LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054144.D
Acq On : 10 May 2023 14:50
Operator : JC/MD
Sample : 02694-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : JREP8

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\SFAMULM042923WMA.M
Title : VOC Analysis

Signal : TIC: VU054144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	98	rVB	95537	116708	10.96%	1.429%
2	1.684	99	107	131	rBV	305731	404734	38.02%	4.955%
3	1.909	169	177	200	rVB	74453	105506	9.91%	1.292%
4	2.372	290	321	361	rBV2	191505	1064555	100.00%	13.032%
5	2.945	497	499	501	rBV2	628	361	0.03%	0.004%
6	3.128	551	556	557	rBV	178	138	0.01%	0.002%
7	3.138	557	559	561	rBV	229	88	0.01%	0.001%
8	3.311	608	613	615	rBV3	464	466	0.04%	0.006%
9	3.440	651	653	656	rBV	322	176	0.02%	0.002%
10	3.475	660	664	669	rVB	229	176	0.02%	0.002%
11	3.494	669	670	671	rBV	119	24	0.00%	0.000%
12	3.575	689	695	697	rBV3	998	1101	0.10%	0.013%
13	3.694	730	732	733	rBV	279	96	0.01%	0.001%
14	3.745	747	748	753	rVB	173	94	0.01%	0.001%
15	3.781	756	759	763	rBV	210	143	0.01%	0.002%
16	3.874	786	788	789	rVB	231	76	0.01%	0.001%
17	3.896	792	795	801	rVV2	372	321	0.03%	0.004%
18	3.983	817	822	823	rBV	305	230	0.02%	0.003%
19	4.134	835	869	895	rBV6	20635	117943	11.08%	1.444%
20	4.620	1009	1020	1042	rBV2	62590	157595	14.80%	1.929%
21	5.057	1138	1156	1176	rBV	159007	351041	32.98%	4.297%
22	5.285	1223	1227	1229	rBV	176	159	0.01%	0.002%
23	5.408	1262	1265	1270	rBV	374	445	0.04%	0.005%
24	5.453	1276	1279	1282	rVB2	129	95	0.01%	0.001%
25	5.504	1293	1295	1300	rVB	175	63	0.01%	0.001%
26	5.626	1331	1333	1334	rBV	226	98	0.01%	0.001%
27	5.645	1338	1339	1340	rBB	102	20	0.00%	0.000%
28	5.719	1340	1362	1390	rBV2	307341	861753	80.95%	10.549%
29	5.912	1420	1422	1429	rVB3	675	623	0.06%	0.008%
30	5.961	1431	1437	1449	rVV5	1575	2909	0.27%	0.036%
31	6.031	1458	1459	1463	rVB2	338	180	0.02%	0.002%
32	6.054	1463	1466	1468	rBV2	277	180	0.02%	0.002%
33	6.112	1481	1484	1486	rBV2	201	152	0.01%	0.002%
34	6.128	1486	1489	1490	rBV	593	376	0.04%	0.005%
35	6.243	1512	1525	1544	rBV	307078	587530	55.19%	7.192%
36	6.465	1591	1594	1598	rBV	191	119	0.01%	0.001%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054144.D
Acq On : 10 May 2023 14:50
Operator : JC/MD
Sample : 02694-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP8

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\SFAMULM042923WMA.M
Title : VOC Analysis

