

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048028.D
 Acq On : 14 Apr 2022 01:04
 Operator : SY/MD
 Sample : N2386-12
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0J13

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_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU048028.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	16	rVB2	5204	5802	0.48%	0.057%
2	1.491	37	47	55	rBV3	25720	57791	4.80%	0.563%
3	1.600	75	81	96	rVB	146309	169381	14.07%	1.650%
4	1.916	172	179	197	rVB	117850	162601	13.51%	1.584%
5	2.571	370	383	398	rBV	243953	398974	33.15%	3.886%
6	2.755	435	440	450	rVV5	1299	2073	0.17%	0.020%
7	2.906	483	487	490	rVB2	357	249	0.02%	0.002%
8	3.012	518	520	526	rVB2	436	404	0.03%	0.004%
9	3.047	526	531	535	rBV5	1060	1051	0.09%	0.010%
10	3.086	538	543	548	rVB4	469	570	0.05%	0.006%
11	3.189	563	575	588	rVB	3558	7550	0.63%	0.074%
12	3.256	593	596	599	rVB2	461	274	0.02%	0.003%
13	3.366	615	630	650	rBV	44682	103982	8.64%	1.013%
14	3.452	652	657	664	rVB5	372	398	0.03%	0.004%
15	3.526	678	680	685	rVB3	327	182	0.02%	0.002%
16	3.697	728	733	737	rVB2	890	920	0.08%	0.009%
17	3.723	737	741	744	rBV	348	388	0.03%	0.004%
18	3.877	782	789	803	rVB4	926	1843	0.15%	0.018%
19	4.176	877	882	887	rBV2	333	380	0.03%	0.004%
20	4.375	939	944	950	rVB3	216	251	0.02%	0.002%
21	4.407	950	954	957	rBV	203	198	0.02%	0.002%
22	4.555	997	1000	1004	rBV2	289	231	0.02%	0.002%
23	4.620	1008	1020	1046	rBV	126804	308237	25.61%	3.002%
24	5.067	1143	1159	1177	rBV	218208	479609	39.85%	4.671%
25	5.211	1201	1204	1207	rVB3	247	184	0.02%	0.002%
26	5.288	1222	1228	1233	rBV2	527	669	0.06%	0.007%
27	5.526	1299	1302	1308	rVB3	331	330	0.03%	0.003%
28	5.568	1308	1315	1317	rBV	210	220	0.02%	0.002%
29	5.729	1343	1365	1397	rBV2	438298	1203621	100.00%	11.723%
30	5.944	1418	1432	1446	rVB3	10572	22766	1.89%	0.222%
31	6.025	1454	1457	1459	rVV	406	318	0.03%	0.003%
32	6.070	1469	1471	1477	rVV2	341	210	0.02%	0.002%
33	6.166	1498	1501	1505	rBV2	284	251	0.02%	0.002%
34	6.250	1512	1527	1549	rBV	388631	741793	61.63%	7.225%
35	6.526	1607	1613	1620	rBV3	1232	1870	0.16%	0.018%
36	6.693	1650	1665	1687	rBV	279844	543477	45.15%	5.293%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048028.D
 Acq On : 14 Apr 2022 01:04
 Operator : SY/MD
 Sample : N2386-12
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0J13

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_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

