

## To know about 2019 Novel Coronavirus (2019 – nCoV)

### Key Facts:

1. 2019 Novel Coronavirus (2019-nCoV) is a virus (more specifically, a coronavirus) identified as the cause of an outburst of respiratory illness first spotted in Wuhan, China.
2. Right off the bat, a significant number of the patients in Wuhan, China reportedly had some link to a large seafood and animal market, signifying animal-to-person spread. Though, a rising patient's number allegedly have not had contact to animal markets, indicating person-to-person spread is occurring.

### Recent Updates:

- A. As per the report published in Worldometer, 10 additional cases confirmed on board the cruise ship in Japan
- B. Recently, 1 new case in the United States (Wisconsin)
- C. Newly, 3 new coronavirus cases in South Korea; 2 men had travelled to Singapore for conference.
- D. Currently, 4 new cases confirmed in Singapore, including a six-month-old child of an infected couple.
- E. As reported, 2 new cases in Malaysia, 1 new case in Australia (Queensland).
- F. As reported, 1 death reported from Tianjin, China: the patient had developed fever and cough after shopping in a department store on January 22. The patient had a history of type 2 diabetes and hypertension.

### Catastrophic Scenario:

- *As reported till 5<sup>th</sup> Feb 2020, Coronavirus Cases: **28,276** of which **3,863 (14%)** in critical condition*
- *Total No. of Deaths: **565**, Total Recovered Patients: **1,173***

### Incubation Period (Symptoms to Appear):

As few as 2 days the symptoms of the novel coronavirus (2019-nCoV) might appear as long as 14 days during this the virus is contagious showing asymptomatic transmission as the patient does not display any symptom.

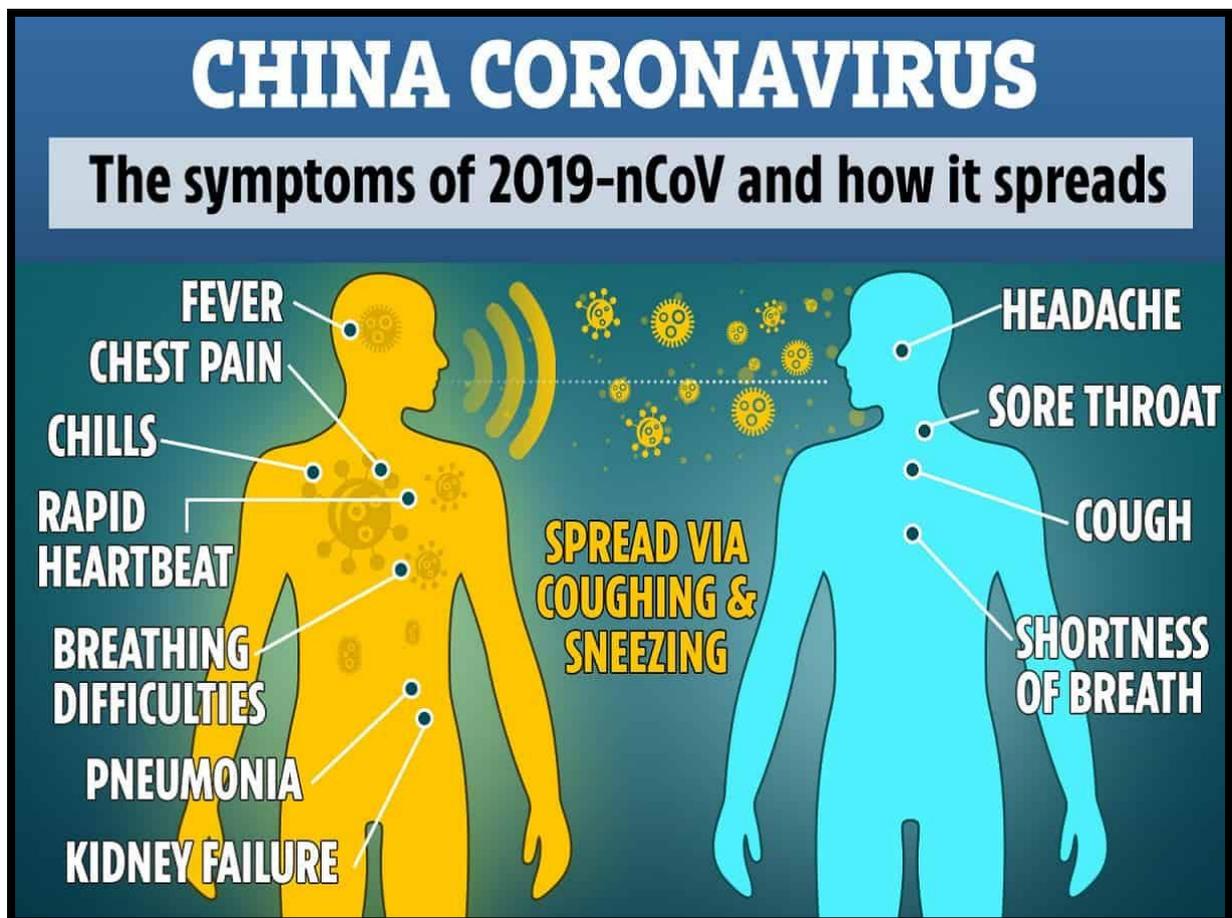
**Treatment and Precautions:** As per the global scenario, the preventive measures published by CDC is as follows

