solid partners
proven solutions

GCXGC SOLUTIONS FOR HYDROCARBON GROUP-TYPE ANALYSIS OF DIESEL AND JET FUELS

Rob de Jong

PAC L.P.

OVER A DECADE OF GCXGC..

- Principal research
- Academic focus on
  - modulation technology,
  - column sets
  - exploring boundaries
  - Methods
  - Further hyphenation
- Poor (practical) application focus

→ How can we get GCxGC to really deliver value?

APPLICATING FOR JET/DIESEL

CHOICES…

- Columns? Modulation? Method? Quantitation?
  - Separation capacity to separate groups over b.p. range
  - Robustness
  - Simplicity. Operator should be able to operate and maintain
  - Repeatability, comparison to other methods

APPLICATING FOR JET/DIESEL

A TURN KEY SOLUTION

- Reverse GCxGC
  - Best peak capacity
- Flow Modulation
  - Very repeatable, simple in design and powerful (enough)
- FID
  - Universal Response, cost effective, familiar and robust
- Application Ready
  - No hardware only, no Engineering. You start work
- Quality control included

APPLICATING FOR JET/DIESEL

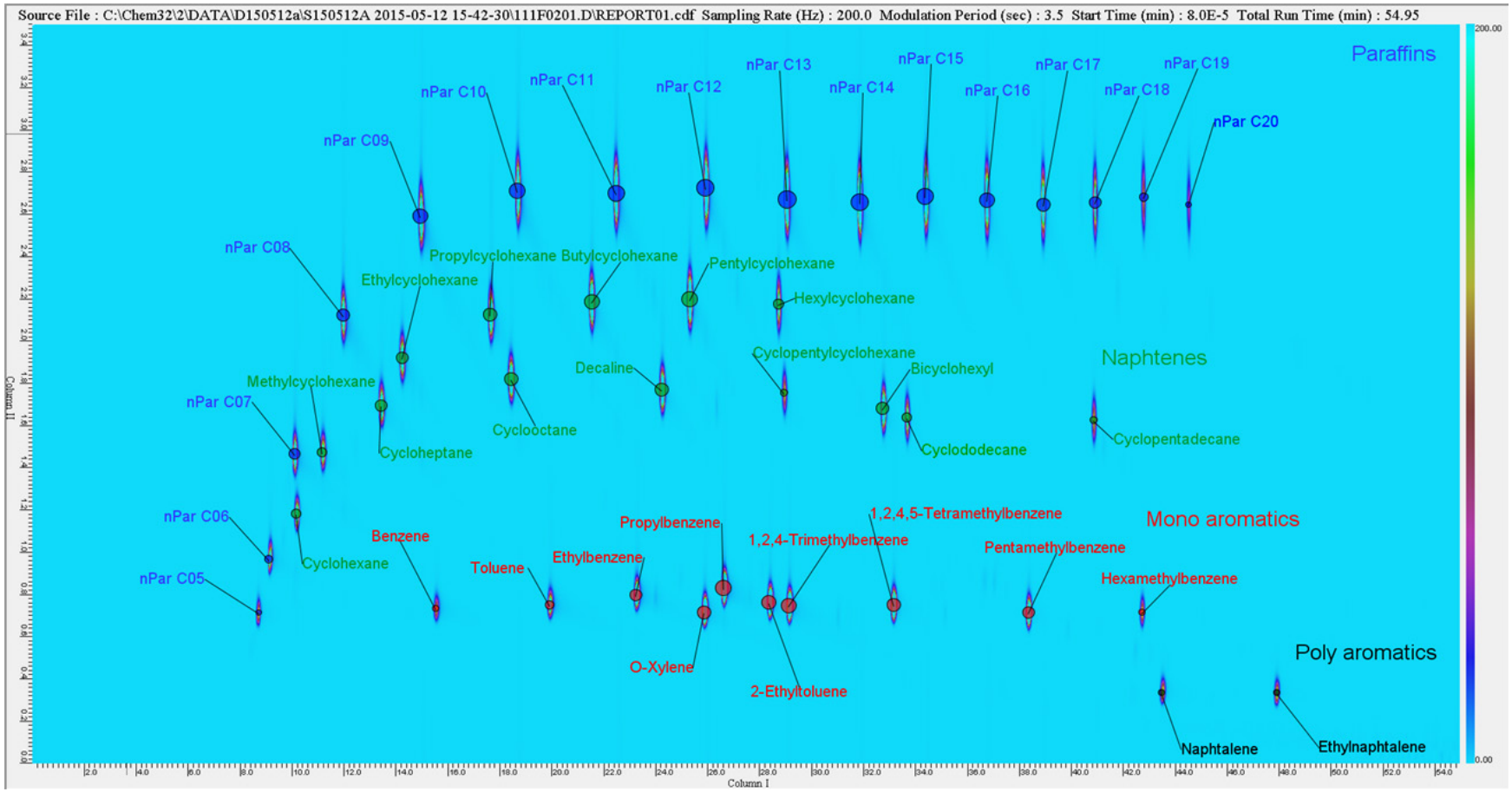
TURN KEY SOLUTION

- Separation by Groups & Selected Individual compounds
  - Paraffin's
  - Iso-paraffins
  - Naphthenes
  - Aromatics
  - FAMES
- 1 method, B.P up to 450C
- Allows for different Fuel types, incl. Biodiesel.
- Robustness, Repeatability, and comparability
- Simplicity that works