37	6.800	1695	1698	1699	rBV3	375	268	0.02%	0.003%
38	7.041	1770	1773	1776	rBV2	275	257	0.02%	0.003%
39	7.150	1804	1807	1810	rVV	296	269	0.02%	0.003%
40	7.182	1810	1817	1828	rVV3	3263	5812	0.48%	0.057%
41	7.282	1846	1848	1851	rBV	316	212	0.02%	0.002%
42	7.388	1878	1881	1885	rVB2	278	206	0.02%	0.002%
43	7.568	1923	1937	1951	rBV	135361	237636	19.74%	2.315%
44	7.687	1966	1974	1986	rVB6	2279	4137	0.34%	0.040%
45	7.822	2013	2016	2020	rVB3	420	294	0.02%	0.003%
46	7.899	2025	2040	2056	rBV	543174	938027	77.93%	9.136%
47	8.179	2115	2127	2148	rBV	96672	168031	13.96%	1.637%
48	8.472	2211	2218	2233	rVB3	3254	5819	0.48%	0.057%
49	8.632	2254	2268	2300	rBV	378779	719546	59.78%	7.008%
50	8.912	2346	2355	2365	rBV5	494	1055	0.09%	0.010%
51	9.070	2401	2404	2408	rVB3	322	287	0.02%	0.003%
52	9.111	2413	2417	2420	rBV2	219	206	0.02%	0.002%
53	9.214	2447	2449	2453	rVB3	278	215	0.02%	0.002%
54	9.327	2481	2484	2487	rBV2	318	200	0.02%	0.002%
55	9.417	2499	2512	2553	rVB	597125	1046668	86.96%	10.194%
56	9.571	2556	2560	2562	rBV2	768	572	0.05%	0.006%
57	9.645	2578	2583	2586	rBV	282	265	0.02%	0.003%
58	9.693	2590	2598	2606	rBV4	1673	2281	0.19%	0.022%
59	9.822	2633	2638	2640	rBV2	259	250	0.02%	0.002%
60	9.861	2644	2650	2654	rVV3	285	276	0.02%	0.003%
61	9.902	2657	2663	2665	rBV3	209	212	0.02%	0.002%
62	10.015	2693	2698	2700	rBV2	359	362	0.03%	0.004%
63	10.044	2703	2707	2711	rVV2	212	246	0.02%	0.002%
64	10.098	2719	2724	2730	rVV4	550	611	0.05%	0.006%
65	10.153	2737	2741	2747	rBV	249	256	0.02%	0.002%
66	10.208	2754	2758	2761	rBV	345	321	0.03%	0.003%
67	10.327	2791	2795	2798	rBV4	480	438	0.04%	0.004%
68	10.346	2798	2801	2807	rVB	459	362	0.03%	0.004%
69	10.420	2821	2824	2827	rBV2	419	295	0.02%	0.003%
70	10.629	2886	2889	2893	rVB2	257	201	0.02%	0.002%
71	10.674	2895	2903	2910	rBV4	1321	1821	0.15%	0.018%
72	10.758	2916	2929	2950	rBV	425441	689625	57.30%	6.717%
73	10.896	2964	2972	2984	rVB2	4962	7772	0.65%	0.076%
74	11.005	3002	3006	3010	rVB2	578	536	0.04%	0.005%
75	11.037	3014	3016	3022	rVB	534	351	0.03%	0.003%
76	11.086	3028	3031	3034	rVB3	331	218	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048028.D
 Acq On : 14 Apr 2022 01:04
 Operator : SY/MD
 Sample : N2386-12
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0J13

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_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

77	11.208	3064	3069	3072	rBV2	463	462	0.04%	0.004%
78	11.320	3100	3104	3108	rVB3	345	330	0.03%	0.003%
79	11.471	3141	3151	3160	rVV7	1009	2311	0.19%	0.023%
80	11.520	3162	3166	3172	rVB2	222	244	0.02%	0.002%
81	11.568	3177	3181	3185	rVB2	361	341	0.03%	0.003%
82	11.696	3215	3221	3224	rBV4	784	705	0.06%	0.007%
83	11.748	3229	3237	3244	rBV3	7762	11272	0.94%	0.110%
84	11.812	3244	3257	3279	rVB	663907	1152071	95.72%	11.221%
85	11.976	3304	3308	3314	rVB3	1521	1292	0.11%	0.013%
86	12.069	3325	3337	3349	rVV4	5895	10652	0.88%	0.104%
87	12.195	3359	3376	3401	rBV	593170	1008877	83.82%	9.826%
88	12.462	3456	3459	3461	rBV2	315	193	0.02%	0.002%
89	12.584	3494	3497	3503	rBV2	256	326	0.03%	0.003%
90	12.703	3531	3534	3535	rBV2	284	190	0.02%	0.002%
91	13.224	3689	3696	3705	rVB5	2852	4348	0.36%	0.042%
92	13.436	3760	3762	3764	rBV	369	192	0.02%	0.002%
93	13.844	3880	3889	3903	rVB4	7756	11871	0.99%	0.116%
94	14.333	4037	4041	4047	rBV2	803	835	0.07%	0.008%
95	14.368	4049	4052	4053	rBV	436	185	0.02%	0.002%
96	14.941	4228	4230	4232	rBV2	311	181	0.02%	0.002%
97	15.102	4278	4280	4283	rBV2	342	204	0.02%	0.002%
98	15.134	4288	4290	4294	rVV3	406	229	0.02%	0.002%
99	15.500	4402	4404	4406	rBV	562	277	0.02%	0.003%
100	15.548	4412	4419	4428	rBV7	3092	4020	0.33%	0.039%

