

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039360.D
 Acq On : 19 Dec 2023 16:41
 Operator : JC/MD
 Sample : 05808-10ME
 Misc : 4.90g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B04ME

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\SFAMXLM120523WMA.M

Title : VOC Analysis

Signal : TIC: VX039360.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	62	rVB	82488	139239	13.78%	1.402%
2	1.648	89	92	100	rBV	27399	51247	5.07%	0.516%
3	2.282	190	196	211	rBV	201304	344708	34.11%	3.471%
4	2.575	242	244	246	rBV	394	299	0.03%	0.003%
5	2.709	264	266	271	rBV5	516	848	0.08%	0.009%
6	2.794	275	280	281	rVV4	2790	4466	0.44%	0.045%
7	2.843	281	288	298	rVV	159909	319891	31.66%	3.221%
8	2.941	300	304	315	rVB2	4766	12090	1.20%	0.122%
9	3.081	326	327	329	rBV2	359	238	0.02%	0.002%
10	3.123	331	334	335	rBV2	474	510	0.05%	0.005%
11	3.197	344	346	349	rBV	440	364	0.04%	0.004%
12	3.300	360	363	364	rBV3	399	437	0.04%	0.004%
13	3.379	374	376	379	rVB	268	256	0.03%	0.003%
14	3.416	380	382	390	rVB3	440	874	0.09%	0.009%
15	3.849	450	453	455	rBV	227	207	0.02%	0.002%
16	4.477	548	556	588	rBV	47695	239623	23.71%	2.413%
17	5.062	638	652	670	rBV	122595	394416	39.03%	3.971%
18	5.263	683	685	688	rBV2	237	294	0.03%	0.003%
19	5.440	712	714	715	rVV2	419	265	0.03%	0.003%
20	5.458	715	717	719	rVV2	316	247	0.02%	0.002%
21	5.556	731	733	735	rBV2	222	236	0.02%	0.002%
22	5.757	764	766	770	rBV2	148	234	0.02%	0.002%
23	5.964	789	800	820	rBV2	348871	1010432	100.00%	10.174%
24	6.233	843	844	849	rBV	434	544	0.05%	0.005%
25	6.757	921	930	955	rVV	253488	646851	64.02%	6.513%
26	7.117	983	989	995	rVB4	1697	3437	0.34%	0.035%
27	7.214	999	1005	1006	rBV2	311	504	0.05%	0.005%
28	7.306	1011	1020	1037	rBV	197780	449596	44.50%	4.527%
29	7.482	1047	1049	1052	rVB2	411	397	0.04%	0.004%
30	7.696	1081	1084	1088	rVB2	365	455	0.05%	0.005%
31	7.732	1088	1090	1092	rBV	283	299	0.03%	0.003%
32	7.781	1096	1098	1100	rVB2	215	208	0.02%	0.002%
33	7.952	1125	1126	1128	rBV2	446	445	0.04%	0.004%
34	8.001	1132	1134	1137	rVV2	211	226	0.02%	0.002%
35	8.116	1151	1153	1156	rBV	206	267	0.03%	0.003%
36	8.324	1181	1187	1203	rBV	123363	219411	21.71%	2.209%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039360.D
 Acq On : 19 Dec 2023 16:41
 Operator : JC/MD
 Sample : 05808-10ME
 Misc : 4.90g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B04ME