37	6.488	1598	1601	1605	rBV3	324	275	0.03%	0.003%
38	6.523	1606	1612	1618	rBV5	2081	3157	0.30%	0.039%
39	6.684	1649	1662	1684	rBV	196892	387484	36.40%	4.743%
40	7.044	1771	1774	1777	rVB	456	319	0.03%	0.004%
41	7.089	1785	1788	1789	rBV	183	83	0.01%	0.001%
42	7.163	1808	1811	1814	rBV	348	310	0.03%	0.004%
43	7.182	1814	1817	1822	rVV3	483	520	0.05%	0.006%
44	7.324	1859	1861	1864	rBV	175	115	0.01%	0.001%
45	7.562	1923	1935	1954	rBV	111269	198672	18.66%	2.432%
46	7.690	1973	1975	1977	rBV2	281	91	0.01%	0.001%
47	7.790	1998	2006	2020	rVB4	5682	9917	0.93%	0.121%
48	7.893	2025	2038	2052	rBV	393812	685817	64.42%	8.396%
49	8.083	2093	2097	2100	rBV2	370	256	0.02%	0.003%
50	8.173	2111	2125	2147	rBV	81595	140587	13.21%	1.721%
51	8.407	2195	2198	2202	rVB3	316	217	0.02%	0.003%
52	8.430	2202	2205	2207	rBV2	181	107	0.01%	0.001%
53	8.465	2209	2216	2222	rBV5	1602	2629	0.25%	0.032%
54	8.629	2256	2267	2297	rBV2	190611	373366	35.07%	4.571%
55	8.780	2311	2314	2316	rBV4	1024	716	0.07%	0.009%
56	8.877	2342	2344	2345	rBV	176	75	0.01%	0.001%
57	8.941	2361	2364	2366	rBV2	213	127	0.01%	0.002%
58	8.951	2366	2367	2369	rBV	188	90	0.01%	0.001%
59	9.018	2386	2388	2389	rBV	172	56	0.01%	0.001%
60	9.063	2400	2402	2403	rBV	128	33	0.00%	0.000%
61	9.263	2461	2464	2467	rBV2	320	198	0.02%	0.002%
62	9.295	2471	2474	2477	rBV	241	194	0.02%	0.002%
63	9.411	2497	2510	2529	rBV	432849	717040	67.36%	8.778%
64	9.616	2571	2574	2577	rBV	329	245	0.02%	0.003%
65	9.661	2586	2588	2590	rBV	201	129	0.01%	0.002%
66	9.919	2665	2668	2671	rBV	327	299	0.03%	0.004%
67	9.960	2679	2681	2684	rVB2	371	136	0.01%	0.002%
68	9.980	2685	2687	2692	rVB	222	112	0.01%	0.001%
69	9.999	2692	2693	2696	rBV	132	51	0.00%	0.001%
70	10.060	2711	2712	2714	rBV	122	68	0.01%	0.001%
71	10.105	2722	2726	2742	rVB8	1823	3538	0.33%	0.043%
72	10.240	2764	2768	2773	rBV2	558	624	0.06%	0.008%
73	10.475	2837	2841	2843	rBV2	237	148	0.01%	0.002%
74	10.748	2915	2926	2941	rBV	268777	439058	41.24%	5.375%
75	10.880	2964	2967	2968	rBV	293	170	0.02%	0.002%
76	11.115	3038	3040	3042	rBV2	406	183	0.02%	0.002%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054144.D
Acq On : 10 May 2023 14:50
Operator : JC/MD
Sample : 02694-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP8

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\SFAMULM042923WMA.M
Title : VOC Analysis

77	11.292	3091	3095	3099	rBV	345	340	0.03%	0.004%
78	11.542	3169	3173	3176	rBV2	423	331	0.03%	0.004%
79	11.591	3185	3188	3191	rBV	365	213	0.02%	0.003%
80	11.806	3243	3255	3273	rBV	459585	728301	68.41%	8.916%
81	11.915	3286	3289	3293	rVB3	762	582	0.05%	0.007%
82	12.063	3331	3335	3336	rBV	399	229	0.02%	0.003%
83	12.189	3360	3374	3398	rBV	424206	694280	65.22%	8.499%
84	12.558	3487	3489	3490	rBV	333	153	0.01%	0.002%
85	13.735	3853	3855	3858	rBV3	379	190	0.02%	0.002%
86	13.793	3869	3873	3878	rBV3	413	443	0.04%	0.005%
87	14.449	4074	4077	4079	rBV	506	299	0.03%	0.004%

