

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042566.D
 Acq On : 25 Jul 2024 15:03
 Operator : JC/MD
 Sample : VX0727MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK697

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: VX042566.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	10	13	16	rBV3	996	1027	0.16%	0.020%
2	1.240	22	25	33	rBV	47410	59103	9.19%	1.124%
3	1.368	42	46	57	rBV	61152	69684	10.84%	1.325%
4	1.660	89	94	110	rVB	40215	63158	9.83%	1.201%
5	1.886	127	131	135	rVB3	878	1425	0.22%	0.027%
6	2.197	180	182	185	rVB	262	204	0.03%	0.004%
7	2.300	193	199	210	rBV	131682	208900	32.50%	3.972%
8	2.386	210	213	217	rVB3	860	1180	0.18%	0.022%
9	2.447	221	223	224	rVB	194	136	0.02%	0.003%
10	2.508	227	233	240	rBV	1524	2838	0.44%	0.054%
11	2.703	264	265	270	rVB2	324	379	0.06%	0.007%
12	2.788	273	279	287	rBV2	2941	6047	0.94%	0.115%
13	2.873	290	293	296	rBV2	156	217	0.03%	0.004%
14	2.941	296	304	317	rVB	4139	9307	1.45%	0.177%
15	3.093	325	329	340	rVB3	1261	3353	0.52%	0.064%
16	3.172	340	342	345	rVB	141	157	0.02%	0.003%
17	3.319	365	366	369	rBV2	117	145	0.02%	0.003%
18	3.367	373	374	378	rBV2	117	160	0.02%	0.003%
19	3.453	386	388	393	rVB	182	205	0.03%	0.004%
20	3.611	408	414	419	rBV2	446	968	0.15%	0.018%
21	3.898	457	461	462	rBV	168	211	0.03%	0.004%
22	3.946	467	469	472	rBV	150	200	0.03%	0.004%
23	4.221	512	514	517	rVB2	142	168	0.03%	0.003%
24	4.459	545	553	571	rBV	49783	147303	22.92%	2.801%
25	4.837	613	615	618	rVB2	164	170	0.03%	0.003%
26	4.910	623	627	631	rVB2	288	517	0.08%	0.010%
27	5.056	638	651	671	rBV	82192	257275	40.02%	4.892%
28	5.275	685	687	690	rVB2	190	193	0.03%	0.004%
29	5.391	700	706	711	rBV5	672	1592	0.25%	0.030%
30	5.464	713	718	725	rVB4	815	1556	0.24%	0.030%
31	5.550	726	732	733	rBV3	520	640	0.10%	0.012%
32	5.672	747	752	754	rBV2	458	736	0.11%	0.014%
33	5.964	788	800	819	rBV2	218117	642819	100.00%	12.223%
34	6.166	831	833	837	rVB3	234	322	0.05%	0.006%
35	6.196	837	838	843	rVB2	151	196	0.03%	0.004%
36	6.556	895	897	902	rVB2	161	209	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042566.D
Acq On : 25 Jul 2024 15:03
Operator : JC/MD
Sample : VX0727MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK697

