LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027839.D
Acq On : 26 Oct 2018 17:24
Operator : MD/SY
Sample : J5668-13
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETBS4

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\SOMULM102218WMA.M
Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.309	26	42	48	rBV2	6357	18046	4.60%	0.519%
2	1.399	64	70	80	rBV	45597	47313	12.07%	1.362%
3	1.682	151	158	170	rVB	35954	46240	11.79%	1.331%
4	2.273	332	342	353	rBV	73467	111721	28.50%	3.215%
5	2.444	386	395	404	rBV	5978	9488	2.42%	0.273%
6	2.624	448	451	456	rVB2	352	356	0.09%	0.010%
7	2.669	461	465	470	rVB2	210	196	0.05%	0.006%
8	2.723	479	482	485	rBV	165	93	0.02%	0.003%
9	2.739	485	487	489	rVV	171	102	0.03%	0.003%
10	2.755	489	492	498	rVB2	169	177	0.05%	0.005%
11	2.833	510	516	518	rBV	486	513	0.13%	0.015%
12	2.990	561	565	567	rVB2	292	190	0.05%	0.005%
13	3.006	567	570	579	rVB	107	133	0.03%	0.004%
14	3.145	611	613	620	rVB	124	99	0.03%	0.003%
15	3.373	681	684	686	rBV	102	76	0.02%	0.002%
16	3.437	695	704	711	rBV4	522	928	0.24%	0.027%
17	3.579	743	748	751	rBV	107	102	0.03%	0.003%
18	3.630	760	764	769	rVB	125	120	0.03%	0.003%
19	3.752	799	802	804	rBV	169	142	0.04%	0.004%
20	4.180	921	935	947	rBV	47335	126061	32.15%	3.628%
21	4.402	1001	1004	1006	rBV	165	136	0.03%	0.004%
22	4.431	1009	1013	1016	rBV	178	200	0.05%	0.006%
23	4.652	1064	1082	1104	rBV2	66977	156495	39.92%	4.503%
24	4.961	1176	1178	1181	rBV	133	87	0.02%	0.003%
25	5.070	1210	1212	1215	rVB	141	76	0.02%	0.002%
26	5.196	1249	1251	1255	rVB	189	153	0.04%	0.004%
27	5.225	1256	1260	1262	rBV	163	162	0.04%	0.005%
28	5.344	1273	1297	1329	rBV2	130327	392060	100.00%	11.282%
29	5.495	1341	1344	1347	rVB2	192	126	0.03%	0.004%
30	5.742	1420	1421	1425	rBV	241	158	0.04%	0.005%
31	5.797	1435	1438	1440	rBV2	155	88	0.02%	0.003%
32	5.887	1452	1466	1493	rBV	149413	293133	74.77%	8.435%
33	5.977	1493	1494	1501	rVB	226	130	0.03%	0.004%
34	6.013	1501	1505	1507	rBV	181	150	0.04%	0.004%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027839.D
Acq On : 26 Oct 2018 17:24
Operator : MD/SY
Sample : J5668-13
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETBS4

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\SOMULM102218WMA.M
Title : VOC Analysis

35	6.054	1515	1518	1523	rVB	230	229	0.06%	0.007%
36	6.080	1524	1526	1528	rBV	168	120	0.03%	0.003%
37	6.250	1576	1579	1582	rBV	159	157	0.04%	0.005%
38	6.331	1591	1604	1624	rBV	95364	187685	47.87%	5.401%
39	6.778	1740	1743	1746	rBV	184	163	0.04%	0.005%
40	6.861	1763	1769	1779	rBV3	950	1834	0.47%	0.053%
41	6.996	1808	1811	1815	rVB	215	203	0.05%	0.006%
42	7.019	1815	1818	1819	rBV	120	88	0.02%	0.003%
43	7.228	1872	1883	1901	rBV	53357	93977	23.97%	2.704%
44	7.328	1913	1914	1918	rVB	163	74	0.02%	0.002%
45	7.389	1929	1933	1934	rBV2	313	236	0.06%	0.007%
46	7.463	1953	1956	1957	rBV	132	94	0.02%	0.003%
47	7.566	1975	1988	2006	rBV	172000	297147	75.79%	8.551%
48	7.746	2041	2044	2048	rVB	266	208	0.05%	0.006%
49	7.771	2049	2052	2054	rBV	155	130	0.03%	0.004%
50	7.787	2054	2057	2061	rVV	173	153	0.04%	0.004%
51	7.852	2065	2077	2096	rVV	37510	62727	16.00%	1.805%
52	7.964	2109	2112	2117	rBV2	148	127	0.03%	0.004%
53	8.051	2136	2139	2142	rVB2	145	102	0.03%	0.003%
54	8.183	2166	2180	2189	rBV	24706	54776	13.97%	1.576%
55	8.312	2211	2220	2255	rVB	166137	292158	74.52%	8.407%
56	8.472	2268	2270	2273	rVB	206	95	0.02%	0.003%
57	8.566	2295	2299	2304	rBV	103	103	0.03%	0.003%
58	8.656	2321	2327	2331	rBV2	313	328	0.08%	0.009%
59	8.684	2333	2336	2339	rVB2	143	80	0.02%	0.002%
60	9.090	2449	2462	2481	rBV	218915	355360	90.64%	10.226%
61	9.193	2491	2494	2496	rBV	168	85	0.02%	0.002%
62	9.308	2525	2530	2534	rBV2	168	146	0.04%	0.004%
63	9.350	2540	2543	2549	rVB	118	101	0.03%	0.003%
64	9.684	2642	2647	2652	rVB	153	151	0.04%	0.004%
65	9.717	2652	2657	2660	rBV	91	100	0.03%	0.003%
66	10.073	2765	2768	2771	rBV	126	101	0.03%	0.003%
67	10.331	2845	2848	2851	rBV	209	100	0.03%	0.003%
68	10.430	2867	2879	2901	rVB	128134	202580	51.67%	5.830%
69	10.527	2906	2909	2914	rBV	106	125	0.03%	0.004%
70	10.614	2925	2936	2951	rBV2	12644	26141	6.67%	0.752%
71	10.729	2968	2972	2976	rBV	107	102	0.03%	0.003%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027839.D
Acq On : 26 Oct 2018 17:24
Operator : MD/SY
Sample : J5668-13
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETBS4

