LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054142.D
Acq On : 10 May 2023 14:03
Operator : JC/MD
Sample : 02694-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP6

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: VU054142.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	96	rVB	94827	115169	10.60%	1.409%
2	1.684	98	107	127	rBV	377384	486904	44.83%	5.959%
3	1.909	169	177	191	rVB	75342	104642	9.63%	1.281%
4	2.347	289	313	354	rBV2	235774	1086149	100.00%	13.292%
5	3.038	523	528	529	rBV	1198	930	0.09%	0.011%
6	3.221	582	585	586	rBV	189	85	0.01%	0.001%
7	3.237	587	590	592	rVV2	303	201	0.02%	0.002%
8	3.263	596	598	599	rBV	206	92	0.01%	0.001%
9	3.501	670	672	676	rVB	167	90	0.01%	0.001%
10	3.527	677	680	682	rBV	195	93	0.01%	0.001%
11	3.562	687	691	692	rBV2	838	511	0.05%	0.006%
12	3.713	733	738	741	rBV2	274	258	0.02%	0.003%
13	3.826	770	773	779	rBV2	235	222	0.02%	0.003%
14	3.855	779	782	784	rBV2	148	128	0.01%	0.002%
15	3.935	804	807	811	rBV	293	285	0.03%	0.003%
16	4.099	833	858	891	rBV8	22901	124848	11.49%	1.528%
17	4.433	954	962	963	rBV3	895	1152	0.11%	0.014%
18	4.536	991	994	995	rBV	718	357	0.03%	0.004%
19	4.617	1009	1019	1041	rBV	66351	159888	14.72%	1.957%
20	5.057	1140	1156	1181	rBV	158438	350684	32.29%	4.292%
21	5.350	1244	1247	1248	rBV	117	51	0.00%	0.001%
22	5.382	1256	1257	1258	rBV	104	25	0.00%	0.000%
23	5.414	1262	1267	1270	rBV3	330	263	0.02%	0.003%
24	5.501	1292	1294	1296	rVB	130	30	0.00%	0.000%
25	5.546	1302	1308	1312	rBV2	146	180	0.02%	0.002%
26	5.565	1312	1314	1317	rBV2	121	67	0.01%	0.001%
27	5.588	1319	1321	1323	rVB	125	30	0.00%	0.000%
28	5.719	1341	1362	1386	rBV2	308469	848533	78.12%	10.384%
29	5.932	1426	1428	1429	rBV	319	137	0.01%	0.002%
30	5.967	1432	1439	1441	rBV3	1412	1497	0.14%	0.018%
31	6.099	1479	1480	1484	rVB	150	46	0.00%	0.001%
32	6.150	1487	1496	1497	rBV4	1554	1986	0.18%	0.024%
33	6.244	1512	1525	1548	rBV	298374	565835	52.10%	6.925%
34	6.453	1588	1590	1597	rVB2	608	647	0.06%	0.008%
35	6.488	1598	1601	1604	rBV	346	276	0.03%	0.003%
36	6.526	1604	1613	1614	rBV4	2599	2892	0.27%	0.035%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054142.D
Acq On : 10 May 2023 14:03
Operator : JC/MD
Sample : 02694-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP6

