**Table 1 ACE2 Target Compound Screening (TCS) Results**

|  |  |  |  |
| --- | --- | --- | --- |
| Name | Rank | Drug Structure | Supporting Evidence In Literature |
| Trandolapril | 3 |  | (Jaberi-Douraki et al. 2021) conducted experiments that show Trandolapril is an ACE2 blocker with minimal pulmonary side effects. Trandolapril is also found in the top hits in the Computational prediction in (Kim et al. 2020). |
| Dimethyl Sulfoxide (DMSO) | 4 |  | (Ferreira et al. 2021) show that DMSO reduces the stability of SARS-Cov2 main protease with recommendations of its use in the treatment of Covid-19 patients and other viral infections (Hoang, Hoang, and Han 2020). |
| Adenosine Triphosphate | 6 |  | Remdesivir is a known SARS-COV-2 drug which is a prodrug of adenosine triphosphate (ATP)(Doyle 2020, 19). Efficient clinical outcome of Inhaled Adenosine Treatment in Hospitalized COVID-19 Patients has also been reported (Caracciolo et al. 2021). (Hashemian, Farhadi, and Velayati 2020, 19) provide direct evidence that Remdesivir is in a clinical trial for SARS-Cov2. There is also direct evidence of binding with ACE2 protein (Geiger et al. 2020; Senger et al. 2020; Xu et al. 2021). |
| Ramipril | 6 |  | Ramipril is also found in the top hits in the Computational prediction in (Kim et al. 2020) |
| N-Acetylglucosamine | 7 | . | Molecular Dynamic analysis shows binding of this compound with ACE2 (Baysal et al. 2021). An observational cohort study for hospitalized patients improves clinical outcomes of SARS-Cov-2 patients (Hassan 2021) |
| Perindopril | 7 |  | Found in the top hits in the Computational prediction in (Kim et al. 2020). |
| Sunitinib | 11 |  | Direct evidence of Sunitinib reducing the infection of SARS-CoV2 moderately by hindering ACE2 is reported in (P.-G. Wang et al. 2020). In vitro study shows that Sunitinib inhibits SARS-CoV2 viral site (Weisberg et al. 2020). |
| Glutathione | 36 |  | Glutathione implicated in affecting ACE2 binding in (Lana et al. 2021). |

**Table 2 Spike-SARS Target Compound Screening (TCS) Results**

|  |  |  |  |
| --- | --- | --- | --- |
| Name | Rank | Drug Structure | Supporting Evidence In Literature |
| N-Acetylglucosamine | 4 |  | Molecular Dynamic analysis shows binding with SARS-Cov-2 Spike Protein (Baysal et al. 2021). An observational cohort study for hospitalized patients improves clinical outcomes of SARS-Cov-2 patients (Hassan 2021) |
| Dimethyl Sulfoxide (DMSO) | 4 |  | (Ferreira et al. 2021) This shows that DMSO reduces the stability of SARS-Cov2 main protease. It is used for the treatment of Covid19 patients and other viral infections (Hoang, Hoang, and Han 2020). PDBID: 5R80 (below) showing DMSO bound to SARS-Cov-2 Spike protein |
| Adenosine Triphosphate | 6 |  | Remdesivir, a known SARS-COV-2 drug, is a prodrug of adenosine triphosphate (ATP)(Doyle 2020, 19).  Efficient clinical outcome of Inhaled Adenosine Treatment in Hospitalized COVID-19 Patients(Caracciolo et al. 2021)  (Hashemian, Farhadi, and Velayati 2020, 19) this review provides direct evidence that Remdesivir is in a clinical trial for the cure of SARS-Cov2.  Direct evidence of binding with Spike protein (Geiger et al. 2020; Senger et al. 2020; Xu et al. 2021). |
| Sunitinib | 6 |  | Direct evidence of Sunitinib reducing the infection of SARS-CoV2 moderately by hindering ACE2 (P.-G. Wang et al. 2020)  The in-vitro study shows that Sunitinib inhibits SARS-CoV2 viral site (Weisberg et al. 2020) |
| Nilotinib | 12 |  | Molecular Dynamic simulation of FDA-approved drugs shows that Nilotinib bind to SARS-Cov-2 Spike protein to restrict the viral site from binding with ACE2(Deganutti, Prischi, and Reynolds 2021)  Site-specific in combination with docking studies using FDA-Approved drugs proposed Nilotinib as an inhibitor of Main Protease of SARS-CoV2 (Singh et al. 2020)  Direct evidence of Nilotinib bind to Spike protein and SARS-CoV2 main protease (Murugan et al. 2020)  The in-vitro study shows tyrosine kinase inhibitors nilotinib inhibit SARS-CoV2 (Cagno et al. 2021) |
| Dasatinib | 12 |  | Serum antibody response study shows that Dastinib along with the combination of other kinase inhibitors for Spike inhibition (Kozak et al. 2021) |
| Sorafenib | 13 |  | The in-vitro study shows that Kinase inhibitor Sorafenib inhibits SARS-CoV2 viral infection(Weisberg et al. 2020) |
| Glutathione | 37 |  | Study of biological effects of glutathione for covid19 patients (Lana et al. 2021) |

