

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039374.D
 Acq On : 19 Dec 2023 22:01
 Operator : JC/MD
 Sample : 05807-12 5X
 Misc : 1.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AZ4

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039374.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	23	25	27	rBV	2262	2372	0.31%	0.038%
2	1.368	43	46	57	rBV	88946	103163	13.28%	1.656%
3	1.648	89	92	102	rVB	60923	89177	11.48%	1.431%
4	2.300	193	199	209	rBV	163418	264057	33.99%	4.238%
5	2.697	260	264	271	rBV4	1529	2742	0.35%	0.044%
6	2.788	274	279	284	rBV2	2065	3686	0.47%	0.059%
7	2.861	284	291	298	rVV2	29042	60494	7.79%	0.971%
8	2.941	299	304	315	rVB2	6352	14028	1.81%	0.225%
9	3.117	329	333	336	rVB3	240	352	0.05%	0.006%
10	3.325	365	367	368	rBV2	297	215	0.03%	0.003%
11	3.520	397	399	401	rBV	257	185	0.02%	0.003%
12	3.550	401	404	407	rVB2	217	281	0.04%	0.005%
13	3.861	454	455	458	rBV2	196	192	0.02%	0.003%
14	3.995	475	477	479	rVB2	209	178	0.02%	0.003%
15	4.154	501	503	508	rVB2	271	331	0.04%	0.005%
16	4.270	519	522	524	rBV	227	261	0.03%	0.004%
17	4.453	544	552	564	rBV	67101	194426	25.03%	3.121%
18	4.733	596	598	601	rBV2	298	406	0.05%	0.007%
19	4.843	613	616	618	rBV	225	341	0.04%	0.005%
20	4.904	624	626	627	rBV2	276	208	0.03%	0.003%
21	4.940	630	632	633	rVV2	279	221	0.03%	0.004%
22	5.056	640	651	669	rVV	95318	297038	38.24%	4.768%
23	5.282	686	688	690	rBV	201	219	0.03%	0.004%
24	5.361	697	701	702	rBV	217	190	0.02%	0.003%
25	5.404	705	708	712	rBV2	307	476	0.06%	0.008%
26	5.562	729	734	735	rBV2	385	432	0.06%	0.007%
27	5.684	751	754	756	rVB2	150	167	0.02%	0.003%
28	5.714	756	759	760	rBV	189	171	0.02%	0.003%
29	5.964	789	800	808	rBV2	255059	776868	100.00%	12.470%
30	6.196	834	838	840	rBV2	279	356	0.05%	0.006%
31	6.434	875	877	879	rVV2	178	163	0.02%	0.003%
32	6.696	918	920	921	rBV	412	234	0.03%	0.004%
33	6.757	921	930	953	rVV	191560	466599	60.06%	7.489%
34	6.995	968	969	970	rBV	398	180	0.02%	0.003%
35	7.117	984	989	995	rBV6	1171	2756	0.35%	0.044%
36	7.306	1012	1020	1038	rBV	158651	350108	45.07%	5.620%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039374.D
 Acq On : 19 Dec 2023 22:01
 Operator : JC/MD
 Sample : 05807-12 5X
 Misc : 1.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AZ4

