LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101221\
Data File : VV022748.D
Acq On : 12 Oct 2021 12:59
Operator : SY/MD
Sample : M4126-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AD0

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_V\Method\SFAMVLM100121WMA.M
Title : VOC Analysis

Signal : TIC: VV022748.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	76	83	98	rVB	105159	107113	15.38%	2.040%
2	1.564	156	163	182	rVB	89791	101056	14.51%	1.924%
3	2.108	322	332	347	rBV	182922	268336	38.53%	5.110%
4	2.506	452	456	463	rVB4	1012	1240	0.18%	0.024%
5	2.593	480	483	485	rBV2	284	205	0.03%	0.004%
6	2.654	500	502	505	rVB2	440	226	0.03%	0.004%
7	2.674	505	508	511	rBV2	265	161	0.02%	0.003%
8	2.973	599	601	603	rBV	212	133	0.02%	0.003%
9	3.066	627	630	631	rBV	282	141	0.02%	0.003%
10	3.098	639	640	646	rBV2	342	230	0.03%	0.004%
11	3.140	650	653	655	rBV2	193	142	0.02%	0.003%
12	3.204	672	673	677	rBV	257	115	0.02%	0.002%
13	3.223	677	679	681	rVB	357	135	0.02%	0.003%
14	3.240	681	684	685	rBV	173	88	0.01%	0.002%
15	3.330	709	712	714	rBV	259	154	0.02%	0.003%
16	3.455	748	751	754	rBV	322	238	0.03%	0.005%
17	3.503	764	766	768	rBV	139	75	0.01%	0.001%
18	3.686	820	823	827	rBV2	224	199	0.03%	0.004%
19	3.786	850	854	855	rBV	516	213	0.03%	0.004%
20	3.883	875	884	928	rBV	51287	151878	21.81%	2.892%
21	4.349	1015	1029	1056	rBV	113108	280011	40.20%	5.332%
22	4.577	1096	1100	1104	rVB2	313	300	0.04%	0.006%
23	4.969	1220	1222	1224	rBV2	177	59	0.01%	0.001%
24	5.050	1230	1247	1274	rBV2	268720	696476	100.00%	13.262%
25	5.410	1358	1359	1366	rVB2	424	376	0.05%	0.007%
26	5.481	1376	1381	1385	rVB2	292	284	0.04%	0.005%
27	5.497	1385	1386	1387	rBV2	118	29	0.00%	0.001%
28	5.516	1388	1392	1394	rBV2	188	166	0.02%	0.003%
29	5.529	1394	1396	1398	rVV	231	63	0.01%	0.001%
30	5.619	1412	1424	1445	rBV	191664	382909	54.98%	7.291%
31	5.908	1502	1514	1535	rBV	27539	58228	8.36%	1.109%
32	6.072	1552	1565	1593	rVB	155568	319490	45.87%	6.084%
33	6.542	1708	1711	1716	rVB2	438	454	0.07%	0.009%
34	6.571	1716	1720	1722	rBV	313	288	0.04%	0.005%
35	6.802	1789	1792	1795	rVB2	144	109	0.02%	0.002%
36	6.818	1795	1797	1798	rBV2	253	84	0.01%	0.002%

LSC Area Percent Report

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Instrument : MSVOA_V
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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_V\Method\SFAMVLM100121WMA.M
Title : VOC Analysis

37	6.863	1809	1811	1812	rBV2	238	86	0.01%	0.002%
38	6.918	1824	1828	1830	rBV2	362	253	0.04%	0.005%
39	6.989	1839	1850	1875	rBV	79879	149337	21.44%	2.844%
40	7.317	1938	1952	1970	rBV	311791	545068	78.26%	10.379%
41	7.625	2038	2048	2072	rBV	53821	98004	14.07%	1.866%
42	7.889	2126	2130	2135	rBV	285	279	0.04%	0.005%
43	7.915	2136	2138	2139	rBV	362	141	0.02%	0.003%
44	7.940	2141	2146	2158	rVV8	1682	2723	0.39%	0.052%
45	7.989	2158	2161	2167	rVB2	352	225	0.03%	0.004%
46	8.014	2167	2169	2174	rBV2	395	313	0.04%	0.006%
47	8.091	2183	2193	2233	rBV2	132271	300315	43.12%	5.719%
48	8.249	2235	2242	2261	rVB4	14500	26536	3.81%	0.505%
49	8.853	2419	2430	2456	rBV	289691	474309	68.10%	9.032%
50	9.516	2632	2636	2638	rBV2	214	145	0.02%	0.003%
51	9.628	2669	2671	2672	rBV2	156	44	0.01%	0.001%
52	9.722	2697	2700	2703	rVB	234	136	0.02%	0.003%
53	9.738	2703	2705	2707	rBV	241	113	0.02%	0.002%
54	9.818	2721	2730	2741	rBV5	2868	5212	0.75%	0.099%
55	10.130	2820	2827	2835	rBV5	2082	2783	0.40%	0.053%
56	10.217	2843	2854	2870	rBV	177791	278338	39.96%	5.300%
57	10.355	2894	2897	2898	rBV	375	220	0.03%	0.004%
58	10.570	2961	2964	2965	rBV3	494	313	0.04%	0.006%
59	10.699	3002	3004	3007	rVB2	252	108	0.02%	0.002%
60	10.802	3034	3036	3038	rBV2	307	102	0.01%	0.002%
61	10.979	3088	3091	3095	rBV4	503	339	0.05%	0.006%
62	11.152	3134	3145	3157	rBV4	15925	24495	3.52%	0.466%
63	11.252	3164	3176	3194	rBV	267088	420698	60.40%	8.011%
64	11.429	3225	3231	3237	rVB6	1715	2500	0.36%	0.048%
65	11.506	3254	3255	3256	rBV6	216	54	0.01%	0.001%
66	11.625	3280	3292	3313	rBV	309794	482325	69.25%	9.184%
67	11.789	3338	3343	3347	rBV4	829	890	0.13%	0.017%
68	11.863	3364	3366	3368	rBV2	313	134	0.02%	0.003%
69	12.088	3433	3436	3439	rBV2	475	383	0.05%	0.007%
70	12.345	3507	3516	3529	rBV	34571	51784	7.44%	0.986%
71	13.008	3720	3722	3723	rBV	256	80	0.01%	0.002%
72	13.300	3811	3813	3815	rBV2	321	182	0.03%	0.003%
73	13.435	3848	3855	3864	rVB6	5598	7738	1.11%	0.147%
74	13.564	3893	3895	3899	rBV	375	307	0.04%	0.006%
75	14.181	4083	4087	4094	rVB6	2522	3012	0.43%	0.057%
76	14.474	4177	4178	4181	rBV2	370	183	0.03%	0.003%