- Wash your hands often with soap and water for at least 20 seconds, especially after going to the bathroom; before eating; and after blowing your nose, coughing, or sneezing.
- If soap and water are not readily available, use an alcohol-based hand sanitizer with at least 60% alcohol. Always wash hands with soap and water if hands are visibly dirty.

- Avoid touching your eyes, nose, and mouth with unwashed hands.
- Avoid close contact with people who are sick.
- Stay home when you are sick.
- Cover your cough or sneeze with a tissue, then throw the tissue in the trash.
- Clean and disinfect frequently touched objects and surfaces using a regular household cleaning spray or wipe.

*For treatment purpose, no specific antiviral treatment recommended for 2019-nCoV infection. Precisely, **Remdesivir** (antiviral drug, nucleotide analog), producing by Gilead, is recently came in existence for the treatment and as report it is in trial phase in China.*

The Omics of (2019-nCoV):



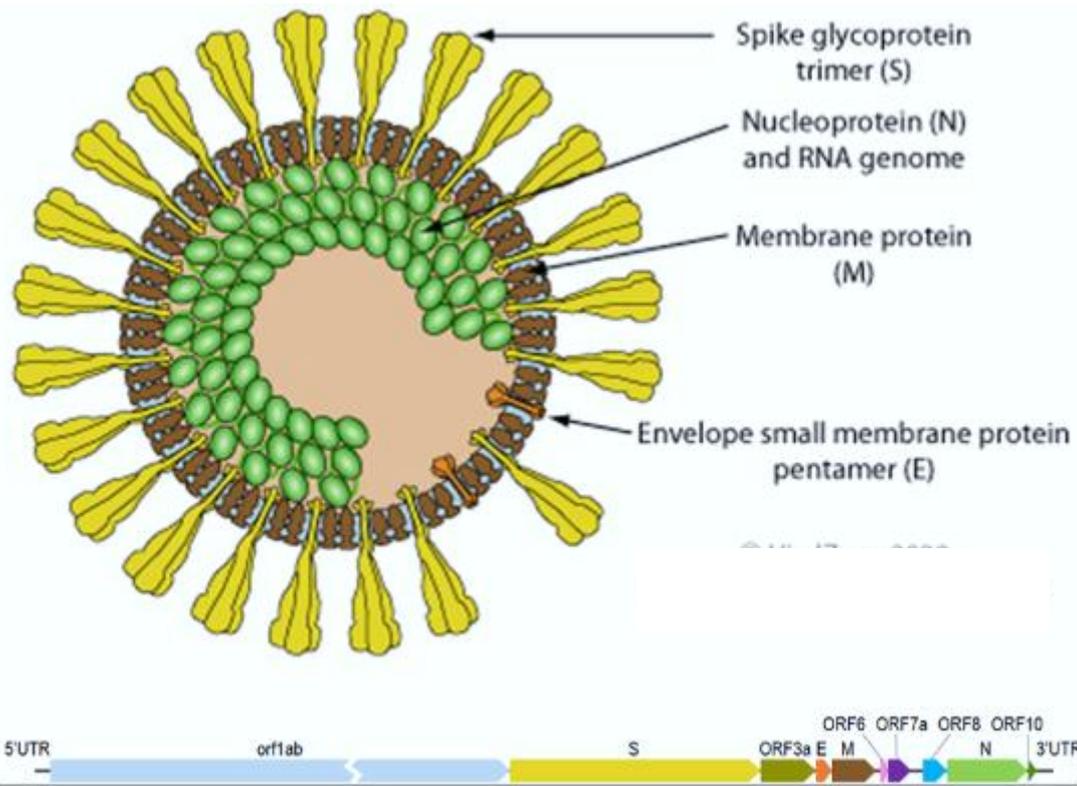


Figure showing 'Structure of Coronavirus' with all Open reading Frames

Coronaviridae Genome Statistics	
Genera	7
Species	1,039
Strains	27,016
3D Protein Structures (PDB)	579
Experimentally Determined Epitopes (IEDB)	5,672
Host Factor Experiments (NIAID Systems Biology, ViPR DBPs)	25
Mature Peptides	755
Proteins with Predicted Epitopes	79,240
Ortholog Groups	1,196
Total Genomes	32,900
Complete Genomes	3,087
Proteins	92,461

### Information about Coronaviridae

Figure showing Coronaviridae Genome Statistics (ViPR)

**Epidemiology:** It was first reported in Wuhan, China, in December 2019. The virus has rapidly spread to other regions of China and other countries, including Australia, Canada, France, Japan, Singapore, South Korea, Taiwan, Thailand, Vietnam, and the US, as in (ViPR)

**Clinical:** As Reported 2019-nCoV cases have ranged from no symptoms to severe pneumonia and death. Symptoms can include fever, cough, & squatness of breath, as in (ViPR)

## Scientific Study Suggested by AKS