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Mathematical and Statistical Study on COVID19- SIR Model

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Method Article

Keywords: Covid19, SARS-COV-2, Random chain biopolymer, SP3 configuration, Molecular simulation, Exponential, Gaussian, Drug intermediate, Drug modeling, Quantum Chemistry, LCAO, Infection fatality rate, Logistic regression, Sigmoid model, Hydrodynamic modeling, Bio-polymer, First order kinetics, SIR compartmental model, p-value, Confidence limit (CI)

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MATHEMATICAL AND STATISTICAL STUDY ON COVID19 – SIR MODEL

Jaydip Datta

ABSTRACT -

In this combinatorial study let us try to simulate the four cases starting from viral spreading kinetics , Gaussian distribution of the infectious disease , mortality statistics like infection fatality ratio (IFR) with the distribution of age of the patient through sigmoid regression method approach and finally the most important modeling of remdesivir on the basis of Molecular bonding method (LCAO). It is an alternative approach to susceptibility – infectivity – recovery (SIR) model .

Keywords – Covid19 ,SARS-COV-2 ,Random chain biopolymer , SP3 configuration ,Molecular simulation , Exponential , Gaussian , Drug intermediate , Drug modeling , Quantum Chemistry , LCAO , Infection fatalality rate , Logistic regression , Sigmoid model , Hydrodynamic modeling , Bio-polymer , First order kinetics , SIR compartmental model , p-value , Confidence limit (CI) .

Literature review –

In my earlier work by ***Datta J*** I have reviewed the three basic mathematical modeling related to Covid19 pointing out exponential series , Gaussian distribution function of one dimension , Probability and Probability density function ,Linear combination of atomic orbital starting from wave function and area under the curve of Gaussian as well as flat Gaussian or Pseudo-Gaussian methods .The fourth work is in continuation of infection fatality rate (IFR) vs Age of ***Mallapaty S*** (Data Source) in different statistical angle of best fit analysis indication logistic or sigmoid probability.

Objective – The main objective of the composite modeling is to correlate the Gaussiun , Pseudo-Gaussiun function as susceptibility , Sigmoid function as spreading and Drug modelling as Recovery compertment of epidemiological SIR model .

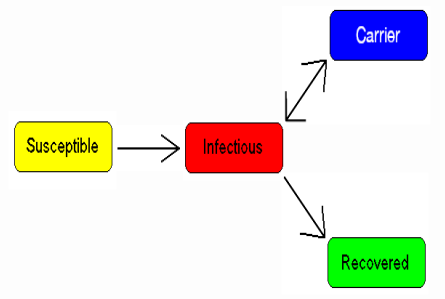
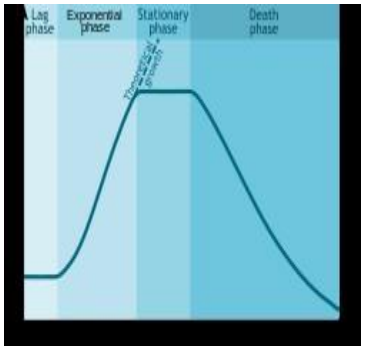


Figure Ref : en.encyclopedia.org

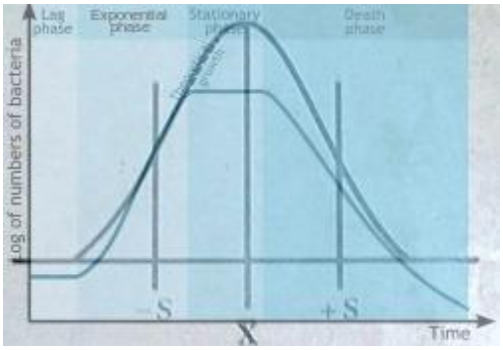
METHODOLOGY -

To start four cases will be discussed as per following order –
Case I – Viral spreading kinetic study :
Most of the microbes including virus should follow four stages namely - lag phase , LOG or exponential phase , stationary phase and death phase . Under this present case of Covid19 the exponential phase is more prominent for spreading of infection as well as sharp one .This exponential phase may be shifted to a flat one by a prolonged lock down may decrease the infection susceptibility. This type of Covid infection then enters to a prolonged static phase of 14days or more depending on mild to severe infection for symptomatic or asymptomatic patients . The declining or death phase will be mathematically an asymptotes ie infinite time will be required to irradiate to

susceptibility of infection .

