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IDENTIFICATION OF SMALL MOLECULE INHIBITORS OF *DESULFOBACTER POSTGATEI* FOR SCALE PREVENTION IN OIL AND GAS WELLS

Abdulmujeeb T. Onawole[1], Hassan I. Nimir[2], Ibnelwaleed A. Hussein[1], Musa E.M. Ahmed[1], Mohammed A. Saad[3]

[1]Gas Processing Center, College of Engineering, PO Box 2713, Qatar University, Doha, Qatar
[2]Chemistry Department, College of Arts and Sciences, Qatar University, Doha, Qatar
[3]Chemical Engineering Department, College of Engineering, PO Box 2713, Qatar University, Doha, Qatar

Sulphate-reducing bacteria (SRB) such as *Desulfobacter postgatei* are often found in oil and gas wells. However, they lead to the release of hydrogen sulfide which in turn leads to the formation of iron sulfide scales. ATP sulfurylase is an enzyme present in SRB which catalyzes the which catalyzes the formation of adenylyl sulfate (APS) and inorganic pyrophosphatase (PPi) from ATP and sulfate which is one of the first steps in hydrogen sulfide production by *D. postgatei*. In the absence of a crystal structure, a homology model was designed for ATP sulfurylase using its genomic sequence. Consensus scoring which combined the virtual screening results from both molecular docking and machine learning was used in identifying three potential inhibitors of ATP sulfurylase from a database of about 40 million compounds. These selected hits are-(S,E)-1-(4-methoxyphenyl)-3-(9-((m-tolylimino)methyl)-9,10-dihydroanthracen-9-yl)pyrrolidine-2,5-dione; methyl 2-[(1S)-5-cyano-2-imino-1-(4-phenylthiazol-2-yl)-3-azaspiro[5.5]undec-4-en-4-yl]sulfanyl] acetate and (4S)-4-(3-chloro-4-hydroxy-phenyl)-1-(6-hydroxypyridazin-3-yl)-3-methyl-4,5-dihydropyrazolo[3,4-b]pyridin-6-ol and hence would be known as compounds A, B and C respectively. The molecular docking results showed that all the compounds have negative binding energies, with compound A having the highest docking score. However, based on the physicochemical and toxicological properties, compound C was the best choice has it does not violate any of the requirements that relate to absorption and distribution. Only compound C was predicted to be both safe and effective as a potential inhibitor of ATP sulfurylase. The binding mode of compound C revealed favorable interactions with the amino residues LEU 213, ASP 308, ARG 307, TRP 347, LEU 224, GLN 212, MET211 and HIS 309. Inhibition of this enzyme is expected to significantly reduce the formation of hydrogen sulfide and consequently prevent scale formation in oil and gas wells.

Biography

ABDULMUJEEB T. ONAWOLE recently completed his master's degree at the King Fahd University of Petroleum and Minerals, Saudi Arabia. He is currently a researcher at the Gas Processing Center, Qatar University, where he is working on applying computational chemistry and biology techniques in solving the challenges facing the oil and gas industry. He published about 10 papers in reputed journals during his master's degree program.

a.onawole@qu.edu.qa