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	8.525	1218	1220	1223	rBV3	446	500	0.05%	0.005%
38	8.647	1234	1240	1250	rBV	479146	777291	76.93%	7.826%
39	8.952	1285	1290	1304	rBV	86153	144071	14.26%	1.451%
40	9.275	1341	1343	1348	rVB2	609	660	0.07%	0.007%
41	9.397	1356	1363	1377	rBV	281559	553449	54.77%	5.572%
42	9.653	1401	1405	1408	rBV3	427	571	0.06%	0.006%
43	9.720	1411	1416	1419	rVB4	708	989	0.10%	0.010%
44	9.860	1434	1439	1441	rBV2	316	597	0.06%	0.006%
45	9.970	1455	1457	1461	rVB	184	220	0.02%	0.002%
46	10.012	1461	1464	1465	rBV	206	263	0.03%	0.003%
47	10.055	1465	1471	1490	rVV	530375	813017	80.46%	8.186%
48	10.195	1492	1494	1500	rVV5	710	977	0.10%	0.010%
49	10.281	1507	1508	1510	rBV	280	204	0.02%	0.002%
50	10.305	1510	1512	1517	rBV2	536	916	0.09%	0.009%
51	10.646	1566	1568	1571	rBV2	252	328	0.03%	0.003%
52	10.823	1594	1597	1599	rVB2	225	274	0.03%	0.003%
53	10.854	1599	1602	1603	rBV	251	251	0.02%	0.003%
54	10.878	1603	1606	1608	rBV2	197	207	0.02%	0.002%
55	10.939	1614	1616	1618	rBV2	517	464	0.05%	0.005%
56	11.061	1631	1636	1637	rBV2	161	243	0.02%	0.002%
57	11.085	1639	1640	1642	rBV	244	233	0.02%	0.002%
58	11.195	1652	1658	1668	rBV	357888	450591	44.59%	4.537%
59	11.311	1673	1677	1683	rVB2	2175	3128	0.31%	0.031%
60	11.366	1683	1686	1688	rBV	243	249	0.02%	0.003%
61	11.482	1703	1705	1710	rVB3	847	1190	0.12%	0.012%
62	11.707	1739	1742	1746	rBV2	240	398	0.04%	0.004%
63	11.756	1747	1750	1755	rVB3	499	748	0.07%	0.008%
64	11.969	1780	1785	1789	rVV	105699	134456	13.31%	1.354%
65	12.024	1789	1794	1806	rVB2	646076	973455	96.34%	9.801%
66	12.152	1814	1815	1818	rVB2	721	423	0.04%	0.004%
67	12.323	1837	1843	1857	rBV3	593758	966681	95.67%	9.733%
68	12.451	1863	1864	1872	rVB3	327	540	0.05%	0.005%
69	12.762	1910	1915	1919	rVB2	3426	5019	0.50%	0.051%
70	12.896	1935	1937	1941	rVB2	310	304	0.03%	0.003%
71	12.939	1941	1944	1945	rBV	275	294	0.03%	0.003%
72	13.061	1959	1964	1970	rVV3	2731	4673	0.46%	0.047%
73	13.116	1970	1973	1977	rVV3	1346	1390	0.14%	0.014%
74	13.201	1983	1987	1992	rVV3	2030	2788	0.28%	0.028%
75	13.268	1996	1998	2000	rVB2	566	432	0.04%	0.004%
76	13.396	2014	2019	2022	rVB2	353	575	0.06%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039360.D
 Acq On : 19 Dec 2023 16:41
 Operator : JC/MD
 Sample : 05808-10ME
 Misc : 4.90g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B04ME

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\SFAMXLM120523WMA.M
 Title : VOC Analysis

77	13.481	2032	2033	2037	rBV2	195	280	0.03%	0.003%
78	13.585	2045	2050	2067	rBV	558505	706892	69.96%	7.117%
79	13.774	2079	2081	2087	rVB	844	1167	0.12%	0.012%
80	13.957	2106	2111	2121	rBV	178805	233026	23.06%	2.346%
81	14.128	2136	2139	2144	rVB2	2407	3380	0.33%	0.034%
82	14.371	2177	2179	2180	rBV2	270	251	0.02%	0.003%
83	14.390	2180	2182	2183	rVV2	409	283	0.03%	0.003%
84	14.627	2218	2221	2225	rVB2	405	402	0.04%	0.004%
85	14.670	2225	2228	2229	rBV	224	243	0.02%	0.002%
86	14.780	2239	2246	2252	rBV2	23984	41160	4.07%	0.414%
87	14.926	2267	2270	2271	rBV3	298	276	0.03%	0.003%
88	14.963	2274	2276	2277	rBV	369	251	0.02%	0.003%
89	15.097	2296	2298	2300	rBV2	267	214	0.02%	0.002%
90	15.243	2317	2322	2330	rBV	167488	241246	23.88%	2.429%
91	15.390	2341	2346	2349	rBV3	766	1235	0.12%	0.012%
92	15.457	2354	2357	2359	rBV2	343	445	0.04%	0.004%
93	15.536	2368	2370	2373	rBV2	265	268	0.03%	0.003%
94	15.737	2401	2403	2404	rBV2	329	267	0.03%	0.003%
95	15.853	2420	2422	2424	rBV2	336	226	0.02%	0.002%
96	16.078	2458	2459	2461	rBV	302	201	0.02%	0.002%
97	16.304	2494	2496	2500	rVB2	352	244	0.02%	0.002%
98	16.505	2522	2529	2535	rVB6	6592	12234	1.21%	0.123%
99	16.615	2544	2547	2548	rBV	424	443	0.04%	0.004%
100	16.688	2558	2559	2561	rVB2	390	227	0.02%	0.002%