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\SOMULM102218WMA.M
Title : VOC Analysis

72	10.791	2987	2991	2993	rBV	128	91	0.02%	0.003%
73	10.877	3009	3018	3025	rBV3	674	1117	0.28%	0.032%
74	11.482	3195	3206	3221	rBV	208594	320022	81.63%	9.209%
75	11.572	3232	3234	3236	rVB	170	91	0.02%	0.003%
76	11.749	3284	3289	3297	rBV3	1228	1771	0.45%	0.051%
77	11.858	3312	3323	3343	rBV	168473	269721	68.80%	7.762%
78	11.948	3346	3351	3357	rBV2	216	339	0.09%	0.010%
79	11.980	3357	3361	3363	rBV	248	139	0.04%	0.004%
80	12.138	3407	3410	3412	rBV	193	113	0.03%	0.003%
81	12.225	3432	3437	3438	rBV3	2002	1577	0.40%	0.045%
82	12.482	3507	3517	3531	rVB	9342	17183	4.38%	0.494%
83	12.546	3534	3537	3542	rBV2	159	191	0.05%	0.005%
84	12.607	3554	3556	3560	rBV	158	92	0.02%	0.003%
85	12.697	3581	3584	3588	rVB	169	112	0.03%	0.003%
86	13.057	3694	3696	3701	rVB	186	91	0.02%	0.003%
87	13.427	3810	3811	3817	rVB	141	74	0.02%	0.002%
88	13.707	3894	3898	3900	rBV2	150	92	0.02%	0.003%
89	13.800	3925	3927	3930	rBV	187	102	0.03%	0.003%
90	13.884	3950	3953	3956	rVB	219	112	0.03%	0.003%
91	14.048	4001	4004	4007	rBV	139	115	0.03%	0.003%
92	14.212	4048	4055	4056	rBV3	613	596	0.15%	0.017%
93	14.279	4066	4076	4091	rVB	12869	21173	5.40%	0.609%
94	14.337	4091	4094	4098	rBV2	306	243	0.06%	0.007%
95	14.388	4107	4110	4114	rVB2	323	217	0.06%	0.006%
96	14.511	4146	4148	4151	rBV	207	148	0.04%	0.004%
97	14.594	4151	4174	4176	rBV5	7719	17502	4.46%	0.504%
98	15.684	4502	4513	4519	rBV7	1274	2397	0.61%	0.069%
99	15.880	4565	4574	4586	rVB	6346	10114	2.58%	0.291%
100	16.456	4738	4753	4765	rBV8	7871	26134	6.67%	0.752%