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

37	7.476	1046	1048	1051	rBV2	508	556	0.07%	0.009%
38	7.537	1057	1058	1061	rVB	327	189	0.02%	0.003%
39	7.964	1123	1128	1129	rBV3	292	319	0.04%	0.005%
40	8.025	1137	1138	1141	rVB2	292	179	0.02%	0.003%
41	8.068	1141	1145	1149	rVB2	265	335	0.04%	0.005%
42	8.214	1166	1169	1171	rBV	207	185	0.02%	0.003%
43	8.324	1179	1187	1197	rBV	102979	169550	21.82%	2.721%
44	8.513	1217	1218	1220	rVB	336	216	0.03%	0.003%
45	8.647	1234	1240	1263	rBV	373157	603398	77.67%	9.685%
46	8.952	1284	1290	1302	rBV	72004	112014	14.42%	1.798%
47	9.055	1306	1307	1311	rBV2	424	359	0.05%	0.006%
48	9.098	1311	1314	1317	rBV	217	287	0.04%	0.005%
49	9.159	1322	1324	1331	rVB2	296	309	0.04%	0.005%
50	9.275	1341	1343	1348	rVV3	858	956	0.12%	0.015%
51	9.385	1356	1361	1383	rBV	334199	485358	62.48%	7.791%
52	9.628	1399	1401	1405	rVB2	284	270	0.03%	0.004%
53	9.714	1413	1415	1418	rBV2	223	180	0.02%	0.003%
54	10.055	1465	1471	1472	rBV	444556	585075	75.31%	9.391%
55	10.500	1541	1544	1545	rBV	239	184	0.02%	0.003%
56	10.653	1565	1569	1574	rBV2	274	436	0.06%	0.007%
57	10.756	1583	1586	1591	rVB2	134	203	0.03%	0.003%
58	10.793	1591	1592	1595	rVB2	202	199	0.03%	0.003%
59	10.964	1618	1620	1622	rVB	326	218	0.03%	0.003%
60	11.189	1652	1657	1666	rVV	296374	388023	49.95%	6.228%
61	11.311	1674	1677	1680	rVB2	668	904	0.12%	0.015%
62	11.409	1690	1693	1696	rBV2	231	284	0.04%	0.005%
63	11.457	1696	1701	1704	rBV2	446	761	0.10%	0.012%
64	11.573	1717	1720	1722	rBV2	183	237	0.03%	0.004%
65	11.604	1724	1725	1728	rVB2	217	181	0.02%	0.003%
66	11.677	1736	1737	1740	rVB	245	195	0.03%	0.003%
67	11.707	1740	1742	1744	rBV	179	181	0.02%	0.003%
68	11.756	1746	1750	1752	rBV	458	559	0.07%	0.009%
69	11.969	1781	1785	1788	rBV3	3992	4990	0.64%	0.080%
70	12.024	1788	1794	1803	rVV	460100	672052	86.51%	10.787%
71	12.195	1819	1822	1824	rBV2	212	220	0.03%	0.004%
72	12.317	1837	1842	1853	rBV	425105	552738	71.15%	8.872%
73	12.488	1868	1870	1873	rVB	282	224	0.03%	0.004%
74	12.713	1902	1907	1908	rVB2	141	183	0.02%	0.003%
75	12.762	1908	1915	1920	rBV2	2407	3119	0.40%	0.050%
76	12.860	1928	1931	1933	rBV2	184	267	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039374.D
 Acq On : 19 Dec 2023 22:01
 Operator : JC/MD
 Sample : 05807-12 5X
 Misc : 1.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AZ4

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

77	13.006	1952	1955	1957	rVV	273	271	0.03%	0.004%
78	13.049	1960	1962	1963	rBV	288	197	0.03%	0.003%
79	13.067	1963	1965	1969	rVB2	160	166	0.02%	0.003%
80	13.110	1970	1972	1974	rVV2	245	236	0.03%	0.004%
81	13.183	1981	1984	1988	rVB2	184	293	0.04%	0.005%
82	13.481	2029	2033	2035	rVV2	168	205	0.03%	0.003%
83	13.597	2048	2052	2057	rVB4	421	594	0.08%	0.010%
84	13.658	2059	2062	2067	rVB2	170	309	0.04%	0.005%
85	13.713	2067	2071	2072	rBV2	198	214	0.03%	0.003%
86	13.786	2081	2083	2085	rVB	264	200	0.03%	0.003%
87	13.969	2109	2113	2116	rVB3	353	415	0.05%	0.007%
88	14.134	2135	2140	2144	rVB	3083	4483	0.58%	0.072%
89	14.292	2165	2166	2169	rVV2	277	204	0.03%	0.003%
90	14.499	2195	2200	2201	rBV2	195	264	0.03%	0.004%
91	14.530	2203	2205	2206	rVV	251	192	0.02%	0.003%
92	14.560	2207	2210	2212	rVV2	220	254	0.03%	0.004%
93	14.615	2215	2219	2220	rBV2	226	254	0.03%	0.004%
94	14.664	2225	2227	2231	rVB	236	259	0.03%	0.004%
95	14.713	2233	2235	2237	rBV	187	189	0.02%	0.003%
96	15.426	2351	2352	2356	rBV2	203	263	0.03%	0.004%
97	16.182	2474	2476	2479	rVB2	300	244	0.03%	0.004%
98	16.286	2491	2493	2495	rVV2	465	281	0.04%	0.005%
99	16.316	2495	2498	2501	rBV2	299	465	0.06%	0.007%
100	16.566	2538	2539	2541	rBV2	311	233	0.03%	0.004%

