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## Exploring Beneficial Structural Features of Ionic Surfactants for Wettability Alteration of Carbonate Rocks using QSPR Modeling Technique

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### Abstract

Surfactant induced wettability alteration of reservoir rocks is an efficient process that enhances oil recovery of carbonate reservoirs. Finding a suitable surfactant for such a process is an interesting challenge in petroleum industry. To this purpose, generating a database of surfactant properties would be a good idea but property measurement of hundreds of surfactants and then screening them is a highly time consuming and expensive method. Therefore, the application of a mathematical model for prediction of surfactant properties may well be so helpful for our purpose. Quantitative structure-property relationship (QSPR) is a mathematical model that relates a specific property of materials to their structural characteristics. For the sake of QSPR modeling a dataset of 24 structurally different surfactants was created through the measurement of contact angles (as the most important surfactant characteristic in the wettability alteration process). Contact angle measurement was carried out through imaging a drop of n-decane as the model oil resting on a carbonate rock which has spent 2 days immersed in surfactant solution. For this dataset a linear QSPR model of oil contact angle on carbonate rocks was derived using genetic algorithm based on multi-linear regression (GA-MLR) and verified by

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