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	6.684	1650	1662	1678	rBV	195340	379584	34.95%	4.645%
38	6.883	1719	1724	1726	rBV3	1082	828	0.08%	0.010%
39	6.935	1735	1740	1742	rBV3	889	869	0.08%	0.011%
40	7.102	1790	1792	1795	rVB2	209	112	0.01%	0.001%
41	7.160	1805	1810	1812	rBV2	563	448	0.04%	0.005%
42	7.189	1817	1819	1825	rVB2	829	615	0.06%	0.008%
43	7.269	1841	1844	1850	rBV	230	187	0.02%	0.002%
44	7.298	1850	1853	1855	rBV2	158	114	0.01%	0.001%
45	7.375	1876	1877	1878	rBV2	137	39	0.00%	0.000%
46	7.398	1883	1884	1885	rBV2	163	51	0.00%	0.001%
47	7.462	1901	1904	1910	rVB2	249	241	0.02%	0.003%
48	7.559	1920	1934	1951	rBV	110753	199078	18.33%	2.436%
49	7.697	1974	1977	1979	rBV2	521	415	0.04%	0.005%
50	7.790	1996	2006	2018	rBV5	5947	10974	1.01%	0.134%
51	7.893	2025	2038	2053	rBV	390385	689069	63.44%	8.433%
52	8.176	2113	2126	2144	rBV	81423	137700	12.68%	1.685%
53	8.356	2179	2182	2183	rBV	187	100	0.01%	0.001%
54	8.420	2199	2202	2206	rBV2	450	277	0.03%	0.003%
55	8.465	2209	2216	2217	rBV3	1592	1550	0.14%	0.019%
56	8.629	2255	2267	2299	rBV2	189463	370364	34.10%	4.532%
57	8.854	2335	2337	2339	rVB	163	48	0.00%	0.001%
58	8.967	2370	2372	2373	rBV	174	78	0.01%	0.001%
59	8.983	2373	2377	2380	rVV3	376	298	0.03%	0.004%
60	9.147	2424	2428	2430	rBV	266	210	0.02%	0.003%
61	9.227	2450	2453	2454	rBV	227	115	0.01%	0.001%
62	9.282	2468	2470	2472	rBV	202	106	0.01%	0.001%
63	9.411	2498	2510	2536	rBV	414779	694600	63.95%	8.500%
64	9.600	2566	2569	2573	rBV3	427	286	0.03%	0.004%
65	9.632	2575	2579	2582	rBV2	477	417	0.04%	0.005%
66	9.694	2590	2598	2602	rBV4	653	925	0.09%	0.011%
67	9.835	2639	2642	2645	rBV	257	207	0.02%	0.003%
68	10.079	2715	2718	2720	rBV	211	143	0.01%	0.002%
69	10.115	2725	2729	2738	rVB5	1466	1955	0.18%	0.024%
70	10.237	2765	2767	2769	rBV	470	185	0.02%	0.002%
71	10.333	2795	2797	2801	rBV2	235	152	0.01%	0.002%
72	10.401	2816	2818	2820	rBV	198	131	0.01%	0.002%
73	10.694	2906	2909	2914	rVB	378	241	0.02%	0.003%
74	10.751	2914	2927	2949	rBV	272346	437932	40.32%	5.359%
75	10.864	2959	2962	2964	rBV	166	131	0.01%	0.002%
76	10.944	2984	2987	2991	rBV	264	219	0.02%	0.003%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054142.D
Acq On : 10 May 2023 14:03
Operator : JC/MD
Sample : 02694-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP6

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	11.806	3243	3255	3276	rBV	448362	700802	64.52%	8.576%
78	11.996	3310	3314	3320	rBV2	505	353	0.03%	0.004%
79	12.189	3361	3374	3396	rBV	417453	682091	62.80%	8.347%
80	12.484	3464	3466	3468	rBV2	265	121	0.01%	0.001%
81	12.648	3515	3517	3519	rBV	291	132	0.01%	0.002%
82	12.822	3568	3571	3575	rBV	298	233	0.02%	0.003%
83	13.021	3630	3633	3636	rBV2	502	448	0.04%	0.005%
84	13.320	3723	3726	3729	rBV2	448	288	0.03%	0.004%
85	13.388	3743	3747	3749	rBV	474	388	0.04%	0.005%
86	13.619	3815	3819	3820	rBV2	492	352	0.03%	0.004%

