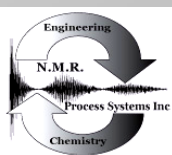




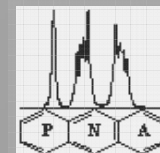
"Analytical Data For Engineering Support: Improving the Lab/Process Interface"

Paul J. Giammatteo* and John C. Edwards



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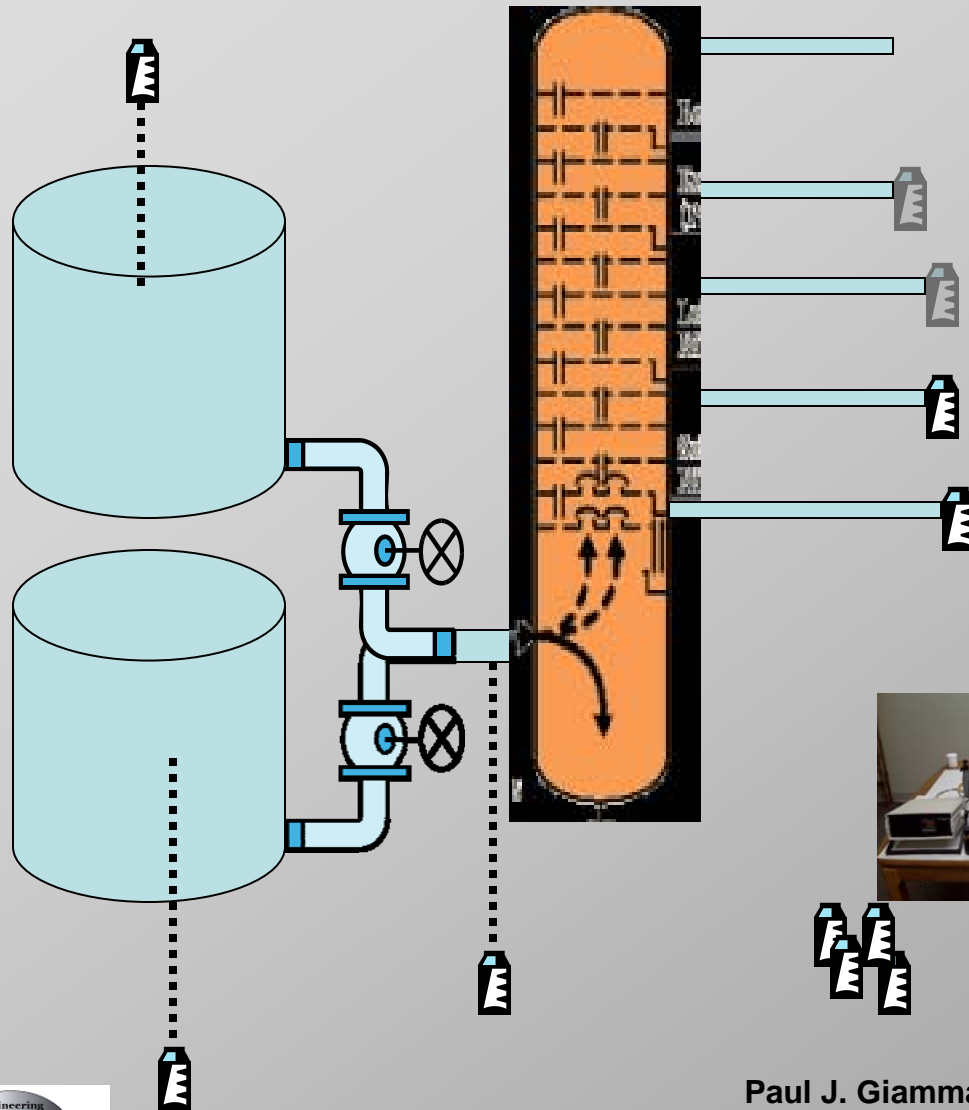
Smith's Detection IdentifyIR-HVP
Mid Infra-Red Spectrometer
Combined with Multi-parameter Prediction

This analyzer utilizes a diamond Attenuated Total Reflectance (ATR) cell. Infra-red/sample interaction occurs at the sample surface thereby eliminating the need to pass the incident beam through the sample. Liquids of all types of viscosity, gels, emulsions and solids are readily available for IR analysis.

The IdentifyIR's rugged design, small footprint, ease of use, and, spectral stability is advantageous in developing chemometric based property predictions on a variety of heavy process streams and/or feeds.

The target application described in the following slides is intended to enable plant engineering to obtain key property measurements as feed/stream inputs into off-line process simulation and planning tools.

Example: Crude Unit



Off-Line Simulation
Planning and Scheduling



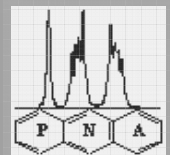
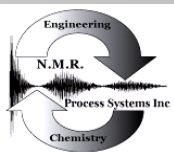
- Distillation (D86, Sim Dis, TBP)
- Flash Point
- Cloud Point
- Pour Point
- Freeze Point
- Chemistry (Aromatics, Benzene)
- API Gravity/Density
- Octane/Cetane

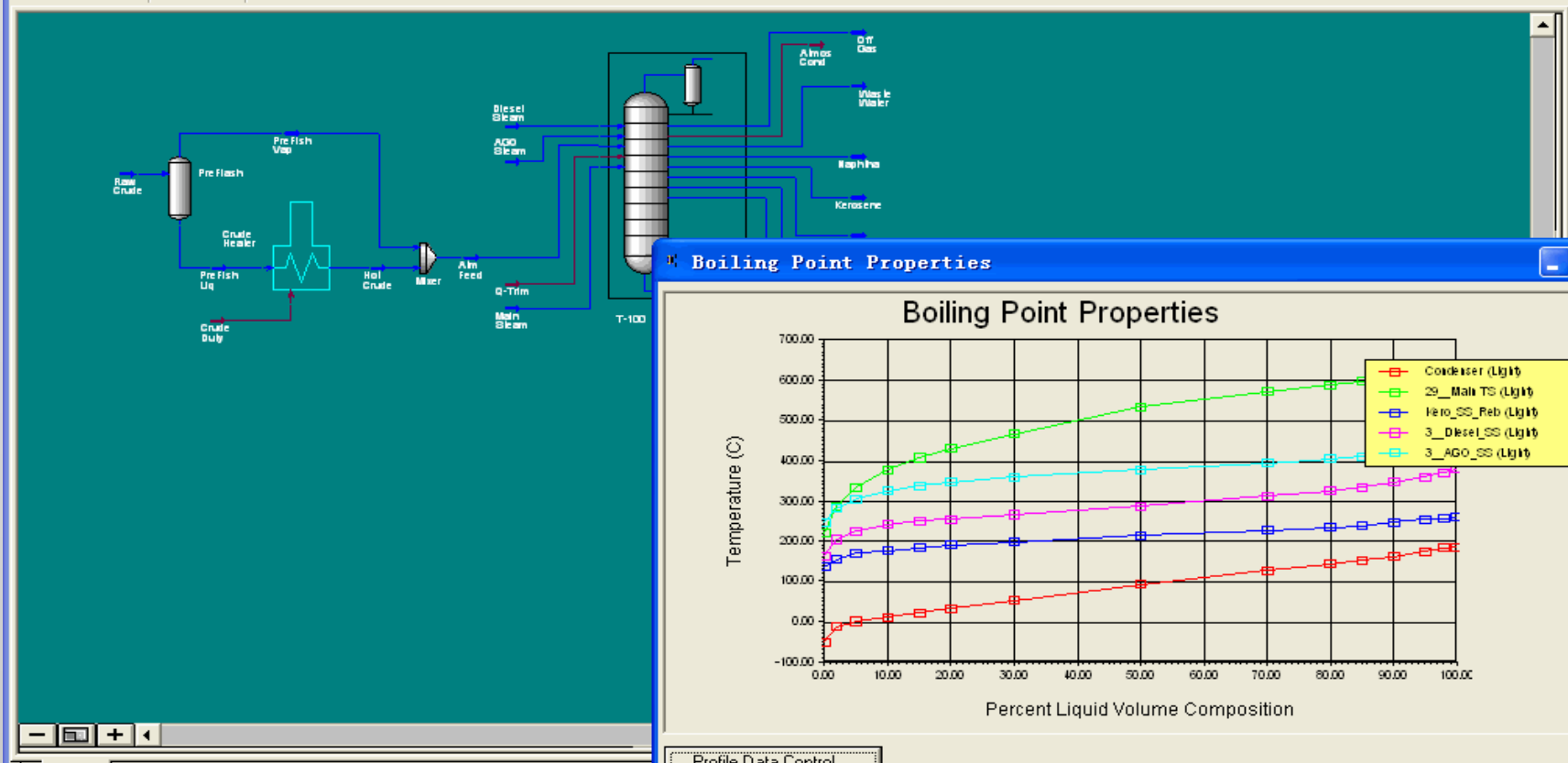


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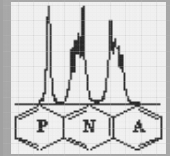
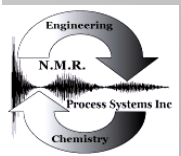
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Calculating Assay Assay-1:
Calculating Blend Blend-1:

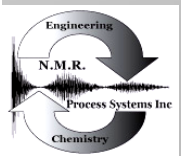
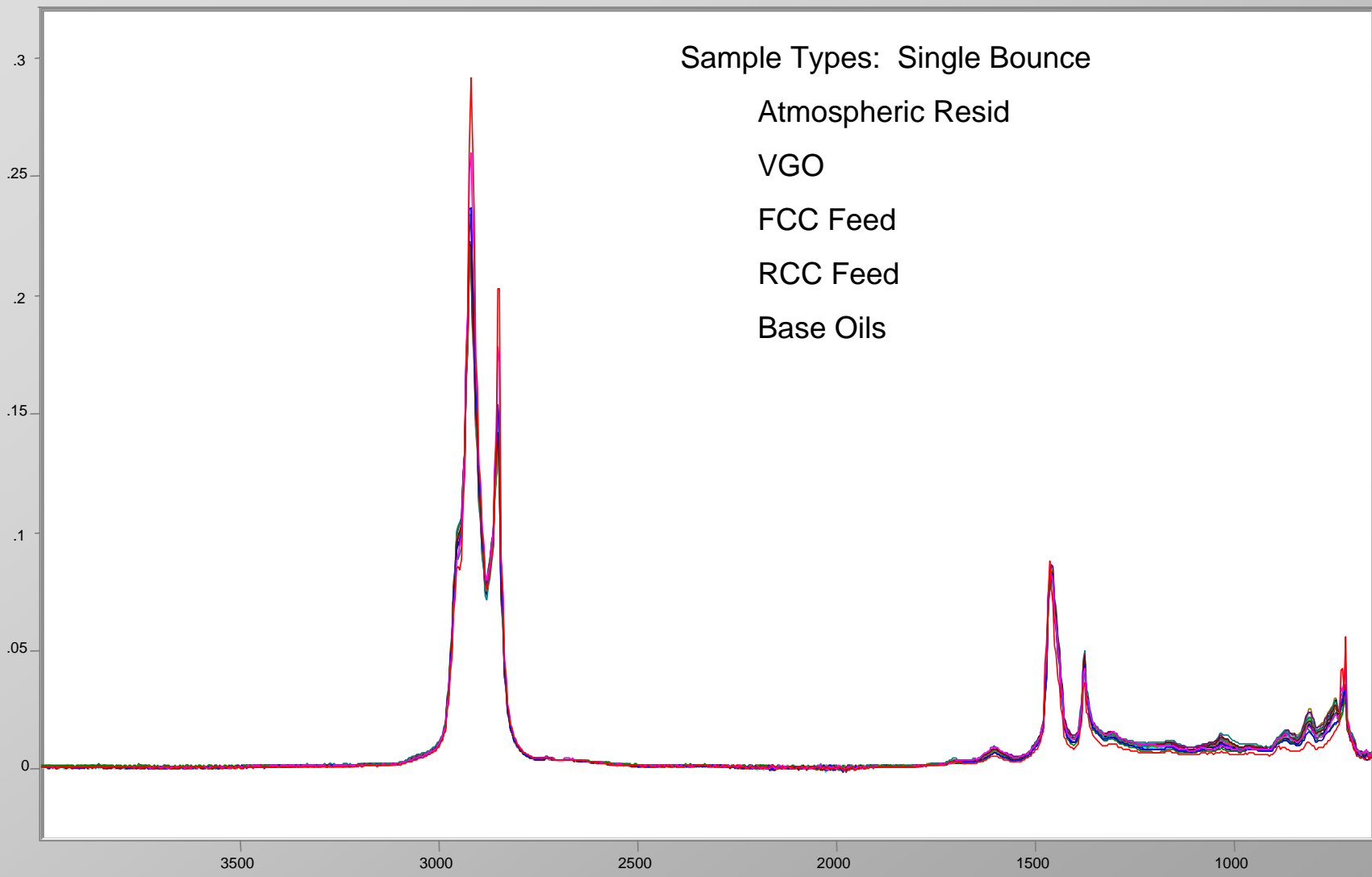




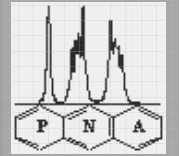
Initial work started on the Smith's Detection IdentifyIR with Diamond ATR single bounce puck.