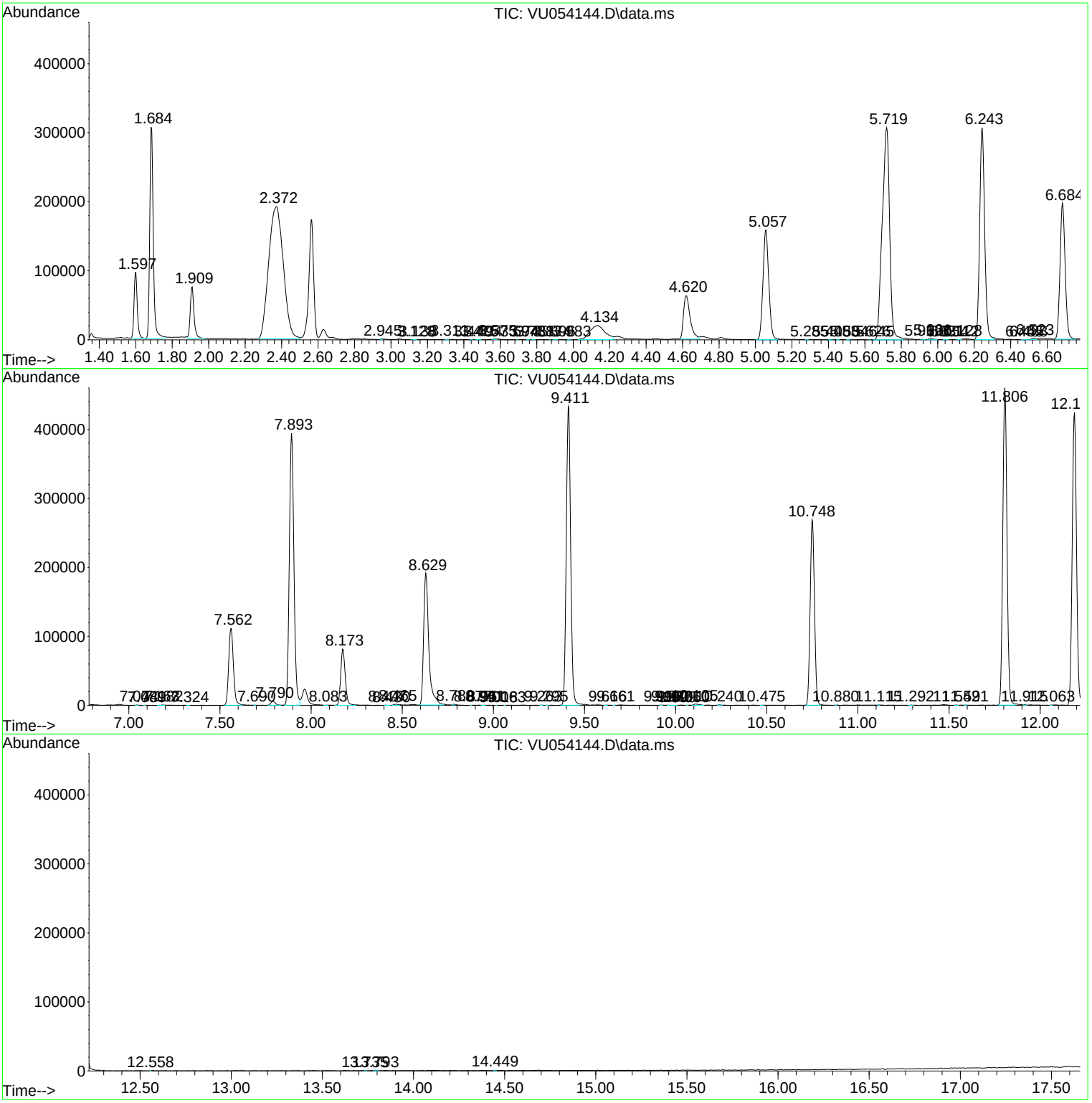
Sum of corrected areas: 8168847

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054144.D
Acq On : 10 May 2023 14:50
Operator : JC/MD
Sample : 02694-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054144.D
Acq On : 10 May 2023 14:50
Operator : JC/MD
Sample : 02694-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

