LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
Data File : VU051985.D
Acq On : 20 Nov 2022 19:58
Operator : JC/MD
Sample : N5710-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0KY9

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\SFAMULM111522WMA.M
Title : VOC Analysis

Signal : TIC: VU051985.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	22	rVB	140688	143209	0.43%	0.186%
2	1.491	42	47	53	rVB3	10989	11403	0.03%	0.015%
3	1.604	71	82	96	rBV	1643158	1990798	5.93%	2.579%
4	1.729	117	121	126	rVB	15569	13928	0.04%	0.018%
5	1.906	167	176	195	rVV	118558	181412	0.54%	0.235%
6	1.986	197	201	212	rVB2	10628	14362	0.04%	0.019%
7	2.154	246	253	261	rBV2	16599	23038	0.07%	0.030%
8	2.202	262	268	275	rVV2	11228	16100	0.05%	0.021%
9	2.244	276	281	288	rVB2	7367	8695	0.03%	0.011%
10	2.578	365	385	420	rBV	3660031	6136828	18.27%	7.950%
11	2.954	499	502	503	rBV2	927	570	0.00%	0.001%
12	3.047	521	531	540	rBV4	3921	7469	0.02%	0.010%
13	3.125	550	555	558	rBV3	752	584	0.00%	0.001%
14	3.186	561	574	591	rVB2	5761	14044	0.04%	0.018%
15	3.353	606	626	645	rBV	21410	42565	0.13%	0.055%
16	3.449	652	656	662	rVB3	552	448	0.00%	0.001%
17	3.594	689	701	711	rVV5	2883	5794	0.02%	0.008%
18	3.703	725	735	742	rVV4	1508	2614	0.01%	0.003%
19	3.867	769	786	810	rBV	137528	329441	0.98%	0.427%
20	3.990	821	824	829	rVB3	427	383	0.00%	0.000%
21	4.192	878	887	889	rBV4	603	683	0.00%	0.001%
22	4.417	954	957	963	rVB3	466	484	0.00%	0.001%
23	4.459	967	970	974	rBV4	697	591	0.00%	0.001%
24	4.523	987	990	992	rVV2	599	315	0.00%	0.000%
25	4.665	1001	1034	1066	rBV2	1750733	4371359	13.01%	5.663%
26	4.803	1069	1077	1102	rVB3	47027	112301	0.33%	0.145%
27	5.060	1141	1157	1180	rBV	284079	632400	1.88%	0.819%
28	5.205	1199	1202	1204	rBV4	837	459	0.00%	0.001%
29	5.314	1219	1236	1259	rVV2	281984	642361	1.91%	0.832%
30	5.517	1295	1299	1303	rVB3	552	329	0.00%	0.000%
31	5.723	1342	1363	1380	rBV2	493754	1415289	4.21%	1.833%
32	5.954	1430	1435	1437	rBV2	499	464	0.00%	0.001%
33	6.022	1445	1456	1468	rVB3	8557	17398	0.05%	0.023%
34	6.128	1484	1489	1494	rBV4	753	749	0.00%	0.001%
35	6.247	1510	1526	1549	rBV	602939	1139302	3.39%	1.476%
36	6.539	1594	1617	1650	rBV	9763302	17973553	53.50%	23.284%

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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0KY9

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\SFAMULM111522WMA.M
Title : VOC Analysis

