Supporting Information

A Rapid ^1H NMR Based Estimation of PONA for Light and Narrow Cut Naphtha Samples of Refinery Streams towards BS-VI Gasoline

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1.0 Estimation of Olefin by ^{1}H NMR

As described in our recent publication [*Energy Fuels*, **33(2)** (2019), pp. 1114–1122] two required parameters for olefin estimation- (i) average absolute number of unsaturated hydrogen (*H*) per average olefinic moiety and (ii) average alkyl chain length (*n)* of the olefins. The *H* is estimated by estimating mol factions of different types of olefinic signals (=CH, =CH2) in the olefinic region (4.4-6.6 ppm) of the 1H NMR spectrum *n* is estimated by SIMDist (or, ^{13}C NMR). The total protons in an average olefins would then be 2*n* leading to %age of oelfinic protons (%UH) as *H*/2*n*. The olefin multiplication factor (f_o) was then obtained (100/UH%) by which the %age of olefin is estimated using a normalized ^{1}H NMR spectrum.

2.0 Correlation Curves of Various Regression Analyses

For Aromatics:

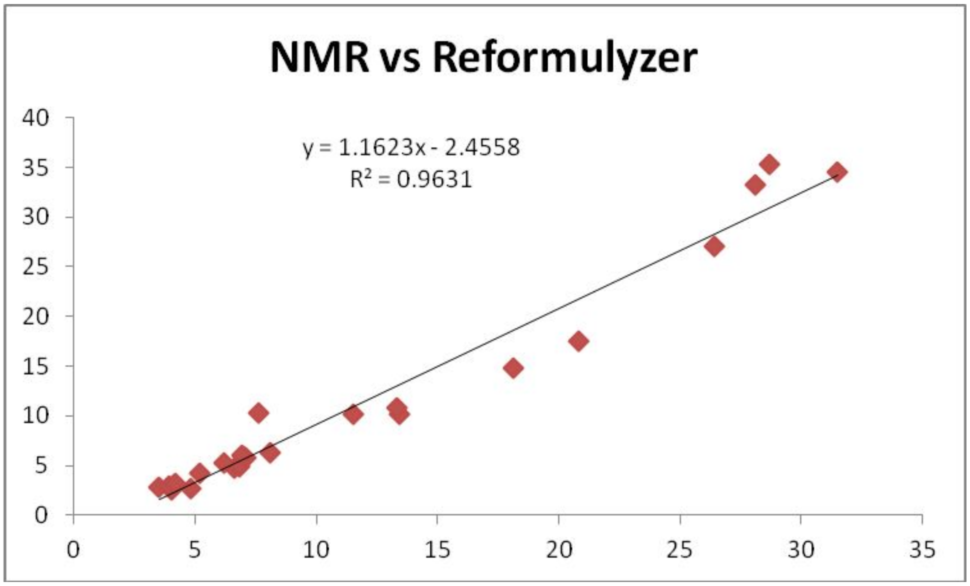

Figure 1S. Correlation Diagram for the Estimation of Aromatics by NMR vs. Refromulizer (ASTM D6839)

