

Proteomic Analysis and Molecular Dynamics Simulation of Effect of Surfactants on SARS–Cov–2 Implications

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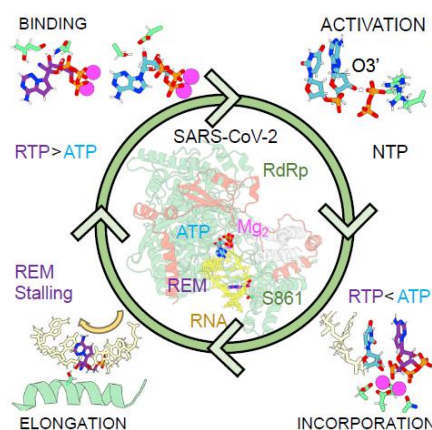
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Abstract



Graphical Abstract

Given that employees in petrochemical industries are exposed to various pollutants and are exposed to serious risks, the need for a comprehensive risk assessment program to determine hazardous chemicals that affect the health of exposed individuals and also to determine hazardous processes and tasks seems essential. Study Method: This cross-sectional-case study was conducted in 3 stages. The first stage included identifying hazardous substances and determining the risk factor of chemicals, the second stage included assessing exposure to benzene, and the third stage included estimating the relative risk of COVID-19 due to exposure to benzene through epidemiological studies. Findings: According to the risk assessment method, 40 chemicals were identified in the entire petrochemical company studied. Benzene was introduced as the most hazardous chemical. The results of the second stage showed that people in the main site during the noon shift and in the aromatic site with an average exposure of 4.29 ppm had the highest exposure to benzene. According to the results of the estimation stage of relative risk of COVID-19 in exposure to benzene, the highest relative risk in workers at my site was found to be related to workers in the aromatic unit, who had a cumulative exposure of 149.4 ppm-years (ppm-years) and a relative risk of 3.2. The statistical test result also showed that there was a significant relationship between the level of exposure to benzene and different work groups ($P < 0.001$). Discussion and Conclusion: This study showed that benzene achieved a risk level of 5 with a risk coefficient of 4.5–5, indicating that corrective measures for this highly hazardous and carcinogenic chemical should be initiated as soon as possible. Schematic of the mechanism analysis and impact of the COVID-19 pandemic and outbreak on petrochemistry and petroleum mechanics.

Keywords: Risk Assessment, Benzene, COVID-19.

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INTRODUCTION

According to studies, living in residential areas adjacent to petrochemical industries increases the risk of COVID-19. These pollutants also cause fertility problems, sterilization, miscarriage, and birth of babies with genetic defects. Oil Knowledge: According to studies and scientific documentation presented in recent years, petrochemical-related industries produce various types of pollutants that are released into the environment in the form of gas, particles, sludge, and liquid effluents [1–23]. These pollutants include polycyclic aromatic hydrocarbons (PAHs), heavy metals, benzene and its derivatives, sulfur dioxide, nitrogen dioxide, hydrogen sulfide, carbon monoxide, and other chemicals, most of which are toxic even at low concentrations and can have irreversible adverse effects on the ecosystem, environment, and human health. So far, various statistics have been presented on the level of various pollutants in the *Southern California Petroleum* region (Southern California) and its side effects on human health and the ecosystem, which sometimes cause concern for people, officials and people working in this region [24–45]. In fact, the statistics presented in the most optimistic form reflect the fact that currently the level of pollutants in this region is at the warning level [46–76]. Although raising these issues may be a little worrying, it is better not to be afraid of saying or hearing the truth, but rather to prevent the crisis from occurring with thinking, decisions and preventive measures. Therefore, it is necessary to conduct comprehensive studies in the field of examining the level of pollutants. Petrochemical industry pollutants enter the body through breathing, eating, drinking or absorption through the skin [77–84]. In this regard, the amount of these pollutants in the air, food and drinks is measured. Different people show different biological responses to a specific pollutant [85–99]. Some people may be exposed to a chemical and never be harmed, while others may be sensitive and become ill quickly. Sometimes, illness only occurs when people are exposed to a pollutant for a long time [100–110]. An important point to note is that pollutants may not directly cause or spread disease, but they may increase the risk of disease through the biological changes they cause in the body [111–121]. Although petrochemical pollutants may not cause disease in the short term, they certainly increase the risk of developing a variety of diseases [122, 123]. Therefore, it is necessary to evaluate the health status of people exposed to these pollutants through long-term studies using modern molecular medicine technologies [124]. One of the most effective strategies available for long-term study of health status and examination of the risk factors and biomarkers specific to diseases associated with pollutants from petrochemical industries is to launch cohort studies and establish biobanks [125–144]. Cohort studies give us the opportunity to assess the health status of a large population of people exposed to pollutants over a long period of time, for example, twenty years or more [145–150]. Today, the establishment of a biobank is recognized as one of the