37	6.687	1652	1663	1687	rVB	369678	731821	2.18%	0.948%
38	6.890	1718	1726	1735	rBV9	2270	4550	0.01%	0.006%
39	6.960	1737	1748	1766	rVB	44518	86187	0.26%	0.112%
40	7.182	1809	1817	1830	rVV2	7729	15489	0.05%	0.020%
41	7.250	1830	1838	1849	rVB5	6151	10062	0.03%	0.013%
42	7.501	1907	1916	1923	rBV4	748	1283	0.00%	0.002%
43	7.565	1923	1936	1958	rBV	159866	281108	0.84%	0.364%
44	7.694	1966	1976	1986	rBV5	4841	8365	0.02%	0.011%
45	7.790	2002	2006	2007	rBV3	465	364	0.00%	0.000%
46	7.896	2026	2039	2056	rBV	525222	908878	2.71%	1.177%
47	8.102	2095	2103	2113	rVB3	4968	8203	0.02%	0.011%
48	8.176	2114	2126	2144	rBV	110009	187042	0.56%	0.242%
49	8.398	2186	2195	2210	rVB3	12378	20318	0.06%	0.026%
50	8.485	2211	2222	2228	rBV3	15356	25169	0.07%	0.033%
51	8.552	2228	2243	2259	rVV	20392256	33594652	100.00%	43.520%
52	8.629	2259	2267	2304	rVB2	569509	1134959	3.38%	1.470%
53	8.787	2309	2316	2331	rVB3	20888	36487	0.11%	0.047%
54	9.041	2382	2395	2409	rBV2	12116	19697	0.06%	0.026%
55	9.230	2452	2454	2457	rVB2	627	350	0.00%	0.000%
56	9.343	2486	2489	2492	rVB4	762	467	0.00%	0.001%
57	9.414	2498	2511	2539	rBV	850596	1418041	4.22%	1.837%
58	9.603	2567	2570	2574	rVB3	874	606	0.00%	0.001%
59	9.761	2609	2619	2629	rVB5	4512	7619	0.02%	0.010%
60	9.870	2649	2653	2658	rBV2	458	553	0.00%	0.001%
61	10.054	2704	2710	2711	rBV3	551	467	0.00%	0.001%
62	10.349	2794	2802	2809	rVV7	2442	3700	0.01%	0.005%
63	10.481	2836	2843	2847	rBV4	528	669	0.00%	0.001%
64	10.536	2856	2860	2863	rBV4	673	500	0.00%	0.001%
65	10.613	2880	2884	2888	rBV2	350	353	0.00%	0.000%
66	10.636	2888	2891	2896	rVV2	700	700	0.00%	0.001%
67	10.674	2900	2903	2907	rVB2	545	401	0.00%	0.001%
68	10.755	2914	2928	2947	rBV	659238	1056349	3.14%	1.368%
69	11.050	3010	3020	3032	rBV5	1250	2638	0.01%	0.003%
70	11.160	3050	3054	3060	rVB2	345	375	0.00%	0.000%
71	11.224	3072	3074	3078	rBV3	377	349	0.00%	0.000%
72	11.523	3156	3167	3177	rBV3	25612	40678	0.12%	0.053%
73	11.690	3211	3219	3233	rVB5	7498	11726	0.03%	0.015%
74	11.809	3243	3256	3279	rBV	676389	1089080	3.24%	1.411%
75	12.057	3323	3333	3356	rBV2	67137	124263	0.37%	0.161%
76	12.189	3361	3374	3398	rVV	654906	1074953	3.20%	1.393%

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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0KY9

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Title : VOC Analysis

77	12.404	3439	3441	3447	rVV3	678	407	0.00%	0.001%
78	12.504	3469	3472	3476	rBV3	506	400	0.00%	0.001%
79	12.574	3492	3494	3499	rBV4	460	317	0.00%	0.000%
80	12.626	3507	3510	3512	rBV2	499	320	0.00%	0.000%
81	12.703	3528	3534	3537	rBV4	555	677	0.00%	0.001%
82	12.742	3543	3546	3551	rVB4	711	523	0.00%	0.001%
83	12.771	3551	3555	3557	rBV2	559	373	0.00%	0.000%
84	12.889	3584	3592	3602	rBV5	12674	20832	0.06%	0.027%
85	12.938	3604	3607	3612	rBV4	430	393	0.00%	0.001%
86	13.063	3643	3646	3649	rBV2	490	318	0.00%	0.000%
87	13.166	3672	3678	3686	rBV4	602	1043	0.00%	0.001%
88	13.201	3686	3689	3693	rVV2	499	386	0.00%	0.001%
89	13.311	3719	3723	3725	rBV2	522	410	0.00%	0.001%
90	13.398	3747	3750	3755	rBV4	444	465	0.00%	0.001%
91	13.436	3758	3762	3764	rBV3	556	405	0.00%	0.001%
92	13.610	3814	3816	3821	rVB2	560	410	0.00%	0.001%
93	13.639	3822	3825	3831	rBV3	556	524	0.00%	0.001%
94	13.680	3836	3838	3843	rVB3	532	409	0.00%	0.001%
95	13.925	3912	3914	3919	rVB2	589	495	0.00%	0.001%
96	13.999	3935	3937	3943	rVB3	517	438	0.00%	0.001%
97	14.182	3991	3994	3998	rVB2	788	651	0.00%	0.001%
98	14.793	4181	4184	4189	rBV4	515	550	0.00%	0.001%
99	15.169	4298	4301	4305	rBV5	426	412	0.00%	0.001%
100	15.616	4438	4440	4445	rBV3	600	536	0.00%	0.001%

