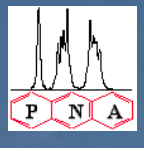


Process NMR Associates

RCC Feedstream Analysis by ^{1}H and ^{13}C NMR: Multivariate Prediction of Chemical and Physical Properties

By

John C. Edwards , Ph.D.
Process NMR Associates, LLC,
87A Sand Pit Rd, Danbury CT USA

Jincheol Kim,
SK Energy Co., Ltd, SK Energy Technology Center,
140-1, Wonchon-dong, Yuseong-gu, Daejeon 305-712, Korea

At the 236th ACS National Meeting, Philadelphia PA, August 17-21, 2008

Process NMR Associates

Company: Process NMR Associates, LLC

Founded : 1997

Personnel: 2 Ph.D. Chemists

Background: Analytical and Process Spectroscopy in Petroleum and Petrochemical Industry
Process NMR Applications and Support Under Contract to Invensys (1997-2003)
Process and Analytical NMR Instrumentation Development
Process NMR Project Suppliers

Facilities: Two Qualion 60 MHz Process MRA Units
300 MHz NMR (Liquids) and 200 MHz NMR (Solids)
Oxford Instruments 20 and 2 MHz Bench-top NMR
Resonance Systems NMR Spectrometer – 20 MHz Bench-top and Surface Analyzer
Shimadzu GC-2010 – Simulated Distillation
Smiths Detection – FTIR-ATR

Business: Application Development for Process NMR Technology
Process NMR Instrumentation Development and Implementation
Analytical NMR Services for 300+ Commercial and Academic Customers
Process and Laboratory NMR Database Development
Licensing of Copyrighted NMR Databases and Patented Applications

Business Partners: TTC Labs, USA (ttclabs.com) Modcon Systems, Israel (modcon-systems.com)
Qualion, Israel (qualion-nmr.com) Smiths Detection, USA (smithsdetection.com)
Resonance Systems, Russia (mobilenmr.com) Swagelok, USA (swagelok.com)
Triangle Analytical, USA (triangleanalytical.com)

Process NMR Associates

NMR Analyzers

Process NMR Associates

Application: Steam Cracking Optimization Installed 2000

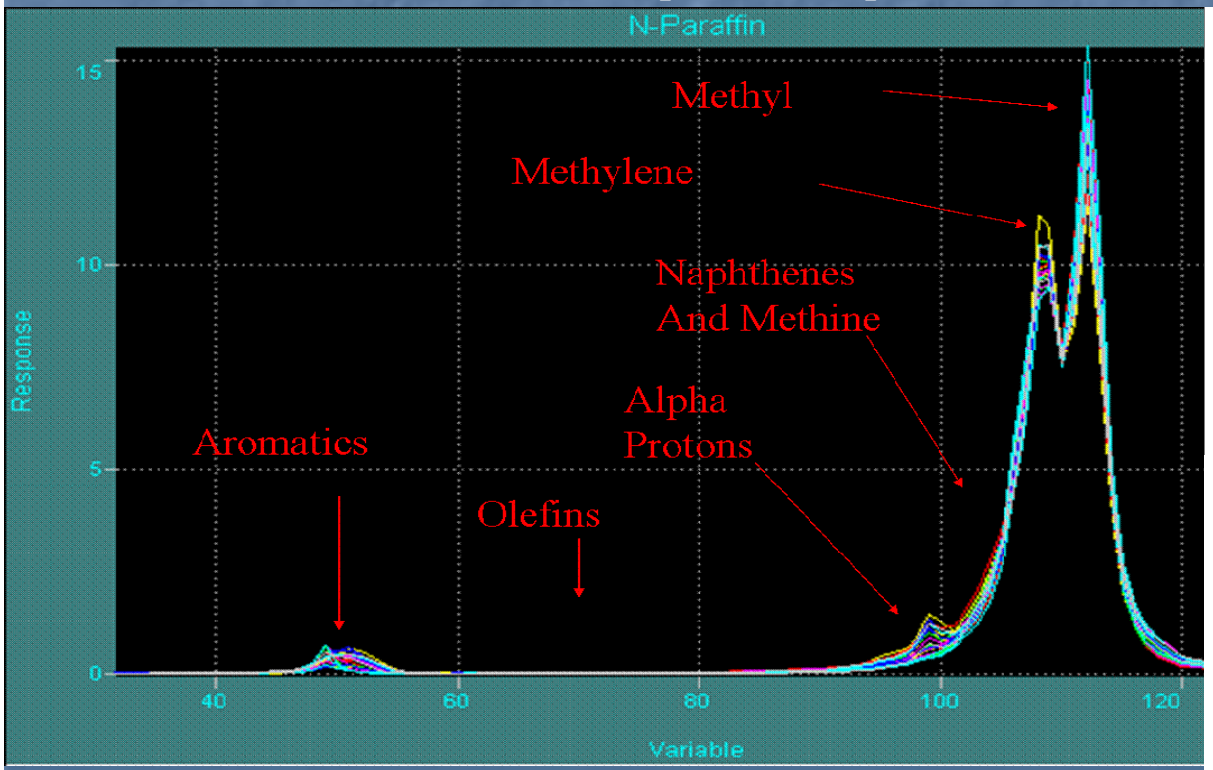
Cracker Facility Capacity: 600,000 Tonnes per Year

Control Strategy: Feed Forward Detailed Hydrocarbon Analysis to SPYRO Optimization

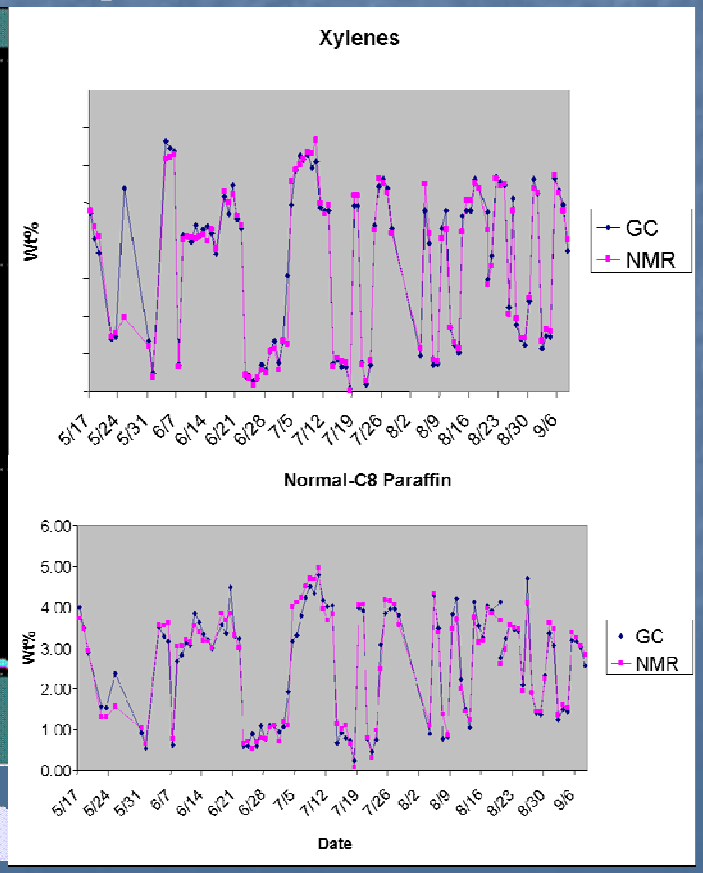
NMR Analysis: 3-4 Minute Cycle (Single Stream)

NMR PLS Outputs: Naphtha – Detailed PIONA

C4-C10 n-paraffin, i-paraffin, aromatics, naphthenes



Spectral Variability Observed in Naphtha Samples



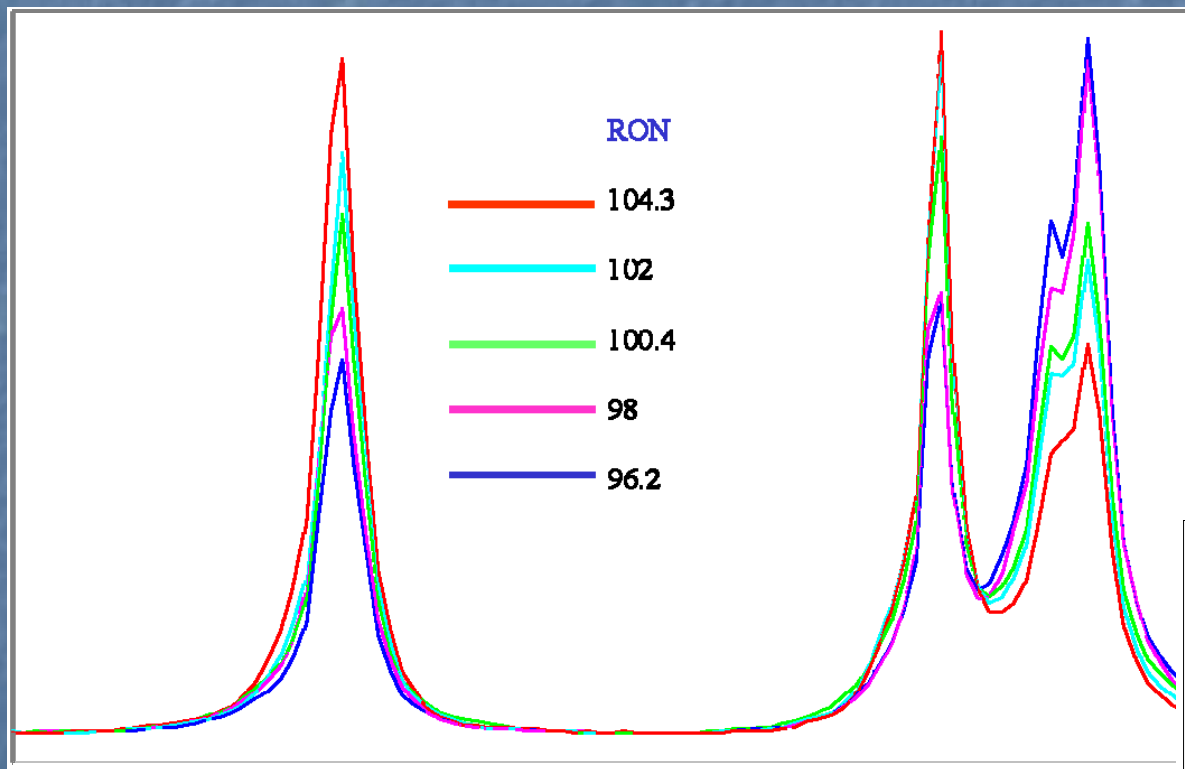
Application: Closed Loop Reformer Control — Installed 1998

Reformer Capacity: 34,000 Barrels per Day

Control Strategy: Control on MON and Benzene Content

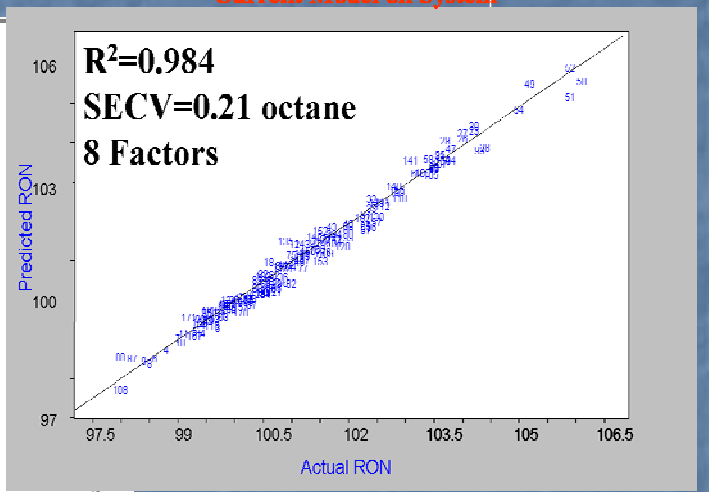
NMR Analysis: 2 Minute Analysis

NMR PLS Outputs: RON, MON, Benzene (Wt%), Total Aromatics (Wt%)

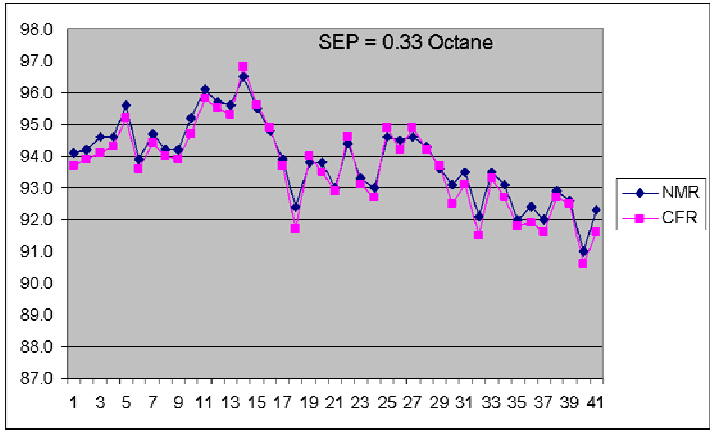


Variation of Reformate Processed ^{1}H NMR Data Observed with Changing Research Octane Number

Current Model on System



NMR Weekly Validation Performance April 2001 – April 2002



US006080301A

United States Patent [19]

Berlowitz et al.

[11] Patent Number: 6,080,301

[45] Date of Patent: Jun. 27, 2000

[54] **PREMIUM SYNTHETIC LUBRICANT BASE STOCK HAVING AT LEAST 95% NON-CYCLIC ISOPARAFFINS**

[75] Inventors: **Paul J. Berlowitz**, E. Windsor; **Jacob J. Habeeb**, Westfield, both of N.J.; **Robert J. Wittenbrink**, Baton Rouge, La.

[73] Assignee: **ExxonMobil Research and Engineering Company**, Florham Park, N.J.

K.I. Zimina, et al, "Method of Comprehensive Investigation of the Composition, Structure and Properties of Oil Hydrocarbons", Scientific Papers of the Prague Institute of Chemical Technology, D 46 (1982), Technology of Fuel, pp. 89–103.

D. Christakudis, et al, "Several Properties of Lubricating Oils Produced by Thermal Diffusion", Organic–Technical Chemistry, Chemistry Dept. at the Bergakademie at Freiberg and presented to the 10th International Symposium "Lubricants, Lubrication and Bearing Engineering" (Aug. 27–31, 1998), pp. 32–41.

G.E. Cranton, "Composition and Oxidation of Petroleum

Col 2, line 8, "These base stocks are premium synthetic lubricating oil base stocks of high purity having a high VI, a low pour point and are iso-paraffinic, in that they comprise at least 95 wt. % of non-cyclic iso-paraffins having a molecular structure in which less than 25% of the total number of carbon atoms are present in the branches, and less than half the branches have two or more carbon atoms."

Col 4, line 5-14, "with at least 50% of the oil molecules containing at least one branch, at least half of which are methyl branches. At least half, and more preferably at least 75% of the remaining branches are ethyl, with less than 25% and preferably less than 15% of the total number of branches having three or more carbon atoms. The total number of branch carbon atoms is typically less than 25%, preferably less than 20% and more preferably no more than 15% (e.g., 10-15%) of the total number of carbon atoms comprising the hydrocarbon molecules."

Col 4, line 24-29, "Thus, the molecular make up of a base stock of the invention comprises at least 95 wt. % isoparaffins having a relatively linear molecular structure, with less than half the branches having two or more carbon atoms and less than 25% of the total number of carbon atoms present in the branches."

Col 12, Line 4-21, "What is claimed is:

1. A lubricant base stock comprising at least 95 wt. % non-cyclic iso-paraffins having a molecular structure in which less than 25% of the total number of carbon atoms of the isoparaffin structure are contained in the branches and less than half of the total iso-paraffin branches contain two or more carbon atoms.