top ten technologies in the world that has the greatest contribution to improving the health of society [151–159]. The development of a biobank for the long-term storage of biological samples related to workers working in polluted areas makes it possible to carefully monitor the biological changes and developments of these people's bodies over the long term. [160–170].

RESULTS AND DISCUSSION

According to studies, living in residential areas adjacent to petrochemical industries increases the risk of COVID-19. These pollutants also cause fertility problems, infertility, miscarriages and the birth of babies with genetic defects. According to a study published in the scientific journal *The Lancet* (2013), people exposed to pollutants from petrochemical industries have a lower life expectancy (which is considered an important health indicator) than people living in areas with an agricultural economy. Despite concerns about the possible effects of pollutants related to petrochemical industries on human health, unfortunately, no comprehensive studies have been conducted to examine the effects of pollutants from petrochemical industries on the health of workers and employees working in petrochemical complexes and people living in areas close to these industries. In a study prepared by a native student of *Southern California Petroleum* (2014) and presented at the Second National Conference on Environmental Hazards, the conclusion was that pollutants from petrochemical industries have affected the physical and mental health of some people in *Southern California Petroleum*. Therefore, it is necessary to first examine the health status of people working in petrochemicals and related industries, and then, based on the level of exposure, the people living in areas close to these industries. Today, it has become clear that general medical examinations and continuous biochemical tests cannot accurately determine the risk of factors and factors affecting the spread of diseases. Therefore, in order to predict or identify various diseases early, we are forced to use advanced technologies, especially "omics" technologies, including "genomics", "proteomics", "metabolomics", "epigenomics" and "transcriptomics". These technologies allow us to determine the risk factors for various diseases at the level of DNA, protein, metabolite and RNA (genome). Today, the category of personalized medicine is considered one of the most important and effective discussions in modern medicine to increase therapeutic efficiency and reduce side effects in the diagnosis and treatment process. Different people show different responses to different pollutants depending on their genetic profile. In fact, the level of resistance or sensitivity of different people to pollutants depends on their genetic profile, mutations or specific polymorphisms of their genes. On the other hand, it has been determined that people show different responses to drugs based on their genetic profile. Before 2007, scientists believed that a limited number of genes were effective in determining the function of drugs in the body and the body's response to drugs, and the science of "pharmacogenetics" was

formed based on this belief. In late 2007, genome-wide association (GWA) studies showed that a large number of genes are involved in this process, and the science of “pharmacogenomics” was introduced. Since pollutants from the petrochemical industry can cause chromosomal instability and widespread genetic mutations, it is necessary to study the “genomic” or at least “exome” profiles of exposed individuals. “Exome” or “genomic”

sequencing helps to determine the risk of genetic factors affecting the occurrence or spread of diseases. This approach also identifies disease-specific genetic “biomarkers” and determines who is vulnerable or resistant to pollutants and quantitatively determines the likelihood of individuals developing various diseases (Figures 1–6).