Sum of corrected areas: 77192887

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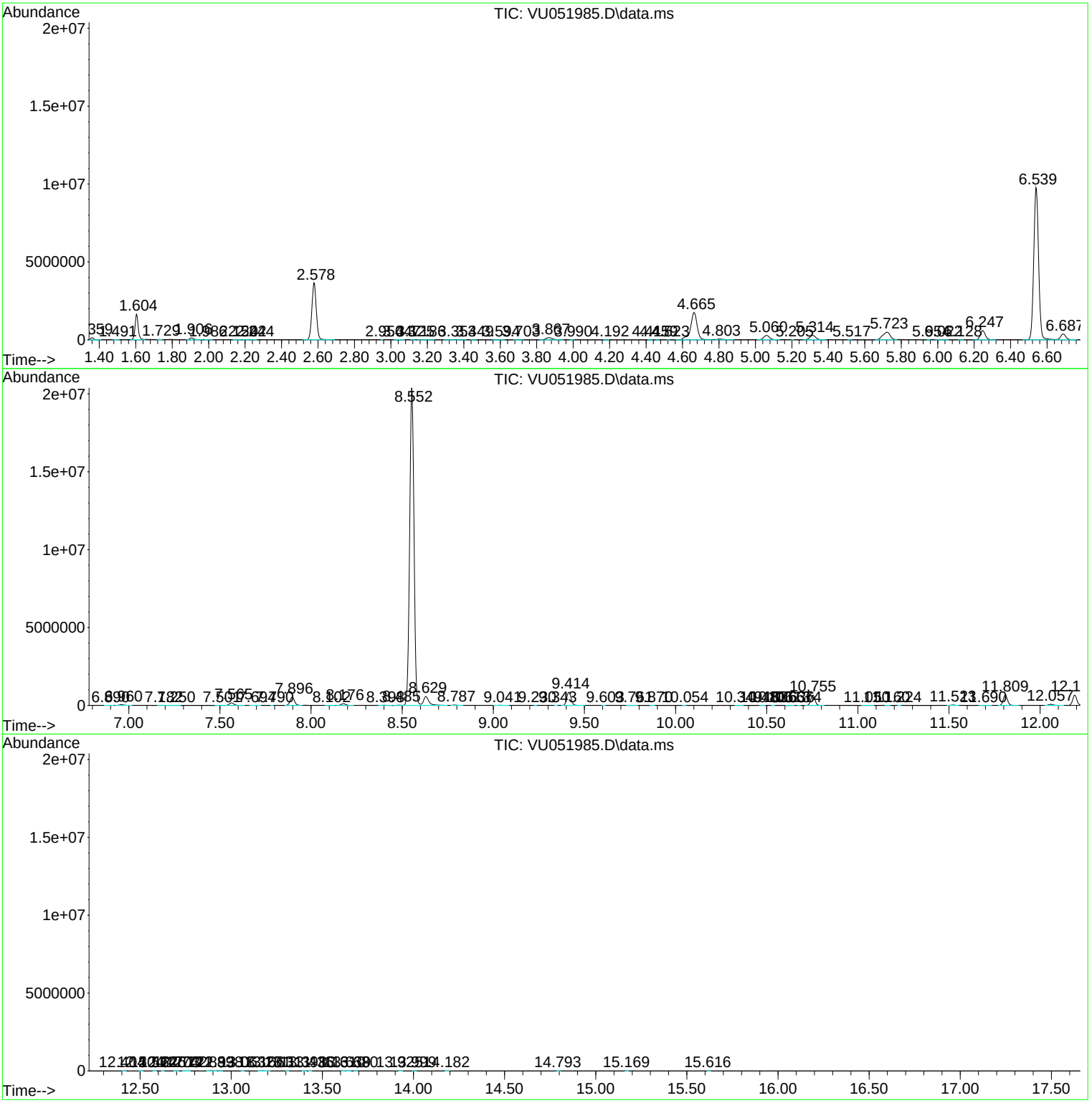
Instrument :
MSVOA_U
ClientSampleId :
C0KY9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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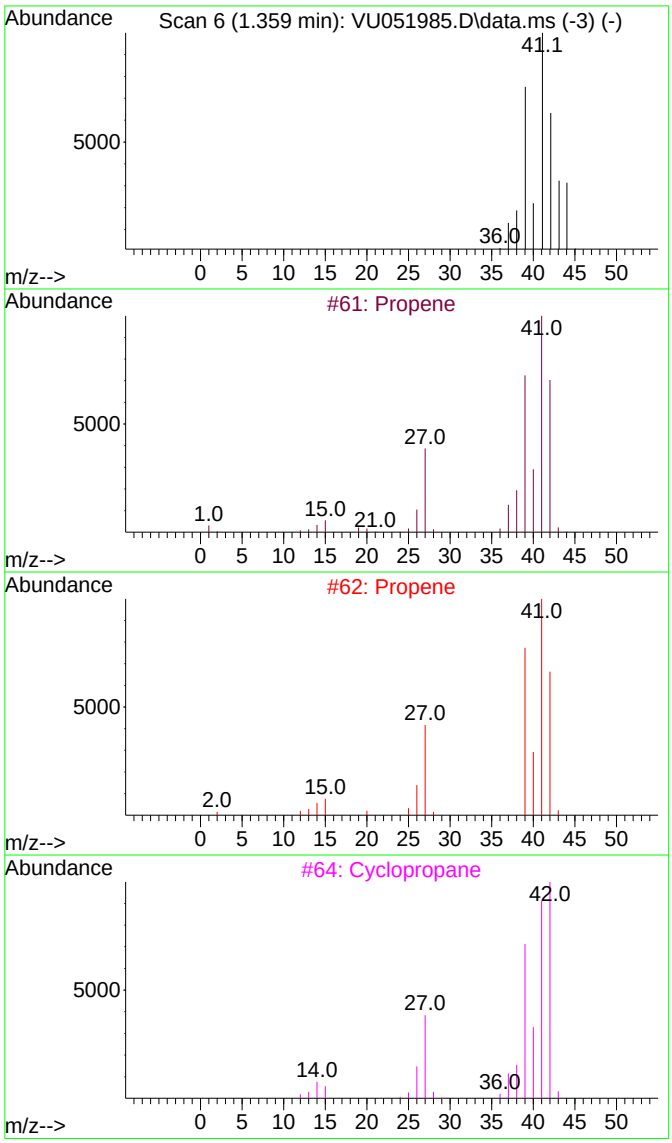
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