JET FUEL

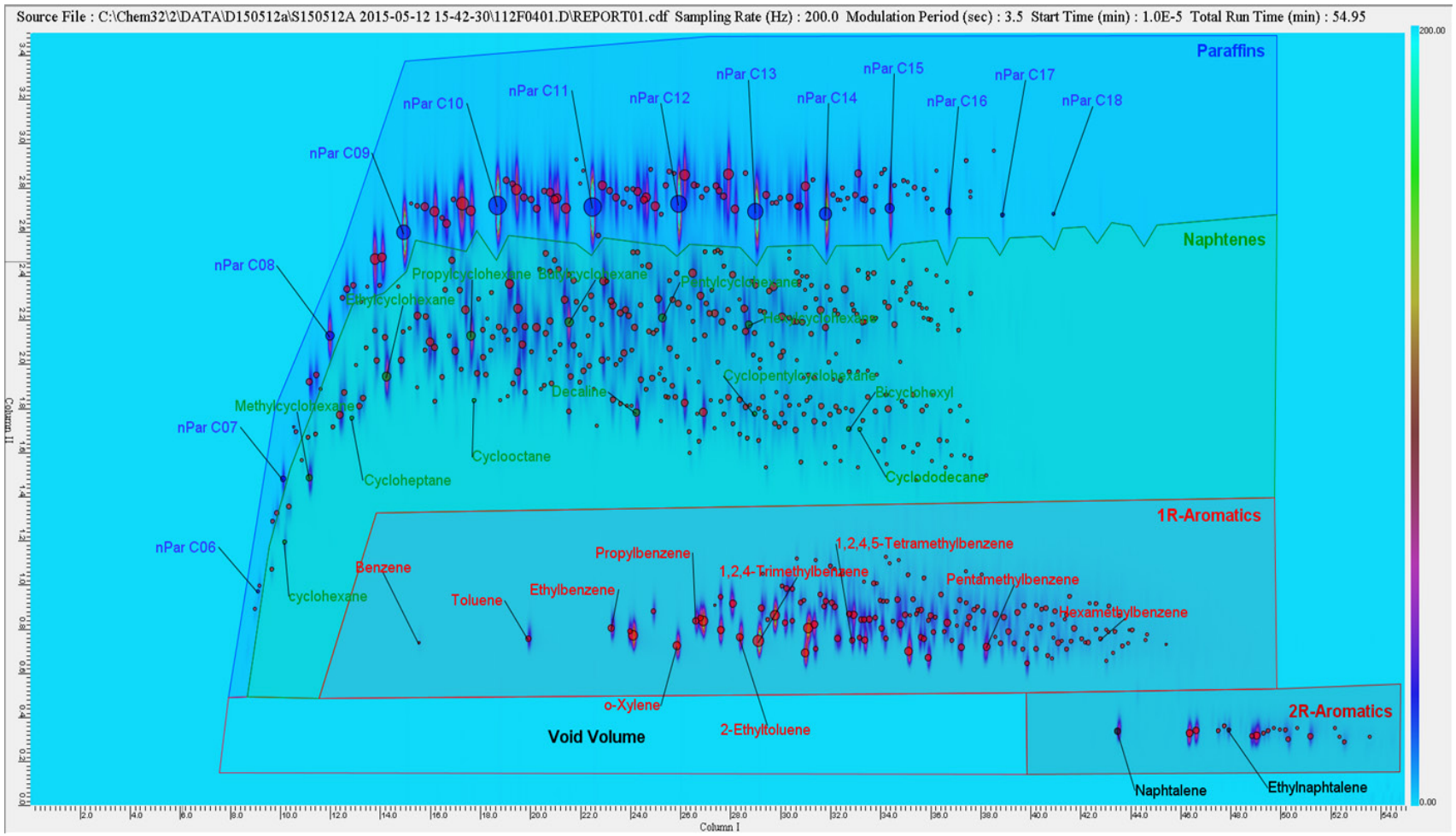
JET FUEL

REFERENCE STD



JET FUEL

PAC QC MATERIAL 00.02.717



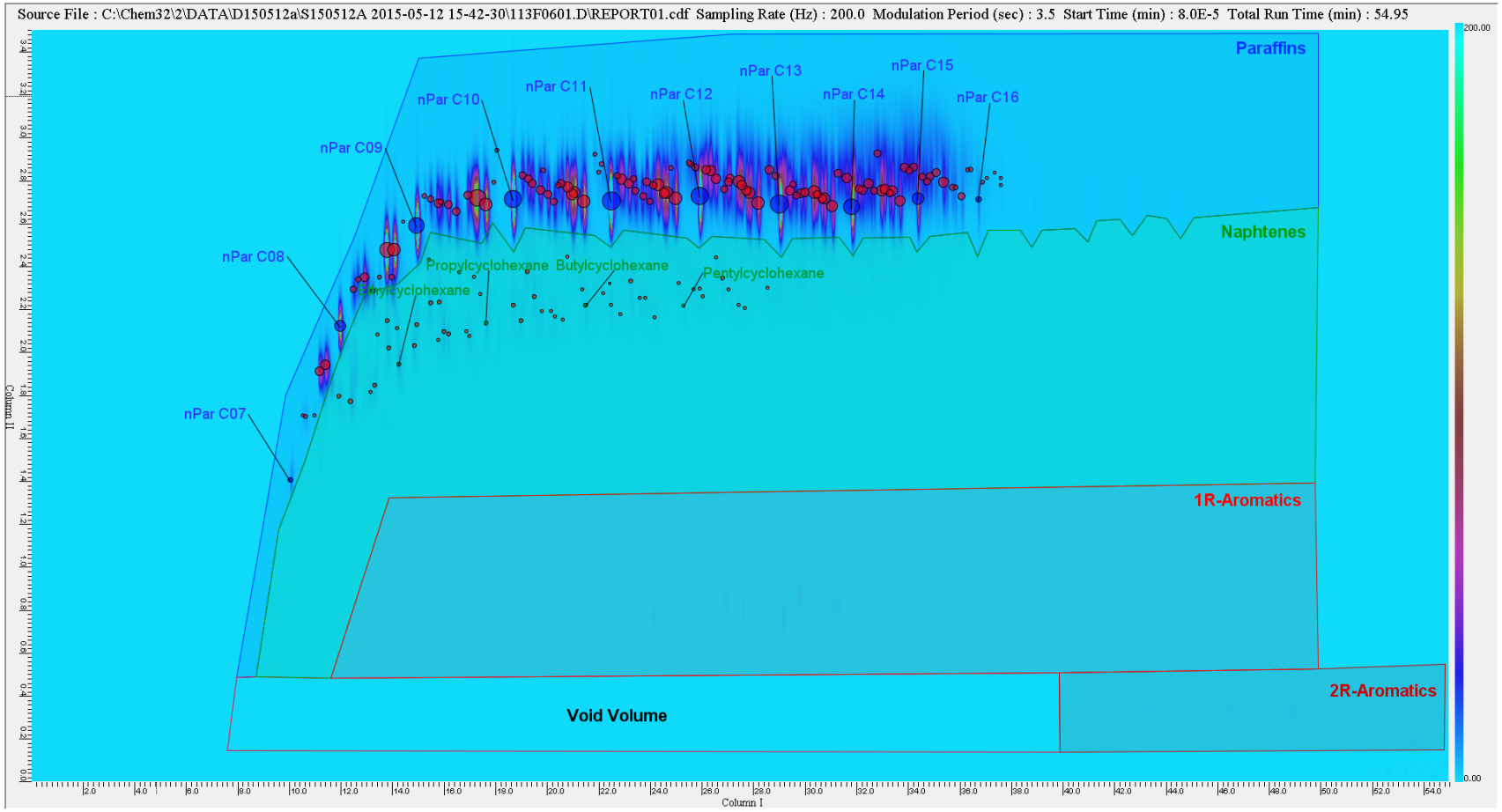
JET FUEL

PAC QC MATERIAL

Component	Mass% standard	Mass% found	Difference
nPar C05	0.51	0.51	0.00
nPar C06	1.00	1.00	0.00
nPar C07	2.00	2.00	0.00
nPar C08	2.50	2.46	0.04
nPar C09	3.50	3.42	0.07
nPar C10	4.00	3.97	0.03
nPar C11	4.75	4.73	0.02
nPar C12	5.25	5.22	0.03
nPar C13	5.50	5.47	0.03
nPar C14	5.00	5.02	0.02
nPar C15	4.25	4.27	0.02
nPar C16	3.50	3.51	0.01
nPar C17	2.75	2.76	0.01
nPar C18	2.00	2.00	0.00
nPar C19	1.00	1.00	0.00
nPar C20	0.50	0.50	0.00
Bicyclohexyl	2.35	2.37	0.02
Butylcyclohexane	3.50	3.52	0.03
Cyclododecane	1.25	1.27	0.02
Cycloheptane	2.00	2.03	0.03
Cyclohexane	1.25	1.28	0.03
Cyclooctane	2.75	2.80	0.05
Cyclopentadecane	0.75	0.76	0.01
Cyclopentylcyclohexane	0.75	0.75	0.00
trans-Decahydronaphtalene	2.75	2.75	0.00
Ethylcyclohexane	2.00	2.02	0.02
Hexylcyclohexane	1.50	1.49	0.01
Methylcyclohexane	1.25	1.29	0.04
Pentylcyclohexane	4.00	3.92	0.07
Propylcyclohexane	2.75	2.75	0.00
1,2,4,5-Tetramethylbenzene	2.75	2.76	0.01
1,2,4-Trimethylbenzene	3.50	3.51	0.01
2-ethyltoluene	3.00	3.01	0.01
Benzene	0.50	0.50	0.00
Ethylbenzene	2.00	2.00	0.01
Hexamethylbenzene	0.50	0.52	0.01
o-Xylene	2.75	2.75	0.00
Pentamethylbenzene	2.00	1.98	0.02
n-Propylbenzene	4.00	4.00	0.00
Toluene	1.05	1.05	0.00
2-Ethylnaphtalene	0.55	0.55	0.00
Naphtalene	0.55	0.55	0.00
Total Paraffins	48.00	47.82	0.18
Total Naphtenes	28.84	29.00	0.16
Total Aromatics	23.16	23.18	0.02
	100.00	100.00	