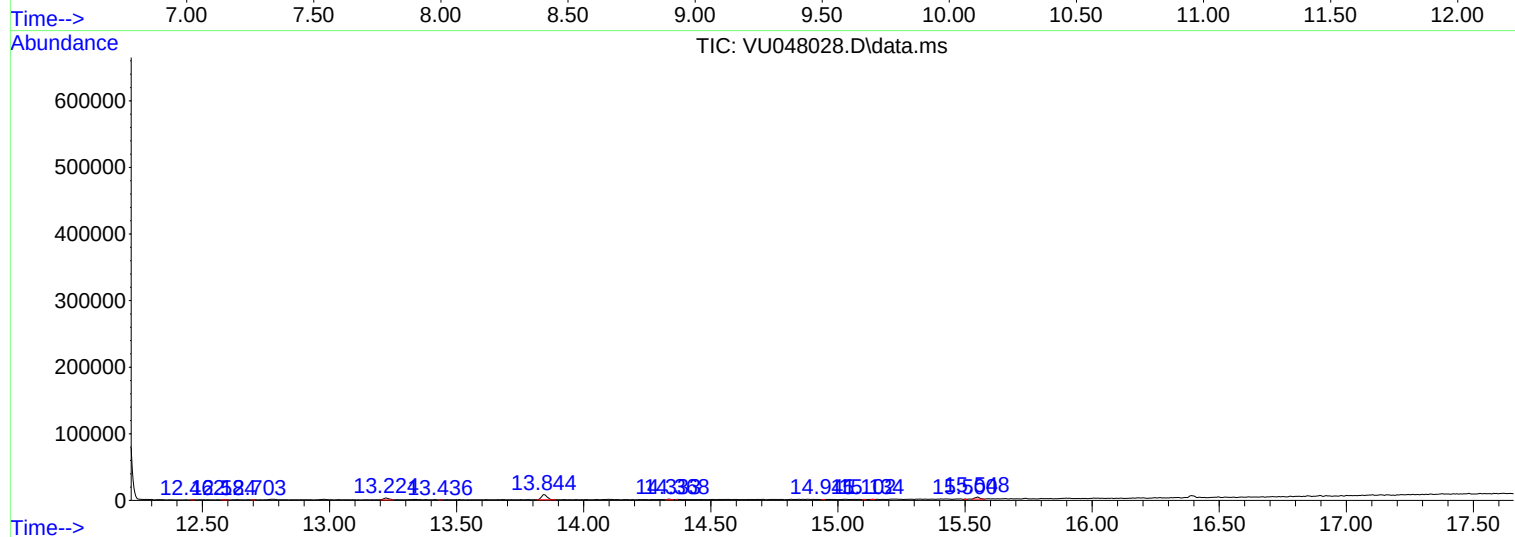
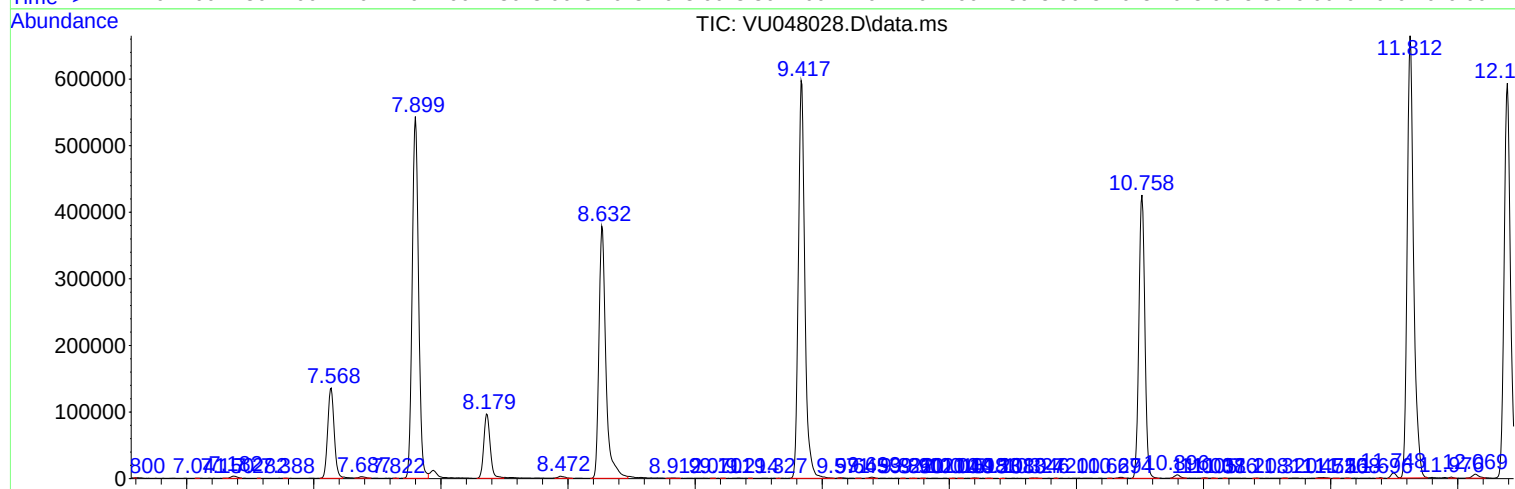