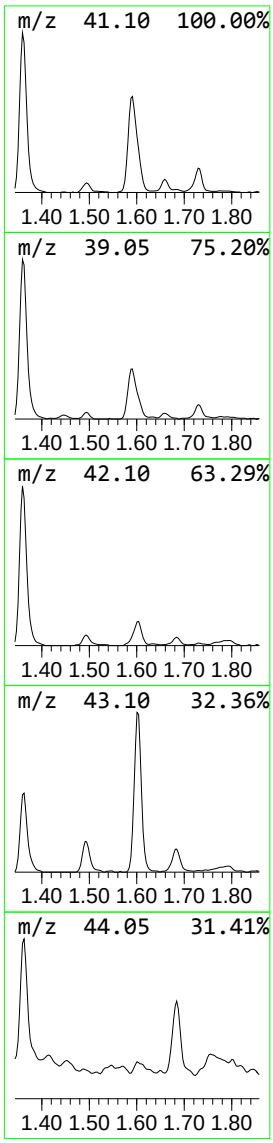
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	6.28 ug/L	143209	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Propene	42	C3H6	000115-07-1	56
3	Cyclopropane	42	C3H6	000075-19-4	10
4	Cyclopropane	42	C3H6	000075-19-4	10
5	Cyclopropane	42	C3H6	000075-19-4	4





