PAMS AutoGC

Lab Quality Analysis in Continuous Ambient Air Monitoring

Monitoring Network Performance for PAMS VOCs Across Over 35 PerkinElmer Ozone Precursor Systems in Texas

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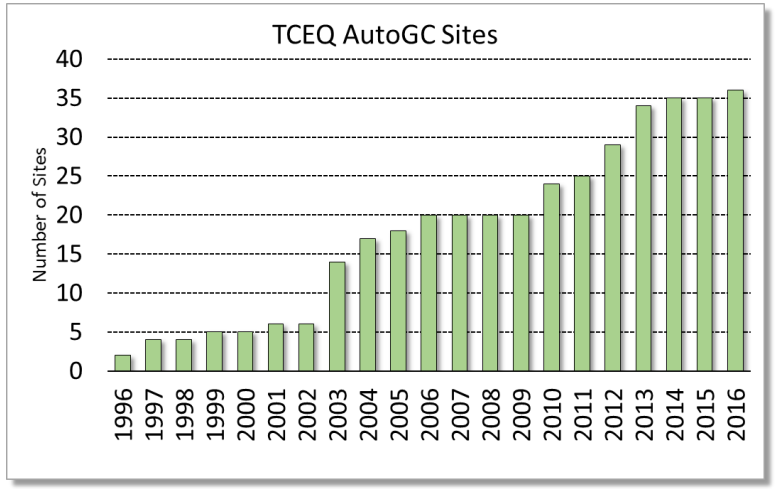
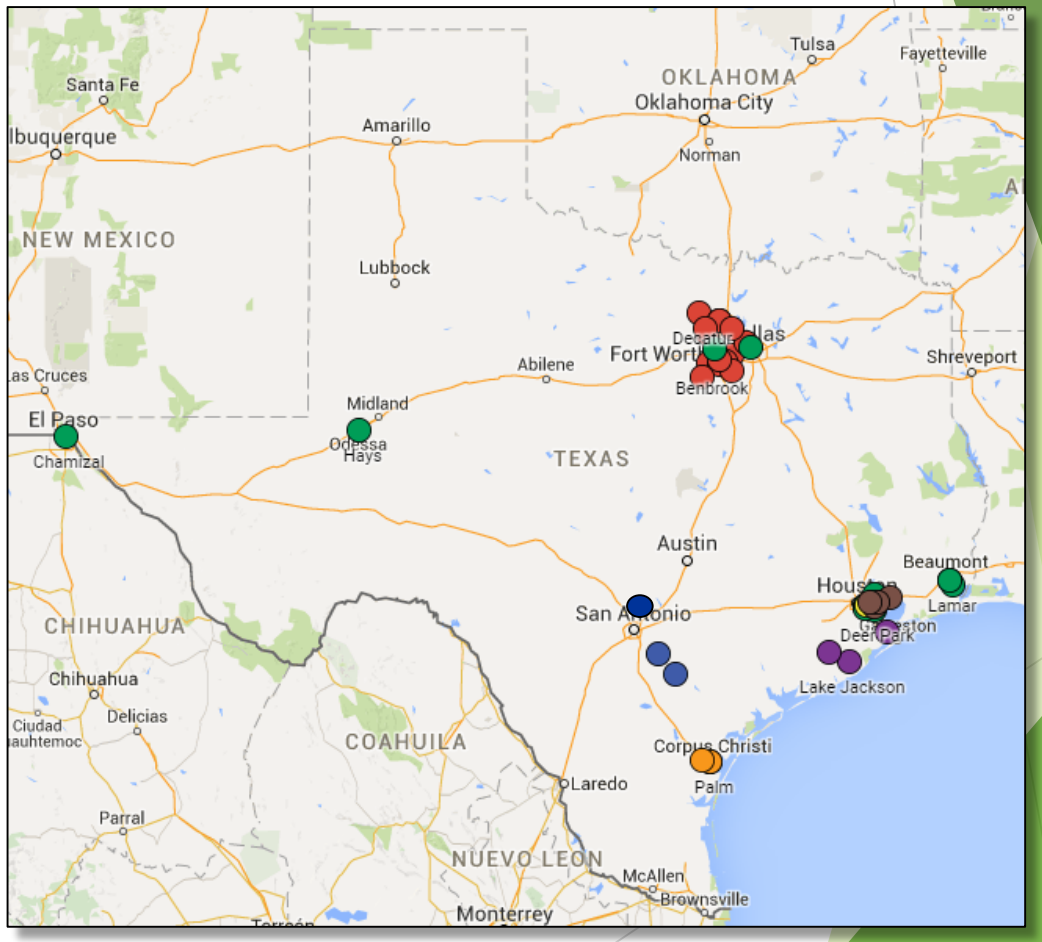
Texas Commission on Environmental Quality AutoGC Networks

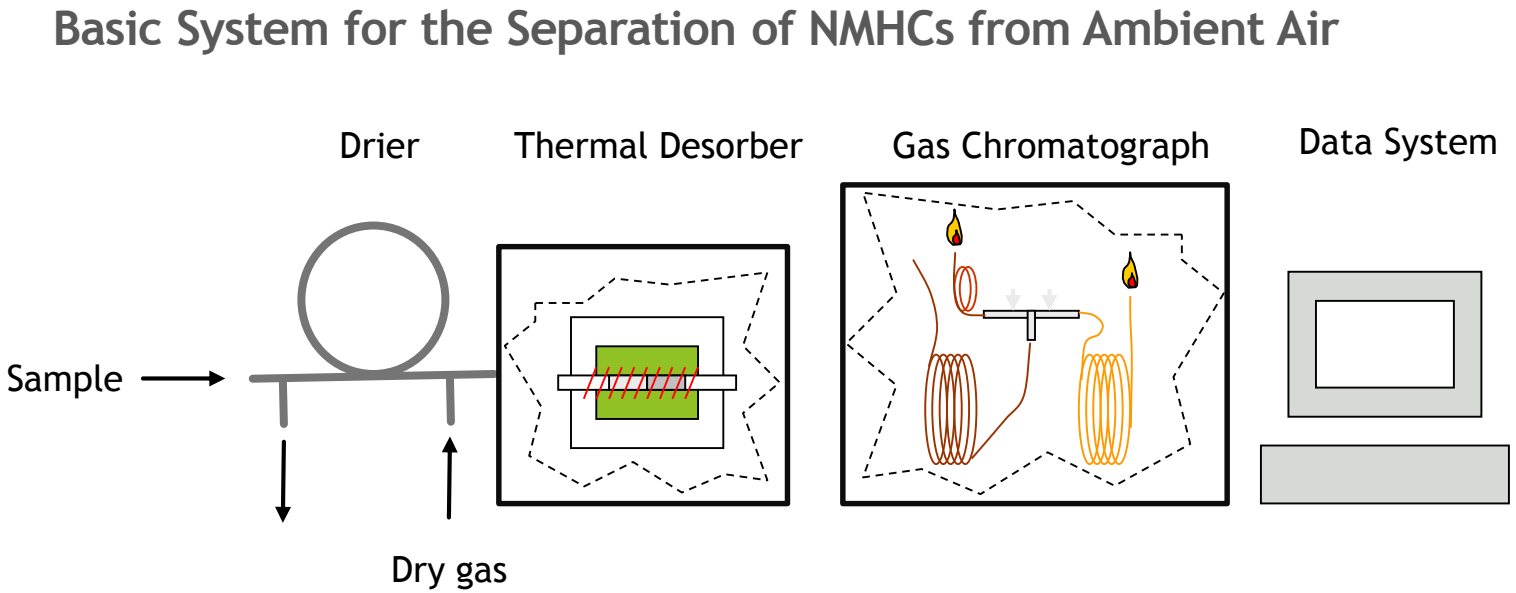
Network	# of Sites
Houston Regional Monitoring Group	4
Extended Industry Monitoring Sites	3
North Texas Commission	13
University of Texas CEER	4
Harris County Pollution Control	1
TCEQ	12
Total AutoGC Sites	37

AutoGC Sites in Operation by Year





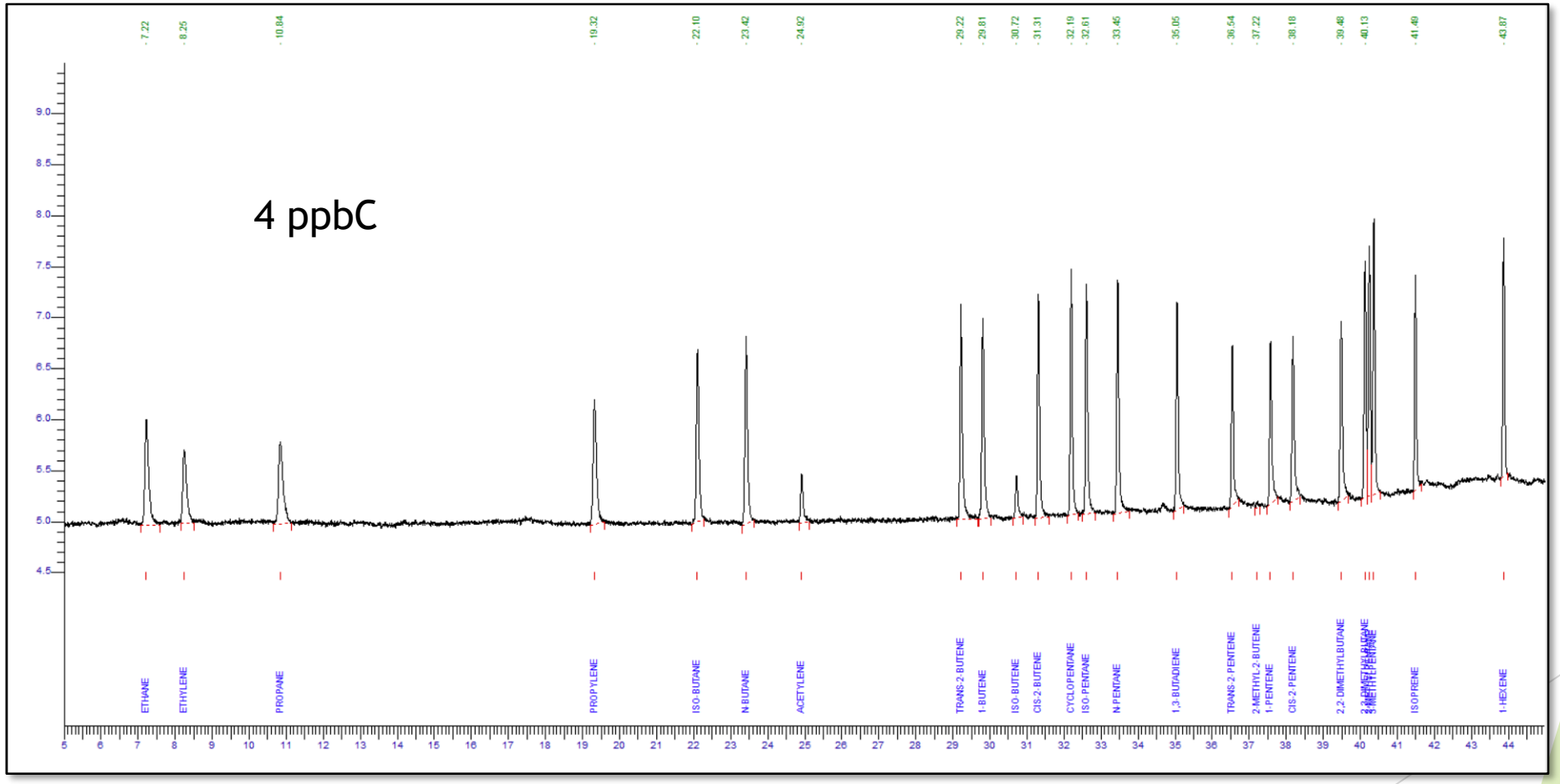
AutoGC Systems: Hourly Sample Collection and Separation



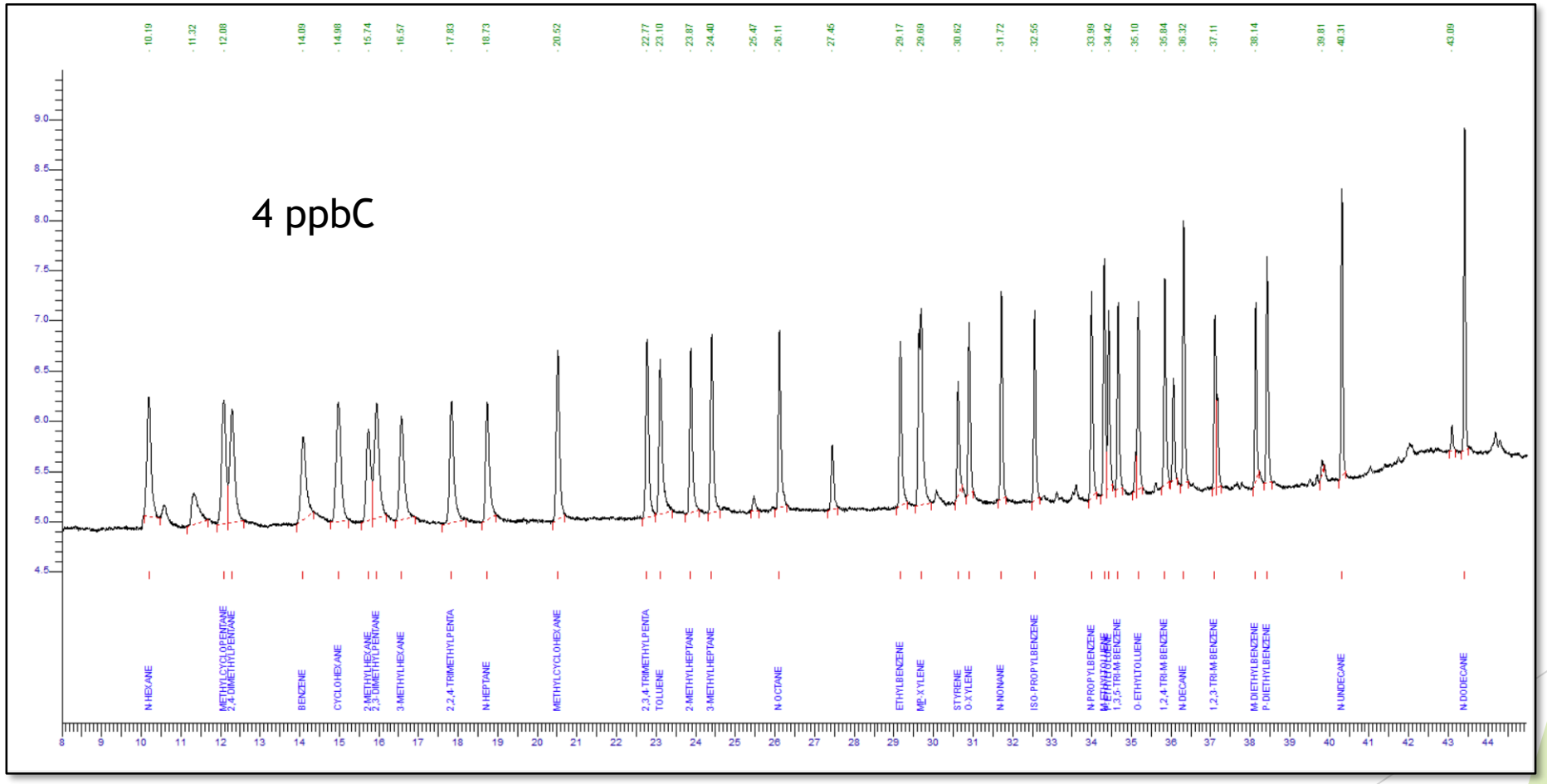
Additional Automation for Introduction of Quality Control Samples

- Automatic introduction of QC samples
  - Dynamically diluted check standard
  - Analytical blank
- Manual dilution of multipoint calibration curve
- Dilution from 100 ppbv or 1 ppmv multi-component standard