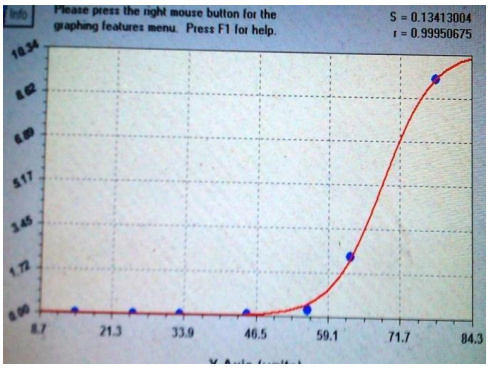


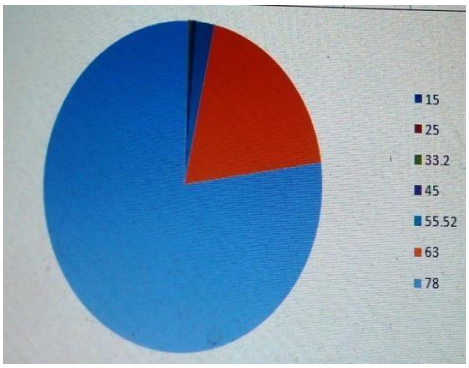
Case II – Viral spreading distribution study :
SARS-COV-2 being a virulent viral biopolymer (like other viruses) the distribution probability is a Gaussian one with conventional exponential phase generates a expo-gaussiun contour or pseudo Gaussiun contour ie why the the infective speed is uncontrollable , epidemic rather pandemic .



The Case I & Case II may be hypothised to susceptibility study of SARS-COV-2 infection.

Case III – Mortality statistics in terms of infection fatality rate (IFR) with age of the patients . The corresponding best fit analysis shows a logistic or sigmoid regression model. The sharp S rise of the model supports the conventional exponential phase .





The best fit analysis plot as well as excel pie chart shows the infectivity or fatality of infection probability vs Age . Obviously the inflection data changes from 46 yrs to an old age patient of more than 70 yrs are having much more prone to death.

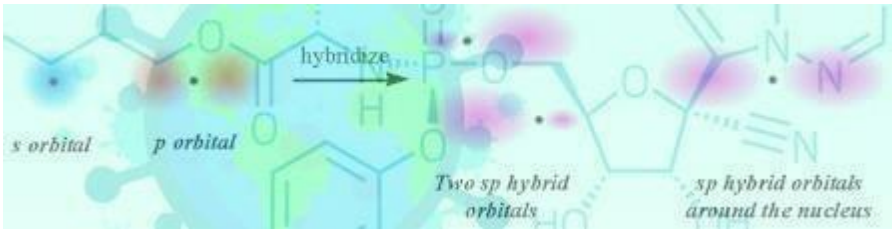
The Case III may be hypothised to infectivity study of SARS-COV-2 .

Cease IV :
It is related to novel drug modelling hypothesis of the most effective use of Covid19 antiviral like Remdesivir . In this hypothesis we will analyse the Linear combination of atomic orbital (LCAO) to overlap S -Orbital and P-Orbital to give rise to a hybrid Sp orbital having 50 % s and 50 % p – Character. Like S–Orbital – spherically symmetrical geometry like spike crown & Remedesivir the most potent synthetic -antiviral may be assumed to dumble shaped P-Orbital in geometry. Here Covid – Remedesivir drug – Protein [DP] intermediate may be considered SP hybridisation analogous to molecular bonding approach .The combined approach of pharmaco-kinetic stability - M.O approach can be simulated as Remdesivir – neucleocapsid protein complex as follows .

MOLECULAR SIMULATION STUDY :

A Combined Model for Covid19 (S-orbital) + Remedesivir (P-orbital)---------- →

Covid -Remedesivir (A SP Hybridized Model Hypothesis) .



Case IV may be hypothised to recovery modeling as a potent antiviral of SARS-COV-2 as mentioned above .

RESULTS -

Basically includes model equations & hypothesis in each case.

The exponential viral growh kinetics shows a Ist order kinetics as mentioned –
Ct = C0 * EXP (- K * t) ----------(1) [Case – I]

[Where C0 = Initial bacterial count, bacterial Colony Count (Ct) at time t & K = Ist order growth const & t= time of growth]

General mathematical expression of Gaussiun Probability distribution of biopolymer can be expressed as :
P (x)= A exp (- B * x ^ 2) .....(2)

A,B are constants depending on the physic-chemical properties of bio-polymer chain .

considering one dimension Gaussian probability P (x) ranging from - infinity to + infinity with mean distribution is zero .For two /three dimension the expression includes dimension factor . To find best fit analysis through Regression method the Gaussian fit is one of the useful one for hydrodynamic modelling of Covid19 considering the flow of viral infection through our blood .

