

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
 Data File : VX044762.D
 Acq On : 29 Jan 2025 12:11
 Operator : JC/MD
 Sample : Q1190-15ME
 Misc : 11.38g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44T4ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
 Title : VOC Analysis

Signal : TIC: VX044762.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	27	rBV	9294	10630	0.91%	0.125%
2	1.368	43	46	50	rBV	79317	91389	7.80%	1.072%
3	1.648	89	92	96	rBV	13359	17906	1.53%	0.210%
4	2.276	190	195	212	rBV	224412	380046	32.42%	4.456%
5	2.721	263	268	274	rVB2	2301	4369	0.37%	0.051%
6	2.837	284	287	295	rVB4	2598	4866	0.42%	0.057%
7	2.947	300	305	314	rVB2	3956	9659	0.82%	0.113%
8	3.075	323	326	330	rBV3	625	685	0.06%	0.008%
9	3.190	343	345	347	rVV2	443	289	0.02%	0.003%
10	3.227	350	351	353	rBV	513	332	0.03%	0.004%
11	3.410	379	381	382	rBV	1404	1131	0.10%	0.013%
12	3.514	396	398	400	rBV	405	350	0.03%	0.004%
13	3.581	407	409	412	rVB	580	515	0.04%	0.006%
14	3.617	412	415	416	rBV	356	382	0.03%	0.004%
15	3.806	444	446	450	rBV3	253	359	0.03%	0.004%
16	3.904	461	462	466	rBV2	361	415	0.04%	0.005%
17	3.934	466	467	470	rVV2	262	285	0.02%	0.003%
18	3.965	470	472	474	rVV2	505	335	0.03%	0.004%
19	3.989	474	476	480	rVV2	473	757	0.06%	0.009%
20	4.038	482	484	487	rVV3	365	502	0.04%	0.006%
21	4.068	487	489	490	rVB	464	259	0.02%	0.003%
22	4.093	492	493	495	rVB	480	346	0.03%	0.004%
23	4.117	495	497	500	rBV2	372	487	0.04%	0.006%
24	4.148	500	502	503	rBV	347	279	0.02%	0.003%
25	4.221	511	514	515	rBV	339	367	0.03%	0.004%
