LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042283.D
Acq On : 05 Feb 2021 17:41
Operator : SY/MD
Sample : M1327-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : X2Z60

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\SFAMULM020521WMA.M
Title : VOC Analysis

Signal : TIC: VU042283.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	75	82	96	rVB	94160	109516	3.17%	0.228%
2	1.935	172	185	200	rVB2	123777	248400	7.18%	0.516%
3	2.584	371	387	404	rBV4	485926	926596	26.79%	1.926%
4	2.784	446	449	450	rBV	199	129	0.00%	0.000%
5	2.945	496	499	500	rBV	330	187	0.01%	0.000%
6	3.054	519	533	561	rVB	166300	319189	9.23%	0.663%
7	3.195	566	577	591	rBV4	2404	5671	0.16%	0.012%
8	3.301	607	610	613	rBV2	168	106	0.00%	0.000%
9	3.372	613	632	656	rBV	506782	1166384	33.73%	2.424%
10	3.588	694	699	702	rBV	240	234	0.01%	0.000%
11	3.665	721	723	727	rVV3	198	110	0.00%	0.000%
12	3.684	727	729	734	rVB	237	168	0.00%	0.000%
13	3.719	734	740	744	rBV	106	122	0.00%	0.000%
14	3.826	768	773	774	rBV	375	280	0.01%	0.001%
15	3.912	795	800	806	rVB2	197	188	0.01%	0.000%
16	4.144	869	872	874	rBV	137	102	0.00%	0.000%
17	4.356	934	938	941	rBV2	203	152	0.00%	0.000%
18	4.375	941	944	947	rVB	168	134	0.00%	0.000%
19	4.395	947	950	953	rVB2	179	128	0.00%	0.000%
20	4.520	986	989	994	rVB	140	115	0.00%	0.000%
21	4.639	1005	1026	1060	rBV	84746	227821	6.59%	0.474%
22	4.948	1119	1122	1126	rBV2	270	189	0.01%	0.000%
23	4.980	1127	1132	1134	rBV3	500	414	0.01%	0.001%
24	5.083	1141	1164	1198	rBV4	186776	583932	16.89%	1.214%
25	5.327	1222	1240	1258	rBV	174237	390633	11.30%	0.812%
26	5.443	1269	1276	1278	rBV	87	114	0.00%	0.000%
27	5.536	1286	1305	1326	rBV	340420	747781	21.62%	1.554%
28	5.639	1335	1337	1339	rVB	252	121	0.00%	0.000%
29	5.735	1344	1367	1373	rBV2	301211	791762	22.90%	1.646%
30	5.964	1436	1438	1442	rVB2	559	336	0.01%	0.001%
31	6.005	1447	1451	1453	rBV2	288	262	0.01%	0.001%
32	6.099	1478	1480	1482	rBV2	526	290	0.01%	0.001%
33	6.260	1517	1530	1552	rVB	245825	459004	13.27%	0.954%
34	6.440	1584	1586	1589	rBV2	287	171	0.00%	0.000%
35	6.494	1601	1603	1606	rBV2	229	141	0.00%	0.000%
36	6.552	1606	1621	1641	rBV	802152	1507084	43.58%	3.132%

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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : X2Z60

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\SFAMULM020521WMA.M
Title : VOC Analysis