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	6.696	919	920	922	rBV	138	145	0.02%	0.003%
38	6.757	922	930	953	rVV	196020	473139	73.60%	8.997%
39	7.123	984	990	1000	rVB4	2192	5884	0.92%	0.112%
40	7.306	1011	1020	1037	rBV	128597	285874	44.47%	5.436%
41	7.434	1037	1041	1046	rVV5	717	1628	0.25%	0.031%
42	7.488	1048	1050	1051	rVV	341	245	0.04%	0.005%
43	7.507	1051	1053	1054	rVB2	229	149	0.02%	0.003%
44	7.830	1100	1106	1111	rVV2	497	823	0.13%	0.016%
45	7.885	1113	1115	1117	rVB	169	139	0.02%	0.003%
46	7.958	1124	1127	1128	rVV2	177	142	0.02%	0.003%
47	7.976	1128	1130	1132	rVV	132	154	0.02%	0.003%
48	8.025	1135	1138	1140	rBV2	98	149	0.02%	0.003%
49	8.281	1178	1180	1181	rBV	163	139	0.02%	0.003%
50	8.324	1181	1187	1204	rVV	83013	141177	21.96%	2.685%
51	8.580	1225	1229	1234	rBV2	1082	1602	0.25%	0.030%
52	8.647	1234	1240	1250	rBV	334868	524121	81.53%	9.966%
53	8.952	1284	1290	1301	rBV	58172	92535	14.40%	1.760%
54	9.153	1321	1323	1328	rVB3	785	1183	0.18%	0.022%
55	9.275	1339	1343	1350	rBV3	2401	3471	0.54%	0.066%
56	9.384	1356	1361	1380	rBV	222345	319366	49.68%	6.073%
57	9.610	1394	1398	1404	rVB2	676	1133	0.18%	0.022%
58	9.702	1409	1413	1419	rVB3	581	983	0.15%	0.019%
59	10.055	1465	1471	1483	rBV	387410	548202	85.28%	10.424%
60	10.195	1491	1494	1499	rVB	2469	2922	0.45%	0.056%
61	10.305	1507	1512	1521	rBV2	2353	3832	0.60%	0.073%
62	10.646	1563	1568	1577	rBV4	2870	6237	0.97%	0.119%
63	10.805	1591	1594	1598	rBV2	517	679	0.11%	0.013%
64	10.963	1615	1620	1626	rVB	2166	3192	0.50%	0.061%
65	11.098	1640	1642	1645	rBB2	209	243	0.04%	0.005%
66	11.189	1652	1657	1664	rBV	259233	335763	52.23%	6.385%
67	11.311	1676	1677	1680	rVB3	295	255	0.04%	0.005%
68	11.378	1687	1688	1692	rBV2	149	201	0.03%	0.004%
69	11.451	1696	1700	1707	rBV	2122	2725	0.42%	0.052%
70	11.713	1740	1743	1745	rVV2	235	256	0.04%	0.005%
71	11.756	1745	1750	1758	rVB2	2138	3298	0.51%	0.063%
72	11.915	1772	1776	1778	rBV2	131	149	0.02%	0.003%
73	11.975	1782	1786	1788	rBV	2402	3116	0.48%	0.059%
74	12.024	1788	1794	1806	rVB	389167	512825	79.78%	9.752%
75	12.207	1822	1824	1825	rBV	194	152	0.02%	0.003%
76	12.232	1825	1828	1831	rVB2	115	141	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042566.D
 Acq On : 25 Jul 2024 15:03
 Operator : JC/MD
 Sample : VX0727MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK697

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	12.317	1837	1842	1854	rBV	359490	474068	73.75%	9.015%
78	12.951	1943	1946	1950	rVB3	436	513	0.08%	0.010%
79	13.116	1969	1973	1979	rVB2	2546	3373	0.52%	0.064%
80	13.323	2006	2007	2011	rVB2	146	170	0.03%	0.003%
81	13.591	2047	2051	2058	rVV2	3124	4237	0.66%	0.081%
82	13.780	2076	2082	2090	rBV2	4463	6790	1.06%	0.129%
83	13.963	2107	2112	2118	rBV2	3671	4728	0.74%	0.090%
84	14.079	2129	2131	2136	rVB2	180	289	0.04%	0.005%
85	14.121	2136	2138	2139	rBV	202	190	0.03%	0.004%
86	14.377	2178	2180	2183	rVB2	151	181	0.03%	0.003%
87	14.646	2222	2224	2227	rVB3	163	151	0.02%	0.003%
88	14.774	2243	2245	2247	rVB2	244	214	0.03%	0.004%
89	14.798	2247	2249	2250	rBV	214	203	0.03%	0.004%
90	14.841	2255	2256	2260	rBV2	194	213	0.03%	0.004%
91	14.914	2266	2268	2271	rBV2	224	299	0.05%	0.006%
92	14.993	2280	2281	2282	rBV	294	152	0.02%	0.003%
93	15.438	2352	2354	2356	rBV3	233	209	0.03%	0.004%
94	15.487	2360	2362	2364	rVB2	338	289	0.04%	0.005%
95	15.676	2391	2393	2394	rBV	244	151	0.02%	0.003%
96	16.066	2455	2457	2459	rBV	317	293	0.05%	0.006%
97	16.292	2493	2494	2499	rBV4	303	408	0.06%	0.008%
98	16.444	2517	2519	2521	rBV2	304	179	0.03%	0.003%
99	16.688	2557	2559	2560	rVB2	341	205	0.03%	0.004%
100	16.712	2561	2563	2566	rBV2	296	341	0.05%	0.006%