26	4.410	541	545	547	rBV3	388	557	0.05%	0.007%
27	4.434	547	549	550	rBV2	381	332	0.03%	0.004%
28	4.489	550	558	580	rBV2	48628	199306	17.00%	2.337%
29	4.843	615	616	617	rBV	659	300	0.03%	0.004%
30	5.050	638	650	667	rBV	141820	448715	38.28%	5.262%
31	5.233	679	680	683	rVB2	530	347	0.03%	0.004%
32	5.312	691	693	695	rBV	433	567	0.05%	0.007%
33	5.531	727	729	730	rBV	524	337	0.03%	0.004%
34	5.666	749	751	754	rVB2	449	558	0.05%	0.007%
35	5.702	754	757	759	rBV2	559	590	0.05%	0.007%
36	5.727	759	761	765	rVV2	425	425	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
 Data File : VX044762.D
 Acq On : 29 Jan 2025 12:11
 Operator : JC/MD
 Sample : Q1190-15ME
 Misc : 11.38g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44T4ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
 Title : VOC Analysis

37	5.830	777	778	780	rVB2	533	280	0.02%	0.003%
38	5.958	788	799	820	rBV2	410107	1172286	100.00%	13.746%
39	6.239	843	845	848	rVB2	699	637	0.05%	0.007%
40	6.586	900	902	904	rBV2	915	836	0.07%	0.010%
41	6.757	920	930	945	rBV	256861	649778	55.43%	7.619%
42	7.037	975	976	980	rBV3	427	304	0.03%	0.004%
43	7.123	983	990	1000	rVV2	19087	44995	3.84%	0.528%
44	7.214	1003	1005	1006	rBV	561	397	0.03%	0.005%
45	7.306	1011	1020	1041	rBV	235395	537784	45.87%	6.306%
46	7.592	1065	1067	1068	rBV2	314	311	0.03%	0.004%
47	7.714	1085	1087	1089	rBV2	368	381	0.03%	0.004%
48	7.769	1094	1096	1099	rVB3	473	339	0.03%	0.004%
49	7.866	1110	1112	1116	rVB3	547	679	0.06%	0.008%
50	7.897	1116	1117	1118	rBV	568	279	0.02%	0.003%
