DETERMINATION OF POTENTIAL DRUG CANDIDATES FOR SARS-COV-2: PART 3

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1. **Cinametic acid**: a food additive approved by the FDA obtained from the cinnamon oil and other kind of plants. It is a neutraceutical with chemical formula C12H14O5. It is a cholinergic agent which is also use to test the function of the liver. Its PubChem CID is 6436159.

![Figure shows 2D structure of cinametic acid.](image)

2. **Doxycycline**: Doxycycline is an antibiotic with chemical formula C22H24N2O8 which is also used for the treatment of malaria. It is used to treat various disease caused by microbes – pneumonia, some infections of eye and skin, infections spread by mites, lice, ticks, infected animals, infections related to the genital, lymphatic and urinary system, also used to treat person having food poison and immune to penicillin, also to treat acne and pimples(Cunha BA, 1982). It was also proposed to use it with the combination of hydroxychloroquine or other medications for the treatment again COVID19 as it has properties of anti-viral and anti-inflammatory activities (Malek AE, 2020). Its PubChem ID is 54671203.

![Figure shows 2D structure of doxycycline.](image)
3. **Guaifenesin**: Guaifenesin is a FDA approved expectorant which is used to treat common cold and cough. Its chemical formula is C10H14O4. It increases the volume of secretion and decreases its viscosity in the bronchi and trachea, hence makes breathing easier (Albrecht HH, 2017). It has proposed that expectorant can be potential to treat COVID19 as it reduces the entry of microbes into the respiratory system by production of mucus in large quantity and also transport the trapped viruses into the stomach (Z., 2020). Its PubChem ID is 3516.

![Guaifenesin 2D structure](image1.png)

**Figures show 2D structure of guaifenesin.**

4. **Nabumetone**: Nabumetone is a FDA approved drug used to treat the rheumatic and inflammatory conditions. It is non-selective anti-inflammatory drug (NSAID) prodrug whose active state is 6-methoxy-2-naphthyl acetic acid and activates in the liver (Friedel HA, 1988). Its chemical formula is C15H16O2. Its PubChem ID is 4409.

![Nabumetone 2D structure](image2.png)

**Figure shows 2D structure of nabumetone**

5. **Nafcillin**: Nafcillin is a semi-synthetic antibiotic just like the penicillin. Its chemical formula is C21H22N2O5S. Its mechanism of action is also similar to the
penicillin but it is used to treat the penicillin resistant Staphylococci strains (Nafcillin., 2020). Its PubChem ID is 8982.

Figure shows 2D structure of nafcillin.

6. **Rutin**: Rutin is a bioflavanoid which is present in many fruits and vegetables such as buckwheat, grapes, apricots, grapefruit, cherries, plums, oranges and many more (Enogieru AB, 2018). Its chemical formula is C27H30O16. It is neuroceutical which shows many pharmacological activities such as anticarcinogenic, cytoprotective, antioxidant, cardioprotective, vasoprotective, and neuroprotective activities (Ganeshpurkar A, 2017). Its PubChem ID is 5280805.
7. **Ritonavir**: Ritonavir has been marketed in China and is commonly used to treat the HIV infections in mainly adults and children above 2 years of age. In vitro experimentations have depicted that ritonavir can inhibit the replication mechanism of SARS-CoV and MERS-CoV and thus, exerting anti-viral effects. This drug is listed under recommended drugs (anti-viral drug section) in the New Coronavirus Infected Pneumonia Diagnosis and Treatment Program (Wu, 2020). Its PubChem CID is 392622 and molecular formula is C37H48N6O5S2.

![Figure shows 2D structure of ritonavir.](image)

8. **Darunavir**: It is a HIV-1 protease nonpeptidic inhibitor and shows activity against HIV. Upon administering it orally, it targets selectively and binds to the active site of HIV-1 protease, thus inhibiting its dimerization and catalytic activity. Due to this, the proteolytic cleavage of polyproteins Gag and Gag-Pol is inhibited in HIV infected cells. Further, this leads to development of immature and non-infectious viral proteins that are not able to form mature virions and prevents HIV replication. Its molecular formula is: C27H37N3O7S and PubChem CID is 213039 (PubChem Compound Summary for CID 213039, Darunavir., 2021).
Figure shows 2D structure of Darunavir.

9. Lopinavir: It is an antiretroviral protease inhibitor which is used in the treatment of human immunodeficiency virus-1 (HIV-1) infection and acquired immunodeficiency syndrome (AIDS) in combination with ritonavir. It causes asymptomatic and transient elevations in serum aminotransferase levels. It retains activity against HIV protease with a Val 82 mutation. It is indicated in combination with other antiretrovirals for treating HIV-1 infection in adults and pediatric patients more than or equal to 14 days old. Its molecular weight is 628.8 g/mol, having chemical formula as C37H48N4O5 and PubChem CID is 92727 (PubChem Compound Summary for CID 92727, Lopinavir, 2021).

Figure shows the 2D structure of lopinavir.

10. Favipiravir: It is a broad spectrum antiviral drug which is used in the treatment of flu. The Shenzhen Health Commission has now initiated clinical studies on the use of favipiravir to treat SARS-CoV-2 infections. Its PubChem CID is 492405 and molecular formula is C5H4FN3O2. It is a pyrazinecarboxamide derivative with
activity against RNA viruses. It gets converted to ribofuranosyltriphosphate derivative by enzymes of the host and selectively binds the influenza viral RdRp (RNA-dependent RNA polymerases) (Wu, 2020).

Figure shows the 2D structure of favipiravir.

11. Ifenprodil: It is an N-methyl-D-aspartate (NDMA) receptor antagonist which is orally bioavailable, with neuroprotective, anti-inflammatory, central nervous system stimulating and anti-fibrotic activities. When administered, it targets and binds to glutamanergic NDMA receptors and also inhibits them, especially the glycine binding NDMA receptor subunit-1 and 2, thereby, preventing NDMAR signaling. It exerts its anti-inflammatory affect by its effect on NDMA and sigma-1 receptors. This agent decreases the infiltration of neutrophils and T-cells into the lungs and prevents the releasing of some pro-inflammatory cytokines, therefore, resulting in the reduction of the lung inflammatory response, inhibit fibrosis in the lungs and may reduce the severity of cough. Its PubChem CID is 3689 and molecular formula is C21H27NO2 (PubChem Compound Summary for CID 3689, Ifenprodil., 2021).

Figure shows the 2D structure of ifenprodil.