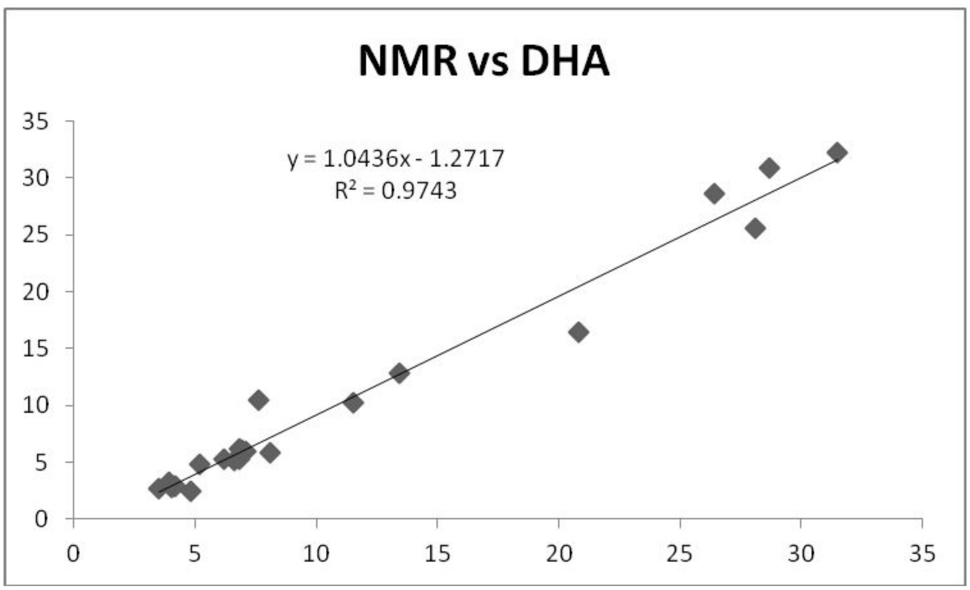

Figure 2S. Correlation Diagram for the Estimation of Aromatics by NMR vs. DHA [ASTM D6730-01(2016)].

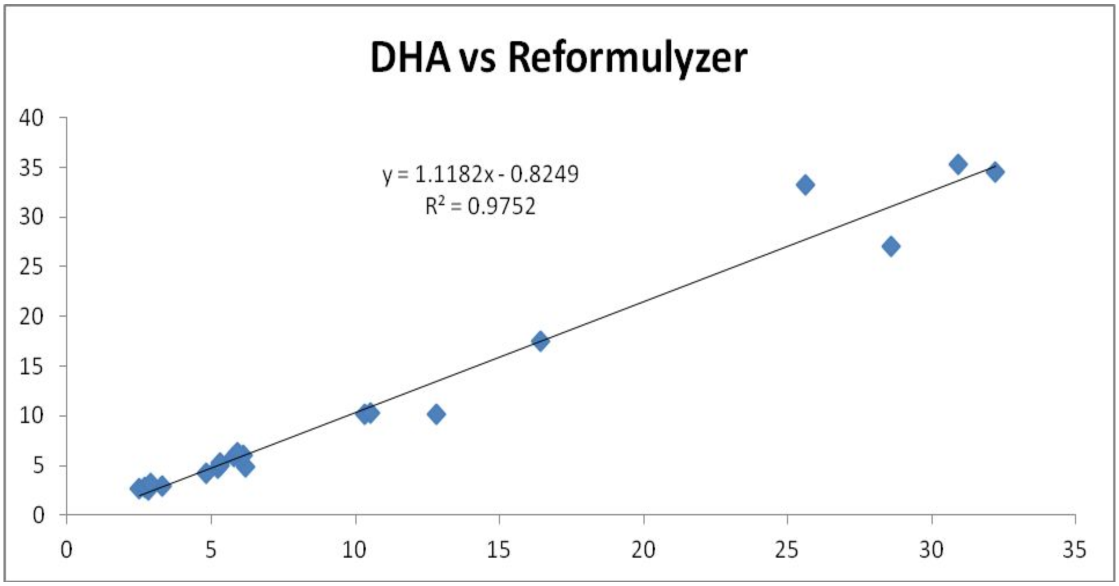

Figure 3S. Correlation Diagram for the Estimation of Aromatics by Refromulizer vs. DHA

For Olefins:

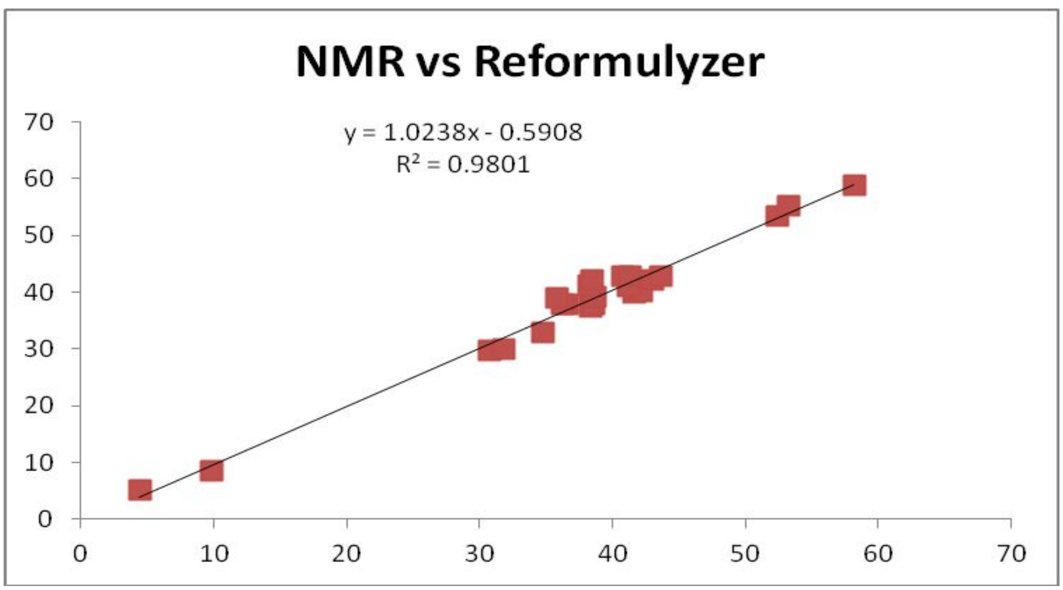

Figure 4S. Correlation Diagram for the Estimation of Olefins by NMR vs. Refromulizer (ASTM D6839)

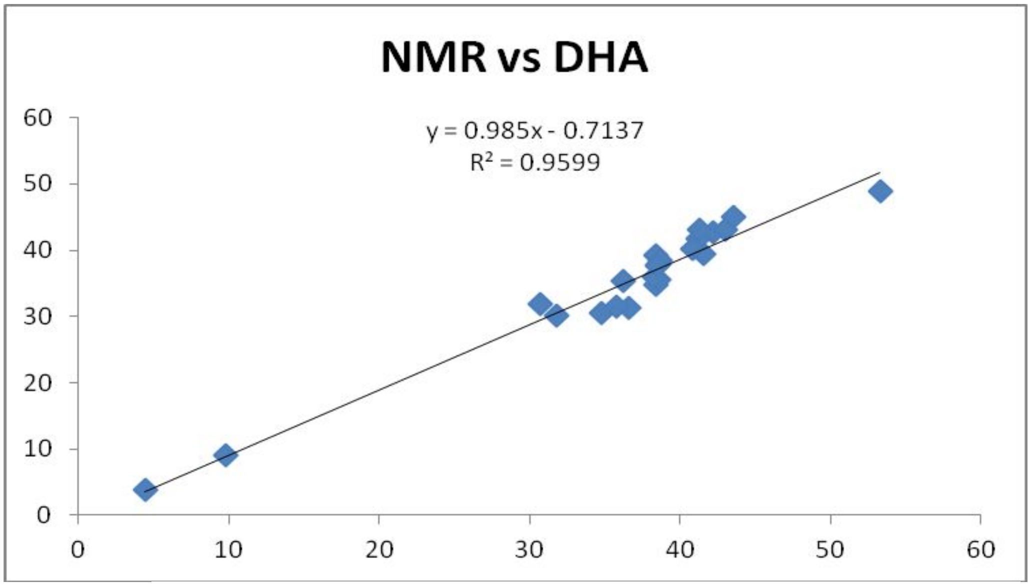

Figure 5S. Correlation Diagram for the Estimation of Olefins by NMR vs. DHA [ASTM D6730-01(2016)].