In this configuration, all samples were run at ambient temperature.

Initial property predictions were developed on a "per stream" basis.



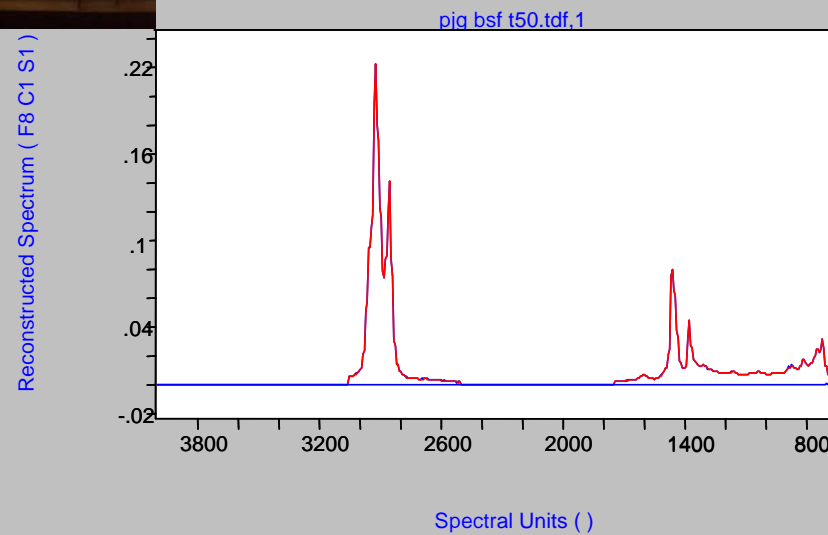
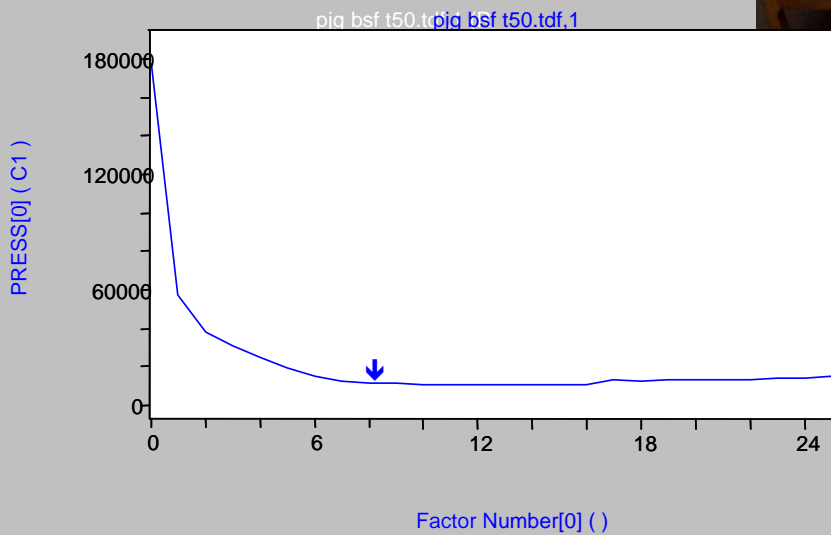
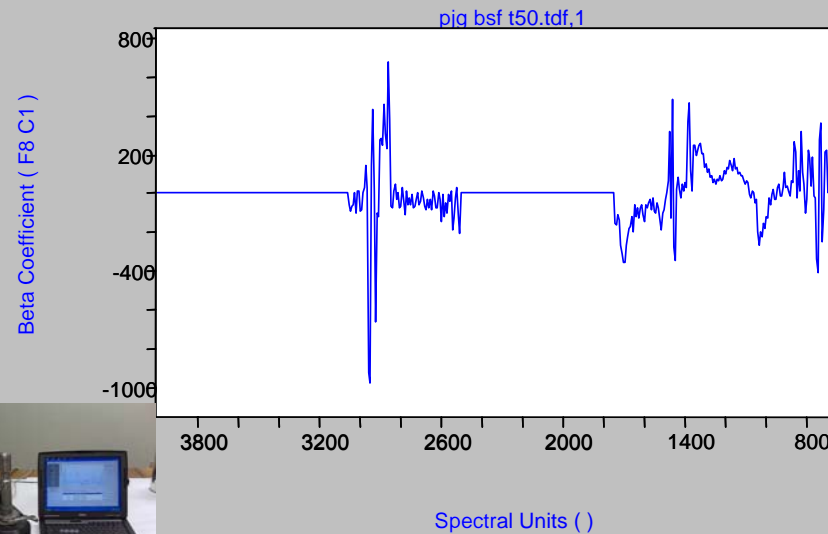
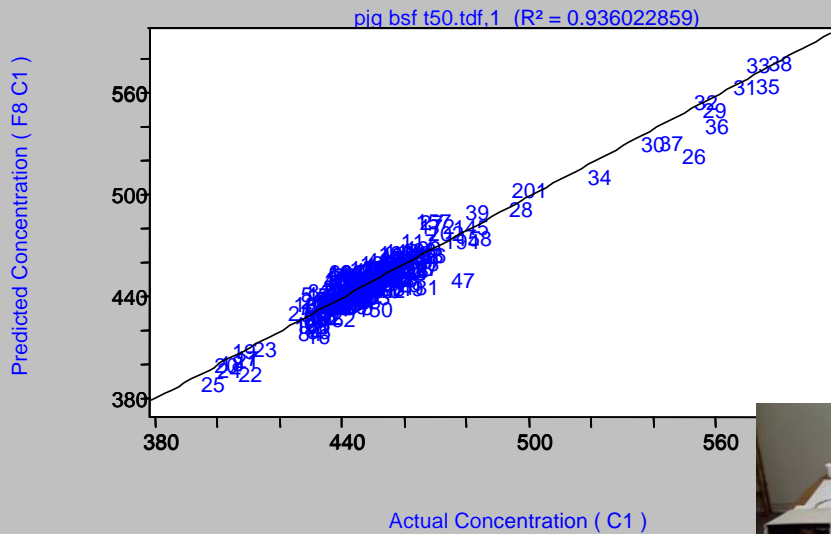
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The following 11 slides show the chemometric modeling protocols and results for several stream dependent properties. This work was performed on the IndentifyIR in it's standard configuration:

- Ambient Temperature Sample Puck
- Single Bounce
- Spectral window 4000 to 650 wave numbers
- 4 wave number resolution

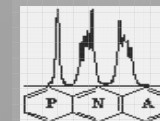
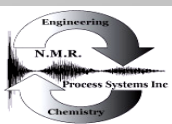
Modeling software Galactic Grams was used in all modeling using Partial Least Squares (PLS1) regression.



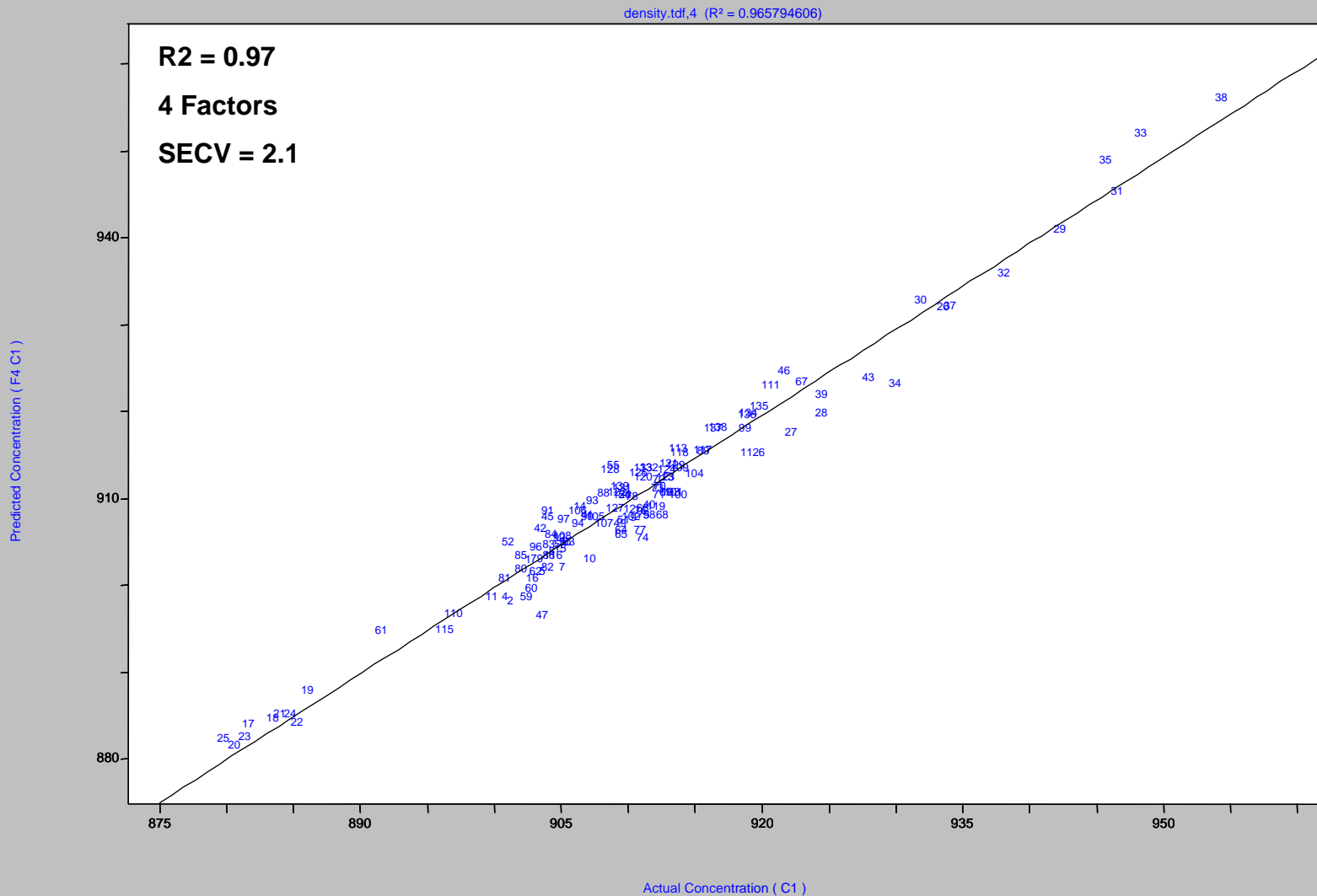
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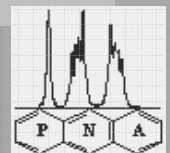
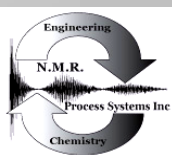
FCC Feed Density