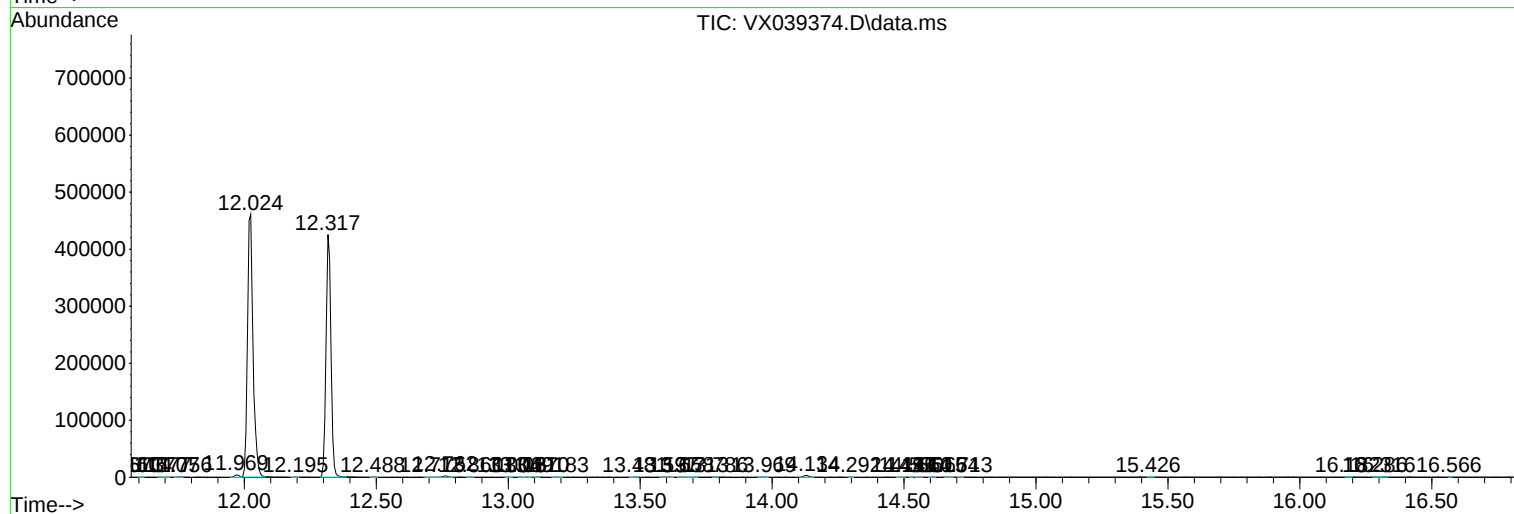
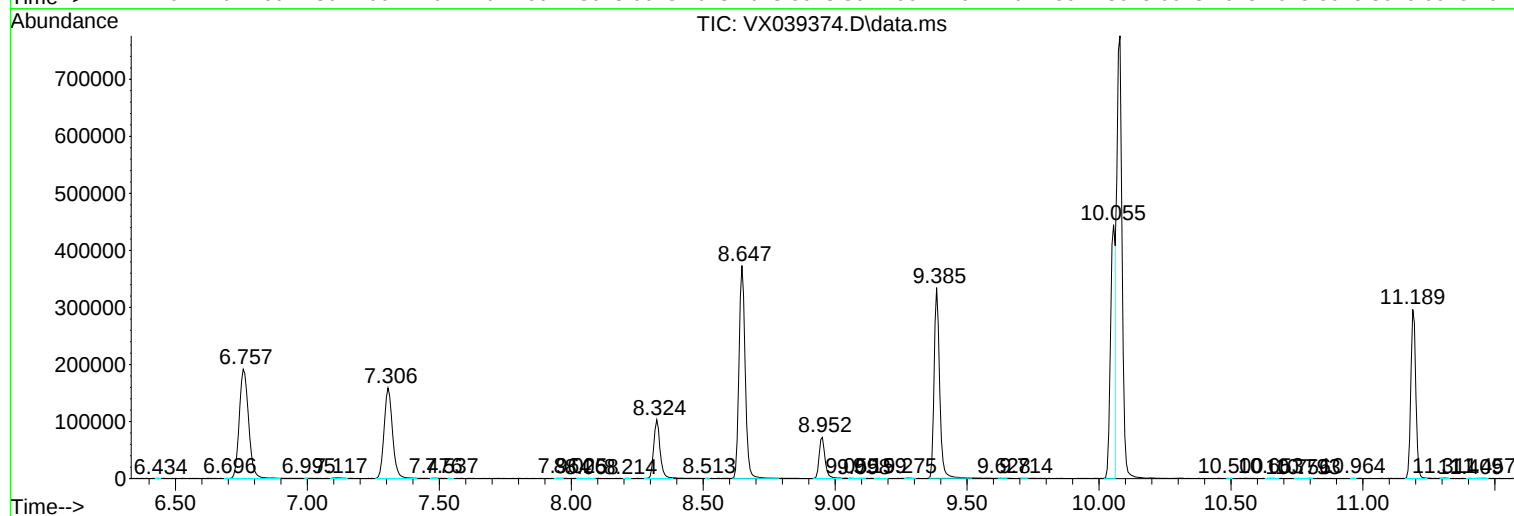