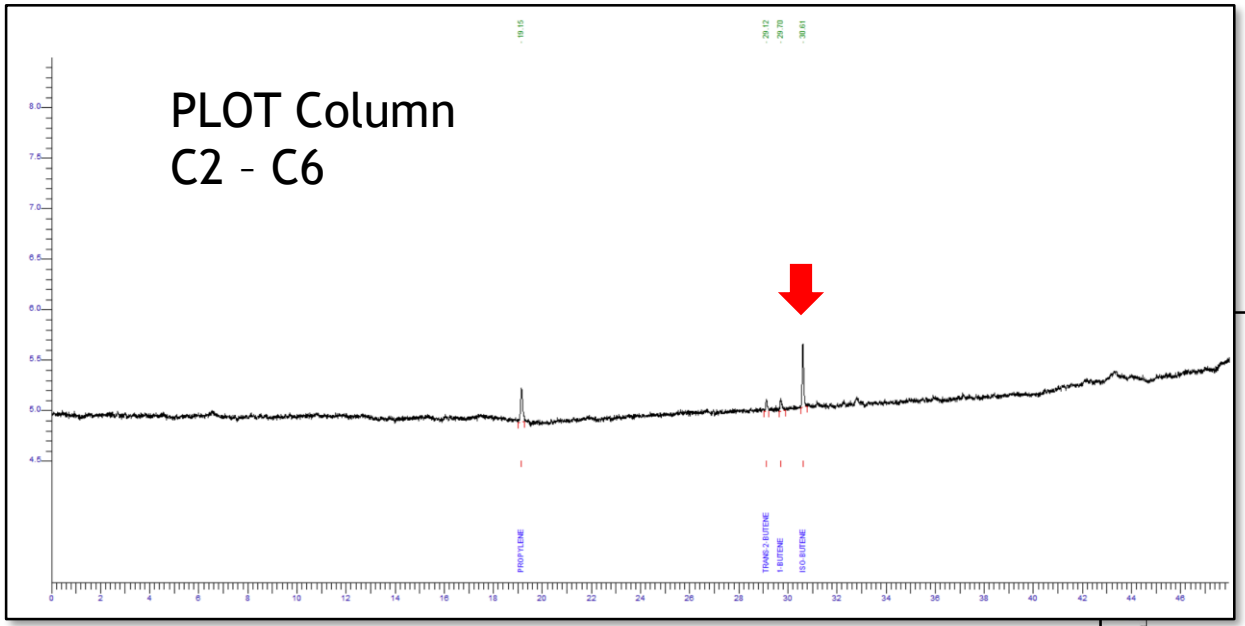
C2-C6 Alumina PLOT Separation

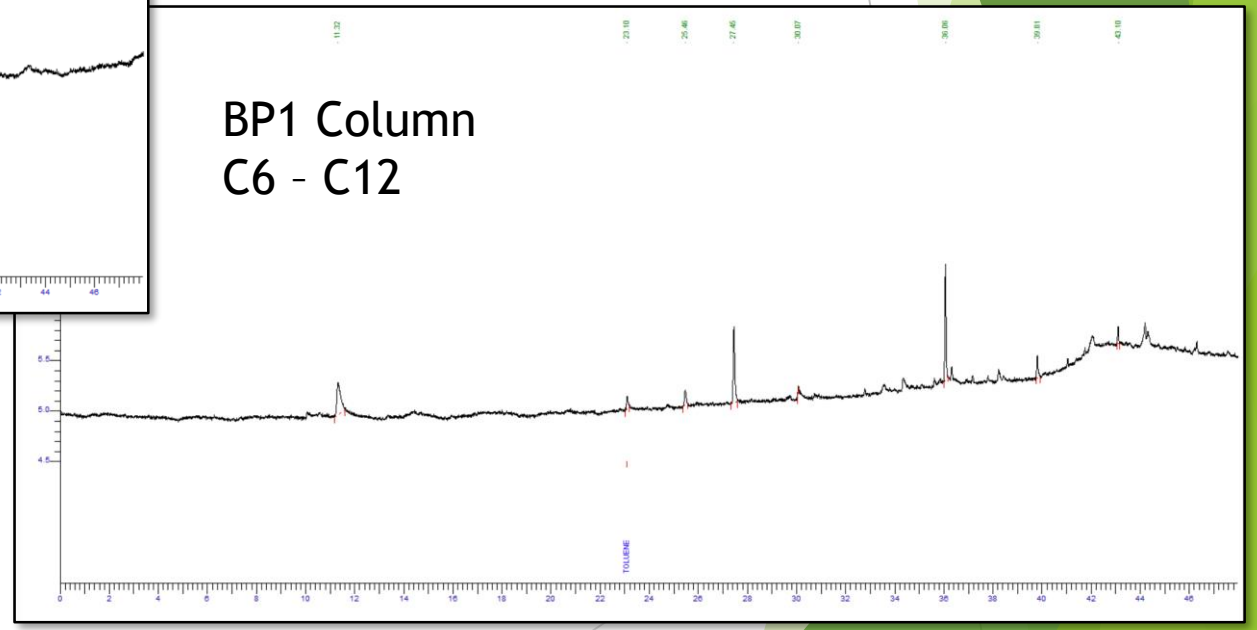


C6+ Dimethylsiloxane (Boiling Point) Separation

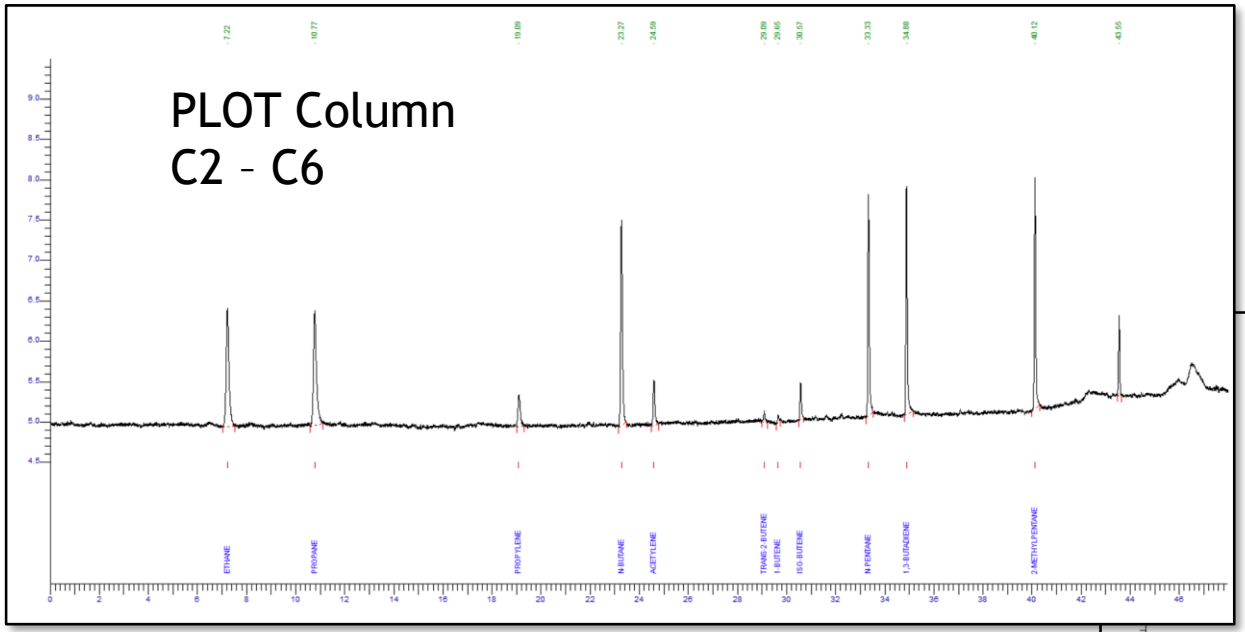


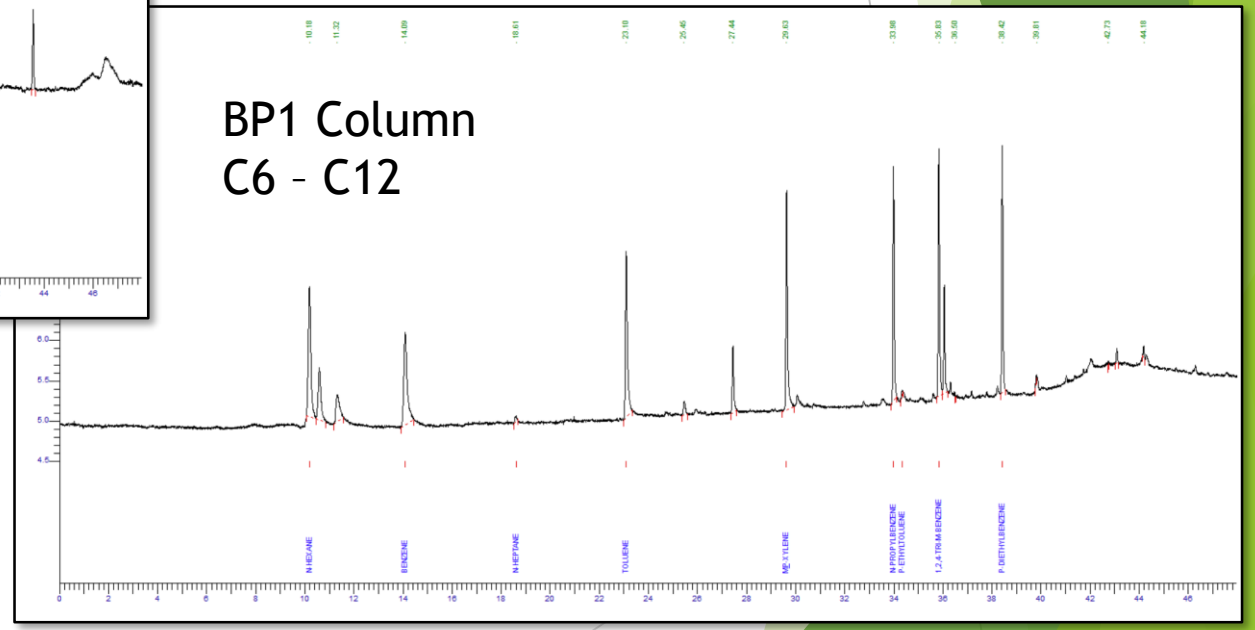
Analytical Blank



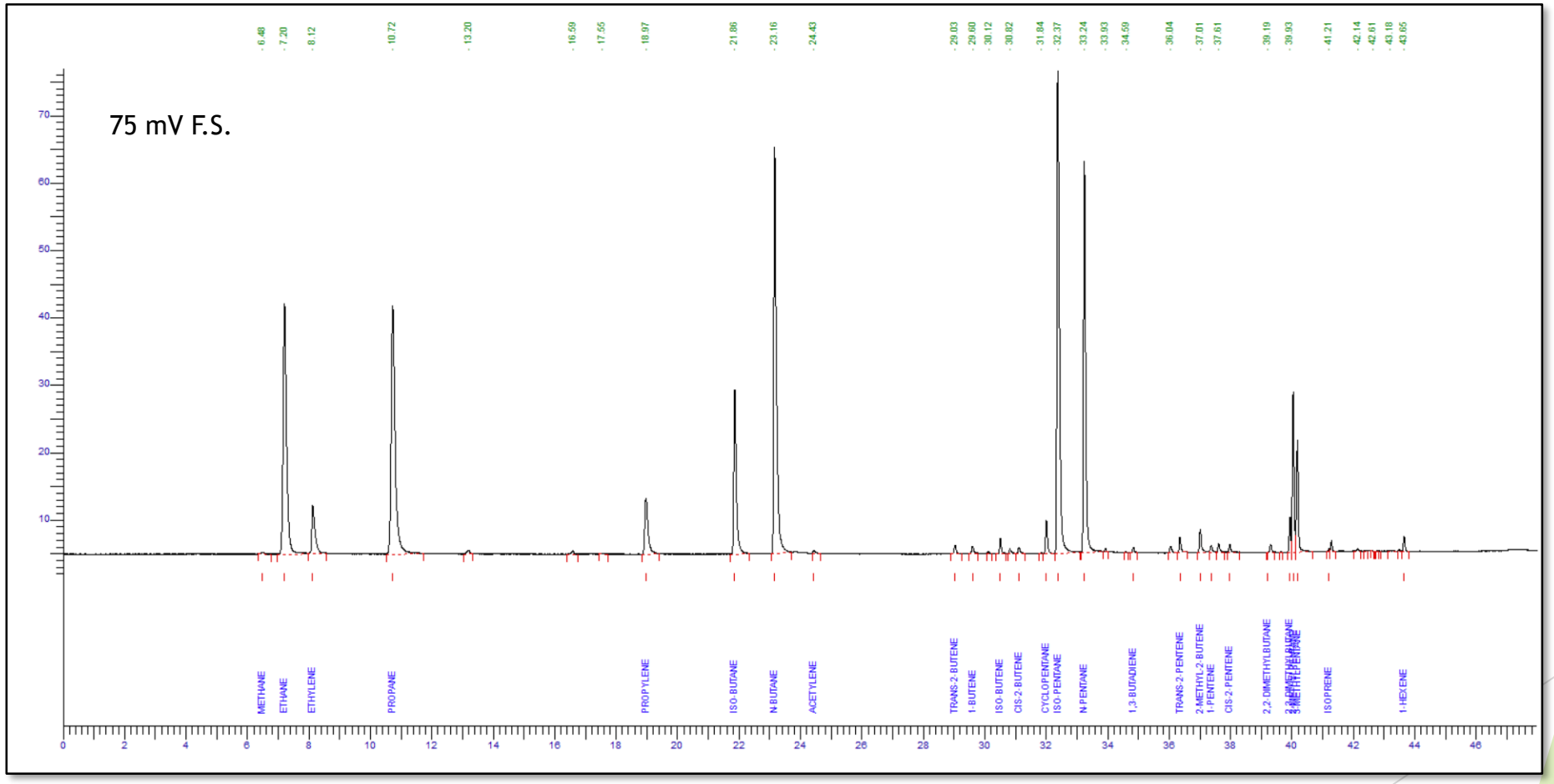


Daily Check Standard – 2-4 ppbC

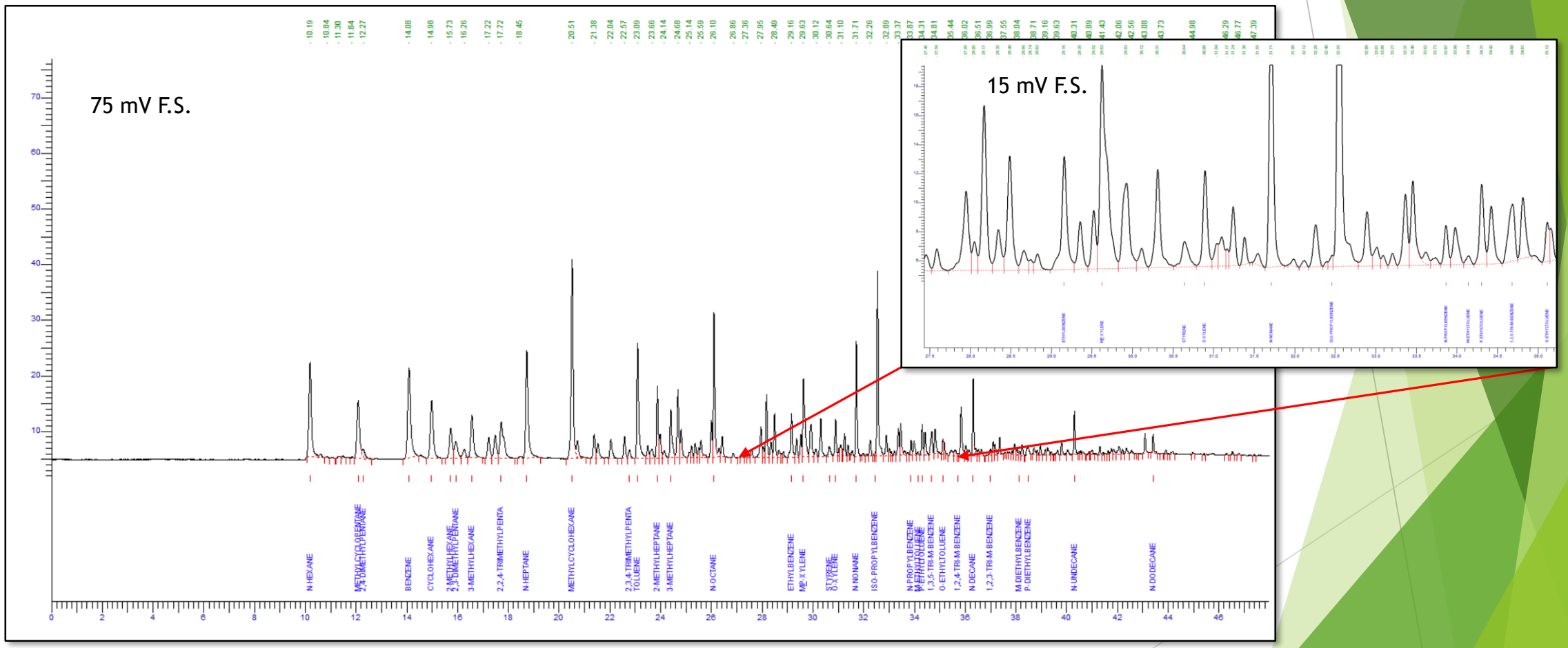




Ambient Air – PLOT Column



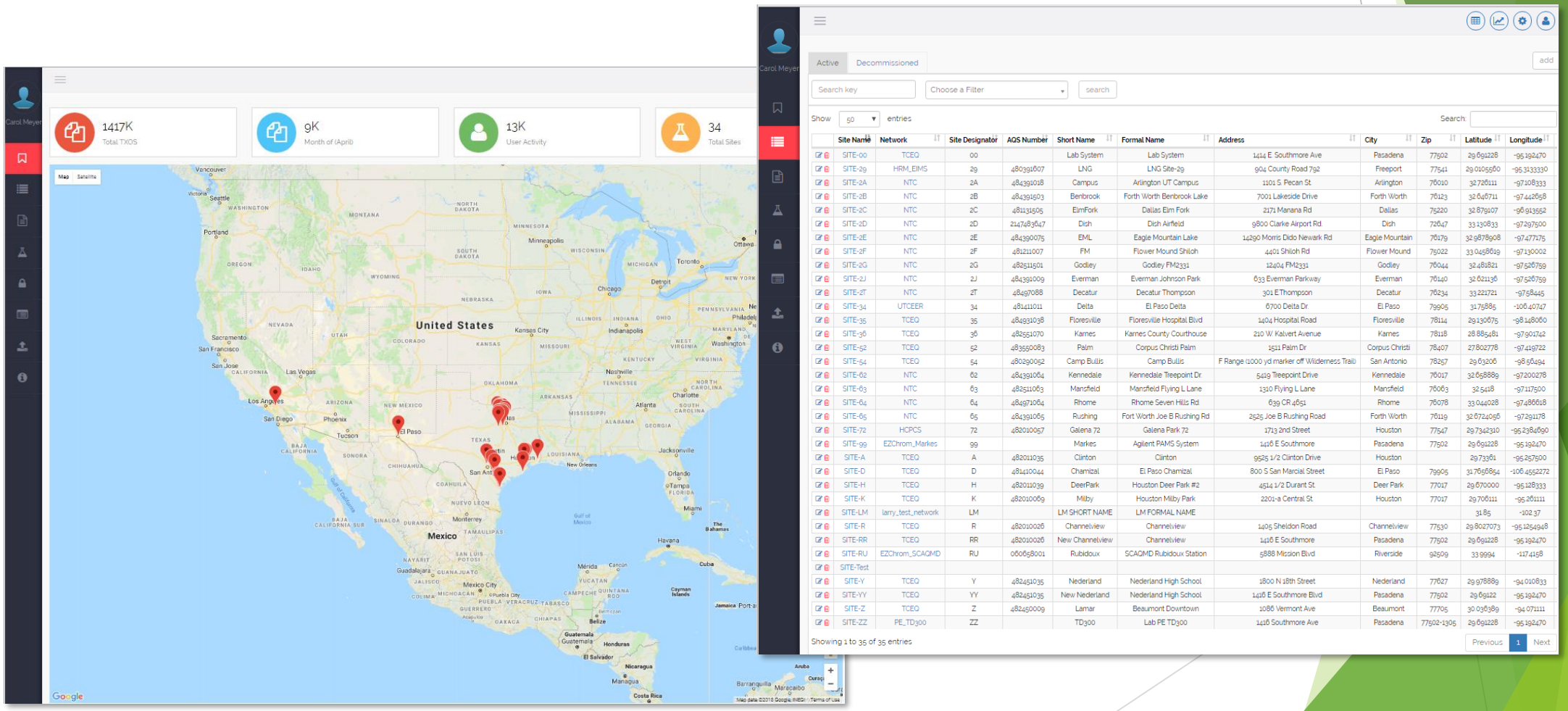
Ambient Air – Boiling Point Column



Network Quality Control

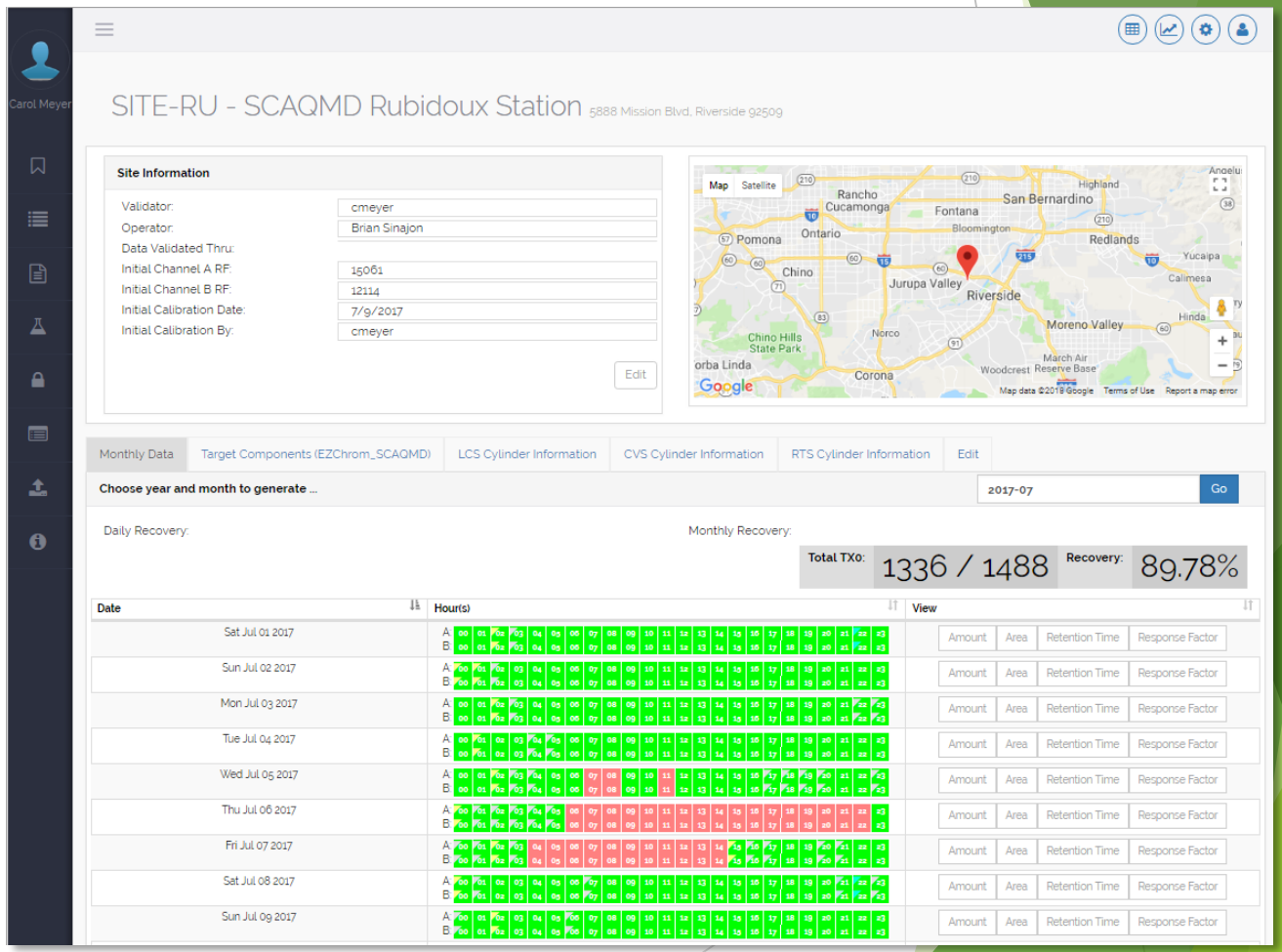
Quality Control Check	Composition	Purpose	Frequency	Acceptance Criteria
Retention Time Standard (RTS)	Mixture containing all target compounds ideally between 1-5 ppbC	To help assess retention time shifts and optimize processing methods	Twice a month or weekly	100% of the compounds are identified correctly in the multicomponent RTS
Calibration Verification Standard (CVS)	Mixture of 15 reference compounds including Propane and Benzene used for calibration	To assess the instrument drift and ensure continued instrument calibration	Daily	1) Propane and Benzene % recoveries within 75% - 125% and all other calibrants within 55 - 145%
				2) Data must be bracketed by valid CVS
Method (Analytical) Blank	Humidified, clean air	To assess system contribution to the measurement	Daily	1) All target compounds < 2.0 ppbC
				2) TNMHC < 20 ppbC
				3) Data must be bracketed by valid blanks
Precision Check	Mixture used for CVS	To assess analytical precision	Weekly	Propane and Benzene %RPD < 20% in two consecutive CVS runs
Laboratory Calibration Standard (LCS)	Mixture of 15 reference compounds including Propane and Benzene used for calibration	Second source standard, statically blended 5 ppbv	Twice a month or weekly	Propane and Benzene % recoveries within 70-130%