37	6.700	1653	1667	1684	rVB	192513	368568	10.66%	0.766%
38	6.845	1710	1712	1715	rVB2	298	175	0.01%	0.000%
39	6.864	1715	1718	1723	rBV2	185	125	0.00%	0.000%
40	6.928	1723	1738	1761	rBV	314461	593036	17.15%	1.233%
41	7.047	1764	1775	1784	rVV	81660	142441	4.12%	0.296%
42	7.115	1785	1796	1814	rVB	356158	645773	18.67%	1.342%
43	7.398	1879	1884	1886	rBV	161	102	0.00%	0.000%
44	7.501	1913	1916	1922	rVB2	157	121	0.00%	0.000%
45	7.575	1923	1939	1945	rBV	120386	210724	6.09%	0.438%
46	7.719	1974	1984	1997	rBV3	50094	104041	3.01%	0.216%
47	7.800	1998	2009	2029	rVV	997304	1776534	51.37%	3.692%
48	7.906	2031	2042	2052	rVV	378801	646888	18.71%	1.345%
49	7.976	2053	2064	2103	rVB	1965048	3370108	97.46%	7.005%
50	8.218	2119	2139	2167	rBV	1035979	1859280	53.77%	3.864%
51	8.407	2185	2198	2214	rBV	1339601	2279686	65.92%	4.738%
52	8.562	2233	2246	2260	rBV	852506	1452441	42.00%	3.019%
53	8.642	2261	2271	2278	rBV	276432	455021	13.16%	0.946%
54	8.693	2279	2287	2296	rBV	760819	1163066	33.63%	2.417%
55	8.819	2315	2326	2346	rVB	414467	721678	20.87%	1.500%
56	8.931	2351	2361	2377	rVB	63342	107652	3.11%	0.224%
57	9.025	2388	2390	2393	rVB2	285	185	0.01%	0.000%
58	9.050	2397	2398	2401	rVB	261	110	0.00%	0.000%
59	9.076	2404	2406	2408	rBV2	224	128	0.00%	0.000%
60	9.118	2417	2419	2421	rBV	230	111	0.00%	0.000%
61	9.218	2437	2450	2467	rBV	83175	131401	3.80%	0.273%
62	9.349	2488	2491	2492	rBV	227	109	0.00%	0.000%
63	9.369	2492	2497	2500	rVV3	371	367	0.01%	0.001%
64	9.456	2502	2524	2539	rVV2	953959	2113985	61.13%	4.394%
65	9.542	2541	2551	2571	rVB	343746	572447	16.55%	1.190%
66	9.703	2586	2601	2630	rVB	1929378	3157741	91.31%	6.563%
67	9.906	2659	2664	2667	rBV2	291	187	0.01%	0.000%
68	9.925	2667	2670	2673	rVB2	214	146	0.00%	0.000%
69	9.989	2687	2690	2694	rVB	233	145	0.00%	0.000%
70	10.121	2711	2731	2759	rBV2	1993811	3321450	96.05%	6.904%
71	10.298	2774	2786	2800	rBV	169162	279891	8.09%	0.582%
72	10.385	2810	2813	2816	rVB2	233	135	0.00%	0.000%
73	10.494	2838	2847	2854	rVV3	2512	3494	0.10%	0.007%
74	10.565	2864	2869	2872	rVB3	317	258	0.01%	0.001%
75	10.594	2875	2878	2881	rBV2	205	175	0.01%	0.000%
76	10.668	2899	2901	2906	rBV	191	114	0.00%	0.000%

LSC Area Percent Report

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Operator : SY/MD
Sample : M1327-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : X2Z60

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\SFAMULM020521WMA.M
Title : VOC Analysis

77	10.716	2913	2916	2919	rBV	172	123	0.00%	0.000%
78	10.790	2919	2939	2962	rVV2	1074821	2098909	60.70%	4.363%
79	10.976	2992	2997	2998	rBV2	205	207	0.01%	0.000%
80	11.005	2999	3006	3014	rVB2	4148	5671	0.16%	0.012%
81	11.095	3020	3034	3053	rBV	2276283	3458116	100.00%	7.188%
82	11.182	3057	3061	3064	rVB	261	183	0.01%	0.000%
83	11.211	3064	3070	3077	rBV3	379	551	0.02%	0.001%
84	11.436	3131	3140	3147	rBV3	15875	25326	0.73%	0.053%
85	11.697	3217	3221	3222	rBV	191	118	0.00%	0.000%
86	11.751	3225	3238	3249	rVV	588082	933844	27.00%	1.941%
87	11.844	3249	3267	3284	rVB2	832135	1859817	53.78%	3.866%
88	12.018	3317	3321	3325	rBV2	226	171	0.00%	0.000%
89	12.221	3365	3384	3401	rBV3	1612540	3022751	87.41%	6.283%
90	12.307	3408	3411	3415	rVB2	550	392	0.01%	0.001%
91	12.330	3415	3418	3420	rBV2	336	242	0.01%	0.001%
92	12.484	3457	3466	3477	rBV2	11925	18731	0.54%	0.039%
93	12.777	3553	3557	3559	rBV2	334	294	0.01%	0.001%
94	12.902	3591	3596	3601	rVB2	260	264	0.01%	0.001%
95	13.230	3692	3698	3704	rVB2	1045	1265	0.04%	0.003%
96	13.848	3876	3890	3915	rBV	1235179	1956871	56.59%	4.067%
97	14.031	3934	3947	3960	rVB	1129733	1750284	50.61%	3.638%
98	14.127	3975	3977	3980	rBV2	294	146	0.00%	0.000%
99	14.301	4028	4031	4034	rBV3	363	270	0.01%	0.001%
100	14.336	4034	4042	4051	rVV3	6274	9586	0.28%	0.020%