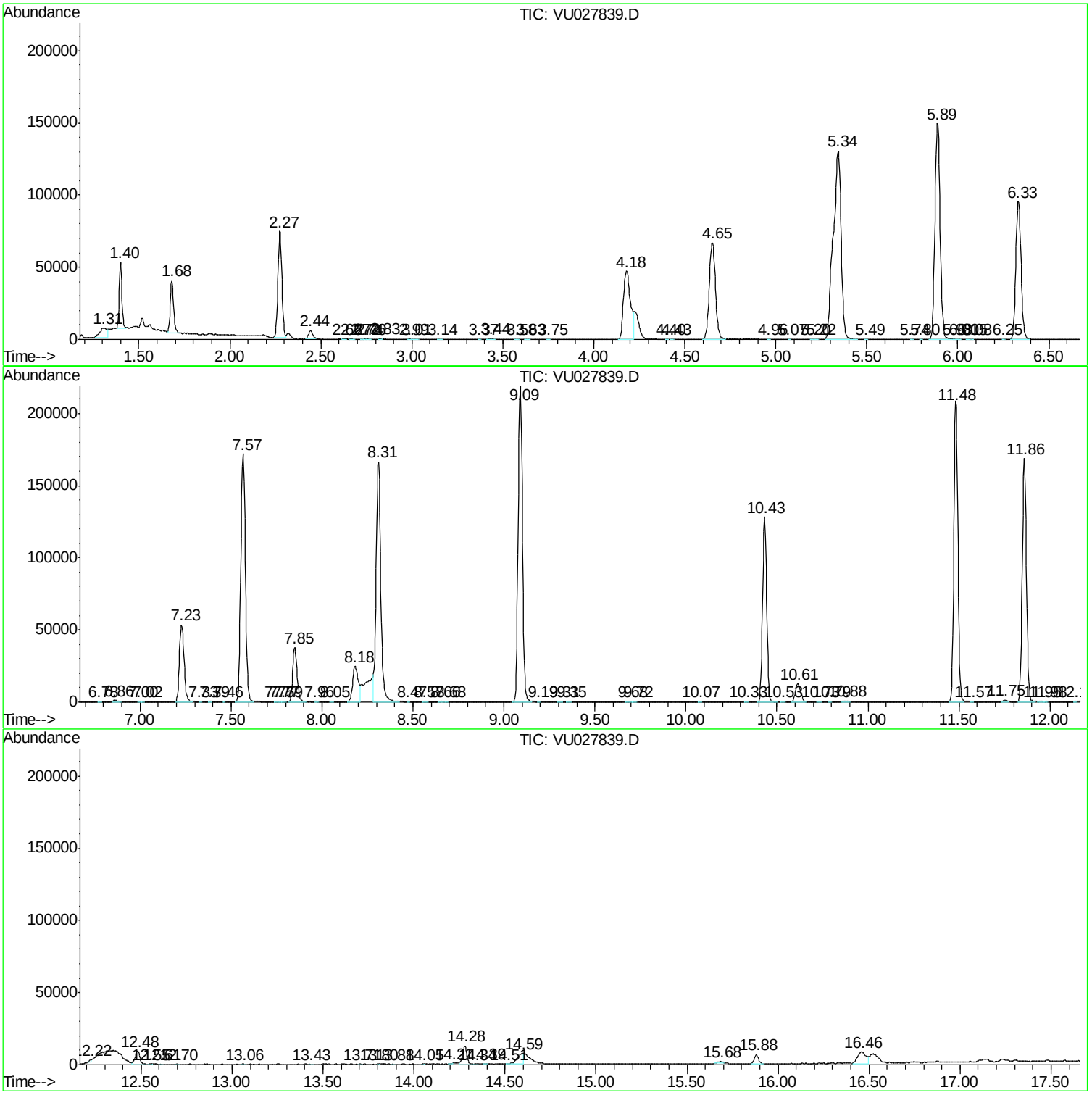
Sum of corrected areas: 3475005

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU102618\
Data File : VU027839.D
Acq On : 26 Oct 2018 17:24
Operator : MD/SY
Sample : J5668-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETBS4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027839.D
Acq On : 26 Oct 2018 17:24
Operator : MD/SY
Sample : J5668-13
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETBS4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