University:

Department of Biotechnology of AKS University had run a “Fast Track Computational Prediction Program” for Coronavirus (2019 – nCoV). The research panel decided to analyze the sequences and further move towards, homology modelling, structure validation and finalize the pipeline as molecular Docking. As treatment, the department of biotechnology had confirmed the biological role of **Cordycepin** (isolated from fungi – *Cordyceps militaris*), **Cordyceps** (*important traditional medicinal mushrooms*) is utilized to prevent coughs, chronic bronchitis, respiratory disorders, kidney disorders and anaemia. It was also suggested in reports that it helps in preventing male sexual problems, irregular heartbeat, high cholesterol, liver disorders and also prevent weight loss. It has been reported that Cordycepin shows anti-carcinogenic activity.

Research wing of department applied “Computational Prediction Model (CPM)” for Cordycepin to validate them acting as **potential inhibitor** for various structural and non-structural proteins of Coronavirus.

On the basis of structure predictions and energy calculations on different structural proteins (S, M, E proteins) mainly, Nucleocapsid N protein, main physical constituent of capsid, that fluxes RNA pack, links the capsid for envelope, helpful in processing viral replication and evasion of the immune system. M protein of coronavirus acts majorly in virus assembly and helpful in turning cellular films into platforms where virus and host factors converge to make new virus particles. ORF5 determined as *RNA Dependent RNA Polymerase* enzyme, enables viral RNA replications in host by virus.

Biotech. Dept. of AKS University, predicted with the help of CPM that Cordycepin is showing inhibition effects on (N, M, E and orf5) structural and non-structural proteins of Coronavirus. The FASTA format sequence were obtained from NCBI and further pipeline of (CPM) were followed to determine the docking and energy calculations. The detailed report were submitted to ‘The Lancet’.