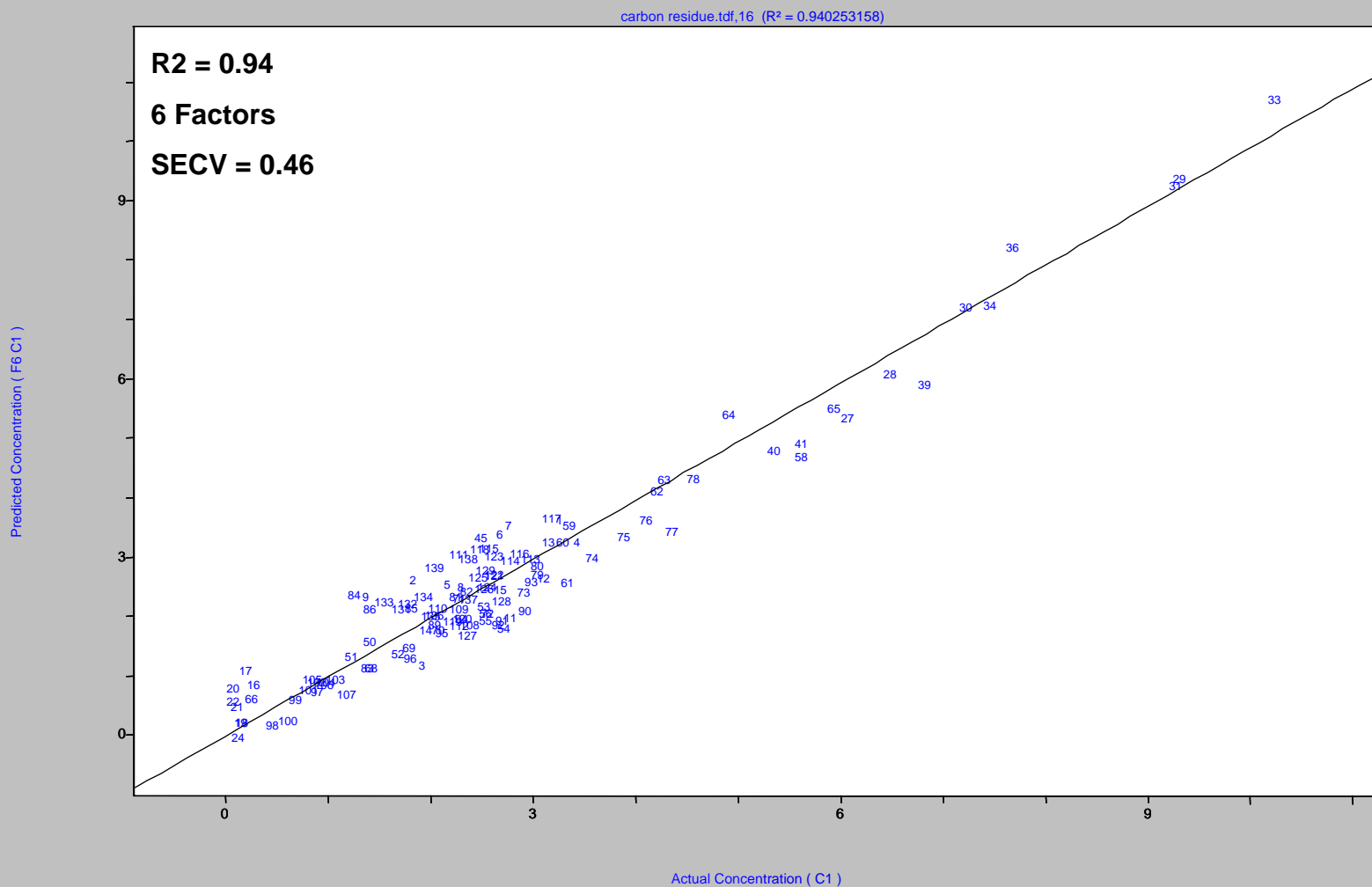
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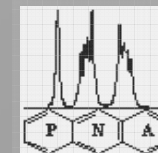
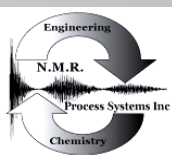
FCC Carbon Residue



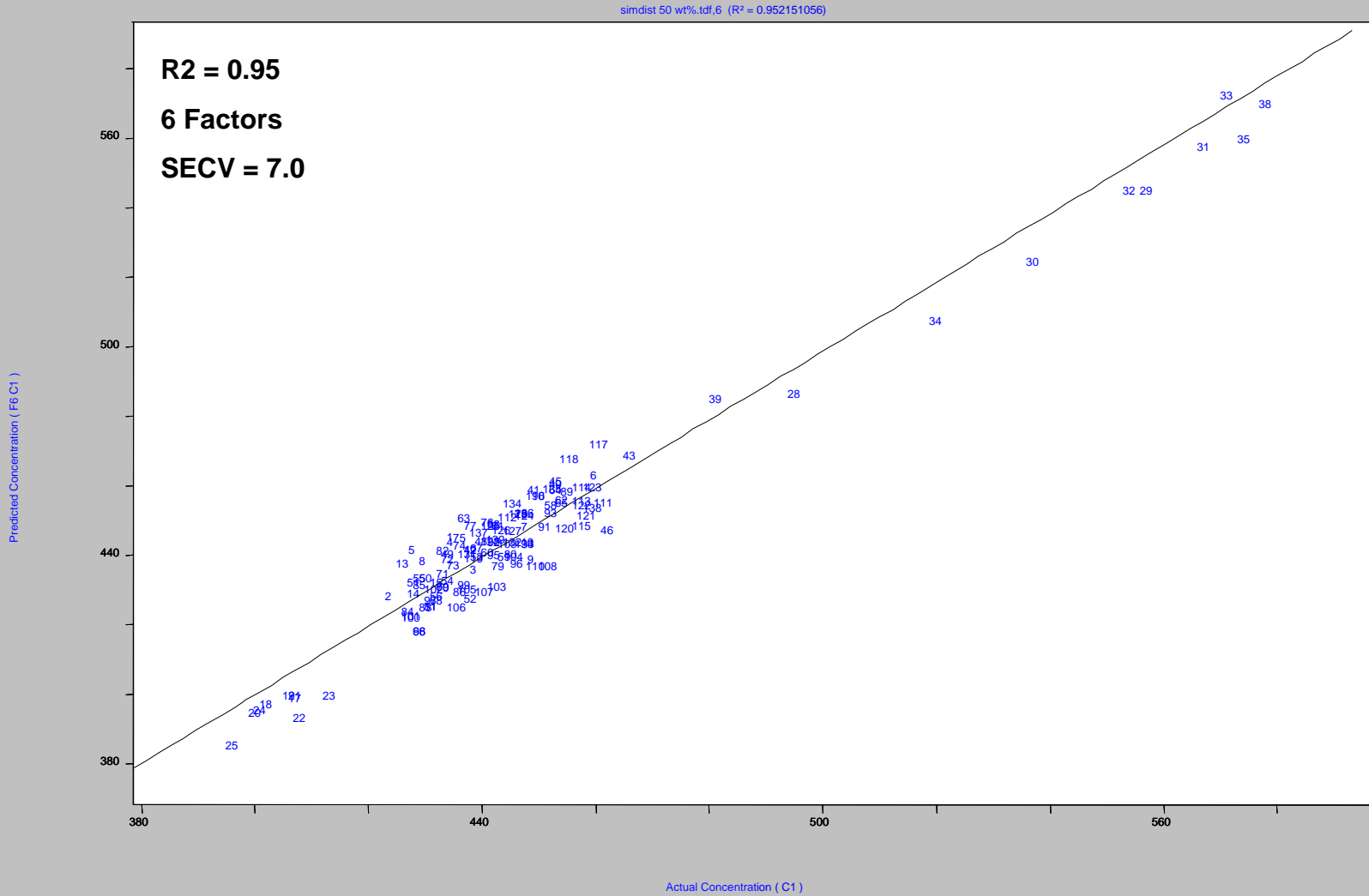
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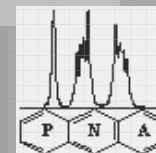
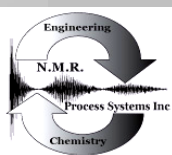
FCC Simulated Distillation 50%



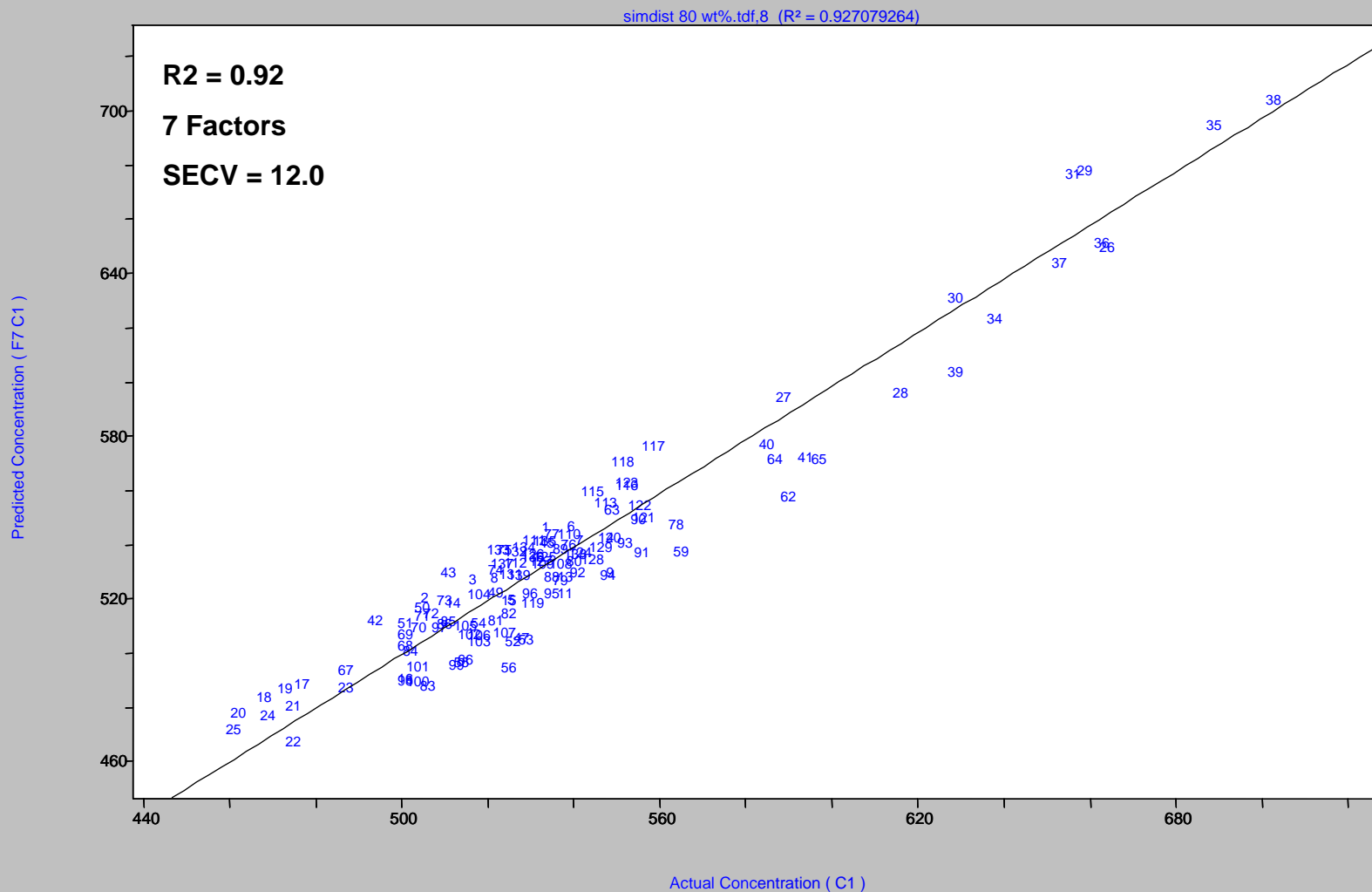
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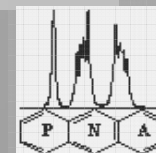
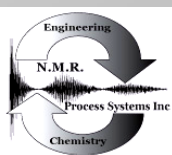
FCC Simulated Distillation 80%