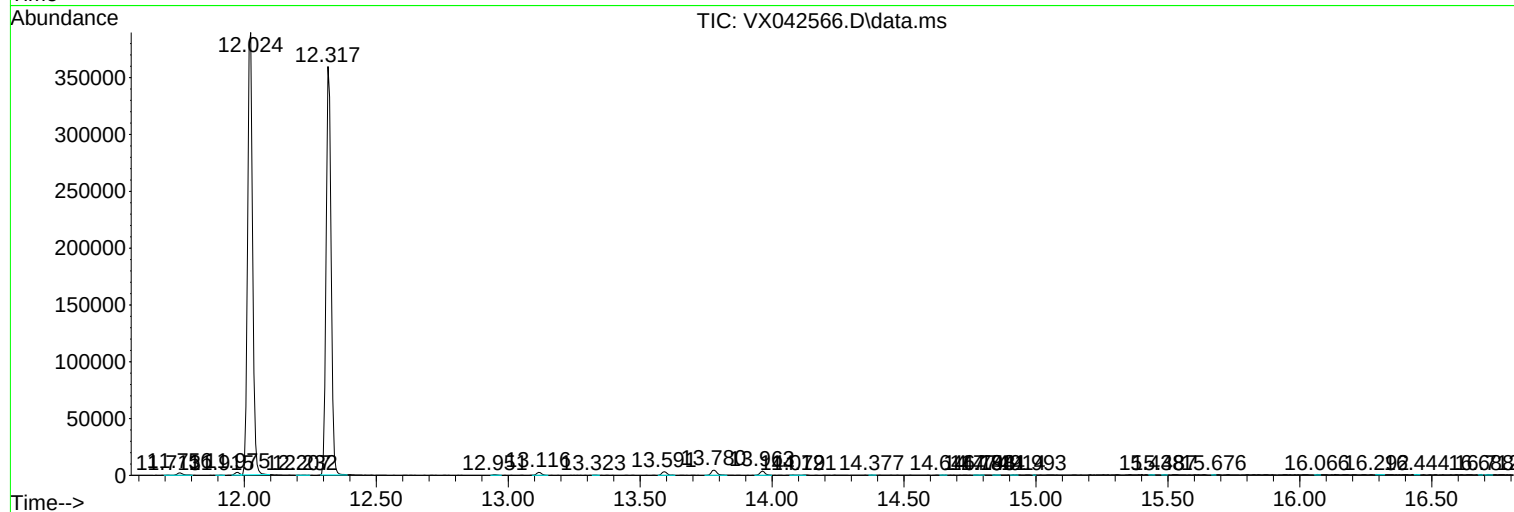
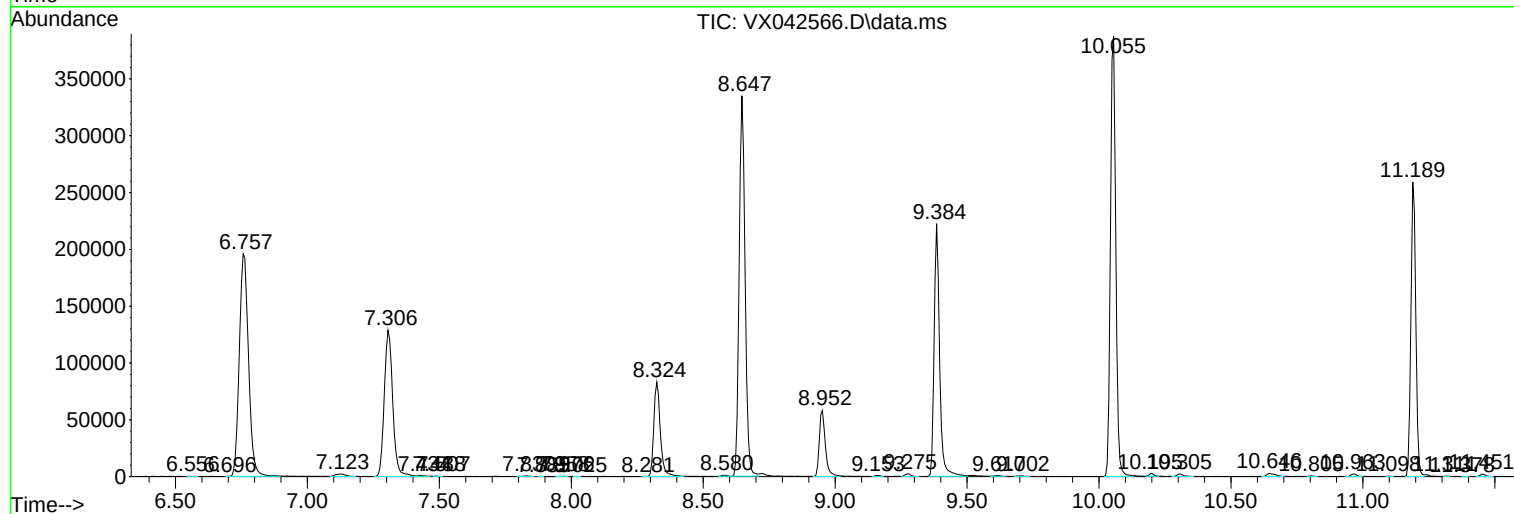