Evaluation of System Performance
Merlin AutoGC Xplorer - MAX

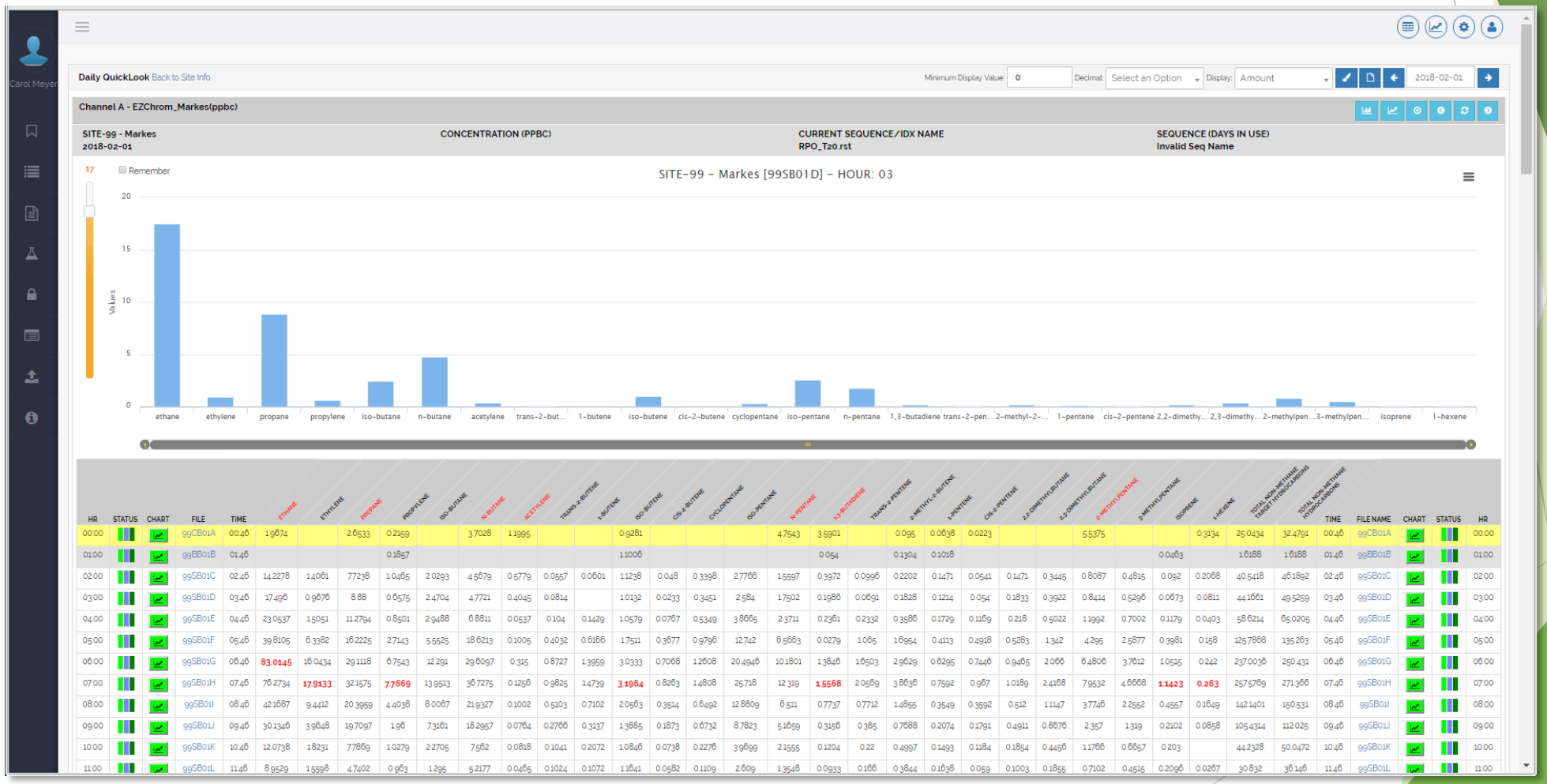


Evaluation of System Performance Data Verification and Validation

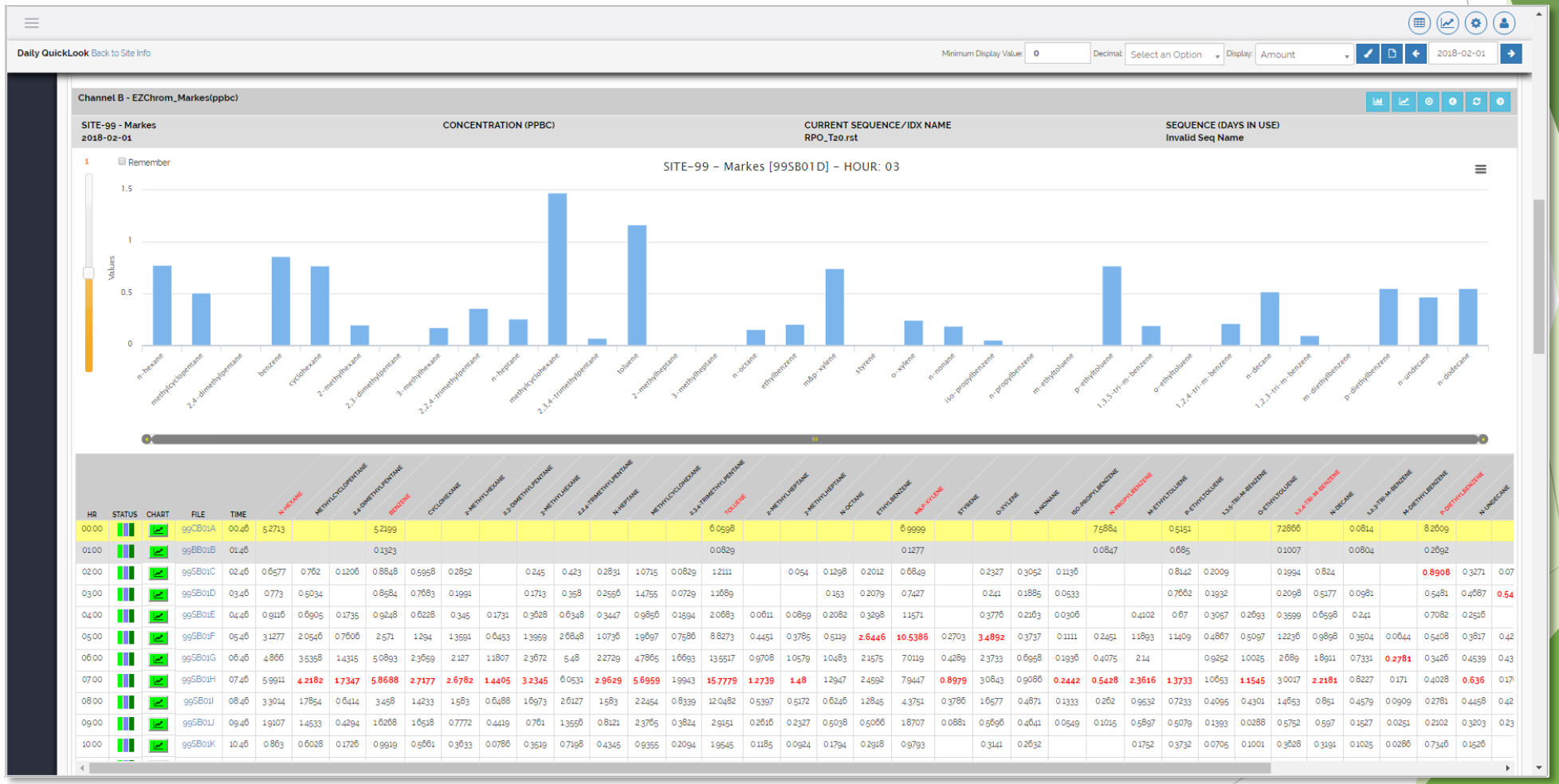
- Verification
  - Routine operator review
    - Instrument operation
    - Data completeness
    - Quality Controls meet criteria
  - Technical Review
    - Quality Controls meet criteria
    - Review operator logs for deviations in procedures
    - Flagging of data based on observed discrepancies
- Data Validation
  - Level 1 – Identify atypical data
  - Level 2 – Compare data set to historical data (if available)
  - Level 3 – Compare dataset within the same population to observe systematic bias



Daily QuickLook

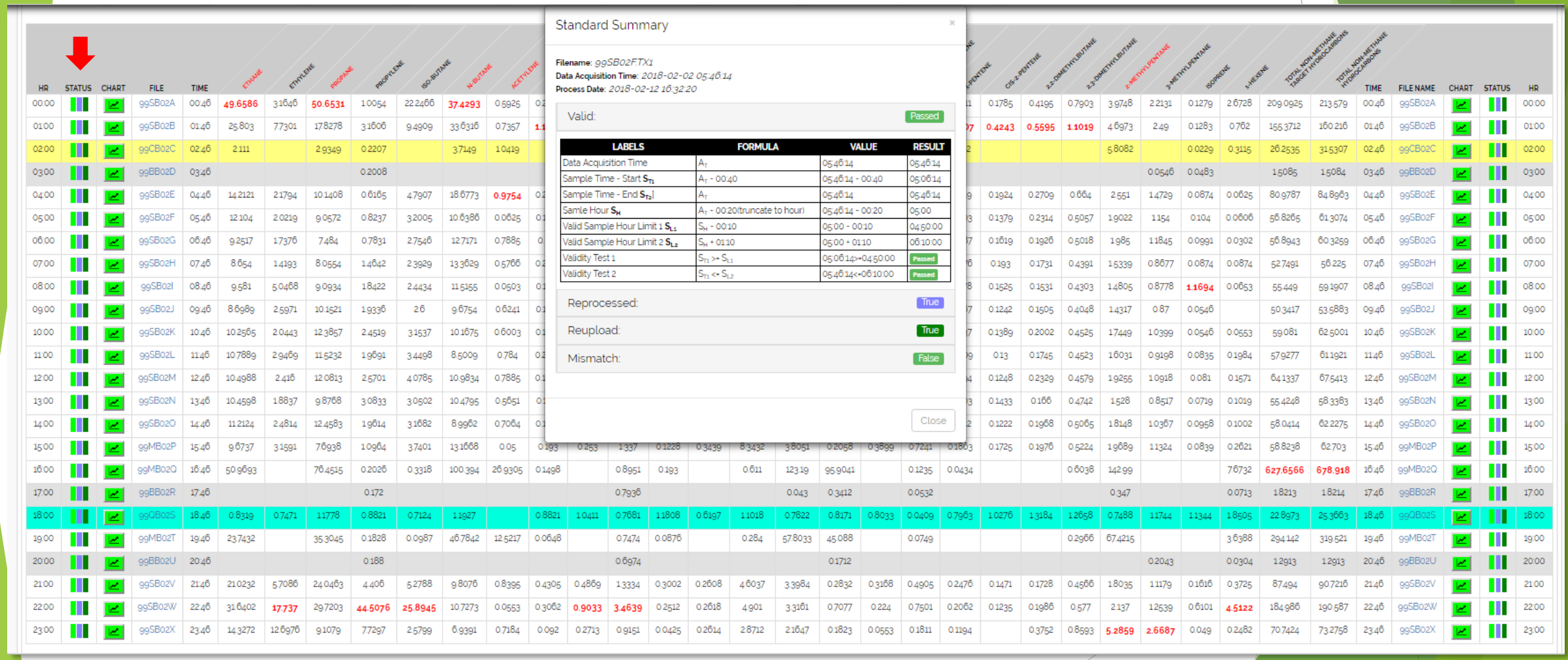


Daily QuickLook



HR	STATUS	CHART	FILE	TIME	N-HEXANE	METHYLCYCLOPENTANE	2,4-DIMETHYLPENTANE	BENZENE	CYCLOHEXANE	2-METHYLHEXANE	2,3-DIMETHYLPENTANE	3-METHYLHEXANE	2,2,4-TRIMETHYLPENTANE	N-HEPTANE	METHYLCYCLOHEXANE	2,3,4-TRIMETHYLPENTANE	TOLUENE	2-METHYLHEPTANE	3-METHYLHEPTANE	N-OCTANE	ETHYLBENZENE	M&P-XYLENE	STYRENE	O-XYLENE	N-NONANE	ISO-PROPYLBENZENE	N-PROPYLBENZENE	M-ETHYLTOLUENE	P-ETHYLTOLUENE	1,3,5-TRI-M-BENZENE	O-ETHYLTOLUENE	1,2,4-TRI-M-BENZENE	N-DECANE	1,2,3-TRI-M-BENZENE	M-DIETHYLBENZENE	P-DIETHYLBENZENE	N-UNDECANE
00:00			99CB01A	00:46	5.2713			5.2199									6.0598					6.9999					7.5884		0.5151			7.2866		0.0814		8.2609		
01:00			99BB01B	01:46				0.1323									0.0829					0.1277					0.0847		0.685			0.1007		0.0804		0.2692		
02:00			99SB01C	02:46	0.6577	0.762	0.1206	0.8848	0.5958	0.2852		0.245	0.423	0.2831	1.0715	0.0829	1.2111		0.054	0.1298	0.2012	0.6849		0.2327	0.3052	0.1136			0.8142	0.2009		0.1994	0.824			0.8908	0.3271	0.07
03:00			99SB01D	03:46	0.773	0.5034		0.8584	0.7683	0.1991		0.1713	0.358	0.2556	1.4755	0.0729	1.1689			0.153	0.2079	0.7427		0.241	0.1885	0.0533			0.7662	0.1932		0.2098	0.5177	0.0981		0.5481	0.4687	0.54
04:00			99SB01E	04:46	0.9116	0.6905	0.1735	0.9248	0.6228	0.345	0.1731	0.3628	0.6348	0.3447	0.9856	0.1594	2.0683	0.0611	0.0859	0.2082	0.3298	1.1571		0.3776	0.2163	0.0306		0.4102	0.67	0.3057	0.2693	0.3699	0.6598	0.241		0.7082	0.2516	
05:00			99SB01F	05:46	3.1277	2.0546	0.7606	2.571	1.294	1.3591	0.6453	1.3959	2.6848	1.0736	1.9697	0.7586	8.8273	0.4451	0.3785	0.5119	2.6446	10.5386	0.2703	3.4892	0.3737	0.1111	0.2451	1.1893	1.1409	0.4867	0.5097	1.2236	0.9898	0.3504	0.0644	0.5408	0.3817	0.42
06:00			99SB01G	06:46	4.866	3.5358	1.4315	5.0893	2.3659	2.127	1.1807	2.3672	5.48	2.2729	4.7865	1.6693	13.5517	0.9708	1.0579	1.0483	2.1575	7.0119	0.4289	2.3733	0.6958	0.1936	0.4075	2.14		0.9252	1.0025	2.689	1.8911	0.7331	0.2781	0.3426	0.4539	0.43
07:00			99SB01H	07:46	5.9911	4.2182	1.7347	5.8688	2.7177	2.6782	1.4405	3.2345	6.0531	2.9629	5.6959	1.9943	15.7779	1.2739	1.48	1.2947	2.4592	7.9447	0.8979	3.0843	0.9086	0.2442	0.5428	2.3616	1.3733	1.0653	1.1545	3.0017	2.2181	0.8227	0.171	0.4028	0.636	0.17
08:00			99SB01I	08:46	3.3014	1.7854	0.6414	3.458	1.4233	1.583	0.6488	1.6973	2.6127	1.583	2.2454	0.8339	12.0482	0.5397	0.5172	0.6246	1.2845	4.3751	0.3786	1.6577	0.4871	0.1333	0.262	0.9532	0.7233	0.4095	0.4301	1.4653	0.851	0.4579	0.0909	0.2781	0.4458	0.42
09:00			99SB01J	09:46	1.9107	1.4533	0.4294	1.6268	1.6518	0.7772	0.4419	0.761	1.3556	0.8121	2.3765	0.3824	2.9151	0.2616	0.2327	0.5038	0.5066	1.8707	0.0881	0.5696	0.4641	0.0549	0.1015	0.5897	0.5079	0.1393	0.0288	0.5752	0.597	0.1527	0.0251	0.2102	0.3203	0.23
10:00			99SB01K	10:46	0.863	0.6028	0.1726	0.9919	0.6661	0.3633	0.0786	0.3519	0.7198	0.4345	0.9355	0.2094	1.9545	0.1185	0.0924	0.1794	0.2918	0.9793		0.3141	0.2632			0.1752	0.3732	0.0705	0.1001	0.3628	0.3191	0.1025	0.0286	0.7346	0.1526	

Sample Status Information



Standard Summary

Filename: 99SB02FTX1
Data Acquisition Time: 2018-02-02 05:46:14
Process Date: 2018-02-12 16:32:20

Valid: Passed

LABELS	FORMULA	VALUE	RESULT
Data Acquisition Time	A_T	05:46:14	05:46:14
Sample Time - Start S_{T1}	A_T - 00:40	05:46:14 - 00:40	05:06:14
Sample Time - End S_{T2}	A_T	05:46:14	05:46:14
Samle Hour S_H	A_T - 00:20(truncate to hour)	05:46:14 - 00:20	05:00
Valid Sample Hour Limit 1 S_{L1}	S_H - 00:10	05:00 - 00:10	04:50:00
Valid Sample Hour Limit 2 S_{L2}	S_H + 01:10	05:00 + 01:10	06:10:00
Validity Test 1	$S_{T1} >= S_{L1}$	05:06:14>=04:50:00	Passed
Validity Test 2	$S_{T1} <= S_{L2}$	05:46:14<=06:10:00	Passed

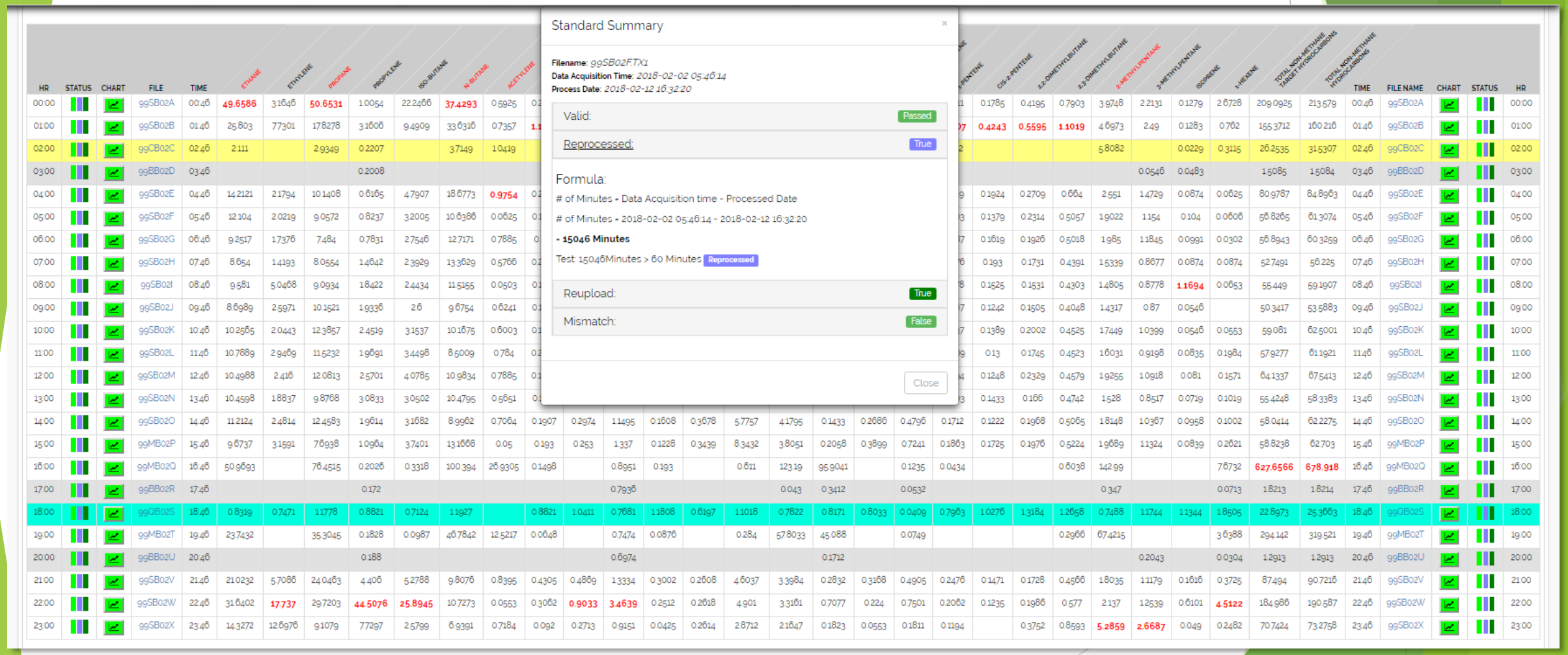
Reprocessed: True

Reupload: True

Mismatch: False

Close

Sample Status Information



Standard Summary

Filename: *99SB02F.TX1*
Data Acquisition Time: *2018-02-02 05:46:14*
Process Date: *2018-02-12 16:32:20*

Valid: Passed

Reprocessed: True

Formula:

# of Minutes - Data Acquisition time - Processed Date

# of Minutes - 2018-02-02 05:46:14 - 2018-02-12 16:32:20

- 15046 Minutes

Test: 15046Minutes > 60 Minutes Reprocessed

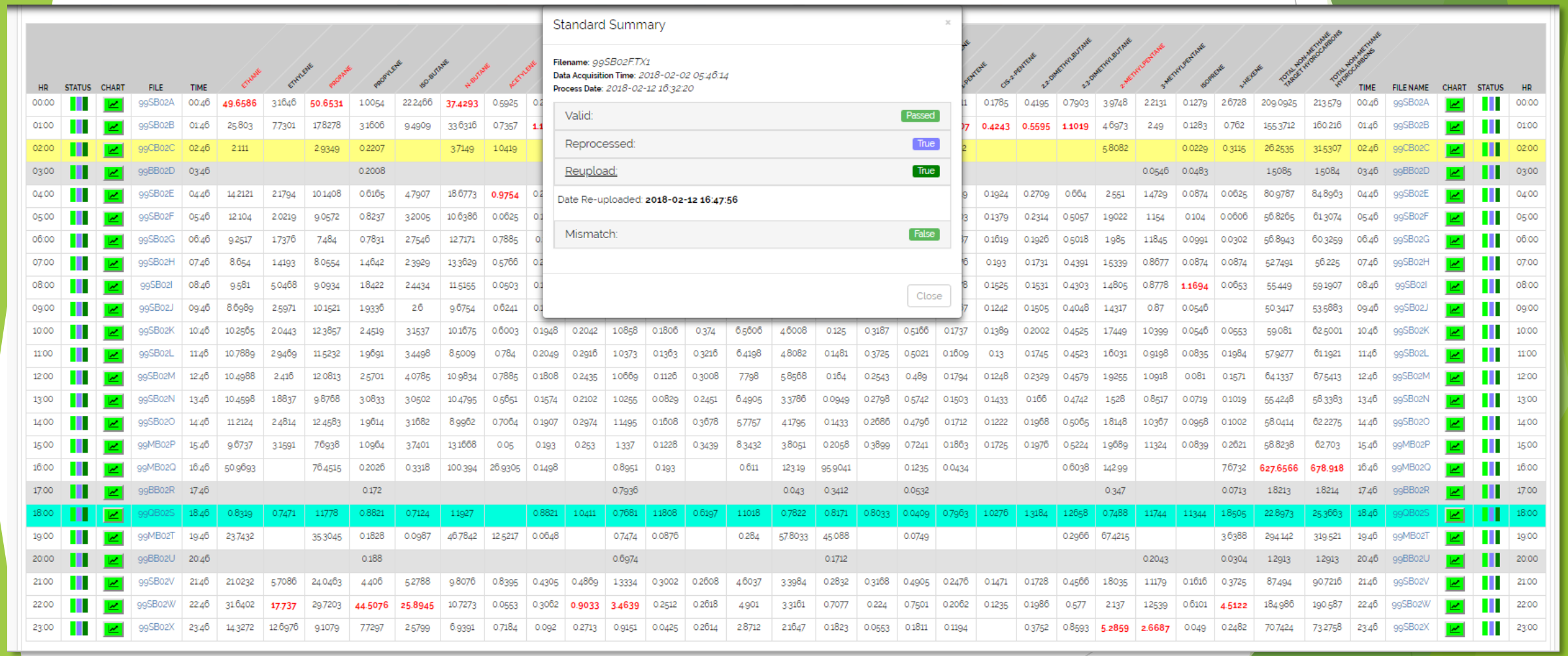
Reupload: True

Mismatch: False

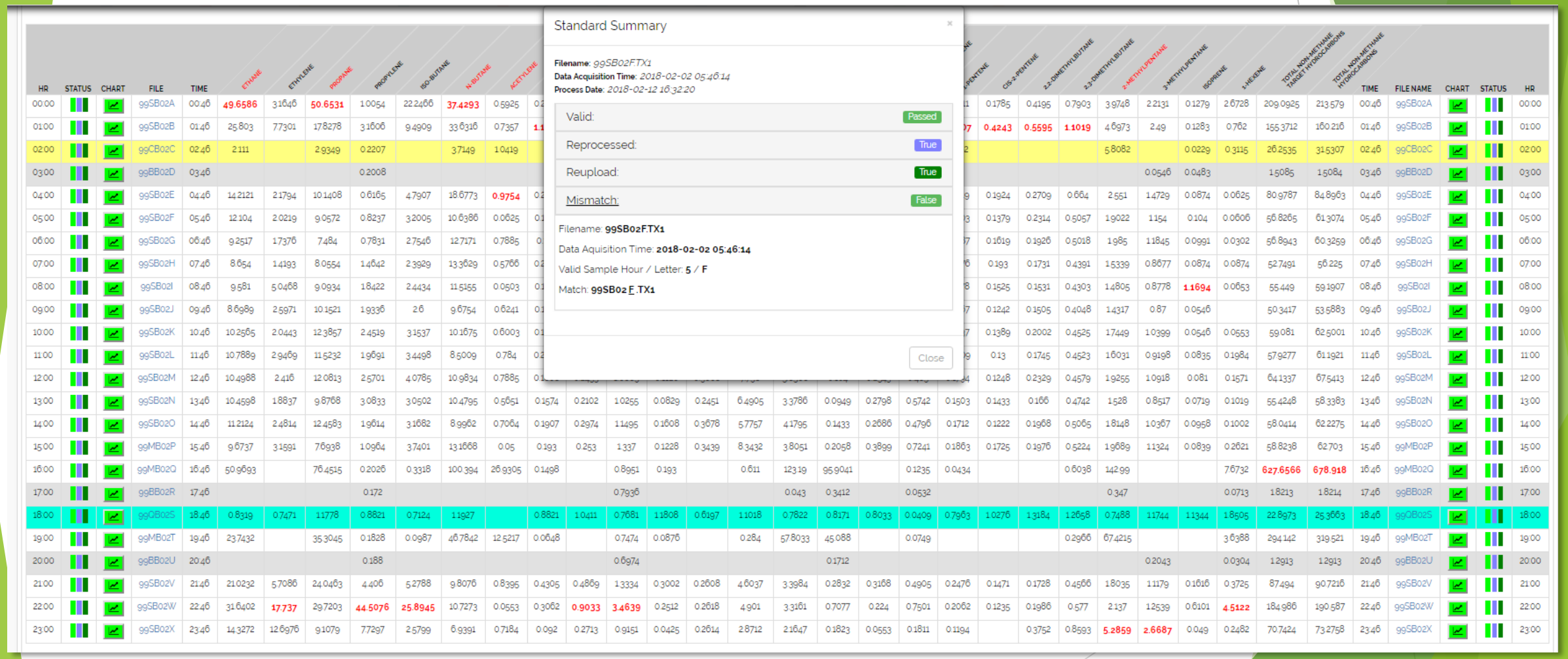
Close

HR	STATUS	CHART	FILE	TIME	ETHANE	ETHYLENE	PROPANE	PROPYLENE	ISO-BUTANE	N-BUTANE	ACETYLENE	CIS-2-PENTENE	2,2-DIMETHYLBUTANE	2,3-DIMETHYLBUTANE	2-METHYLPENTANE	3-METHYLPENTANE	ISOPRENE	1-HEXENE	TOTAL NON-METHANE TARGET HYDROCARBONS	TOTAL NON-METHANE HYDROCARBONS	TIME	FILE NAME	CHART	STATUS	HR
00:00			99SB02A	00:46	49.6586	3.1646	50.6531	1.0054	22.2466	37.4293	0.5925	0.1785	0.4195	0.7903	3.9748	2.2131	0.1279	2.6728	209.0925	213.579	00:46	99SB02A			00:00
01:00			99SB02B	01:46	25.803	7.7301	17.8278	3.1606	9.4909	33.6316	0.7357	0.4243	0.5595	1.1019	4.6973	2.49	0.1283	0.762	155.3712	160.216	01:46	99SB02B			01:00
02:00			99CB02C	02:46	2.111		2.9349	0.2207		3.7149	1.0419				5.8082		0.0229	0.3115	26.2535	31.5307	02:46	99CB02C			02:00
03:00			99BB02D	03:46				0.2008									0.0546	0.0483		1.5085	1.5084	03:46	99BB02D			03:00
04:00			99SB02E	04:46	14.2121	2.1794	10.1408	0.6165	4.7907	18.6773	0.9754	0.1924	0.2709	0.664	2.551	1.4729	0.0874	0.0625	80.9787	84.8963	04:46	99SB02E			04:00
05:00			99SB02F	05:46	12.104	2.0219	9.0572	0.8237	3.2005	10.6386	0.0625	0.1379	0.2314	0.5057	1.9022	1.154	0.104	0.0606	56.8265	61.3074	05:46	99SB02F			05:00
06:00			99SB02G	06:46	9.2517	1.7376	7.484	0.7831	2.7546	12.7171	0.7885	0.1619	0.1926	0.5018	1.985	1.1845	0.0991	0.0302	56.8943	60.3259	06:46	99SB02G			06:00
07:00			99SB02H	07:46	8.654	1.4193	8.0554	1.4642	2.3929	13.3629	0.5766	0.193	0.1731	0.4391	1.5339	0.8677	0.0874	0.0874	52.7491	56.225	07:46	99SB02H			07:00
08:00			99SB02I	08:46	9.581	5.0468	9.0934	1.8422	2.4434	11.5155	0.0503	0.1525	0.1531	0.4303	1.4805	0.8778	1.1694	0.0653	55.449	59.1907	08:46	99SB02I			08:00
09:00			99SB02J	09:46	8.6989	2.5971	10.1521	1.9336	2.6	9.6754	0.6241	0.1242	0.1505	0.4048	1.4317	0.87	0.0546		50.3417	53.5883	09:46	99SB02J			09:00
10:00			99SB02K	10:46	10.2565	2.0443	12.3857	2.4519	3.1537	10.1675	0.6003	0.1389	0.2002	0.4525	1.7449	1.0399	0.0546	0.0553	59.081	62.5001	10:46	99SB02K			10:00
11:00			99SB02L	11:46	10.7889	2.9469	11.5232	1.9691	3.4498	8.5009	0.784	0.13	0.1745	0.4523	1.6031	0.9198	0.0835	0.1984	57.9277	61.1921	11:46	99SB02L			11:00
12:00			99SB02M	12:46	10.4988	2.416	12.0813	2.5701	4.0785	10.9834	0.7885	0.1248	0.2329	0.4579	1.9255	1.0918	0.081	0.1571	64.1337	67.5413	12:46	99SB02M			12:00
13:00			99SB02N	13:46	10.4598	1.8837	9.8768	3.0833	3.0502	10.4795	0.5651	0.1433	0.166	0.4742	1.528	0.8517	0.0719	0.1019	55.4248	58.3383	13:46	99SB02N			13:00
14:00			99SB02O	14:46	11.2124	2.4814	12.4583	1.9614	3.1682	8.9962	0.7064	0.1907	0.2974	1.1495	0.1608	0.3678	5.7757	4.1795	0.1433	0.2686	0.4796	0.1712	0.1222	0.1968	0.5065	1.8148	1.0367	0.0958	0.1002	58.0414	62.2275	14:46	99SB02O			14:00
15:00			99MB02P	15:46	9.6737	3.1591	7.6938	1.0964	3.7401	13.1668	0.05	0.193	0.253	1.337	0.1228	0.3439	8.3432	3.8051	0.2058	0.3899	0.7241	0.1863	0.1725	0.1976	0.5224	1.9689	1.1324	0.0839	0.2621	58.8238	62.703	15:46	99MB02P			15:00
16:00			99MB02Q	16:46	50.9693		76.4515	0.2026	0.3318	100.394	26.9305	0.1498		0.8951	0.193		0.611	12.319	95.9041		0.1235	0.0434			0.6038	14.299			7.6732	627.6566	678.918	16:46	99MB02Q			16:00
17:00			99BB02R	17:46				0.172						0.7936				0.043	0.3412		0.0532					0.347			0.0713	1.8213	1.8214	17:46	99BB02R			17:00
18:00			99GB02S	18:46	0.8319	0.7471	1.1778	0.8821	0.7124	1.1927		0.8821	1.0411	0.7681	1.1808	0.6197	1.1018	0.7822	0.8171	0.8033	0.0409	0.7963	1.0276	1.3184	1.2658	0.7488	1.1744	1.1344	1.8505	22.8973	25.3663	18:46	99GB02S			18:00
19:00			99MB02T	19:46	23.7432		35.3045	0.1828	0.0987	46.7842	12.5217	0.0648		0.7474	0.0876		0.284	57.8033	45.088		0.0749				0.2966	67.4215			3.6388	29.4142	31.9521	19:46	99MB02T			19:00
20:00			99BB02U	20:46				0.188						0.6974					0.1712									0.0304	1.2913	1.2913	20:46	99BB02U			20:00
21:00			99SB02V	21:46	21.0232	5.7086	24.0463	4.406	5.2788	9.8076	0.8395	0.4305	0.4869	1.3334	0.3002	0.2608	4.6037	3.3984	0.2832	0.3168	0.4905	0.2476	0.1471	0.1728	0.4566	1.8035	1.1179	0.1616	0.3725	8.7494	9.0721	21:46	99SB02V			21:00
22:00			99SB02W	22:46	31.6402	17.737	29.7203	44.5076	25.8945	10.7273	0.0553	0.3062	0.9033	3.4639	0.2512	0.2618	4.901	3.3161	0.7077	0.224	0.7501	0.2062	0.1235	0.1986	0.577	2.137	1.2539	0.6101	4.5122	18.4986	19.0587	22:46	99SB02W			22:00
23:00			99SB02X	23:46	14.3272	12.6976	9.1079	7.7297	2.5799	6.9391	0.7184	0.092	0.2713	0.9151	0.0425	0.2614	2.8712	2.1647	0.1823	0.0553	0.1811	0.1194		0.3752	0.8593	5.2859	2.6687	0.049	0.2482	7.0742	7.3275	23:46	99SB02X			23:00

Sample Status Information



Sample Status Information



Standard Summary

Filename: *99SB02F.TX1*
Data Acquisition Time: *2018-02-02 05:46:14*
Process Date: *2018-02-12 16:32:20*

Valid:	Passed
Reprocessed:	True
Reupload:	True
Mismatch:	False

Filename: **99SB02F.TX1**
Data Aquisition Time: **2018-02-02 05:46:14**
Valid Sample Hour / Letter: **5 / F**
Match: **99SB02F.TX1**

Close

HR	STATUS	CHART	FILE	TIME	ETHANE	ETHYLENE	PROPANE	PROPYLENE	ISO-BUTANE	N-BUTANE	ACETYLENE	CIS-2-PENTENE	2,2-DIMETHYLBUTANE	2,3-DIMETHYLBUTANE	2-METHYLPENTANE	3-METHYLPENTANE	ISOPRENE	1-HEXENE	TOTAL NON-METHANE TARGET HYDROCARBONS	TOTAL NON-METHANE HYDROCARBONS	TIME	FILE NAME	CHART	STATUS	HR
00:00			99SB02A	00:46	49.6586	3.1646	50.6531	1.0054	22.2466	37.4293	0.5925	0.1785	0.4195	0.7903	3.9748	2.2131	0.1279	2.6728	209.0925	213.579	00:46	99SB02A			00:00
01:00			99SB02B	01:46	25.803	7.7301	17.8278	3.1606	9.4909	33.6316	0.7357	0.4243	0.5595	1.1019	4.6973	2.49	0.1283	0.762	155.3712	160.216	01:46	99SB02B			01:00
02:00			99CB02C	02:46	2.111		2.9349	0.2207		3.7149	1.0419				5.8082		0.0229	0.3115	26.2535	31.5307	02:46	99CB02C			02:00
03:00			99BB02D	03:46				0.2008									0.0546	0.0483		1.5085	1.5084	03:46	99BB02D			03:00
04:00			99SB02E	04:46	14.2121	2.1794	10.1408	0.6165	4.7907	18.6773	0.9754	0.1924	0.2709	0.664	2.551	1.4729	0.0874	0.0625	80.9787	84.8963	04:46	99SB02E			04:00
05:00			99SB02F	05:46	12.104	2.0219	9.0572	0.8237	3.2005	10.6386	0.0625	0.1379	0.2314	0.5057	1.9022	1.154	0.104	0.0606	56.8265	61.3074	05:46	99SB02F			05:00
06:00			99SB02G	06:46	9.2517	1.7376	7.484	0.7831	2.7546	12.7171	0.7885	0.1619	0.1926	0.5018	1.985	1.1845	0.0991	0.0302	56.8943	60.3259	06:46	99SB02G			06:00
07:00			99SB02H	07:46	8.654	1.4193	8.0554	1.4642	2.3929	13.3629	0.5766	0.193	0.1731	0.4391	1.5339	0.8677	0.0874	0.0874	52.7491	56.225	07:46	99SB02H			07:00
08:00			99SB02I	08:46	9.581	5.0468	9.0934	1.8422	2.4434	11.5155	0.0503	0.1525	0.1531	0.4303	1.4805	0.8778	1.1694	0.0653	55.449	59.1907	08:46	99SB02I			08:00
09:00			99SB02J	09:46	8.6989	2.5971	10.1521	1.9336	2.6	9.6754	0.6241	0.1242	0.1505	0.4048	1.4317	0.87	0.0546		50.3417	53.5883	09:46	99SB02J			09:00
10:00			99SB02K	10:46	10.2565	2.0443	12.3857	2.4519	3.1537	10.1675	0.6003	0.1389	0.2002	0.4525	1.7449	1.0399	0.0546	0.0553	59.081	62.5001	10:46	99SB02K			10:00
11:00			99SB02L	11:46	10.7889	2.9469	11.5232	1.9691	3.4498	8.5009	0.784	0.13	0.1745	0.4523	1.6031	0.9198	0.0835	0.1984	57.9277	61.1921	11:46	99SB02L			11:00
12:00			99SB02M	12:46	10.4988	2.416	12.0813	2.5701	4.0785	10.9834	0.7885	0.1248	0.2329	0.4579	1.9255	1.0918	0.081	0.1571	64.1337	67.5413	12:46	99SB02M			12:00
13:00			99SB02N	13:46	10.4598	1.8837	9.8768	3.0833	3.0502	10.4795	0.5651	0.1574	0.2102	1.0255	0.0829	0.2451	6.4905	3.3786	0.0949	0.2798	0.5742	0.1503	0.1433	0.166	0.4742	1.528	0.8517	0.0719	0.1019	55.4248	58.3383	13:46	99SB02N			13:00
14:00			99SB02O	14:46	11.2124	2.4814	12.4583	1.9614	3.1682	8.9962	0.7064	0.1907	0.2974	1.1495	0.1608	0.3678	5.7757	4.1795	0.1433	0.2686	0.4796	0.1712	0.1222	0.1968	0.5065	1.8148	1.0367	0.0958	0.1002	58.0414	62.2275	14:46	99SB02O			14:00
15:00			99MB02P	15:46	9.6737	3.1591	7.6938	1.0964	3.7401	13.1668	0.05	0.193	0.253	1.337	0.1228	0.3439	8.3432	3.8051	0.2058	0.3899	0.7241	0.1863	0.1725	0.1976	0.5224	1.9689	1.1324	0.0839	0.2621	58.8238	62.703	15:46	99MB02P			15:00
16:00			99MB02Q	16:46	50.9693		76.4515	0.2026	0.3318	100.394	26.9305	0.1498		0.8951	0.193		0.611	12.319	95.9041		0.1235	0.0434			0.6038	14.299			7.6732	627.6566	678.918	16:46	99MB02Q			16:00
17:00			99BB02R	17:46				0.172						0.7936				0.043	0.3412		0.0532					0.347			0.0713	1.8213	1.8214	17:46	99BB02R			17:00
18:00			99GB02S	18:46	0.8319	0.7471	1.1778	0.8821	0.7124	1.1927		0.8821	1.0411	0.7681	1.1808	0.6197	1.1018	0.7822	0.8171	0.8033	0.0409	0.7963	1.0276	1.3184	1.2658	0.7488	1.1744	1.1344	1.8505	22.8973	25.3663	18:46	99GB02S			18:00
19:00			99MB02T	19:46	23.7432		35.3045	0.1828	0.0987	46.7842	12.5217	0.0648		0.7474	0.0876		0.284	57.8033	45.088		0.0749				0.2966	67.4215			3.6388	29.4142	31.9521	19:46	99MB02T			19:00
20:00			99BB02U	20:46				0.188						0.6974					0.1712								0.2043		0.0304	1.2913	1.2913	20:46	99BB02U			20:00
21:00			99SB02V	21:46	21.0232	5.7086	24.0463	4.406	5.2788	9.8076	0.8395	0.4305	0.4869	1.3334	0.3002	0.2608	4.6037	3.3984	0.2832	0.3168	0.4905	0.2476	0.1471	0.1728	0.4566	1.8035	1.1179	0.1616	0.3725	8.7494	9.0721	21:46	99SB02V			21:00
22:00			99SB02W	22:46	31.6402	17.737	29.7203	44.5076	25.8945	10.7273	0.0553	0.3062	0.9033	3.4639	0.2512	0.2618	4.901	3.3161	0.7077	0.224	0.7501	0.2062	0.1235	0.1986	0.577	2.137	1.2539	0.6101	4.5122	18.4986	19.0587	22:46	99SB02W			22:00
23:00			99SB02X	23:46	14.3272	12.6976	9.1079	7.7297	2.5799	6.9391	0.7184	0.092	0.2713	0.9151	0.0425	0.2614	2.8712	2.1647	0.1823	0.0553	0.1811	0.1194		0.3752	0.8593	5.2859	2.6687	0.049	0.2482	7.0.7424	7.3.2758	23:46	99SB02X			23:00

Daily and Weekly Quality Control Checks

Daily Dynamic Dilution Check Standard

Channel A: CVS Concentration (2018-02-03)

Cylinder	Date On	Date Off	Dilution Factor
CC-80844	2017-10-17 09:00:00	In Use	0.00077

[Propane RF = 6818]

NAME	CARBON NUMBER	CERT CONC (PPMV)	CALC DILUTED 1 (PPBC)	MEASURED CONC 1 (PPBC)	RUN 1 % RECOVERY (99CB03A.TX1)	RECOVERY MIN/MAX
ETHANE	2	110	169	202	119.27	75 | 125
PROPANE	3	110	254	289	113.8	75 | 125
N-BUTANE	4	107	330	372	112.99	75 | 125
ACETYLENE	2	110	169	106	62.74	75 | 125
N-PENTANE	5	107	412	470	114.18	75 | 125
1,3-BUTADIENE	4	107	330	369	111.88	75 | 125
2-METHYLPENTANE	6	104	480	574	119.38	75 | 125

Blank Run: (99BB03B.TX1) 1.0345

Channel B: CVS Concentration (2018-02-03)

Cylinder	Date On	Date Off	Dilution Factor
CC-80844	2017-10-17 09:00:00	In Use	0.00077

[Benzene RF = 7163]

NAME	CARBON NUMBER	CERT CONC (PPMV)	CALC DILUTED 1 (PPBC)	MEASURED CONC 1 (PPBC)	RUN 1 % RECOVERY (99CB03A.TX1)	RECOVERY MIN/MAX
N-HEXANE	6	103	476	536	112.68	75 | 125
BENZENE	6	106	490	541	110.49	75 | 125
TOLUENE	7	106	571	609	106.51	75 | 125
M&P-XYLENE	8	109	671	702	104.54	75 | 125
N-PROPYLBENZENE	9	107	742	763	102.94	75 | 125
1,2,4-TRI-M-BENZENE	9	106	735	724	98.62	75 | 125
P-DIETHYLBENZENE	10	101	778	782	100.52	75 | 125

Blank Run: (99BB03B.TX1) 0.9102

Weekly Static 2nd Source Check Standard

Channel A: LCS Concentration (2018-02-03)

Cylinder	Date On	Date Off	Dilution Factor
CC-126878	2017-10-16 09:00:00	In Use	0.005

[Propane RF = 6818]

NAME	CARBON NUMBER	CERT CONC (PPMV)	CALC DILUTED 1 (PPBC)	MEASURED CONC 1 (PPBC)	RUN 1 % RECOVERY (99EB03V.TX1)	RECOVERY MIN/MAX
ETHANE	2	101	10.10	10.39	102.85	70 | 130
PROPANE	3	0.95	14.25	15.64	109.79	70 | 130
N-BUTANE	4	0.96	19.20	20.37	106.08	70 | 130
ACETYLENE	2	101	10.10	10.22	101.15	70 | 130
N-PENTANE	5	1.00	25.00	27.31	109.23	70 | 130
1,3-BUTADIENE	4	0.97	19.40	20.27	104.49	70 | 130
2-METHYLPENTANE	6	101	30.30	33.55	110.72	70 | 130

Blank Run: (99BB03B.TX1) 1.0345

Channel B: LCS Concentration (2018-02-03)

Cylinder	Date On	Date Off	Dilution Factor
CC-126878	2017-10-16 09:00:00	In Use	0.005

[Benzene RF = 7163]

NAME	CARBON NUMBER	CERT CONC (PPMV)	CALC DILUTED 1 (PPBC)	MEASURED CONC 1 (PPBC)	RUN 1 % RECOVERY (99EB03V.TX1)	RECOVERY MIN/MAX
N-HEXANE	6	1.02	30.60	31.11	101.66	70 | 130
BENZENE	6	1.04	31.20	31.12	99.73	70 | 130
TOLUENE	7	1.04	36.40	36.06	99.05	70 | 130
M&P-XYLENE	8	1.04	41.60	41.49	99.75	70 | 130
N-PROPYLBENZENE	9	1.00	45.00	46.22	102.7	70 | 130
1,2,4-TRI-M-BENZENE	9	1.02	45.90	44.42	96.77	70 | 130

Blank Run: (99BB03B.TX1) 0.9102

Retention Time Checks

Channel A: RTS Concentration (2018-02-03)

Cylinder	Date On	Date Off	Dilution Factor
CC-361828	2017-12-12 00:00:00	In Use	0.025

[Propane RF = 6818]

NAME	CARBON NUMBER	CERT CONC (PPBC)	CALC DILUTED 1 (PPBC)	MEASURED CONC 1 (PPBC)	RUN 1 % RECOVERY (99QB03W.TX1)	RECOVERY MIN/MAX
ETHANE	2	24.00	0.60	0.72	120.63	75 | 125
ETHYLENE	2	19.00	0.47	0.70	147.73	75 | 125
PROPANE	3	41.00	1.02	1.07	104.59	75 | 125
PROPYLENE	3	25.00	0.63	0.87	138.99	75 | 125
ISO-BUTANE	4	26.00	0.65	0.75	114.92	75 | 125
N-BUTANE	4	41.00	1.02	1.10	107.47	75 | 125
ACETYLENE	2	39.00	0.98	0.00	0	75 | 125
TRANS-2-BUTENE	4	26.00	0.65	0.85	130.72	75 | 125
1-BUTENE	4	31.00	0.78	0.96	123.97	75 | 125
CIS-2-BUTENE	4	37.00	0.93	1.06	114.28	75 | 125
CYCLOPENTANE	4	20.00	0.50	0.55	110	75 | 125
ISO-PENTANE	5	40.00	1.00	1.00	99.81	75 | 125
N-PENTANE	5	25.00	0.63	0.70	112.18	75 | 125
1,3-BUTADIENE	4	0.00	0.00	0.71	0	75 | 125
TRANS-2-PENTENE	5	27.00	0.68	0.73	108.56	75 | 125
1-PENTENE	5	25.00	0.63	0.77	123.1	75 | 125
CIS-2-PENTENE	5	34.00	0.85	0.97	114.44	75 | 125
2,2-DIMETHYLBUTANE	6	41.00	1.02	1.23	119.97	75 | 125
2,3-DIMETHYLBUTANE	6	52.00	1.30	1.22	93.75	75 | 125
2-METHYLPENTANE	6	21.00	0.53	0.64	121.77	75 | 125
3-METHYLPENTANE	6	41.00	1.02	1.09	105.94	75 | 125
ISOPRENE	5	27.00	0.68	1.05	155.36	75 | 125
1-HEXENE	6	61.00	1.52	1.74	113.88	75 | 125

