Subject: r
Date: Tuesday, October 27, 2015 at 1:43:14 PM Pacific Daylight Time
From: Tfaily, Malak
To: Todd-Brown, Katherine E, Smith, Peyton

Please find below some useful information.

NEW BOUNDARIES that we have been using:

class	O:C(low)	O:C(high)	H:C(low)
lipid	>0	0.3	1.5
unsatHC	0	0.125	0.8
condHC	0	0.95	0.2
protein	>0.3	0.55	1.5
aminosugar	>0.55	0.7	1.5
carb	>0.7	1.5	1.5
lignin	>0.125	0.65	0.8
tannin	>0.65	1.1	0.8

$$DBE = 1 + \frac{1}{2}(2C - H + N + P)$$ reference: http://epic.awi.de/13820/1/Koc2005f.pdf

$$AI = \frac{DBE_{AI}}{C_{AI}} = \frac{1 + C - O - S - 0.5H}{C - O - S - N - P}$$ Aromaticity index . reference: http://epic.awi.de/13820/1/Koc2005f.pdf

$$AI_{mod} = \frac{1 + C - 0.5\,O - S - 0.5\,H}{C - 0.5\,O - S - N - P}$$ modified Aromaticity index. reference: http://epic.awi.de/13820/1/Koc2005f.pdf

Kendrick plot (reference http://www.ingenieria-analitica.com/downloads/dl/file/id/1468/product/150/s05_kendrick_mass_defect_spectrum_hughey_and_marshall.pdf):

$$\text{Kendrick mass} = \text{IUPAC mass} \times (14/14.01565)$$

$$\text{Kendrick mass defect} = (\text{nominal Kendrick mass} - \text{exact Kendrick mass}) \quad (2)$$