

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042469.D
 Acq On : 23 Jul 2024 14:10
 Operator : JC/MD
 Sample : P3263-18ME
 Misc : 5.56g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CK8ME

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\SFAMXML070324WMA.M

Title : VOC Analysis

Signal : TIC: VX042469.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	21	25	27	rBV	37694	43383	7.09%	0.828%
2	1.368	43	46	69	rVB	17828	61055	9.98%	1.166%
3	2.276	189	195	210	rBV	77569	141170	23.08%	2.695%
4	2.727	262	269	283	rBV	23952	56657	9.26%	1.082%
5	2.947	300	305	311	rVB2	2180	4980	0.81%	0.095%
6	3.343	364	370	371	rBV2	124	163	0.03%	0.003%
7	3.410	379	381	383	rVV	209	213	0.03%	0.004%
8	3.556	403	405	407	rBV2	153	172	0.03%	0.003%
9	3.587	408	410	411	rVV	242	186	0.03%	0.004%
10	3.605	411	413	417	rVV3	336	554	0.09%	0.011%
11	3.642	417	419	423	rVB	216	253	0.04%	0.005%
12	3.764	437	439	442	rBV	177	150	0.02%	0.003%
13	3.843	446	452	463	rBV3	1438	4046	0.66%	0.077%
14	3.983	469	475	477	rBV2	209	386	0.06%	0.007%
15	4.233	513	516	519	rBV2	92	161	0.03%	0.003%
16	4.331	530	532	535	rVB	212	161	0.03%	0.003%
17	4.501	551	560	579	rBV	41288	147051	24.05%	2.808%
18	5.062	641	652	666	rBV	76086	234731	38.38%	4.482%
19	5.397	699	707	714	rBV4	1003	2671	0.44%	0.051%
20	5.452	714	716	717	rVB	249	149	0.02%	0.003%
21	5.556	728	733	744	rVB4	1280	3677	0.60%	0.070%
22	5.721	759	760	763	rBV2	194	215	0.04%	0.004%
23	5.812	770	775	776	rBV2	123	172	0.03%	0.003%
24	5.964	790	800	817	rBV2	211092	611539	100.00%	11.677%
25	6.245	844	846	850	rVB2	193	213	0.03%	0.004%
26	6.294	850	854	857	rBV2	111	208	0.03%	0.004%
27	6.385	864	869	871	rBV2	395	495	0.08%	0.009%
28	6.537	890	894	896	rBV2	164	213	0.03%	0.004%
29	6.678	913	917	918	rBV2	286	349	0.06%	0.007%
30	6.763	922	931	947	rBV	210335	510737	83.52%	9.752%
31	7.117	984	989	995	rVV3	1102	2333	0.38%	0.045%
32	7.220	1002	1006	1013	rBV3	484	986	0.16%	0.019%
33	7.312	1013	1021	1043	rBV	125926	279039	45.63%	5.328%
34	7.513	1052	1054	1056	rVB2	273	211	0.03%	0.004%
35	7.617	1069	1071	1075	rBV2	164	173	0.03%	0.003%
36	7.684	1080	1082	1086	rVB	321	275	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042469.D
 Acq On : 23 Jul 2024 14:10
 Operator : JC/MD
 Sample : P3263-18ME
 Misc : 5.56g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CK8ME

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\SFAMXML070324WMA.M
 Title : VOC Analysis

