

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
 Data File : VX029649.D
 Acq On : 21 Jun 2022 08:28
 Operator : JC/MD
 Sample : N3354-12
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-56

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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\82X061822W.M
 Title : SW846 8260

Signal : TIC: VX029649.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	23	30	39	rBV	33665	83926	6.23%	0.981%
2	2.568	230	243	258	rBV3	4672	19384	1.44%	0.227%
3	2.782	270	278	285	rBV2	12680	27841	2.07%	0.325%
4	4.215	504	513	521	rBV4	5132	15411	1.14%	0.180%
5	5.391	695	706	716	rBV	151101	443311	32.89%	5.180%
6	5.556	723	733	758	rVB2	282252	816866	60.61%	9.546%
7	5.958	788	799	812	rBV	159505	425377	31.56%	4.971%
8	6.257	831	848	860	rVB3	20815	65842	4.89%	0.769%
9	6.763	922	931	944	rBV	426377	1023503	75.94%	11.960%
10	7.982	1124	1131	1142	rVB	23003	47179	3.50%	0.551%
11	8.110	1144	1152	1162	rBV2	50041	105578	7.83%	1.234%
12	8.653	1230	1241	1251	rBV	856855	1347779	100.00%	15.750%
13	8.958	1286	1291	1299	rVB	47940	77035	5.72%	0.900%
14	9.049	1299	1306	1312	rBV2	42696	65826	4.88%	0.769%
15	9.165	1320	1325	1334	rVB	11795	19390	1.44%	0.227%
16	10.055	1465	1471	1477	rBV	854356	1134708	84.19%	13.260%
17	10.280	1504	1508	1517	rVB6	6518	13754	1.02%	0.161%
18	10.963	1616	1620	1625	rBV	11876	16873	1.25%	0.197%
19	11.079	1634	1639	1646	rBV	625753	830304	61.61%	9.703%
20	11.171	1650	1654	1661	rVB2	15904	24102	1.79%	0.282%
21	11.305	1672	1676	1683	rVB	19236	24055	1.78%	0.281%
22	11.866	1761	1768	1778	rVB2	20089	30440	2.26%	0.356%
23	12.024	1788	1794	1806	rBV	829137	1040788	77.22%	12.162%
24	12.244	1823	1830	1837	rBV	76037	102956	7.64%	1.203%
25	12.317	1837	1842	1848	rVB2	10850	16128	1.20%	0.188%
26	12.469	1862	1867	1872	rBV2	13952	19178	1.42%	0.224%
27	12.615	1881	1891	1894	rBV3	13963	22494	1.67%	0.263%
28	12.701	1901	1905	1911	rVV2	30763	49051	3.64%	0.573%
29	12.841	1919	1928	1934	rVB2	23564	37224	2.76%	0.435%
30	12.920	1934	1941	1947	rBV	33849	52945	3.93%	0.619%
31	13.292	1998	2002	2007	rVB2	20533	27042	2.01%	0.316%
32	13.426	2021	2024	2030	rVB2	10326	14123	1.05%	0.165%
33	13.579	2045	2049	2053	rVV3	20022	30124	2.24%	0.352%
34	13.621	2053	2056	2058	rVV	13355	17937	1.33%	0.210%
35	13.853	2089	2094	2099	rBV2	32082	40231	2.98%	0.470%
36	13.926	2103	2106	2111	rVB3	12522	17269	1.28%	0.202%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029649.D
Acq On : 21 Jun 2022 08:28
Operator : JC/MD
Sample : N3354-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-56

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % 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\82X061822W.M
Title : SW846 8260

37	14.225	2149	2155	2163	rVB6	6815	17451	1.29%	0.204%
38	14.322	2163	2171	2174	rBV	36470	48723	3.62%	0.569%
39	14.371	2176	2179	2184	rVB5	12774	18240	1.35%	0.213%
40	14.481	2192	2197	2201	rBV2	11188	16175	1.20%	0.189%
41	14.615	2211	2219	2220	rBV5	10431	20210	1.50%	0.236%
42	14.670	2225	2228	2233	rVV4	10498	14775	1.10%	0.173%
43	14.786	2241	2247	2252	rBV3	39938	62830	4.66%	0.734%
44	15.115	2295	2301	2308	rBV	43004	66873	4.96%	0.781%
45	15.182	2308	2312	2318	rVV2	25012	39282	2.91%	0.459%
46	15.255	2318	2324	2331	rVB6	9033	15017	1.11%	0.175%
47	15.731	2396	2402	2409	rBV4	8652	18412	1.37%	0.215%
48	15.810	2409	2415	2419	rBV3	17047	27142	2.01%	0.317%
49	15.993	2438	2445	2457	rVB2	16255	31117	2.31%	0.364%
50	16.328	2490	2500	2505	rVB4	6447	15270	1.13%	0.178%