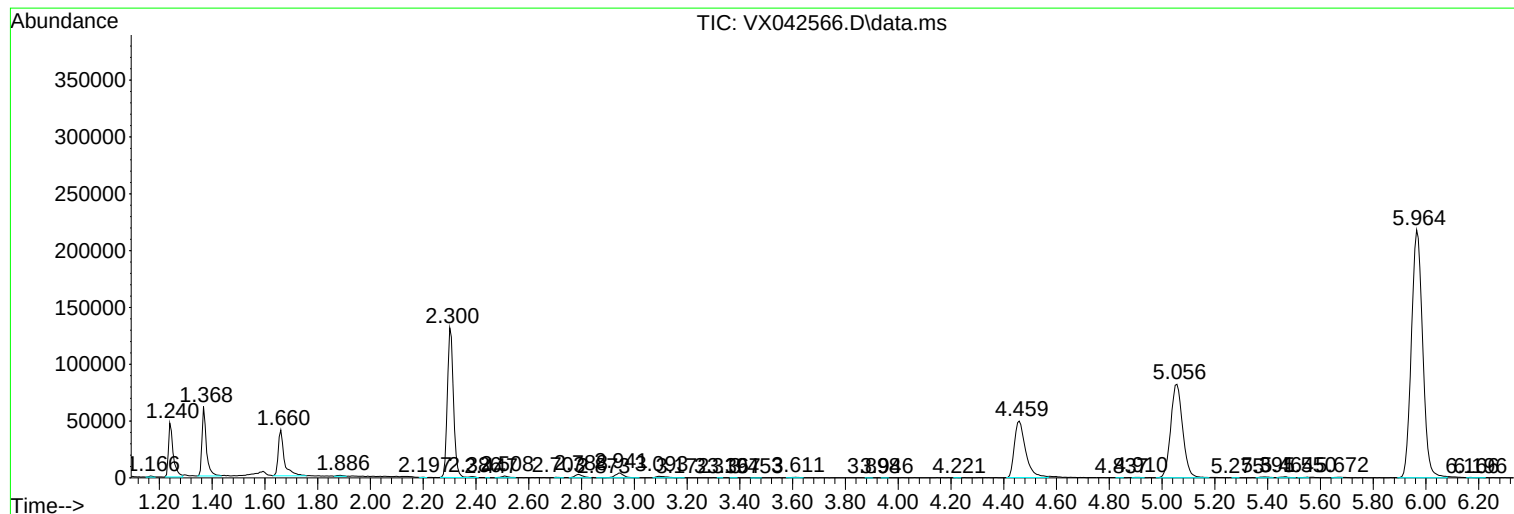
Sum of corrected areas: 5258915