Sum of corrected areas: 48112137

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Data File : VU042283.D
Acq On : 05 Feb 2021 17:41
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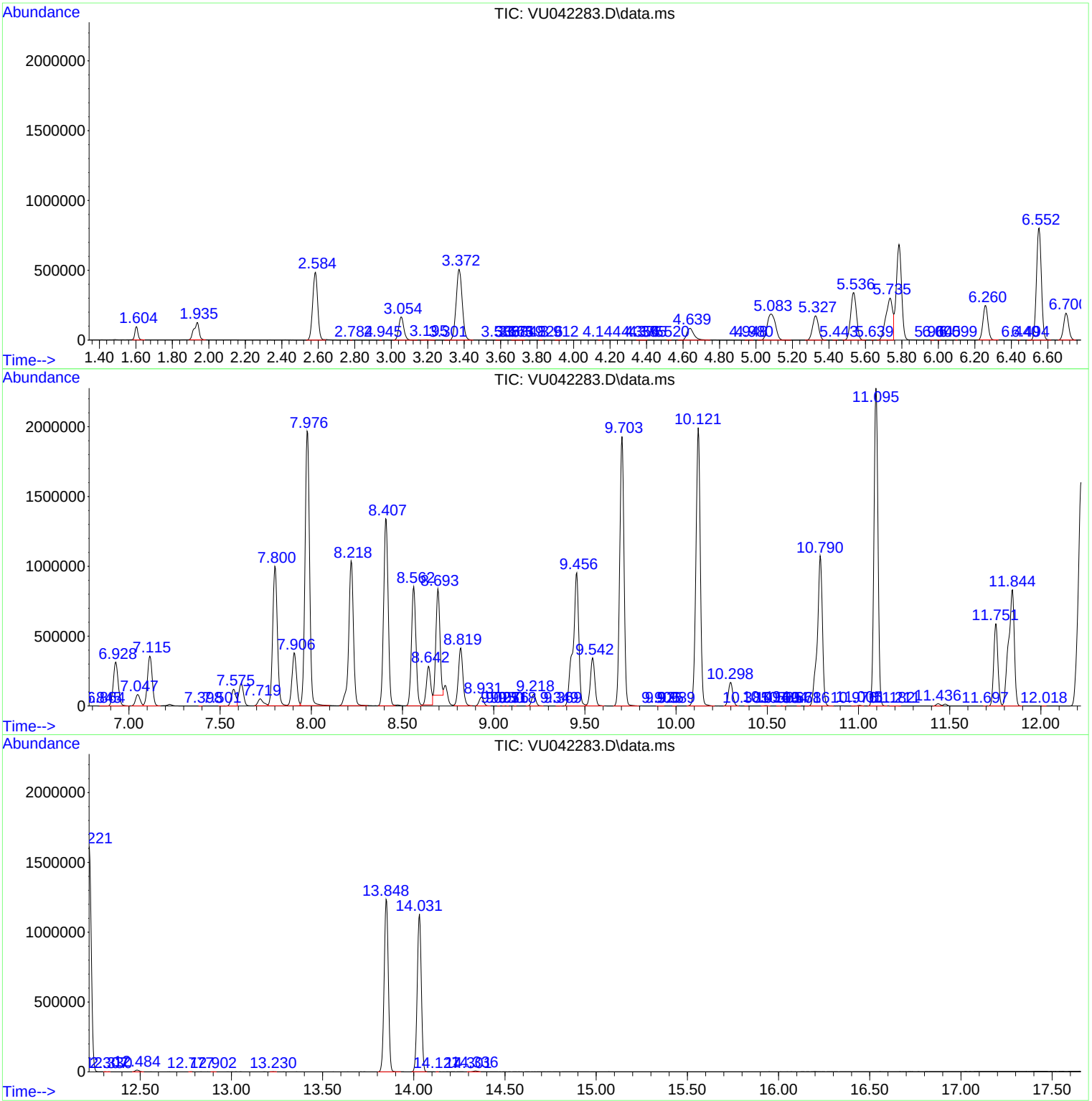
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
X2Z60

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042283.D
Acq On : 05 Feb 2021 17:41
Operator : SY/MD
Sample : M1327-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : X2Z60