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0KY9

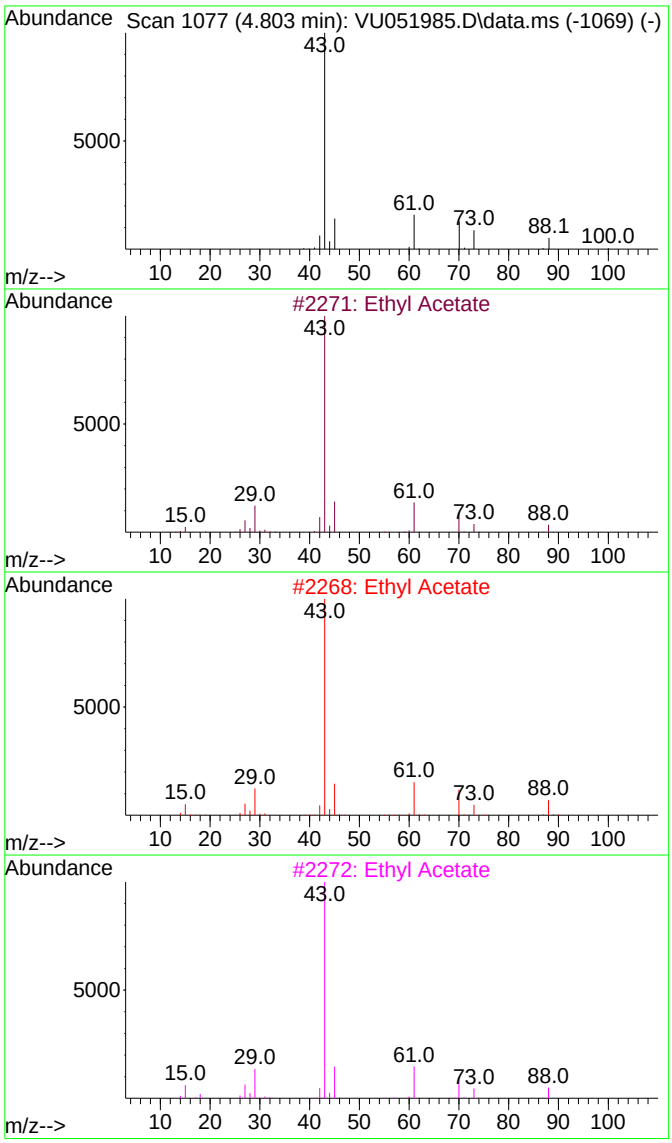
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

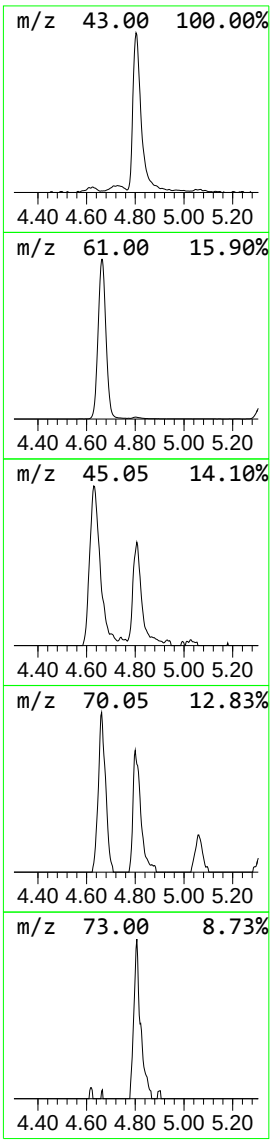
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethyl Acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.803	4.93 ug/L	112301	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2	Ethyl Acetate	88	C4H8O2	000141-78-6	86
3	Ethyl Acetate	88	C4H8O2	000141-78-6	86
4	Ethyl Acetate	88	C4H8O2	000141-78-6	64
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	42