The Gaussiun probality can be represented as randomisation of monomer chain of biopolymers (including virus like Covid19) (N=Number of Monomers vs Rrms = An Important Statistical parameters like Root mean square end to end separation as a F(X) of Radius of gyration (Rg) . The representative equation is as follows .The Rg of SARS-COV-2 biopolymer with a tremendous SP3 monomer leads to the virus more and more virulent as well as genetically recombinant .
P (N, x) = A * exp (- 0.042 * Rrms ^ 2)..... (3) [Case – II]

X = distribution chain length of random biopolymer coil

Rrms = Root mean square end to end separation of

bio-polymer chain .

Cuver finder V.1.4 run mode gives the best fit logistic

regression as bellow :

Y (IFR) = Sigmoid f [X(Age)] = [a / (1 + b* exp (-cx)] ---------(4) [Case –III]
a , b , c are the coefficients obtained from best fit analysis **.**
The equation (4) represents the desired model equation and the measure of a sigmoid probability of Covid infection with a significant correlation (r) value [0 < r < 1] .The pearson –coefficiant (r) in this case is 0.9995 with SE = 0.1341 , p < 0.00001 , CI > 95 % , with p < 0.05 makes the sigmoid statistics more significant .

Hypothesis regarding Remdesivir antiviral drug-neucleocapsid protein of Covid19 –Quantum Molecular bonding approach of drug-design. (Case –IV)

The Theorem of Normalisation - Integration of Shi (Shi *)dV = Unity . Very useful in quantum chemistry. dv = volume element for a probability Shi*Shi .Considering Covid19 as an uniform sphere we can compare with the spherical symmetrical s - Orbital in Atomic structure . Wave particle duality hypothesis assumes a wave nature for quick viral spreading as well as crown like particle . We can apply the probability density theory on s - Orbital where dv = 4/3 * pie * R^3 .
Applying Cylindrical polar symmetry on spike crown (R, Theta , Phi) - The cylindrical probability can be calculated as usual.
Now considering Remedesivir as p-orbital , we can assume the [Drug- Protein] Complex as SP hybridisation for linear overlap .

The modelling relationship from LCAO (Linear combination of Atomic Orbital) –
Shi (Covid19) + Shi (Remedesivir) = Shi (Drug- Protein Intermediate) . [Where Shi represents the Corresponding wave functional probability] correlating the stability of [R-P] complex intermediate through the approach of molecular bonding .

CONCLUSION –

Between four cases I – II (may be simulated as **Susceptibility** , case-III may be simulated as **Infectivity** of Covid19 and IV may be considered as probability of Remdesivir- Covid19 complex resulting **Recovery approach** of the patient .It is an alternative approach to study SIR model .