51	7.958	1123	1127	1128	rBV2	662	698	0.06%	0.008%
52	8.013	1134	1136	1140	rVB3	547	485	0.04%	0.006%
53	8.269	1175	1178	1181	rBV2	578	620	0.05%	0.007%
54	8.324	1181	1187	1207	rVV	166433	288205	24.58%	3.379%
55	8.537	1221	1222	1225	rBV	477	284	0.02%	0.003%
56	8.598	1227	1232	1233	rVV3	1567	2156	0.18%	0.025%
57	8.647	1234	1240	1265	rVB	558172	961029	81.98%	11.269%
58	8.909	1279	1283	1285	rBV4	2458	3692	0.31%	0.043%
59	8.952	1285	1290	1303	rVB	110815	184445	15.73%	2.163%
60	9.177	1326	1327	1329	rBV2	430	298	0.03%	0.003%
61	9.238	1333	1337	1339	rVB3	681	845	0.07%	0.010%
62	9.275	1339	1343	1348	rBV2	5407	9056	0.77%	0.106%
63	9.391	1357	1362	1385	rBV	218472	407688	34.78%	4.781%
64	9.610	1396	1398	1403	rVB3	1884	2051	0.17%	0.024%
65	9.708	1411	1414	1417	rVB3	1703	2379	0.20%	0.028%
66	9.823	1429	1433	1440	rBB4	964	1474	0.13%	0.017%
67	9.939	1450	1452	1454	rBV2	398	331	0.03%	0.004%
68	9.994	1456	1461	1462	rBV3	671	723	0.06%	0.008%
69	10.049	1465	1470	1487	rVV	506182	761790	64.98%	8.933%
70	10.275	1503	1507	1508	rBV4	1008	1296	0.11%	0.015%
71	10.305	1508	1512	1517	rVV3	4913	8176	0.70%	0.096%
72	10.360	1517	1521	1527	rVB2	3990	4982	0.42%	0.058%
73	10.561	1549	1554	1555	rBV2	1106	1696	0.14%	0.020%
74	10.646	1564	1568	1576	rVB5	2019	4109	0.35%	0.048%
75	10.750	1581	1585	1587	rBV4	705	990	0.08%	0.012%
76	10.823	1595	1597	1598	rBV	575	440	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
 Data File : VX044762.D
 Acq On : 29 Jan 2025 12:11
 Operator : JC/MD
 Sample : Q1190-15ME