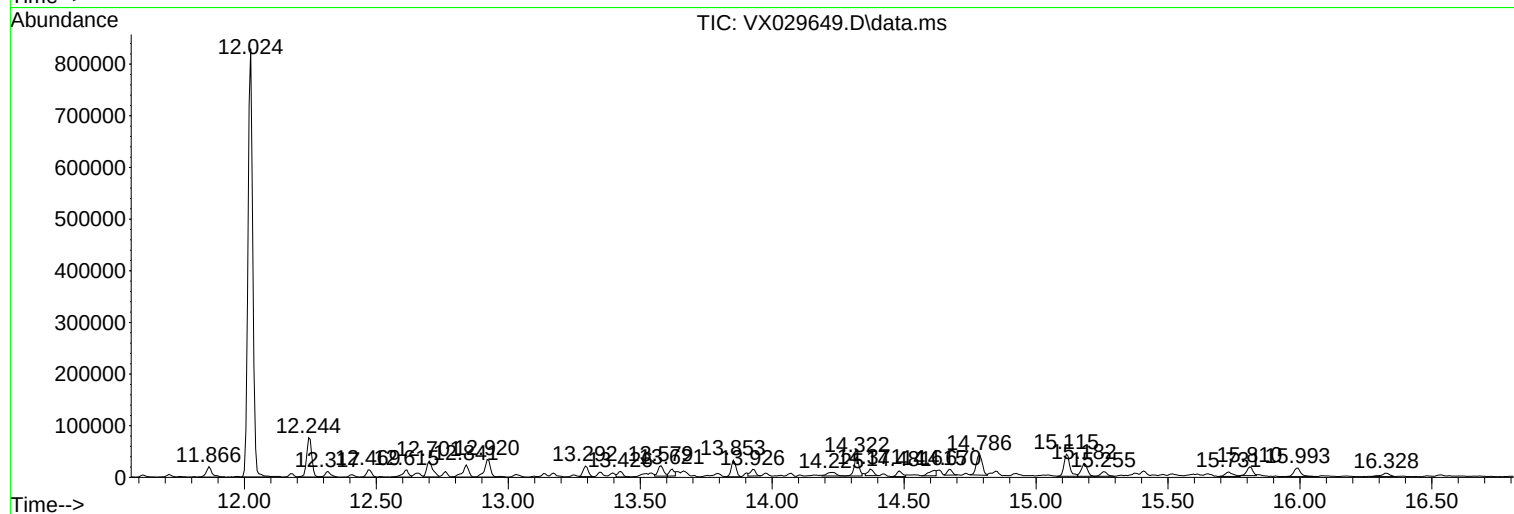
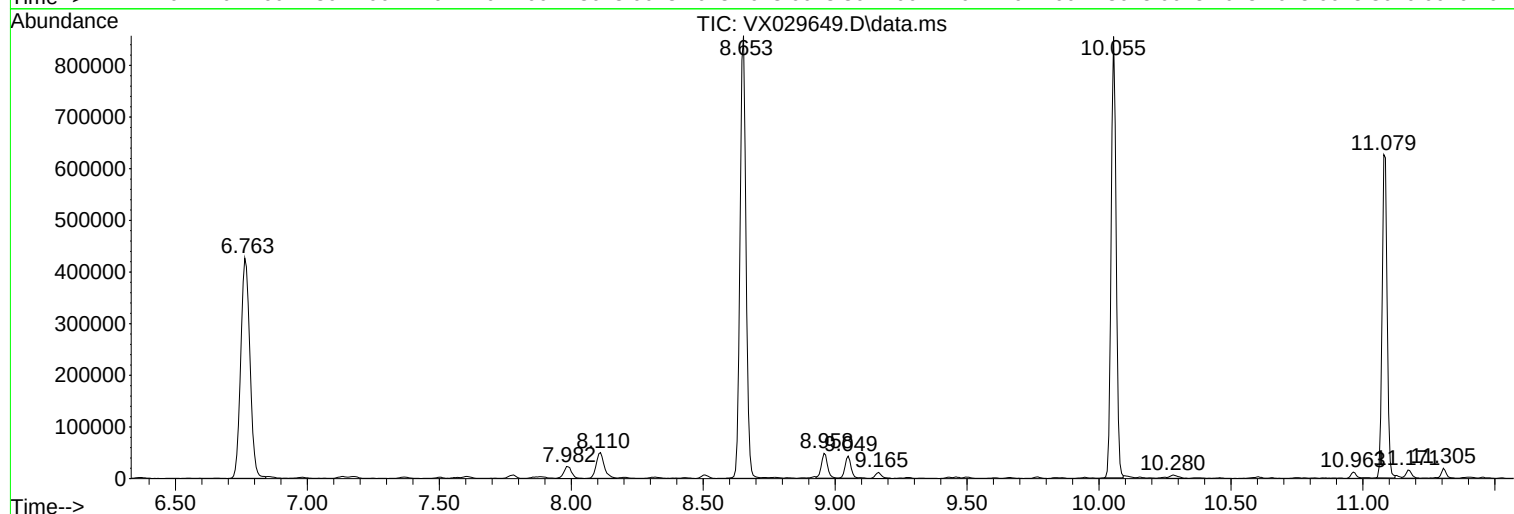