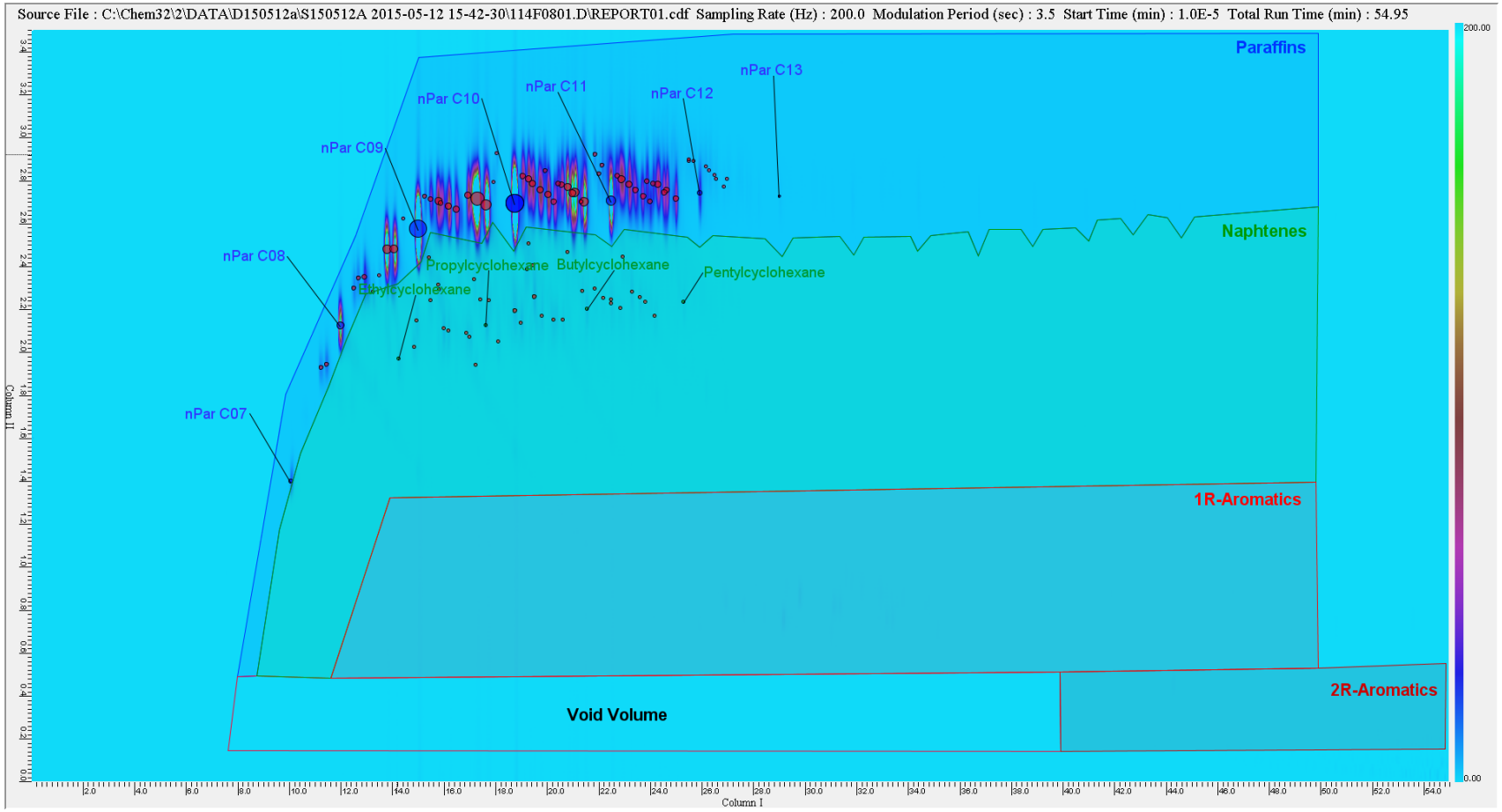
JET FUEL

SPK 5018



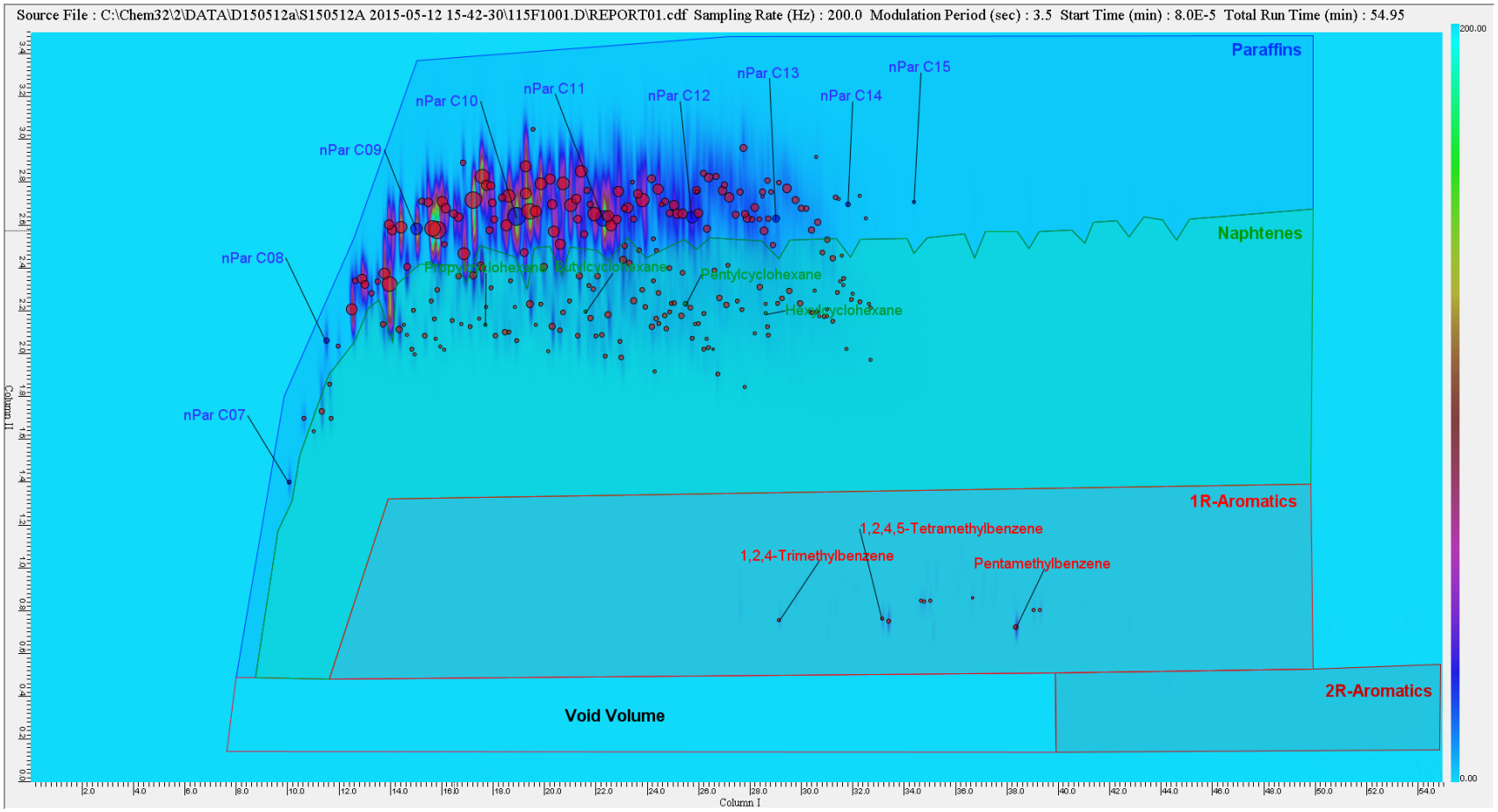
JET FUEL

SPK 5172



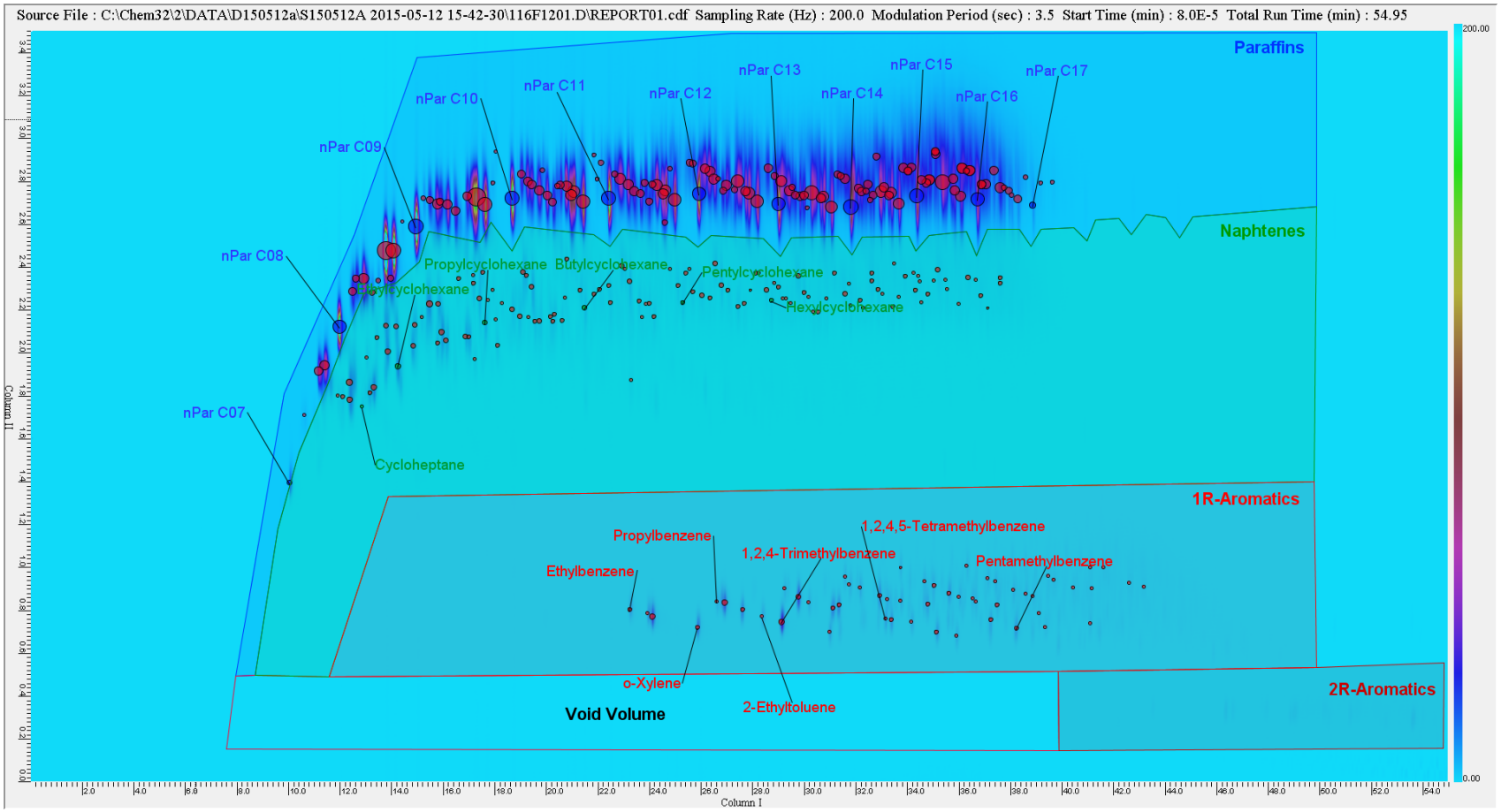
JET FUEL

SPK 5642



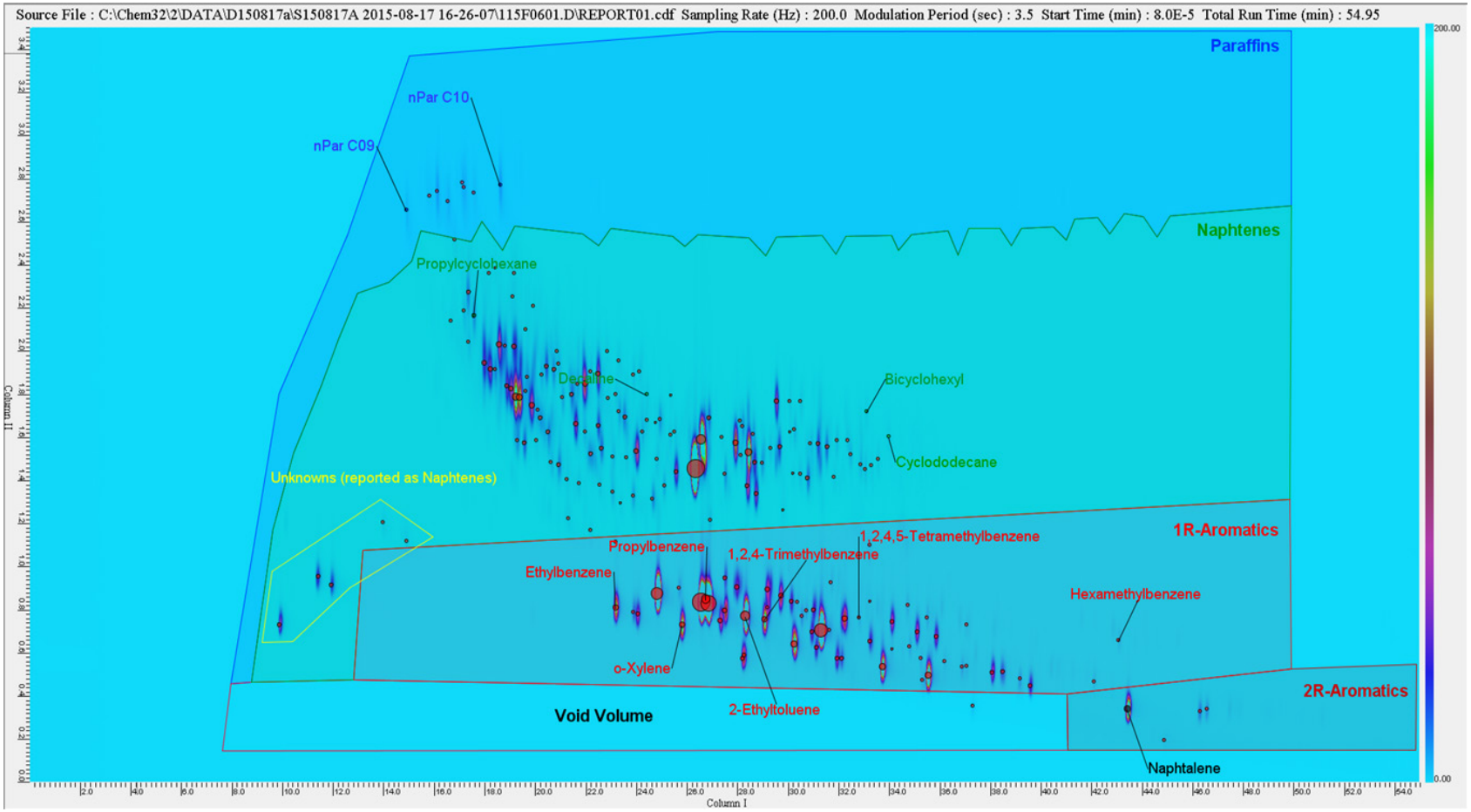
JET FUEL

SPK 5698



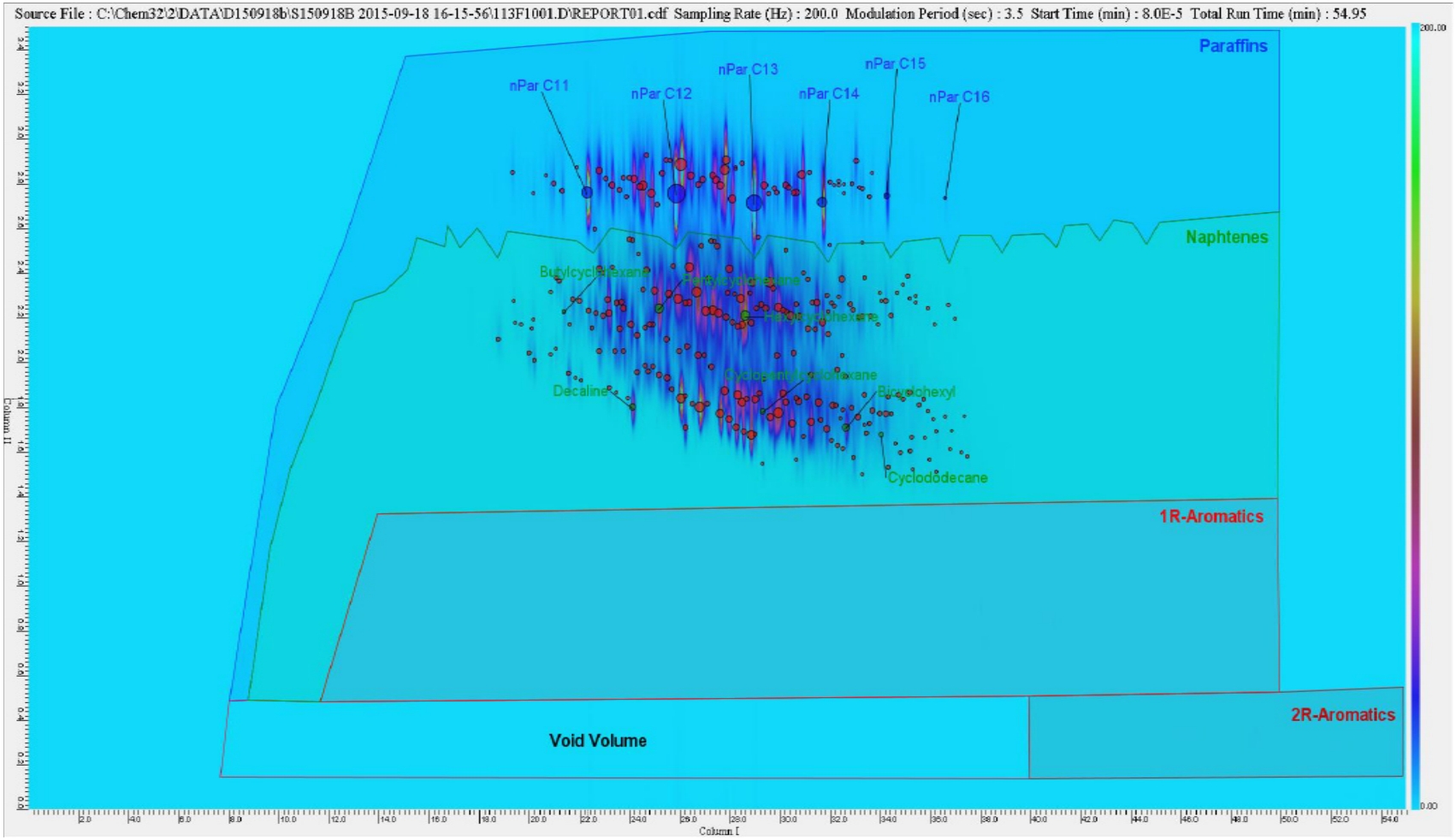
JET FUEL

'KERO' 1



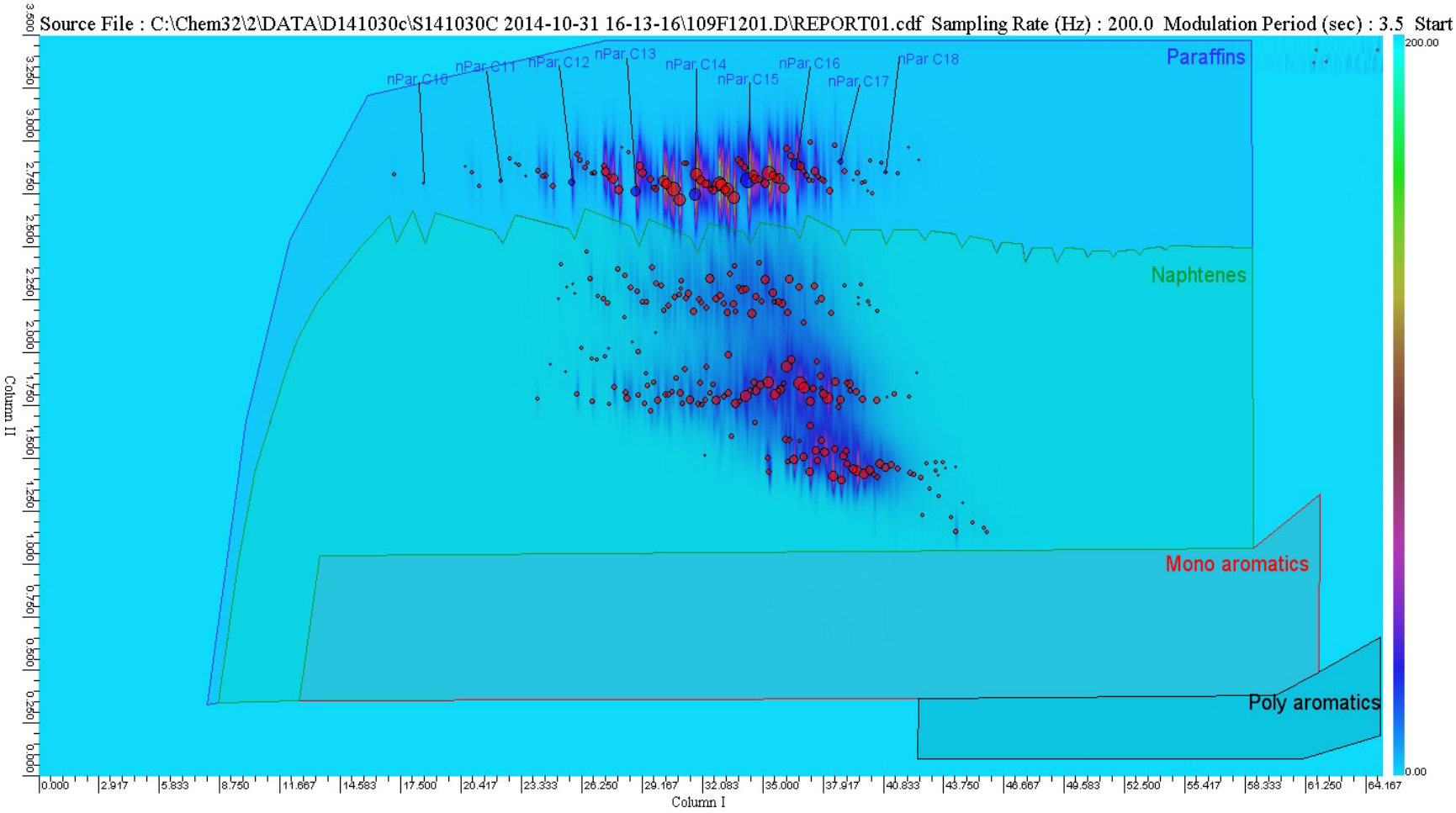
JET FUEL

JET W/O AROMATICS



JET FUEL

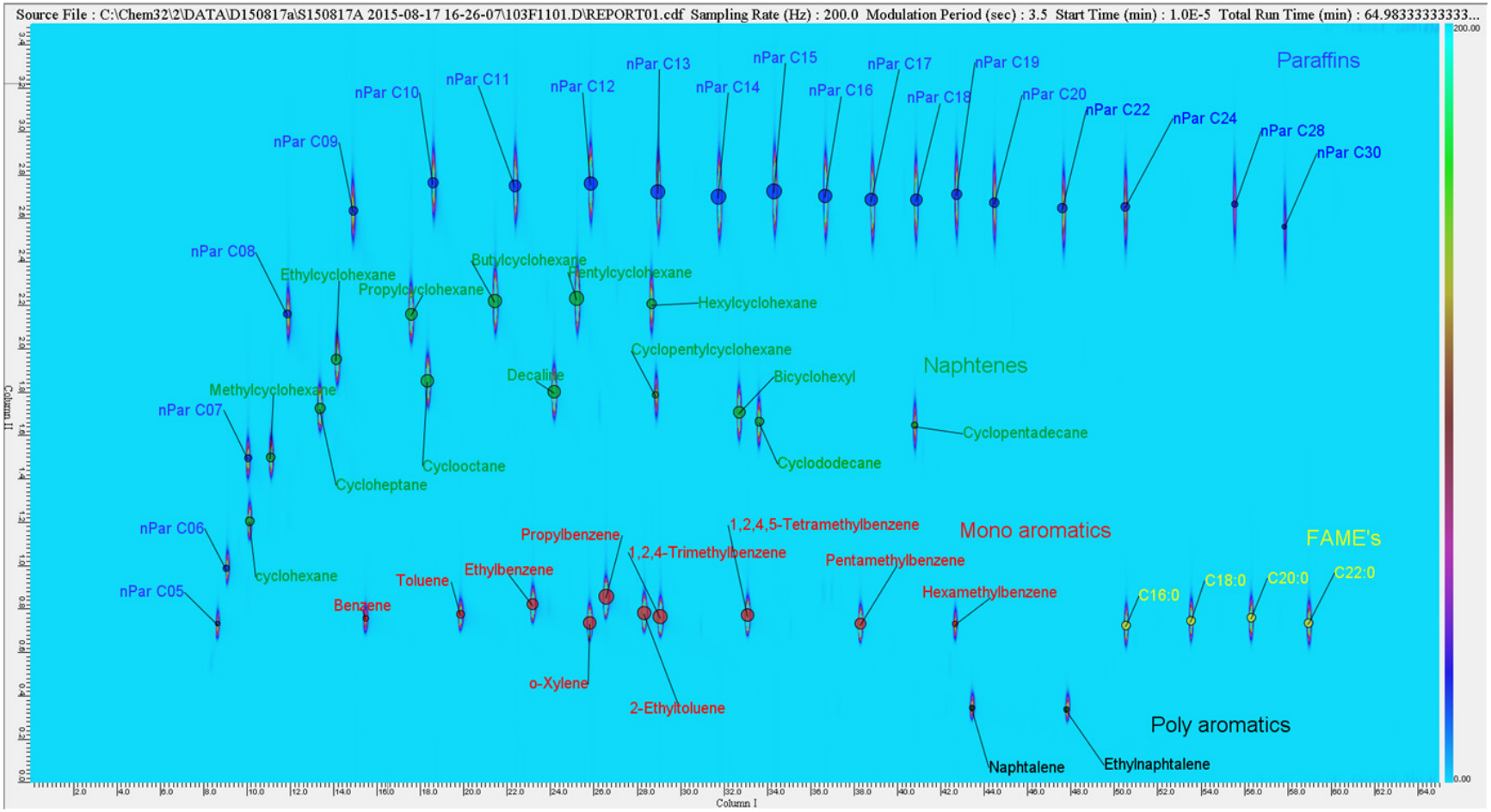
BASE FLUID



DIESEL

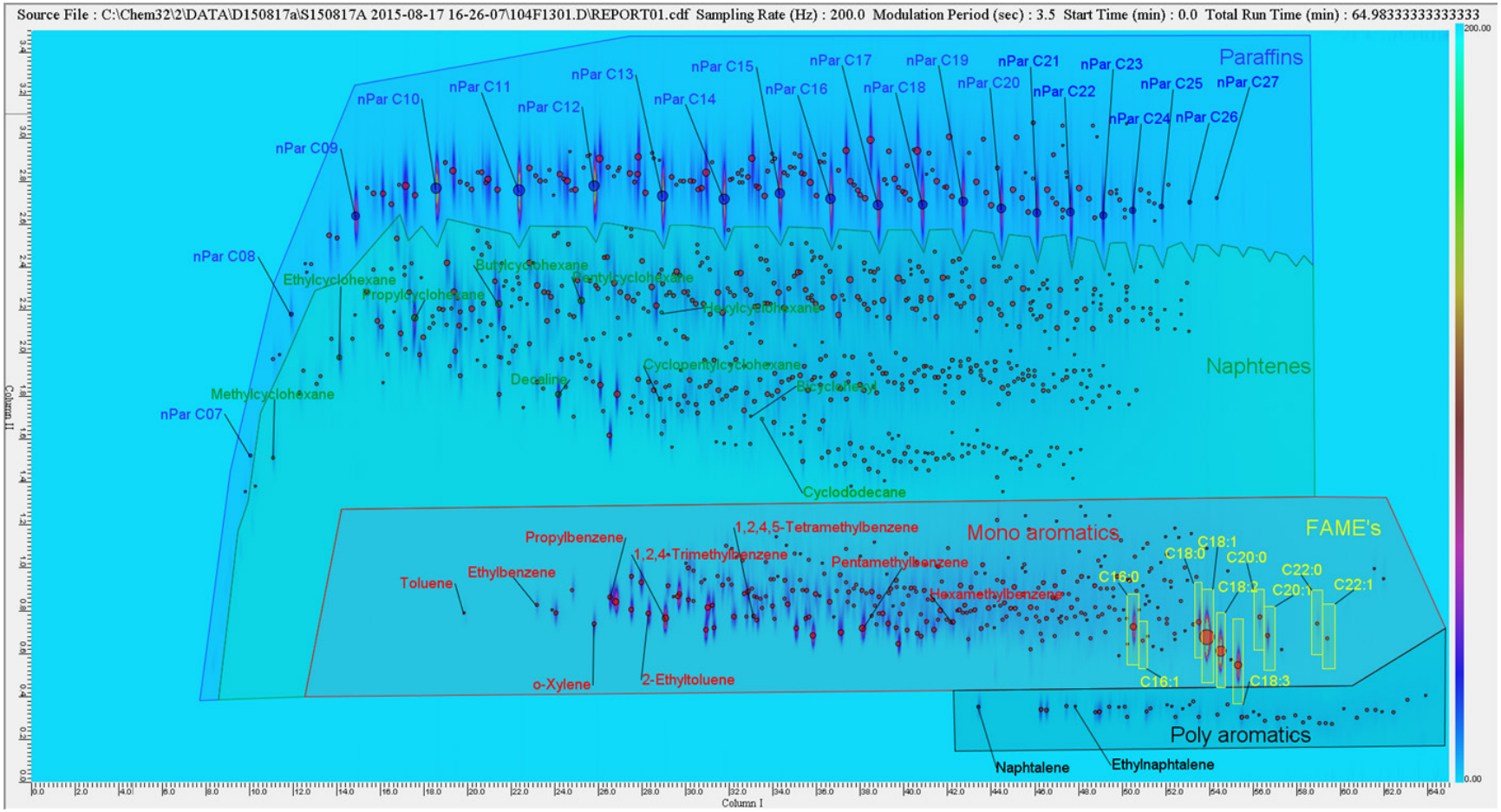
DIESEL

REFERENCE STD



DIESEL FUEL

PAC QC MATERIAL 00.02.719