37	7.958	1123	1127	1128	rBV2	840	871	0.14%	0.017%
38	8.001	1133	1134	1135	rVB	384	152	0.02%	0.003%
39	8.159	1156	1160	1166	rBV3	190	424	0.07%	0.008%
40	8.257	1172	1176	1177	rBV2	155	195	0.03%	0.004%
41	8.330	1182	1188	1205	rVV	68468	117184	19.16%	2.237%
42	8.464	1209	1210	1213	rVB2	327	196	0.03%	0.004%
43	8.525	1215	1220	1224	rBV5	665	1507	0.25%	0.029%
44	8.647	1234	1240	1250	rBV	293184	494817	80.91%	9.448%
45	8.915	1279	1284	1286	rBV5	589	901	0.15%	0.017%
46	8.958	1286	1291	1302	rVV	45800	75135	12.29%	1.435%
47	9.275	1339	1343	1349	rBV2	5967	9318	1.52%	0.178%
48	9.397	1357	1363	1383	rBV	163823	336061	54.95%	6.417%
49	9.714	1411	1415	1423	rBV4	905	1622	0.27%	0.031%
50	9.823	1431	1433	1437	rVB2	238	268	0.04%	0.005%
51	9.854	1437	1438	1441	rBV2	206	168	0.03%	0.003%
52	9.982	1455	1459	1460	rBV2	131	181	0.03%	0.003%
53	9.994	1460	1461	1465	rBV	212	156	0.03%	0.003%
54	10.055	1465	1471	1482	rBV	432247	593515	97.05%	11.332%
55	10.311	1509	1513	1514	rBV3	775	972	0.16%	0.019%
56	10.439	1532	1534	1536	rBV	231	205	0.03%	0.004%
57	10.482	1540	1541	1546	rBV2	131	161	0.03%	0.003%
58	10.555	1551	1553	1556	rBV2	182	162	0.03%	0.003%
59	10.646	1566	1568	1571	rBV2	377	489	0.08%	0.009%
60	10.671	1571	1572	1574	rVB	291	162	0.03%	0.003%
61	10.878	1602	1606	1615	rVB4	748	1596	0.26%	0.030%
62	10.970	1617	1621	1631	rBV4	1883	3154	0.52%	0.060%
63	11.067	1634	1637	1639	rVB2	423	383	0.06%	0.007%
64	11.098	1639	1642	1647	rBV2	366	564	0.09%	0.011%
65	11.140	1647	1649	1652	rBV	139	179	0.03%	0.003%
66	11.195	1652	1658	1671	rBV	254981	339818	55.57%	6.488%
67	11.439	1694	1698	1701	rVV3	1538	2128	0.35%	0.041%
68	11.482	1702	1705	1716	rVV3	2411	3965	0.65%	0.076%
69	11.579	1719	1721	1725	rVV2	154	221	0.04%	0.004%
70	11.622	1727	1728	1731	rVB2	186	170	0.03%	0.003%
71	11.713	1740	1743	1745	rBV2	345	298	0.05%	0.006%
72	11.762	1745	1751	1763	rBV	26940	46608	7.62%	0.890%
73	11.939	1776	1780	1784	rBV3	1449	2240	0.37%	0.043%
74	11.976	1784	1786	1789	rBV2	2668	3440	0.56%	0.066%
75	12.024	1789	1794	1803	rVB	465596	579493	94.76%	11.065%
76	12.225	1824	1827	1832	rBV3	966	1138	0.19%	0.022%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042469.D
 Acq On : 23 Jul 2024 14:10
 Operator : JC/MD
 Sample : P3263-18ME
 Misc : 5.56g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CK8ME

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\SFAMXML070324WMA.M
 Title : VOC Analysis

77	12.323	1837	1843	1856	rBV	366872	472784	77.31%	9.027%
78	12.555	1876	1881	1883	rBV	301	360	0.06%	0.007%
79	12.597	1885	1888	1894	rBV3	531	1017	0.17%	0.019%
80	12.768	1912	1916	1920	rBV2	741	1019	0.17%	0.019%
81	12.872	1928	1933	1938	rBV3	9025	12687	2.07%	0.242%
82	13.036	1957	1960	1962	rBV3	279	249	0.04%	0.005%
83	13.116	1971	1973	1976	rVB	267	253	0.04%	0.005%
84	13.164	1976	1981	1983	rBV3	381	528	0.09%	0.010%
85	13.268	1995	1998	2001	rBV2	734	886	0.14%	0.017%
86	13.390	2014	2018	2019	rBV2	247	319	0.05%	0.006%
87	13.408	2019	2021	2027	rVB3	1017	1255	0.21%	0.024%
88	13.506	2034	2037	2039	rVB2	204	192	0.03%	0.004%
89	13.597	2049	2052	2054	rVV2	420	520	0.09%	0.010%
90	13.689	2062	2067	2073	rVB3	1167	1644	0.27%	0.031%
91	13.780	2078	2082	2090	rBV2	2558	3858	0.63%	0.074%
92	13.884	2096	2099	2105	rVB2	868	1175	0.19%	0.022%
93	13.945	2105	2109	2110	rBV3	323	301	0.05%	0.006%
94	13.963	2110	2112	2115	rVV2	294	375	0.06%	0.007%
95	13.993	2115	2117	2122	rVB3	498	585	0.10%	0.011%
96	14.042	2122	2125	2129	rBV4	529	693	0.11%	0.013%
97	14.134	2136	2140	2144	rVB2	1350	1983	0.32%	0.038%
98	14.207	2151	2152	2155	rBV2	178	197	0.03%	0.004%
99	14.426	2185	2188	2196	rVB2	2077	2942	0.48%	0.056%
100	14.646	2219	2224	2229	rBV3	1163	2149	0.35%	0.041%