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

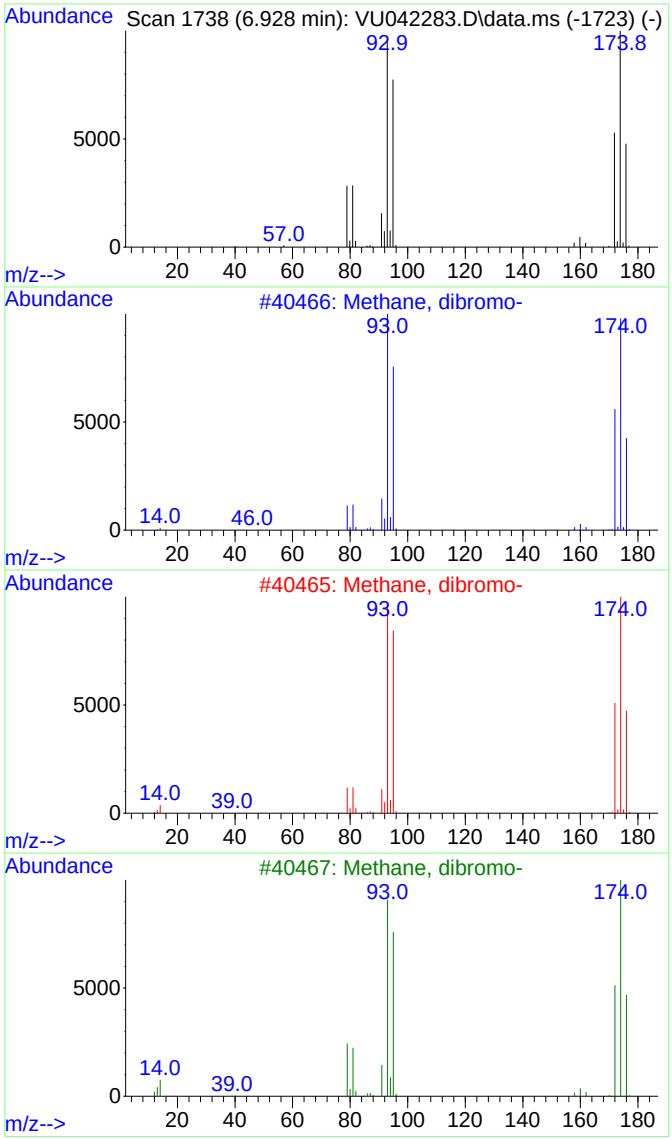
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

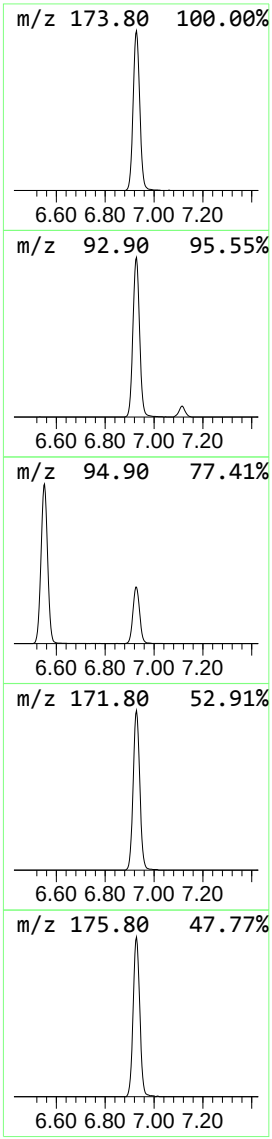
****

Peak Number 1 Methane, dibromo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.928	64.60 ug/L	593036	1,4-Difluorobenzene	6.260

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methane, dibromo-	172	CH2Br2	000074-95-3	96
2	Methane, dibromo-	172	CH2Br2	000074-95-3	95
3	Methane, dibromo-	172	CH2Br2	000074-95-3	94
4	1-Hydroxymethyl-2-methyl-1-cyclo...	126	C8H14O	029474-11-1	9
5	(4-Methyl-cyclohex-3-enyl)-methanol	126	C8H14O	089690-46-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042283.D
Acq On : 05 Feb 2021 17:41
Operator : SY/MD
Sample : M1327-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : X2Z60

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

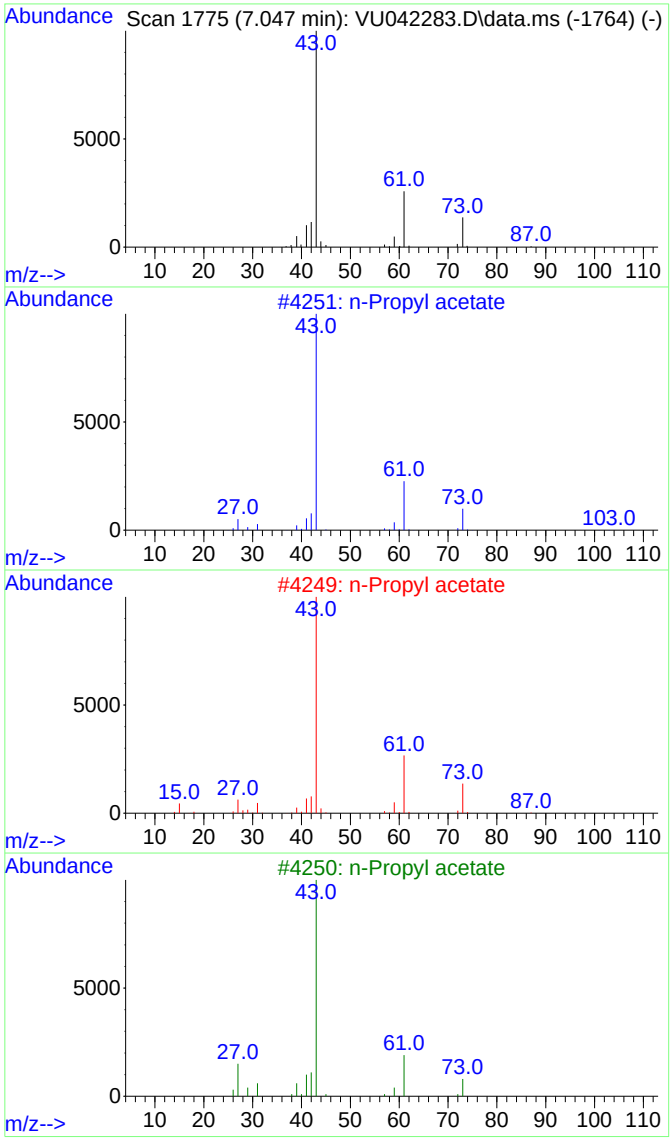
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