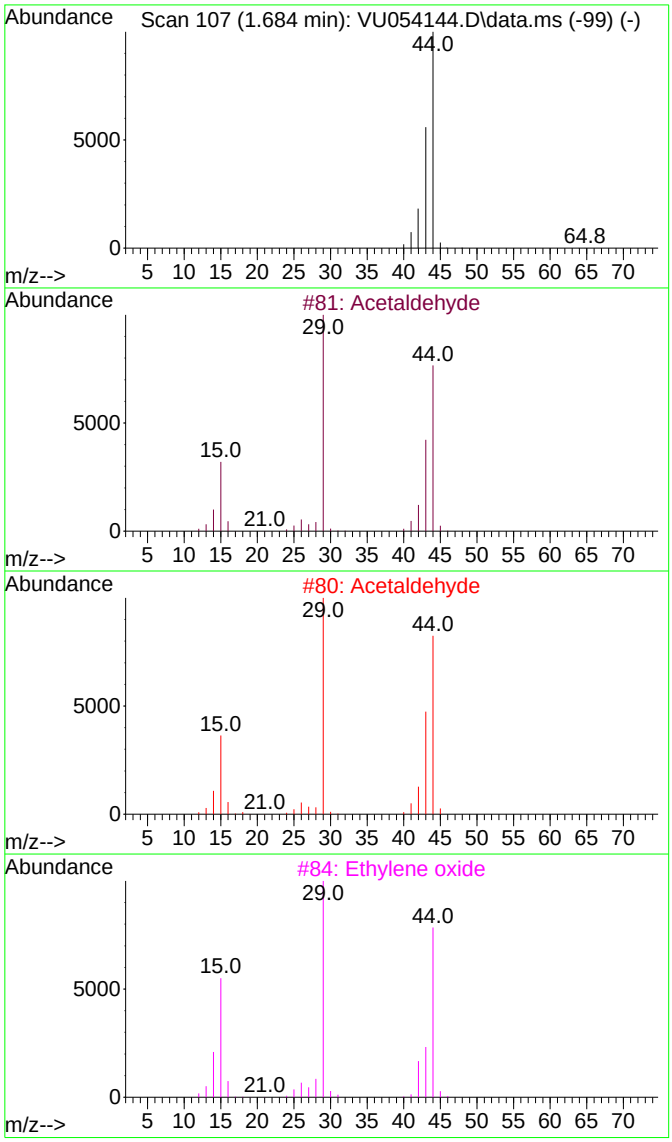
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

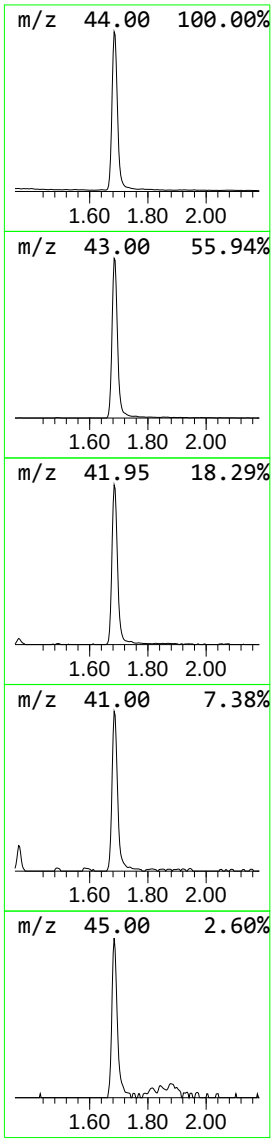
****

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.684	34.44 ug/L	404734	1,4-Difluorobenzene	6.243

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Acetaldehyde	44	C2H4O	000075-07-0	74
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Ethylene oxide	44	C2H4O	000075-21-8	5
5	Ethylene oxide	44	C2H4O	000075-21-8	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054144.D
Acq On : 10 May 2023 14:50
Operator : JC/MD
Sample : 02694-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP8