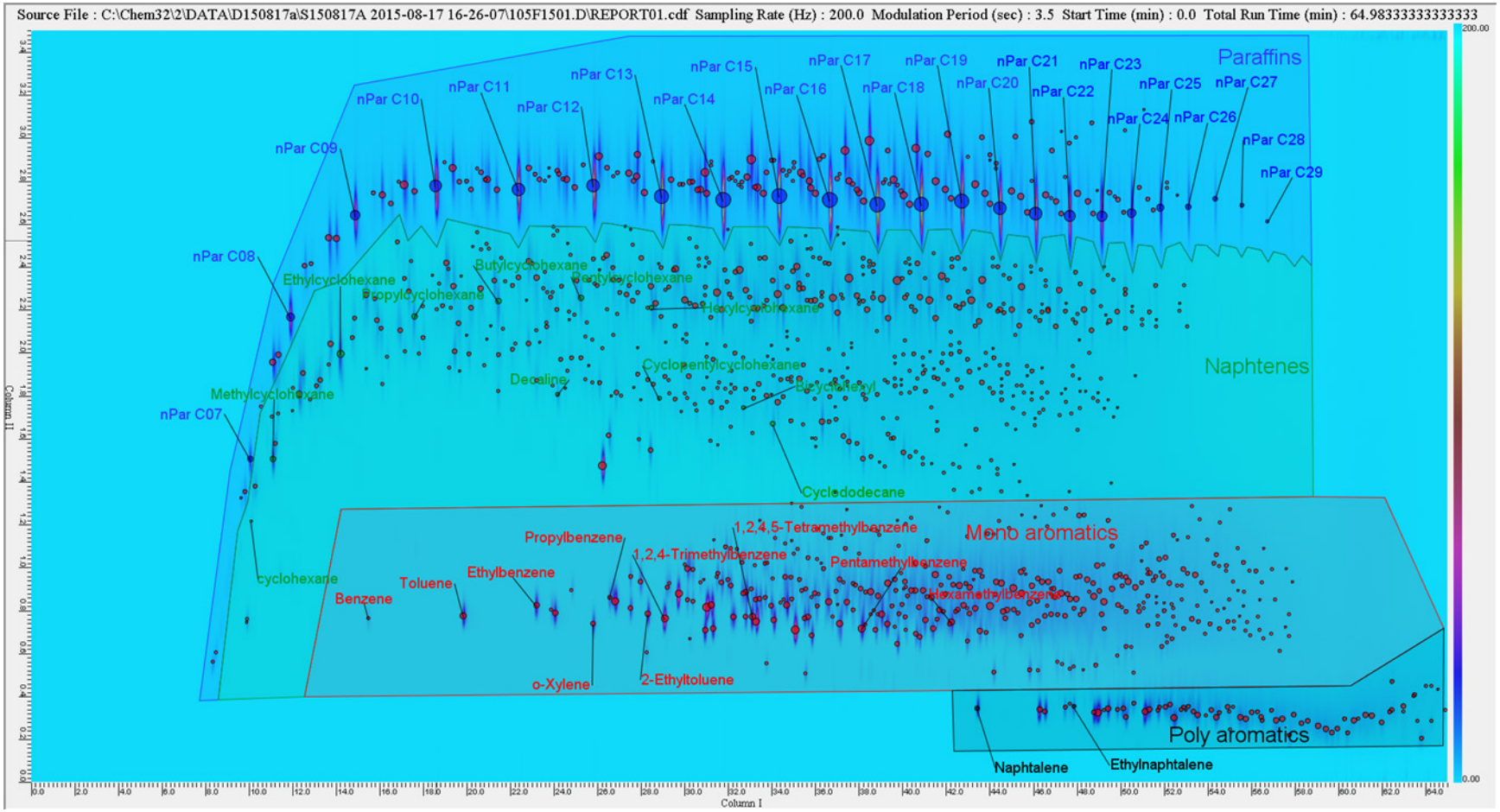
DIESEL FUEL

PAC REFERENCE MATERIAL

Component	Mass% standard	Mass% found	Difference
nPar C05	0.50	0.51	0.01
nPar C06	0.75	0.73	0.02
nPar C07	1.00	0.98	0.02
nPar C08	1.25	1.19	0.06
nPar C09	1.50	1.43	0.07
nPar C10	2.00	1.96	0.04
nPar C11	2.50	2.47	0.03
nPar C12	3.25	3.23	0.02
nPar C13	4.00	3.99	0.01
nPar C14	4.50	4.53	0.03
nPar C15	4.25	4.27	0.02
nPar C16	3.50	3.55	0.04
nPar C17	3.00	3.04	0.04
nPar C18	2.50	2.55	0.04
nPar C19	2.00	2.02	0.02
nPar C20	1.50	1.51	0.01
nPAr C22	1.50	1.52	0.02
nPar C24	1.25	1.26	0.01