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Figures

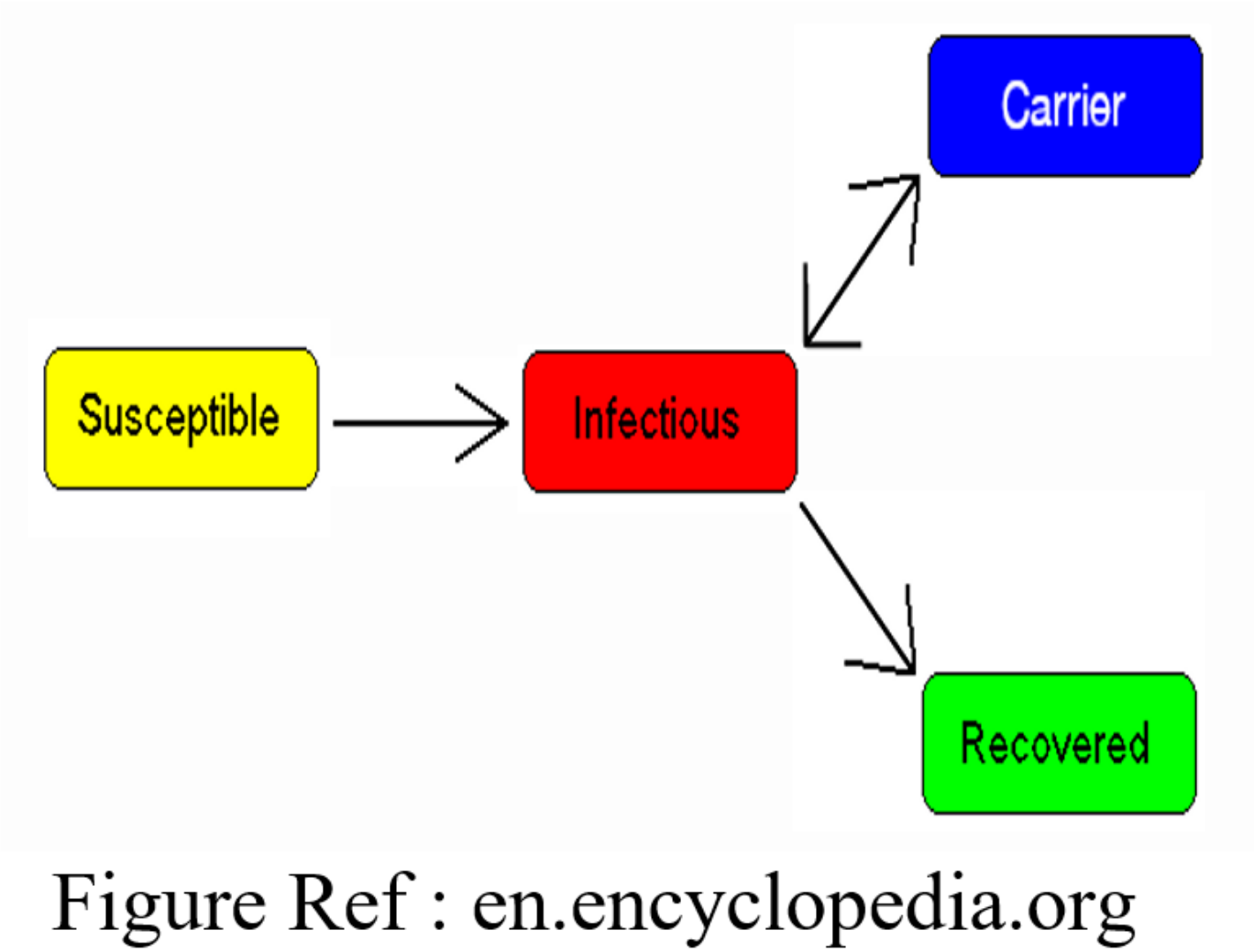


Figure 1

The main objective of the composite modeling is to correlate the Gaussiun, Pseudo-Gaussiun function as susceptibility, Sigmoid function as spreading and Drug modelling as Recovery compertment of epidemiological SIR model.