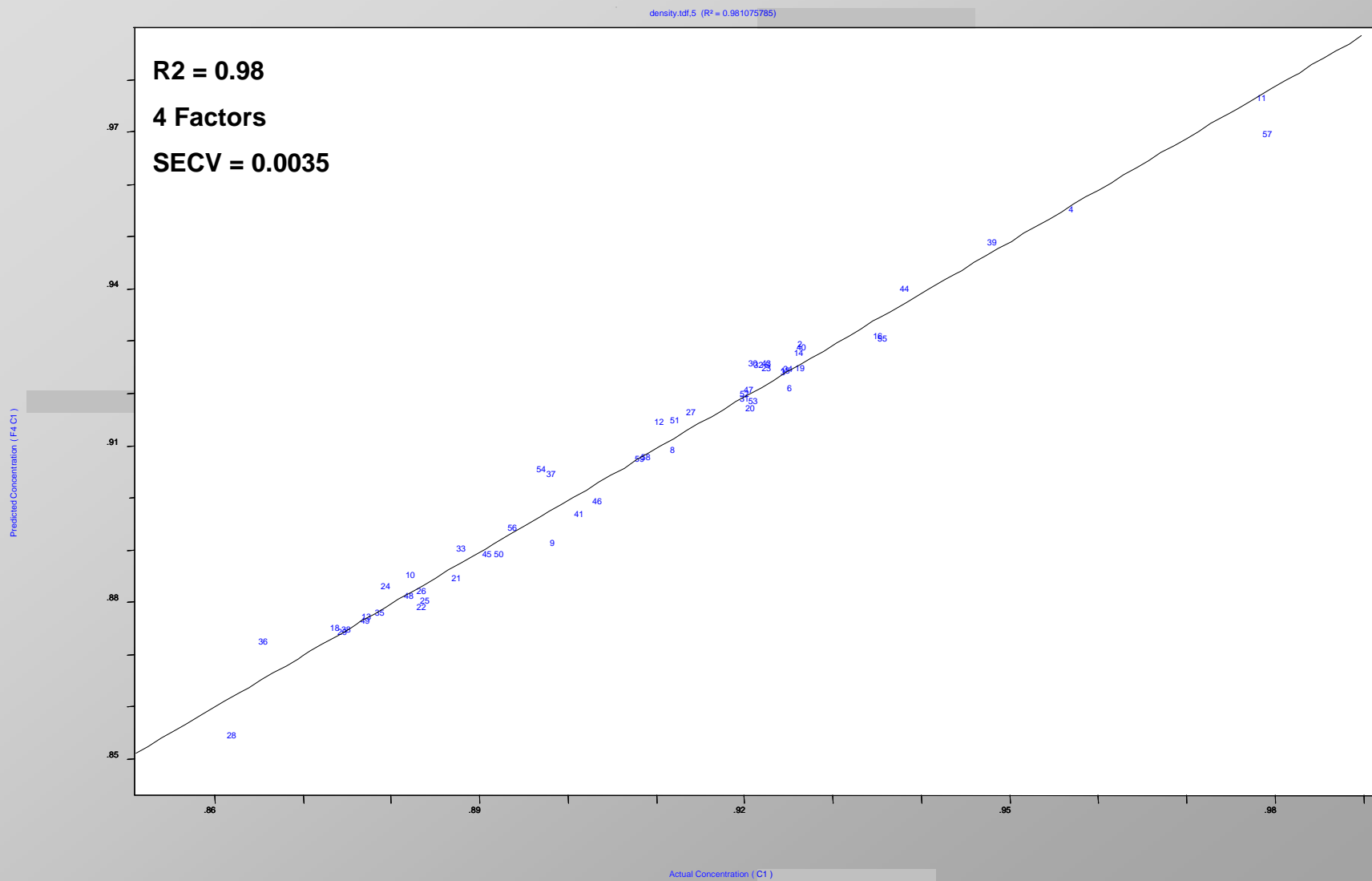
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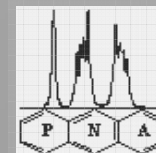
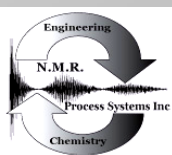
Vacuum Gas Oil Density



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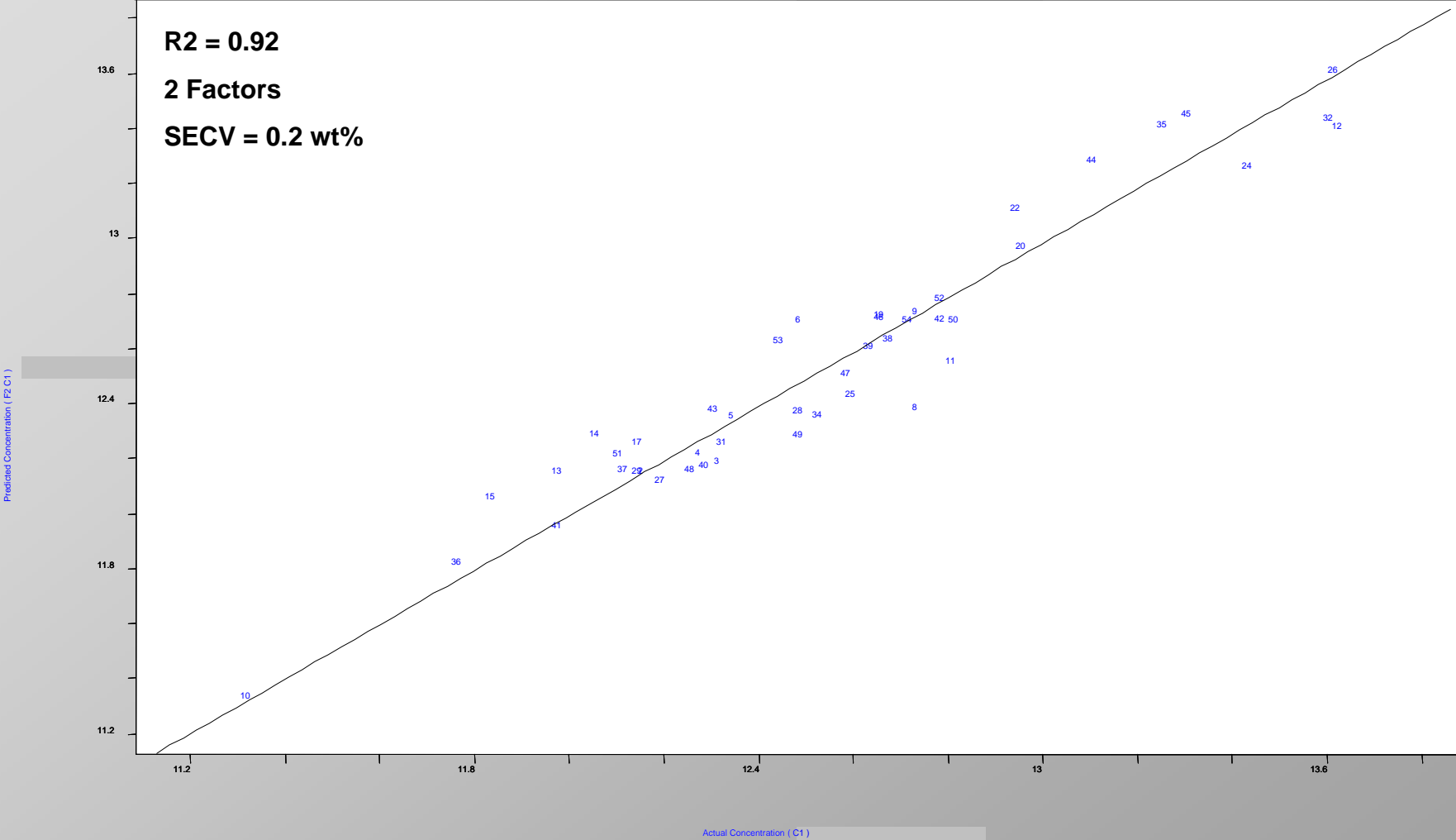
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Vacuum Gas Oil Hydrogen Content

hydrogen.tdf.5 (R² = 0.926313065)

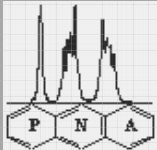
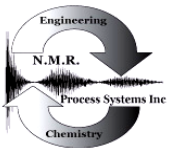
R2 = 0.92
2 Factors
SECV = 0.2 wt%



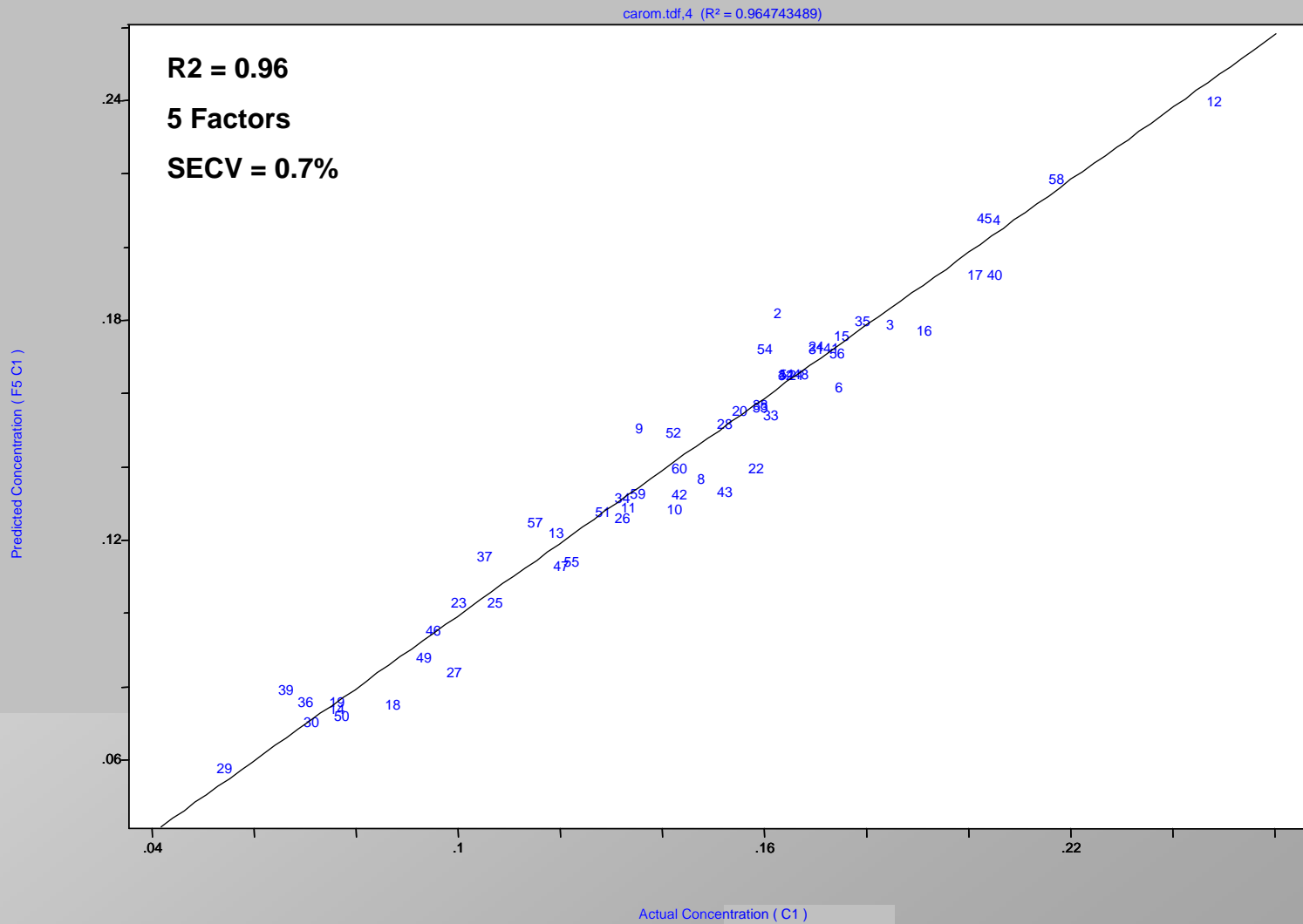
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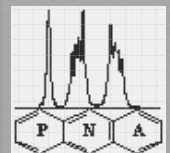
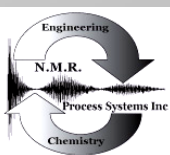
Vacuum Gas Oil Total Carbon Aromaticity