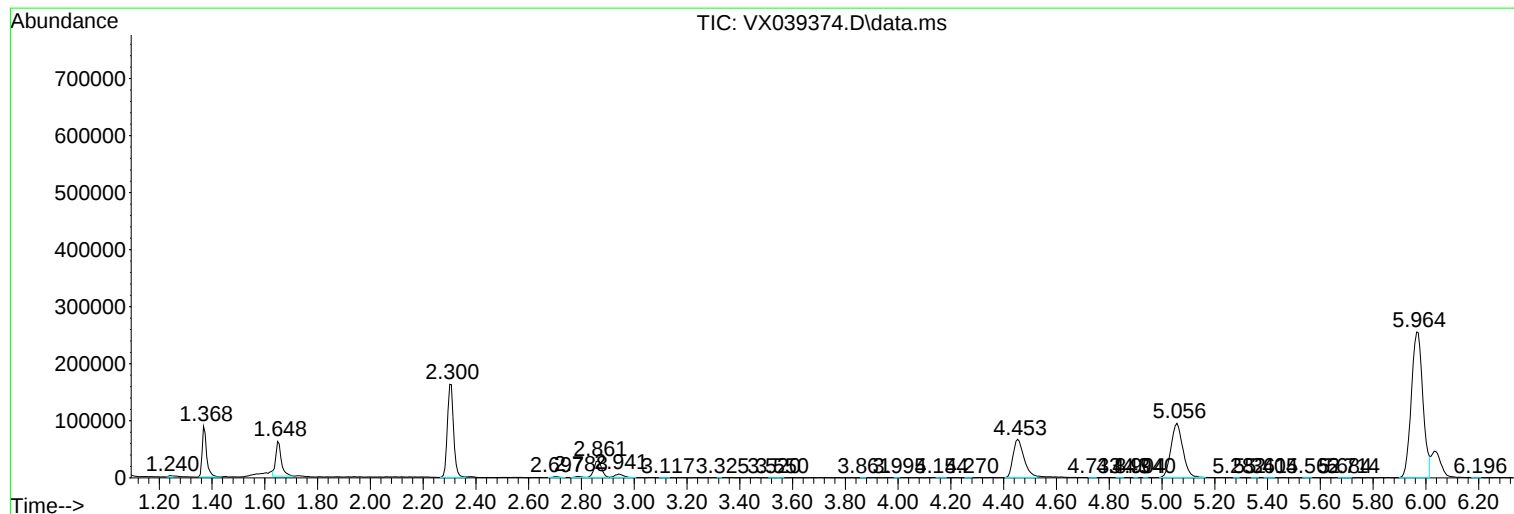
Sum of corrected areas: 6230051