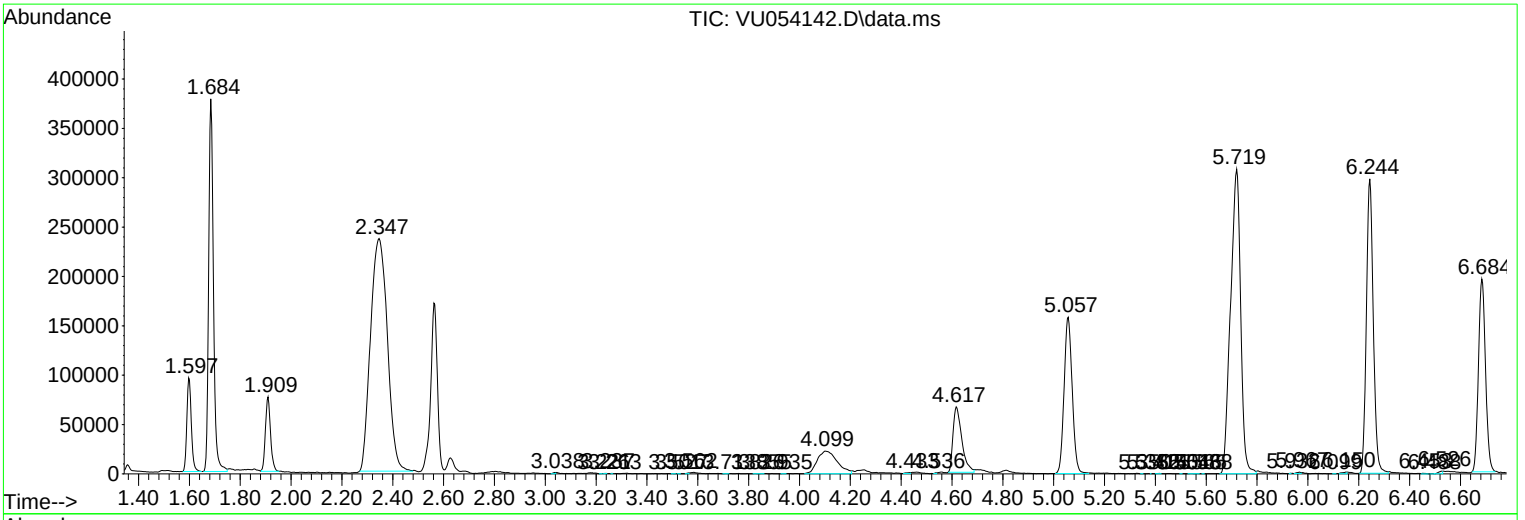
Sum of corrected areas: 8171385

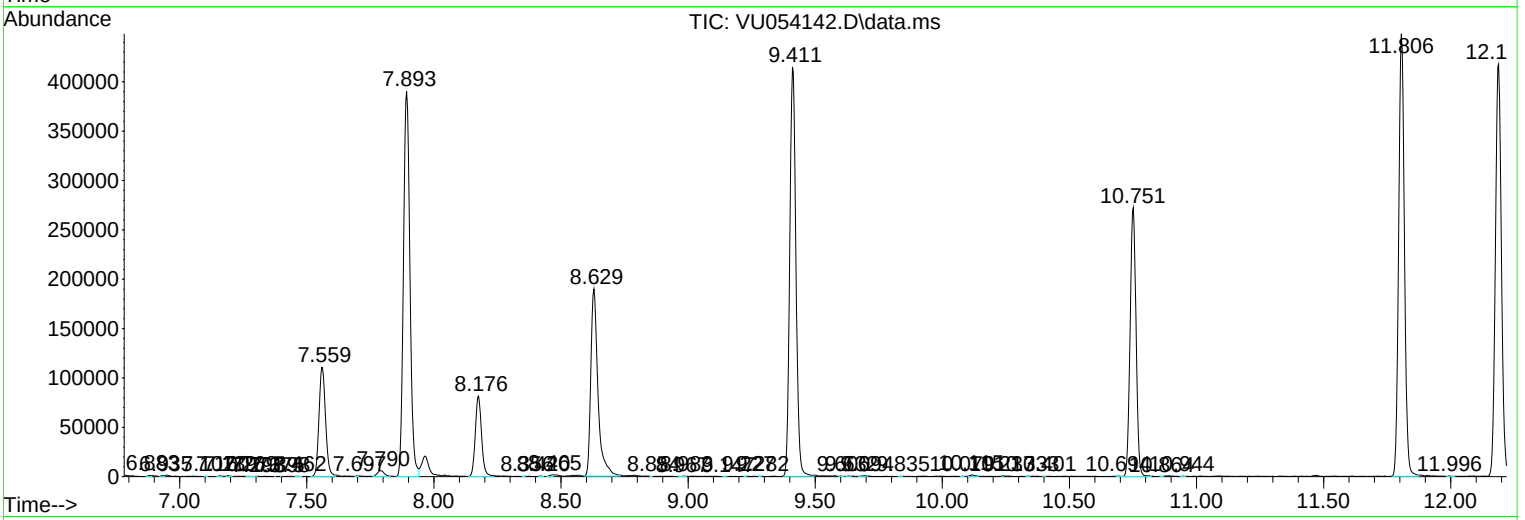
Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054142.D
Acq On : 10 May 2023 14:03
Operator : JC/MD
Sample : 02694-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