2. A base stock according to claim 1 wherein at least half of the iso-paraffin branches are methyl branches.

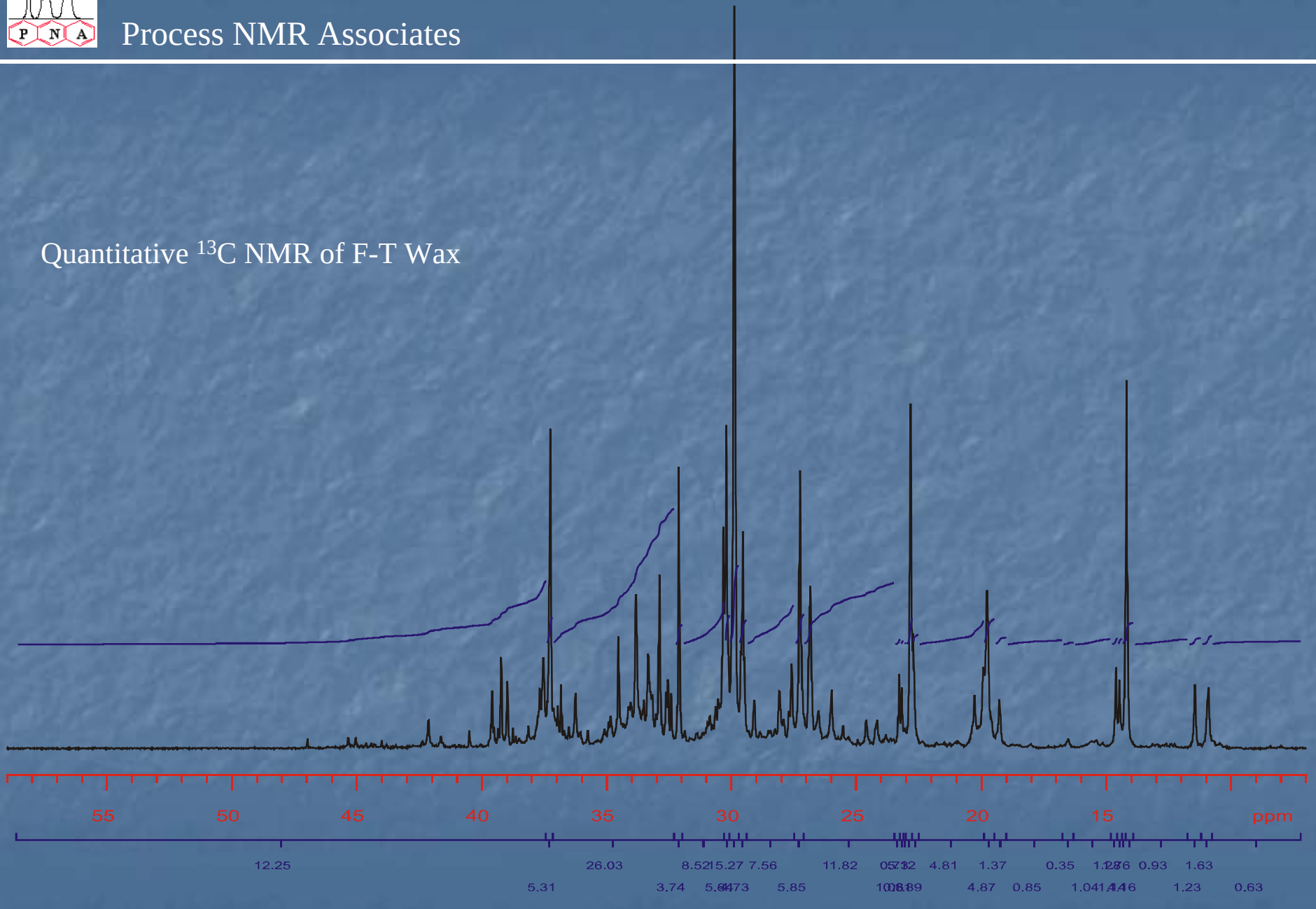
3. A base stock according to claim 2 wherein at least half of the remaining, non-methyl branches are ethyl, with less than 25% of the total number of branches having three or more carbon atoms.

4. A base stock according to claim 3 wherein at least 75% of the non-methyl branches are ethyl.

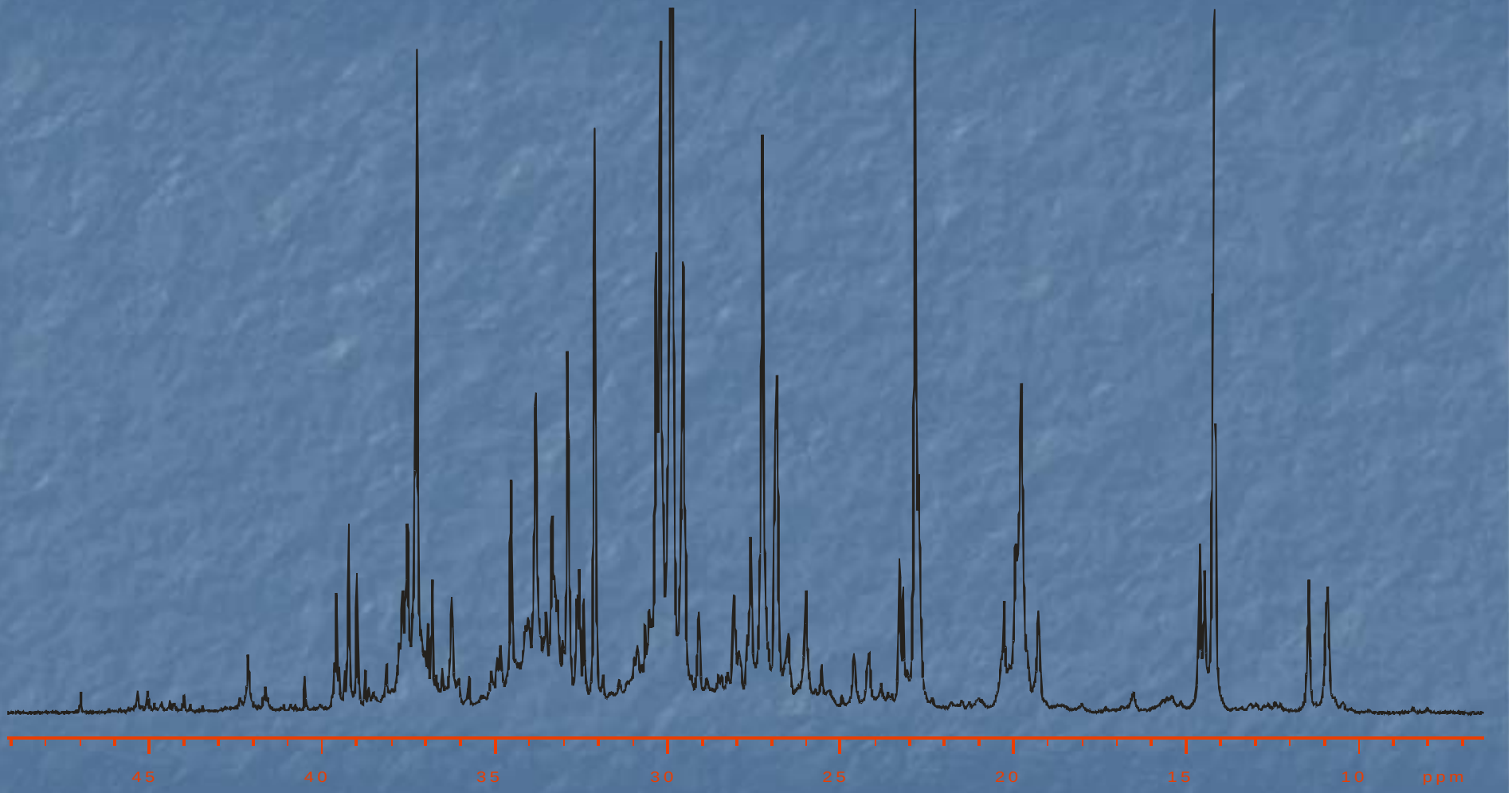
5. A base stock according to claim 4 wherein of the total number of carbon atoms contained in the iso-paraffin molecule, 10-15% of the carbon atoms are located in the branches."

Process NMR Associates

Quantitative ^{13}C NMR of F-T Wax



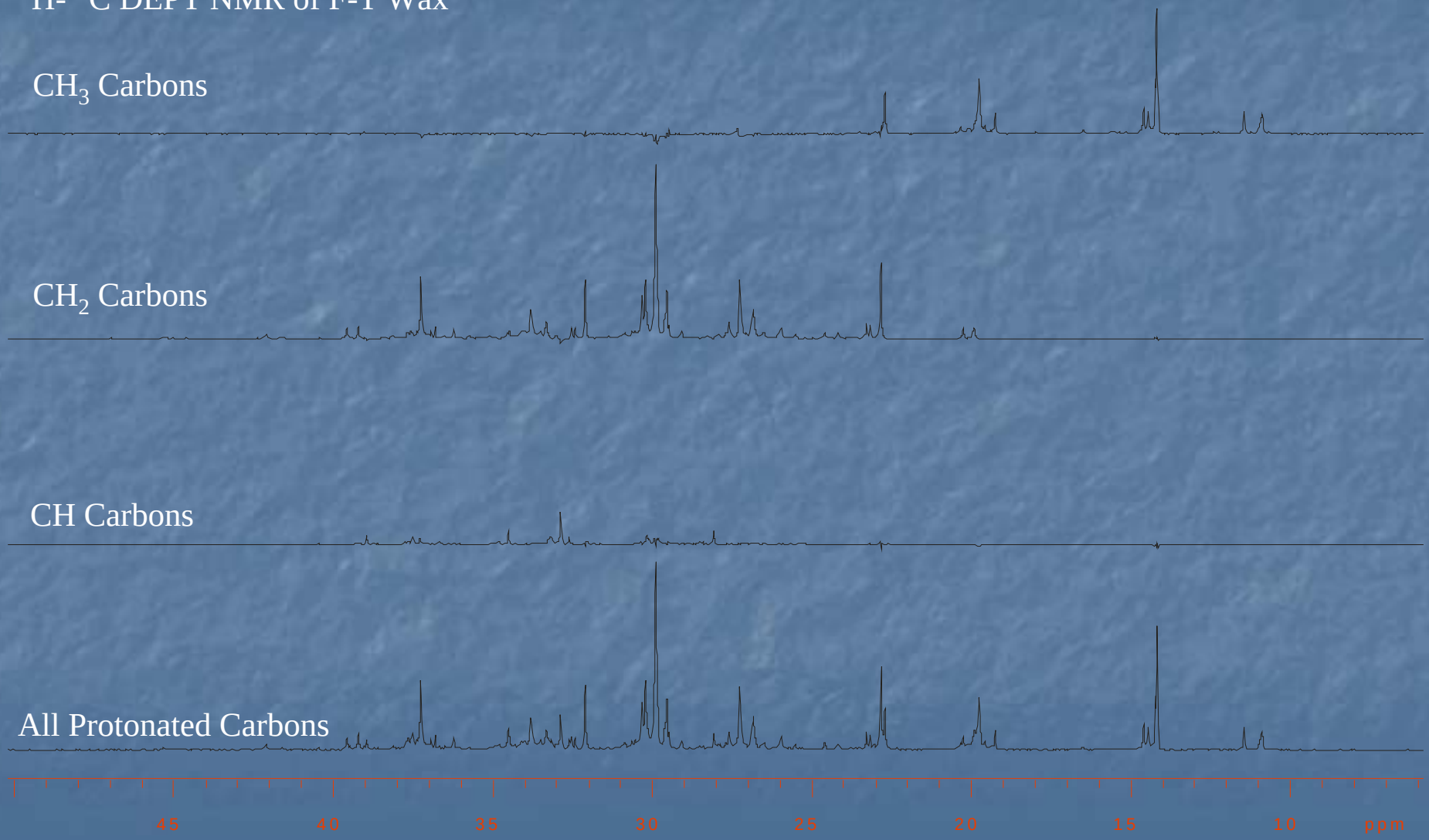
Process NMR Associates



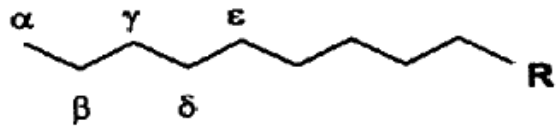
Quantitative ^{13}C NMR of F-T Wax - Vertical Expansion

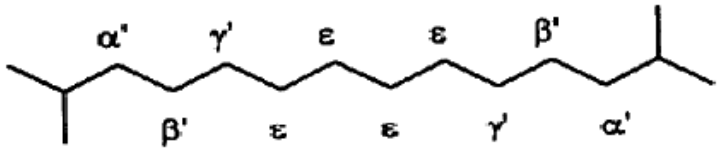
Process NMR Associates

^{1}H-^{13}C DEPT NMR of F-T Wax



^{13}C NMR Assignments for Various Paraffins Structure Types

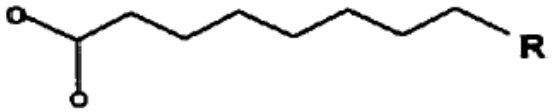




α = 14.0 ppm
β = 22.8 ppm
γ = 32.0 ppm
δ = 29.5 ppm
ε = 29.8 ppm

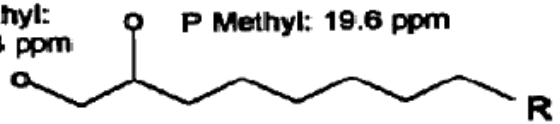
α' = 37.4 ppm
β' = 27.4 ppm
γ' = 30.3 ppm