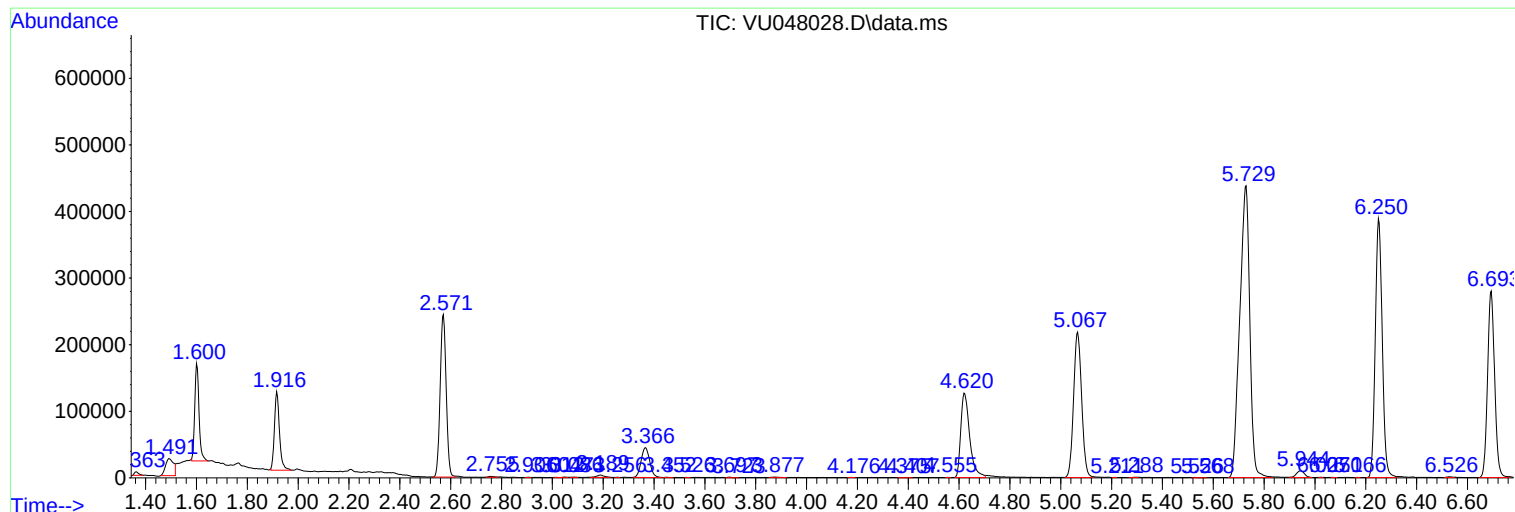
Sum of corrected areas: 10267072