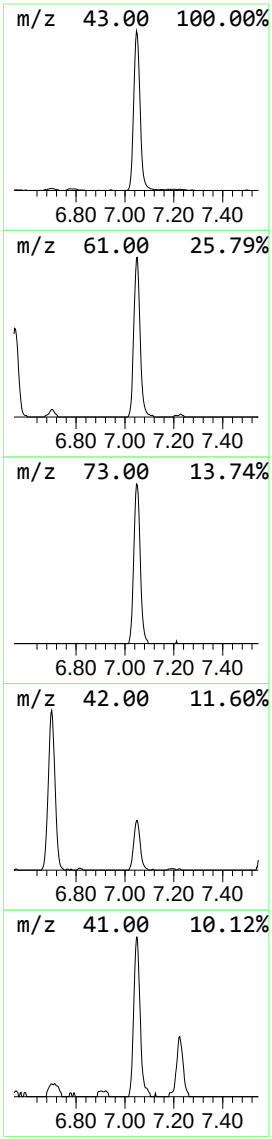
****

Peak Number 2 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.047	15.52 ug/L	142441	1,4-Difluorobenzene	6.260

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	n-Propyl acetate	102	C5H10O2	000109-60-4	83
3	n-Propyl acetate	102	C5H10O2	000109-60-4	78
4	Isopropyl acetate	102	C5H10O2	000108-21-4	36
5	Isobutyl acetate	116	C6H12O2	000110-19-0	9





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Operator : SY/MD
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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : X2Z60

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

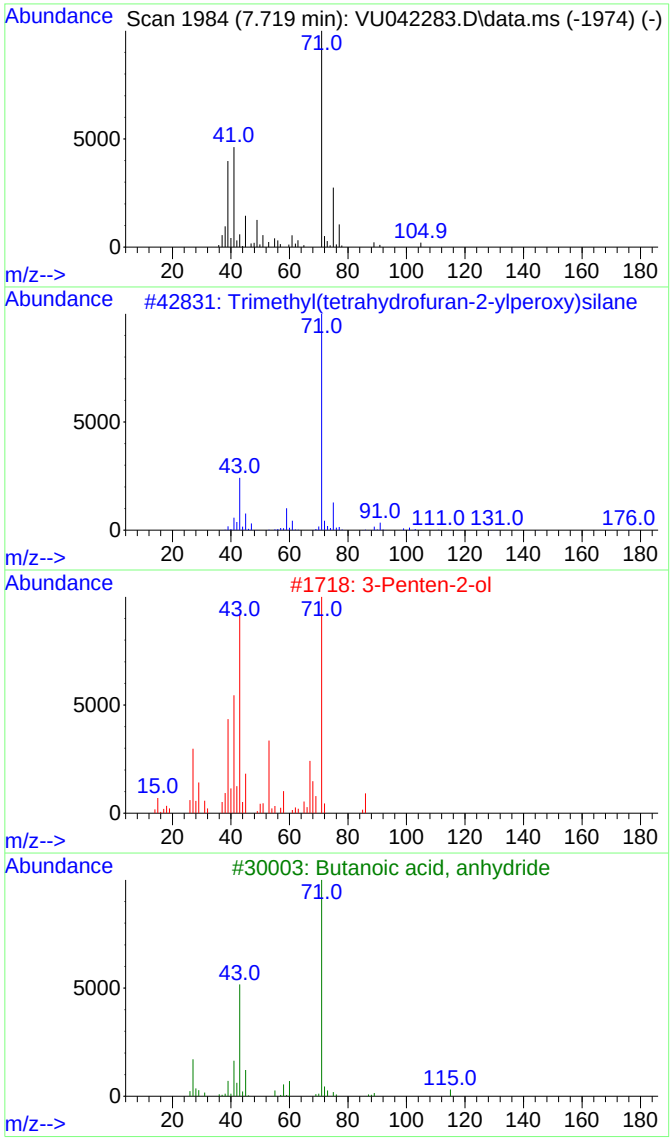
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

