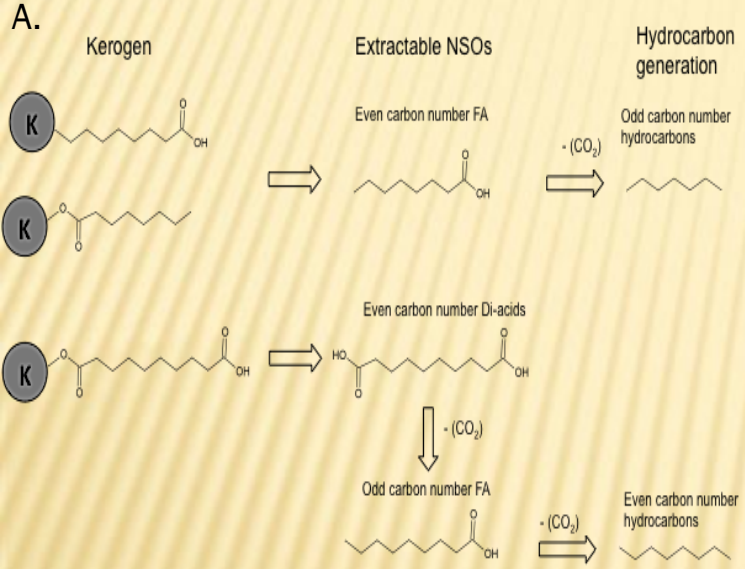
Revisiting Chemical Mechanisms Of Petroleum Generation In Sedimentary Basins : Role Of Asphaltenes During Kerogen Cracking

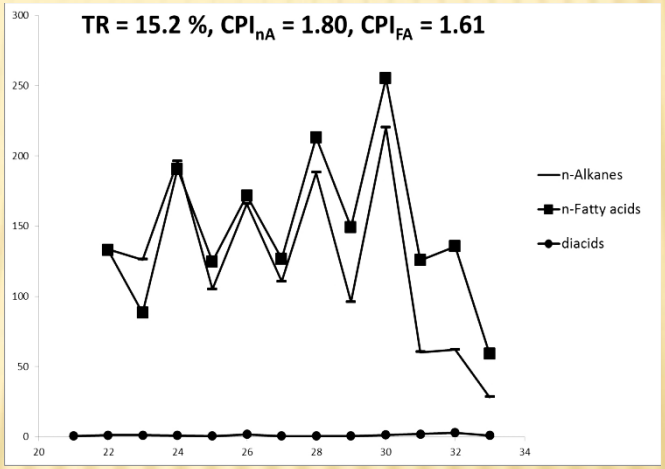
Patrick G. Hatcher, Department of Chemistry and biochemistry, Old Dominion University, Norfolk, VA

Our aim is to identify the major chemical mechanism for petroleum formation. We compare the chemical structures of NSO's generated in artificial simulations of petroleum formation with the chemical structure of precursor kerogen and the chemical structure of the hydrocarbons formed with a molecular-scale specificity involving Fourier transform mass spectrometry (FTMS). We propose a new decarboxylation reaction pathway of carboxylic acid-containing compounds that are responsible for the generation of hydrocarbons found in petroleum.

A.



B.



TR = Transformation ratio = Maturation level of Kerogen
CPI = Carbon preference

Carboxylic acids, are the major components of the NSO's generated in closed system pyrolysis of a Type I kerogen from the Mahogany Zone of the Green River Formation. By calibrating the FTICR-MS with internal standard, it is possible to quantify mono-carboxylic acids (CA) and dicarboxylic acids (DA).

Figure A shows the reaction pathway for carboxylic acids in the NSOs from artificial maturation. The odd carbon number hydrocarbons (HC) are generated from CA directly released by kerogen. DA generated from kerogen form predominantly odd-numbered CA that subsequently decarboxylate to form predominantly even-numbered HC.

Figure B shows the correlation between long chain HC and long chain CA released at the same kerogen maturation level. The Carbon Preference Indexes (CPI) of the odd-dominant HC and the even-dominant CA are very close. This suggests a genetic link between these long chain HC and these long chain CA. The minor abundance of DA (diacids) indicates that they have a small contribution to the production of HC and may also have an effect on the CPI since even DA can produce odd HC after single decarboxylation or even CA after double decarboxylation.