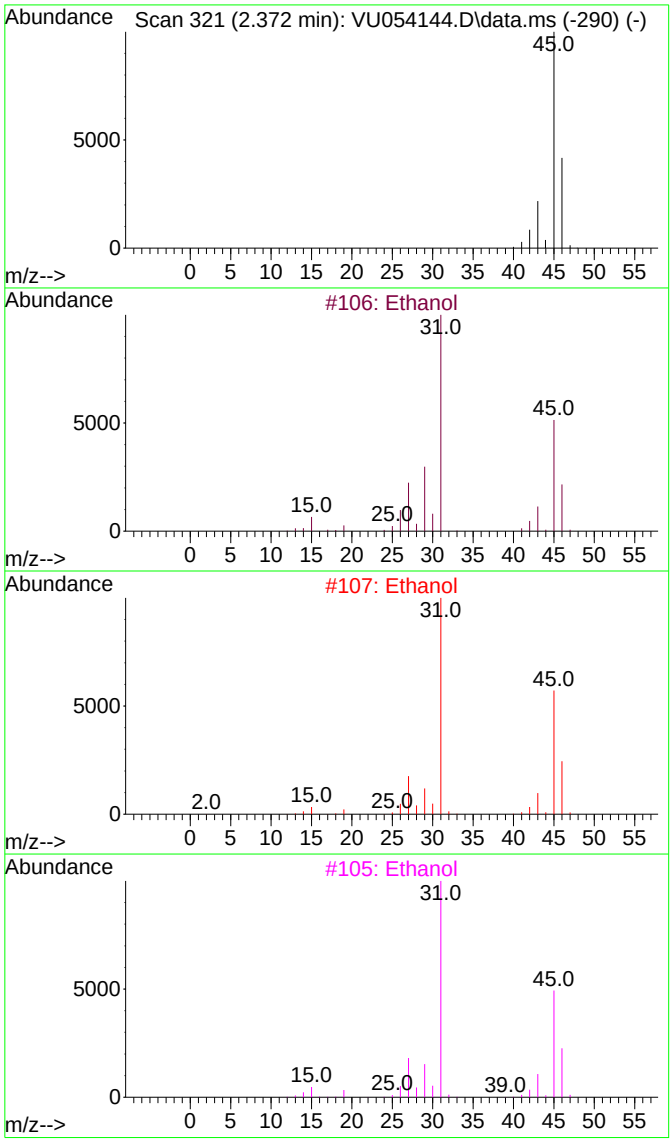
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

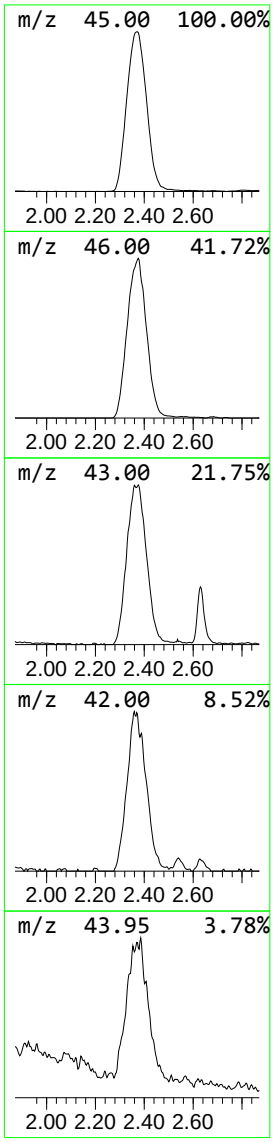
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.372	90.60 ug/L	1064560	1,4-Difluorobenzene	6.243

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
2	Ethanol	46	C2H6O	000064-17-5	74
3	Ethanol	46	C2H6O	000064-17-5	64
4	Dimethyl ether	46	C2H6O	000115-10-6	9
5	Ethanol	46	C2H6O	000064-17-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054144.D
Acq On : 10 May 2023 14:50
Operator : JC/MD
Sample : 02694-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