P and T Methyl: 22.5 ppm

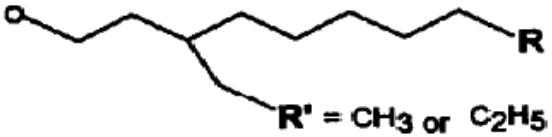


T Ethyl: 11.3 ppm

P Methyl: 19.6 ppm

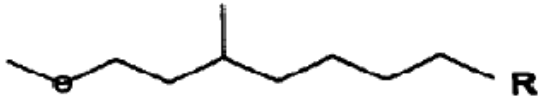


T Propyl: 14.4 ppm

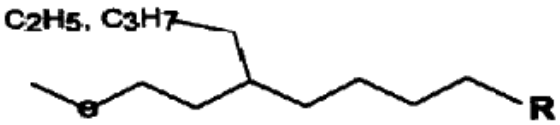


T Propyl: 14.3 ppm

P Methyl: 19.6 ppm



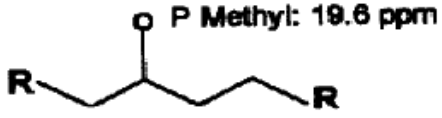
R' = CH3, C2H5, C3H7



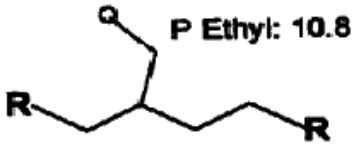
β T Butyl: 23.2 ppm

β T Butyl: 23.1 ppm

P Methyl: 19.6 ppm

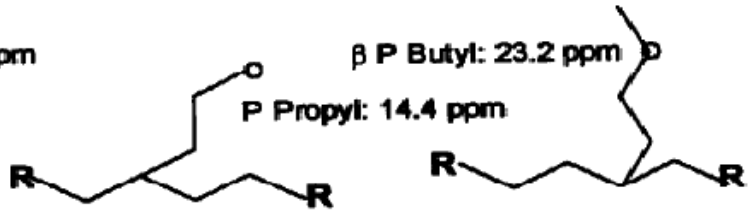


P Ethyl: 10.8 ppm

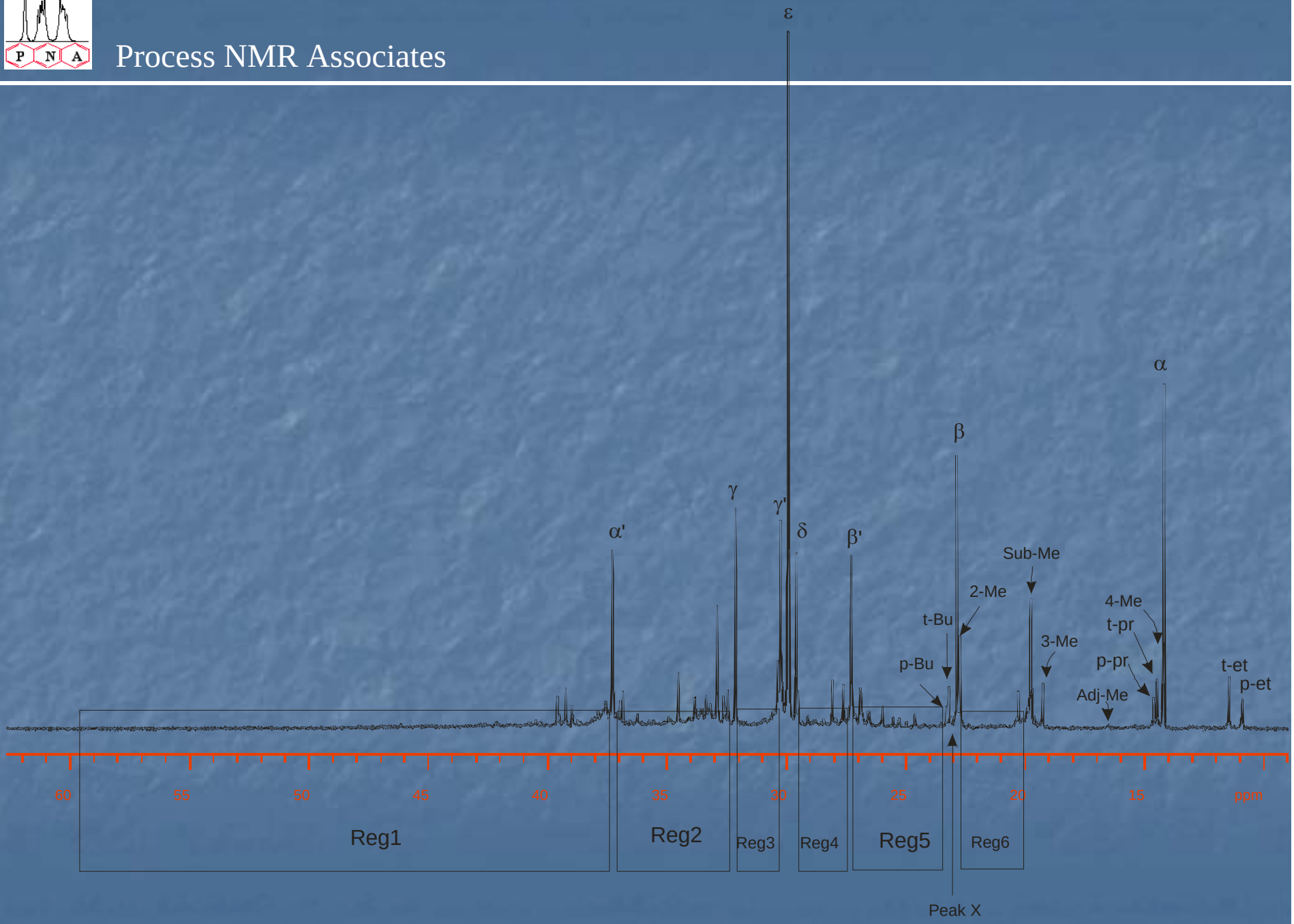


β P Butyl: 23.2 ppm

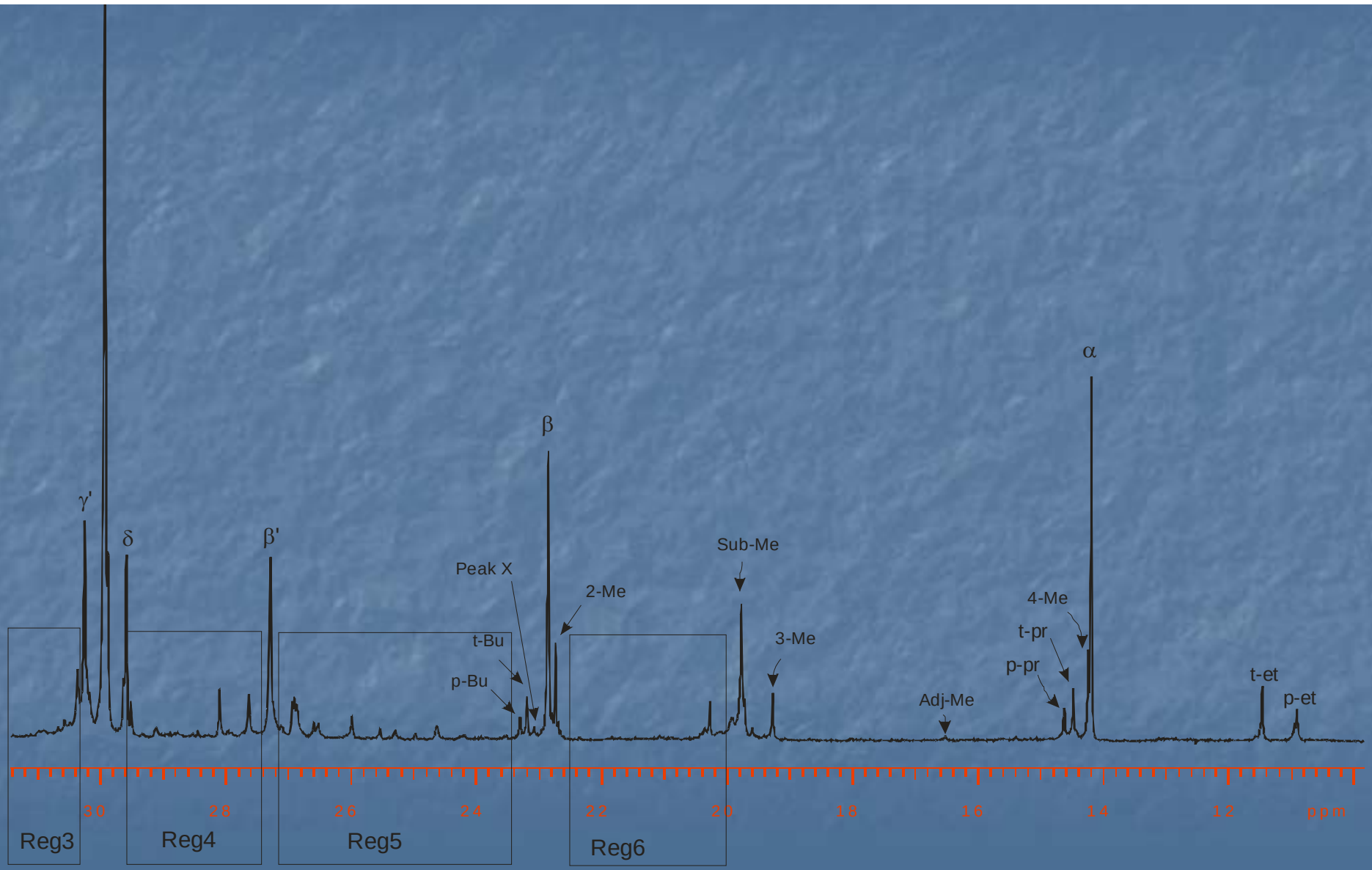
P Propyl: 14.4 ppm



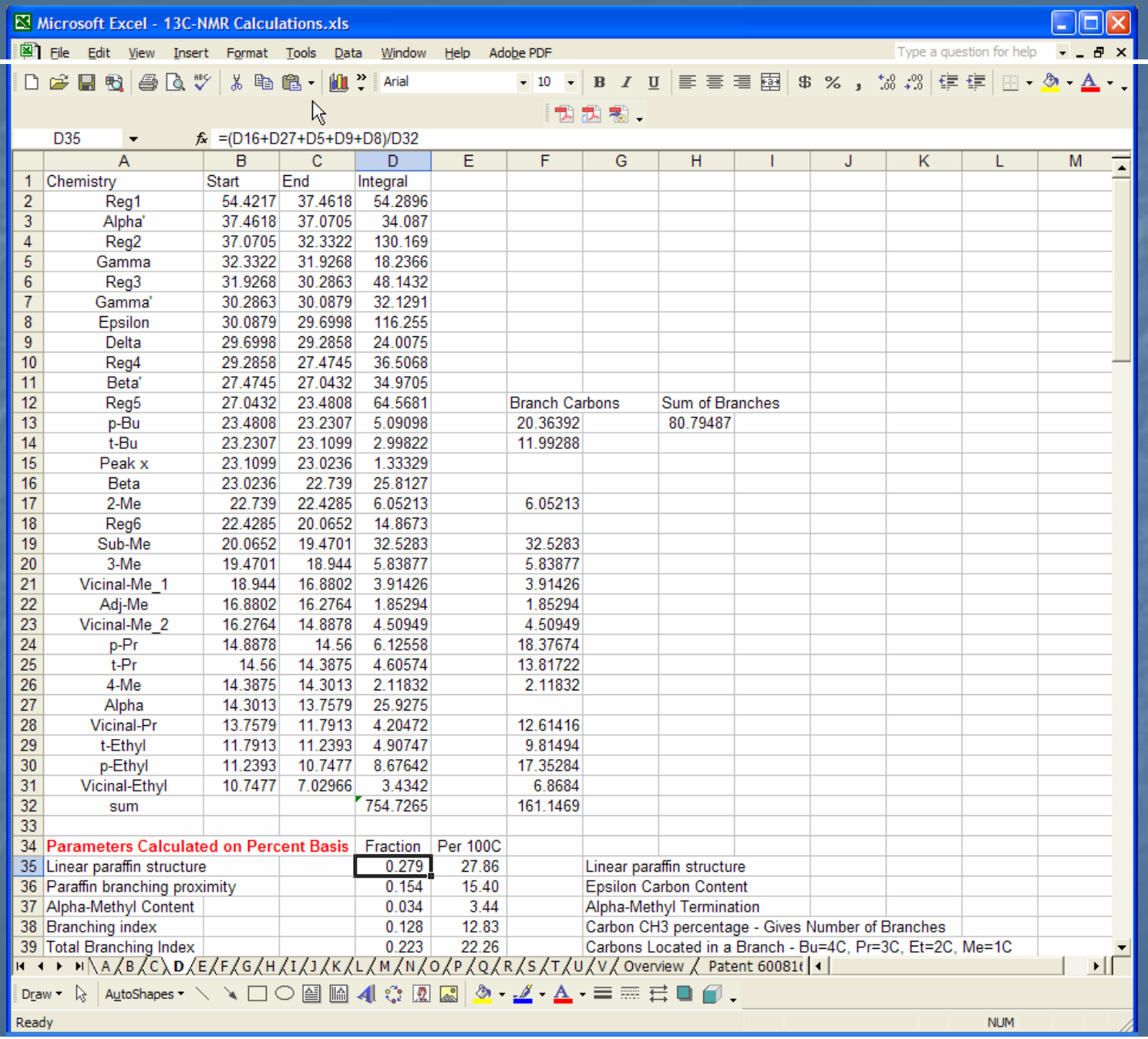
Process NMR Associates



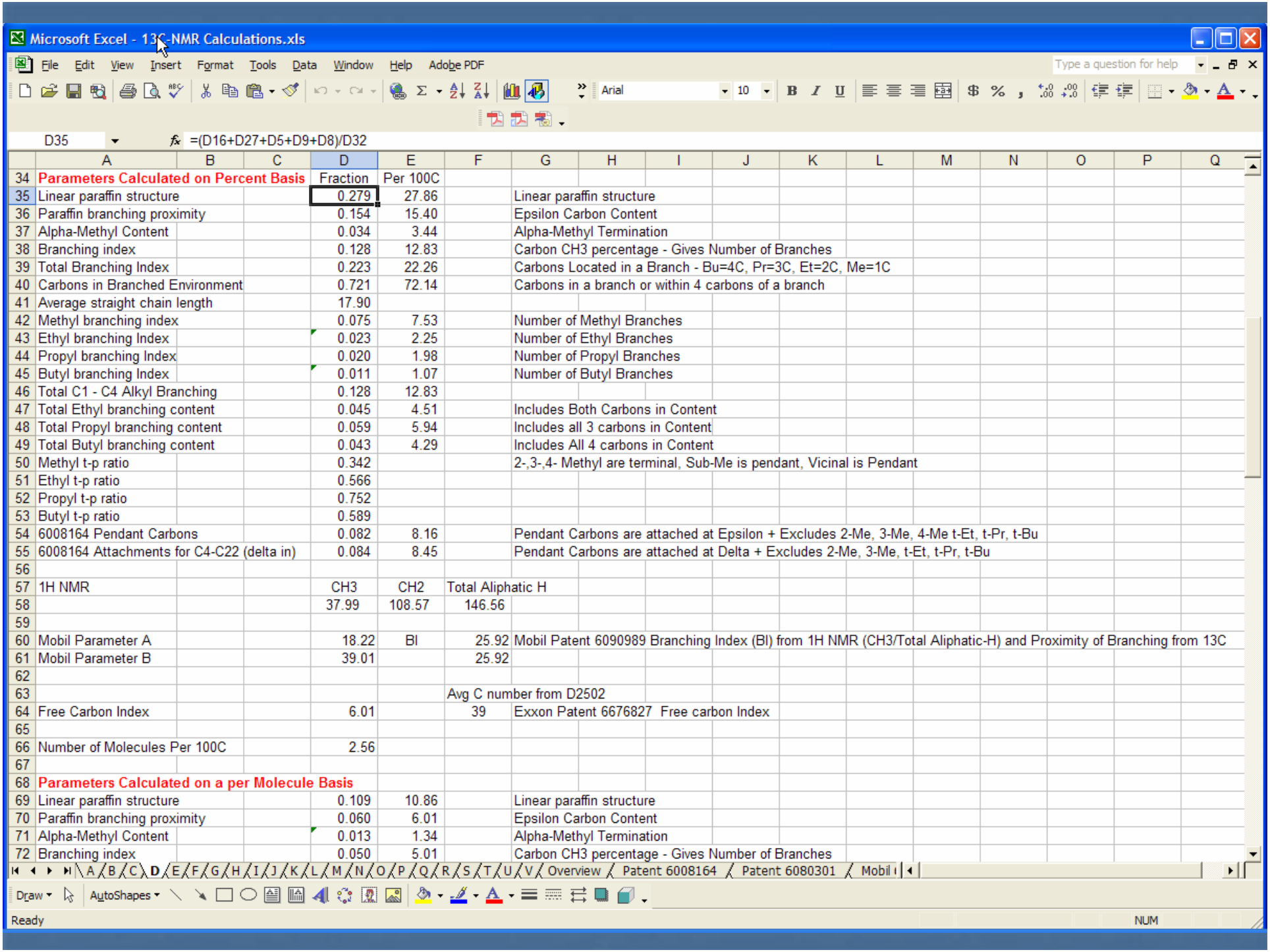
Process NMR Associates



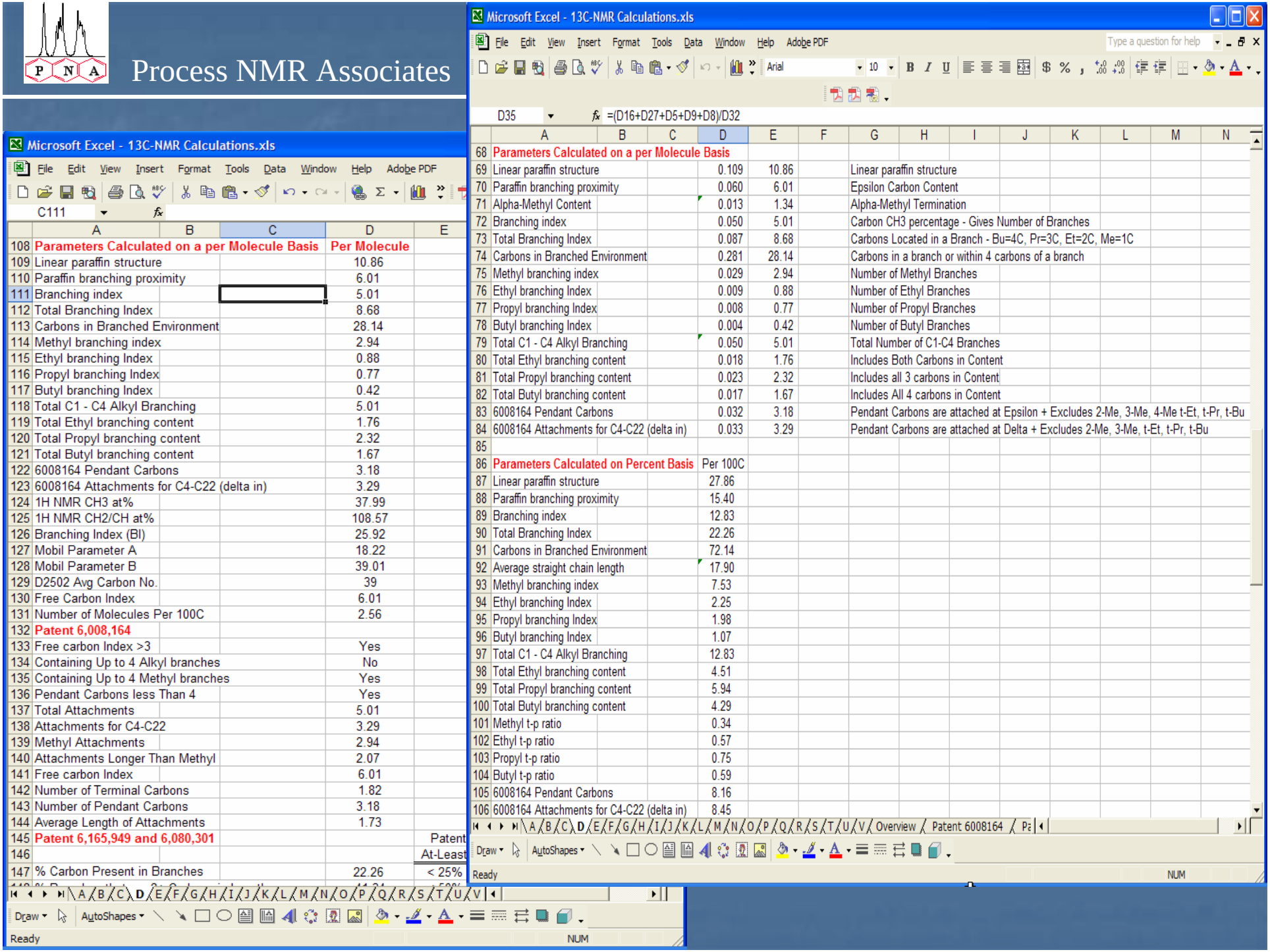
Process NMR Associates



	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Chemistry	Start	End	Integral									
2	Reg1	54.4217	37.4618	54.2896									
3	Alpha'	37.4618	37.0705	34.087									
4	Reg2	37.0705	32.3322	130.169									
5	Gamma	32.3322	31.9268	18.2366									
6	Reg3	31.9268	30.2863	48.1432									
7	Gamma'	30.2863	30.0879	32.1291									
8	Epsilon	30.0879	29.6998	116.255									
9	Delta	29.6998	29.2858	24.0075									
10	Reg4	29.2858	27.4745	36.5068									
11	Beta'	27.4745	27.0432	34.9705									
12	Reg5	27.0432	23.4808	64.5681		Branch Carbons		Sum of Branches					
13	p-Bu	23.4808	23.2307	5.09098		20.36392		80.79487					
14	t-Bu	23.2307	23.1099	2.99822		11.99288							
15	Peak x	23.1099	23.0236	1.33329									
16	Beta	23.0236	22.739	25.8127									
17	2-Me	22.739	22.4285	6.05213		6.05213							
18	Reg6	22.4285	20.0652	14.8673									
19	Sub-Me	20.0652	19.4701	32.5283		32.5283							
20	3-Me	19.4701	18.944	5.83877		5.83877							
21	Vicinal-Me_1	18.944	16.8802	3.91426		3.91426							
22	Adj-Me	16.8802	16.2764	1.85294		1.85294							
23	Vicinal-Me_2	16.2764	14.8878	4.50949		4.50949							
24	p-Pr	14.8878	14.56	6.12558		18.37674							
25	t-Pr	14.56	14.3875	4.60574		13.81722							
26	4-Me	14.3875	14.3013	2.11832		2.11832							
27	Alpha	14.3013	13.7579	25.9275									
28	Vicinal-Pr	13.7579	11.7913	4.20472		12.61416							
29	t-Ethyl	11.7913	11.2393	4.90747		9.81494							
30	p-Ethyl	11.2393	10.7477	8.67642		17.35284							
31	Vicinal-Ethyl	10.7477	7.02966	3.4342		6.8684							
32	sum			754.7265		161.1469							
33													
34	**Parameters Calculated on Percent Basis**			Fraction	Per 100C								
35	Linear paraffin structure			0.279	27.86		Linear paraffin structure						
36	Paraffin branching proximity			0.154	15.40		Epsilon Carbon Content						
37	Alpha-Methyl Content			0.034	3.44		Alpha-Methyl Termination						
38	Branching index			0.128	12.83		Carbon CH3 percentage - Gives Number of Branches						
39	Total Branching Index			0.223	22.26		Carbons Located in a Branch - Bu=4C, Pr=3C, Et=2C, Me=1C						



