

Abstract

Data Science Framework to Select Corrosion Inhibitors [†]

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Organic corrosion inhibitors embedded in coatings play a crucial role in substituting for traditional anti-corrosion pigments, which can cause acute toxicity problems to human health and the environment. However, it is still not well understood why some organic compounds inhibit corrosion and others do not. Therefore, we are currently developing two complementary technological approaches to help corrosion scientists and engineers working in academia and across different industries choose the optimal inhibitor for each specific problem. We (1) build an interactive exploratory data tool for the selection of the ideal corrosion inhibitor, taking into account different conditions (type of alloy, electrolyte, pH, etc.) based on previously published information (<https://datacor.shinyapps.io/cordata/> accessed on 7 May 2021), and (2) develop machine learning models and an online tool to perform an initial virtual screen of potential molecules for the design of more efficient organic corrosion inhibitors [1]. These two approaches will contribute to the digitalization of the search for inhibitors, helping to speed up research in corrosion science and tailor corrosion-protective technologies in a more efficient and condition specific manner.

Supplementary Materials: The conference poster is available at <https://www.mdpi.com/article/10.3390/CMDWC2021-09935/s1>.

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