 Misc : 11.38g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44T4ME

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\SFAMXML012825WMA.M
 Title : VOC Analysis

77	10.854	1598	1602	1605	rVV6	1347	2152	0.18%	0.025%
78	10.939	1614	1616	1621	rVB4	849	1134	0.10%	0.013%
79	11.189	1652	1657	1666	rBV	386764	525312	44.81%	6.160%
80	11.384	1685	1689	1693	rBV6	1921	3378	0.29%	0.040%
81	11.476	1701	1704	1709	rVB3	8422	10588	0.90%	0.124%
82	11.713	1740	1743	1746	rBV2	4879	4979	0.42%	0.058%
83	11.756	1746	1750	1761	rVV	74356	115365	9.84%	1.353%
84	12.018	1788	1793	1804	rBV	524778	693612	59.17%	8.133%
85	12.317	1837	1842	1850	rBV	603659	774235	66.04%	9.079%
86	12.427	1856	1860	1864	rVB	11489	13460	1.15%	0.158%
87	12.902	1931	1938	1947	rBV	28503	51355	4.38%	0.602%
88	13.268	1994	1998	2001	rBV	13209	15112	1.29%	0.177%
89	13.353	2008	2012	2014	rBV3	1011	1363	0.12%	0.016%
90	13.384	2014	2017	2020	rBV3	4693	6285	0.54%	0.074%
91	13.591	2050	2051	2054	rBV2	941	724	0.06%	0.008%
92	13.780	2078	2082	2085	rBV4	2962	4985	0.43%	0.058%
93	13.841	2089	2092	2096	rVB2	5269	6468	0.55%	0.076%
94	14.036	2121	2124	2128	rBV	11729	12906	1.10%	0.151%
95	14.438	2186	2190	2198	rVB	15532	22244	1.90%	0.261%
96	14.609	2216	2218	2222	rBV4	2163	2730	0.23%	0.032%
97	14.755	2239	2242	2245	rBV	7245	8518	0.73%	0.100%
98	15.389	2342	2346	2350	rBV2	4012	7779	0.66%	0.091%
99	15.493	2359	2363	2368	rBV4	3087	4836	0.41%	0.057%
100	16.237	2483	2485	2486	rBV2	565	388	0.03%	0.005%

Sum of corrected areas: 8528106

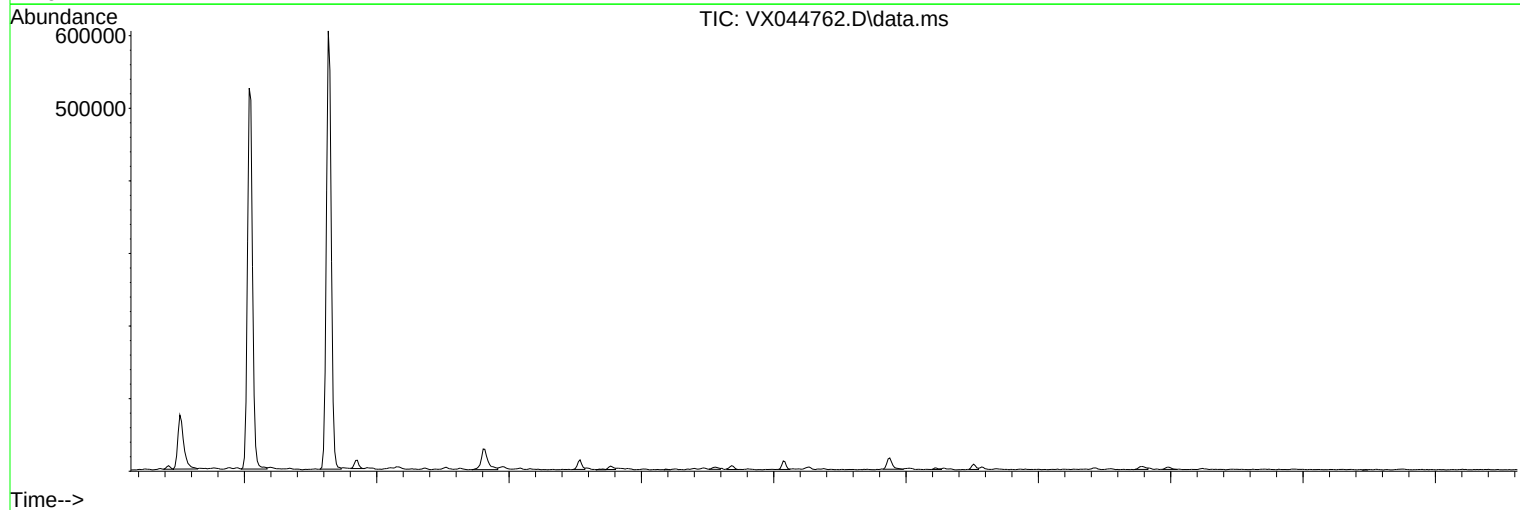