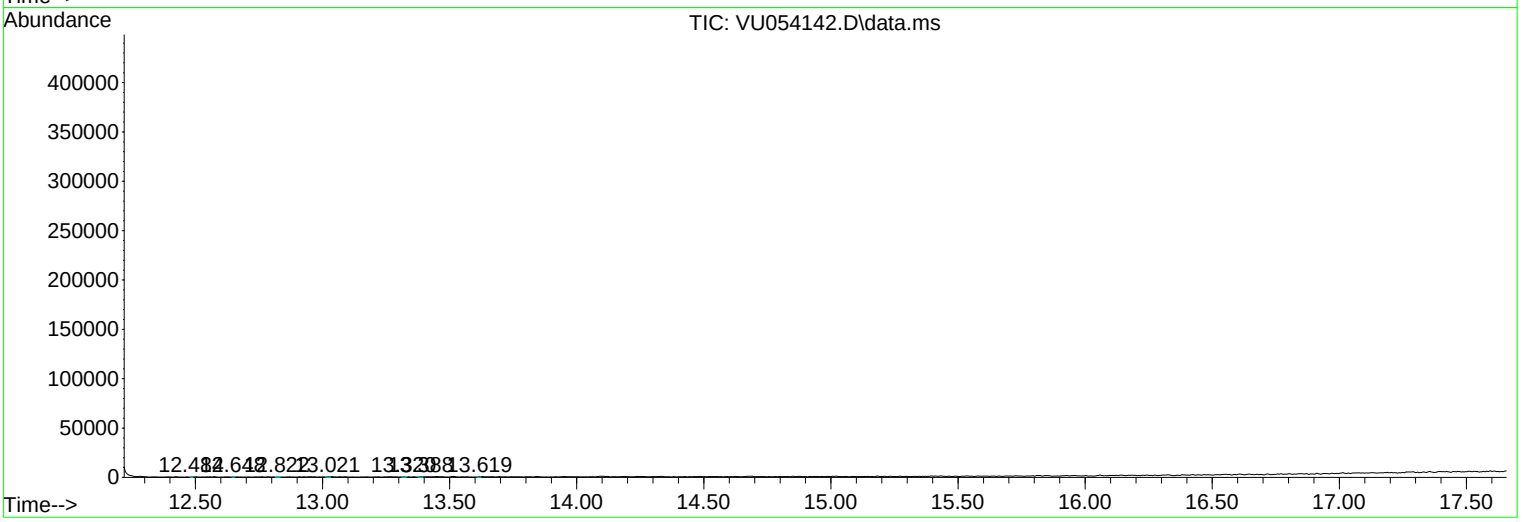
Instrument :
MSVOA_U
ClientSampleId :
JREP6

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 : VU054142.D
Acq On : 10 May 2023 14:03
Operator : JC/MD
Sample : 02694-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP6