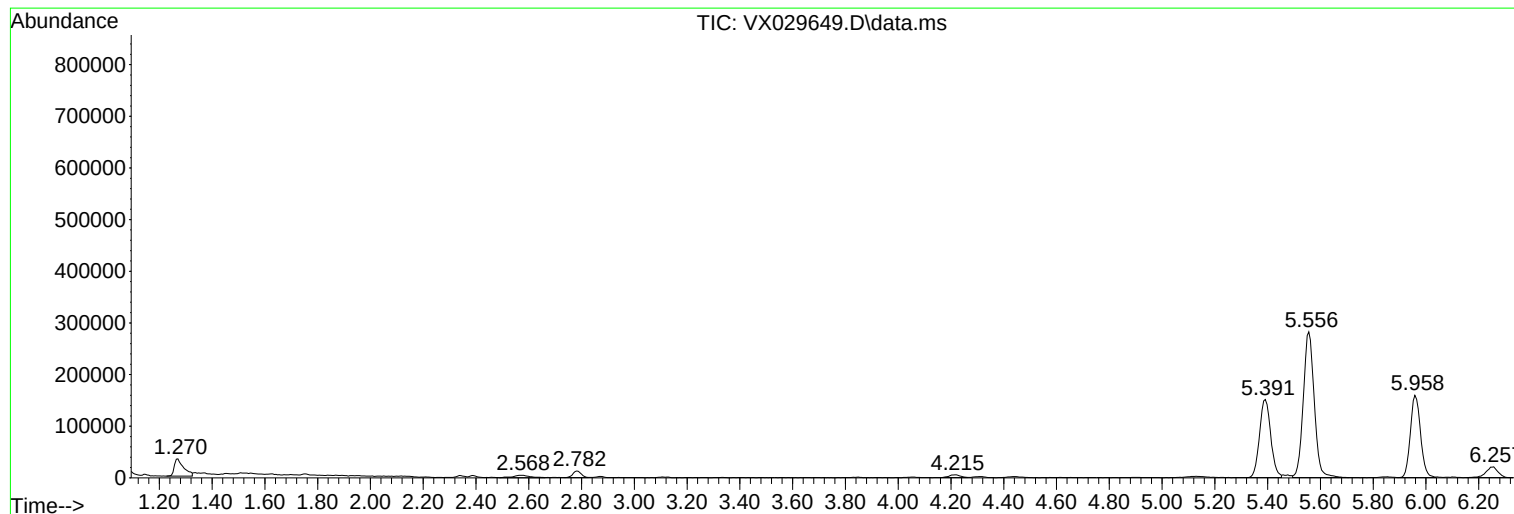
Sum of corrected areas: 8557491