Blank Run: (99BB03B.TX1) 1.0345

Channel B: RTS Concentration (2018-02-03)

Cylinder	Date On	Date Off	Dilution Factor
CC-361828	2017-12-12 00:00:00	In Use	0.025

[Benzene RF = 7163]

NAME	CARBON NUMBER	CERT CONC (PPBC)	CALC DILUTED 1 (PPBC)	MEASURED CONC 1 (PPBC)	RUN 1 % RECOVERY (99QB03W.TX1)	RECOVERY MIN/MAX
N-HEXANE	6	31.00	0.78	0.85	110.03	75 | 125
METHYLCYCLOPENTANE	6	26.00	0.65	0.63	97.02	75 | 125
2,4-DIMETHYLPENTANE	7	41.00	1.02	1.11	108.04	75 | 125
BENZENE	6	31.00	0.78	0.96	123.39	75 | 125
CYCLOHEXANE	6	42.00	1.05	0.84	79.57	75 | 125
2-METHYLHEXANE	7	26.00	0.65	0.67	103.11	75 | 125
2,3-DIMETHYLPENTANE	7	53.00	1.32	1.39	105.19	75 | 125
3-METHYLHEXANE	7	26.00	0.65	0.61	93.77	75 | 125
2,2,4-TRIMETHYLPENTANE	8	31.00	0.78	0.79	101.96	75 | 125
N-HEPTANE	7	26.00	0.65	0.64	98.58	75 | 125
METHYLCYCLOHEXANE	7	31.00	0.78	0.93	120.28	75 | 125
2,3,4-TRIMETHYLPENTANE	8	26.00	0.65	0.67	103.75	75 | 125
TOLUENE	7	41.00	1.02	1.29	125.9	75 | 125
2-METHYLHEPTANE	8	25.00	0.63	0.67	107.33	75 | 125
3-METHYLHEPTANE	8	25.00	0.63	0.68	109.42	75 | 125
N-OCTANE	8	31.00	0.78	0.86	111.12	75 | 125
ETHYLBENZENE	8	26.00	0.65	0.65	99.6	75 | 125
M&P-XYLENE	8	40.00	1.00	1.51	151.07	75 | 125
STYRENE	8	37.00	0.93	0.81	87.43	75 | 125
O-XYLENE	8	25.00	0.63	0.70	112.29	75 | 125
N-NONANE	9	25.00	0.63	0.71	113.04	75 | 125
ISO-PROPYLBENZENE	9	39.00	0.98	1.12	114.53	75 | 125
N-PROPYLBENZENE	9	29.00	0.73	1.19	164.18	75 | 125
M-ETHYLTOLUENE	9	25.00	0.63	0.71	113.98	75 | 125
P-ETHYLTOLUENE	9	41.00	1.02	1.28	124.63	75 | 125
1,3,5-TRI-M-BENZENE	9	25.00	0.63	0.65	104.27	75 | 125
O-ETHYLTOLUENE	9	30.00	0.75	0.82	109.37	75 | 125
1,2,4-TRI-M-BENZENE	9	40.00	1.00	1.70	169.58	75 | 125
N-DECANE	10	32.00	0.80	0.86	107.13	75 | 125
1,2,3-TRI-M-BENZENE	9	26.00	0.65	0.66	101.78	75 | 125
M-DIETHYLBENZENE	10	41.00	1.02	1.01	98.72	75 | 125
P-DIETHYLBENZENE	10	25.00	0.63	1.73	276.37	75 | 125
N-UNDECANE	11	32.00	0.80	0.81	101.21	75 | 125
N-DODECANE	12	48.00	1.20	0.87	72.25	75 | 125

Blank Run: (99BB03B.TX1) 0.9102

Daily Analytical Blanks

Channel A: BLANK Concentration (2018-02-03)

NAME	RUN 1 (PPBC) AMOUNT (99BB03B.TX1)	MAX
PROPYLENE	0.1929	0.5
1-PENTENE	0.0409	0.5
3-METHYLPENTANE	0.0349	0.5
CHANNEL A TNMTC :	**0.2687**	

Channel B: BLANK Concentration (2018-02-03)

NAME	RUN 1 (PPBC) AMOUNT (99BB03B.TX1)	MAX
TOLUENE	0.0490	0.5
M&P-XYLENE	0.1753	0.5
N-PROPYLBENZENE	0.1044	0.5
1,2,4-TRI-M-BENZENE	0.1765	0.5
P-DIETHYLBENZENE	0.4050	0.5
CHANNEL B TNMTC :	**0.9102**	

TOTAL BLANKS (TNMTC)

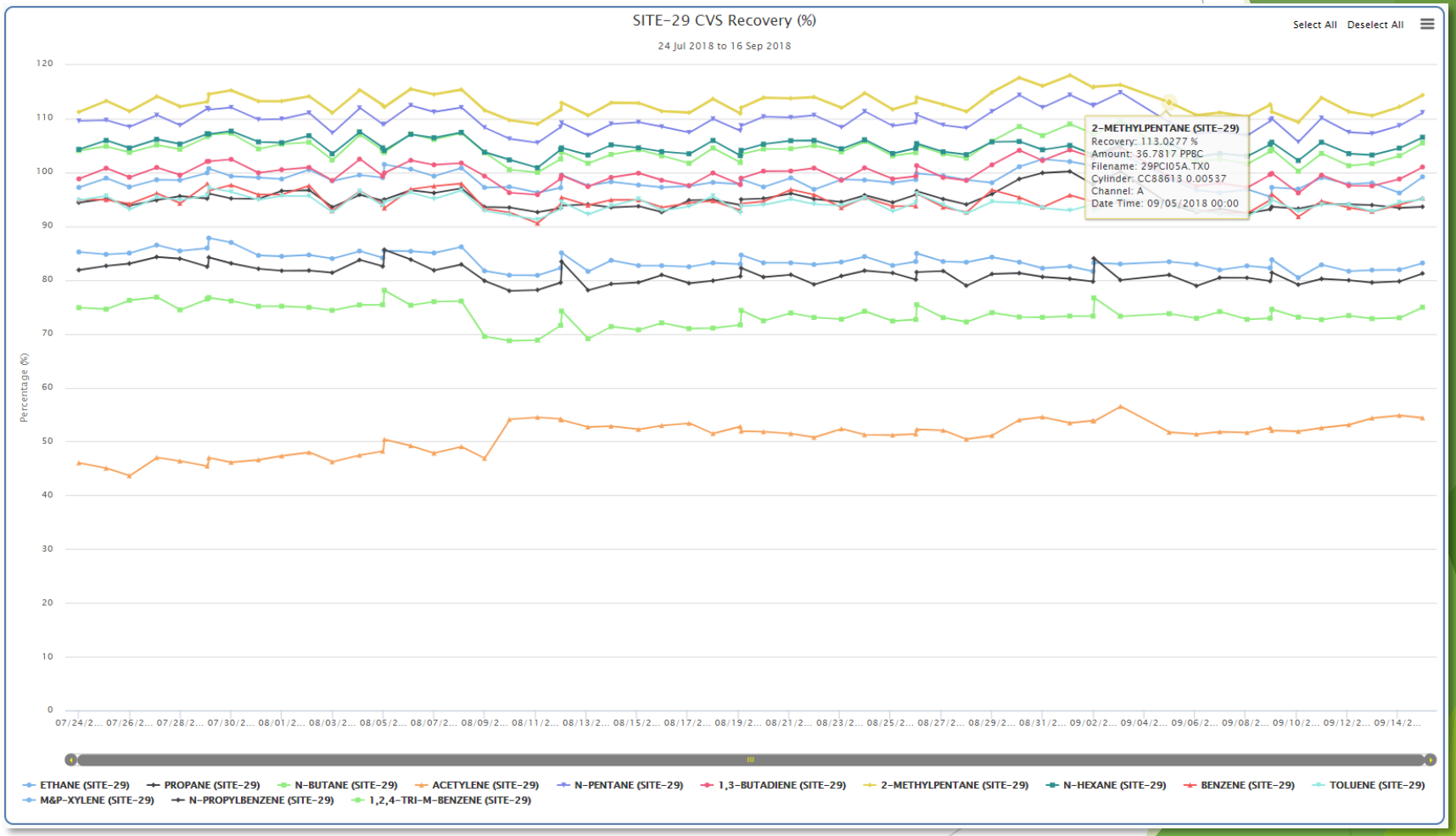
	RUN 1 (PPBC) AMOUNT (99BB03B.TX1)
TNMTC CHANNEL A:	0.2687
TNMTC CHANNEL B:	0.9102
TOTAL TNMTC:	**1.1789**

TOTAL BLANKS (TNMHC)

	RUN 1 (PPBC) AMOUNT
TNMHC CHANNEL A:	1.0345
TNMHC CHANNEL B:	0.9102
TOTAL TNMHC:	**1.9447**

Quality Control Charts

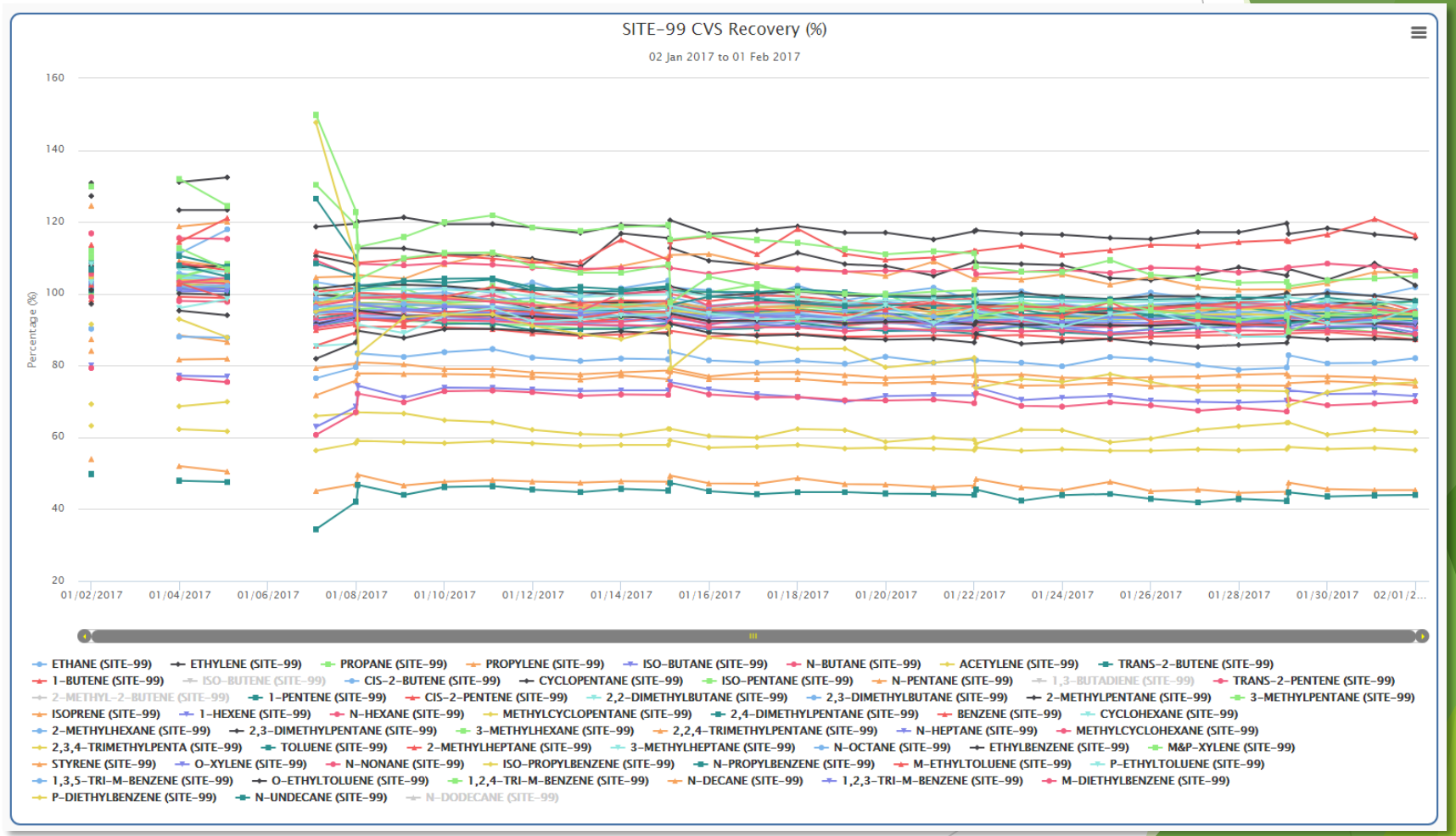
Daily Check Standard
CVS – CCV
1 ppbv



Quality Control Charts

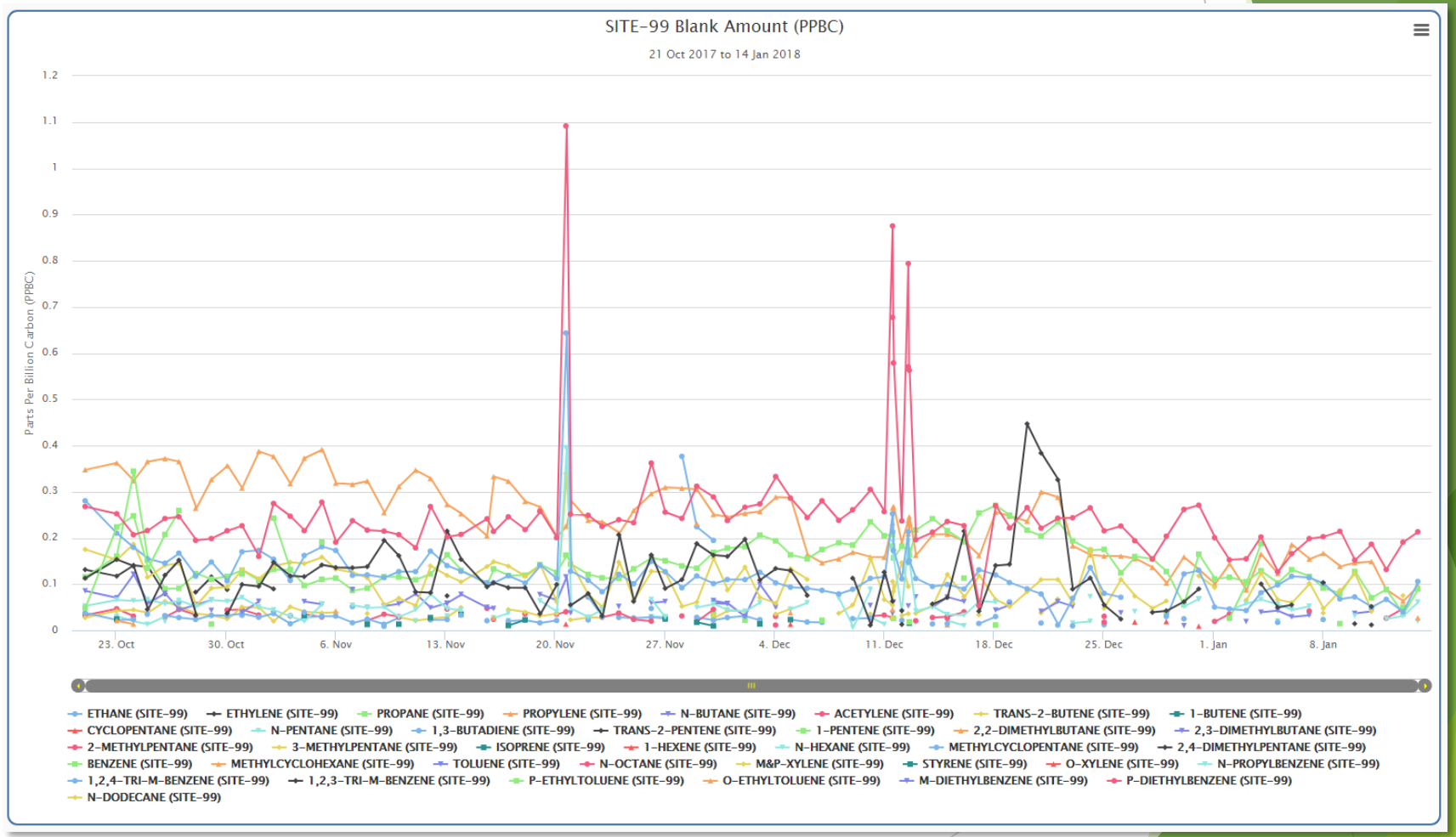
Weekly Check Standard
LCS – SSQC
5 ppbv

Daily Check Standard
CVS – CCV
56 component
0.5 ppbv



Quality Control Charts

Daily Blank



Quality Control Charts

CSV or Excel output of graphed data

Hide Data Table

CSV Excel

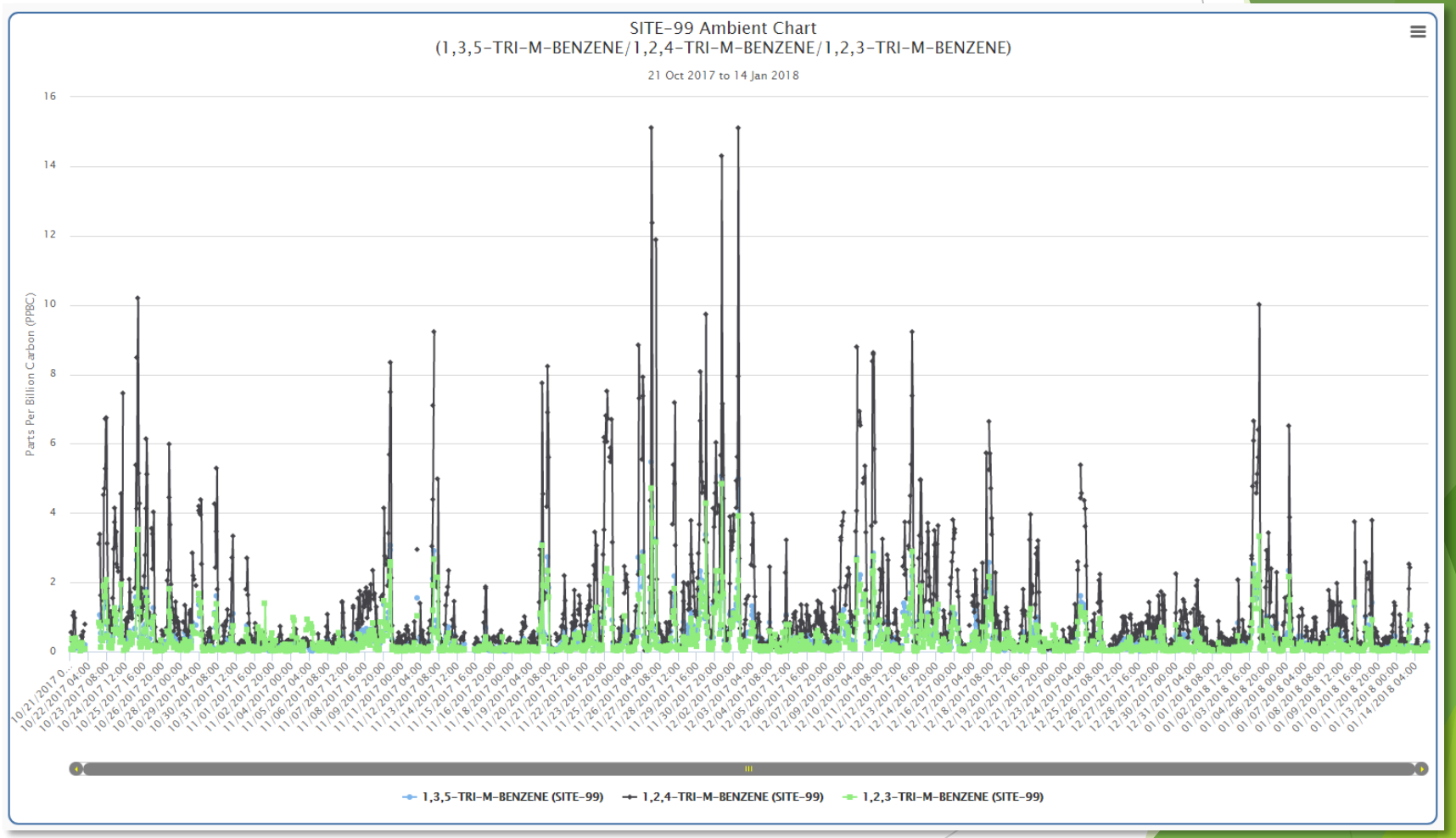
DATE TIME	ETHANE (SITE-99) PPBC	ETHYLENE (SITE-99) PPBC	PROPANE (SITE-99) PPBC	PROPYLENE (SITE-99) PPBC	N-BUTANE (SITE-99) PPBC	ACETYLENE (SITE-99) PPBC	TRANS-2-BUTENE (SITE-99) PPBC	1-BUTENE (SITE-99) PPBC	CYCLOPENTANE (SITE-99) PPBC	N-PENTANE (SITE-99) PPBC	1,3-BUTADIENE (SITE-99) PPBC	TRANS-2-PENTENE (SITE-99) PPBC	1-PENTENE (SITE-99) PPBC	2,2-DIMETHYLBUTANE (SITE-99) PPBC	2,3-DIMETHYLBUTANE (SITE-99) PPBC	2-METHYLPENTANE (SITE-99) PPBC	3-METHYLPENTANE (SITE-99) PPBC	ISOPRENE (SITE-99) PPBC	1-HEXENE (SITE-99) PPBC	N-HEXANE (SITE-99) PPBC	METHYLCYCLOPENTANE (SITE-99) PPBC	2,4-DIMETHYLPENTANE (SITE-99) PPBC	BENZENE (SITE-99) PPBC	METHYLCYCLOHEXANE (SITE-99) PPBC	TOLUENE (SITE-99) PPBC	N-OCTANE (SITE-99) PPBC	M&P-XYLENE (SITE-99) PPBC	STYRENE (SITE-99) PPBC	O-XYLENE (SITE-99) PPBC	N-PROPYLBENZENE (SITE-99) PPBC	1,2,4-TRI-M-BENZENE (SITE-99) PPBC	1,2,3-TRI-M-BENZENE (SITE-99) PPBC	P-ETHYLTOLUENE (SITE-99) PPBC	O-ETHYLTOLUENE (SITE-99) PPBC	M-DIETHYLBENZENE (SITE-99) PPBC	P-DIETHYLBENZENE (SITE-99) PPBC	N-DODECANE (SITE-99) PPBC
10/21/2017 01:00		0.1312		0.3475		0.0326	0.0275				0.0376												0.1155		0.0855		0.1752			0.0527	0.2804	0.1128	0.0487			0.2680	
10/23/2017 01:00		0.1173		0.3625		0.0468	0.0422			0.0308	0.0225							0.0247					0.1607		0.0704		0.1527			0.0658	0.2103	0.1535	0.2238	0.0209		0.2523	
10/24/2017 03:00		0.1407		0.3241		0.0306	0.0444			0.0197	0.0235												0.3445		0.1214		0.1869			0.0639	0.1796	0.1391	0.2478	0.0134		0.2069	
10/25/2017 01:00		0.1370		0.3653			0.0382			0.0130											0.0348		0.1521		0.0586		0.1149			0.0667	0.1551	0.0454	0.1346			0.2161	
10/26/2017 03:00		0.0792		0.3720		0.0290	0.0624			0.0304	0.0318									0.0191			0.0899		0.0800		0.1408			0.0574	0.1454	0.1191	0.2075			0.2420	
10/27/2017 01:00				0.3651		0.0451	0.0511				0.0276										0.0604		0.0910		0.0446		0.1452			0.0646	0.1672	0.1522	0.2594			0.2458	
10/28/2017 03:00		0.0828		0.2643		0.0332	0.0364				0.0236												0.1229		0.0556		0.0542			0.0512	0.1172	0.0330				0.1950	
10/29/2017 02:00		0.1157		0.3268	0.0431		0.0326				0.0325		0.0135										0.1107		0.0660		0.0910			0.0657	0.1479					0.1986	
10/30/2017 03:00		0.0881		0.3565		0.0440	0.0247				0.0322												0.1170				0.0941			0.0630	0.1070	0.0367				0.2156	
10/31/2017 01:00				0.3082		0.0450	0.0503				0.0362										0.0326		0.1303		0.0389		0.1311			0.0707	0.1701	0.0990	0.1220			0.2264	