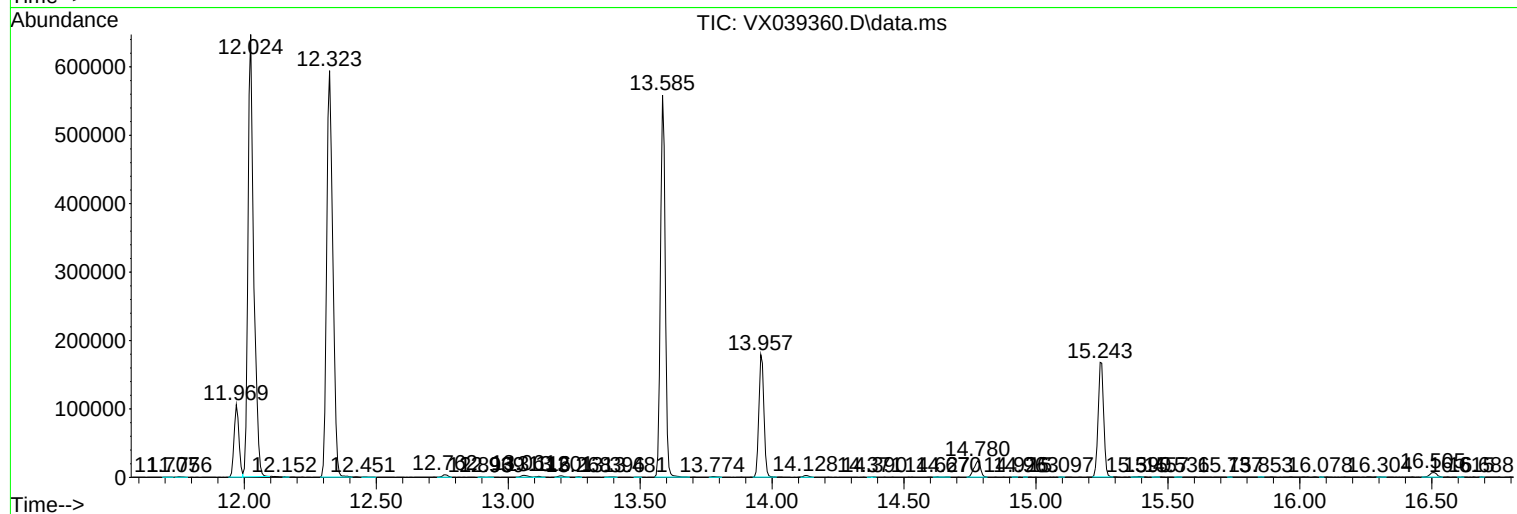
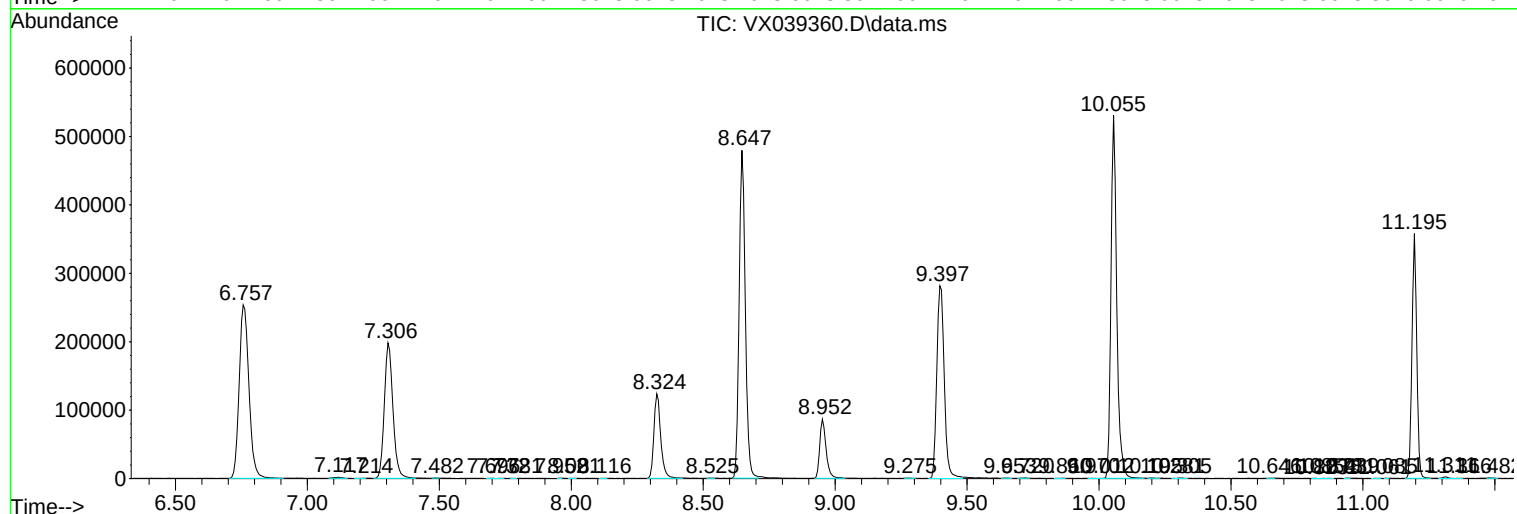