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ClientSampleId :
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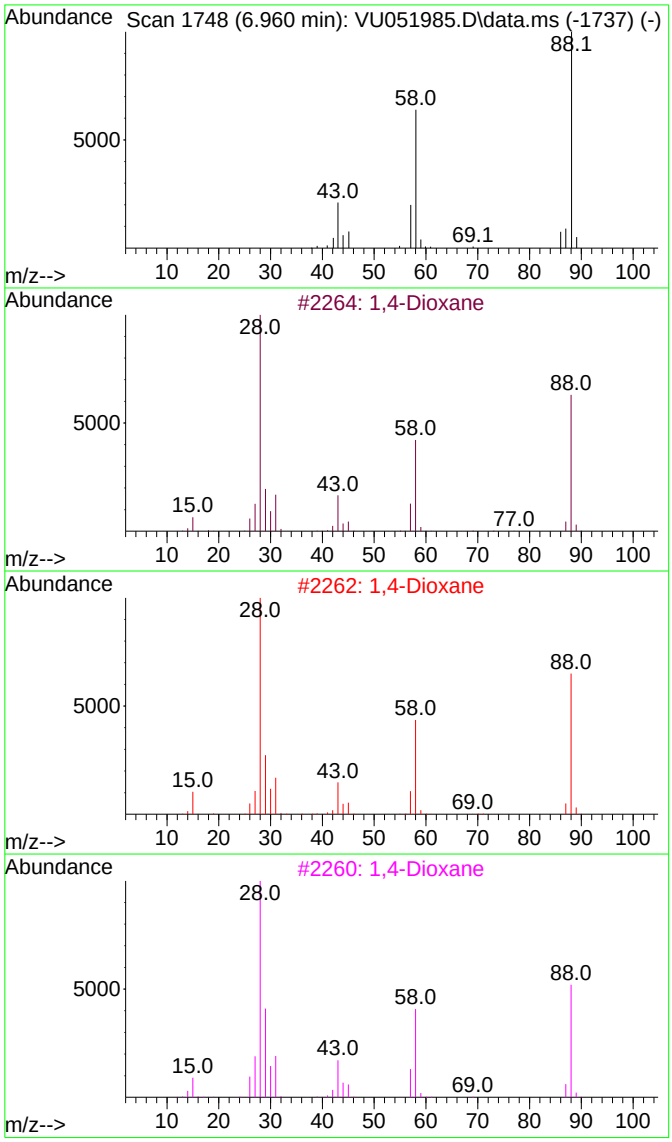
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

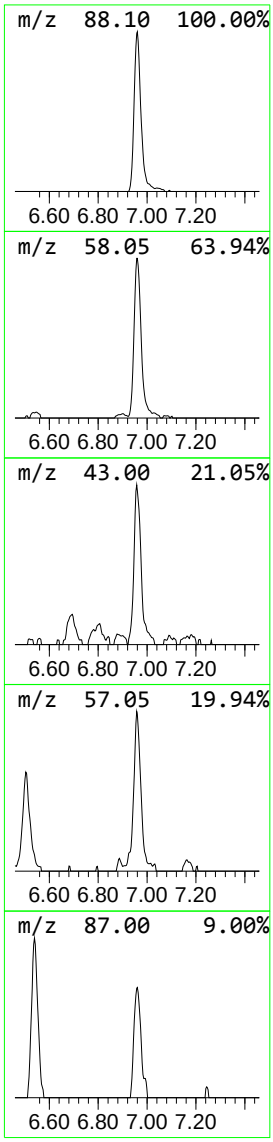
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,3,6-Trioxocane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.960	3.78 ug/L	86187	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxane	88	C4H8O2	000123-91-1	91
2	1,4-Dioxane	88	C4H8O2	000123-91-1	90
3	1,4-Dioxane	88	C4H8O2	000123-91-1	86
4	1,4-Dioxane	88	C4H8O2	000123-91-1	83
5	1,3,6-Trioxocane	118	C5H10O3	001779-19-7	56