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039374.D
Acq On : 19 Dec 2023 22:01
Operator : JC/MD
Sample : 05807-12 5X
Misc : 1.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AZ4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039374.D
Acq On : 19 Dec 2023 22:01
Operator : JC/MD
Sample : 05807-12 5X
Misc : 1.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AZ4

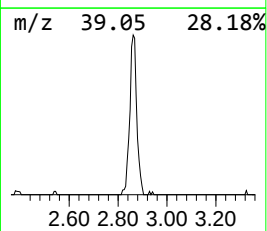
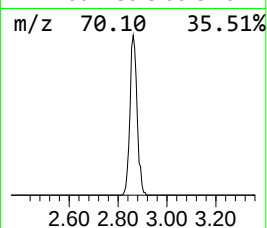
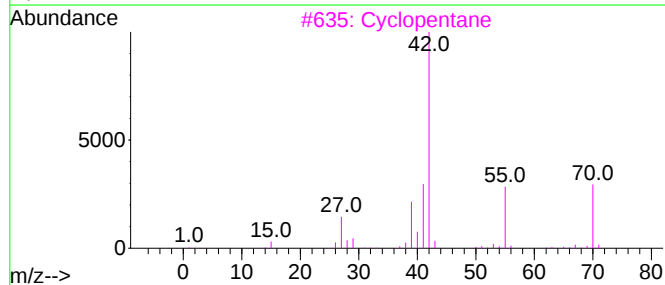
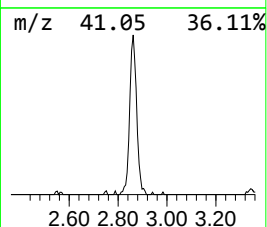
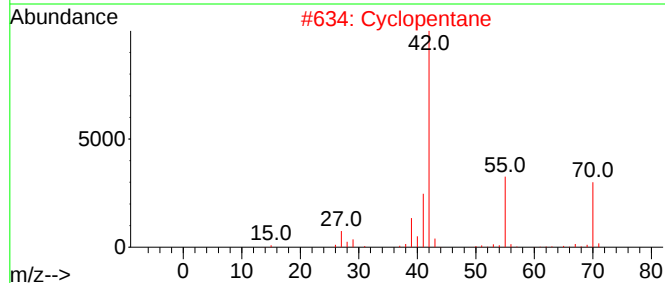
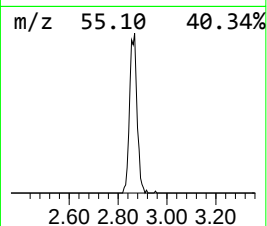
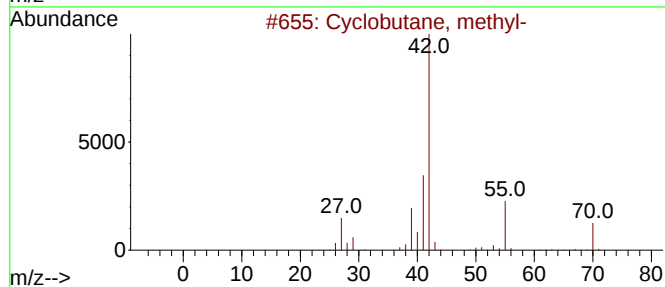
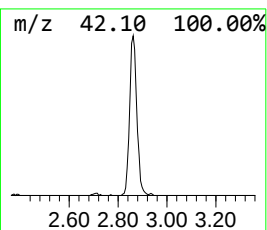
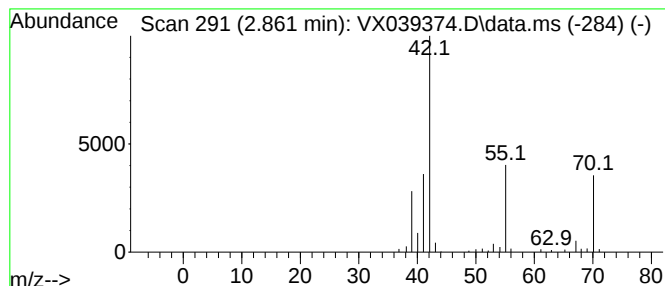
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (DEL) Alkane: Cyclic2.861 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.861	6.48 ug/L	60494	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	86
2			Cyclopentane	70	C5H10	000287-92-3	86
3			Cyclopentane	70	C5H10	000287-92-3	86
4			1-Pentene	70	C5H10	000109-67-1	64
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039374.D
Acq On : 19 Dec 2023 22:01
Operator : JC/MD
Sample : 05807-12 5X
Misc : 1.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AZ4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	2.861	6.5	ug/L	60494	1	6.757	466599	50.0