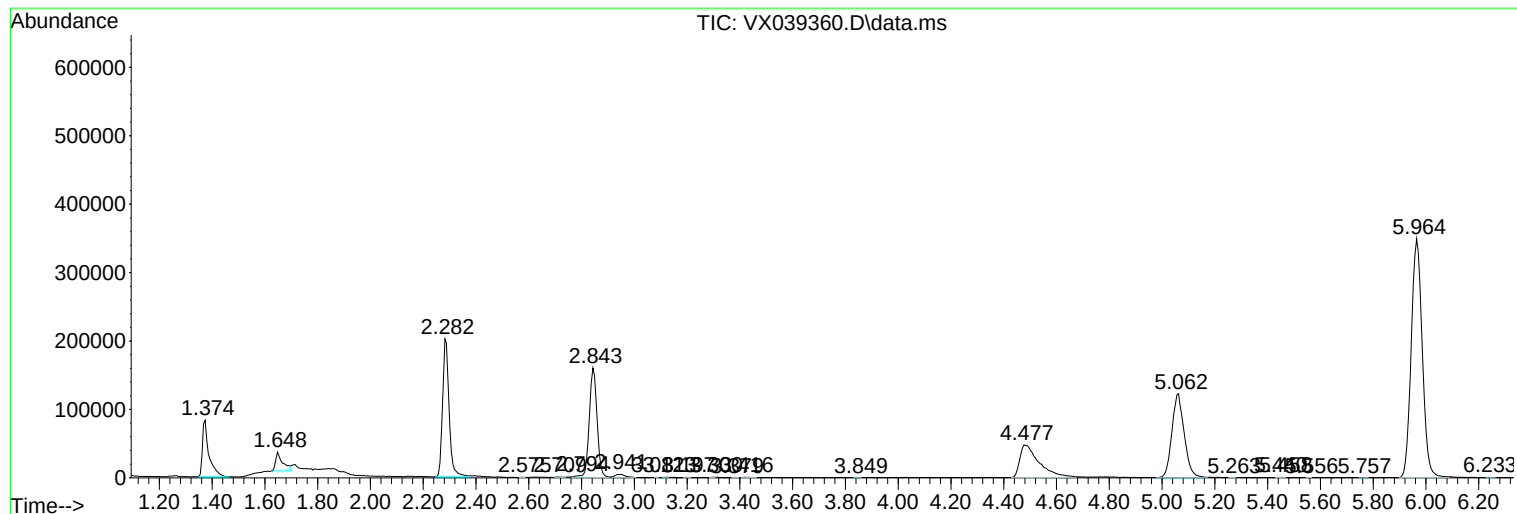
Sum of corrected areas: 9931981