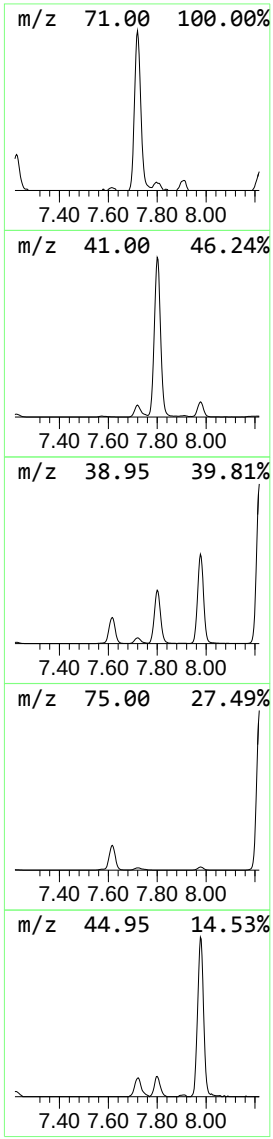
****

Peak Number 3 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.719	11.33 ug/L	104041	1,4-Difluorobenzene	6.260

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trimethyl(tetrahydrofuran-2-ylpe...	176	C7H16O3Si	1000368-50-8	47
2	3-Penten-2-ol	86	C5H10O	001569-50-2	36
3	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	23
4	Methoxyacetic acid, 2-tetrahydro...	174	C8H14O4	1000282-41-3	23
5	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	17





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Instrument : MSVOA_U
ClientSampleId : X2Z60

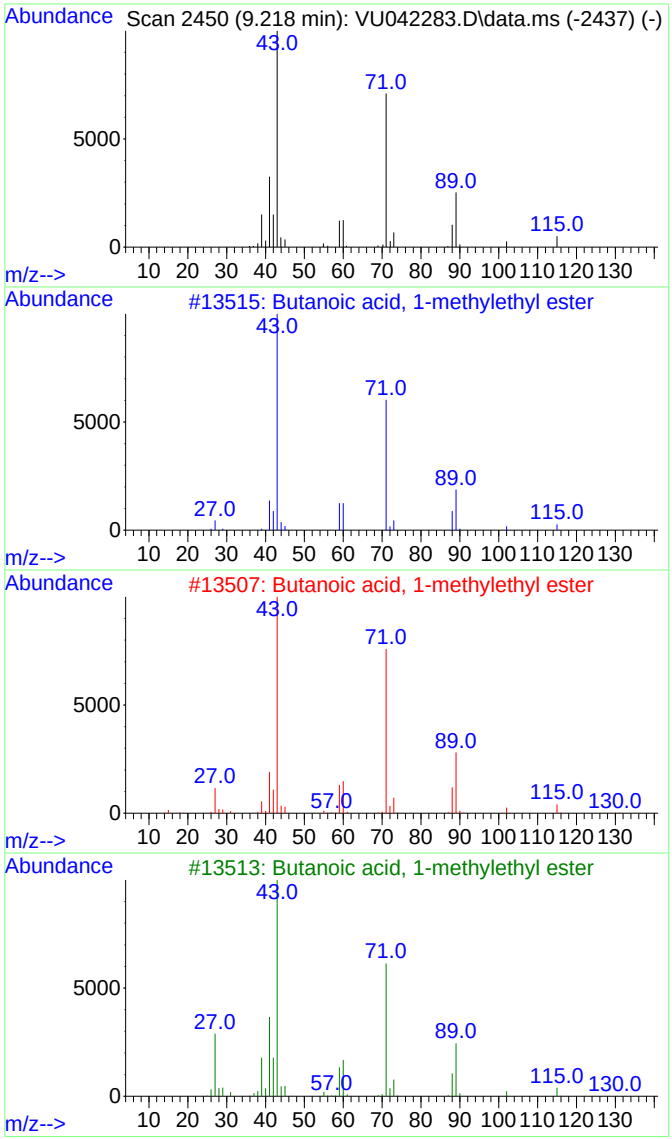
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