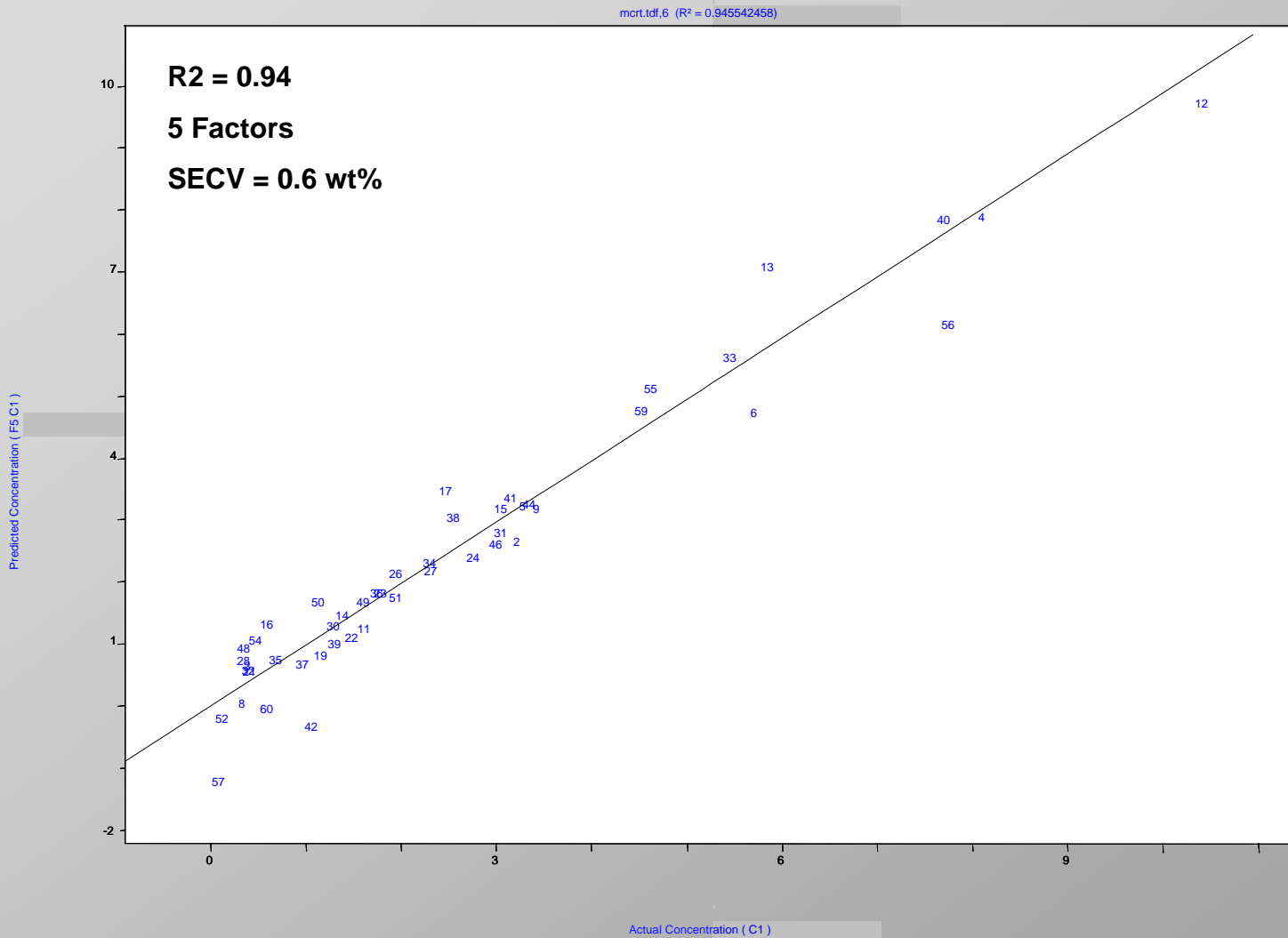
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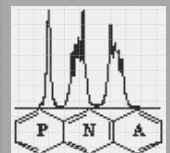
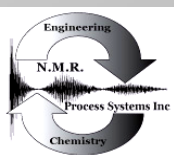
Vacuum Gas Oil MCRT



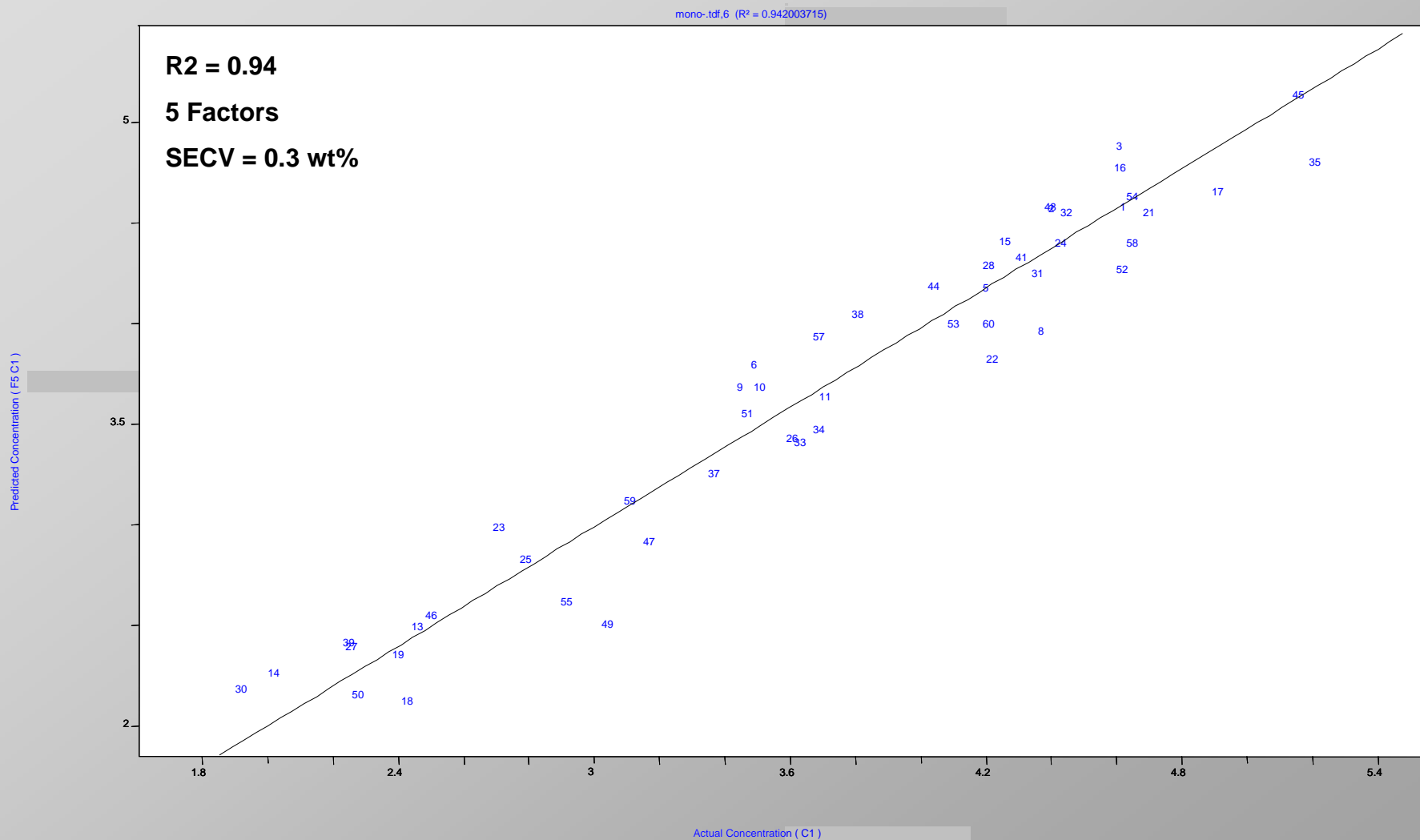
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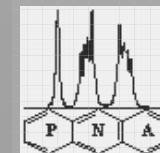
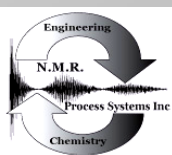
Vacuum Gas Oil Mono Aromatics



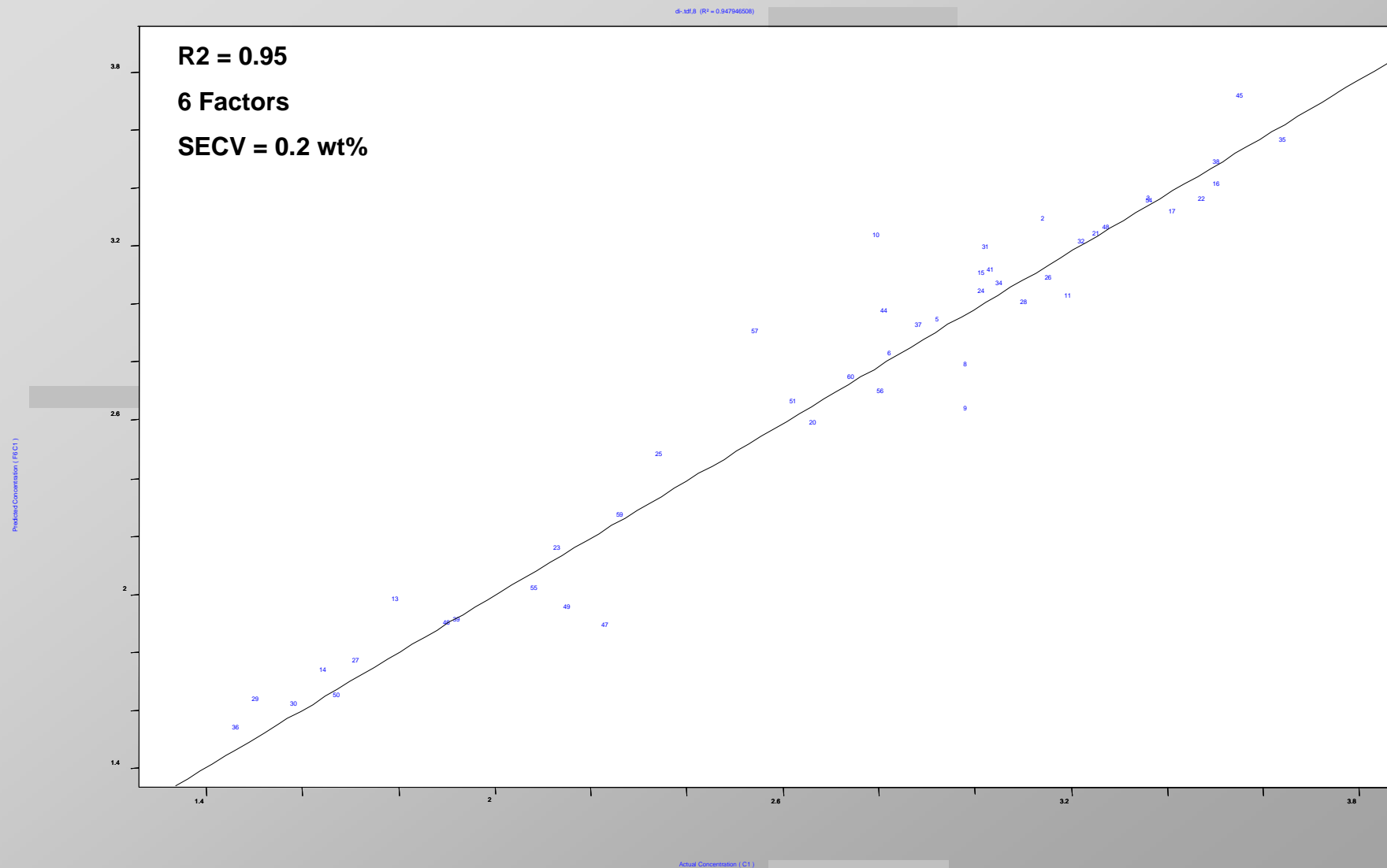
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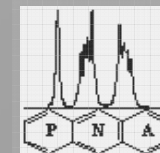
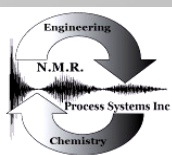
Vacuum Gas Oil Di Aromatics



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Based on the initial work, the IdentifyIR was modified with:

- Heated puck controllable to less than ± 0.5 deg C. This ensures sample uniformity especially for waxy samples.
- 3 bounce puck to enhance signal to noise.
- Allows for extending models to include range of sample types.