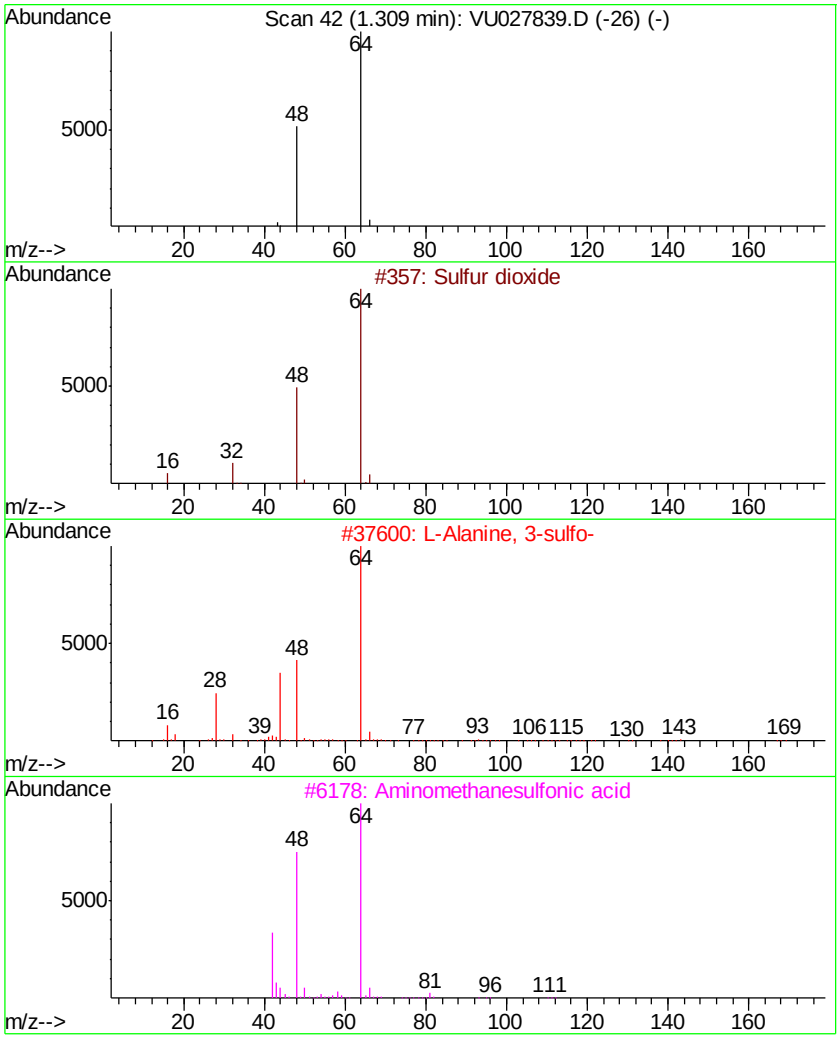
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

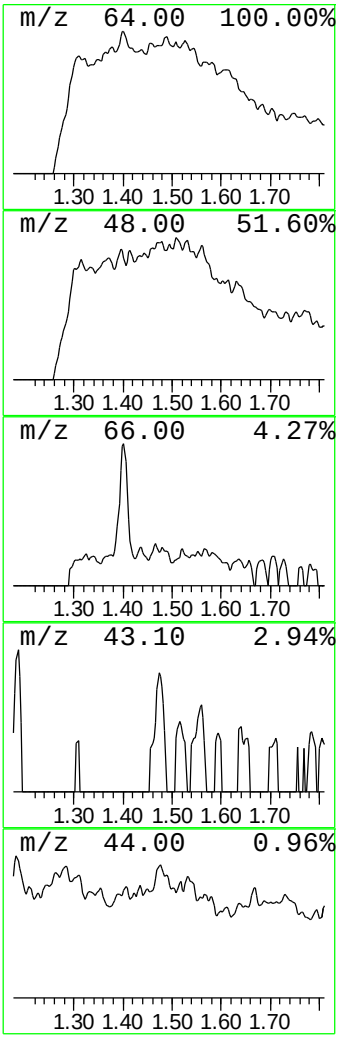
****

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.31	3.08 ug/L	18046	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	74
2	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU102618\
Data File : VU027839.D
Acq On : 26 Oct 2018 17:24
Operator : MD/SY
Sample : J5668-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETBS4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

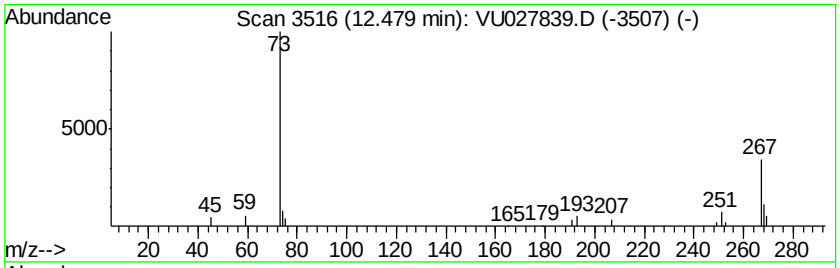
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