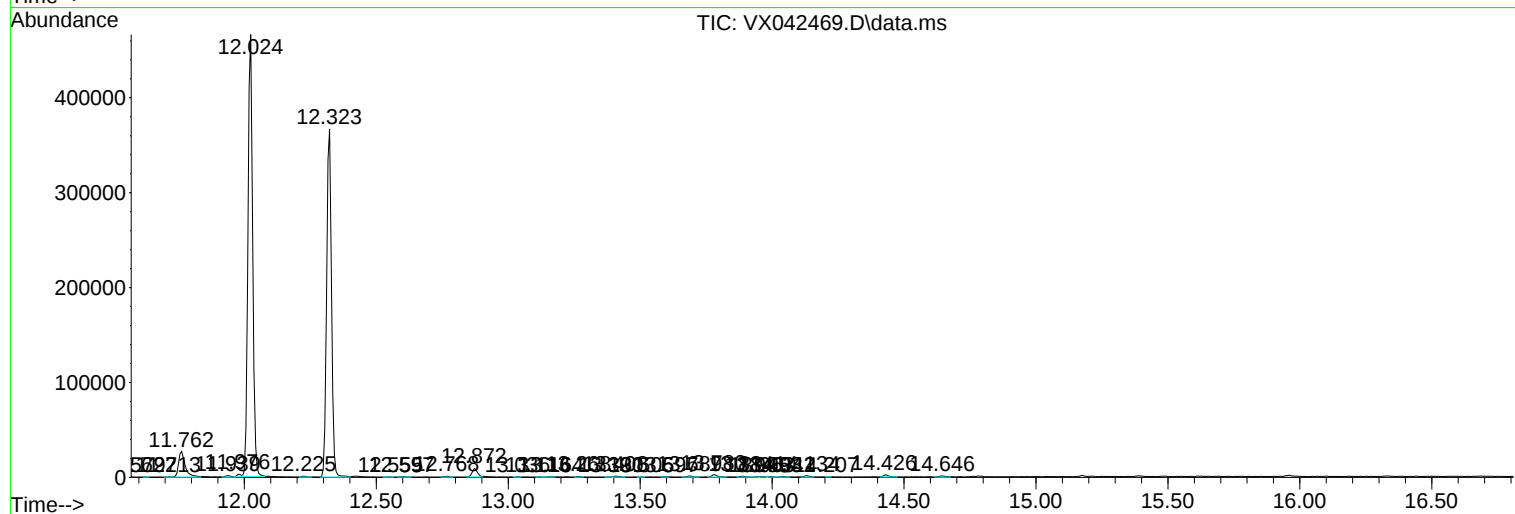
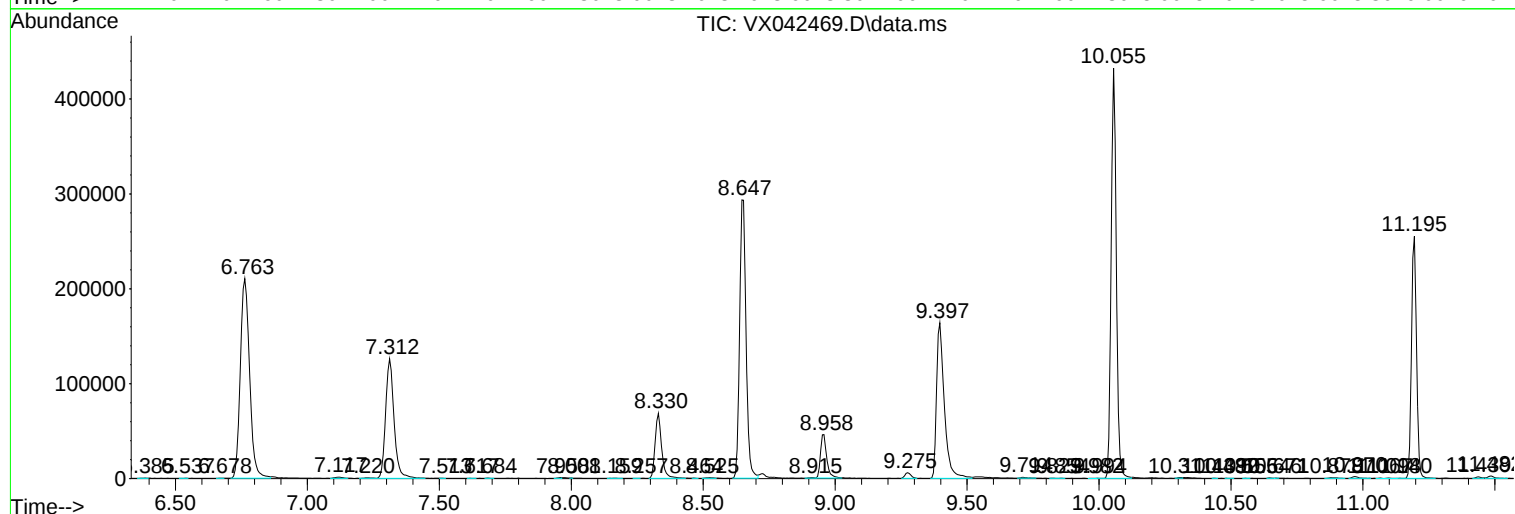