nPar C28	0.75	0.75	0.00
nPar C30	0.50	0.49	0.01
C16:0 FAME	1.50	1.50	0.00
C18:0 FAME	1.50	1.50	0.00
C20:0 FAME	1.50	1.49	0.01
C22:0 FAME	1.50	1.48	0.02
Bicyclohexyl	2.35	2.39	0.04
Butylcyclohexane	3.50	3.52	0.02
Cyclododecane	1.25	1.27	0.02
Cycloheptane	2.00	2.01	0.01
Cyclooctane	2.75	2.78	0.03
Cyclopentadecane	0.75	0.76	0.01
Cyclopentylcyclohexane	0.75	0.75	0.00
trans-Decahydronaphtalene	2.75	2.75	0.00
Ethylcyclohexane	2.00	1.99	0.00
Hexylcyclohexane	1.50	1.50	0.00
Methylcyclohexane	1.25	1.27	0.02
Pentylcyclohexane	4.00	3.93	0.07
Propylcyclohexane	2.75	2.73	0.02
Cyclohexane	1.25	1.26	0.01
1,2,4,5-Tetramethylbenzene	2.75	2.77	0.02
1,2,4-Trimethylbenzene	3.50	3.51	0.01
2-ethyltoluene	3.00	3.01	0.01
Benzene	0.50	0.49	0.01
Ethylbenzene	2.00	1.98	0.02
Hexamethylbenzene	0.50	0.52	0.02
Pentamethylbenzene	2.00	1.99	0.01
n-Propylbenzene	4.00	3.99	0.01
Toluene	1.05	1.03	0.02
o-Xylene	2.75	2.74	0.01
2-Ethylnaphtalene	0.55	0.55	0.00
Naphtalene	0.55	0.55	0.00
Total Paraffins	42.008	41.99	0.02
Total FAME	6.001	5.963	0.04
Total Naphtenes	28.85	28.93	0.08
Total Aromatics	23.14	23.12	0.02
	100.000	100.00	