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029649.D
Acq On : 21 Jun 2022 08:28
Operator : JC/MD
Sample : N3354-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-56

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029649.D
Acq On : 21 Jun 2022 08:28
Operator : JC/MD
Sample : N3354-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-56

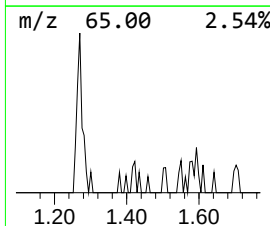
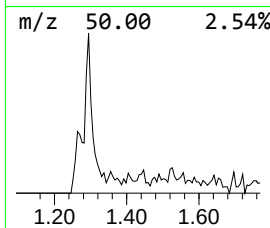
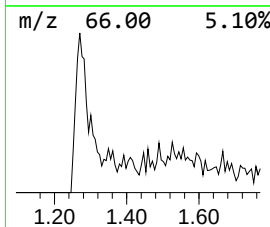
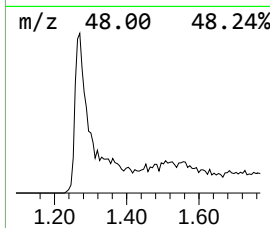
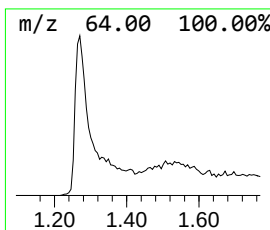
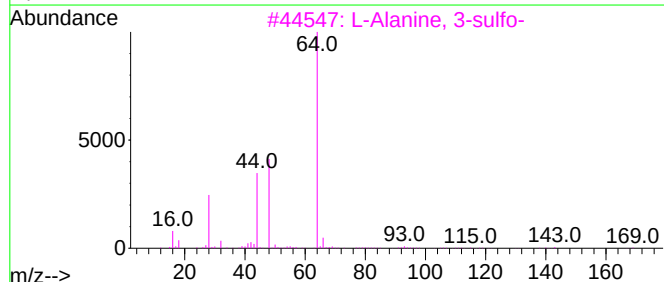
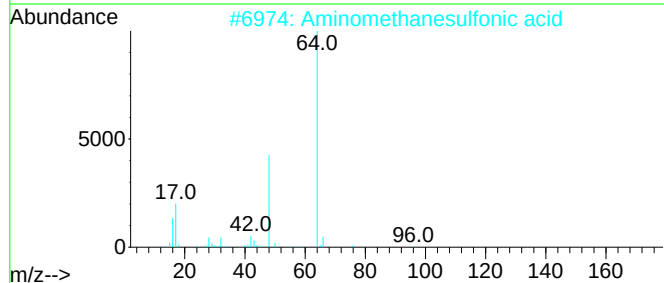
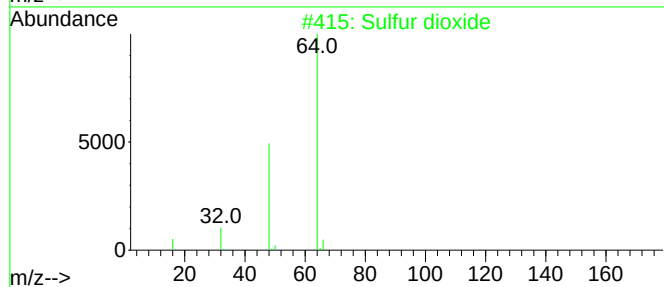
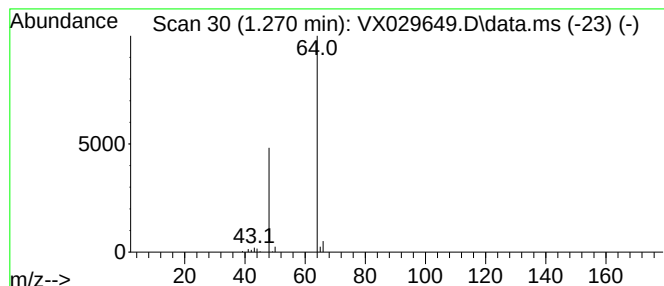
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	5.14 ug/l	83926	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029649.D
Acq On : 21 Jun 2022 08:28
Operator : JC/MD
Sample : N3354-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-56