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

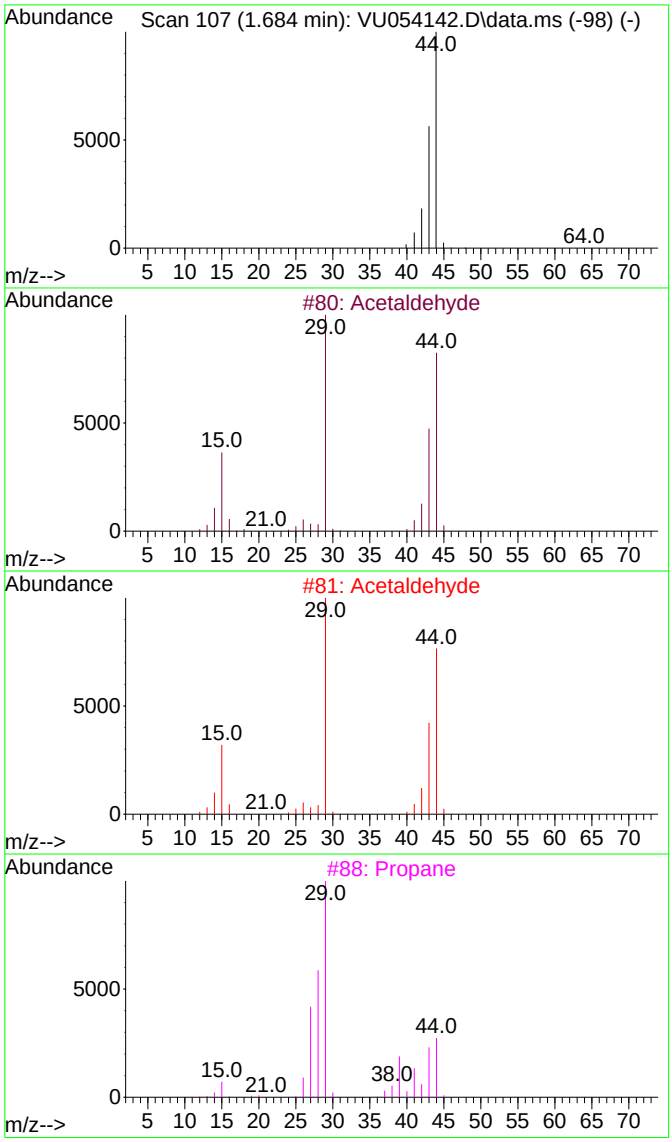
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

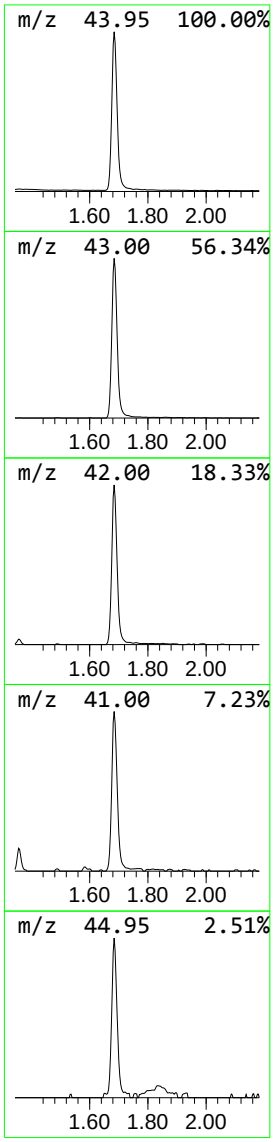
****

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.684	43.03 ug/L	486904	1,4-Difluorobenzene	6.244

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	9
2	Acetaldehyde	44	C2H4O	000075-07-0	9
3	Propane	44	C3H8	000074-98-6	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 : VU054142.D
Acq On : 10 May 2023 14:03
Operator : JC/MD
Sample : 02694-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP6