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**Table 4 ACE2’s top 100 Compounds predicted by our proposed model**

|  |  |
| --- | --- |
| ACE2 Median Rank | ACE2Names |
| 1 | glycerol |
| 2 | dexfosfoserine |
| 3 | trandolapril |
| 4 | dimethyl sulfoxide |
| 6 | adenosine triphosphate |
| 6 | ramipril |
| 7 | N-Acetylglucosamine |
| 7 | perindopril |
| 8 | cysteine |
| 9 | cacodylic acid |
| 10 | glycine |
| 11 | sunitinib |
| 12 | mercaptamine |
| 15 | octanoic acid |
| 16 | 1-Octacosanol |
| 16 | diiodohydroxypropane |
| 17 | cetyl alcohol |
| 18 | docosanol |
| 18 | ferric hydroxide |
| 21 | xenon (127Xe) gas |
| 22 | Molybdenum Mo-99 |
| 23 | thallous chloride Tl-201 |
| 23 | glycolic acid |
| 23 | propylene glycol |
| 24 | dimercaprol |
| 25 | cystine |
| 27 | itramin tosilate |
| 29 | dasatinib |
| 30 | krypton (81mKr) gas |
| 30 | inositol |
| 31 | xenon |
| 32 | cholic acid |
| 34 | lactic acid |
| 34 | iodine |
| 35 | trichloroacetic acid |
| 35 | succimer |
| 36 | glutathione |
| 38 | glutamic acid |
| 38 | iodoform |
| 39 | xenon (133Xe) gas |
| 40 | mercuric amidochloride |
| 42 | glucose |
| 43 | galactose |
| 43 | iopydol |
| 44 | bromoform |
| 46 | vorinostat |
| 47 | dodecanoic acid |
| 47 | xylitol |
| 48 | docosanoic acid |
| 48 | sulfur hexafluoride |
| 48 | tetrachloroethylene |
| 49 | stearic acid |
| 49 | ethambutol |
| 52 | aminohydroxybutyric acid |
| 54 | cupric chloride |
| 55 | aluminium oxide |
| 57 | trichloroethylene |
| 58 | mercuric chloride |
| 62 | sorafenib |
| 62 | carbocloral |
| 62 | stannous fluoride |
| 63 | zinc oxide |
| 63 | imatinib |
| 64 | fomepizole |
| 65 | carbon tetrachloride |
| 67 | trometamol |
| 67 | migalastat |
| 68 | thiram |
| 69 | chromic chloride |
| 70 | glucose-1-phosphate |
| 73 | sucrose |
| 74 | algeldrate |
| 74 | fosfestrol |
| 74 | cupric oxide |
| 74 | ferrous chloride |
| 75 | methylpentynol |
| 76 | phenylalanine |
| 77 | lactose |
| 77 | perflunafene |
| 77 | mecysteine |
| 78 | maltose |
| 80 | symclosene |
| 81 | chloralodol |
| 83 | flurotyl |
| 83 | tribromoethanol |
| 84 | pyridoxal phosphate |
| 85 | unithiol |
| 86 | mercuric iodide |
| 87 | aspartic acid |
| 88 | mitolactol |
| 89 | phenol |
| 89 | mitobronitol |
| 90 | pentaerithrityl tetranitrate |
| 93 | pentaerythritol |
| 94 | streptozocin |
| 94 | fytic acid |
| 94 | propiolactone |
| 95 | isosorbide |
| 96 | moroxydine |