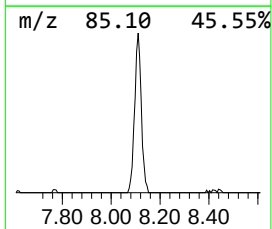
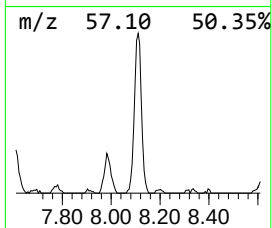
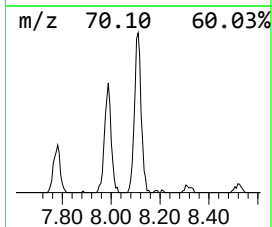
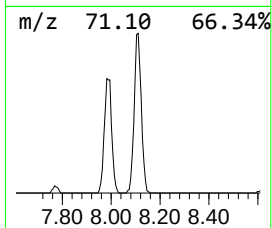
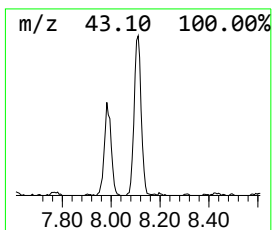
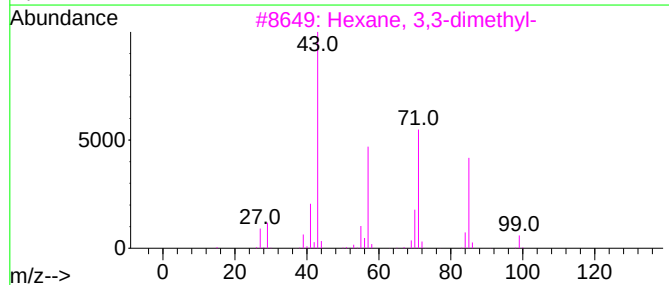
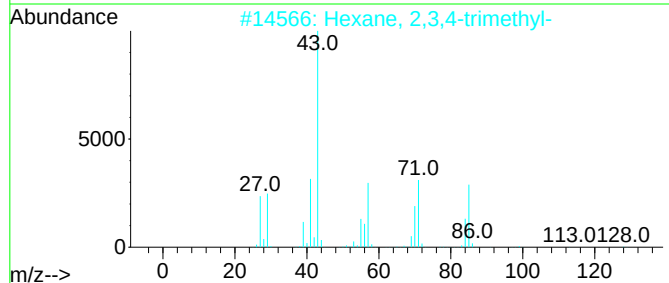
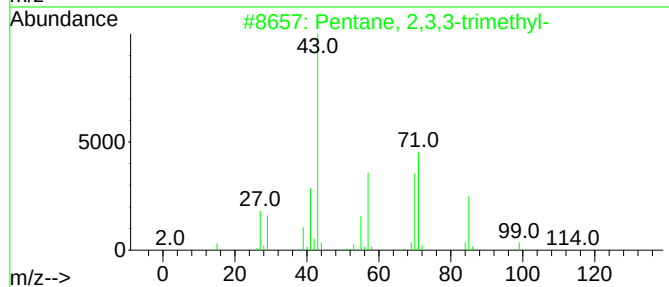
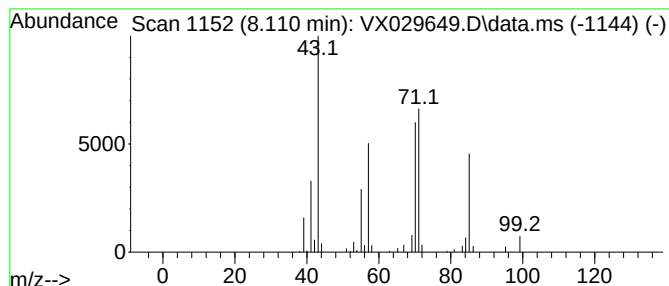
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	5.16 ug/l	105578	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029649.D
Acq On : 21 Jun 2022 08:28
Operator : JC/MD
Sample : N3354-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-56

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.270	5.1	ug/l	83926	1	5.556	816866	50.0
Pentane, 2,3,3-...	8.110	5.2	ug/l	105578	2	6.763	1023500	50.0