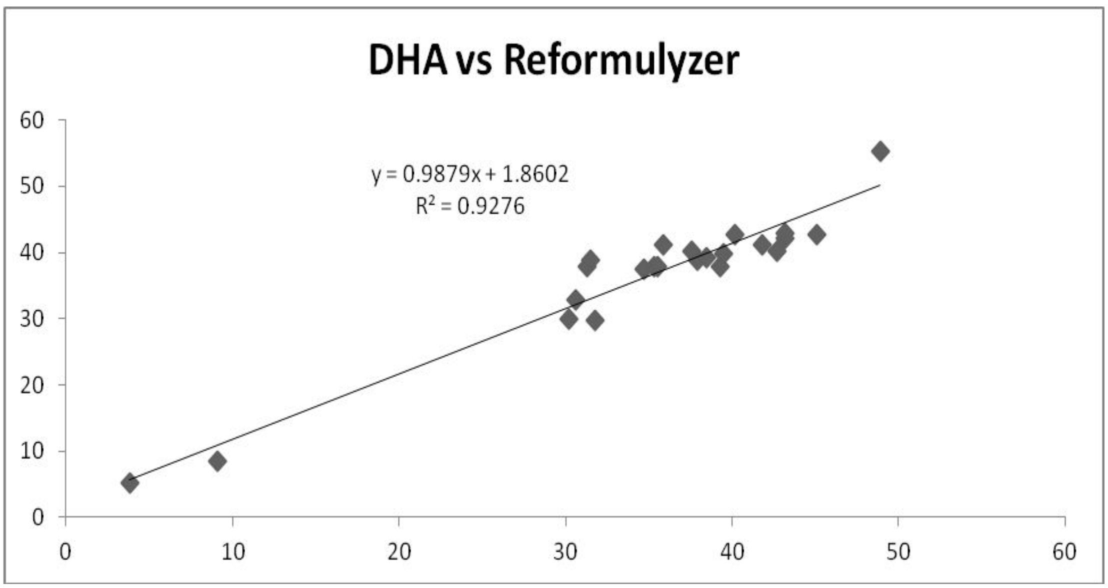

Figure 6S. Correlation Diagram for the Estimation of Olefins by Refromulizer vs. DHA.

For Naphthenes:

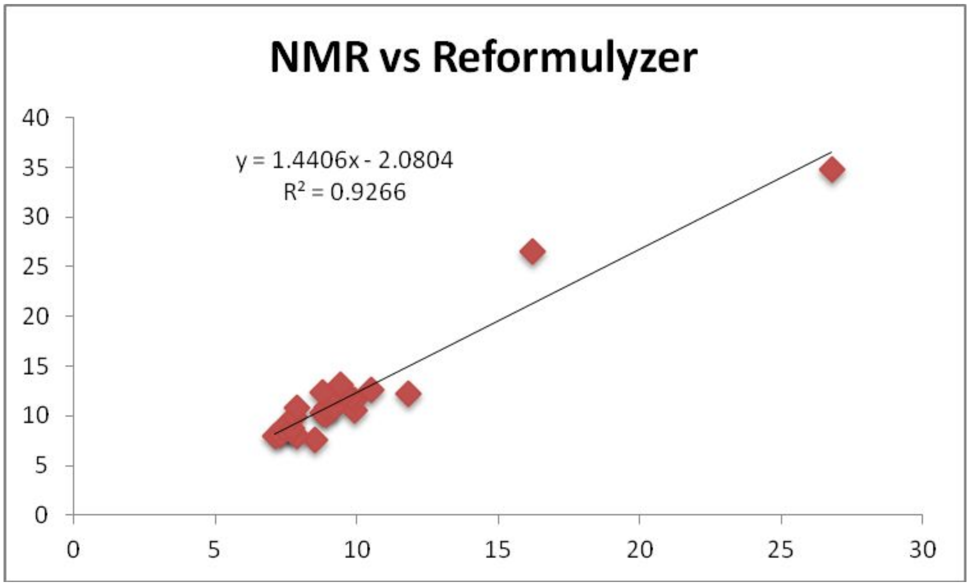

Figure 7S. Correlation Diagram for the Estimation of Naphthenes by NMR vs. Refromulizer (ASTM D6839)

