., 2023. |
| Epigallocatechin | Molecular docking | Spike Protein, ACE2 receptor | Inhibits viral entry | Antiviral | Investigational | Dinata, R., Nisa, N., Arati, C., et al., 2023. |

Note: The "Identified through" column indicates the in-silico method used to identify the drug candidate's potential against SARS-CoV-2. The "Target Protein" column indicates the protein targeted by the drug candidate. The "Mechanism of Action" column describes how the drug candidate inhibits viral replication or entry. The "Potential Use" column indicates the proposed use of the drug candidate.

**Table 2:** Drug candidates or in silico analysis methods used in the search for COVID-19 treatments

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Drug Candidate | Target Receptor | In Silico Analysis | Result | Reference |
| Remdesivir | Viral RNA Polymerase | Molecular docking, molecular dynamics simulations | Strong binding affinity, stable complex formation | Shahabadi, N., Zendehcheshm, S., Mahdavi, M. and Khademi, F., 2023. |
| Hydroxychloroquine | Viral Spike Protein | Molecular docking | Moderate binding affinity, potential inhibition of viral entry | Oner, E., Demirhan, I., Miraloglu, M., Yalin, S. and Kurutas, E.B., 2023 |
| Camostat Mesylate | Human ACE2 Receptor | Molecular docking, molecular dynamics simulations | Strong binding affinity, potential inhibition of viral entry | Wang, C., Ye, X., Ding, C., Zhou, M., et al., 2023 |
| Ivermectin | Viral NSP14 Protein | Molecular docking | Moderate binding affinity, potential inhibition of viral replication | Kumar, S. and Choudhary, M., 2023. |
| Favipiravir | Viral RNA Polymerase | Molecular docking | Moderate binding affinity, potential inhibition of viral replication | Nath, A., Rani, M., Rahim, A., et al., 2023. |
| Baricitinib | Host Cell ACE2 Receptor | Molecular docking | Strong binding affinity, potential anti-inflammatory effects | Pirolli, D., Righino, B., Camponeschi, C., Ria, F., Di Sante, G. and De Rosa, M.C., 2023. |
| Tocilizumab | Host Cell IL-6 Receptor | Machine learning algorithms | Potential anti-inflammatory effects, may reduce cytokine storm | Zielińska, A., Eder, P., Karczewski, J., et al., 2023. |
| Lopinavir | Viral Protease | Molecular docking, molecular dynamics simulations | Moderate binding affinity, potential inhibition of viral replication | Oner, E., Demirhan, I., Miraloglu, M., Yalin, S. and Kurutas, E.B., 2023 |
| Ritonavir | Viral Protease | Molecular docking, molecular dynamics simulations | Moderate binding affinity, potential inhibition of viral replication | Miatmoko, A., Sulistyowati, M.I., Setyawan, D. and Cahyani, D.M., 2023. |
| Nitazoxanide | Viral Protease | Molecular docking | Moderate binding affinity, potential inhibition of viral replication | Shoaib, S., Ansari, M.A., Kandasamy, G., et al., 2023. |
| Nelfinavir | Viral Protease | Molecular docking, molecular dynamics simulations | Moderate binding affinity, potential inhibition of viral replication | Ghasemlou, A., Uskoković, V. and Sefidbakht, Y., 2023. |
| Oseltamivir | Viral Neuraminidase | Molecular docking | Moderate binding affinity, potential inhibition of viral release | Oner, E., Demirhan, I., Miraloglu, M., Yalin, S. and Kurutas, E.B., 2023. |
| Zanamivir | Viral Neuraminidase | Molecular docking | Moderate binding affinity, potential inhibition of viral release | Devi, R.N., Pounraj, P., Kumar, S.B., et al., 2023. |
| Darunavir | Viral Protease | Molecular docking | Moderate binding affinity, potential inhibition of viral replication | Makhloufi, A., Ghemit, R., El Kolli, M. and Baitiche, M., 2023. |
| Sofosbuvir | Viral RNA Polymerase | Molecular docking | Moderate binding affinity, potential inhibition of viral replication | Mohamed, E.A., Abdel-Rahman, I.M., et al., 2023. |
| Ribavirin | Viral RNA Polymerase | Molecular docking | Moderate binding affinity, potential inhibition of viral replication | Oner, E., Demirhan, I., Miraloglu, M., Yalin, S. and Kurutas, E.B., 2023. |
| Tenofovir | Viral Reverse Transcriptase | Molecular docking | Moderate binding affinity, potential inhibition of viral replication | Mohandoss, S., Velu, K.S., Stalin, T., Ahmad, N., Alomar, S.Y. and Lee, Y.R., 2023. |
| Emtricitabine | Viral Reverse Transcriptase | Molecular docking | Moderate binding affinity, potential inhibition of viral replication | Oner, E., Demirhan, I., Miraloglu, M., Yalin, S. and Kurutas, E.B., 2023. |
| Atazanavir | Viral Protease | Molecular docking | Moderate binding affinity, potential inhibition of viral replication | Solanki, R., Shankar, A., Modi, U. and Patel, S., 2023. |
| Remdesivir | Viral RNA Polymerase | Molecular docking, molecular dynamics simulations | Strong binding affinity, stable complex formation | Oner, E., Demirhan, I., Miraloglu, M., Yalin, S. and Kurutas, E.B., 2023. |

Note: This is just an example table and is not an exhaustive list of drug candidates or in silico analysis methods used in the search for COVID-19 treatments. The results presented in this table should be validated by further experimental studies.