	A	D	E	F	G
34	**Parameters Calculated on Percent Basis**	Fraction	Per 100C		
35	Linear paraffin structure	0.279	27.86		Linear paraffin structure
36	Paraffin branching proximity	0.154	15.40		Epsilon Carbon Content
37	Alpha-Methyl Content	0.034	3.44		Alpha-Methyl Termination
38	Branching index	0.128	12.83		Carbon CH3 percentage - Gives Number of Branches
39	Total Branching Index	0.223	22.26		Carbons Located in a Branch - Bu=4C, Pr=3C, Et=2C, Me=1C
40	Carbons in Branched Environment	0.721	72.14		Carbons in a branch or within 4 carbons of a branch
41	Average straight chain length	17.90			
42	Methyl branching index	0.075	7.53		Number of Methyl Branches
43	Ethyl branching Index	0.023	2.25		Number of Ethyl Branches
44	Propyl branching Index	0.020	1.98		Number of Propyl Branches
45	Butyl branching Index	0.011	1.07		Number of Butyl Branches
46	Total C1 - C4 Alkyl Branching	0.128	12.83		
47	Total Ethyl branching content	0.045	4.51		Includes Both Carbons in Content
48	Total Propyl branching content	0.059	5.94		Includes all 3 carbons in Content
49	Total Butyl branching content	0.043	4.29		Includes All 4 carbons in Content
50	Methyl t-p ratio	0.342			2-,3-,4- Methyl are terminal, Sub-Me is pendant, Vicinal is Pendant
51	Ethyl t-p ratio	0.566			
52	Propyl t-p ratio	0.752			
53	Butyl t-p ratio	0.589			
54	6008164 Pendant Carbons	0.082	8.16		Pendant Carbons are attached at Epsilon + Excludes 2-Me, 3-Me, 4-Me t-Et, t-Pr, t-Bu
55	6008164 Attachments for C4-C22 (delta in)	0.084	8.45		Pendant Carbons are attached at Delta + Excludes 2-Me, 3-Me, t-Et, t-Pr, t-Bu
56					
57	1H NMR	CH3	CH2	Total Aliphatic H	
58		37.99	108.57	146.56	
59					
60	Mobil Parameter A	18.22	BI	25.92	Mobil Patent 6090989 Branching Index (BI) from 1H NMR (CH3/Total Aliphatic-H) and Proximity of Branching from 13C
61	Mobil Parameter B	39.01		25.92	
62					
63				Avg C number from D2502	
64	Free Carbon Index	6.01		39	Exxon Patent 6676827 Free carbon Index
65					
66	Number of Molecules Per 100C	2.56			
67					
68	**Parameters Calculated on a per Molecule Basis**				
69	Linear paraffin structure	0.109	10.86		Linear paraffin structure
70	Paraffin branching proximity	0.060	6.01		Epsilon Carbon Content
71	Alpha-Methyl Content	0.013	1.34		Alpha-Methyl Termination
72	Branching index	0.050	5.01		Carbon CH3 percentage - Gives Number of Branches


Process NMR Associates
Microsoft Excel - 13C-NMR Calculations.xls
File Edit View Insert Format Tools Data Window Help Adobe PDF
C111
Parameters Calculated on a per Molecule Basis | Per Molecule
Linear paraffin structure | 10.86
Paraffin branching proximity | 6.01
Branching index | 5.01
Total Branching Index | 8.68
Carbons in Branched Environment | 28.14
Methyl branching index | 2.94
Ethyl branching Index | 0.88
Propyl branching Index | 0.77
Butyl branching Index | 0.42
Total C1 - C4 Alkyl Branching | 5.01
Total Ethyl branching content | 1.76
Total Propyl branching content | 2.32
Total Butyl branching content | 1.67
6008164 Pendant Carbons | 3.18
6008164 Attachments for C4-C22 (delta in) | 3.29
1H NMR CH3 at% | 37.99
1H NMR CH2/CH at% | 108.57
Branching Index (BI) | 25.92
Mobil Parameter A | 18.22
Mobil Parameter B | 39.01
D2502 Avg Carbon No. | 39
Free Carbon Index | 6.01
Number of Molecules Per 100C | 2.56
Patent 6,008,164
Free carbon Index >3 | Yes
Containing Up to 4 Alkyl branches | No
Containing Up to 4 Methyl branches | Yes
Pendant Carbons less Than 4 | Yes
Total Attachments | 5.01
Attachments for C4-C22 | 3.29
Methyl Attachments | 2.94
Attachments Longer Than Methyl | 2.07
Free carbon Index | 6.01
Number of Terminal Carbons | 1.82
Number of Pendant Carbons | 3.18
Average Length of Attachments | 1.73
Patent 6,165,949 and 6,080,301 | Patent
At-Least
% Carbon Present in Branches | 22.26 | < 25%
Draw AutoShapes
Ready NUM
Microsoft Excel - 13C-NMR Calculations.xls
File Edit View Insert Format Tools Data Window Help Adobe PDF
D35 =(D16+D27+D5+D9+D8)/D32
Parameters Calculated on a per Molecule Basis
Linear paraffin structure | 0.109 | 10.86 | Linear paraffin structure
Paraffin branching proximity | 0.060 | 6.01 | Epsilon Carbon Content
Alpha-Methyl Content | 0.013 | 1.34 | Alpha-Methyl Termination
Branching index | 0.050 | 5.01 | Carbon CH3 percentage - Gives Number of Branches
Total Branching Index | 0.087 | 8.68 | Carbons Located in a Branch - Bu=4C, Pr=3C, Et=2C, Me=1C
Carbons in Branched Environment | 0.281 | 28.14 | Carbons in a branch or within 4 carbons of a branch
Methyl branching index | 0.029 | 2.94 | Number of Methyl Branches
Ethyl branching Index | 0.009 | 0.88 | Number of Ethyl Branches
Propyl branching Index | 0.008 | 0.77 | Number of Propyl Branches
Butyl branching Index | 0.004 | 0.42 | Number of Butyl Branches
Total C1 - C4 Alkyl Branching | 0.050 | 5.01 | Total Number of C1-C4 Branches
Total Ethyl branching content | 0.018 | 1.76 | Includes Both Carbons in Content
Total Propyl branching content | 0.023 | 2.32 | Includes all 3 carbons in Content
Total Butyl branching content | 0.017 | 1.67 | Includes All 4 carbons in Content
6008164 Pendant Carbons | 0.032 | 3.18 | Pendant Carbons are attached at Epsilon + Excludes 2-Me, 3-Me, 4-Me t-Et, t-Pr, t-Bu
6008164 Attachments for C4-C22 (delta in) | 0.033 | 3.29 | Pendant Carbons are attached at Delta + Excludes 2-Me, 3-Me, t-Et, t-Pr, t-Bu
Parameters Calculated on Percent Basis | Per 100C
Linear paraffin structure | 27.86
Paraffin branching proximity | 15.40
Branching index | 12.83
Total Branching Index | 22.26
Carbons in Branched Environment | 72.14
Average straight chain length | 17.90
Methyl branching index | 7.53
Ethyl branching Index | 2.25
Propyl branching Index | 1.98
Butyl branching Index | 1.07
Total C1 - C4 Alkyl Branching | 12.83
Total Ethyl branching content | 4.51
Total Propyl branching content | 5.94
Total Butyl branching content | 4.29
Methyl t-p ratio | 0.34
Ethyl t-p ratio | 0.57
Propyl t-p ratio | 0.75
Butyl t-p ratio | 0.59
6008164 Pendant Carbons | 8.16
6008164 Attachments for C4-C22 (delta in) | 8.45
Overview Patent 6008164
Draw AutoShapes
Ready NUM

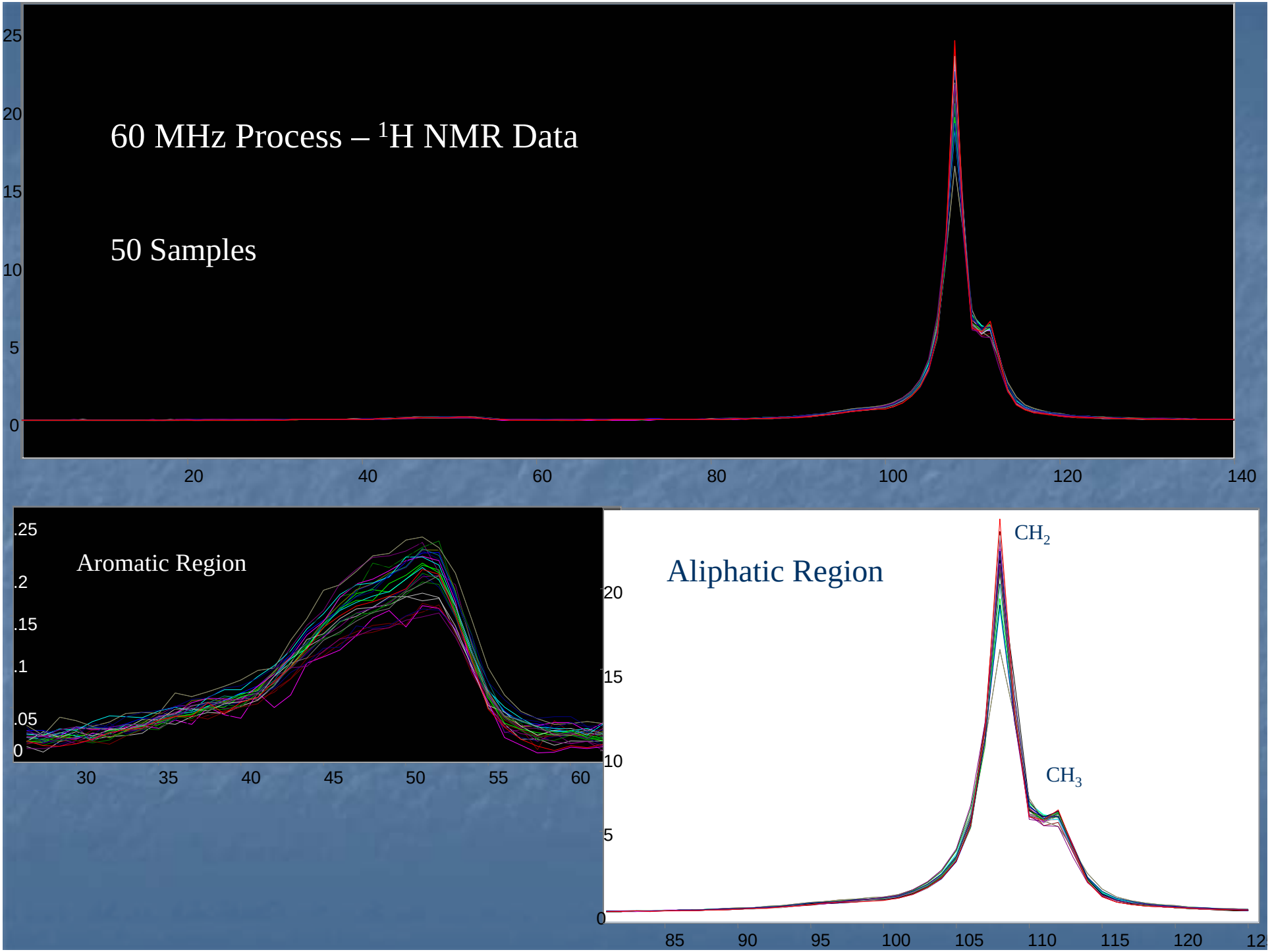
Residual Catalytic Cracking – Feed-stream Analysis