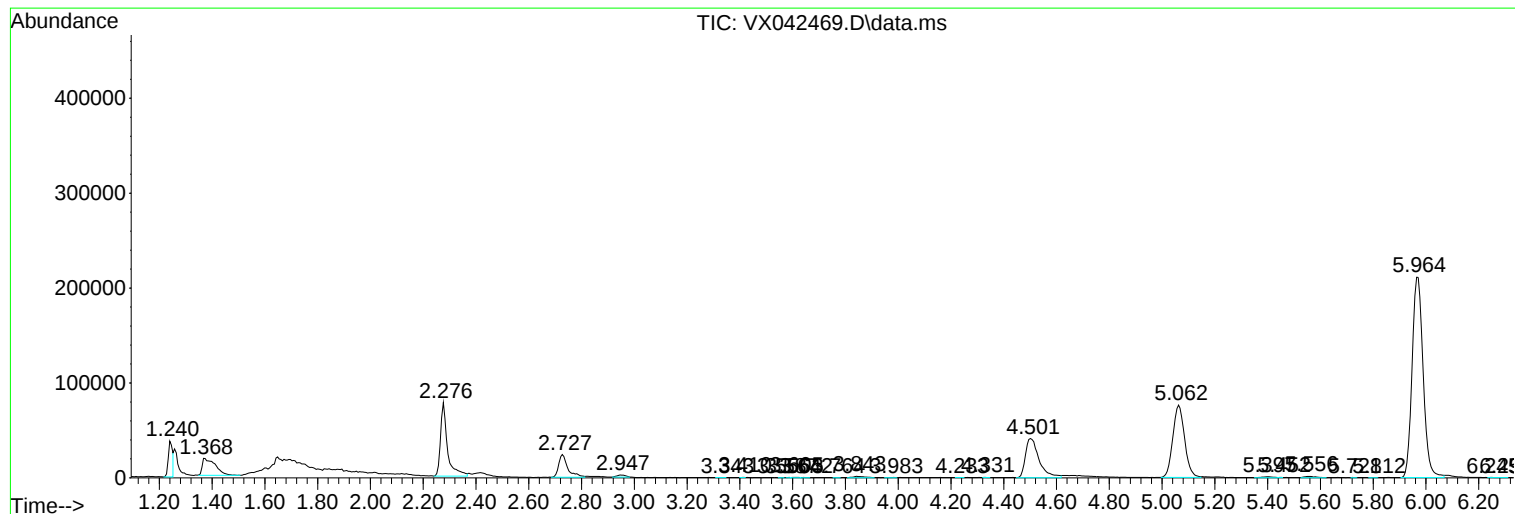
Sum of corrected areas: 5237315