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU048028.D
Acq On : 14 Apr 2022 01:04
Operator : SY/MD
Sample : N2386-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J13

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU048028.D
Acq On : 14 Apr 2022 01:04
Operator : SY/MD
Sample : N2386-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J13

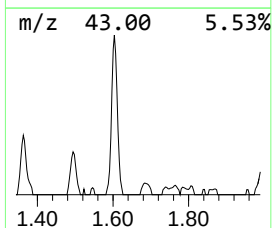
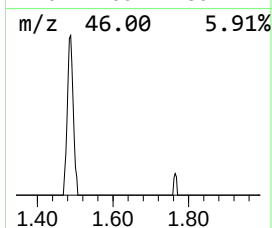
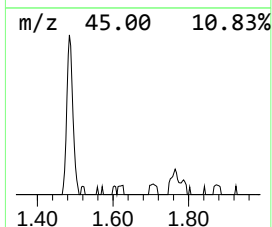
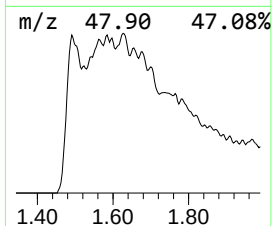
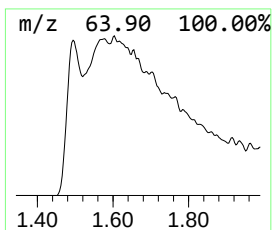
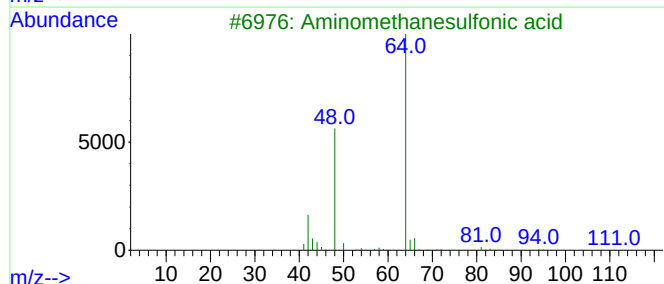
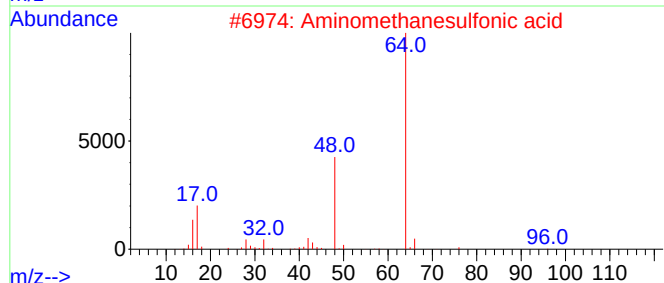
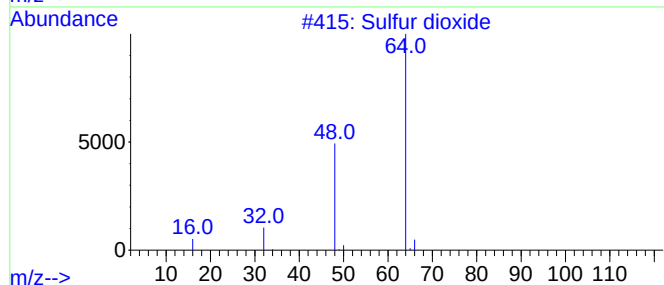
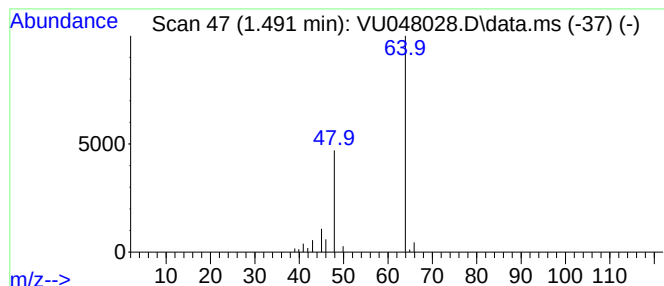
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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.
1.491	3.90 ug/L	57791	1,4-Difluorobenzene	6.250

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	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU048028.D
Acq On : 14 Apr 2022 01:04
Operator : SY/MD
Sample : N2386-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J13

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.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	1.491	3.9	ug/L	57791	1	6.250	741793	50.0