Showing 1 to 10 of 92 entries

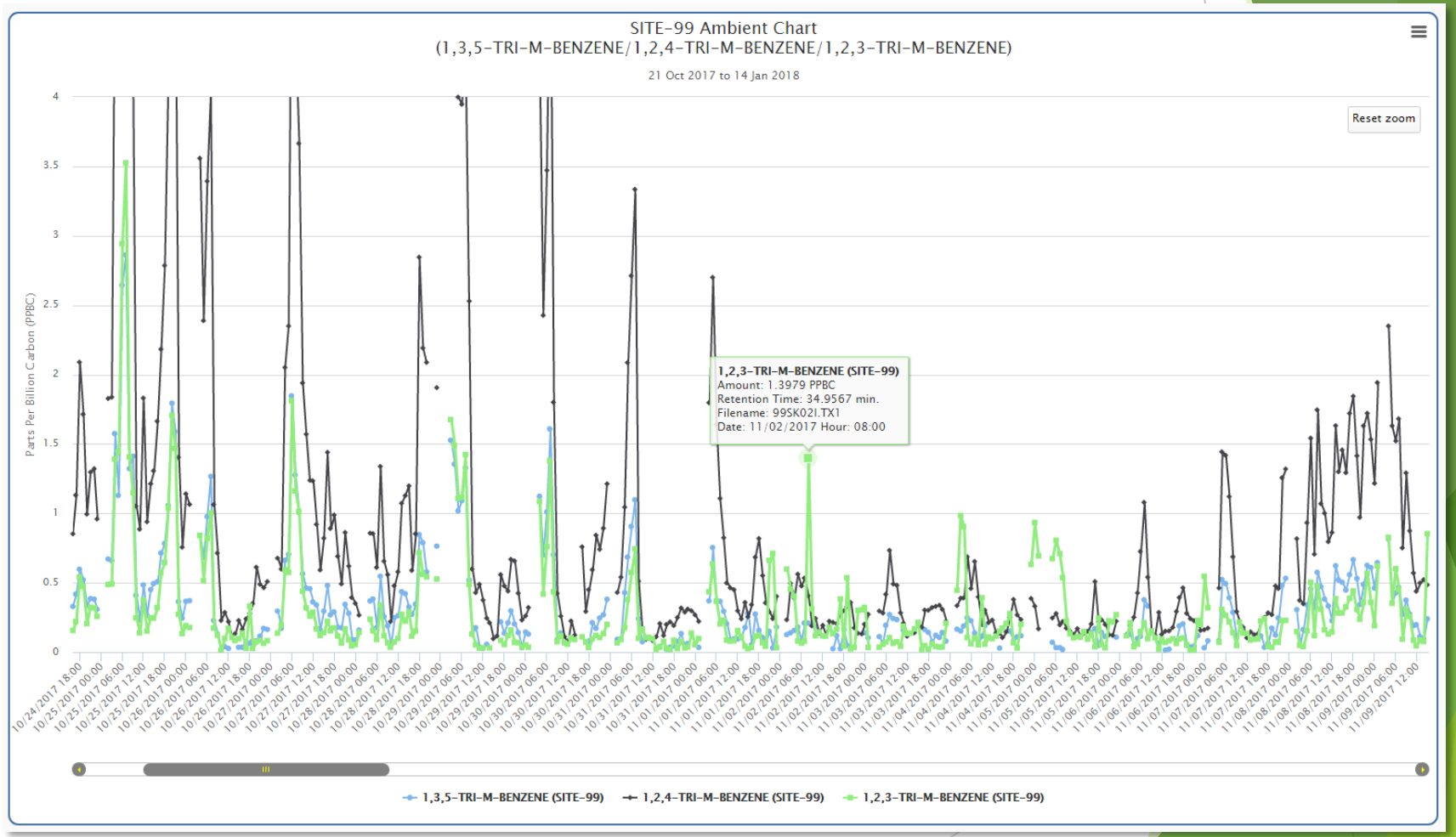
Previous 1 2 3 4 5 … 10 Next

Ambient Data Time Series

Trimethylbenzenes



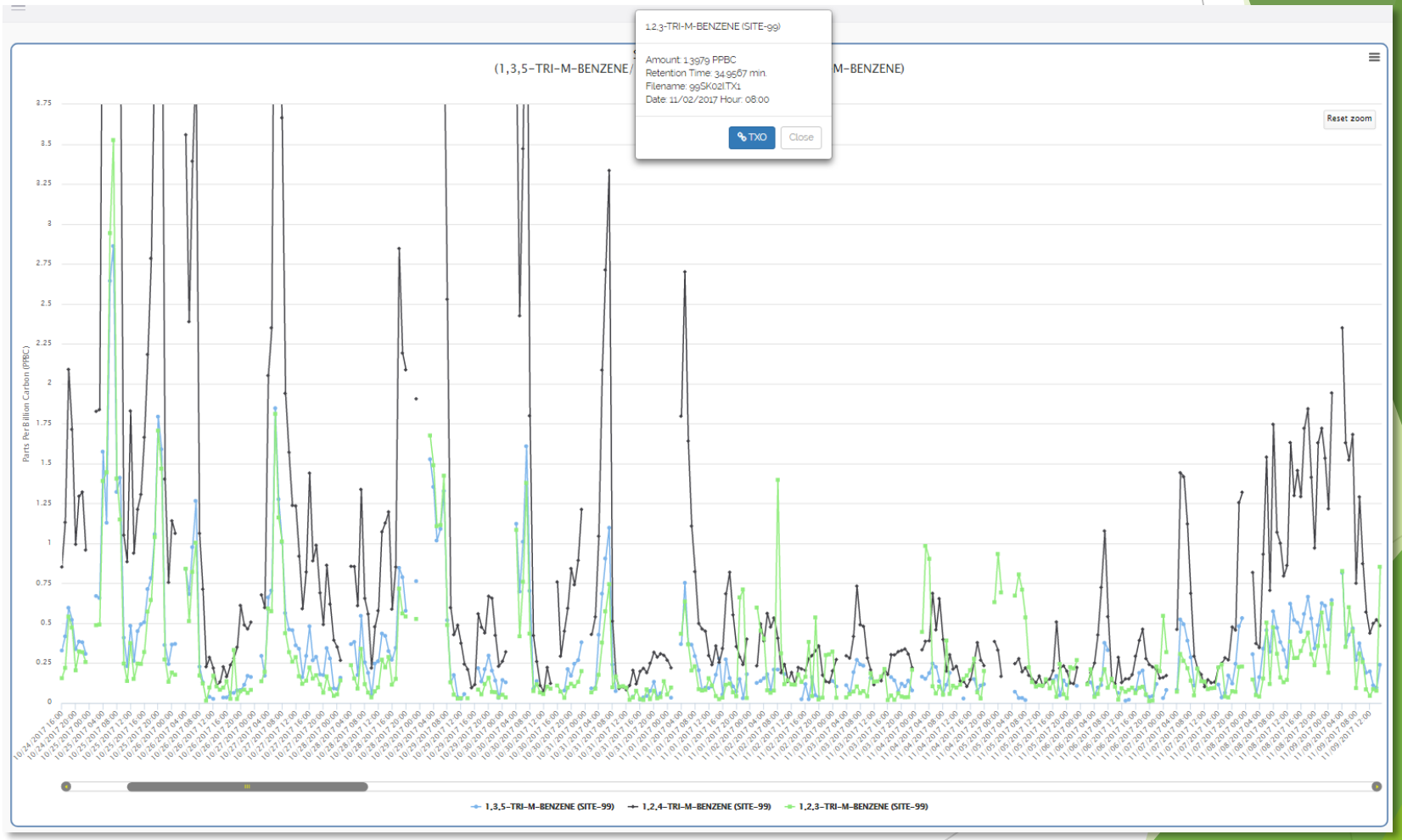
Ambient Data Time Series



- Expand to inspect
- Locate outliers
- Identification of data file

Ambient Data Time Series

ASCII File information

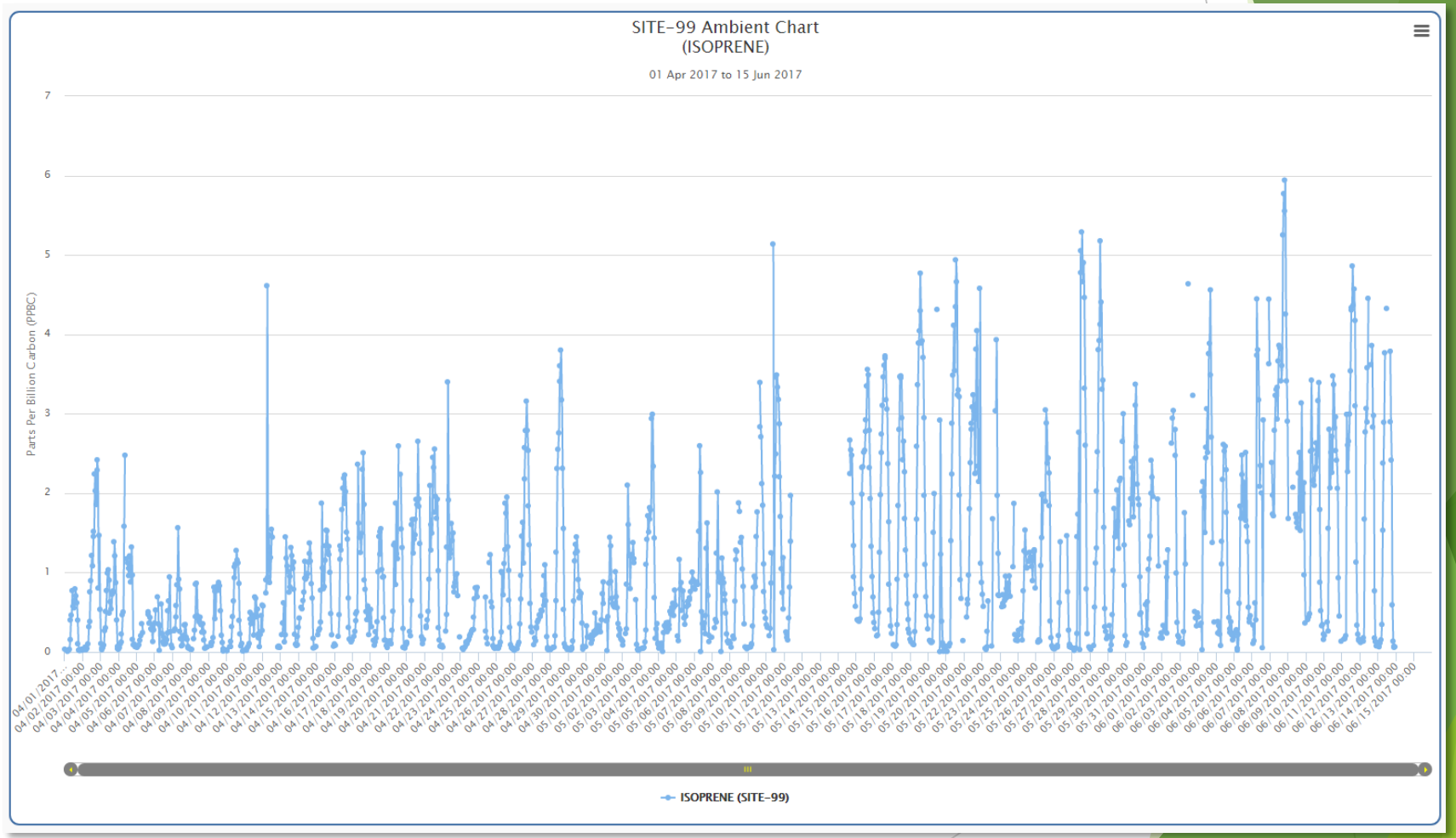


Ambient Data Time Series

ASCII File information

Ambient Data Time Series

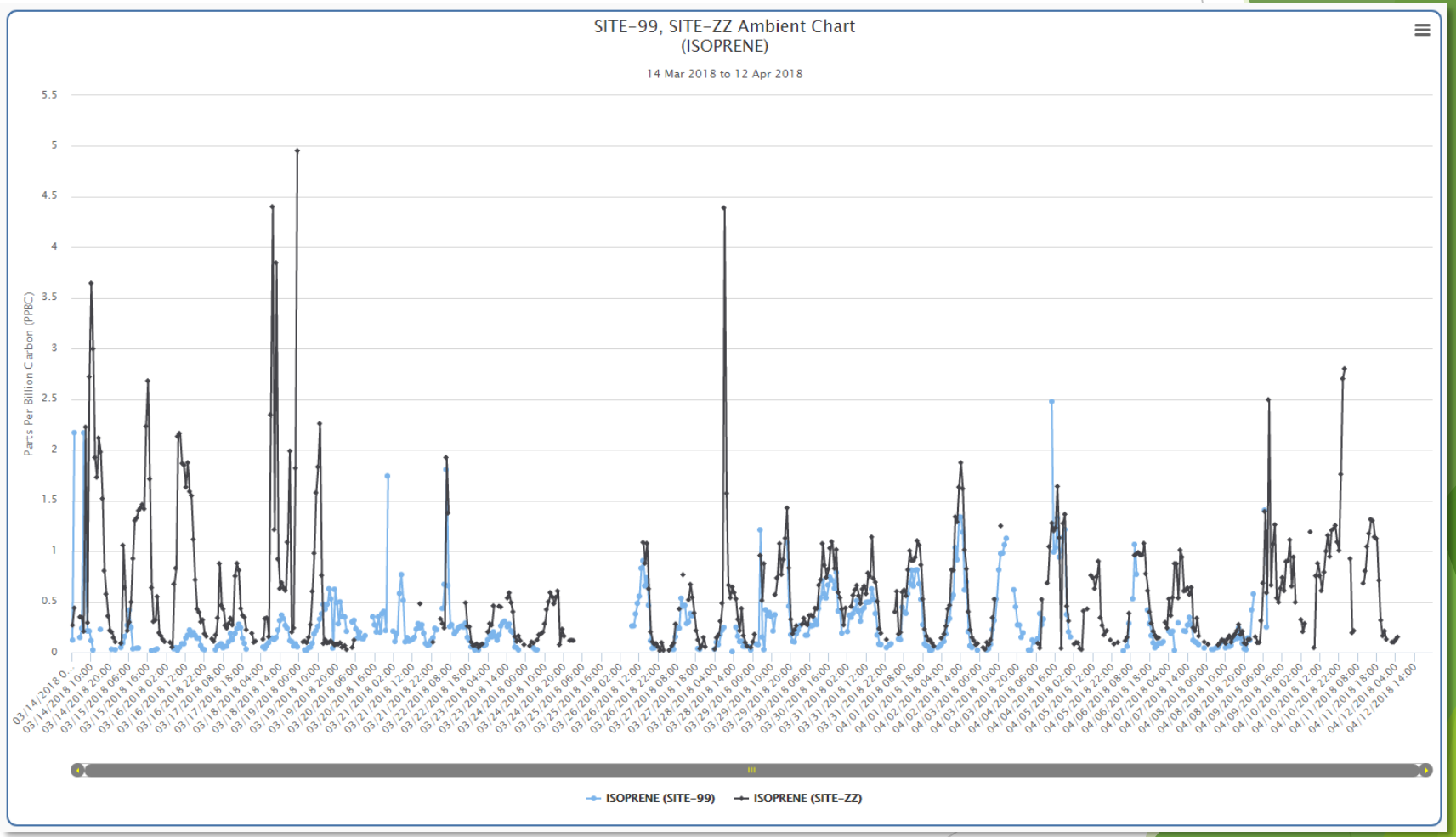
Diurnal Patterns
Isoprene



Ambient Data Time Series

Diurnal Patterns
Isoprene

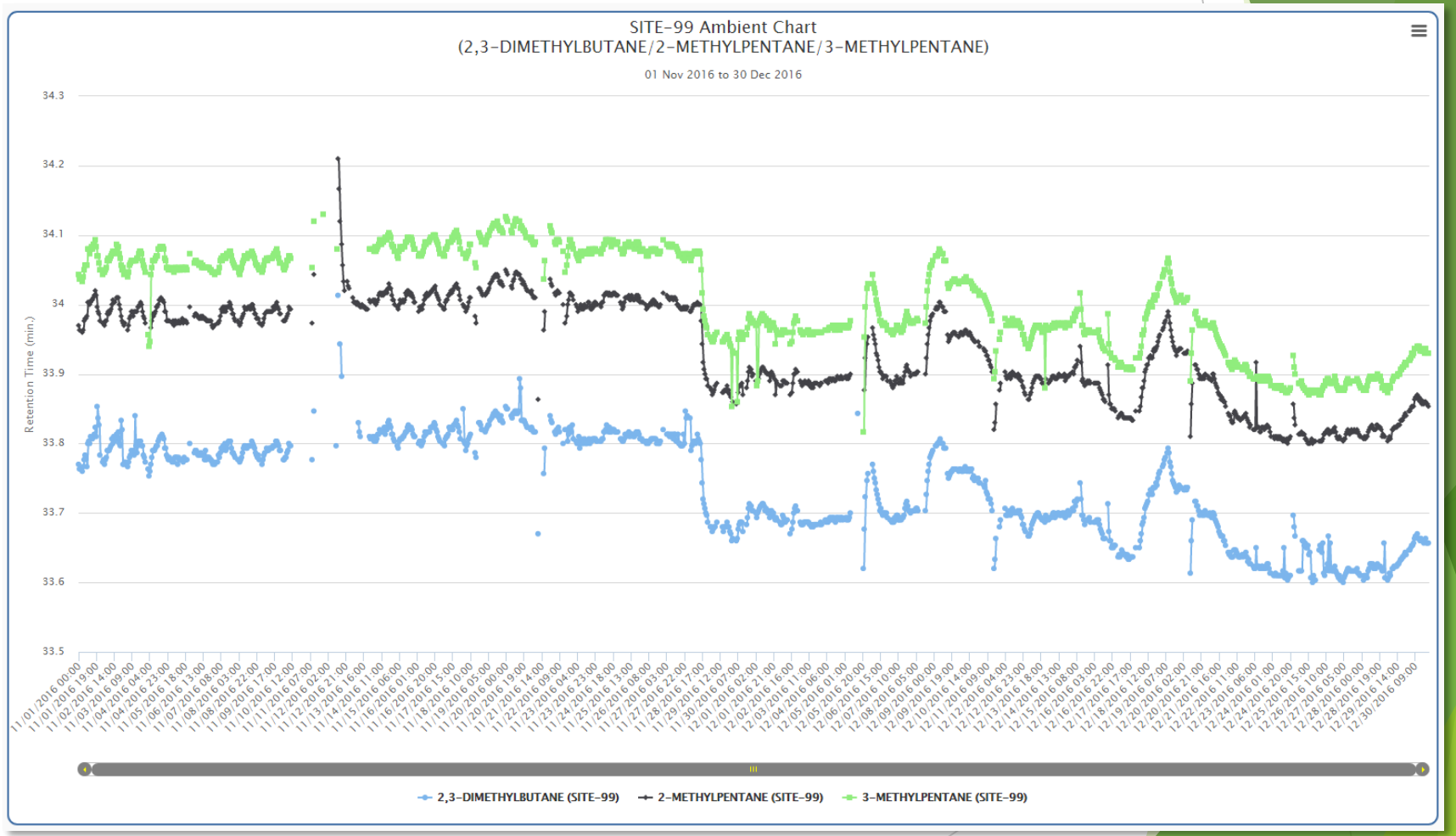
Comparison between Sites



Ambient Data Time Series

Time Series of component retention times to identify missidentifications

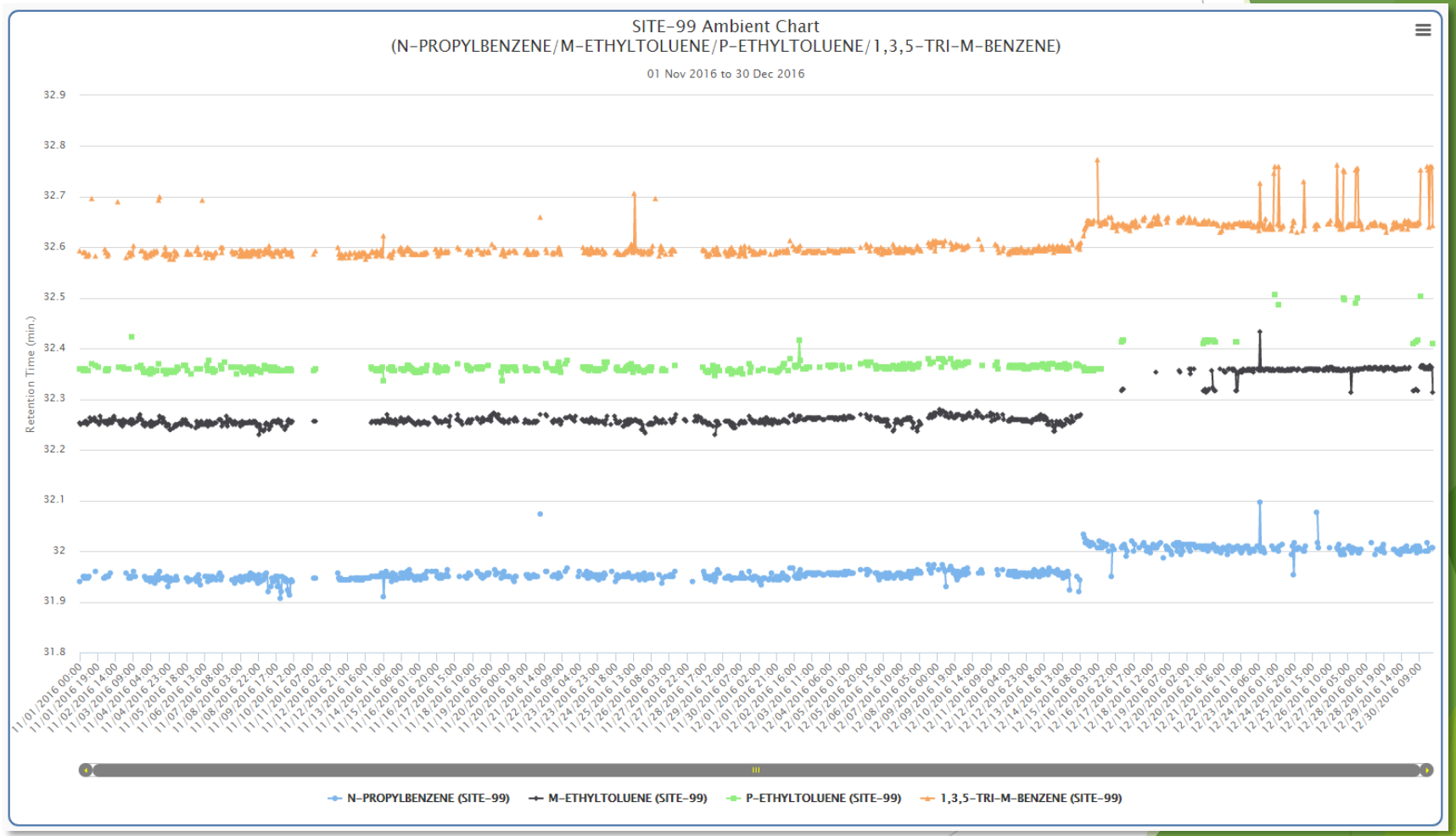
Plot column
- 2,3-Dimethylbutane
- 2-Methylpentane
- 3-Methylpentane