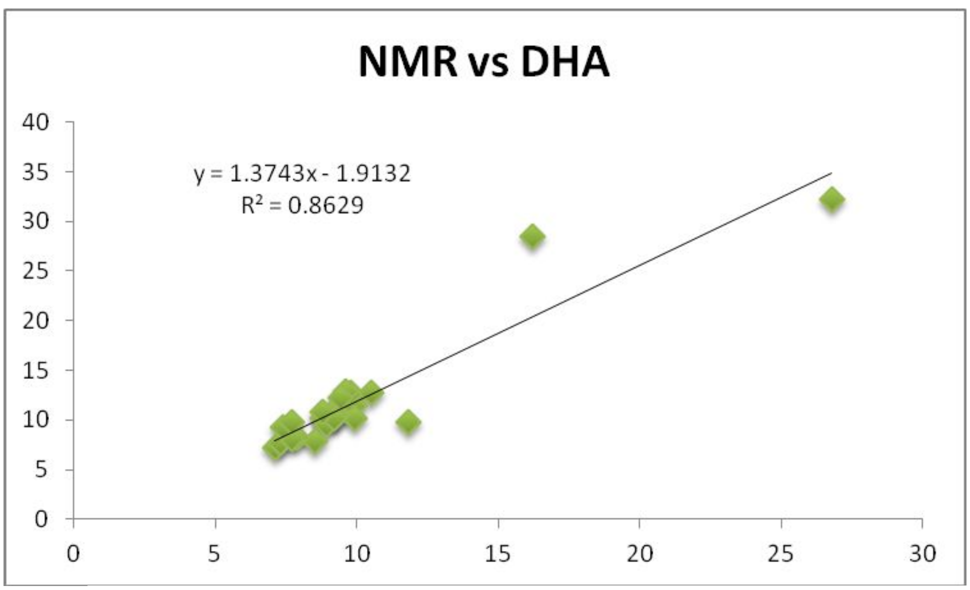

Figure 8S. Correlation Diagram for the Estimation of Naphthenes by NMR vs. DHA [ASTM D6730-01(2016)].

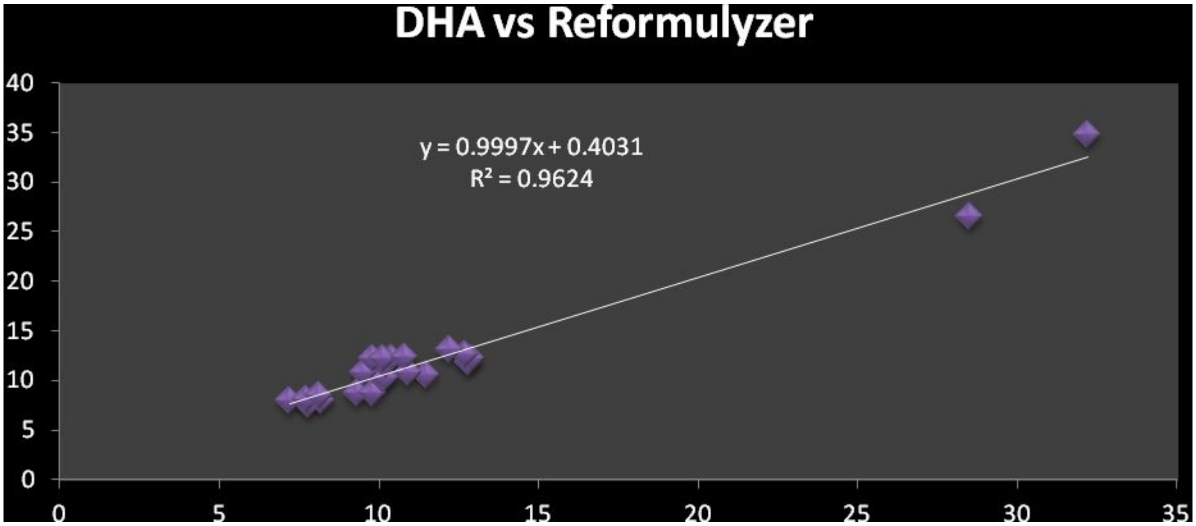

Figure 9S. Correlation Diagram for the Estimation of Naphthenes by Refromulizer vs. DHA.