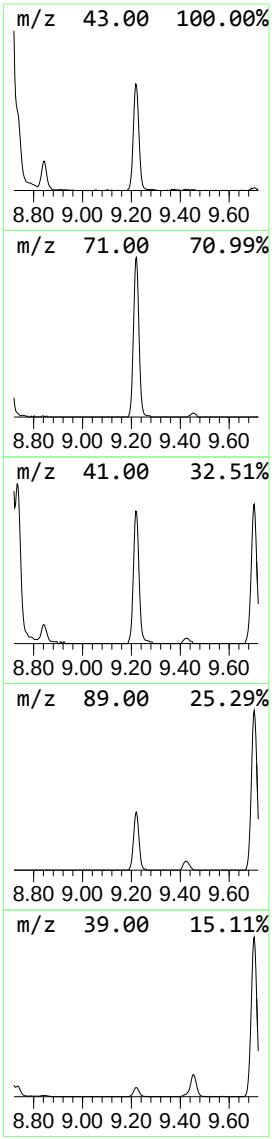
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.218	3.11 ug/L	131401	Chlorobenzene-d5	9.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
4	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	86
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042283.D
Acq On : 05 Feb 2021 17:41
Operator : SY/MD
Sample : M1327-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
X2Z60

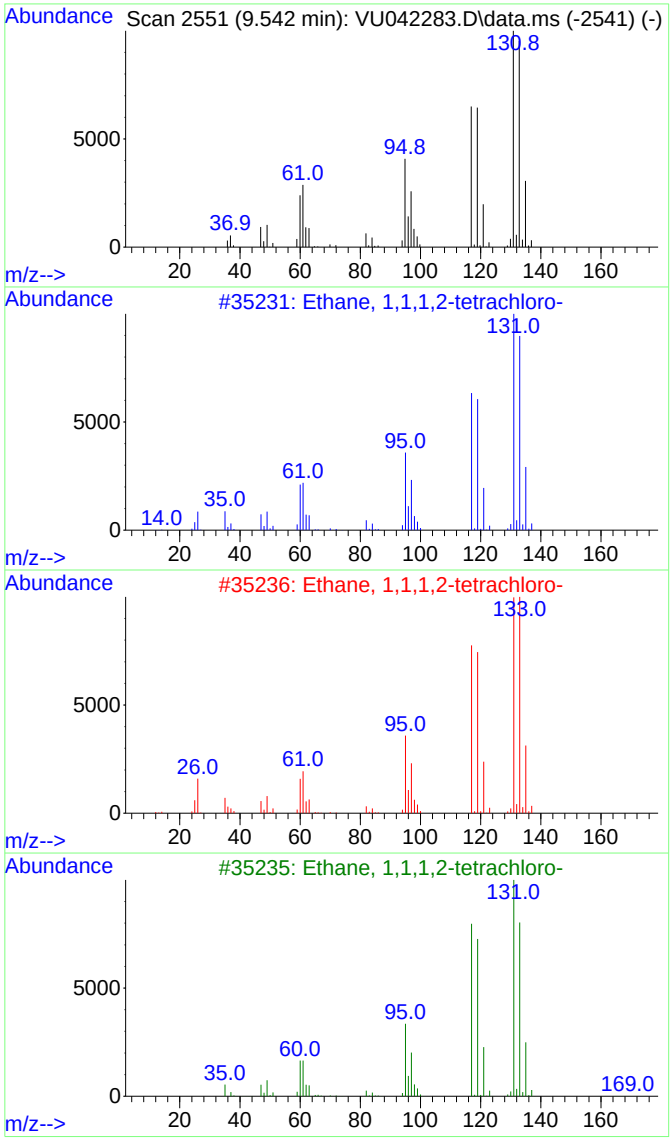
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

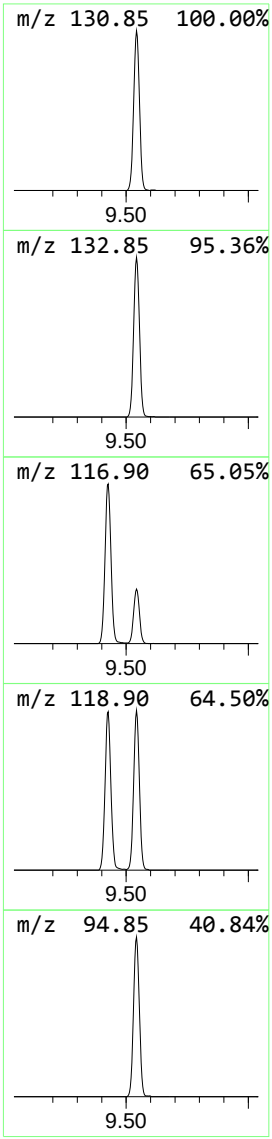
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethane, 1,1,1,2-tetrachloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.542	13.54 ug/L	572447	Chlorobenzene-d5	9.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	90
2	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	83
3	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	72
4	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	50
5	Carbon Tetrachloride	152	CCl4	000056-23-5	11