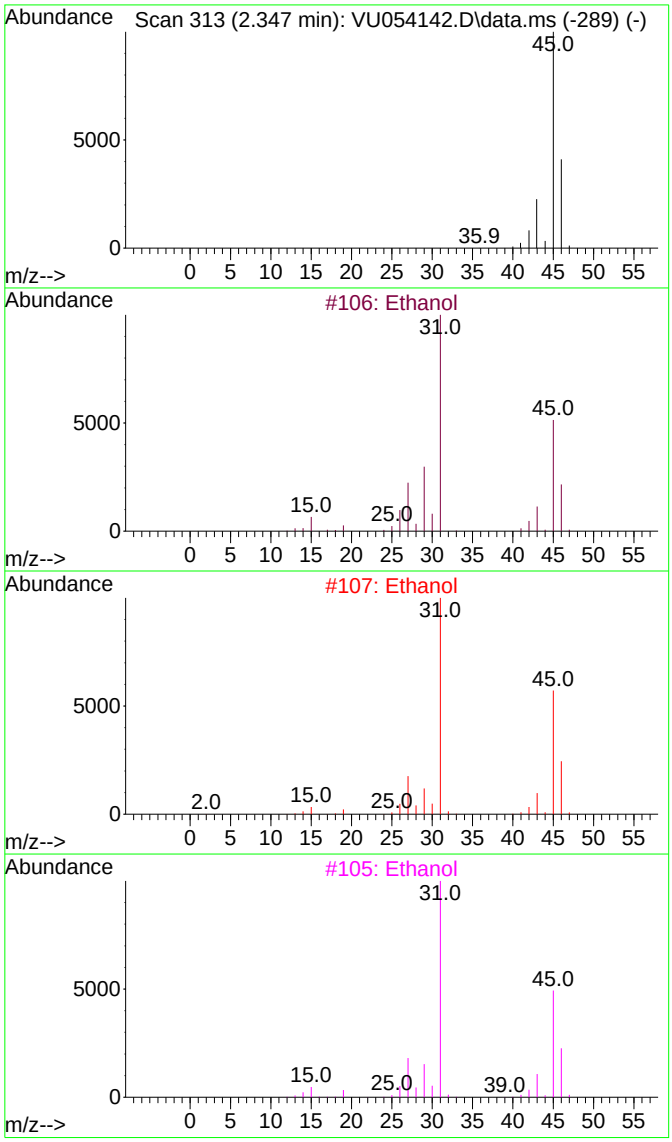
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

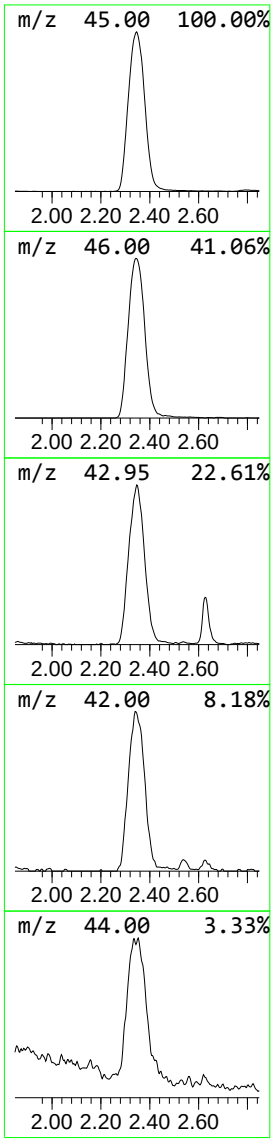
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.347	95.98 ug/L	1086150	1,4-Difluorobenzene	6.244

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	Ethanol	46	C2H6O	000064-17-5	9
5	Dimethyl ether	46	C2H6O	000115-10-6	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054142.D
Acq On : 10 May 2023 14:03
Operator : JC/MD
Sample : 02694-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP6