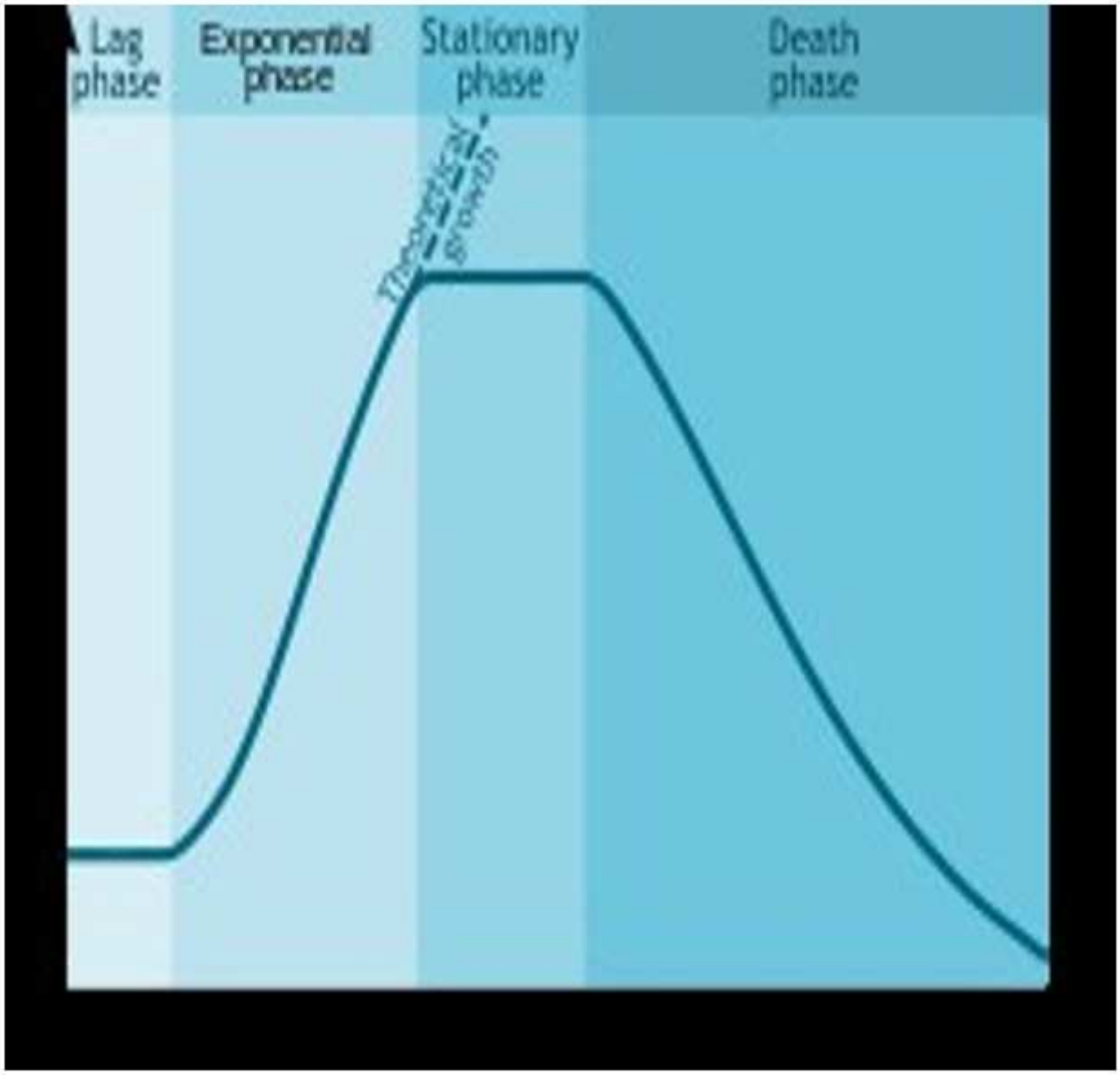


Figure 2

Case I – Viral spreading kinetic study

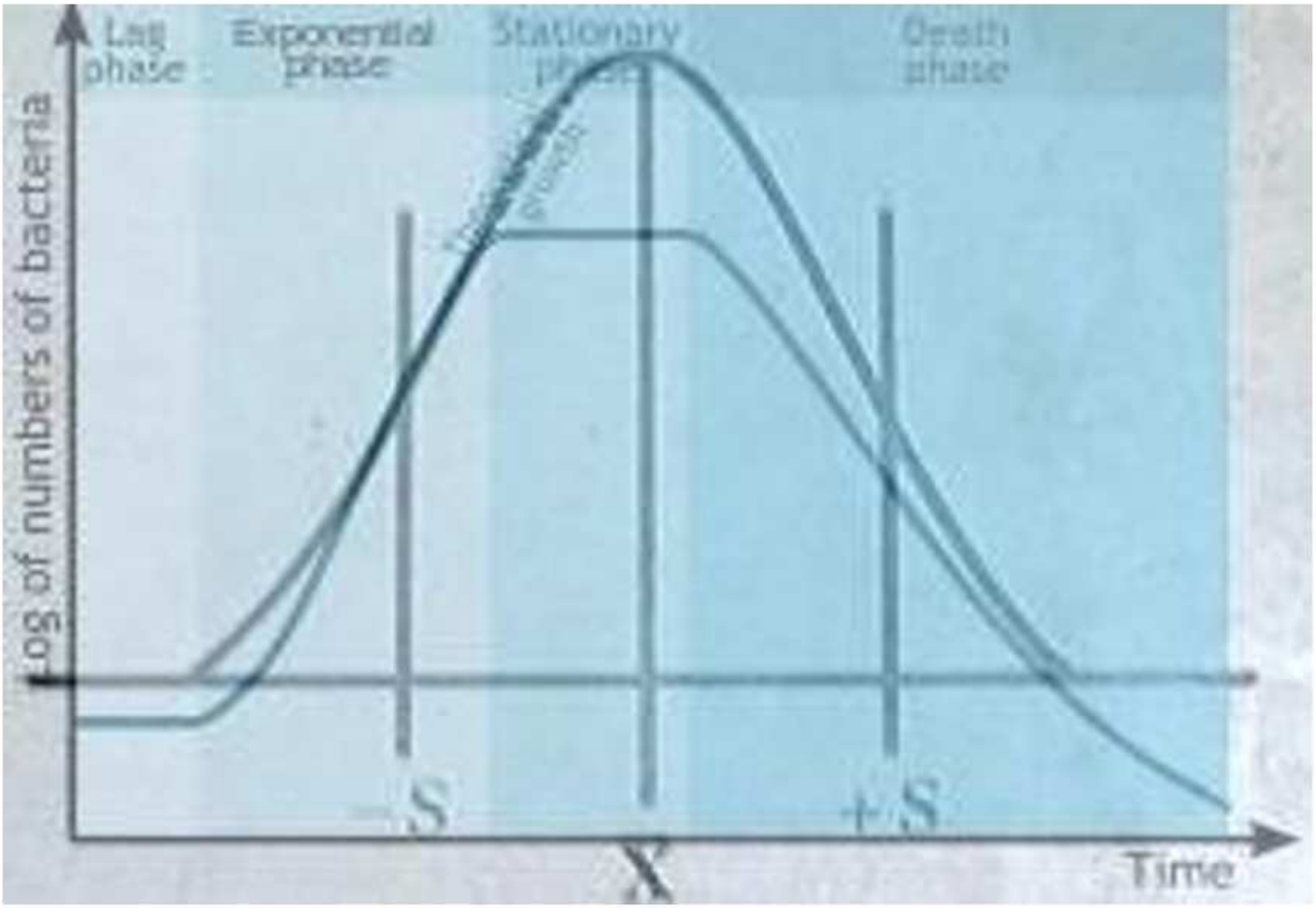
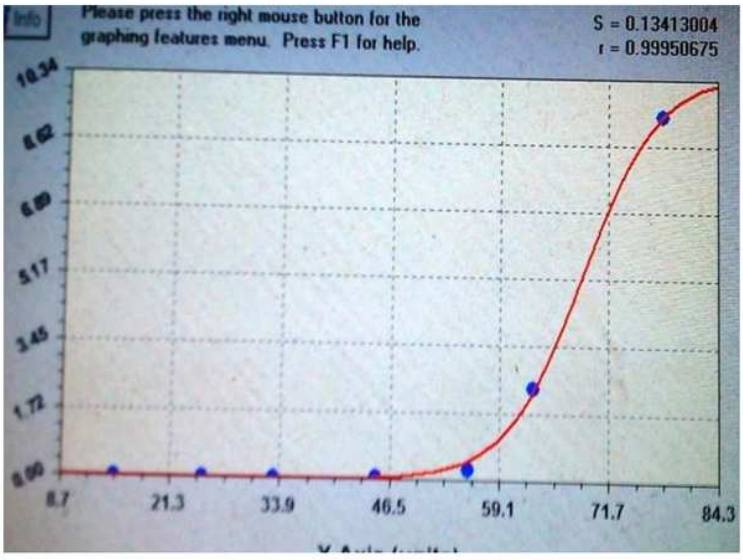


Figure 3

Case II – Viral spreading distribution study



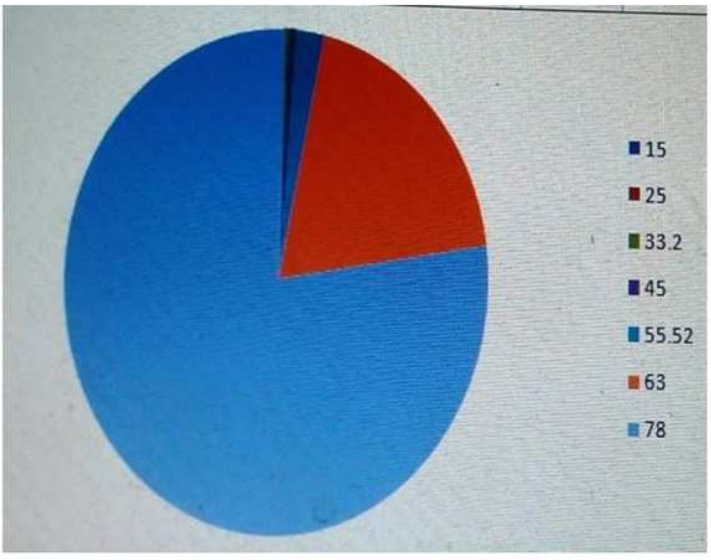


Figure 4

Case III – Mortality statistics in terms of infection fatality rate (IFR) with age of the patients.

Figure 5

Molecular Simulation Study

Supplementary Files

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- Supplymentaryfile.pdf