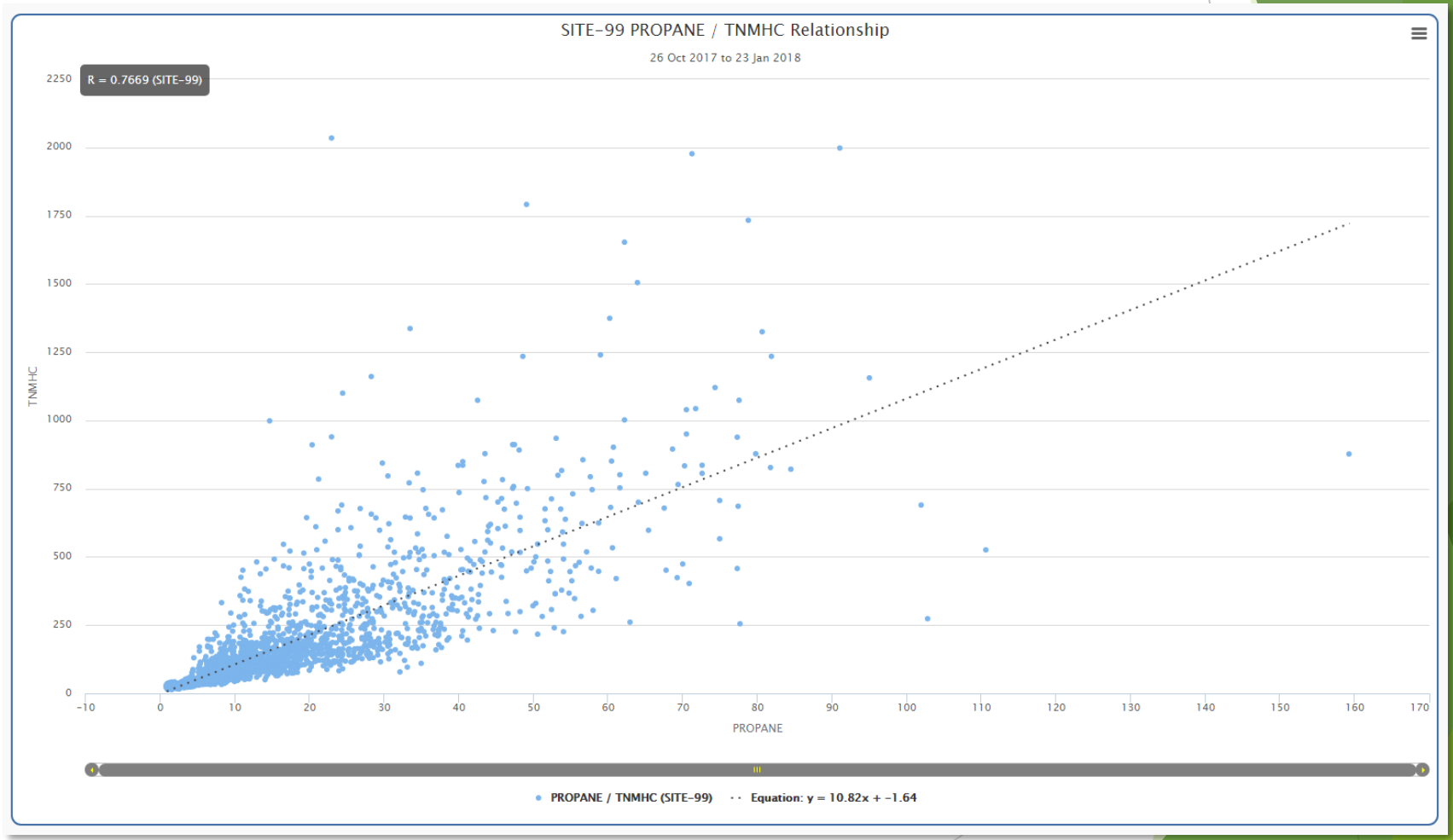
Ambient Data Time Series

Time Series of component retention times to identify missidentifications

BP column
- n-Propylbenzene
- m-Ethyltoluene
- p-Ethyltoluene
- 1,3,5-Trimethylbenzene



Scatter Plot of Propane and TNMHC to identify outliers



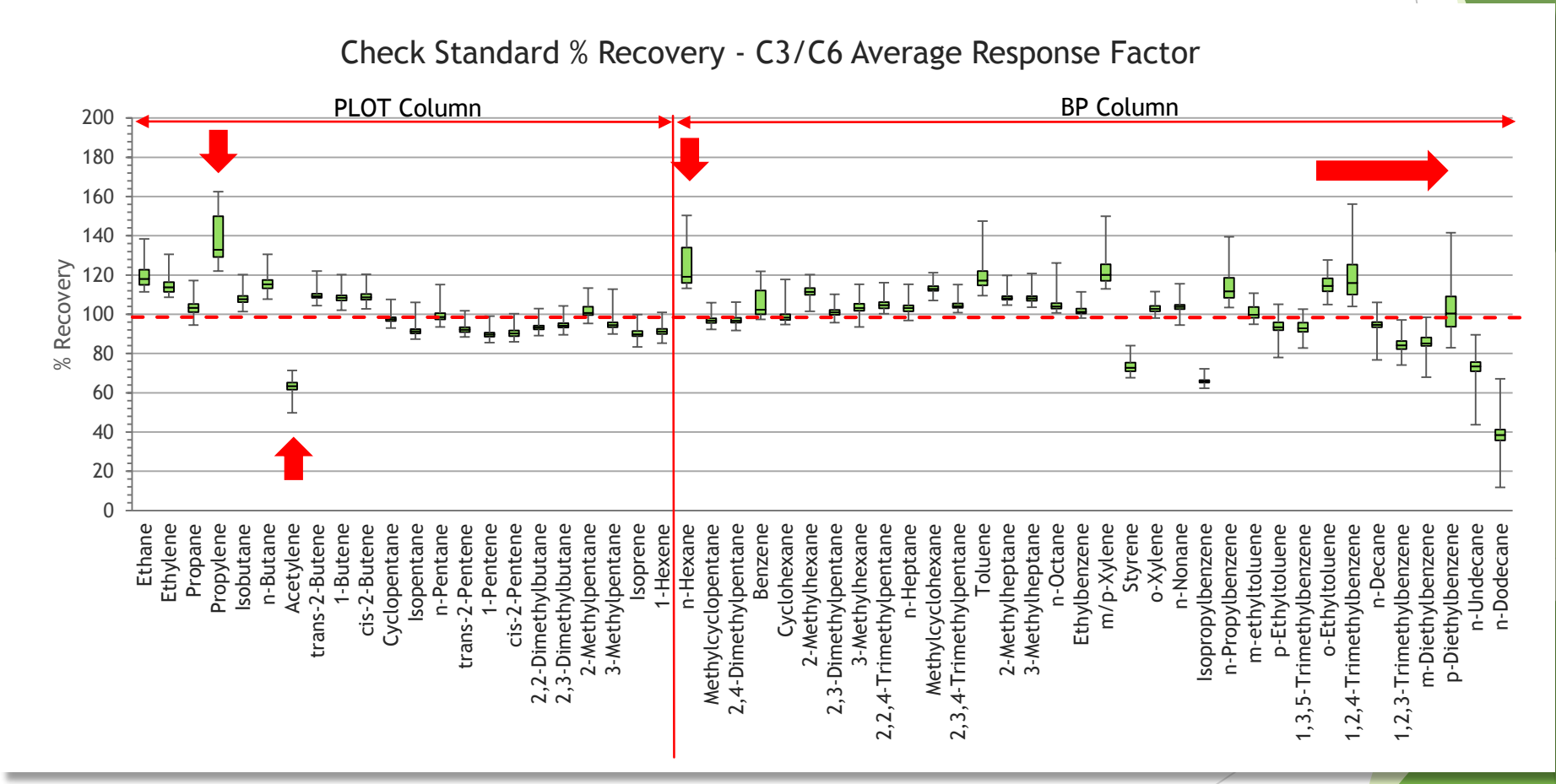
Merlin AutoGC Xplorer

- Ingestion of ASCII Text files from the PerkinElmer PAMS VOC AutoGC Systems
  - Format specific native output files from Totalchrom or EZChrom data systems
  - Data loaded from zip files or individual hourly files
  - Re-loading of reprocessed data accepted and flagged as reprocessed
- Database capable of holding multiple years of data
  - Users are responsible for archiving original raw data
  - Graphing of large data sets
  - Automatic association with AQS parameter codes
  - User configured site parameters
    - Target list user defined
    - Quality control components, concentrations and pass/fail limits
    - Tracks Certificates of Analysis concentrations for each new quality control across years
- Cloud based secure server
  - User defined access levels for operators, validators and administrators
  - User defined site access

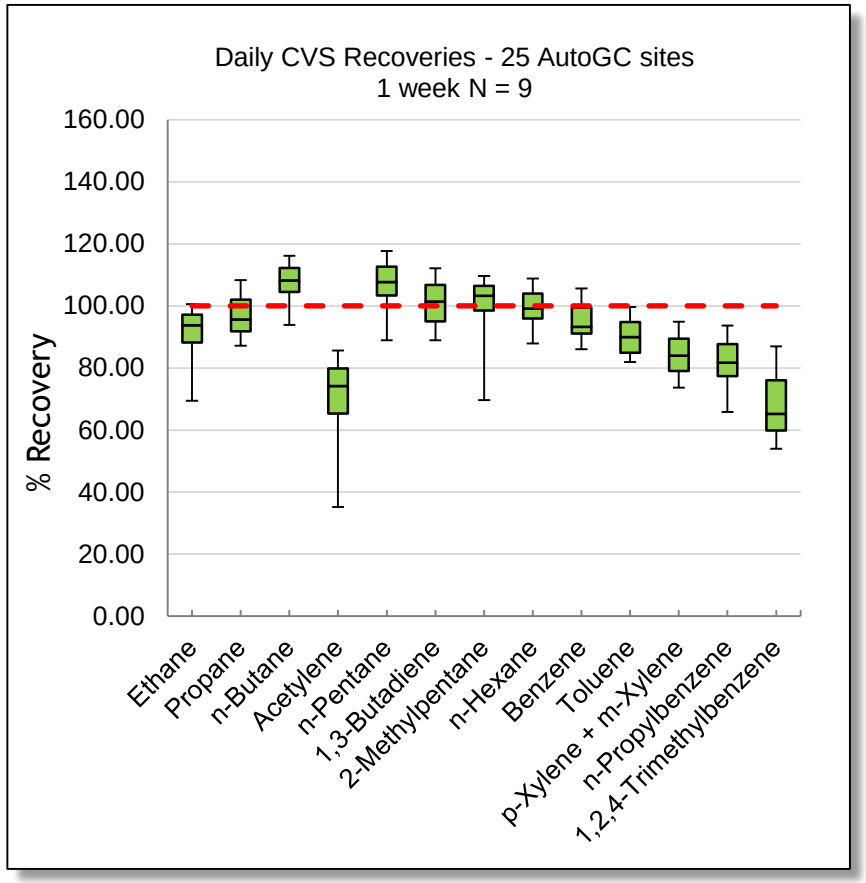
Value of Quality Assurance in AutoGC Networks

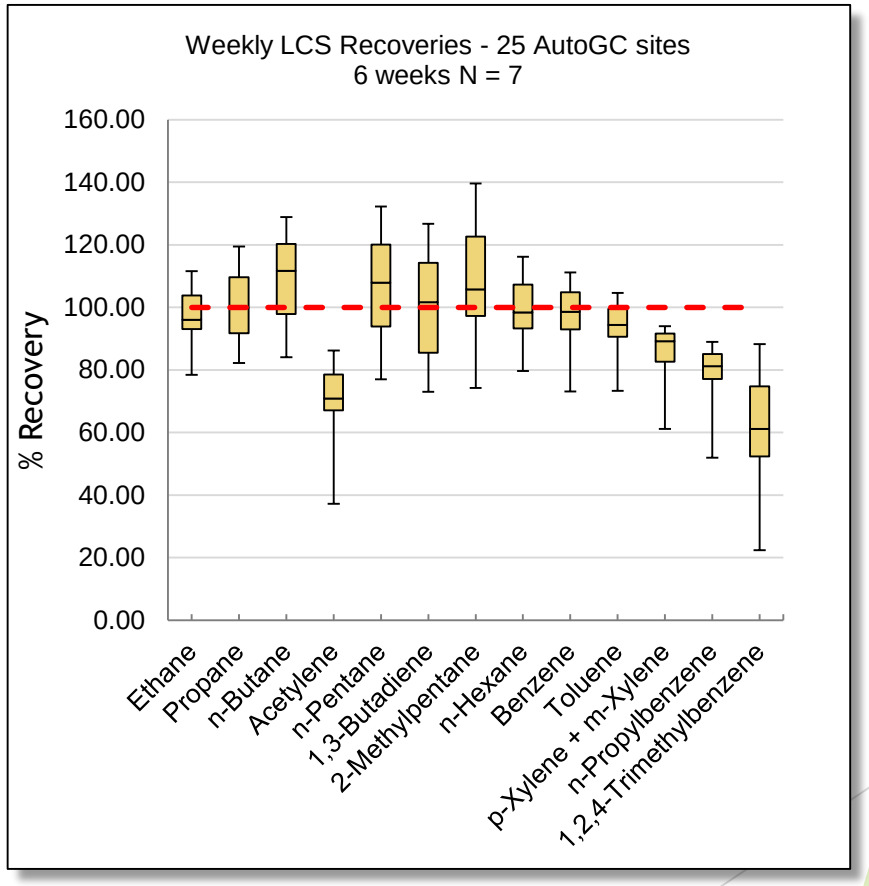
- Maintain consistent operating procedures and methods
  - All instruments operating under similar methods and conditions
  - All instrument performance evaluated with the same quality controls
- Quality Controls designed to insure consistent data quality
  - QC failures trigger actions which insure against poor quality data
  - Common QC rules insure similar quality of data for all sites
- Measurements of Network performance
  - Network-wide Audits to verify inter-site performance within the network
  - Evaluations of site data over time for intra-site performance.