**Table 5 Sars-Cov-2 Spike protein’s top 100 Compounds predicted by our proposed model**

|  |  |
| --- | --- |
| Spike Median Rank | SpikeNames |
| 1 | glycerol |
| 2 | dexfosfoserine |
| 4 | N-Acetylglucosamine |
| 4 | dimethyl sulfoxide |
| 6 | sunitinib |
| 6 | adenosine triphosphate |
| 7 | glycine |
| 9 | cacodylic acid |
| 11 | cysteine |
| 11 | glutamic acid |
| 12 | dasatinib |
| 12 | nilotinib |
| 13 | mercaptamine |
| 13 | sorafenib |
| 14 | cetyl alcohol |
| 15 | docosanol |
| 16 | 1-Octacosanol |
| 20 | cystine |
| 21 | lovastatin |
| 23 | ferric hydroxide |
| 24 | Molybdenum Mo-99 |
| 24 | xenon (127Xe) gas |
| 25 | thallous chloride Tl-201 |
| 25 | glucose |
| 26 | itramin tosilate |
| 26 | galactose |
| 27 | glycolic acid |
| 28 | octanoic acid |
| 29 | trichloroacetic acid |
| 29 | diiodohydroxypropane |
| 30 | xenon |
| 35 | pyridoxal phosphate |
| 37 | aminohydroxybutyric acid |
| 37 | glutathione |
| 38 | iopydol |
| 38 | inositol |
| 40 | krypton (81mKr) gas |
| 41 | glucose-1-phosphate |
| 42 | mercuric amidochloride |
| 42 | streptozocin |
| 43 | dimercaprol |
| 43 | xenon (133Xe) gas |
| 44 | cholic acid |
| 44 | sucrose |
| 44 | voglibose |
| 47 | succimer |
| 48 | iodine |
| 49 | iodoform |
| 50 | lactic acid |
| 50 | lactose |
| 50 | propylene glycol |
| 51 | bromoform |
| 51 | maltose |
| 52 | imatinib |
| 53 | sulfur hexafluoride |
| 54 | stearic acid |
| 54 | aluminium oxide |
| 55 | docosanoic acid |
| 55 | fosfestrol |
| 56 | dodecanoic acid |
| 57 | phenol |
| 59 | propiolactone |
| 60 | aspartic acid |
| 62 | zinc oxide |
| 63 | aminolevulinic acid |
| 63 | mercuric chloride |
| 64 | erlotinib |
| 69 | xylitol |
| 69 | trometamol |
| 72 | fomepizole |
| 73 | migalastat |
| 74 | ethambutol |
| 75 | algeldrate |
| 77 | stannous fluoride |
| 79 | cupric chloride |
| 80 | flurotyl |
| 80 | fludeoxyglucose (18F) |
| 81 | carbon tetrachloride |
| 81 | perflunafene |
| 83 | carbocloral |
| 83 | symclosene |
| 85 | monoctanoin |
| 85 | tetrachloroethylene |
| 85 | thiram |
| 86 | norethisterone |
| 86 | phenelzine |
| 89 | trichloroethylene |
| 89 | mercuric iodide |
| 90 | fludarabine phosphate |
| 91 | chromic chloride |
| 91 | isosorbide |
| 93 | DL-Alanine |
| 94 | alanine |
| 94 | cupric oxide |
| 95 | mitolactol |
| 95 | chloralodol |
| 96 | pentaerythritol |
| 96 | mitobronitol |
| 96 | pentaerithrityl tetranitrate |