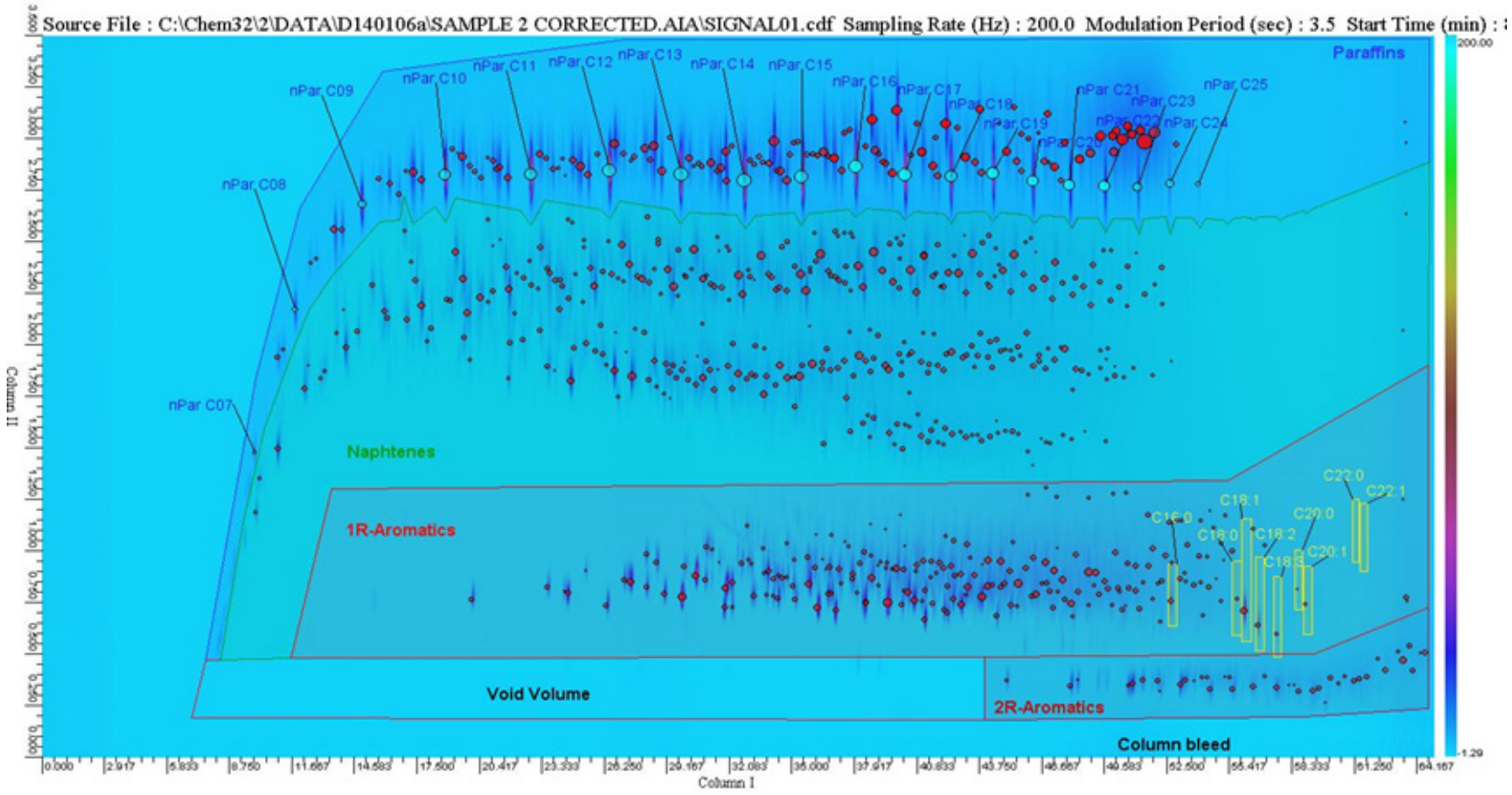
DIESEL FUEL

REGULAR DIESEL 1



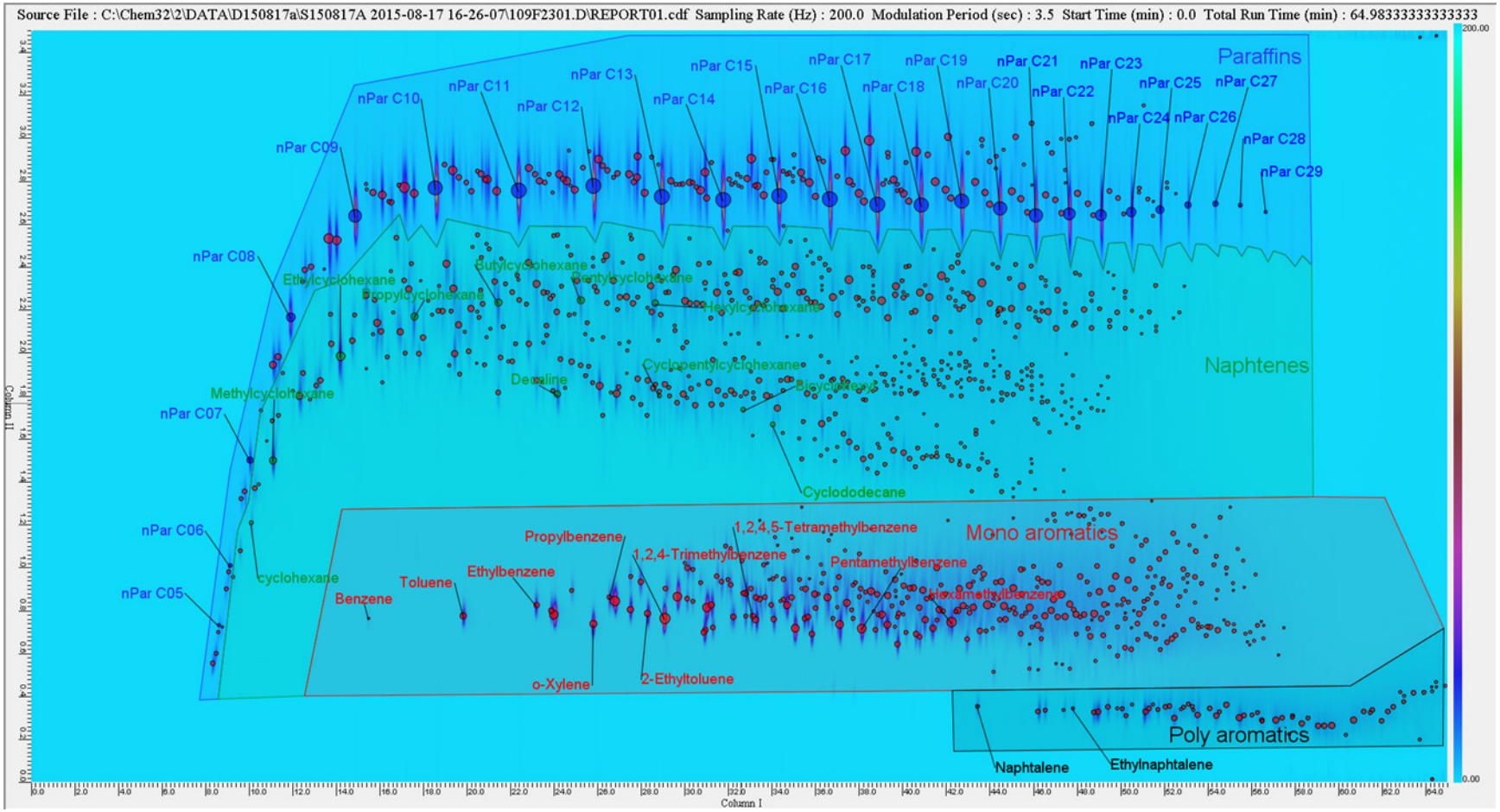
DIESEL FUEL

SHELL V-POWER DIESEL



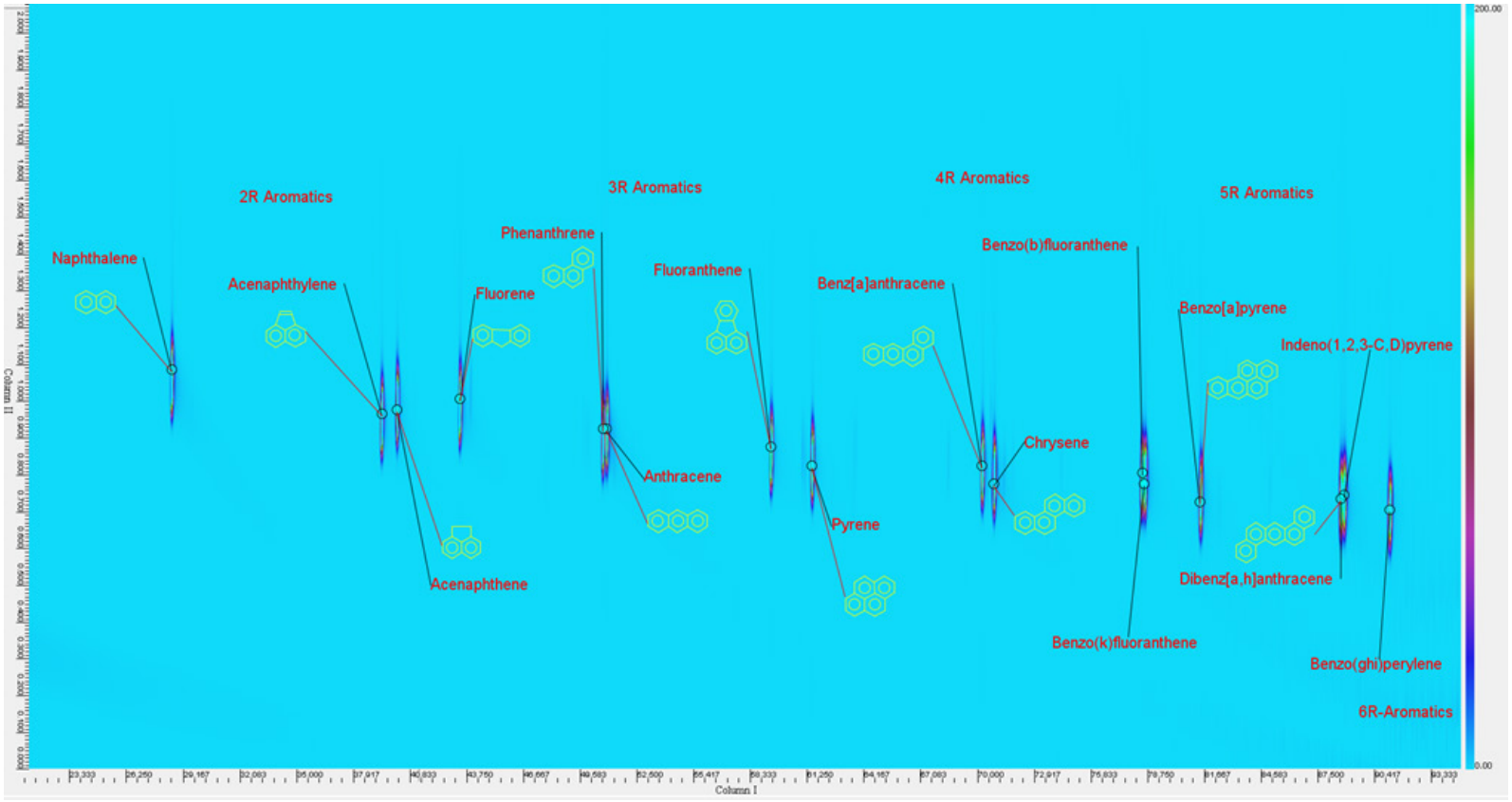
DIESEL FUEL

DIESEL "R5"