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0KY9

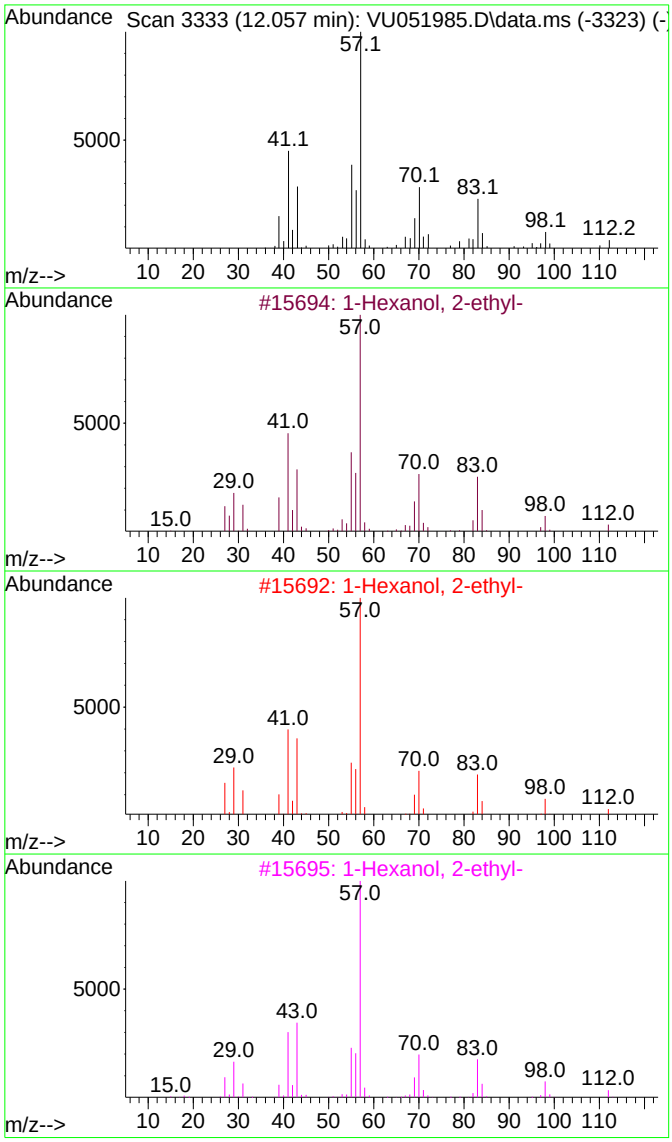
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

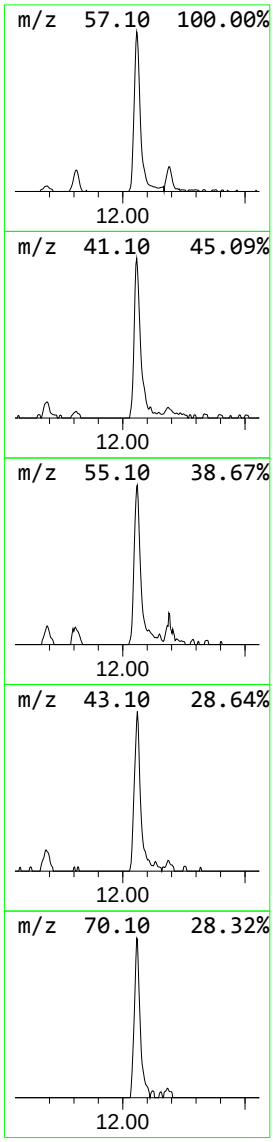
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	5.70 ug/L	124263	1,4-Dichlorobenzene-d4	11.809

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53





Tentatively Identified Compound (LSC) summary

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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0KY9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.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
(DEL) Alkane: S...	1.359	6.3	ug/L	143209	1	6.247	1139300	50.0
Ethyl Acetate	4.803	4.9	ug/L	112301	1	6.247	1139300	50.0
1,3,6-Trioxocane	6.960	3.8	ug/L	86187	1	6.247	1139300	50.0
1-Hexanol, 2-et...	12.057	5.7	ug/L	124263	3	11.809	1089080	50.0