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042283.D
Acq On : 05 Feb 2021 17:41
Operator : SY/MD
Sample : M1327-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
X2Z60

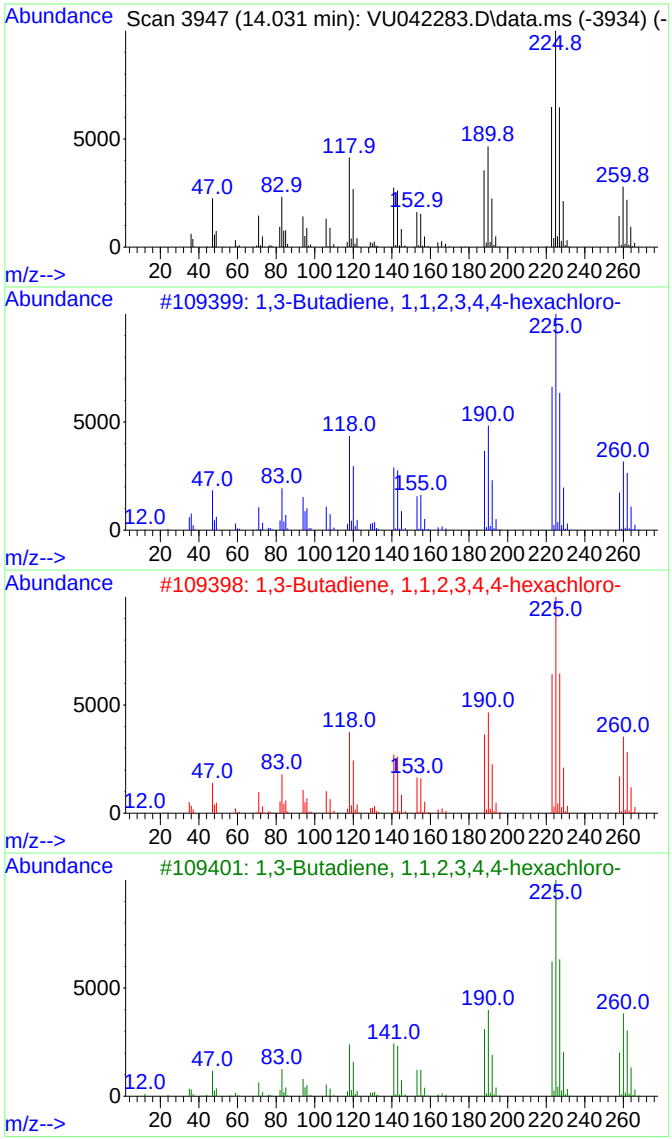
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

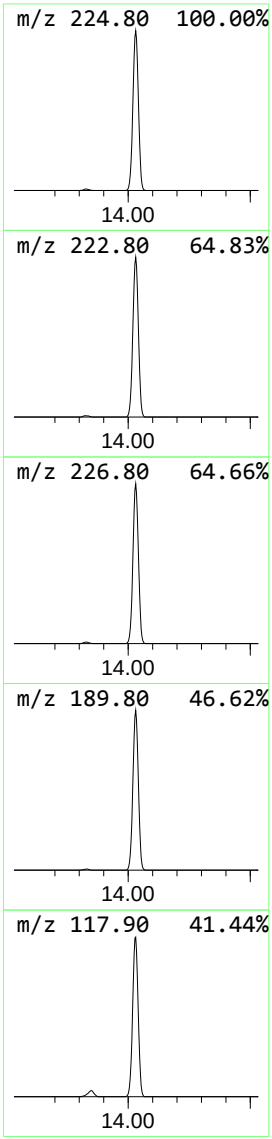
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Butadiene, 1,1,2,3,4,4-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.031	47.06 ug/L	1750280	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
2	1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
3	1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
4	1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
5	Tin(IV) chloride	260	Cl4Sn	007646-78-8	12





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042283.D
Acq On : 05 Feb 2021 17:41
Operator : SY/MD
Sample : M1327-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : X2Z60

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.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
Methane, dibromo-	6.928	64.6	ug/L	593036	1	6.260	459004	50.0
n-Propyl acetate	7.047	15.5	ug/L	142441	1	6.260	459004	50.0
unknown-01	7.719	11.3	ug/L	104041	1	6.260	459004	50.0
Butanoic acid, ...	9.218	3.1	ug/L	131401	2	9.427	2113990	50.0
Ethane, 1,1,1,2...	9.542	13.5	ug/L	572447	2	9.427	2113990	50.0
1,3-Butadiene, ...	14.031	47.1	ug/L	1750280	3	11.819	1859820	50.0