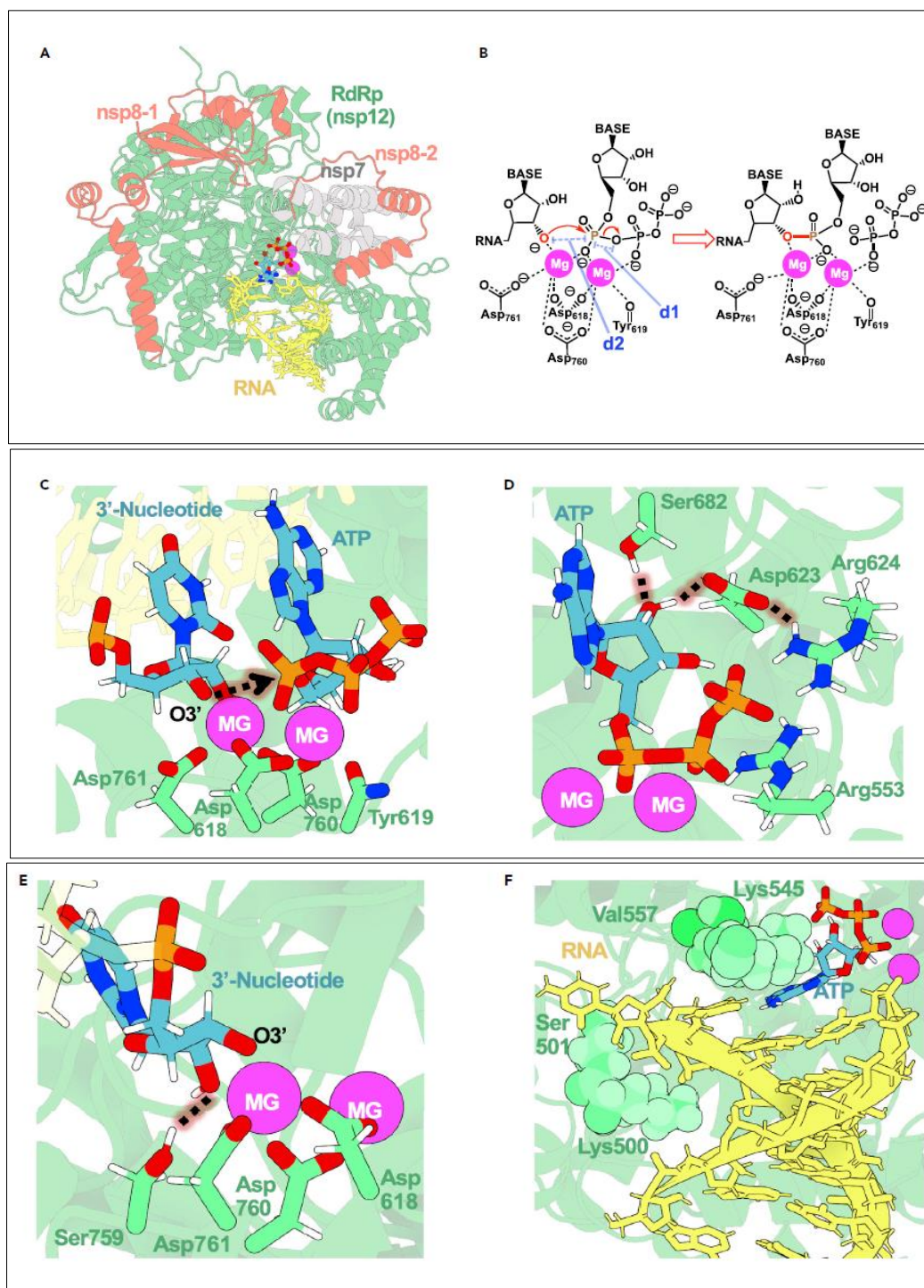


Figure 1: Active site of SARS-CoV-2 RdRp makes it an efficient polymerase

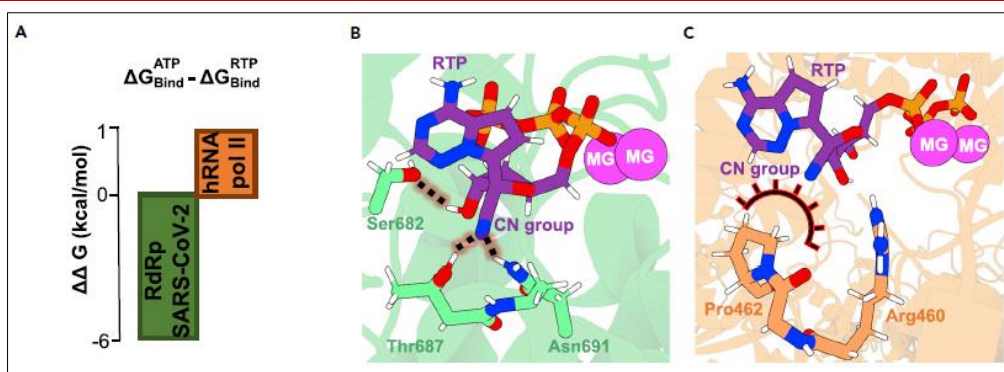


Figure 2: Binding preferences in viral and human RNA polymerases

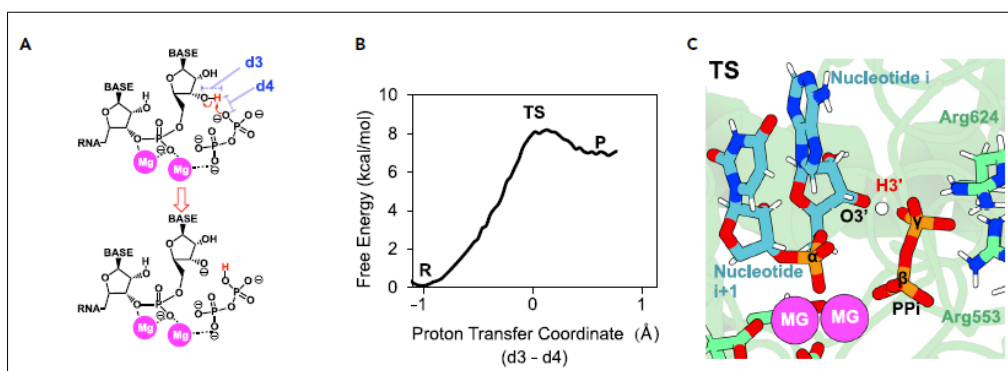


Figure 3: Mechanism of activation through O3' deprotonation inside RdRp

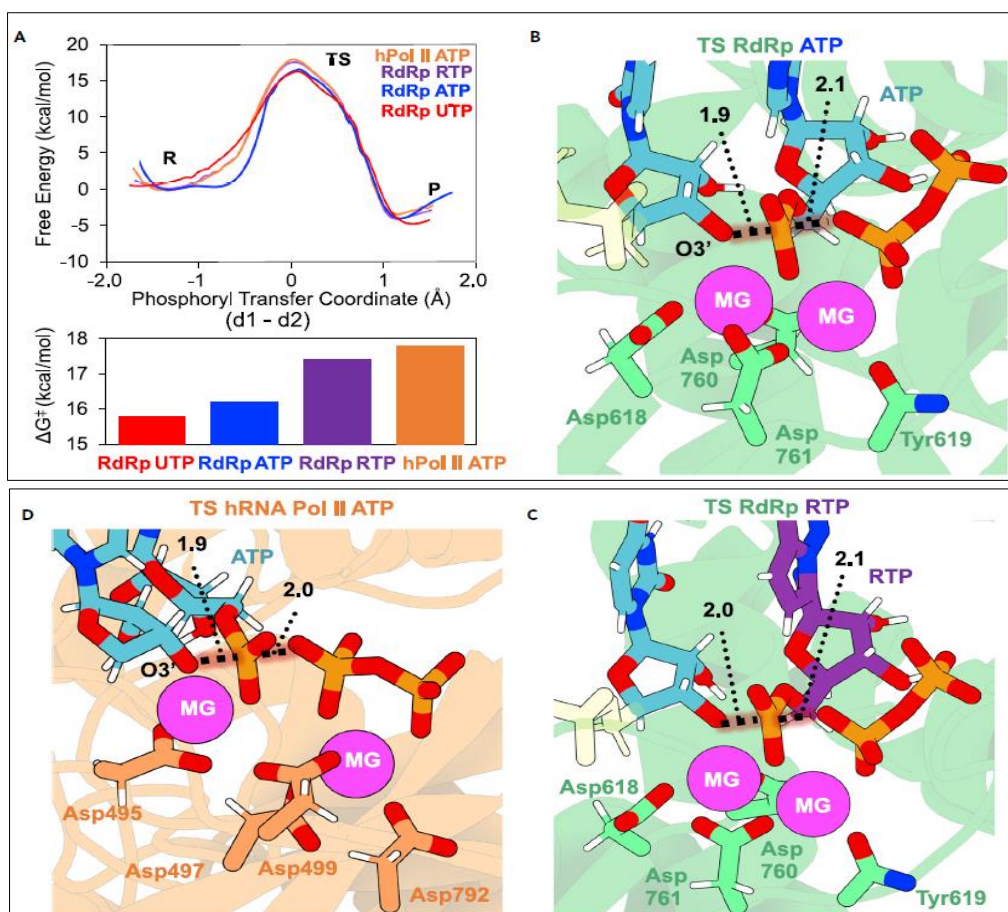


Figure 4: RNA elongation inside RdRp of SARS-CoV-2 and human RNA Pol II

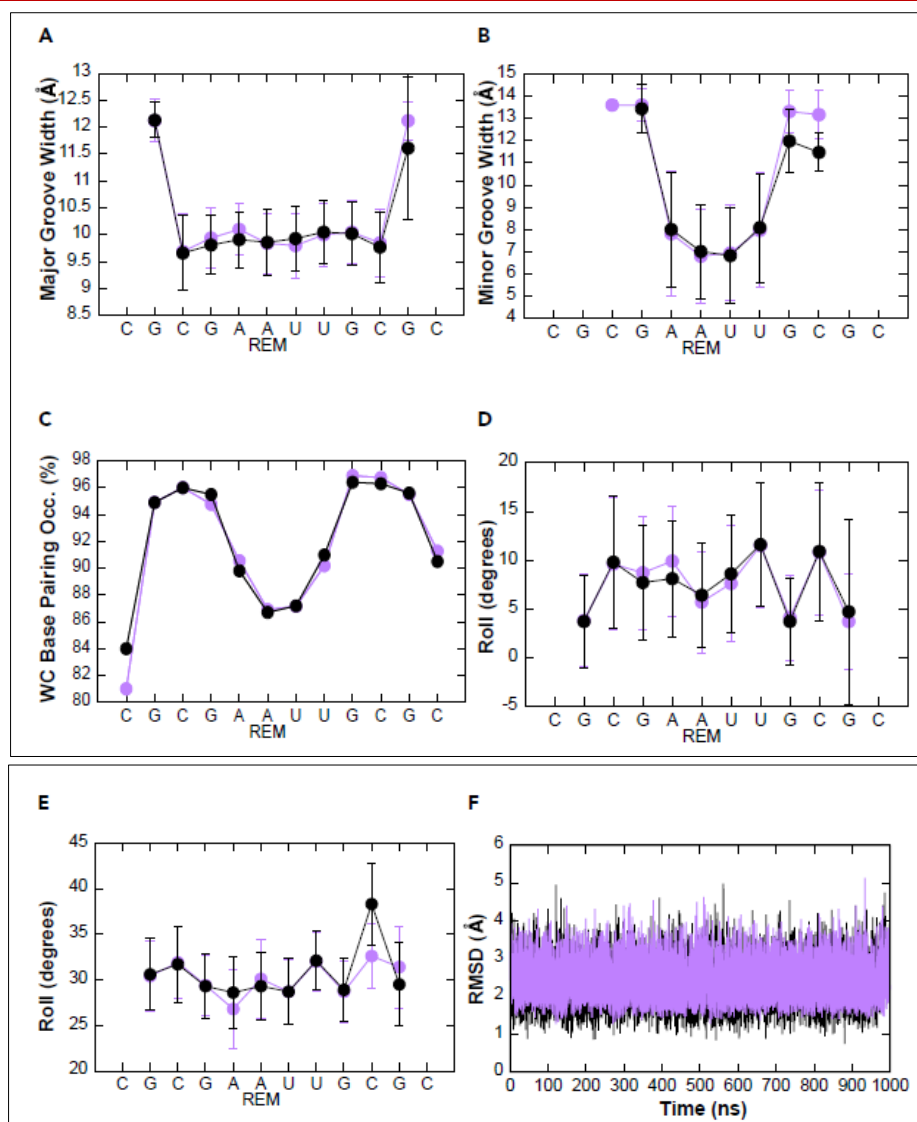