Analysis – Refractive Index, Distillation, Specific Gravity

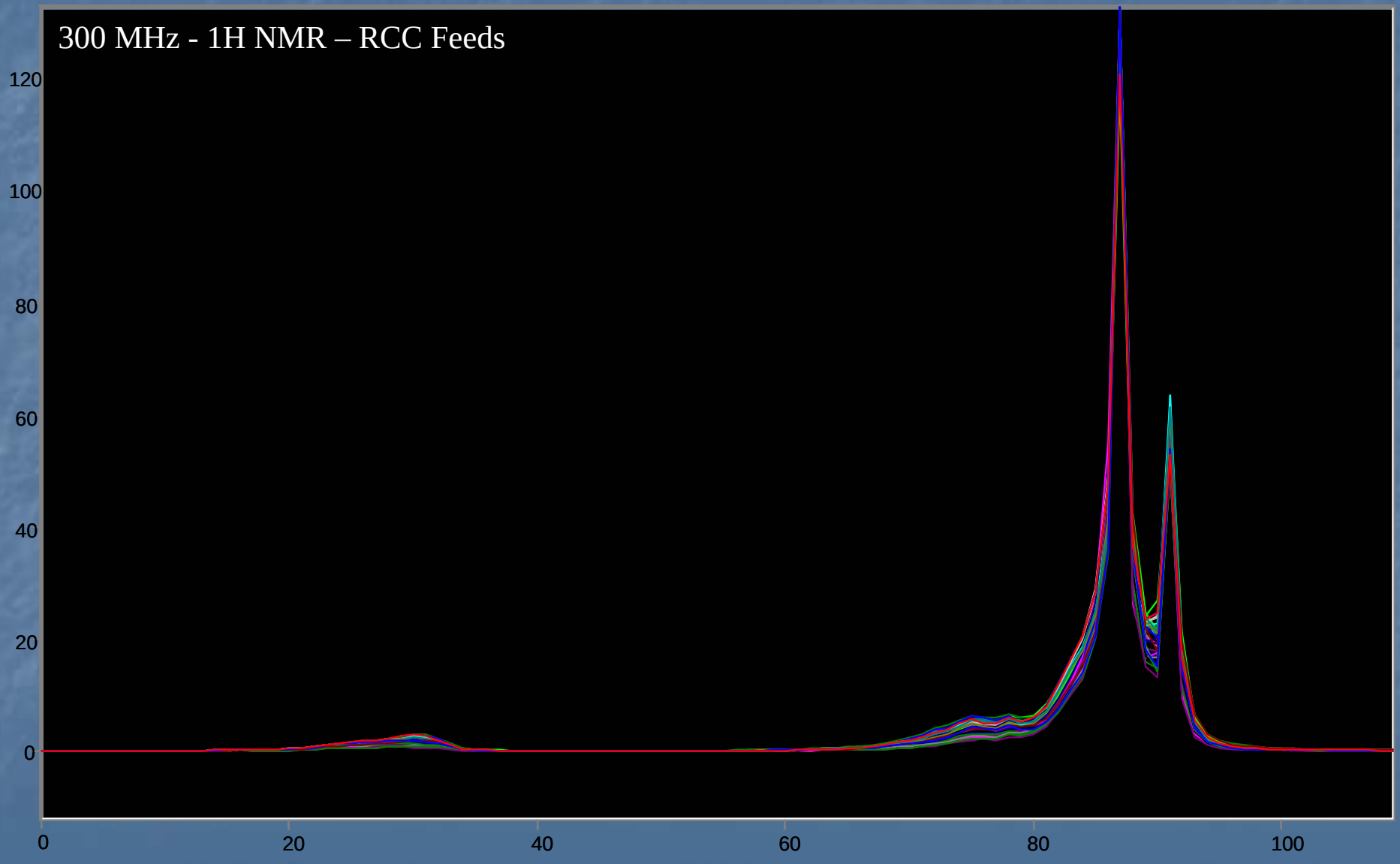
Calculation – Watson K-Factor

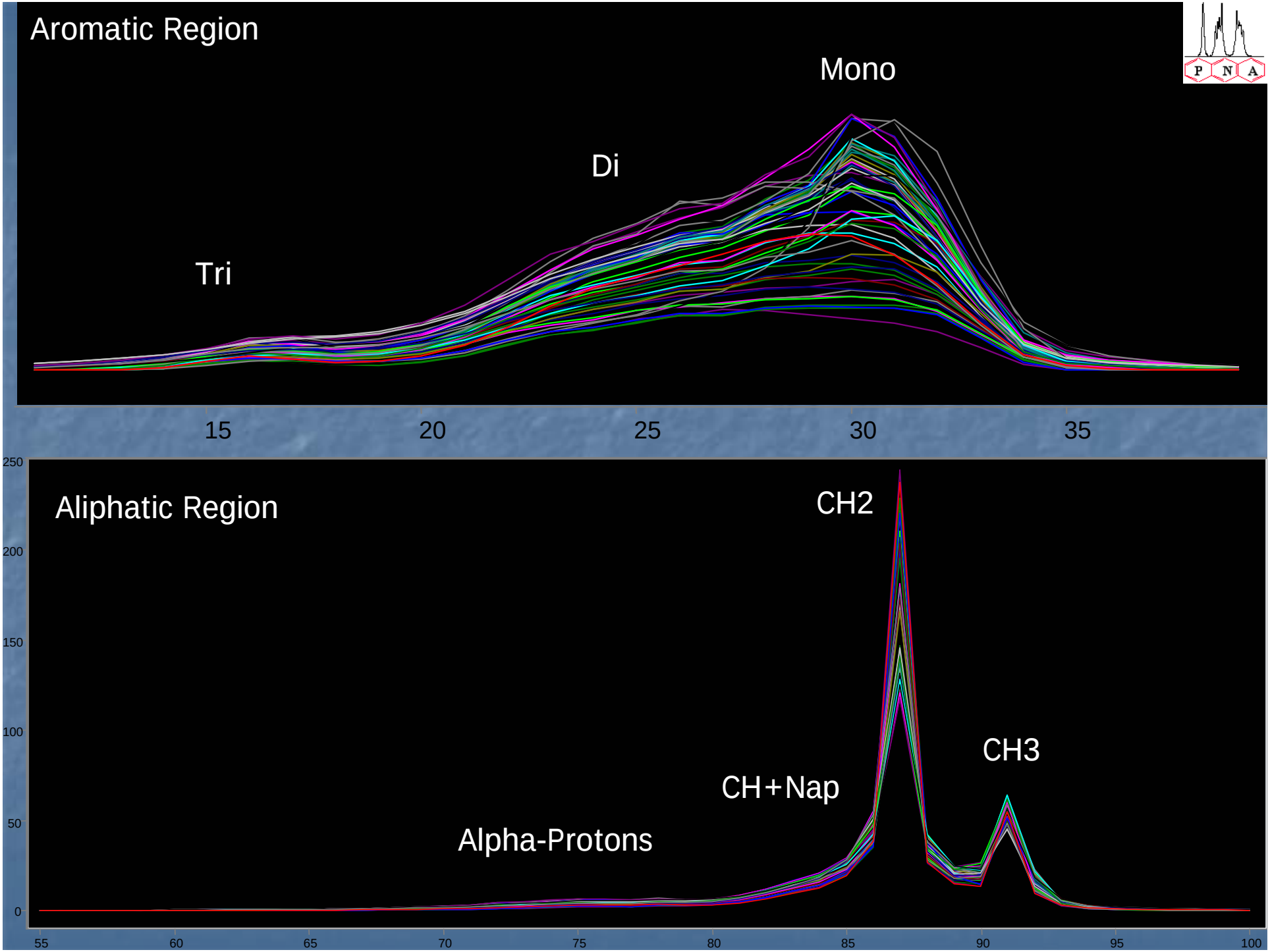
Outcome: aromatic carbon number
aromatic hydrogen number
total hydrogen content

Proposition: Detailed hydrocarbon analysis for kinetic model development

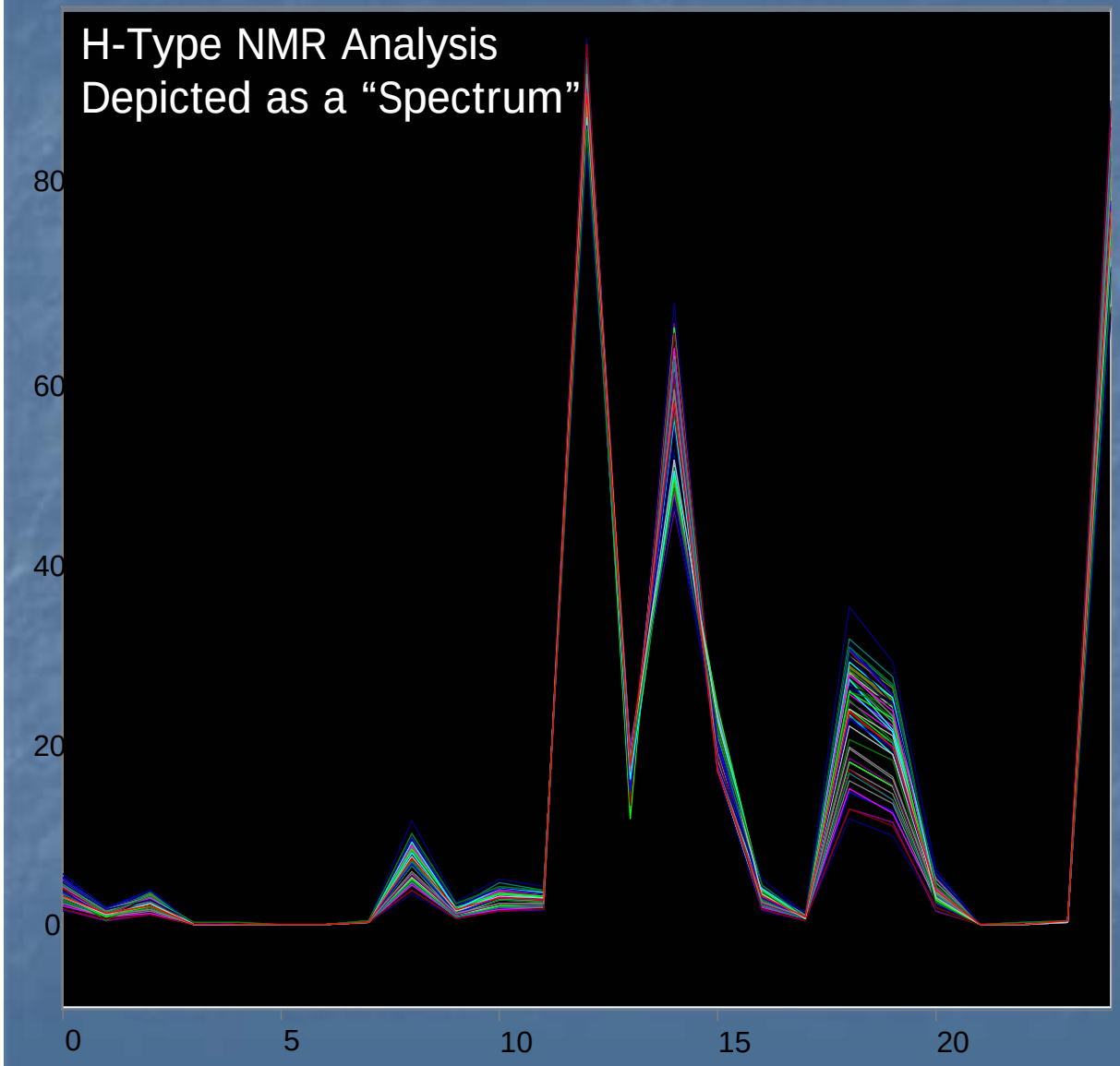

60 MHz Process – ^{1}H NMR Data
50 Samples
Aromatic Region
Aliphatic Region
CH_2
CH_3

Process NMR Associates



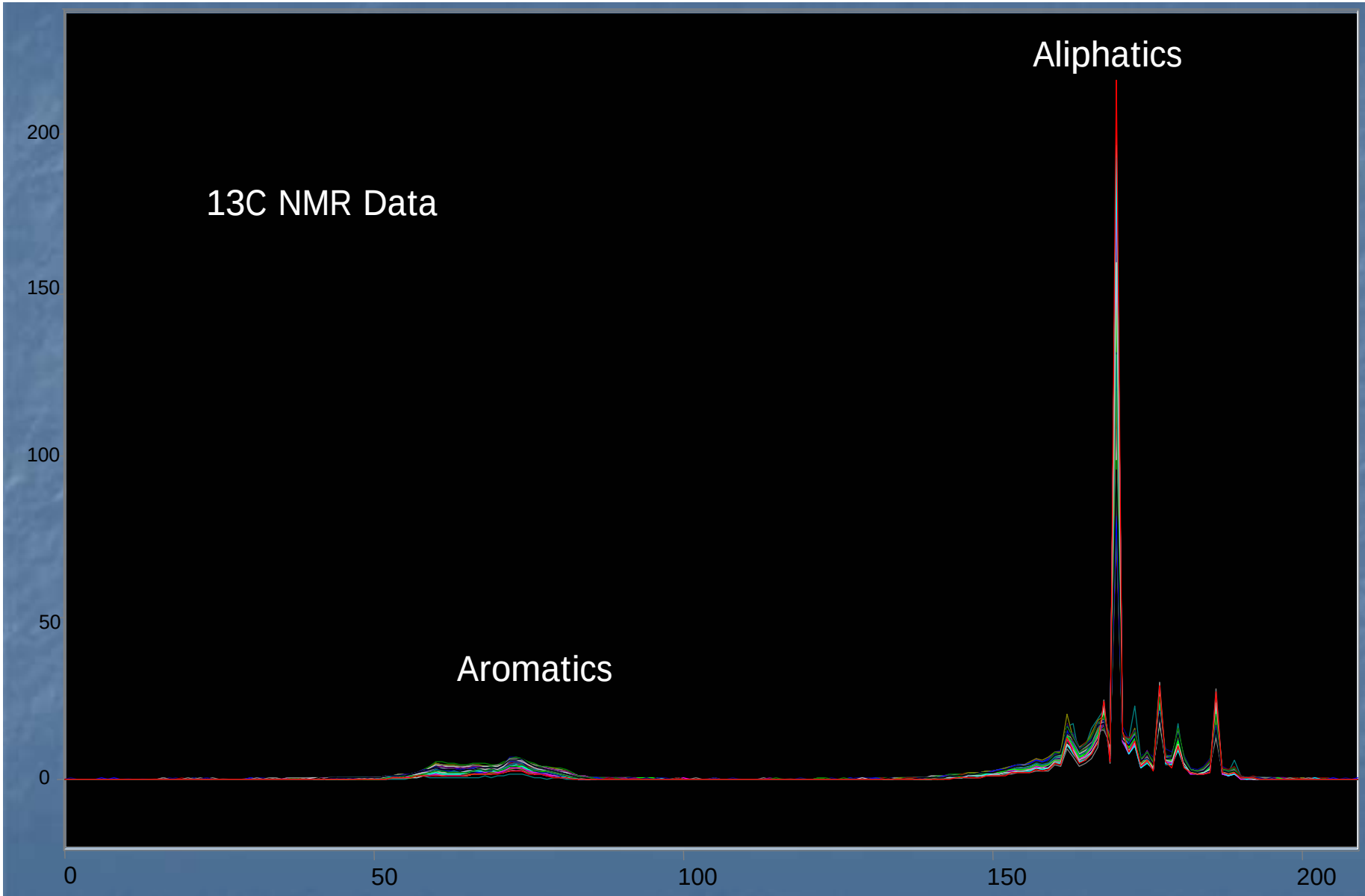

Aromatic Region
Mono
Di
Tri
15
20
25
30
35
Aliphatic Region
CH2
CH3
CH+Nap
Alpha-Protons
250
200
150
100
50
0
55
60
65
70
75
80
85
90
95
100

Process NMR Associates

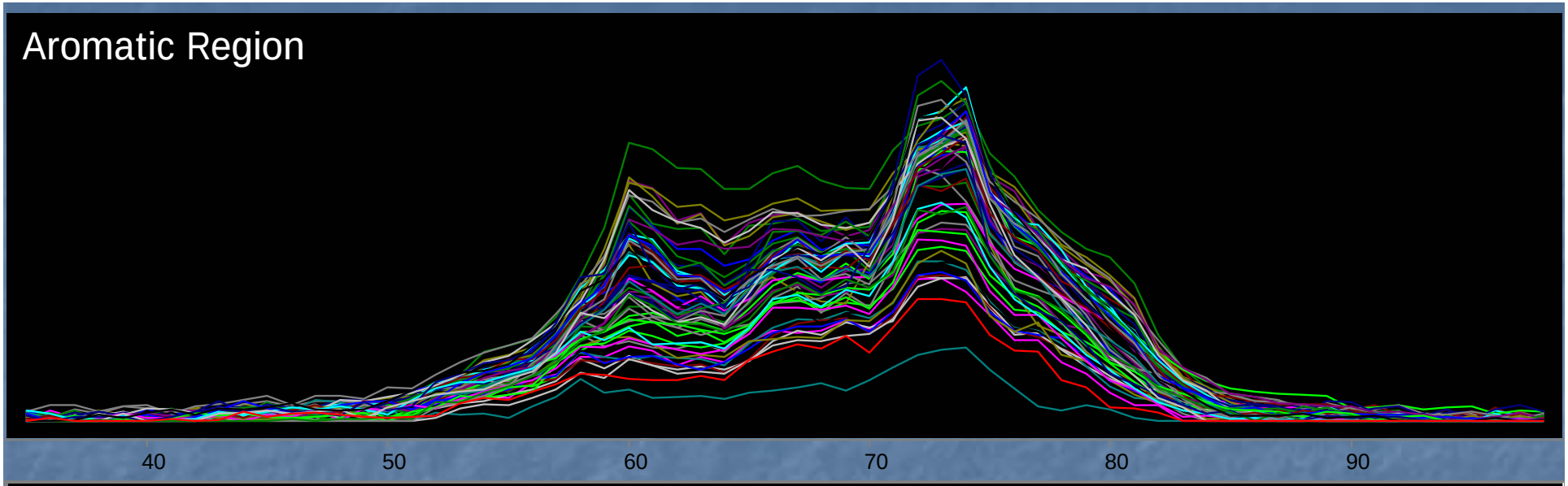


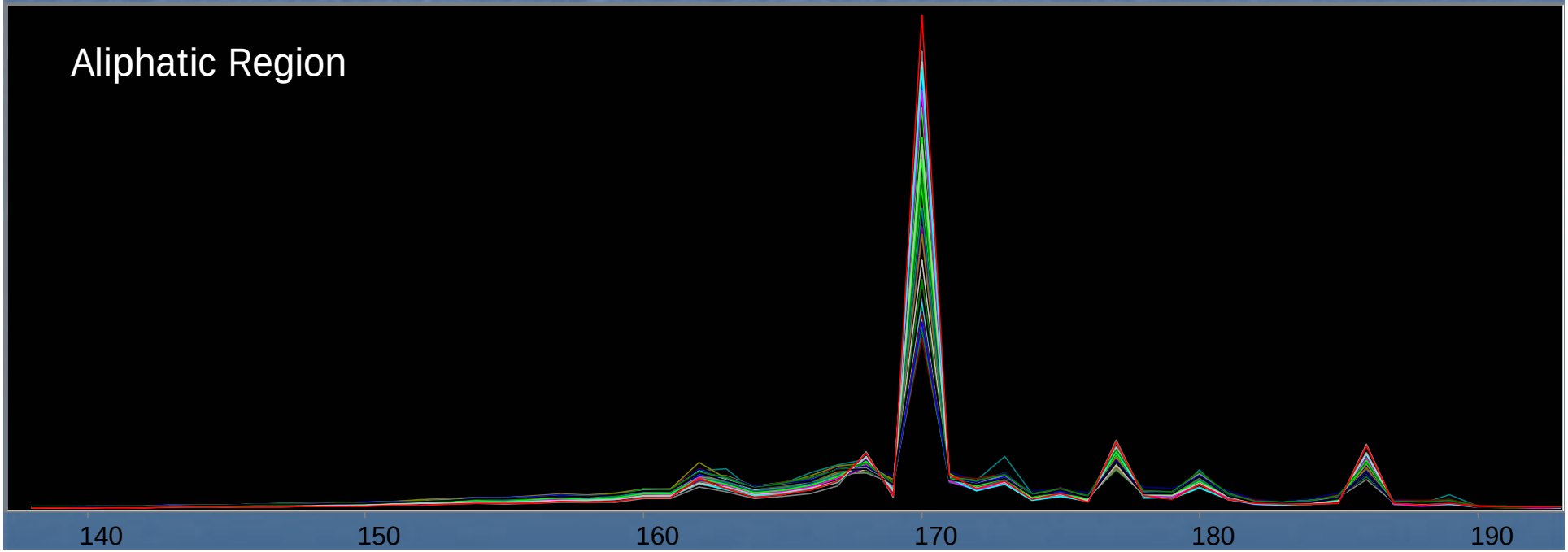
Parameter	1H - Type Analysis
1	Total aromatic
2	Diaromatic+ protons
3	Monoaromatic protons
4	Total olefinic
5	R**H**C=CH_2
6	R**H**C=C**H**R
7	RHC=C$\mathbf{H}_2$
8	Oxygenates protons
9	Total α protons to aromatics
10	a-CH to aromatics
11	a-CH_2 to aromatics
12	a-CH_3 to aromatics
13	Saturates
14	Paraffinic CH
15	Paraffinic CH_3
16	Paraffinic CH_3
17	Substituted aromatic carbon
18	Bridgehead carbons
19	Total aromatics (wt %)
20	Mono aromatics (wt %)
21	Di+ aromatics (wt %)
22	Benzene (wt %)
23	Olefin functions (wt %)
24	Oxygenates (wt %)
25	Saturates (wt %)