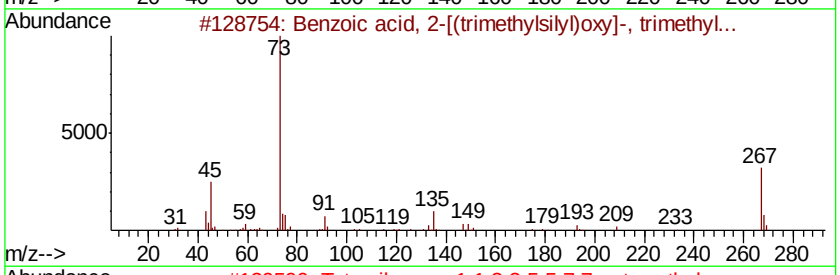
****

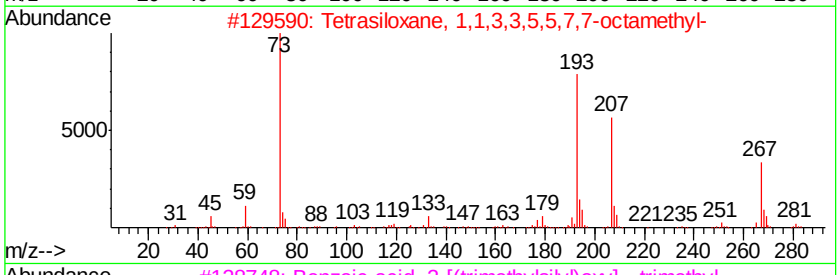
Peak Number 5 unknown-01 Concentration Rank 8

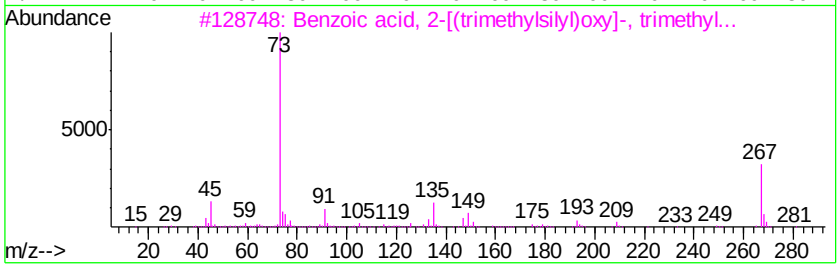
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	2.68 ug/L	17183	1,4-Dichlorobenzene-d4	11.48

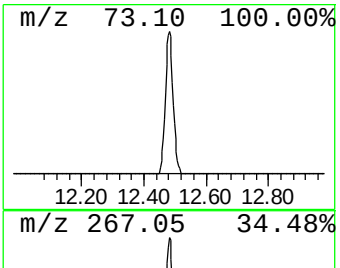
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	42
2	Tetrasiloxane, 1,1,3,3,5,5,7,7-o...	282	C8H26O3Si4	001000-05-1	38
3	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	36
4	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	36
5	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	9

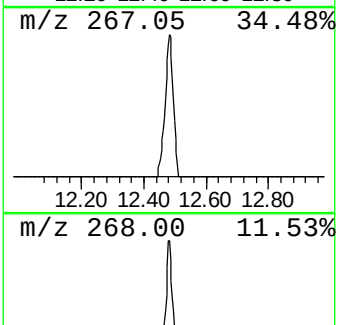


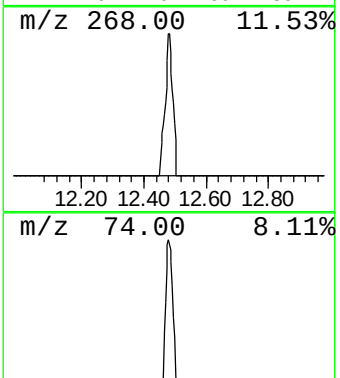


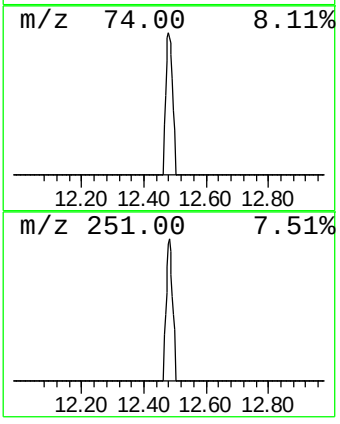












Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027839.D
Acq On : 26 Oct 2018 17:24
Operator : MD/SY
Sample : J5668-13
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETBS4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