Temp Controller
(± 0.5 deg C)

Heated Puck
(3 bounce diamond ATR)

Automated Analysis and
and Chemometrics

Sample Types: 3 Bounce (heated)

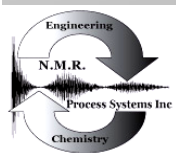
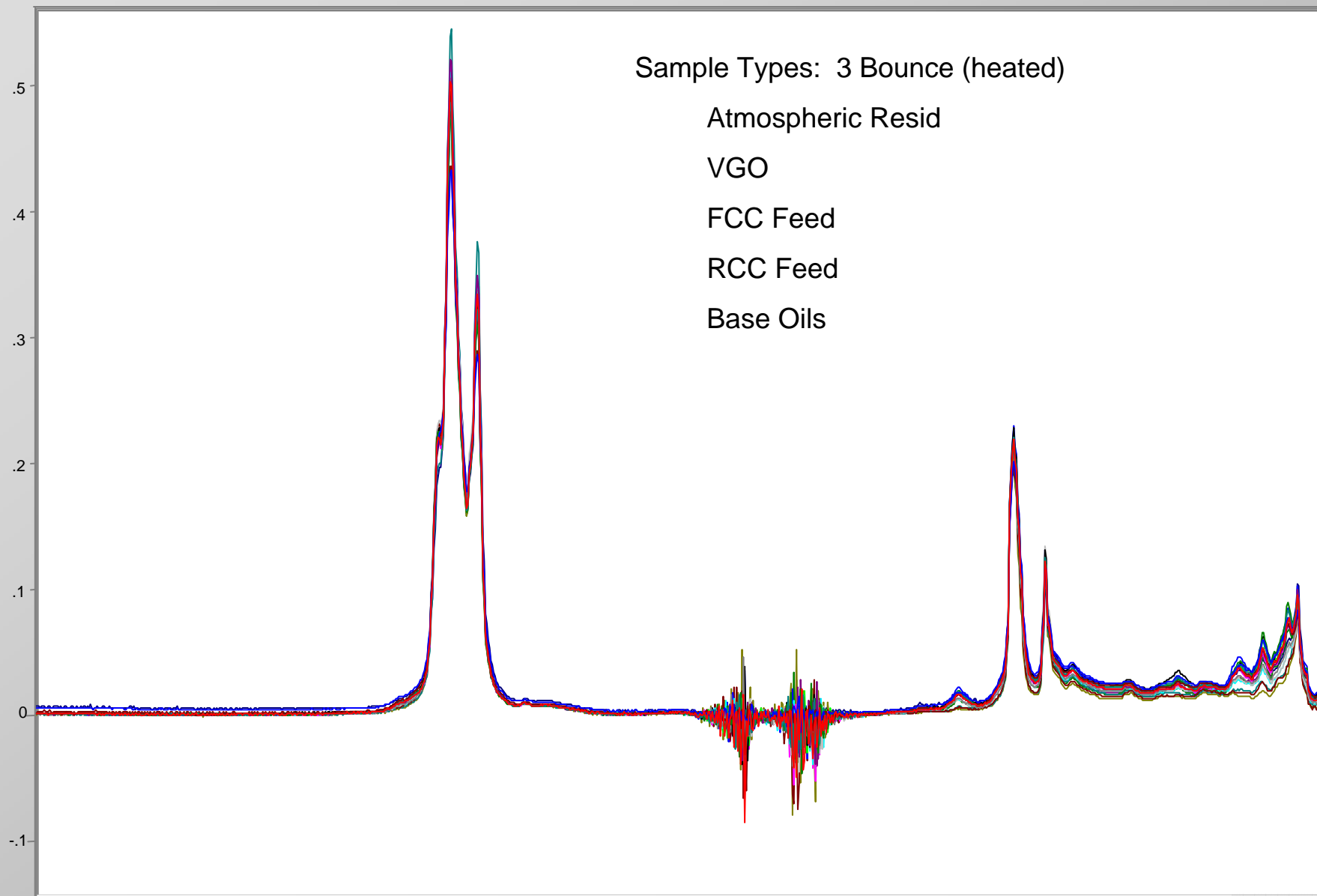
Atmospheric Resid

VGO

FCC Feed

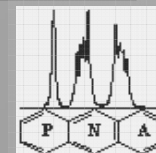
RCC Feed

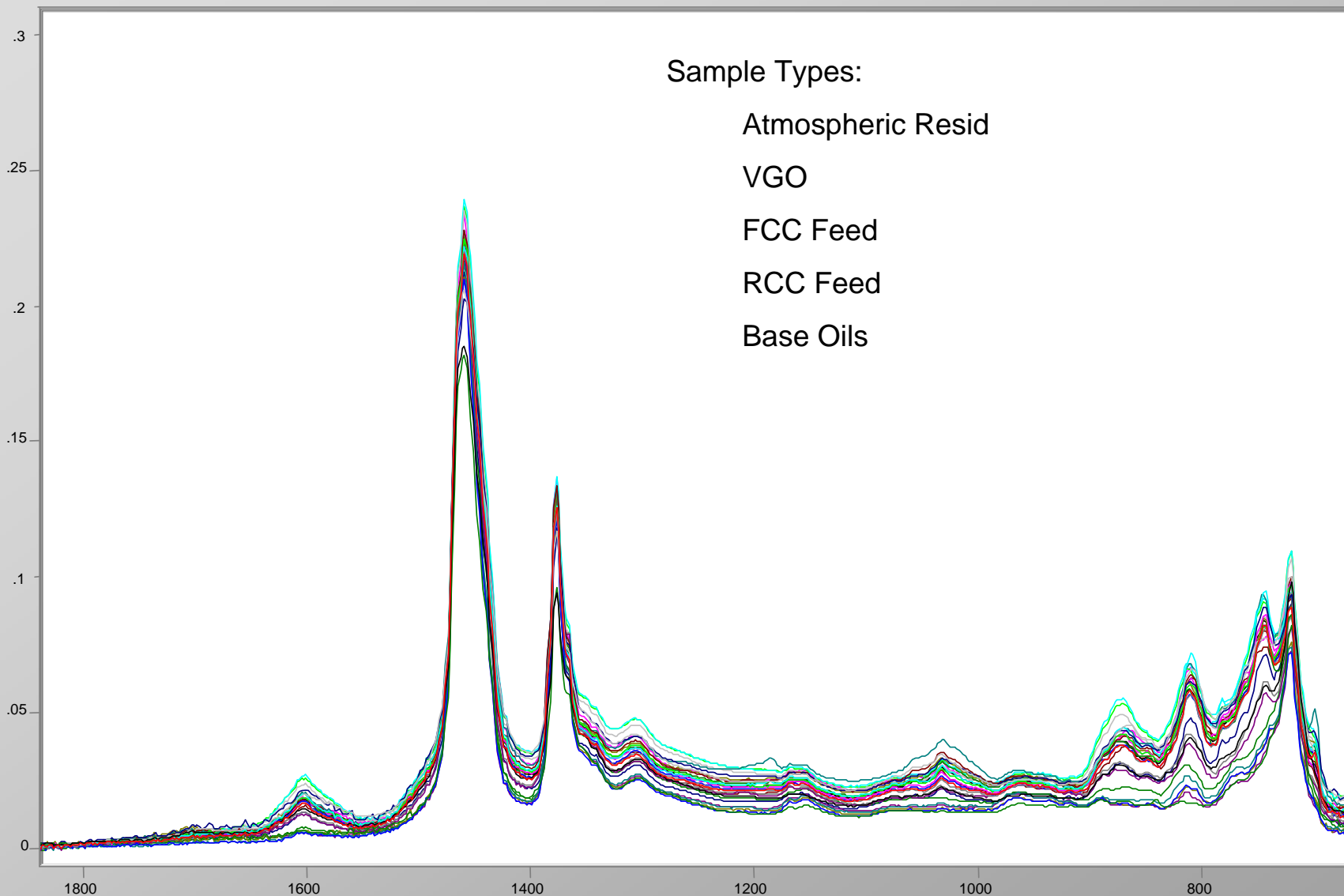
Base Oils



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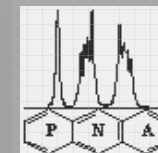
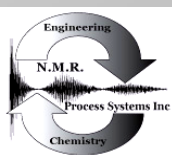


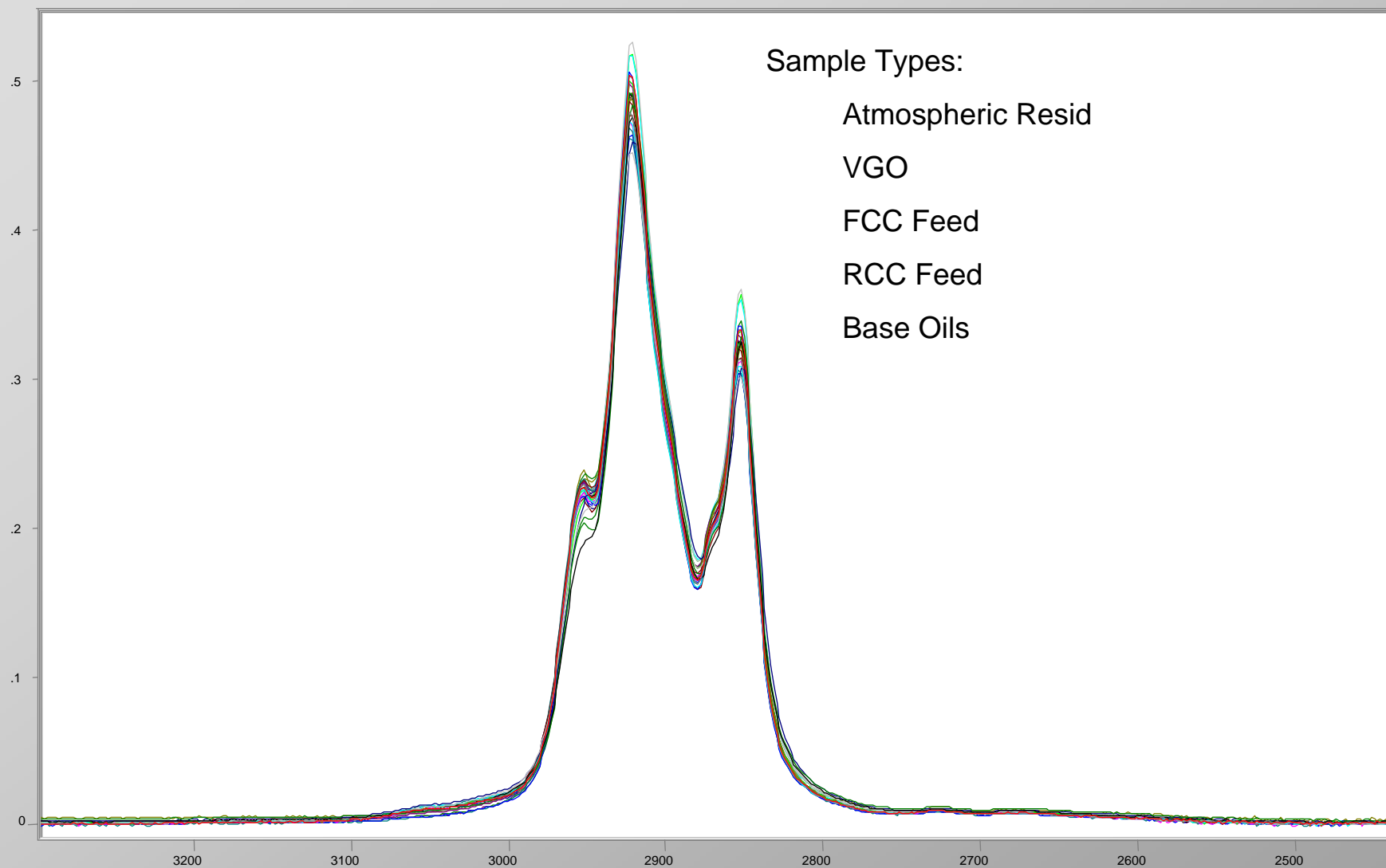


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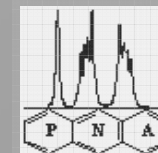
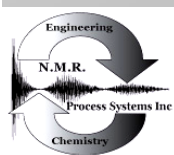