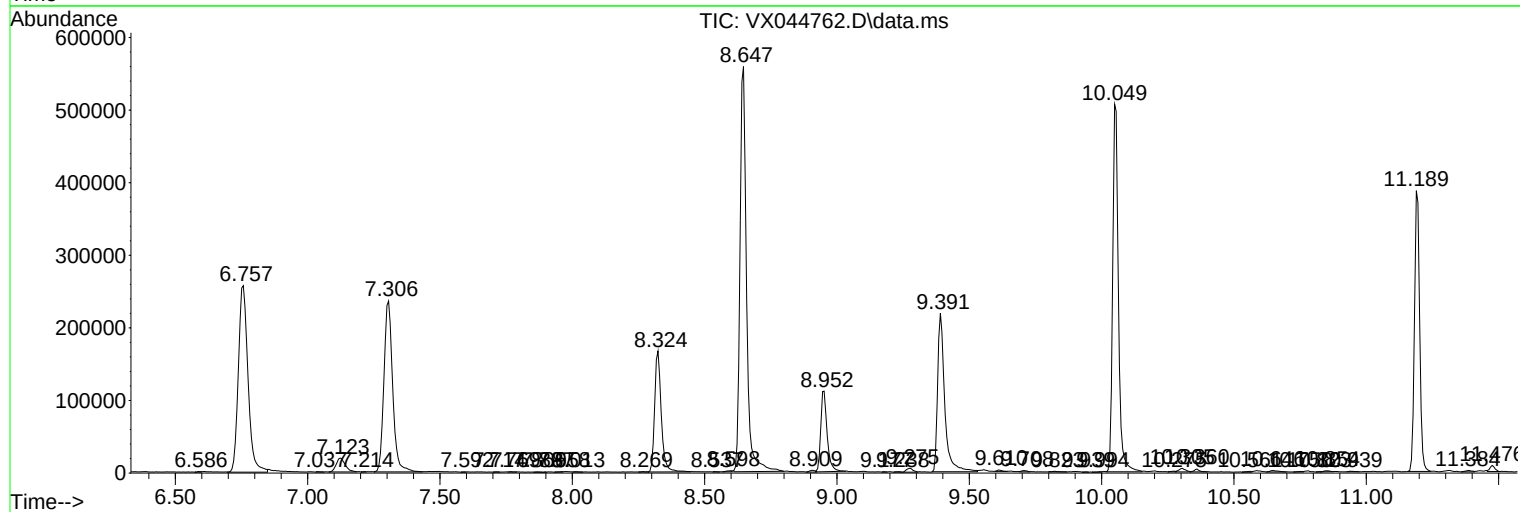
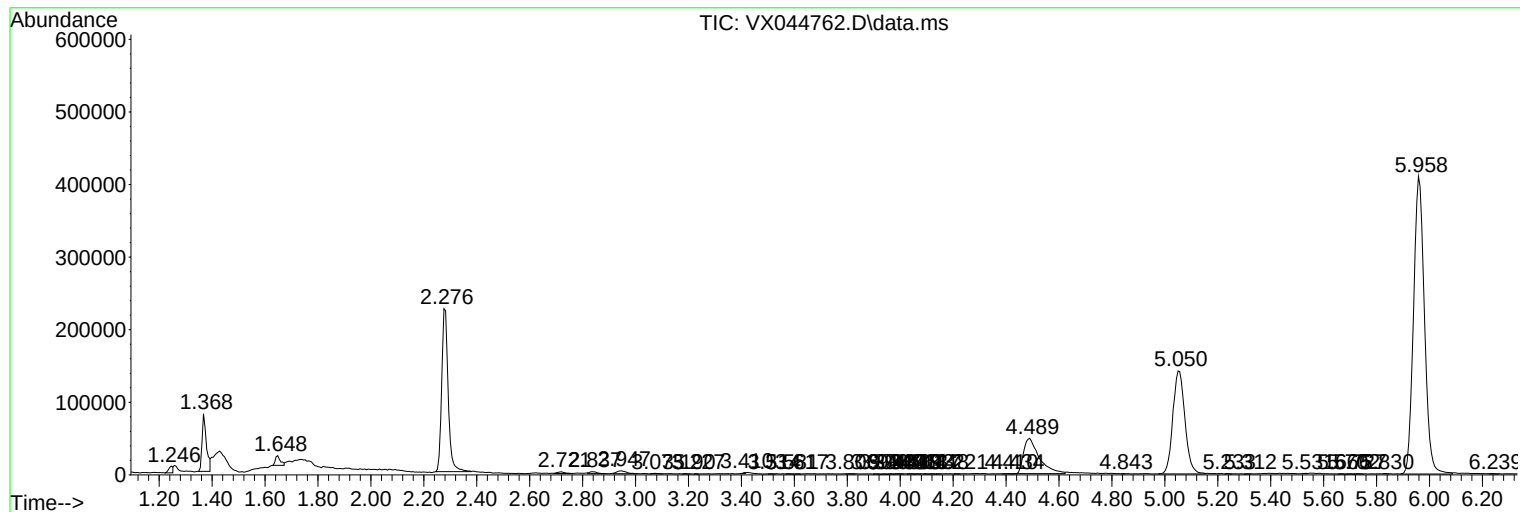
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044762.D
Acq On : 29 Jan 2025 12:11
Operator : JC/MD
Sample : Q1190-15ME
Misc : 11.38g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXM012825WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044762.D
Acq On : 29 Jan 2025 12:11
Operator : JC/MD
Sample : Q1190-15ME
Misc : 11.38g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

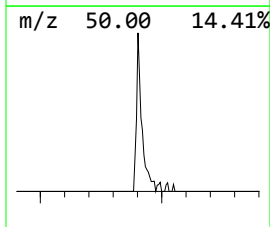
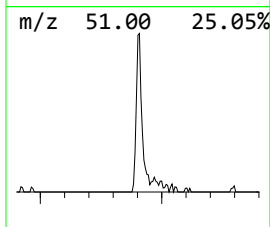
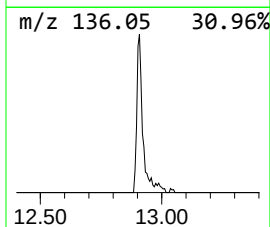
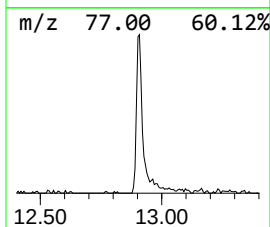
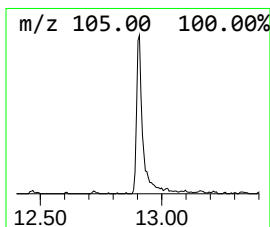
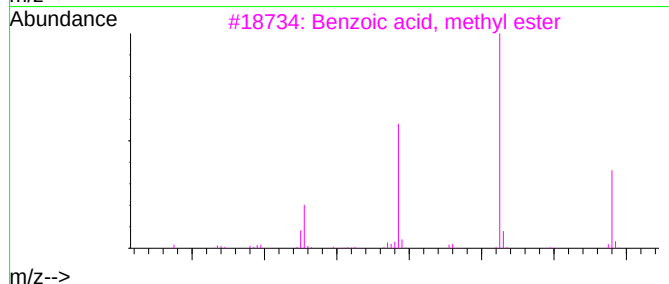
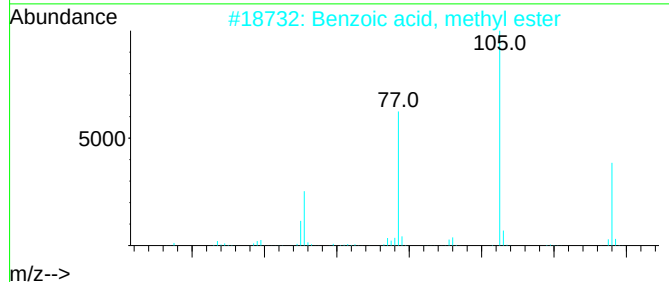
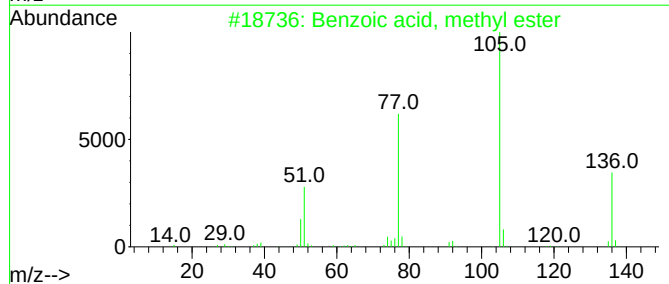
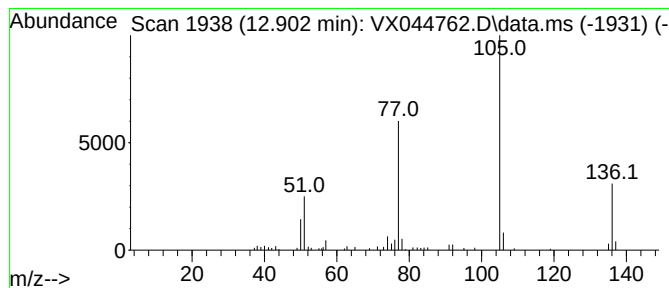
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.902	3.70 ug/L	51355	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, methyl ester	136	C8H8O2	000093-58-3	97
2	Benzoic acid, methyl ester	136	C8H8O2	000093-58-3	95
3	Benzoic acid, methyl ester	136	C8H8O2	000093-58-3	94
4	Benzoic acid, methyl ester	136	C8H8O2	000093-58-3	91
5	Benzoic acid, hydrazide	136	C7H8N2O	000613-94-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044762.D
Acq On : 29 Jan 2025 12:11
Operator : JC/MD
Sample : Q1190-15ME
Misc : 11.38g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.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
Benzoic acid, m...	12.902	3.7	ug/L	51355	3	12.024	693612	50.0