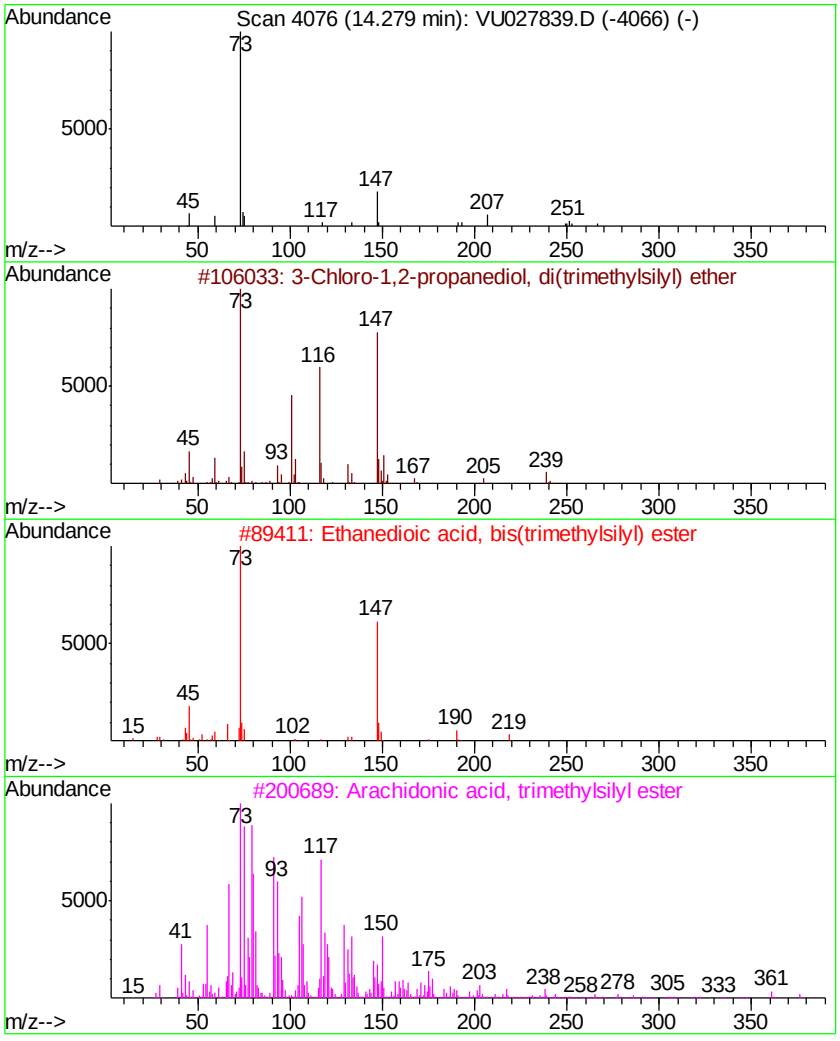
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

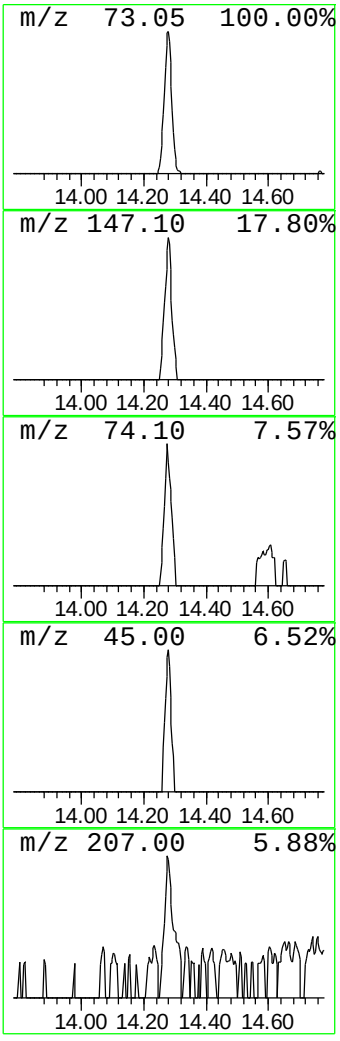
****

Peak Number 6 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	3.31 ug/L	21173	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-1,2-propanediol, di(tri...	254	C9H23ClO2Si2	073639-52-8	17
2	Ethanedioic acid, bis(trimethyls...	234	C8H18O4Si2	018294-04-7	17
3	Arachidonic acid, trimethylsilyl...	376	C23H40O2Si	113516-18-0	12
4	Spiro[2.4]hept-5-ene, 5-trimethy...	252	C14H28Si2	1000153-96-9	9
5	3,6,9-Trioxa-2,10-disilaundecane...	250	C10H26O3Si2	016654-74-3	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU102618\
Data File : VU027839.D
Acq On : 26 Oct 2018 17:24
Operator : MD/SY
Sample : J5668-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETBS4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