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042566.D
Acq On : 25 Jul 2024 15:03
Operator : JC/MD
Sample : VX0727MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK697

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\VX072724\
Data File : VX042566.D
Acq On : 25 Jul 2024 15:03
Operator : JC/MD
Sample : VX0727MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK697

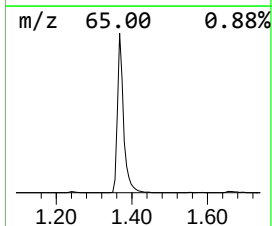
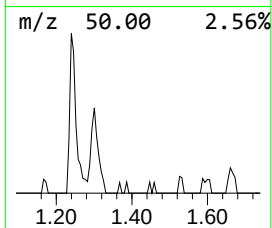
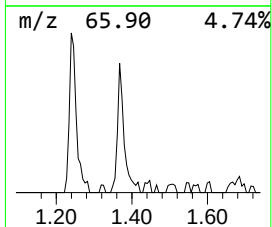
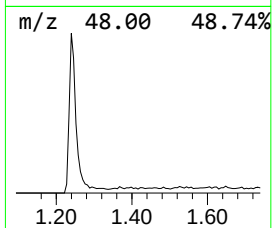
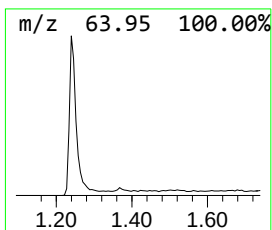
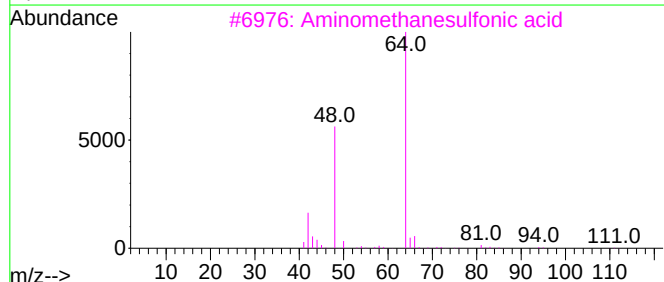
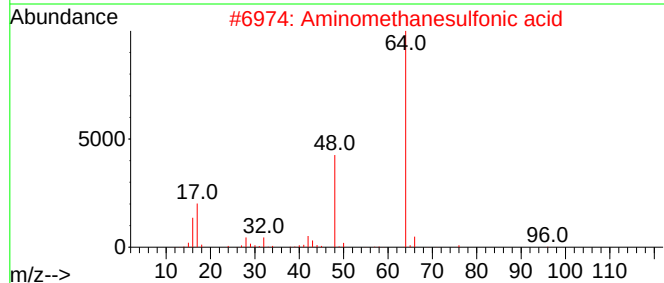
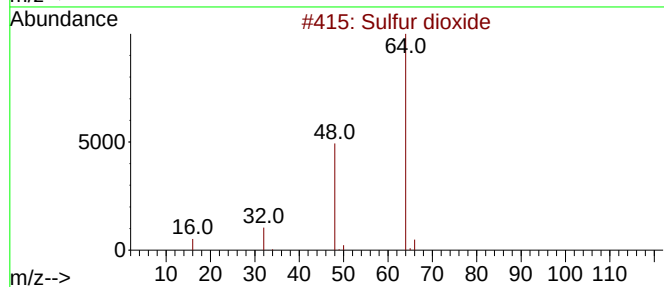
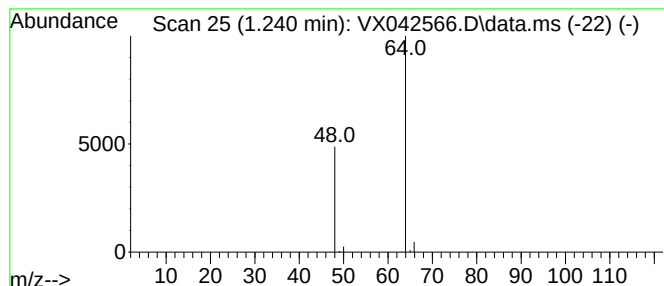
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	6.25 ug/L	59103	1,4-Difluorobenzene	6.757

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			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042566.D
Acq On : 25 Jul 2024 15:03
Operator : JC/MD
Sample : VX0727MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK697

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	6.3	ug/L	59103	1	6.757	473139	50.0