Process NMR Associates



Process NMR Associates

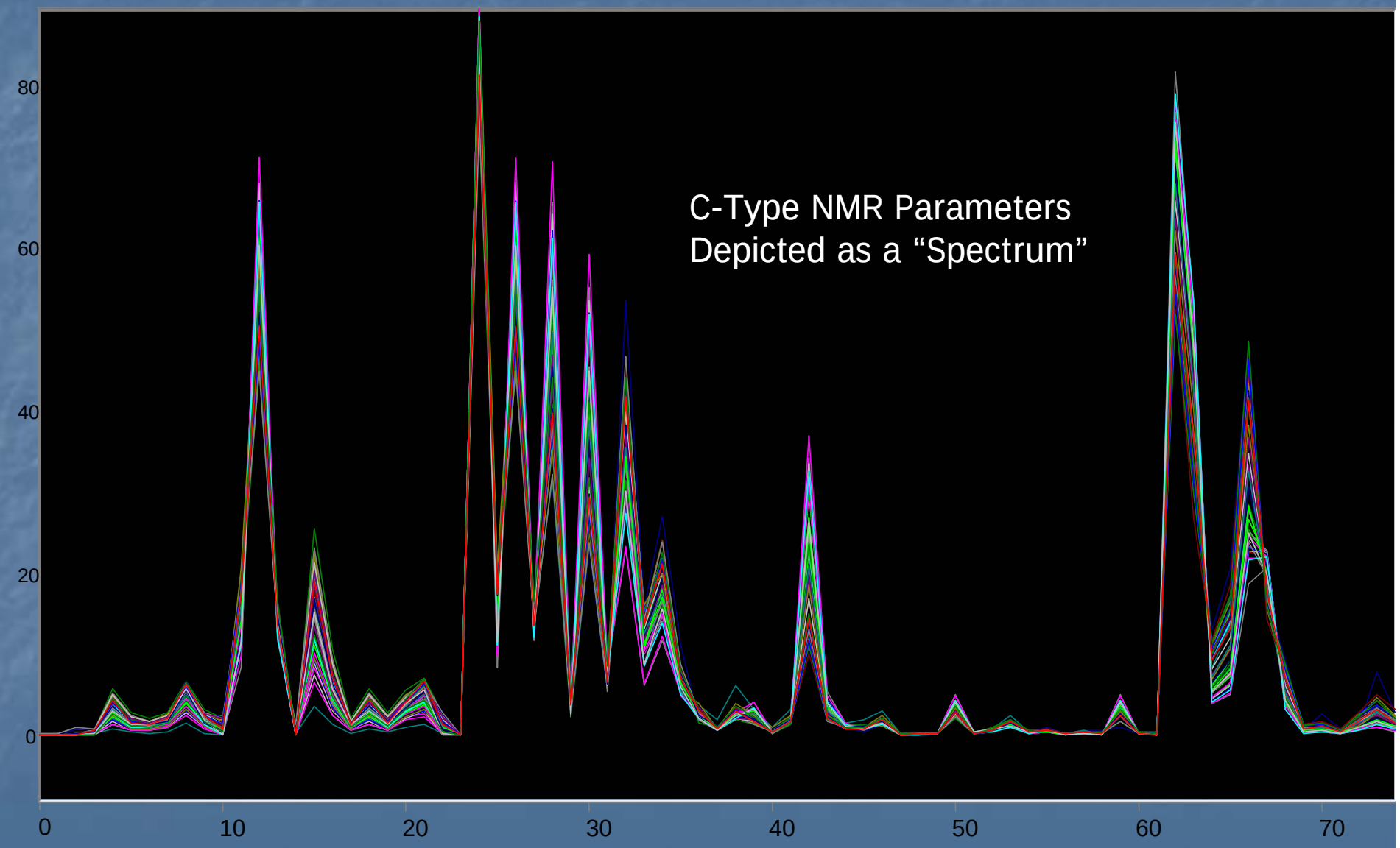




Calculated C-Type Parameters

Index	Carbon Type Parameters (%C Unless Otherwise Listed)	Index	Carbon Type Parameters (%C Unless Otherwise Listed)	Index	Carbon Type Parameters (%C Unless Otherwise Listed)
1	Ketone carbonyl carbon %c	26	Aliphatic methine carbon (CH)	51	b
2	Aldehyde carbonyl carbon	27	Aliphatic methylene carbon (CH2)	52	2-Me
3	Carboxylic acids, esters and amides carbonyl carbon	28	Aliphatic methyl carbon (CH3)	53	Aromatic a methyl carbon
4	Phenoxy carbon	29	Total paraffinic carbon	54	All other-Me
5	CH2 & CH sub aromatic carbon	30	Paraffinic methine carbon (CH)	55	3-Me
6	Naphthenic sub aromatic carbon	31	Paraffinic methylene carbon (CH2)	56	Reg7
7	CH3 sub aromatic carbon	32	Paraffinic methyl carbon (CH3)	57	p-Pr
8	Half of internal aromatic carbon	33	Total naphthenic carbon	58	t-Pr
9	Protonated Internal aromatic C+ 1/2 internal aromatic C	34	Naphthenic methine carbon (CH)	59	4-Me
10	Protonated aromatic carbon	35	Naphthenic methylene carbon (CH2)	60	a
11	Heteroaromatic other than phenoxy carbon	36	Naphthenic methyl carbon (CH3)	61	t-Ethyl
12	Methine carbon	37	Reg1	62	p-Ethyl
13	Methylene carbon	38	a'	63	Linear Paraffin Structure: % Linear Paraffin/Total Paraffin
14	Methyl carbon	39	Reg2	64	Waxiness : % Epsilon C/Total Paraffin
15	Total carbonyl carbon	40	g	65	Branching Index: %Branching CC/Total Paraffin
16	Total aromatic carbon	41	Reg3	66	Total Branching Content: % C Near Branching C/Total C
17	Aliphatic sub aromatic carbon	42	g'	67	C in Branched Environment: % 1-linear paraffin structure
18	Methyl-substituted aromatic carbon	43	e	68	Average Straight Chain Length (C No.)
19	CH2 & CH substituted aromatic carbon	44	d	69	Methyl branching index
20	Naphthenic substituted aromatic carbon	45	Reg4	70	Ethyl branching Index
21	Internal aromatic carbon	46	b'	71	Propyl branching Index
22	Peripheral unsubstituted aromatic carbon	47	Reg5	72	Butyl branching Index
23	Total heteroaromatic carbon	48	p-Bu	73	Total ethyl branching content
24	Total olefinic carbon	49	t-Bu	74	Total propyl branching content
25	Total aliphatic carbon	50	Peak x	75	Total butyl branching content

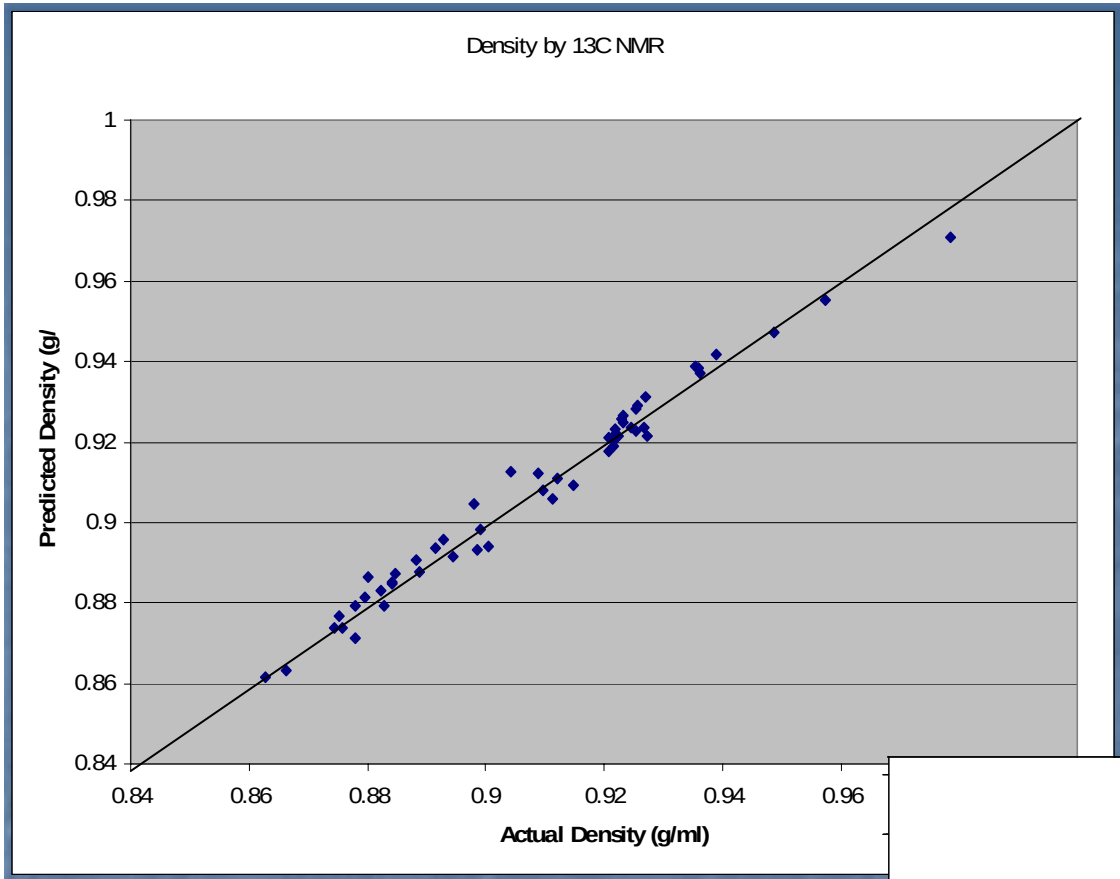
Process NMR Associates

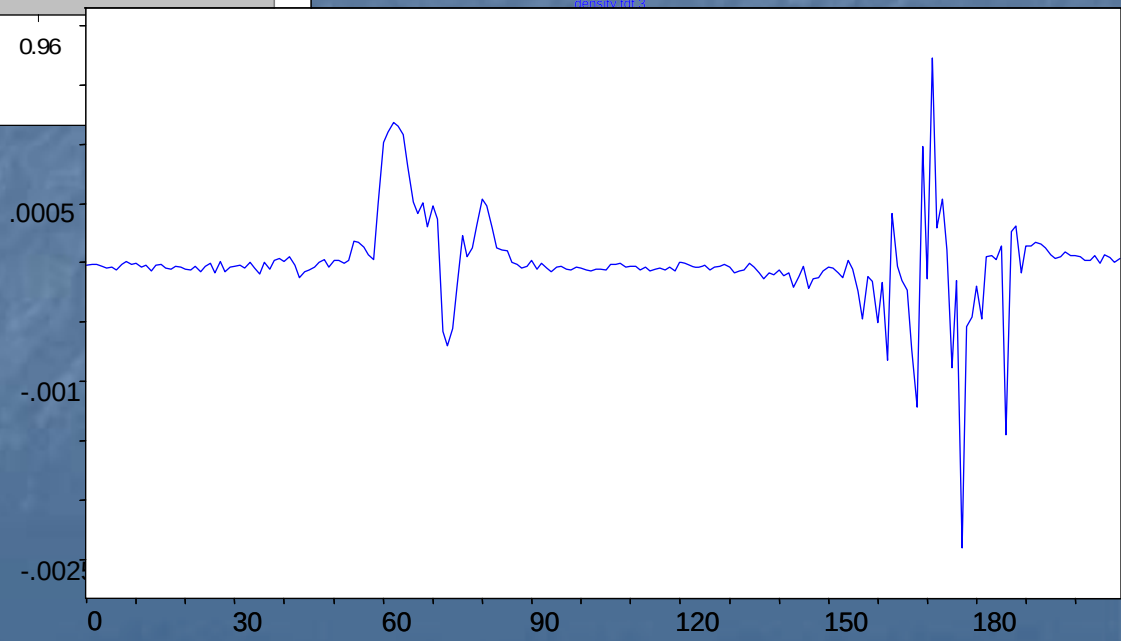


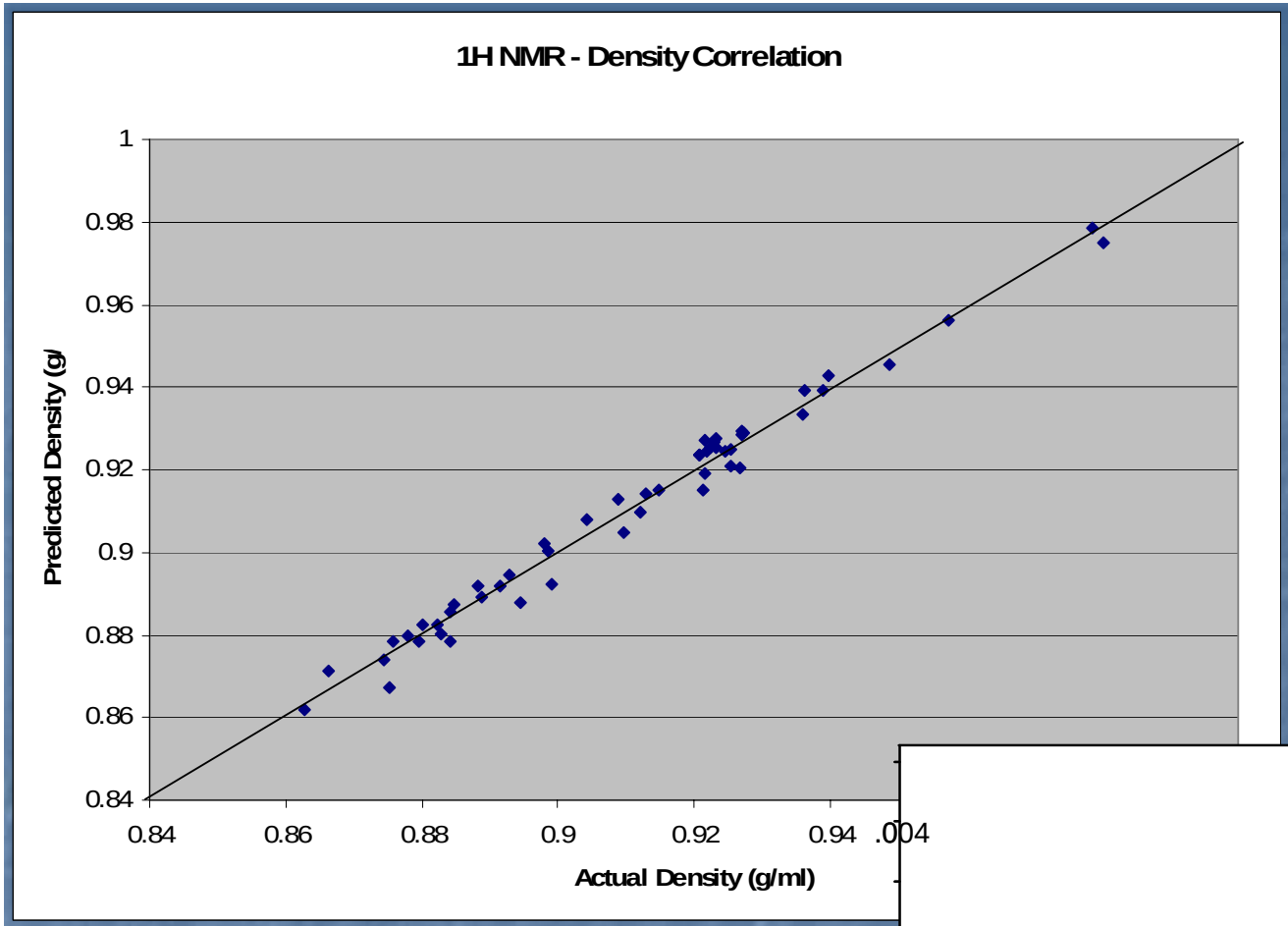
Summary of RCC Feed NMR Analysis – Correlations to Physical/Chemical Properties

Resonance Frequency	60 MHz Proton	300 MHz Proton		75 MHz Carbon-13	
Parameter	1H NMR 0.1 ppm Bin	1H NMR - 0.1 ppm Bin	H-Type Spectrum	13C NMR- 1 ppm Bin	C-Type Spectrum
Density at 15°C	0.961	0.983	0.924	0.982	0.974
Viscosity Index	-	0.951	-	0.935	-
MCRT	0.940	0.952	0.727	0.931	0.875
SULPHUR	0.931	0.964	0.855	0.979	0.962
Carbon Aromaticity	0.958	0.951	0.926	0.998	0.997
HYDROGEN	0.925	0.914	0.819	0.922	0.862
Total Aromatics	0.936	0.946	0.904	0.965	0.941
Monoaromatics	0.930	0.941	0.912	0.954	0.897
Diaromatics	0.927	0.945	0.866	0.951	0.897
TriAromatics	0.941	0.911	0.862	0.939	0.863
Tetra+ aromatics	0.913	0.921	0.656	0.912	0.934