Recoveries in Daily Check Standard at 0.5 ppbv

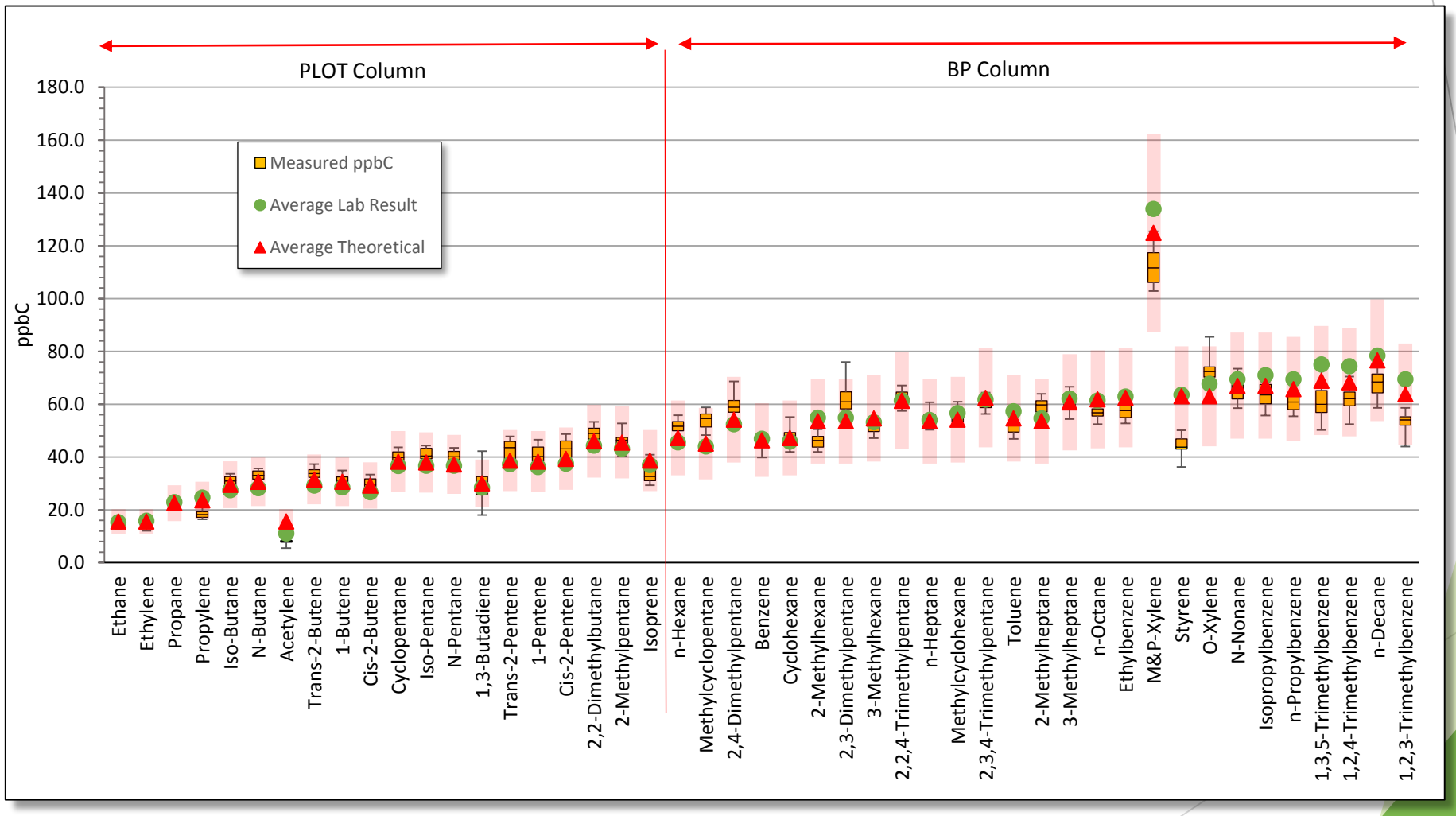


Network Quality Control – 25 AutoGC Sites

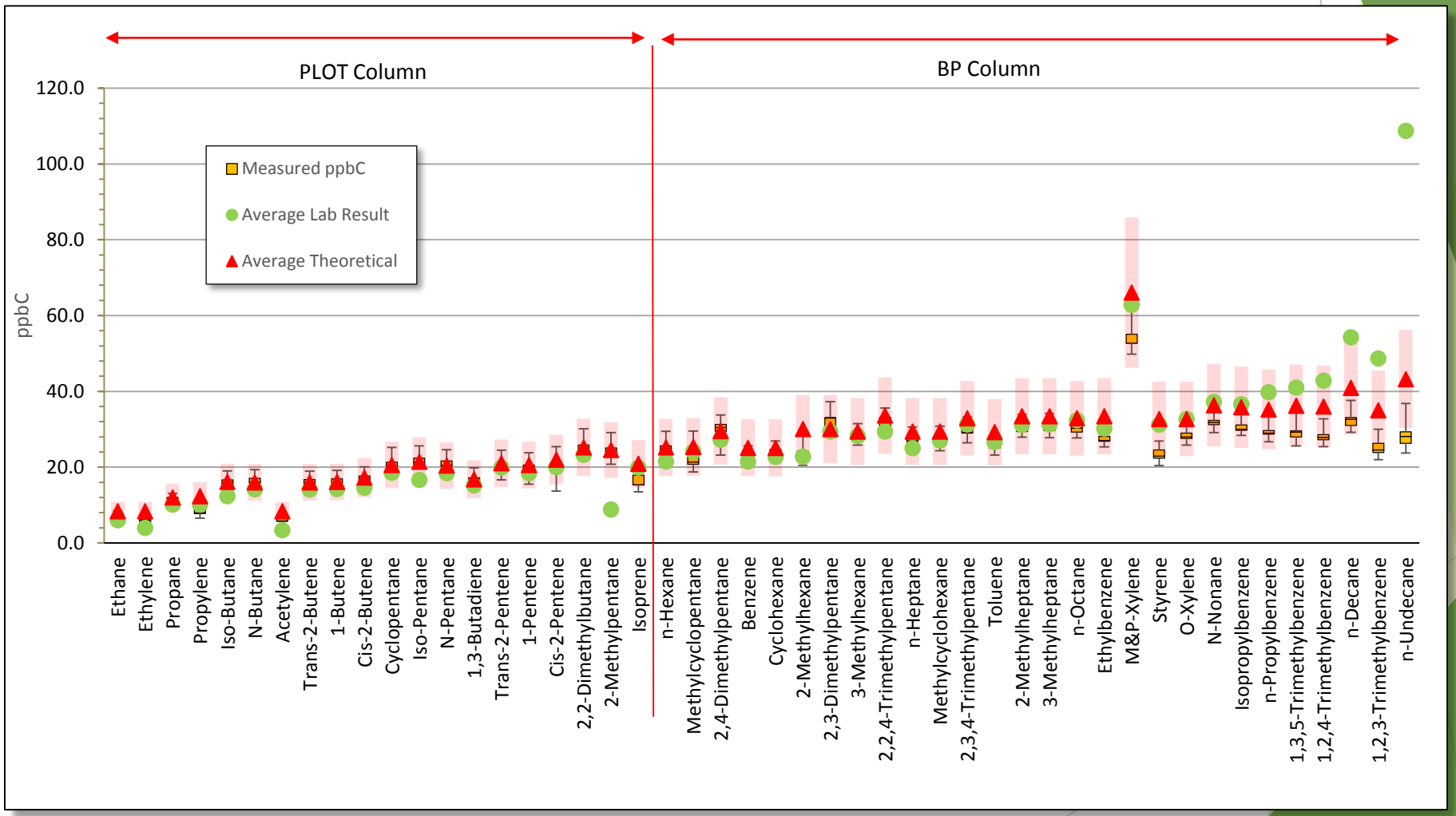




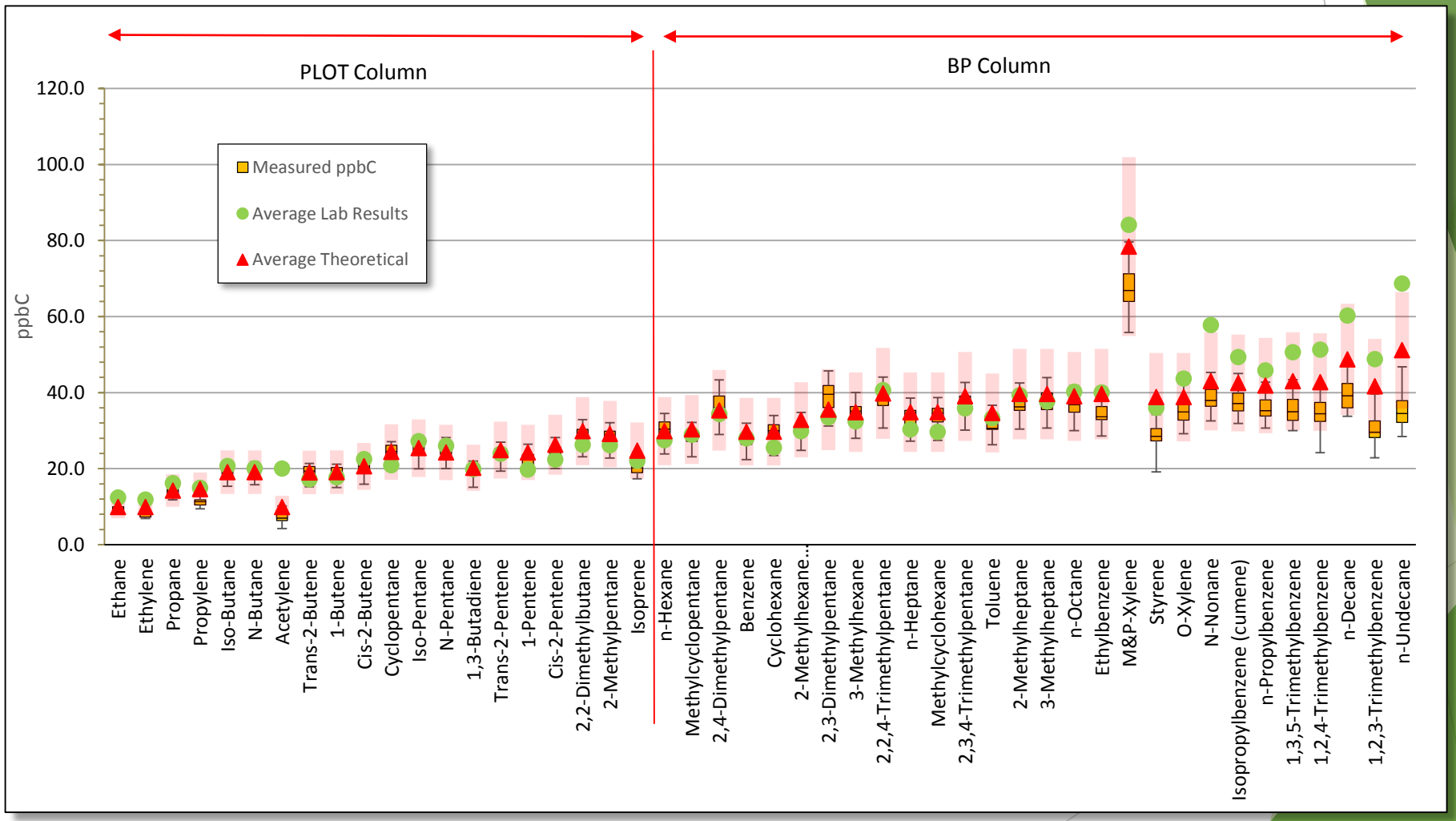
TCEQ Performance Evaluation Audit
Fall 2014 - 12 AutoGCs



AECOM Performance Evaluation Audits
Q2 & Q4 2015 - 13 AutoGCs North Texas Network

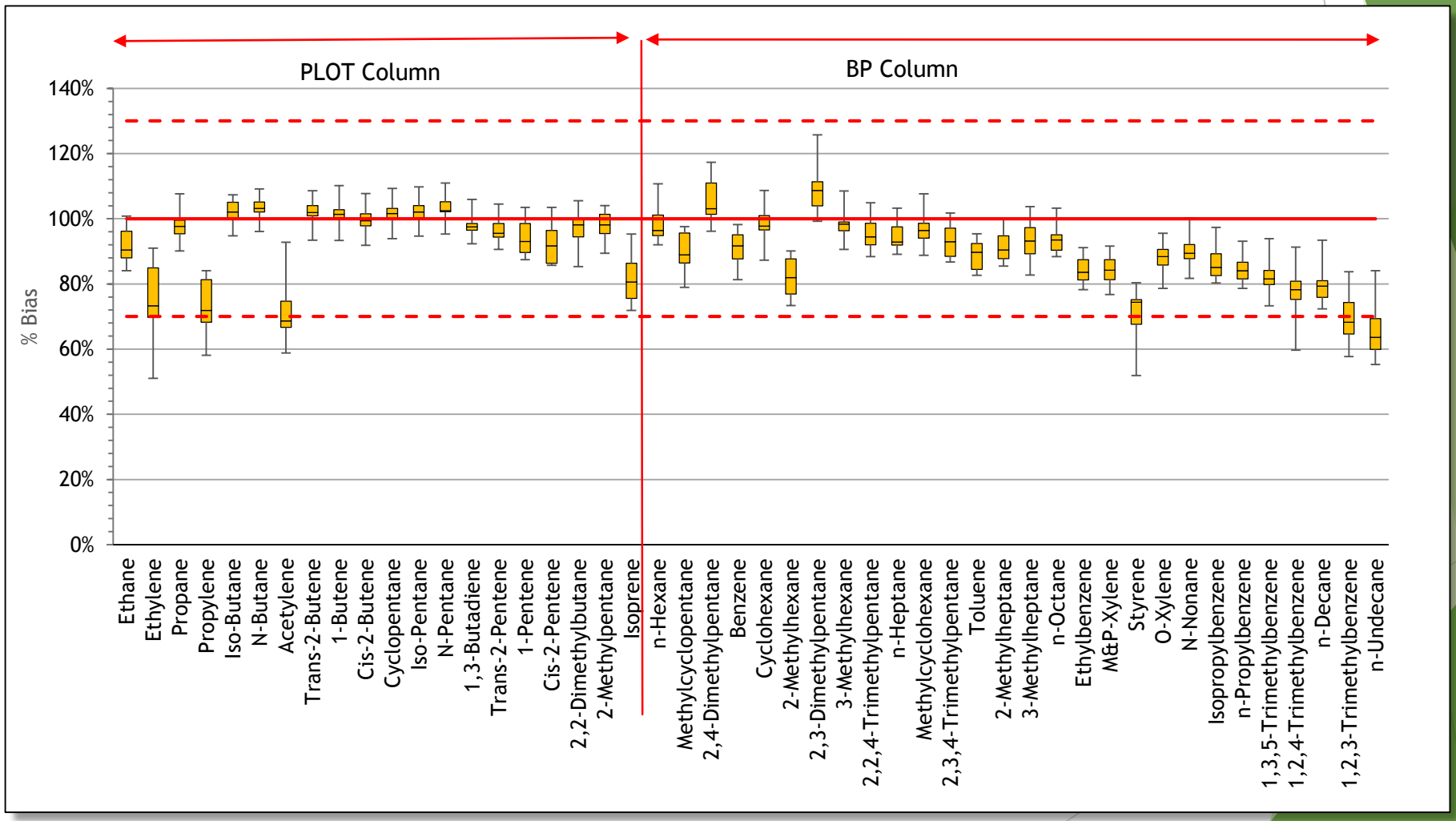


AECOM Performance Evaluation Audits
Q2 & Q3 2015 - 7 AutoGCs Houston/Galveston Network



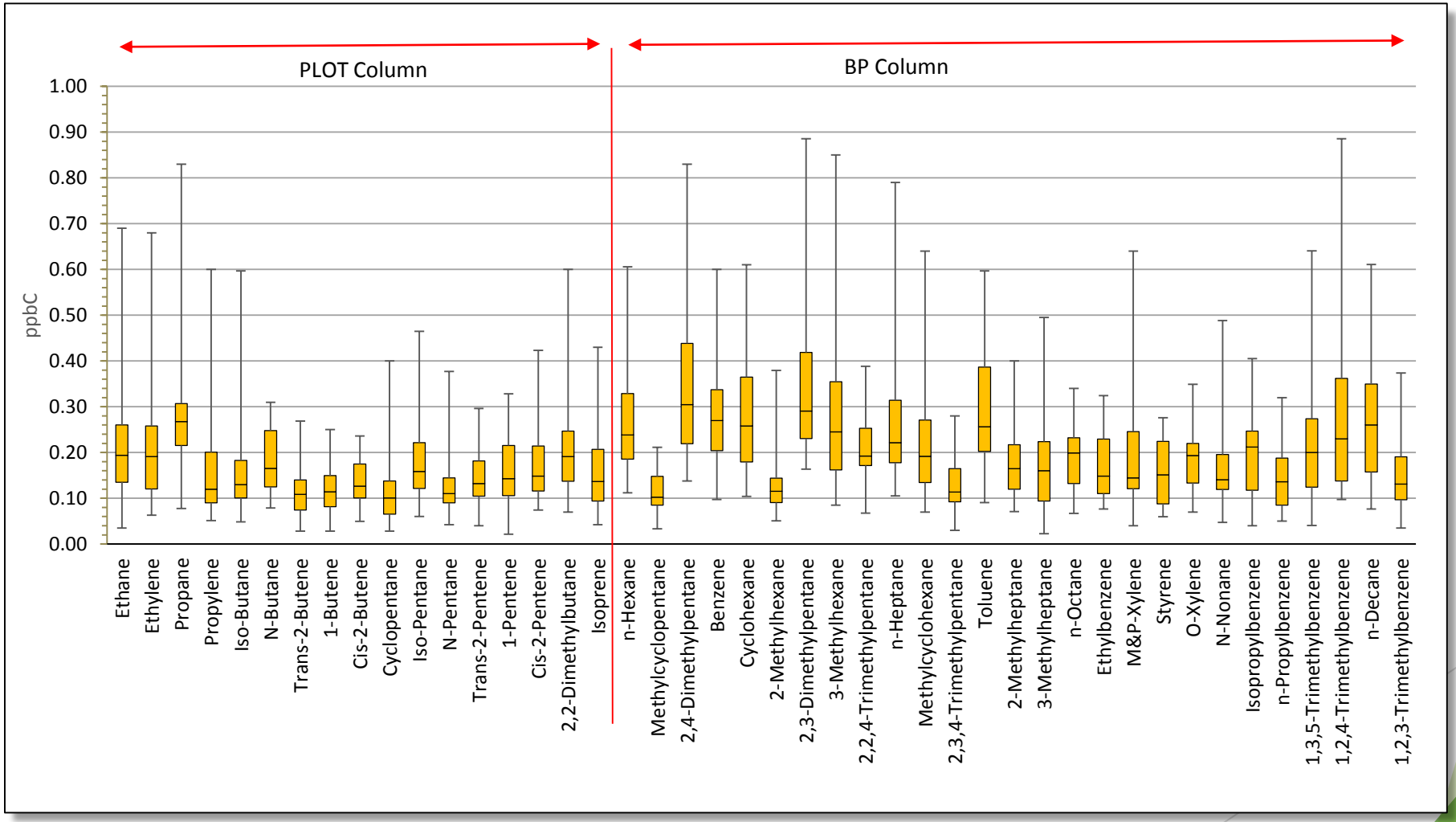
Normalized Performance Audit Data
Fall 2014 - Spring 2015 – 32 AutoGC Sites

Network	# of Sites	Nominal ppbv
NTC	13	5
EIMS	7	5
TCEQ	12	7



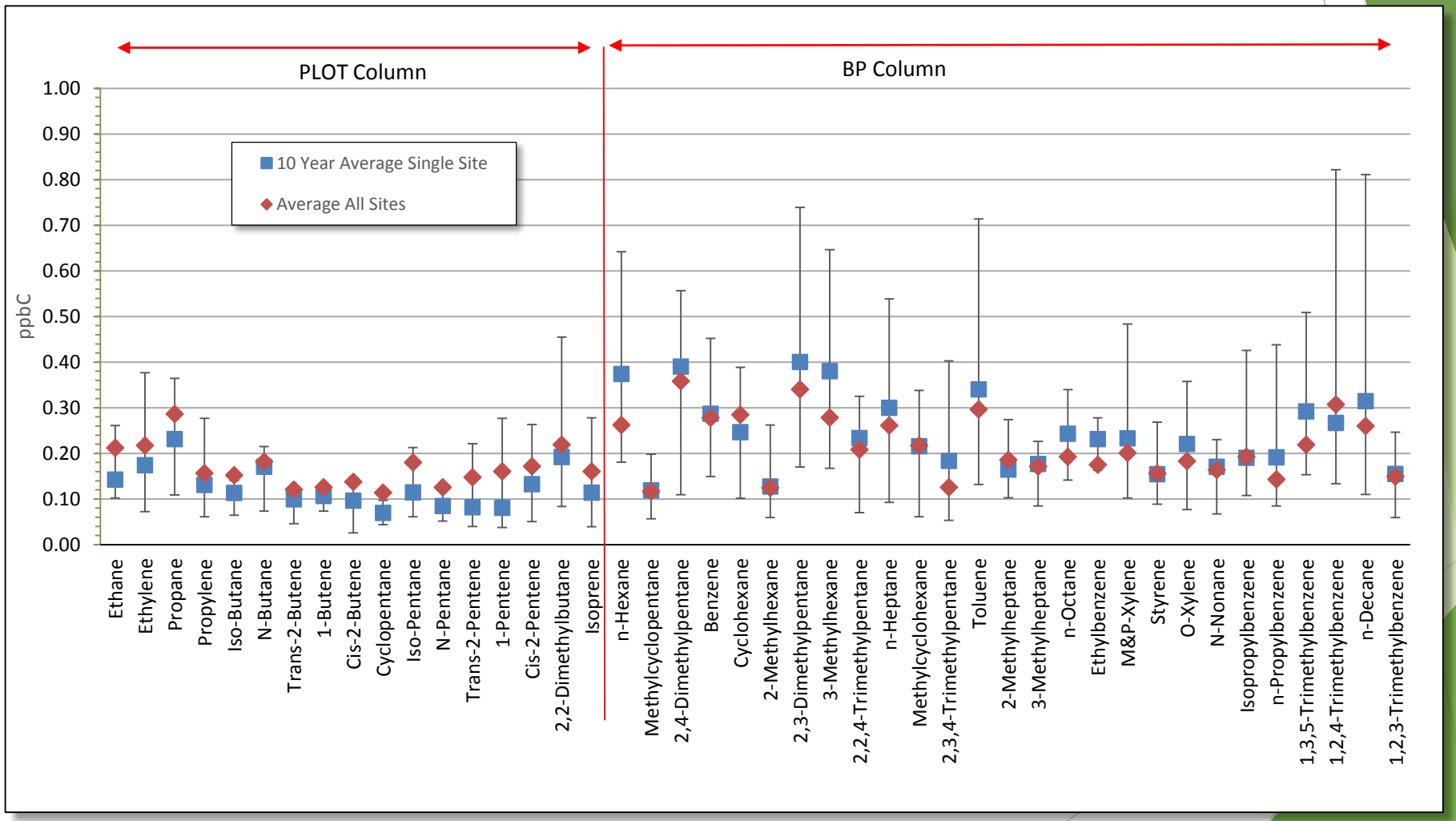
Minimum Detection Limits across 34 AutoGC Systems

40 CFR part 136 Appendix B

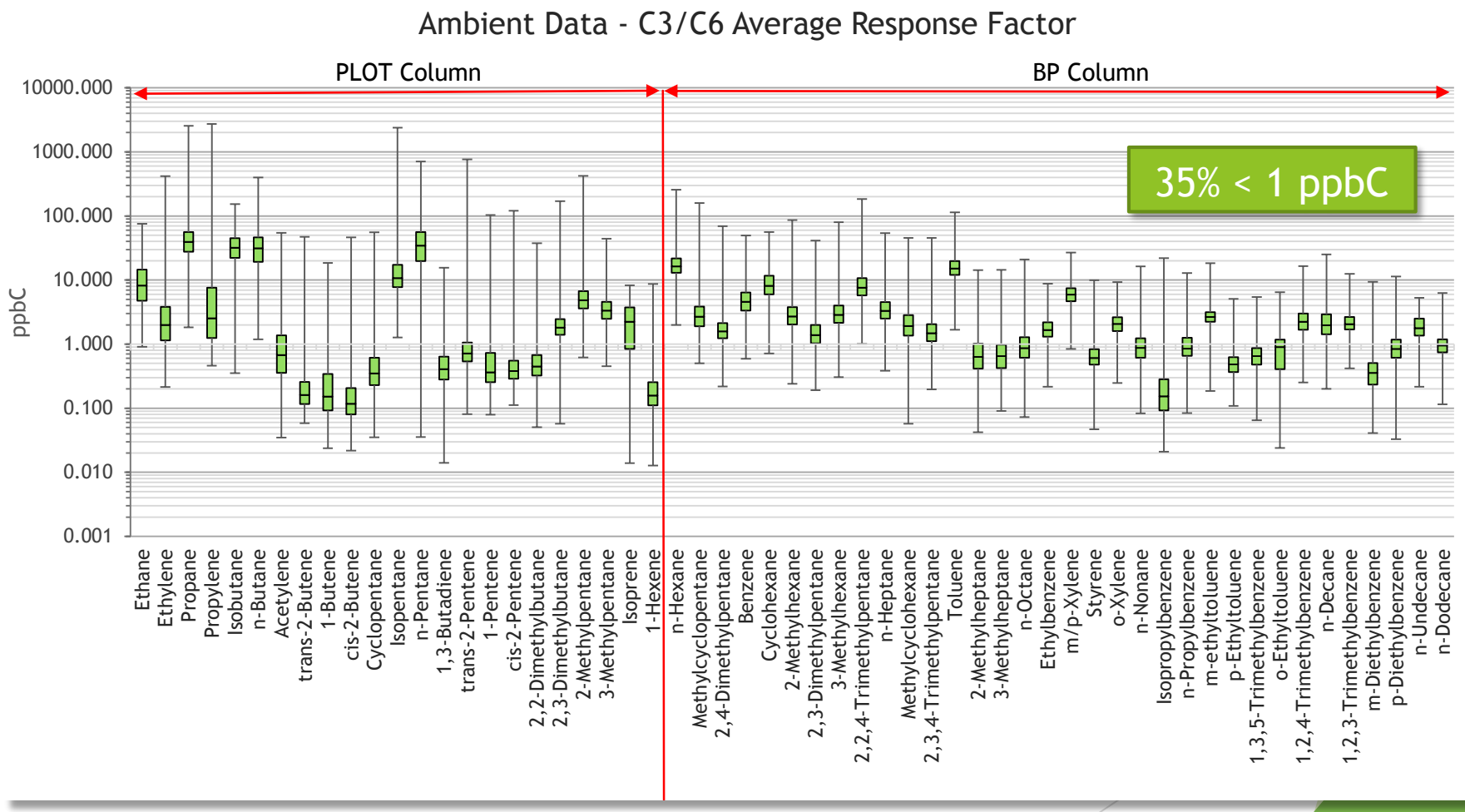


Network	# of Sites
NTC	13
EIMS	5
TCEQ	11
UT	4
HCPCS	1

Minimum Detection Limits over 10 years on a Single AutoGC System 40 CFR part 136 Appendix B



Distribution of Ambient Data
3.5 Months – over 1900 measurements



Summary
Requirements for Successful AutoGC

- Chromatographic Data System
  - Capable of identification and quantitation of complex samples
  - Robust and simple calibration strategy
  - Output format for easy review of data
  - Event control for automation of quality control checks
- Standard Operating Procedures
  - Daily operations for consistent data collection
  - Validation to handle deviations consistently
- Data Quality Objectives
  - Well defined control limits
  - System for identifying and correcting failures

FIFTY SIX
NON-METHANE
HYDROCARBONS
TWENTY FOUR
HOURS A DAY
SEVEN
DAYS A WEEK

Acknowledgements

"Without data you are just another person with an opinion." ---W. Edwards Deming

AECOM

Marty Hale

Scott Jenkins

✦✦✦

University of Texas Austin

Dr. Dave Sullivan

✦✦✦

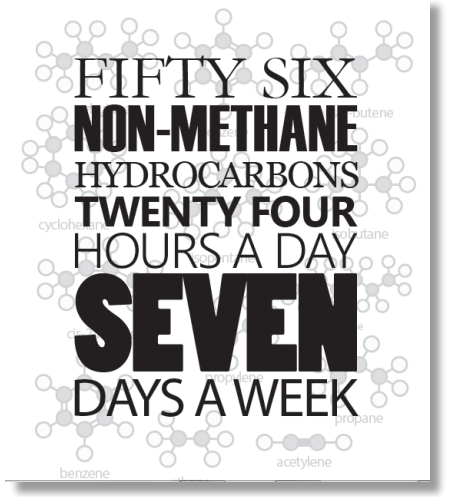
Texas Commission on Environmental Quality

Cory Chism

Cindy Maresh

Melanie Hotchkiss

Questions?

Carol J. Meyer
carol@orsat.com

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