S. No.	Parameters for CORDYCEPIN	Description
1	Accession Number	DB12156
2	Type	Small Molecule
3	Weight	Average: 251.2419 Mono-isotopic: 251.101839307
4	Chemical Formula	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>3</sub>
5	Water Solubility	11.3 mg/mL
6	Rule of Five	YES

Description of Cordycepin reported in Drugbank Database

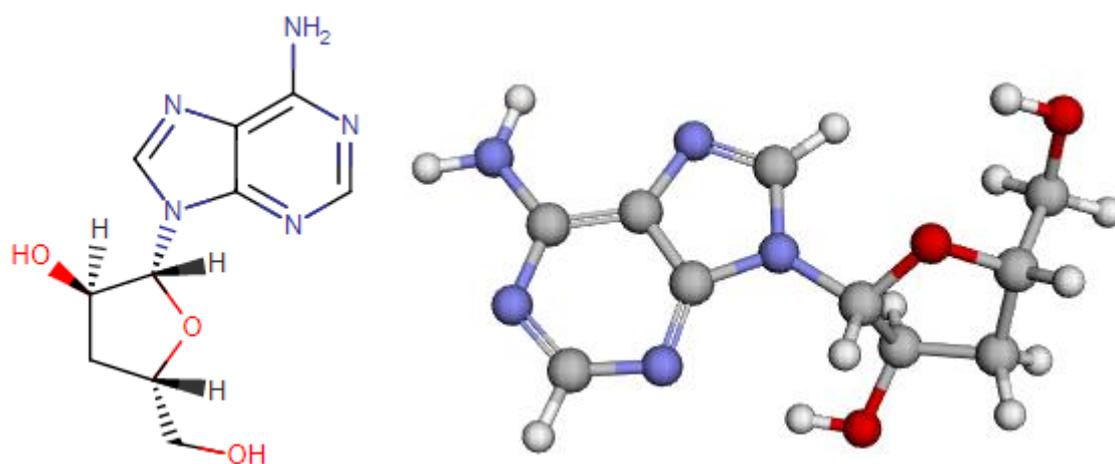


Figure representing 2D/3D structure of Cordycepin (DrugBank Database)

### Predicted Properties of Cordycepin:

PROPERTY	VALUE
Water Solubility	11.3 mg/mL
logP	-0.85
logP	-1.4
logS	-1.4
pKa (Strongest Acidic)	13.53
pKa (Strongest Basic)	4.99
Physiological Charge	0
Hydrogen Acceptor Count	7
Hydrogen Donor Count	3
Polar Surface Area	119.31 Å <sup>2</sup>
Rotatable Bond Count	2
Refractivity	62.1 m <sup>3</sup> ·mol <sup>-1</sup>
Polarizability	24.15 Å <sup>3</sup>
Number of Rings	3
Bioavailability	1
Rule of Five	Yes
Ghose Filter	No
Veber's Rule	No
MDDR-like Rule	No
Polar Surface Area	119.31 Å <sup>2</sup>
Rotatable Bond Count	2
Refractivity	62.1 m <sup>3</sup> ·mol <sup>-1</sup>
Polarizability	24.15 Å <sup>3</sup>

Predicted Properties of Cordycepin reported in Drugbank Database

Department of Biotechnology of AKS University, had made a useful step to setback the stone in leading research over Coronavirus majorly (2019-nCoV). The aim of department is to dedicate possibilities of conceptual research for scientists and to scientific communities so to utilize (mushrooms) *Cordyceps sp.* or its purine nucleoside antimetabolite (cordycepin) which has been known to have various pharmacological and therapeutic applications, especially, as far as human wellbeing making it a reasonable candidate as inhibitor to restrict the viral mechanism of Coronavirus.

## Contributions:

Department of Biotechnology, AKS University

Dr. Kamlesh Choure

Er. Arpit Srivastava

Mr. Shreyansh Parsai

Mr. Vivek Agnihotri

Mr. Saurabh Singh Gour