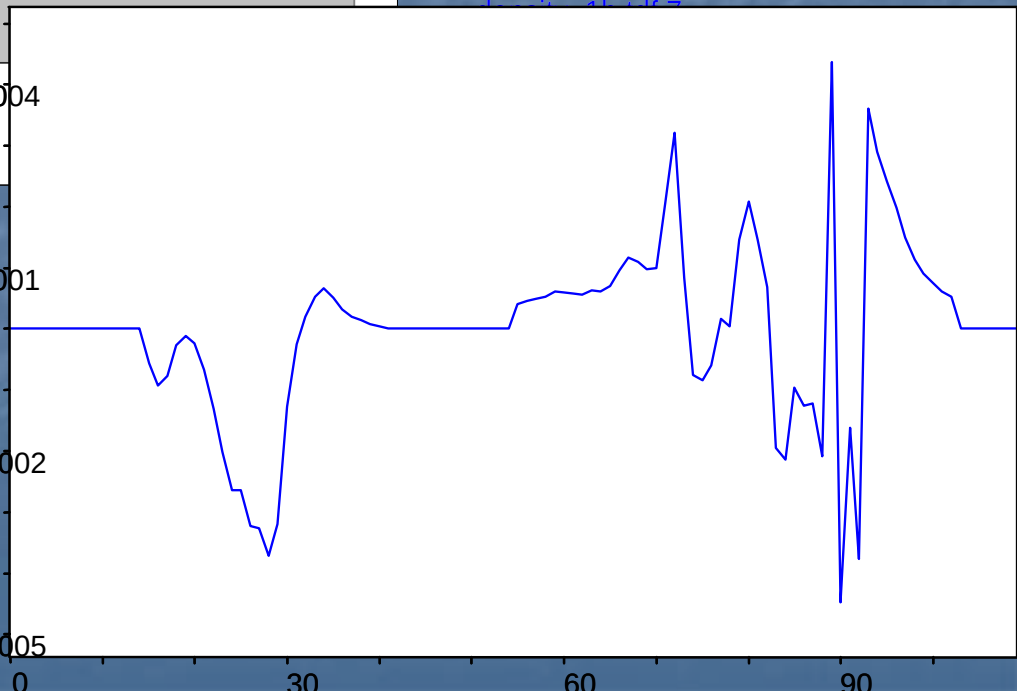
^{13}C NMR Correlation to Density

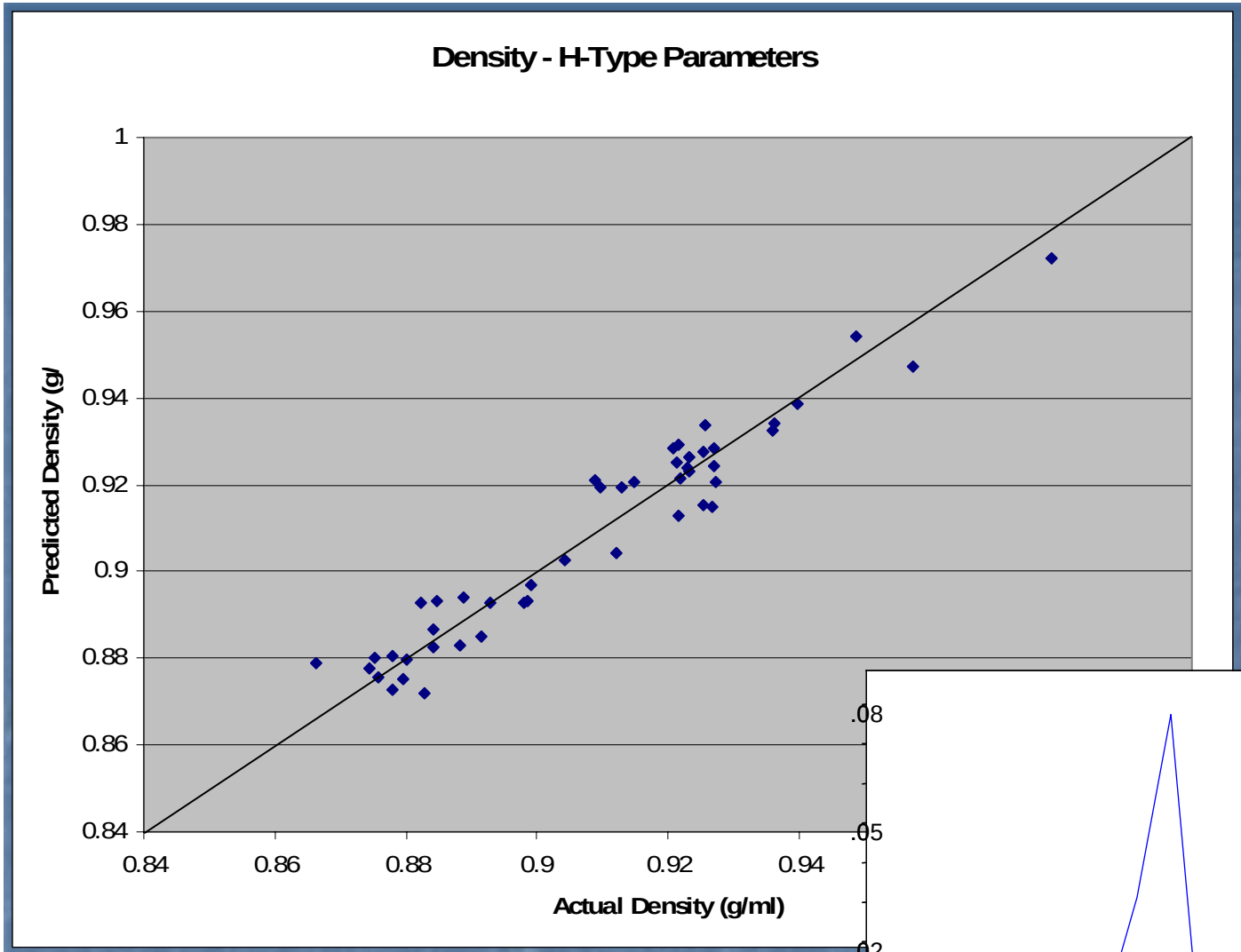


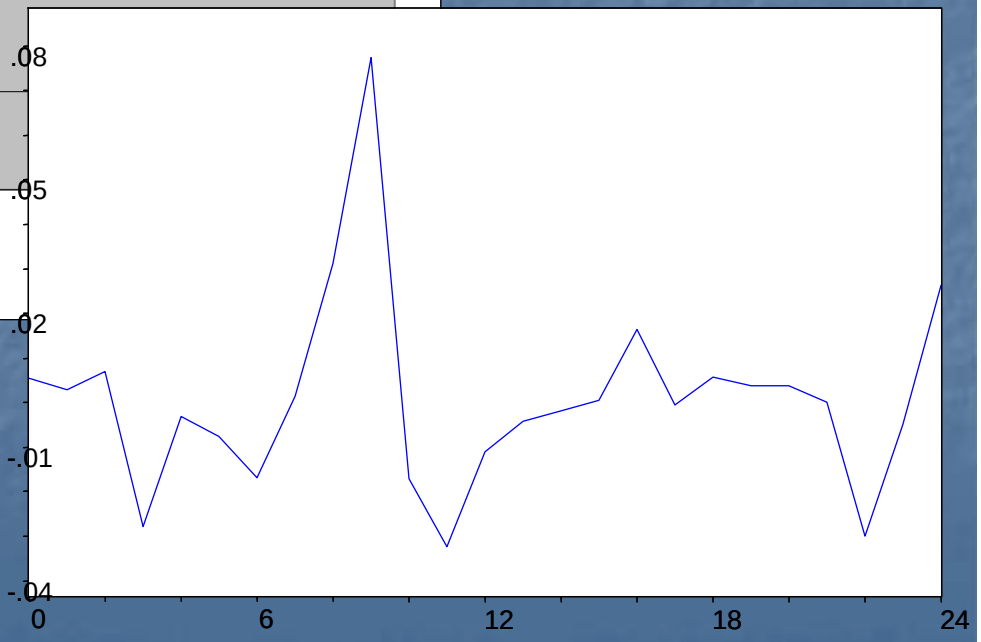




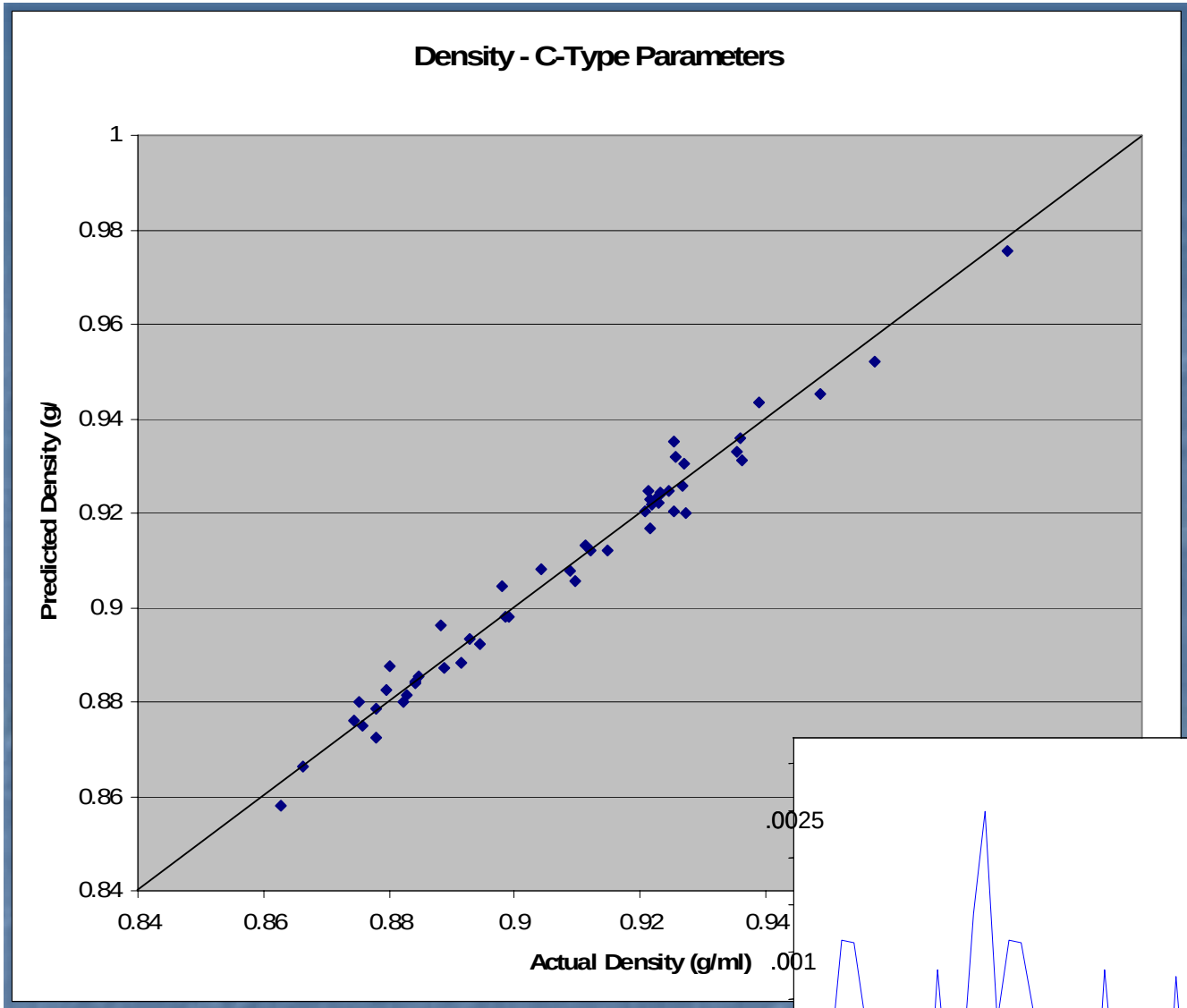
1H NMR Correlation to Density

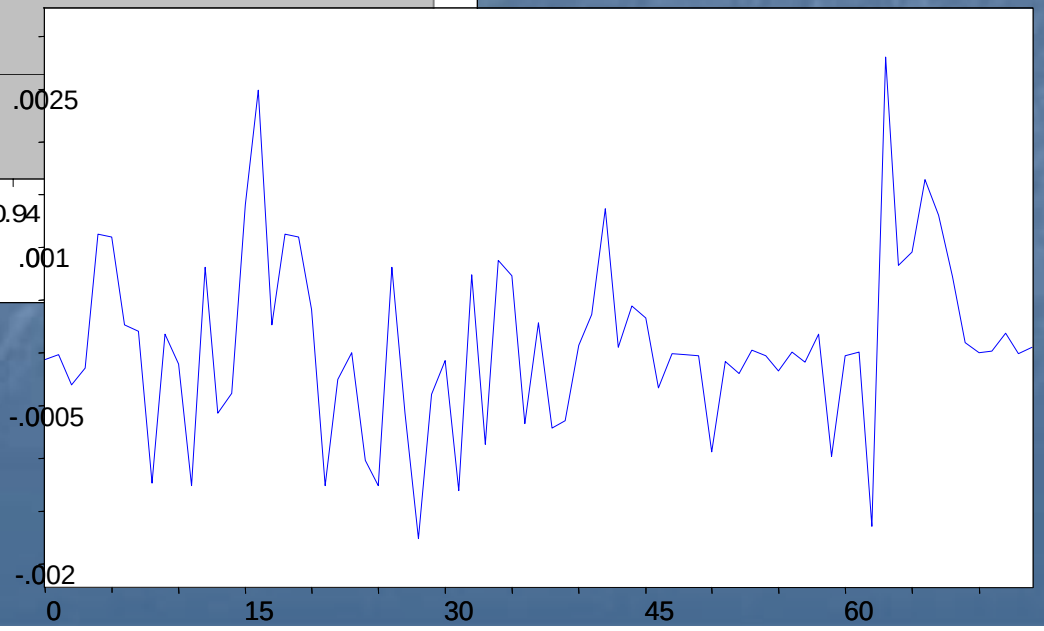




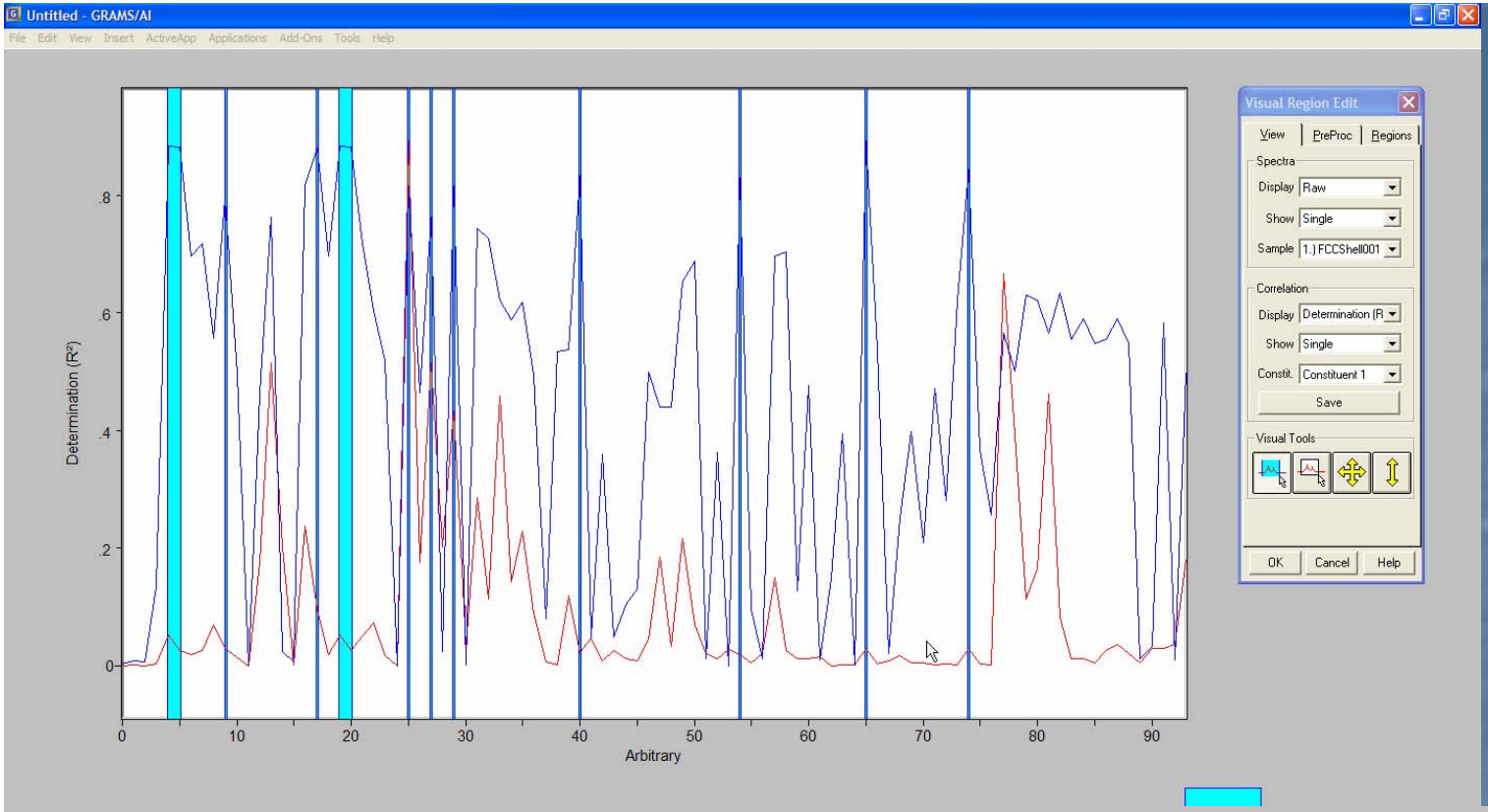


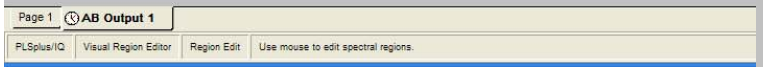
Density Correlation with
Proton Type Parameters