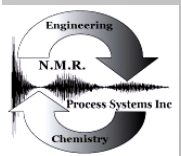
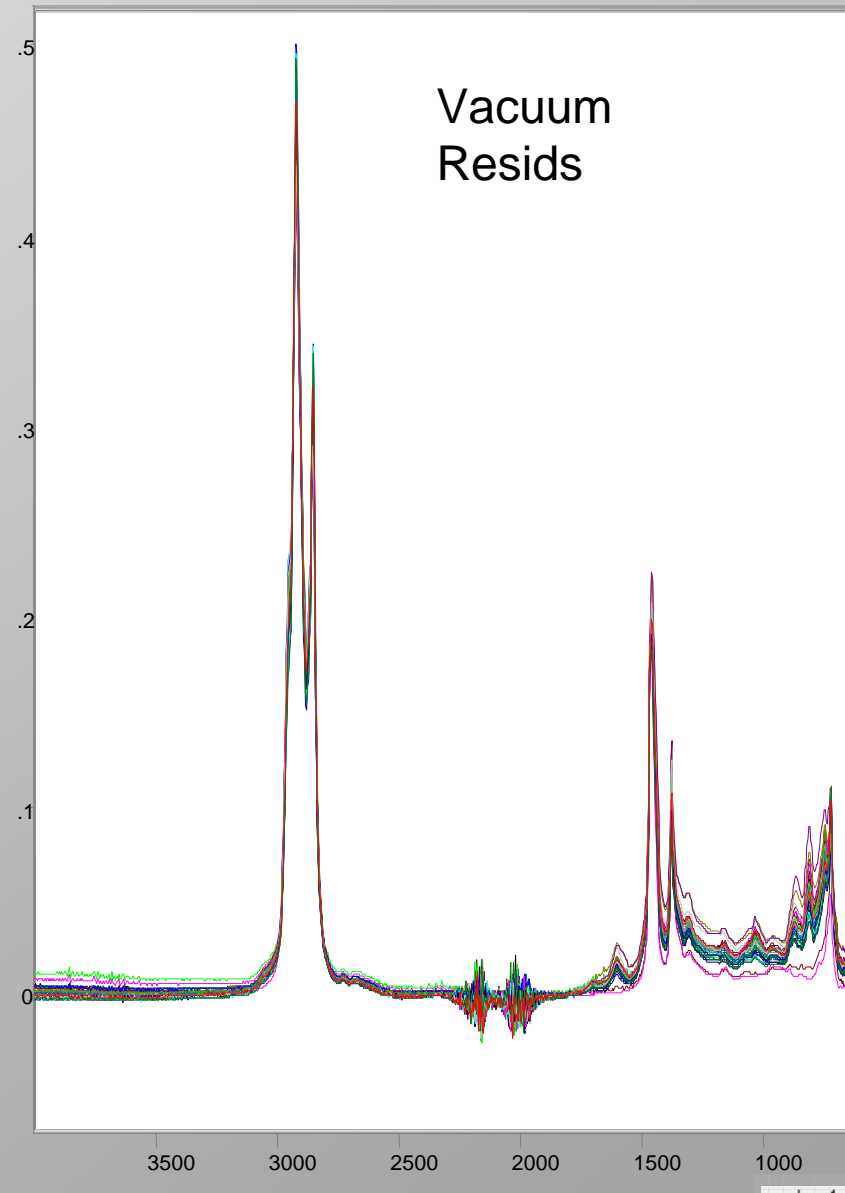
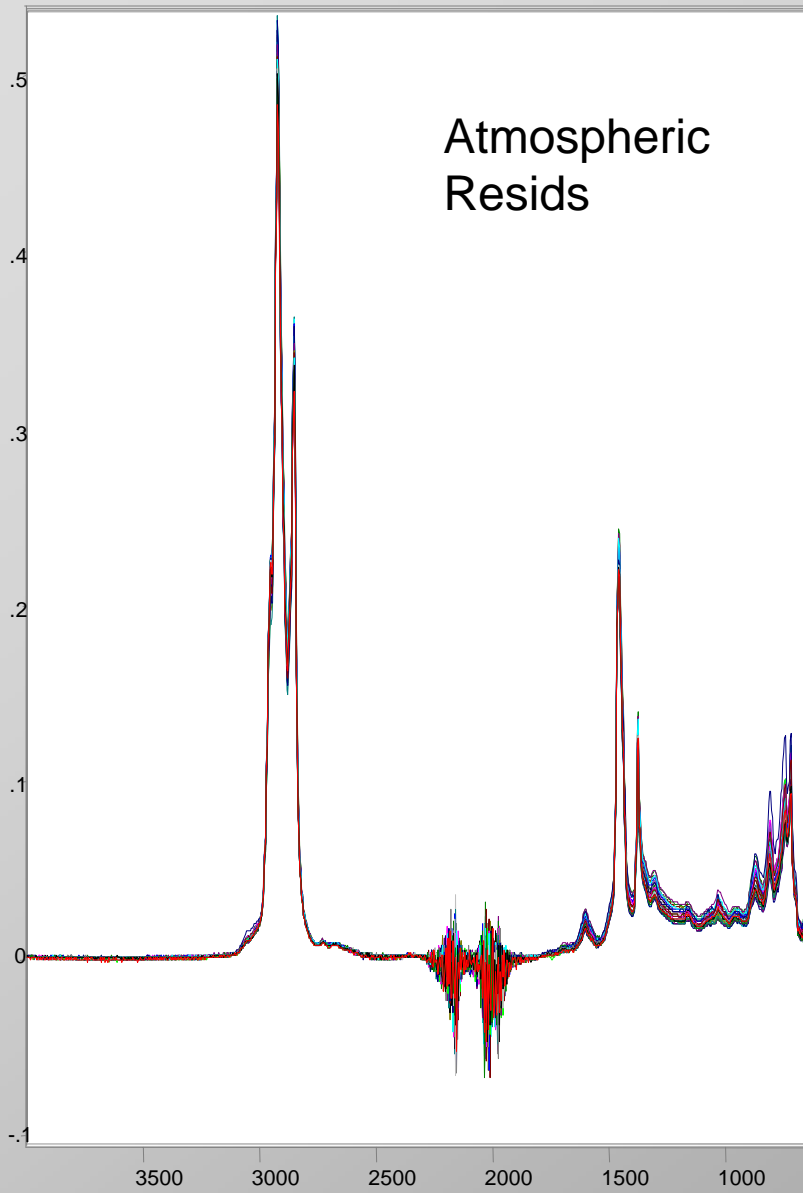


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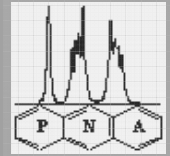
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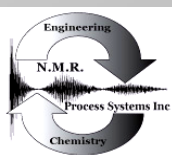




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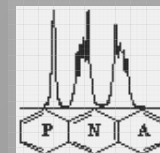


- Expanded Sample Sets (hundreds of samples)
 - Atmospheric Resid
 - VGO
 - FCC Feed
 - RCC Feed
 - Base Oils
 - Crude
- Improved Sample Interface
 - Heated (less than +/- 0.5 deg C at sample)
 - Heavy samples heated at 55 deg C
 - Three bounce reflection across sample surface
 - Samples placed on cell using a disposable wooden spatula
 - Samples wipe clean without solvent
- Uses full infra red spectrum (4000 – 675 wave numbers)
 - 4 wave number resolution
- Flow Cell Attachment for “light” samples (naphtha, kero, diesel)
 - Applies same ATR measurement. Fixes path length to 100 um
 - Flow cell id approximately 4 mm.



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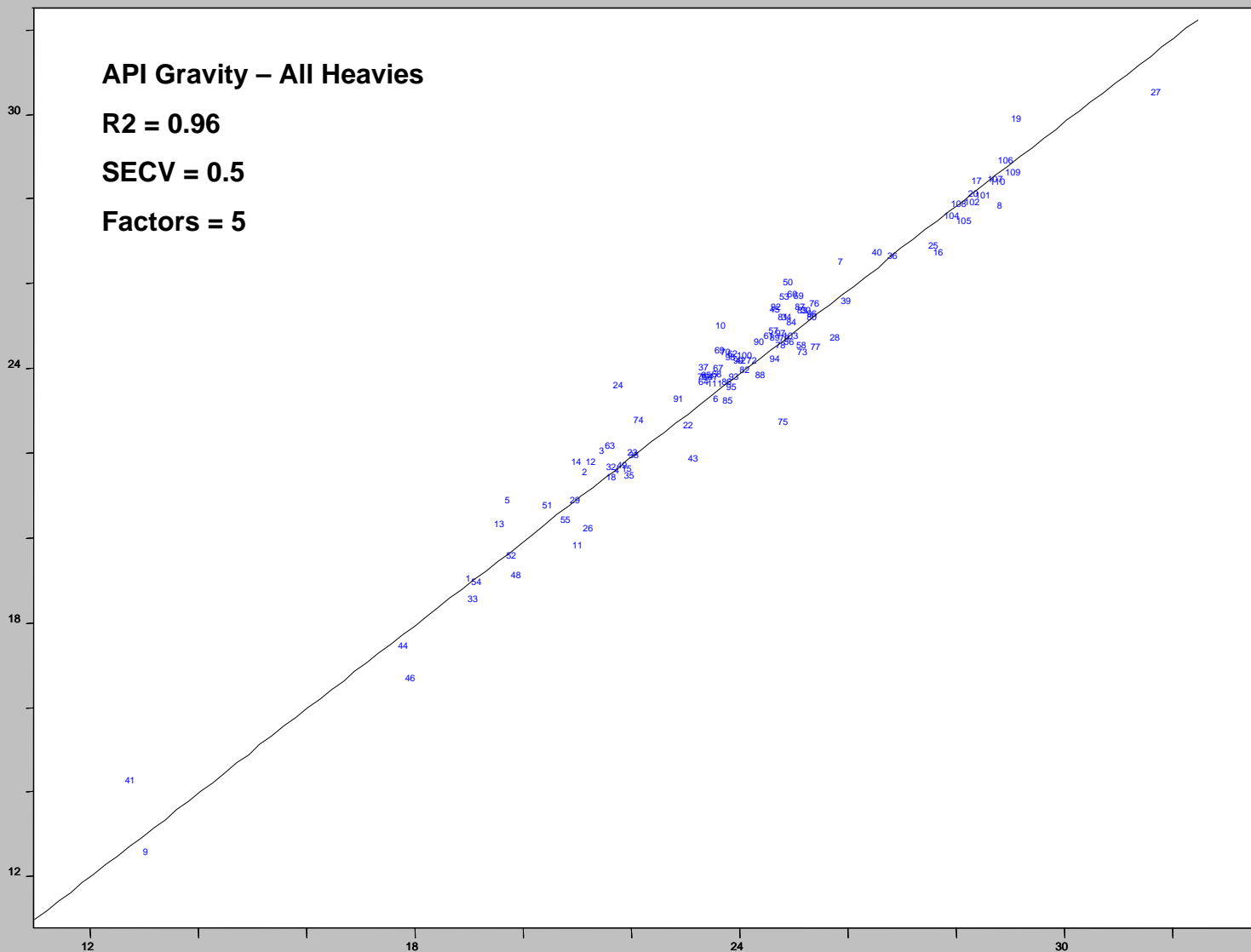
API Gravity – All Heavies

R² = 0.96

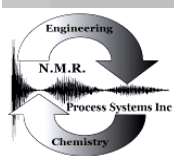
SECV = 0.5

Factors = 5

Predicted Concentration (F4 C1)

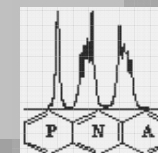


Actual Concentration (C1)