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
Data File : VX042469.D
Acq On : 23 Jul 2024 14:10
Operator : JC/MD
Sample : P3263-18ME
Misc : 5.56g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CK8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
Data File : VX042469.D
Acq On : 23 Jul 2024 14:10
Operator : JC/MD
Sample : P3263-18ME
Misc : 5.56g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CK8ME

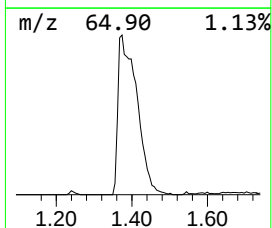
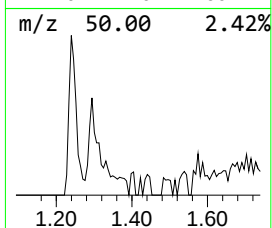
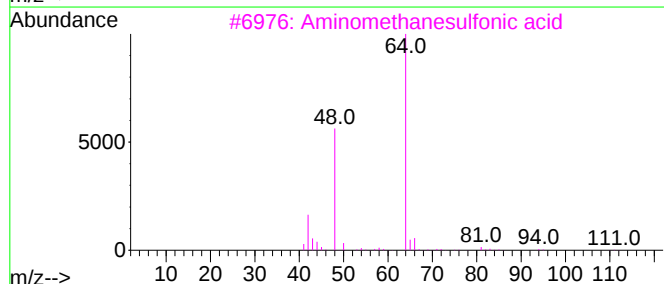
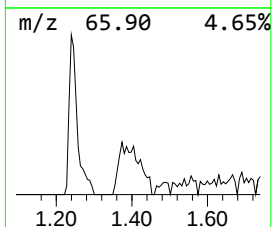
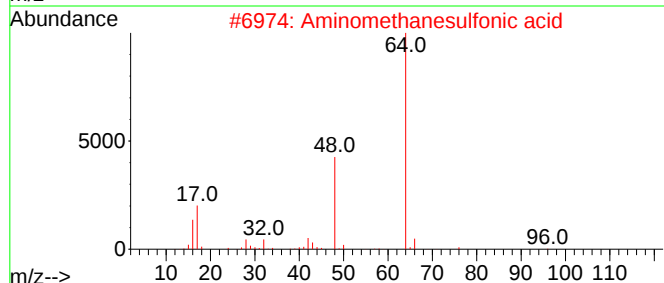
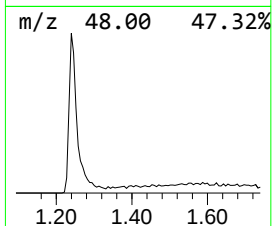
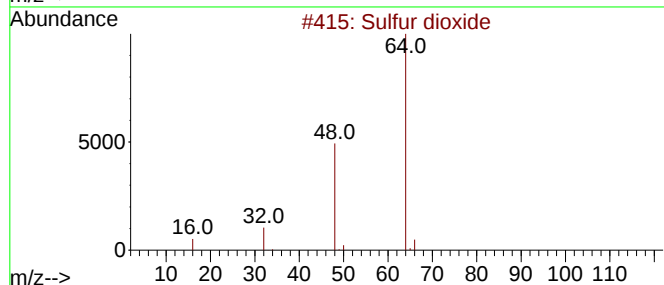
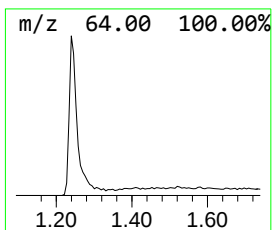
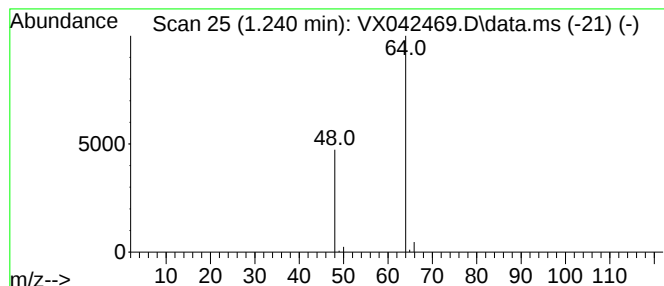
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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.
1.240	4.25 ug/L	43383	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
Data File : VX042469.D
Acq On : 23 Jul 2024 14:10
Operator : JC/MD
Sample : P3263-18ME
Misc : 5.56g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CK8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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
Sulfur dioxide	1.240	4.3	ug/L	43383	1	6.763	510737	50.0