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CHEMOMETRIC RESTORATION OF SOURCE-ROCK PALEOGEOGRAPHY USING BIOMARKER AND ISOTOPE COMPOSITIONS OF CRUDE OILS

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Biomarker and stable carbon isotope ratios were measured for >550 crude oil samples expelled from Upper Jurassic source rock in West Siberia, the North Sea, and offshore Labrador. A unique, multi-tiered chemometric (multivariate statistical) decision tree was used to classify seven genetically distinct Upper Jurassic oil families among these samples. The method, which we call decision-tree chemometrics, utilizes PCA (principal components analysis), multiple tiers of KNN (K-Nearest Neighbor), and SIMCA (soft independent modeling of class analogy) to classify and assign confidence limits for newly acquired oil samples and source-rock extracts.

Present-day geographic locations for each collected oil sample were restored to the paleo-latitude and paleo-longitude of the source rock during Late Jurassic time using the PALEOMAP Project© tectonic restoration program AutoPointTracker. Remarkably, predicted paleo-latitude and paleo-longitude based on partial least squares (PLS) analysis of the geochemical data closely correspond to those determined by tectonic restoration. For example, Family 3212 consists of 16 oil samples from the Norwegian and United Kingdom sectors of the North Sea. Tectonic restoration yields paleo-latitudes for these samples in range 48.0 to 56.8°N. Predicted paleo-latitudes based on PLS of the geochemical data for these samples correlate with the tectonic paleo-latitudes (correlation coefficient, $r^2 = 0.98$). Likewise, Family 3214 consists of 68 oil samples from West Siberia and offshore Norway, Denmark, United Kingdom, and Newfoundland. Tectonic paleo-latitudes are in the range 45.8 to 67.0°N and correlate with paleo-latitudes predicted by PLS of the geochemical data ($r^2 = 0.90$).