Figure 5: Remdesivir does not distort RNA structure

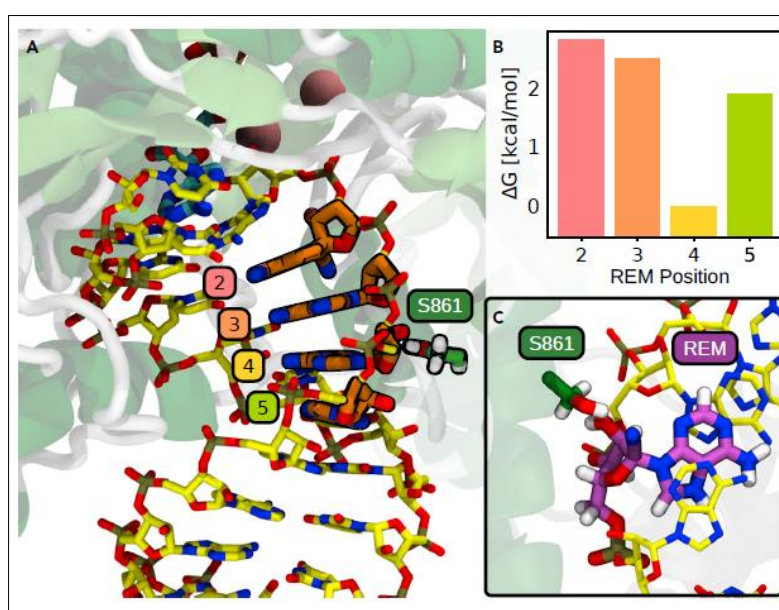


Figure 6: Remdesivir elongation along RdRp's exit channel

CONCLUSIONS

Petrochemical products are all compounds that can be obtained from oil refineries. Petrochemical industries play a vital role in the food, pharmaceutical, agricultural and technological industries and, in general, the national economy. However, environmental issues have received special attention today due to the harmful effects of chemical emissions. Chemical emissions may be due to improper production processes, incorrect storage methods and problems related to the operation process. Plastics and microplastics, volatile organic compounds, acid rain, oil spills, waste oil and pure water discharge are some of these environmental pollutants. In addition, petrochemical products cause acute and chronic diseases in living organisms such as allergies, COVID-19 and liver and kidney problems. Therefore, in recent years, measures such as providing subsidies for renewable energies, using clean energies such as biodiesel and biomass, as well as using technology to reduce safety and health risks caused by petrochemical products have been considered in different countries. In this review, problems related to petrochemical industries and their products are discussed and alternative solutions are presented.

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