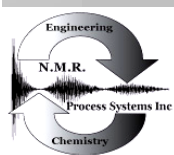
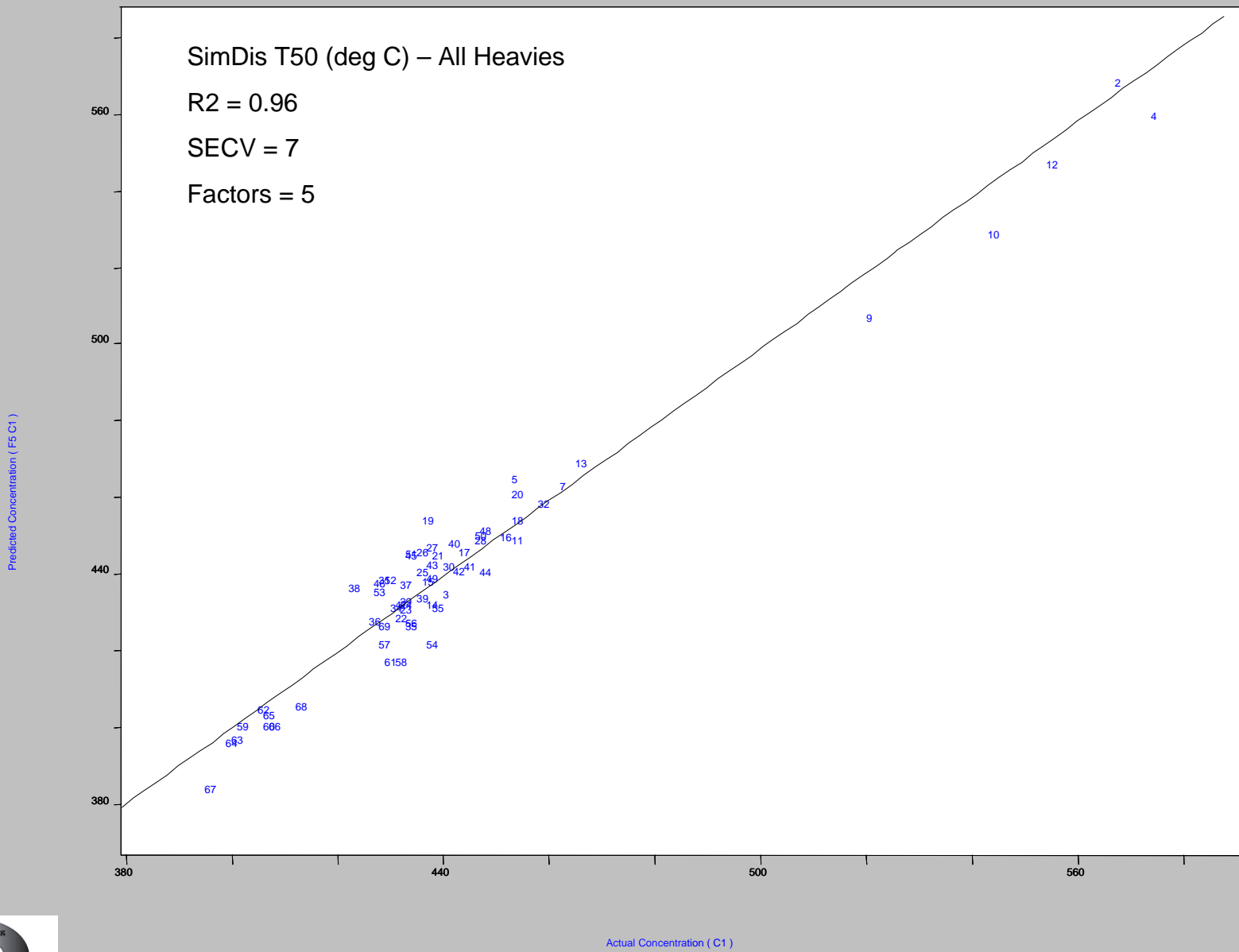


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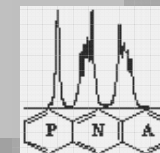


pna_identifyir_hvp_simdis_t50 (c) 100808.1 (R² = 0.954725293)

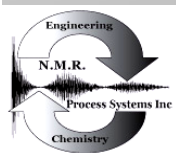
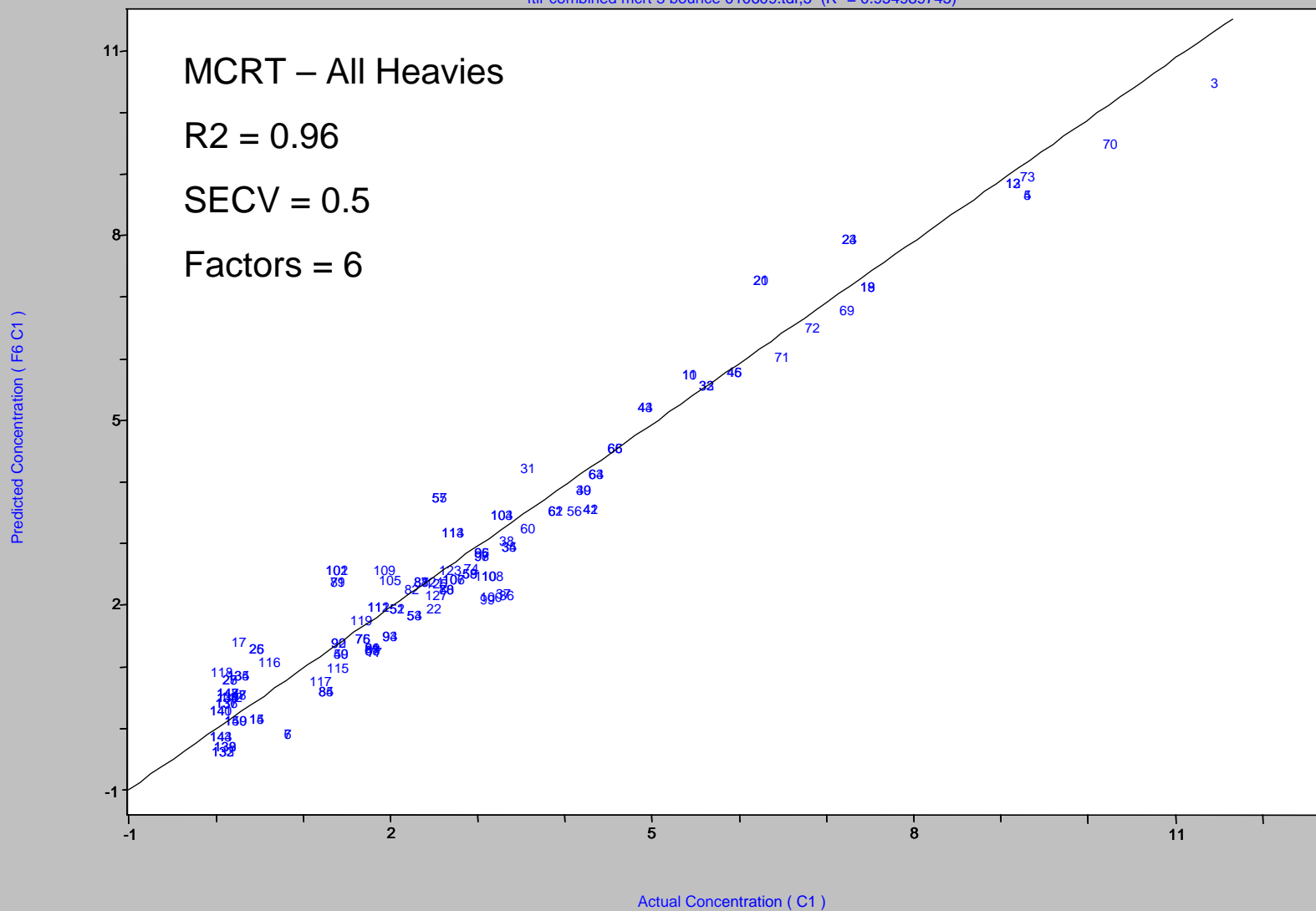


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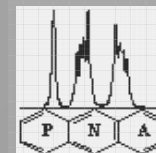
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ftir combined mcrt 3 bounce 010609.tdf,5 (R² = 0.954989745)



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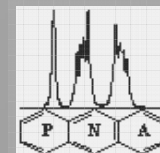
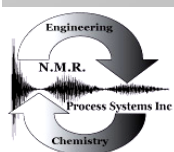
Benefits

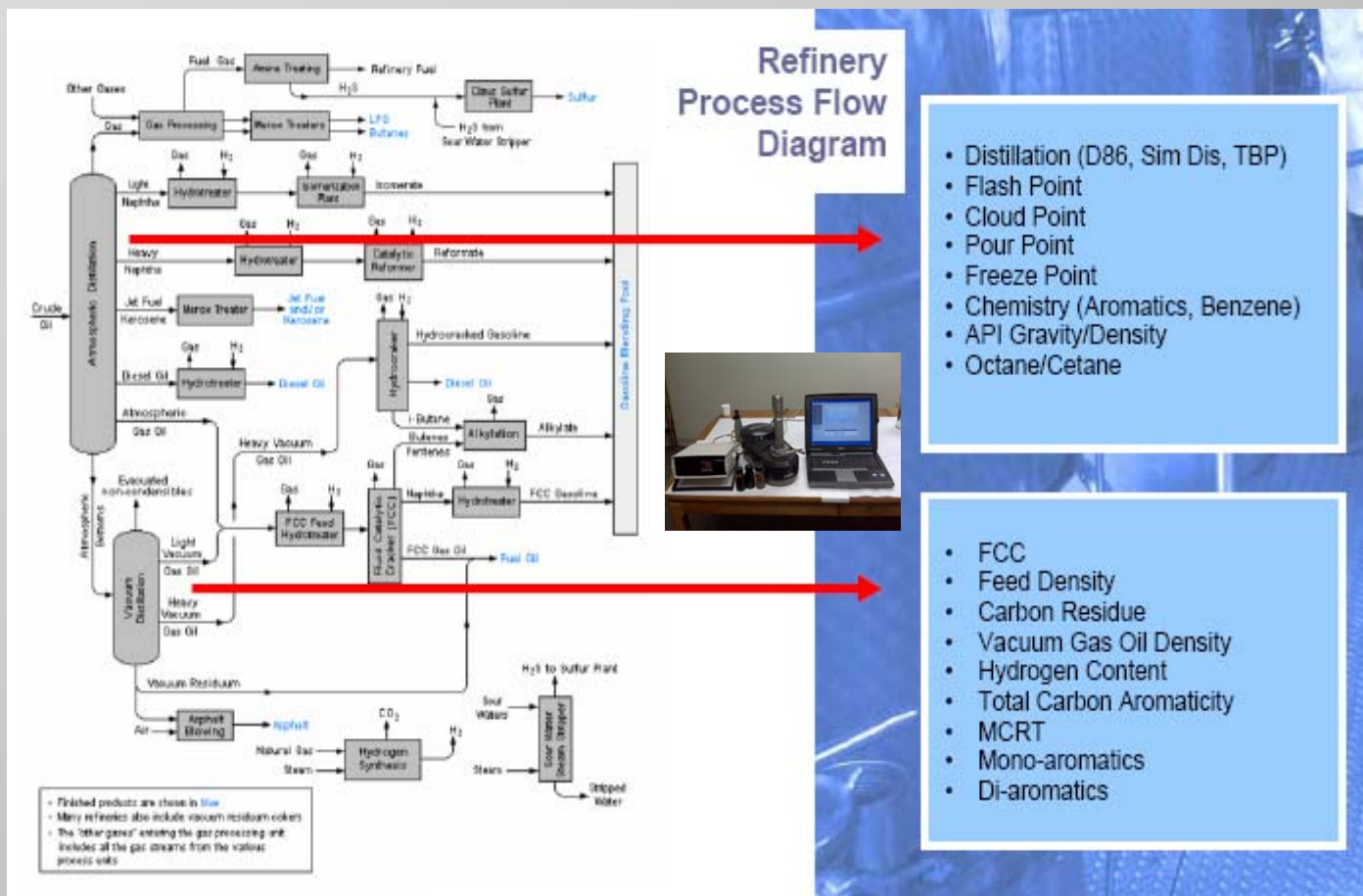
- Ease of Sample Application – Swipe'n Go.
- Dark, opaque, viscous samples not a problem.
- Simple, straight forward, simultaneous, multi-parameter predictions using standard chemometrics.
- Easy to use, accurate database matching.
- Training packages available.
- Allows input of actual data into simulation, optimization, and planning software without delay.
- Pre-qualify new feeds, blends, and/or mid-stream components quickly and reliably.

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NMR Process Systems, Inc www.nmr-automation.com

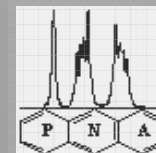
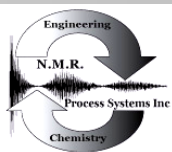




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The hardware configuration is finalized. We are finishing a software interface that will allow for “walk up, walk in” utilization of the system. Features of this software will be:

- Automatic prompting for sample information:
 - Sample ID
 - User ID
 - Time, Date, etc
- Automatic selection of chemometric application including multi-parameter predictions, results reporting and logging.
- LIMS compatible

Complete system (hardware and software) will be available on or before March 1.