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039360.D
Acq On : 19 Dec 2023 16:41
Operator : JC/MD
Sample : 05808-10ME
Misc : 4.90g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B04ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039360.D
Acq On : 19 Dec 2023 16:41
Operator : JC/MD
Sample : 05808-10ME
Misc : 4.90g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B04ME

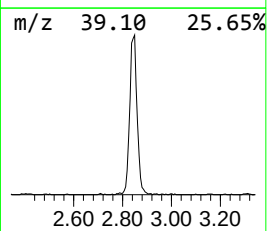
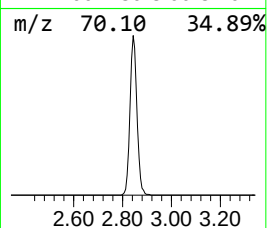
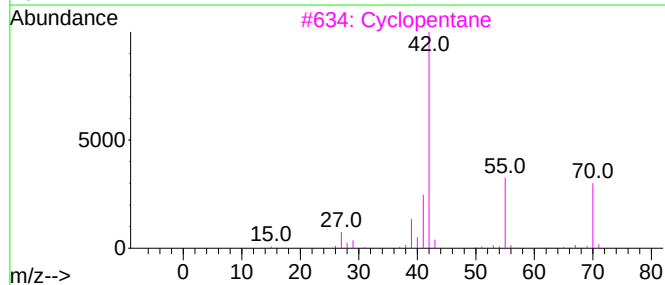
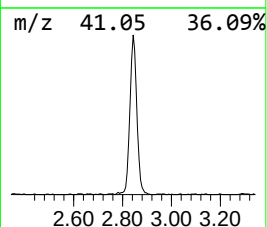
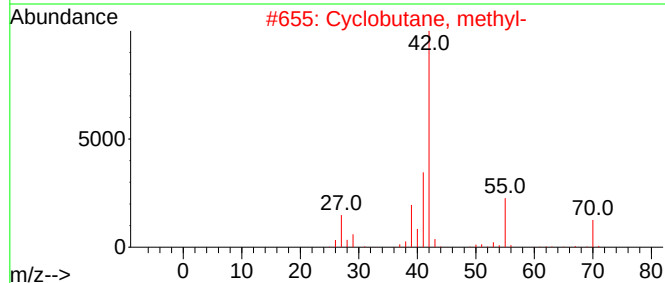
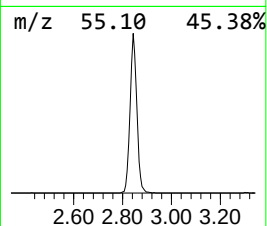
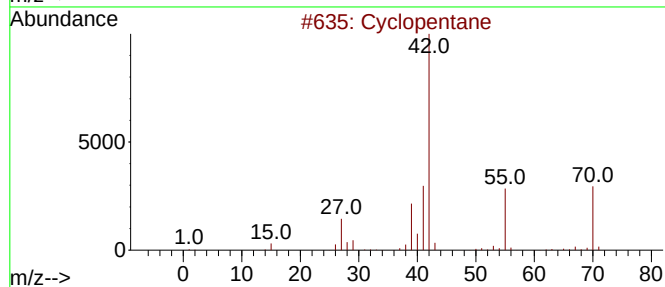
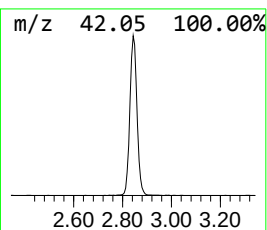
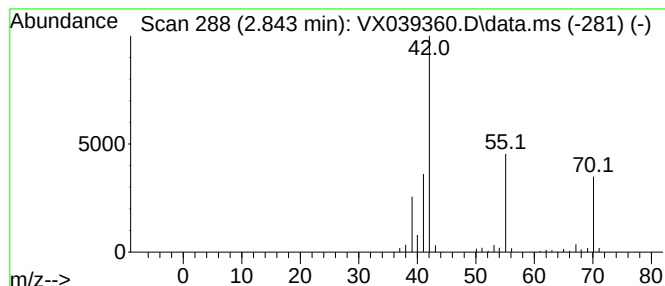
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic2.843 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.843	24.73 ug/L	319891	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	80
2			Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3			Cyclopentane	70	C5H10	000287-92-3	78
4			Cyclopentane	70	C5H10	000287-92-3	56
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039360.D
Acq On : 19 Dec 2023 16:41
Operator : JC/MD
Sample : 05808-10ME
Misc : 4.90g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B04ME

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...	2.843	24.7	ug/L	319891	1	6.757	646851	50.0