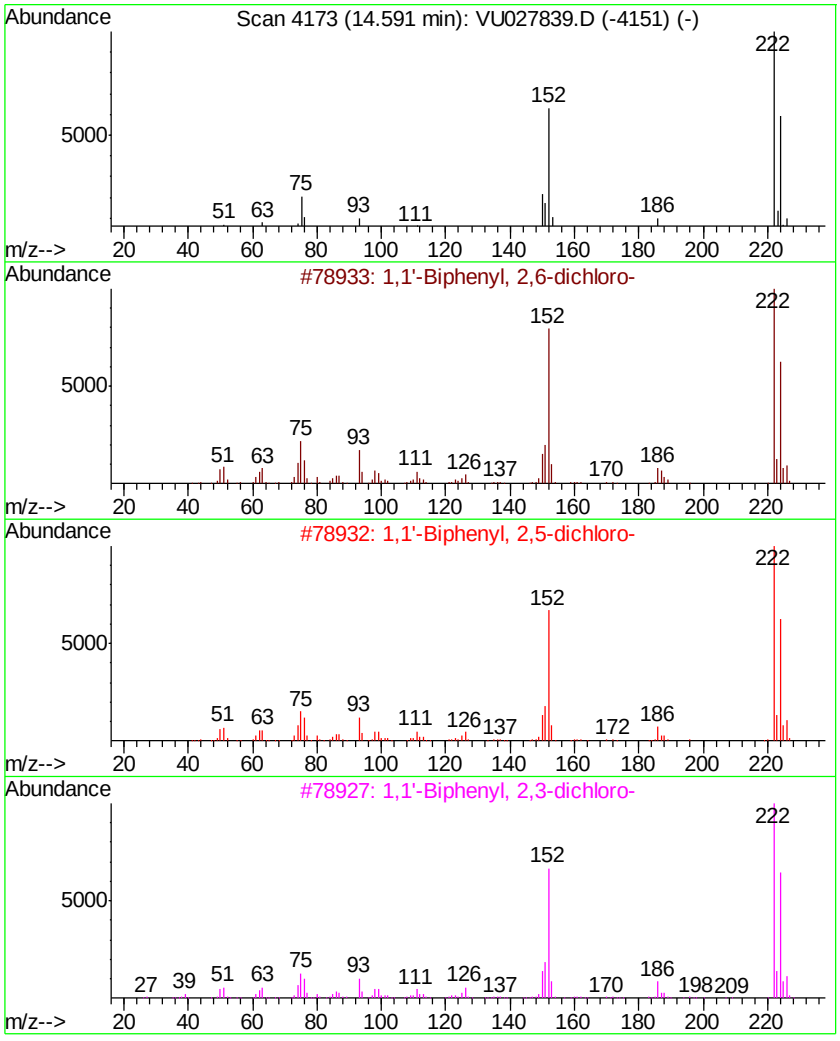
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

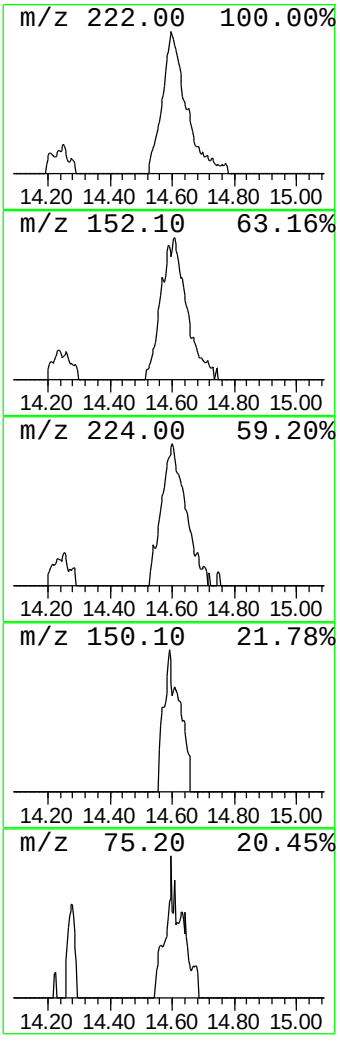
****

Peak Number 7 1,1'-Biphenyl, 2,6-dichloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.73 ug/L	17502	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,6-dichloro-	222	C12H8Cl2	033146-45-1	98
2	1,1'-Biphenyl, 2,5-dichloro-	222	C12H8Cl2	034883-39-1	97
3	1,1'-Biphenyl, 2,3-dichloro-	222	C12H8Cl2	016605-91-7	97
4	1,1'-Biphenyl, 3,3'-dichloro-	222	C12H8Cl2	002050-67-1	97
5	1,1'-Biphenyl, 4,4'-dichloro-	222	C12H8Cl2	002050-68-2	96





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027839.D
Acq On : 26 Oct 2018 17:24
Operator : MD/SY
Sample : J5668-13
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETBS4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