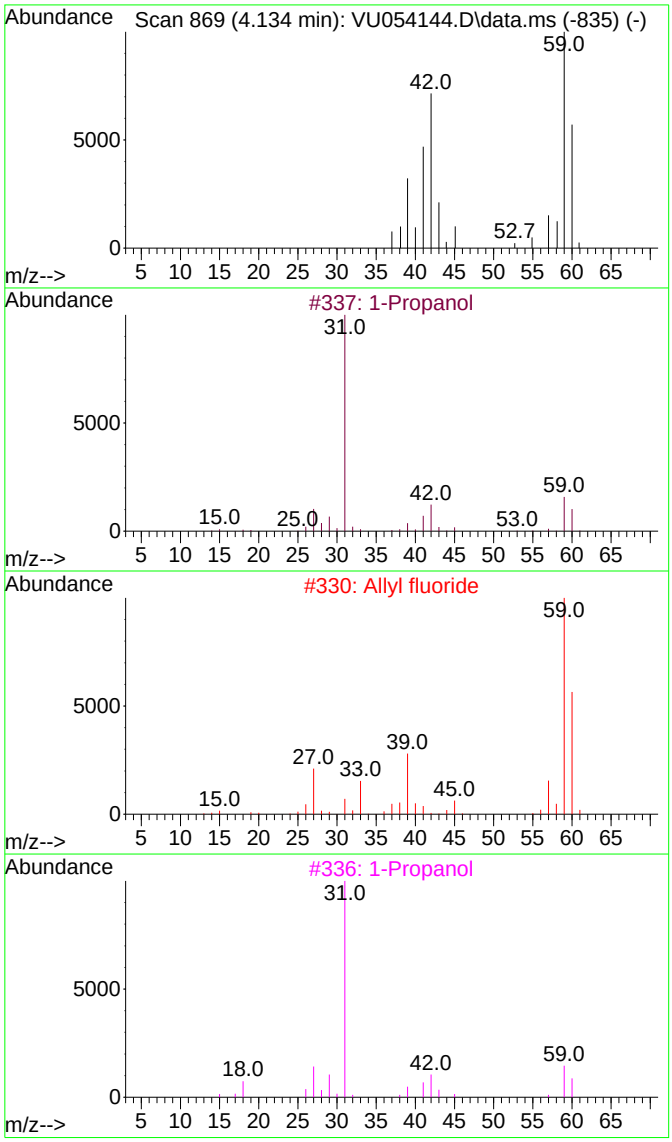
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

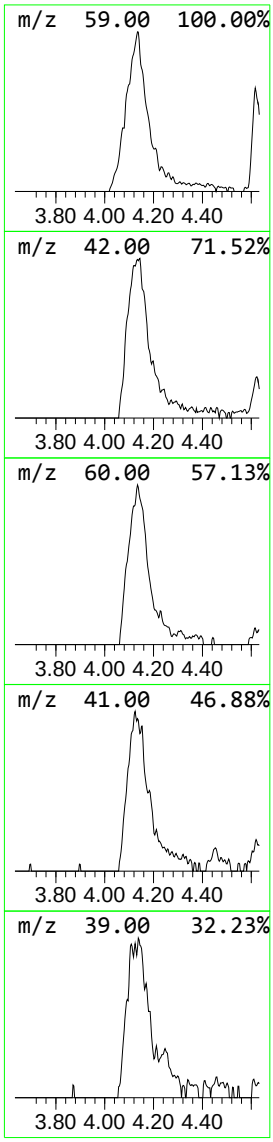
****

Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.134	10.04 ug/L	117943	1,4-Difluorobenzene	6.243

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	64
2	Allyl fluoride	60	C3H5F	000818-92-8	64
3	1-Propanol	60	C3H8O	000071-23-8	64
4	2-Fluoropropene	60	C3H5F	001184-60-7	58
5	1-Propanol	60	C3H8O	000071-23-8	56





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054144.D
Acq On : 10 May 2023 14:50
Operator : JC/MD
Sample : 02694-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetaldehyde	1.684	34.4	ug/L	404734	1	6.243	587530	50.0
Ethanol	2.372	90.6	ug/L	1064560	1	6.243	587530	50.0
1-Propanol	4.134	10.0	ug/L	117943	1	6.243	587530	50.0