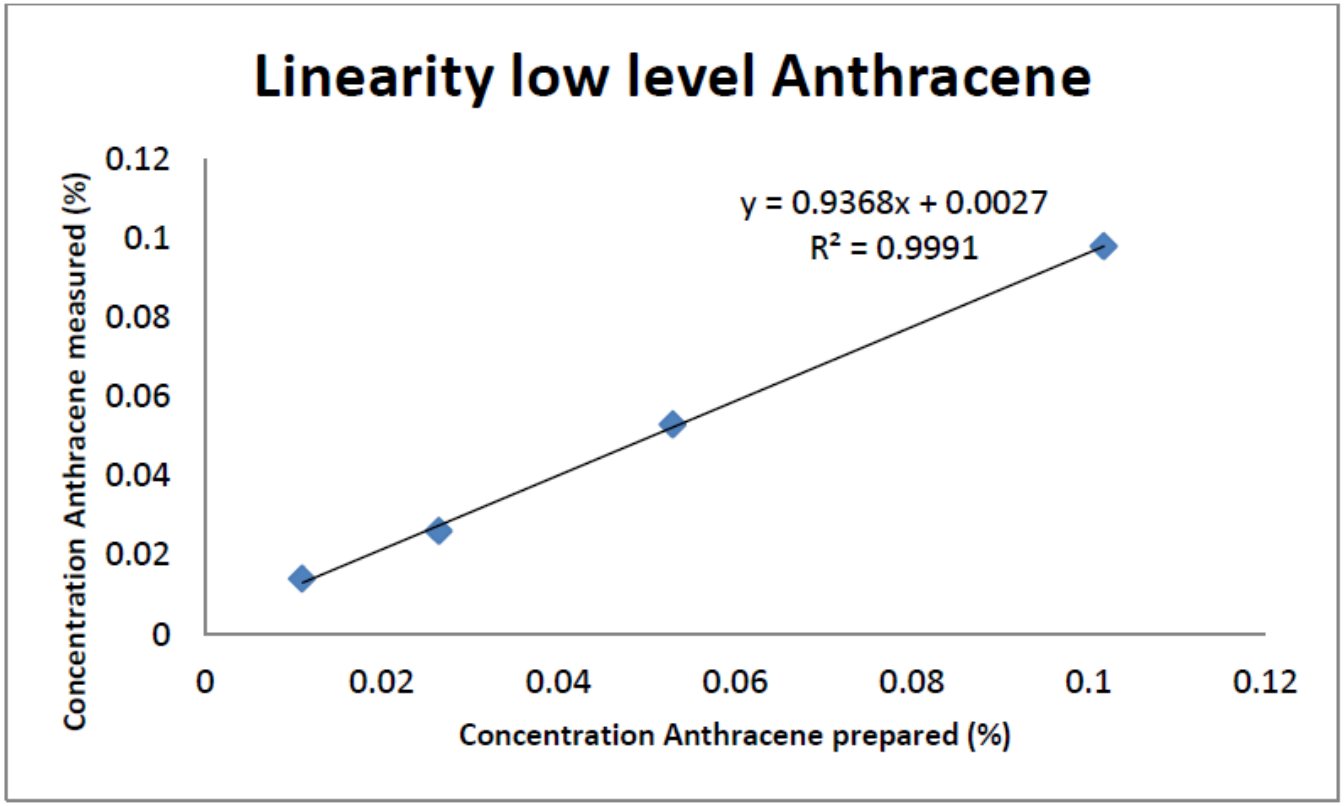
OTHER APPLICATIONS

POLY NUCLEAR AROMATICS



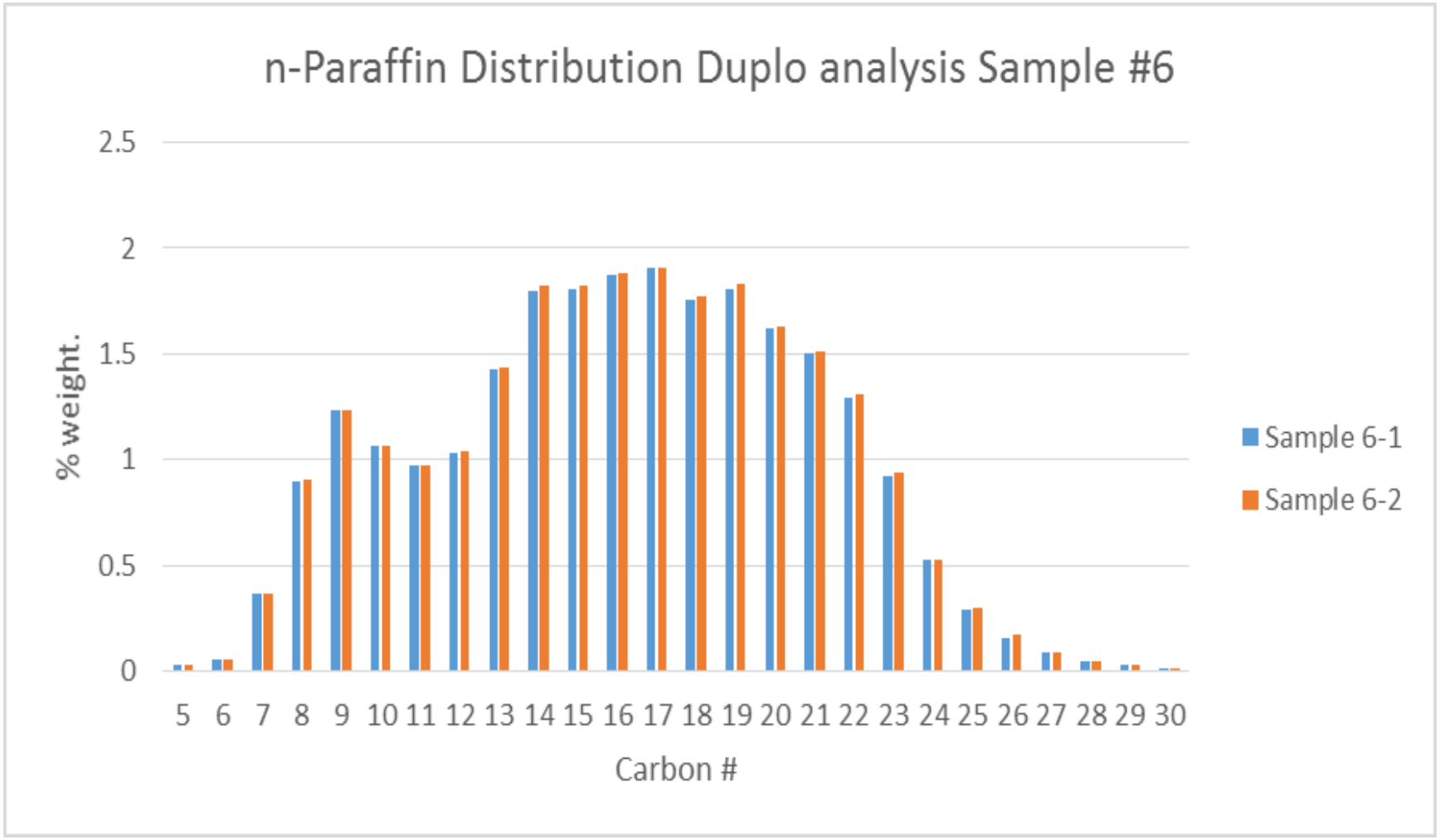
LINEARITY & DETECTION LIMIT

POLY NUCLEAR AROMATICS



REPEATABILITY

DIESEL

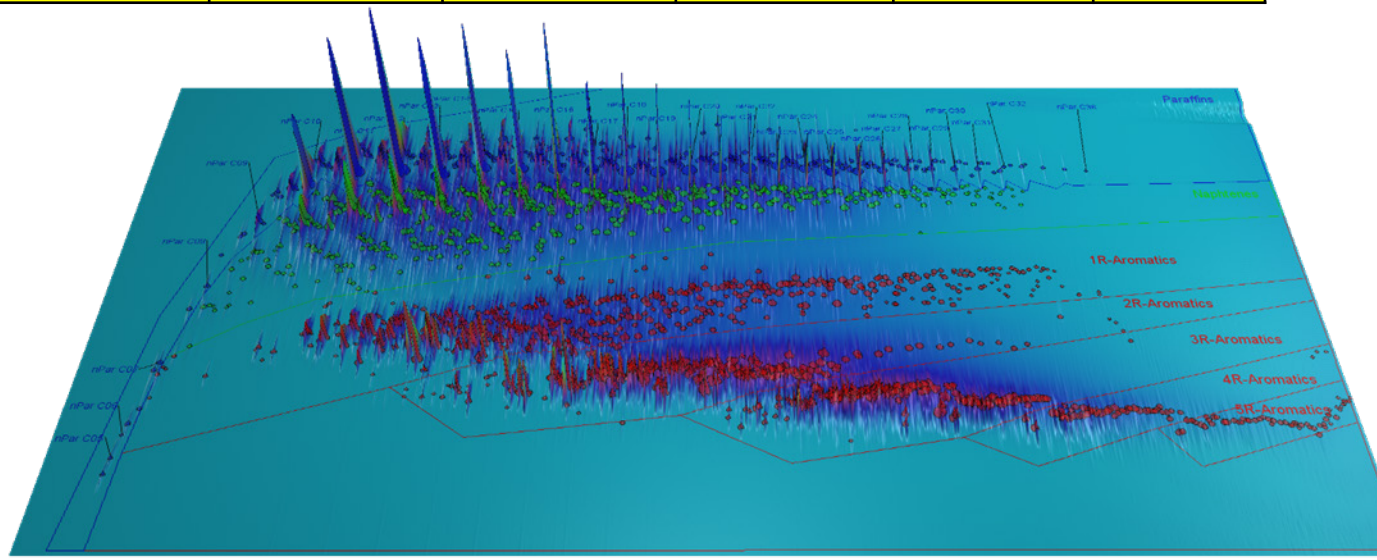


REPEATABILITY

LIGHT CYCLE OIL

Run	1R aromatics (% m/m)	2R aromatics (% m/m)	3R aromatics (% m/m)	4R aromatics (% m/m)	Naphthenes (% m/m)	n-Paraffins (% m/m)	Paraffins (% m/m)
1	14.89	26.03	22.59	0.80	10.18	7.44	25.51
2	14.80	26.05	22.65	0.81	9.98	7.56	25.72
3	14.88	25.89	22.70	0.83	9.83	7.40	25.87
4	14.86	25.81	22.78	0.84	9.97	7.40	25.74
5	14.84	25.99	22.73	0.71	9.87	7.43	25.86
6	14.84	25.64	22.59	0.74	9.86	7.35	26.17
7	14.92	25.74	22.72	0.79	10.11	7.39	25.72
8	14.87	25.99	22.55	0.75	9.63	7.42	26.19
9	14.77	25.92	22.73	0.74	9.86	7.45	25.99
10	14.69	26.12	22.67	0.76	9.74	7.43	26.02
MIN	14.69	25.64	22.55	0.71	9.63	7.35	25.51
MAX	14.92	26.12	22.78	0.84	10.18	7.56	26.19
Average	14.84	25.92	22.67	0.77	9.90	7.43	25.88
stdev	0.0677	0.1498	0.0744	0.0439	0.1631	0.0554	0.2184
RSD	**0.46%**	**0.58%**	**0.33%**	**5.7%**	**1.7%**	**0.75%**	**0.84%**

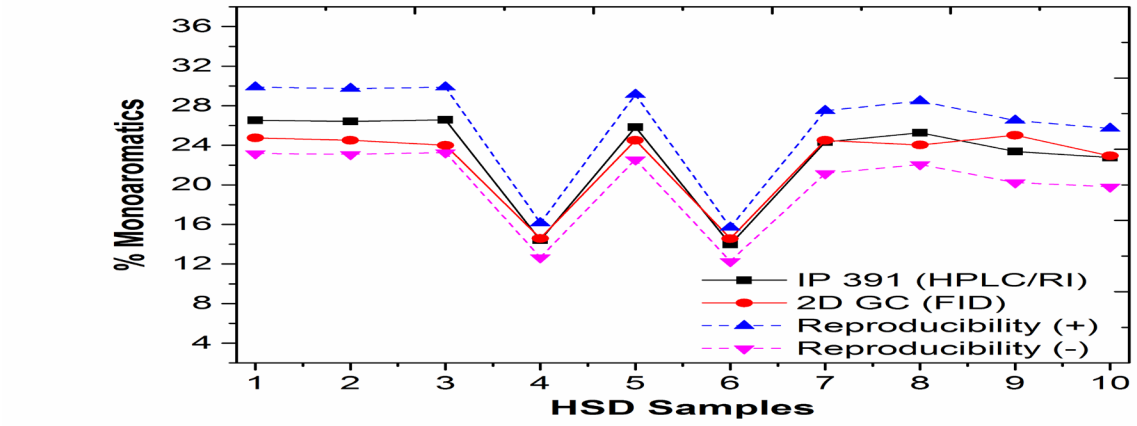
Sample: Light Cycle Oil sample



ACCURACY/PRECISION/BIAS

GCXGC VS IP391 - MONOAROMATICS

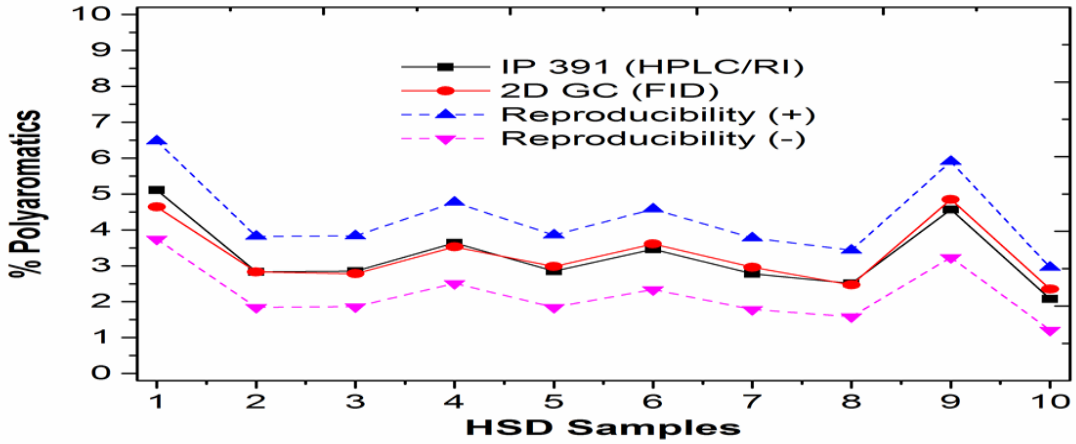
Sample	Monoaromatics, % by mass		Reproducibilty calculation as per IP 391 method	
	IP 391 method (HPLC/RI detection)	2D GC method	Reproducibiility (+)	Reproducibiility (-)
HSD -1	26.53	24.75	29.88	23.18
HSD -2	26.42	24.51	29.74	23.10
HSD -3	26.57	24	29.87	23.27
HSD -4	14.41	14.59	16.15	12.67
HSD -5	25.85	24.51	29.13	22.57
HSD -6	13.99	14.57	15.70	12.28
HSD -7	24.33	24.5	27.50	21.16
HSD -8	25.27	24.03	28.48	22.06
HSD -9	23.37	25.02	26.51	20.23
HSD -10	22.76	22.93	25.71	19.81



ACCURACY/PRECISION/BIAS

GCXGC VS IP391 - POLY-AROMATICS

Sample	Polyaromatics, % by mass		Reproducibilty calculation as per IP 391 method	
	IP 391 method (HPLC/RI detection)	2D GC method	Reproducibiility (+)	Reproducibiility (-)
HSD -1	5.11	4.64	6.48	3.74
HSD -2	2.83	2.83	3.82	1.84
HSD -3	2.85	2.78	3.84	1.86
HSD -4	3.64	3.53	4.77	2.51
HSD -5	2.85	2.98	3.85	1.85
HSD -6	3.46	3.61	4.58	2.34
HSD -7	2.78	2.96	3.78	1.78
HSD -8	2.51	2.47	3.44	1.58
HSD -9	4.57	4.85	5.91	3.23
HSD -10	2.08	2.35	2.95	1.21



SUMMARY
GCXGC ANALYZER

- 1 system, 1 method
  - Simple hardware: Flow Modulation + FID
- Reports all relevant groups including FAMES
- Sample range Jet/Diesel/Biodiesel (450C FBP)
- Standards and Reference Materials
- Robust, comparable and actionable data

GCxGC can be simple and performed in routine.

GCXGC

FUTURE CHALLENGES

- Widen implementation, produce more real sample data in routine use.
- Standardization

PAC | solid partners proven solutions

Contacts for more information:
Salessupport@paclp.com
rob.dejong@paclp.com