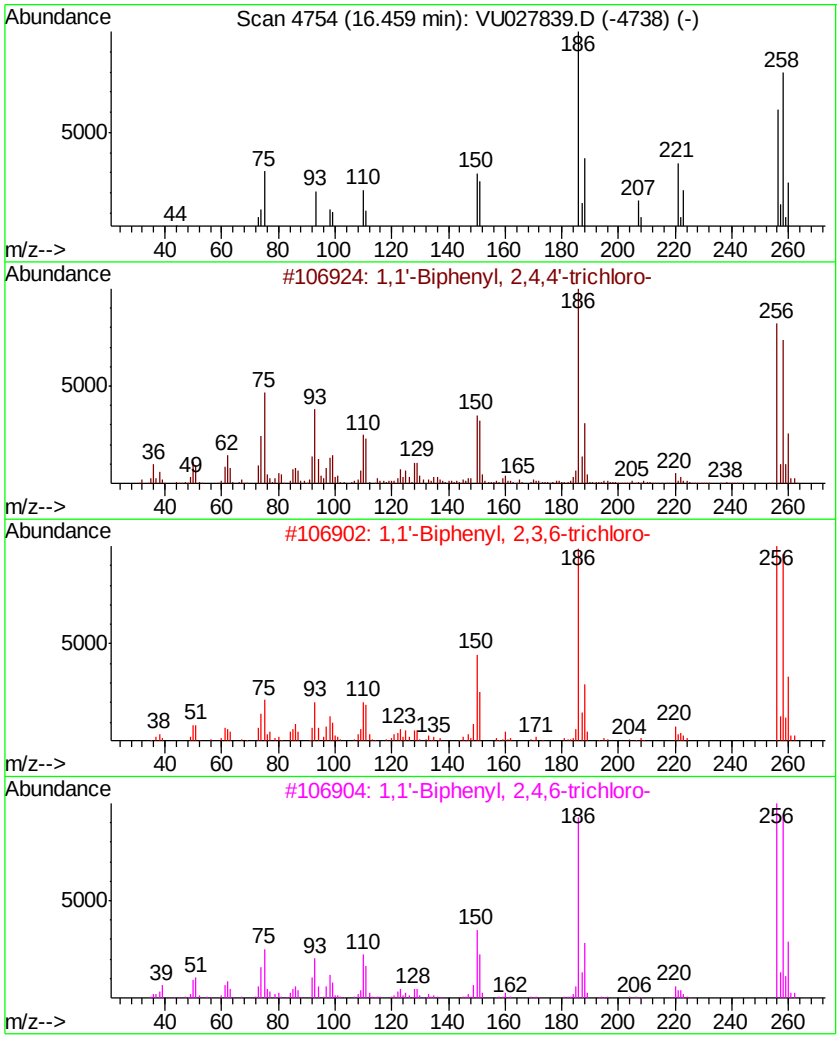
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

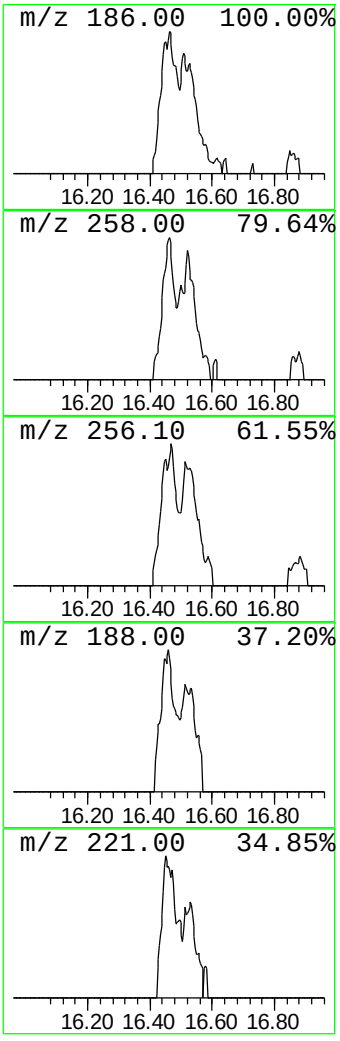
****

Peak Number 8 1,1'-Biphenyl, 2,4,4'-trich... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	4.08 ug/L	26134	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,4,4'-trichloro-	256	C12H7Cl3	007012-37-5	94
2	1,1'-Biphenyl, 2,3,6-trichloro-	256	C12H7Cl3	055702-45-9	89
3	1,1'-Biphenyl, 2,4,6-trichloro-	256	C12H7Cl3	035693-92-6	89
4	1,1'-Biphenyl, 2,4',5-trichloro-	256	C12H7Cl3	016606-02-3	86
5	1,1'-Biphenyl, 2,2',5-trichloro-	256	C12H7Cl3	037680-65-2	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU102618\
Data File : VU027839.D
Acq On : 26 Oct 2018 17:24
Operator : MD/SY
Sample : J5668-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETBS4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.31	3.1	ug/L	18046	1	5.89	293133	50.0
unknown-01	12.48	2.7	ug/L	17183	3	11.48	320022	50.0
unknown-02	14.28	3.3	ug/L	21173	3	11.48	320022	50.0
1,1'-Biphenyl, 2,...	14.59	2.7	ug/L	17502	3	11.48	320022	50.0
1,1'-Biphenyl, 2,...	16.46	4.1	ug/L	26134	3	11.48	320022	50.0