Density Correlation with Carbon Type Parameters

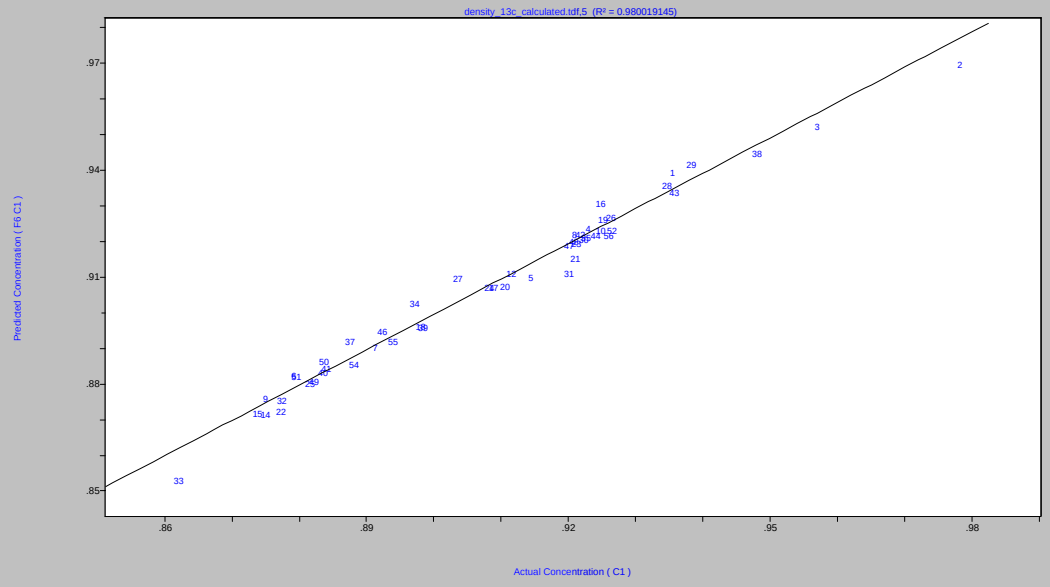




Variable Selection Process

Reduces Number of Variables

Linear Equations that Describe Density in terms of 13 Carbon Type Parameters



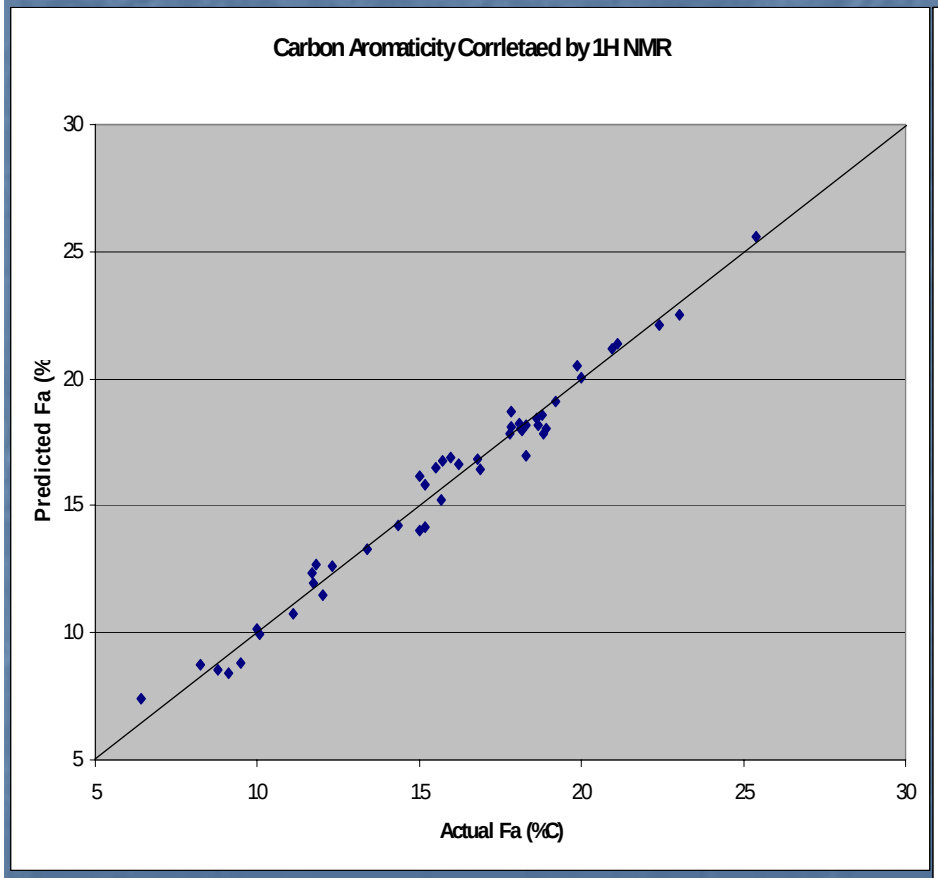
Correlation of ^{1}H and ^{13}C NMR Spectra to ^{13}C Derived Parameters

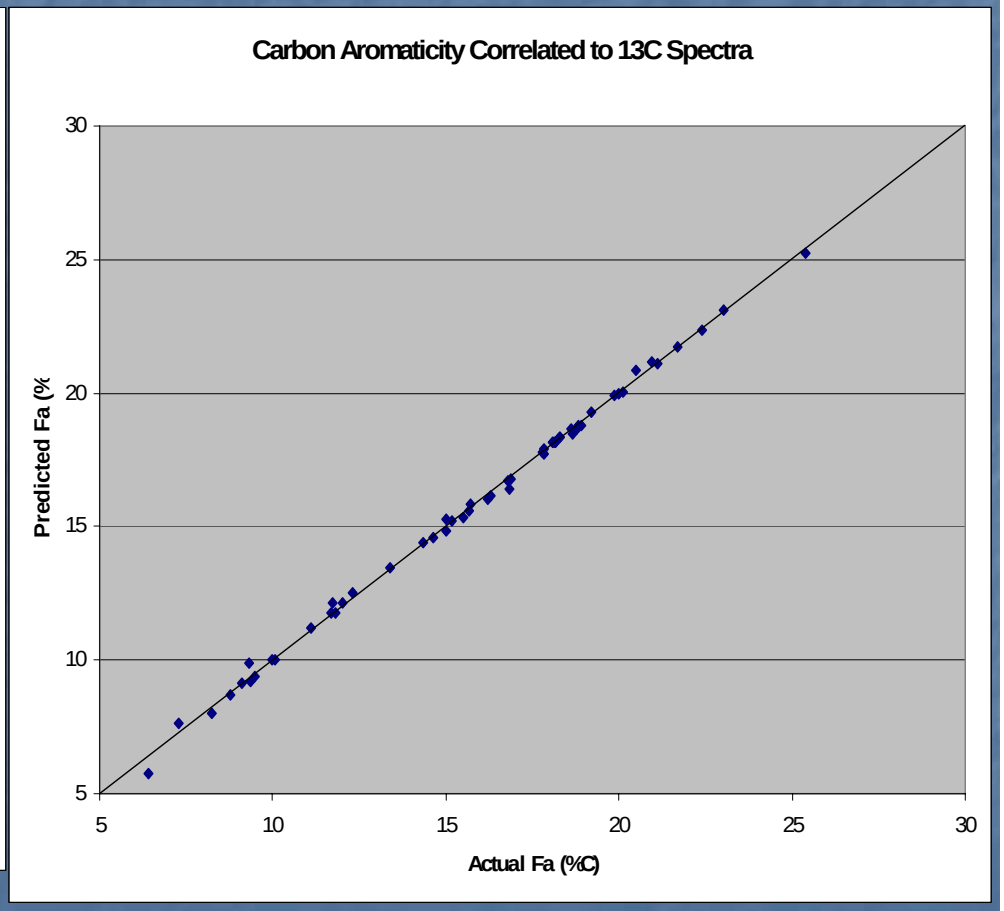
13C Parameter	1H NMR	13C NMR
Total aromatic carbon	0.980	0.996
Aliphatic substituted aromatic carbon	0.962	0.999
Methyl-substituted aromatic carbon	0.970	0.994
CH2 & CH substituted aromatic carbon	0.935	0.996
Naphthenic substituted aromatic carbon	0.973	0.996
Internal aromatic carbon	0.949	0.994
Peripheral unsubstituted aromatic carbon	0.950	0.996
Total heteroaromatic carbon	0.275	0.976
Total aliphatic carbon	0.952	0.997
Aliphatic methine carbon (CH)	0.932	0.999
Aliphatic methylene carbon (CH2)	0.976	1.000
Aliphatic methyl carbon (CH3)	0.610	0.996
Total paraffinic carbon	0.984	0.995
P methine carbon (CH)	0.876	0.940
P methylene carbon (CH2)	0.987	0.998
P methyl carbon (CH3)	0.810	0.960
Total naphthenic carbon	0.964	0.989
N methine carbon (CH)	0.927	0.996
N methylene carbon (CH2)	0.957	0.987
N methyl carbon (CH3)	0.809	0.966
N methine/N methylene ratio	0.085	0.878
Mole fraction of bridgehead aromatic carbon	0.448	0.899
Aromatic carbons per aromatic group	0.697	0.895

13C Parameter	1H NMR	13C NMR
Cluster number (=aromatic group number)	0.941	0.995
Aliphatic substitutions per cluster	0.087	0.906
Methyl-substitutions per cluster	0.379	0.909
CH2 & CH substitutions per cluster	0.063	0.899
Naphthenic substitutions per cluster	0.227	0.910
Heteroatoms per cluster	0.032	0.926
Naphthenic CH3 per cluster	0.449	0.906
# of naphthenic ring carbons per cluster	0.524	0.924
Naphthenic rings per cluster	0.317	0.939
# of paraffinic carbons per cluster	0.892	0.934
Average chain length of paraffinic substitutions	0.913	0.932
Linear paraffin structure	0.972	0.976
Waxiness : e/total paraffin	0.977	0.983
Branching index	0.973	0.972
Total branching content	0.964	0.972
Carbons in branched environment	0.972	0.976
Average straight chain length	0.967	0.986
Methyl branching index	0.972	0.962
Ethyl branching Index	0.945	0.945
Propyl branching Index	0.919	0.932
Butyl branching Index	0.919	0.951
Total ethyl branching content	0.946	0.946
Total propyl branching content	0.919	0.933
Total butyl branching content	0.917	0.950

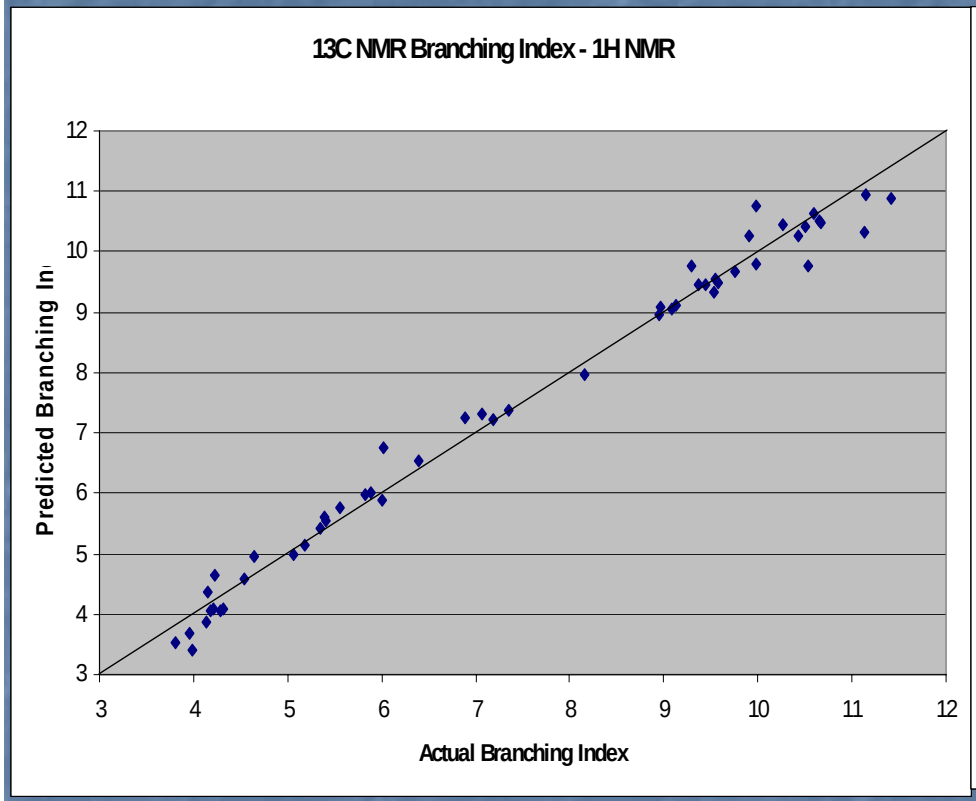
Process NMR Associates

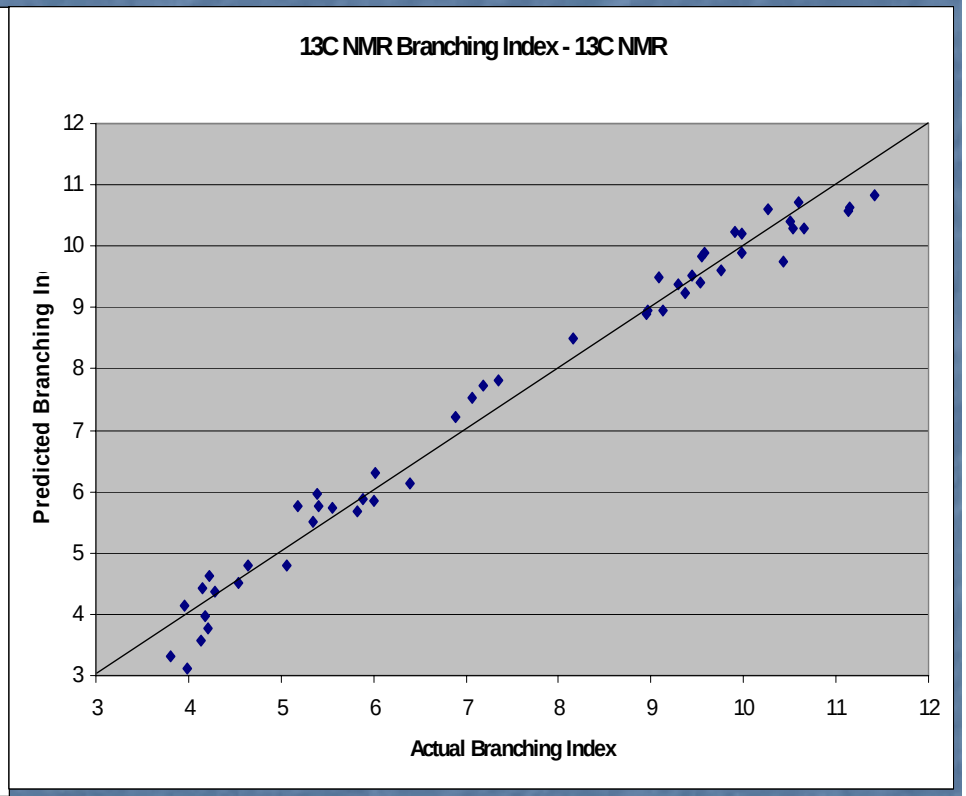
^{1}H and ^{13}C NMR Correlation to Carbon Aromaticity





1H and 13C NMR Correlation to Branching Index





Branching Carbons/Total Paraffinic Carbons

Summary

Chemical and Physical Properties of RCC Feedstreams can be determined by ^{1}H NMR (at 60 and 300 MHz) and by ^{13}C NMR

H-Type and C-Type Parameters do not provide as good a correlation as is observed by full spectrum regression. This is due to loss of resolved chemical shift information when the spectrum is reduced to larger integral areas.

^{1}H NMR can be combined with PLS regression modeling to provide detailed carbon type analysis for RCC Feeds

Regression analysis of ^{13}C NMR data can be utilized to fully automate the prediction of ^{13}C NMR type analysis : reducing the necessity for considerable knowledge and analysis time on the part of the analyst.

Parallel Work

Similar analysis has been performed on:

Crude Oil - TBP, Density, Water
Canadian Syncrude - Olefins, Density, Distillation
Vacuum Residues – Distillation, Density, ^{13}C Parameters
Naphtha – Density, PIONA, Distillation
Gasoline – Octane, Benzene, Oxygenates, Distillation, Aromatics
Kerosene – Distillation, Smoke Point
Jet Fuel – Cloud Point, Freeze Point, Distillation, Density
Diesel – Density, Cloud point, Flash, Distillation, Cetane Index
Reformate – Octanes, Benzene, Aromatics
Alkylate – Octane, Distillation
Lubricant Oil – Pour, VI, Distillation, ^{13}C Parameters
FT-Waxes – ^{13}C Parameters
VGO – FCC Feeds (Same as RCC Feeds)
Biodiesel