Computational engineering of efficient enzyme catalysts for biodesulfurization of sour crude oil through 4S pathway

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In the last decades, the 4S metabolic pathway of bacterium *Rhodococcus erythropolis* strain IGTS8 has been discussed as an efficient and greener way to desulfurize organic sulfur compounds without degrading their carbon skeleton. This alternative is increadibly appealing as about 70% of the crude oil available worldwide is rich in organic sulfur compounds (mercaptans, thiols, sulfides, disulfides and thiophenes) that lead to high emissions of sulfur oxides (SO_X) after combustion, with repercussions in environment, health and industrial maintenance. More importantly, as regulatory agencies now demand for lower sulfur content fuels, we lack efficient methods to remove the abundant dibenzothiophene (DBT) and its alkylated derivatives. Two enzymes are referred to be the bottleneck of the 4S pathway: the $FMNH_2$-dependent monooxygenase DszC (k_{cat} = 1.6±0.3 min^{-1}, K_M = 1.4±0.3 μM) and the desulfinase DszB (k_{cat} = 1.7±0.2 min^{-1}, K_M = 1.3±0.3 μM).[1] Since the rate of the pathway has to be increased at least 500 fold to be of use in oil refining plants, we have been studying the reaction mechanism of these enzymes and attempted rational enzyme engineering protocols aiming at DszC and DszB, combining hybrid quantum mechanics/molecular mechanics methods and molecular dynamics simulations.[2-4]

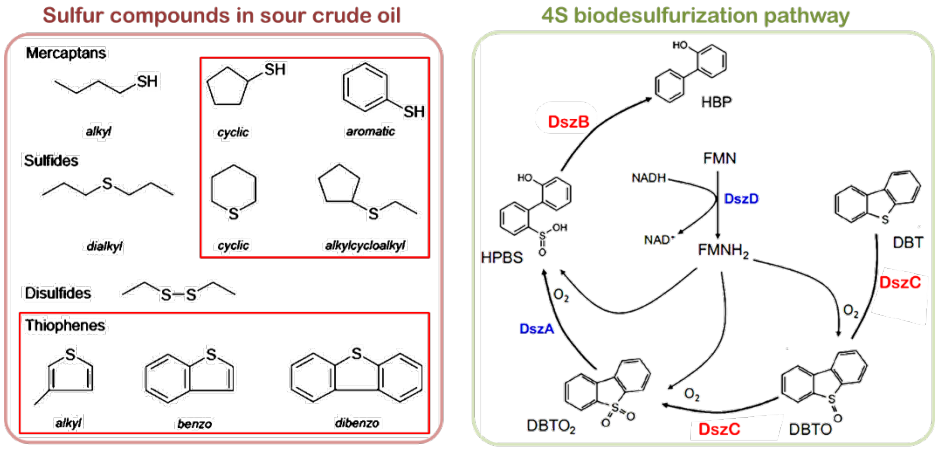

Figure 1: On the left, most common sulfur-containing organic molecules in sour crude oil, with the most abundant highlighted in red. On the right, depiction of 4S pathway, with the rate-limiting enzymes highlighted in red.

References

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