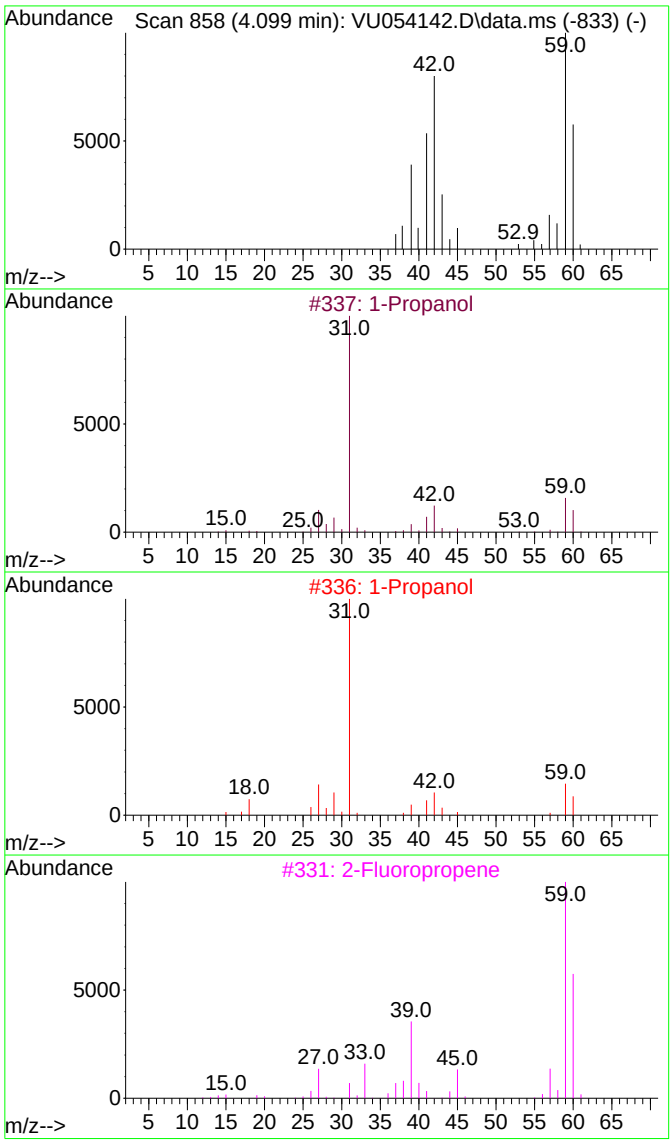
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

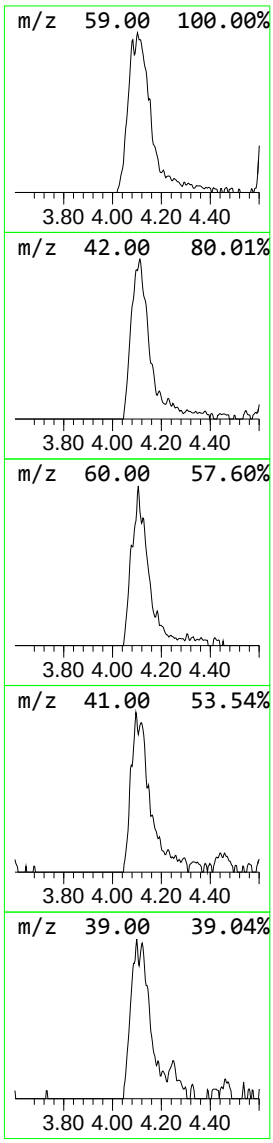
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.099	11.03 ug/L	124848	1,4-Difluorobenzene	6.244

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	64
2	1-Propanol	60	C3H8O	000071-23-8	59
3	2-Fluoropropene	60	C3H5F	001184-60-7	52
4	2-Fluoropropene	60	C3H5F	001184-60-7	50
5	Allyl fluoride	60	C3H5F	000818-92-8	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
Data File : VU054142.D
Acq On : 10 May 2023 14:03
Operator : JC/MD
Sample : 02694-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JREP6

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
unknown-01	1.684	43.0	ug/L	486904	1	6.244	565835	50.0
Ethanol	2.347	96.0	ug/L	1086150	1	6.244	565835	50.0
1-Propanol	4.099	11.0	ug/L	124848	1	6.244	565835	50.0