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Determination of boiling point of petrochemicals by gas chromatography-mass spectrometry and multivariate regression analysis of structural activity relationship

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The utility of petroleum is highly dependent on its boiling point (BP), necessitating the need for the development of analytical techniques, capable of crude oil separation into its various components. Accurate understanding of analyte boiling points (BP) is therefore of critical importance in separation science and crude oil refinery operation in petrochemical industries. Separation of crude petroleum typically involves a conventional fractional distillation (FD) technique based on differences in petrochemicals BP distribution. However, FD has significant challenges and drawbacks including, large sample size requirement, lengthy analysis time, and relatively poor accuracy. This study explored the possible combined use of gas chromatography (GC) separation and partial-least-square (PLS1) multivariate regression analysis of petrochemical structural activity relationship (SAR) for accurate BP determination of two commercially available (D3710 and MA VHP) calibration gas mix samples. The results of the BP determination using PLS1 multivariate regression were further compared with the results of traditional simulated distillation method of BP determination. The developed PLS1 regression was able to accurately predict analytes BP in D3710 and MA VHP calibration gas mix samples, with a root-mean-square-%-relative-error (*RMS%RE*) of 6.4%, and 10.8% respectively. In contrast, the overall *RMS%RE* of 32.9% and 40.4%, respectively obtained for BP determination in D3710 and MA VHP using a traditional simulated distillation method were approximately four times larger than the corresponding *RMS%RE* of BP prediction using MRA, demonstrating the better predictive ability of MRA. The method is also rapid, robust, and promising, and can be potentially used routinely for fast analysis, pattern recognition, and analyte BP determination in petrochemical industries.

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