LSC Area Percent Report

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Operator : SY/MD
Sample : M4126-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AD0

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_V\Method\SFAMVLM100121WMA.M
Title : VOC Analysis

Sum of corrected areas: 5251611

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101221\
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Acq On : 12 Oct 2021 12:59
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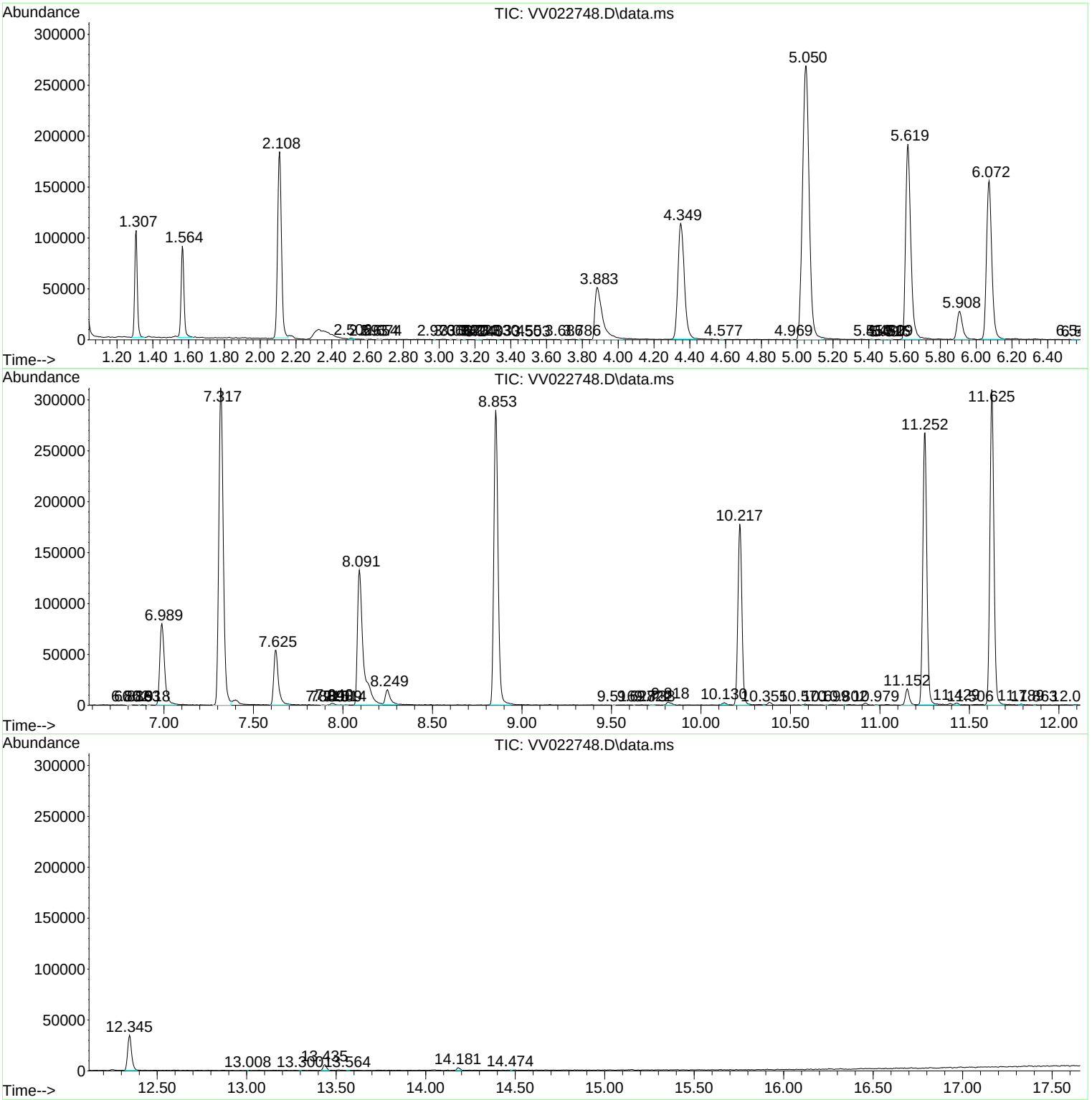
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AD0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101221\
Data File : VV022748.D
Acq On : 12 Oct 2021 12:59
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Instrument : MSVOA_V
ClientSampleId : C0AD0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

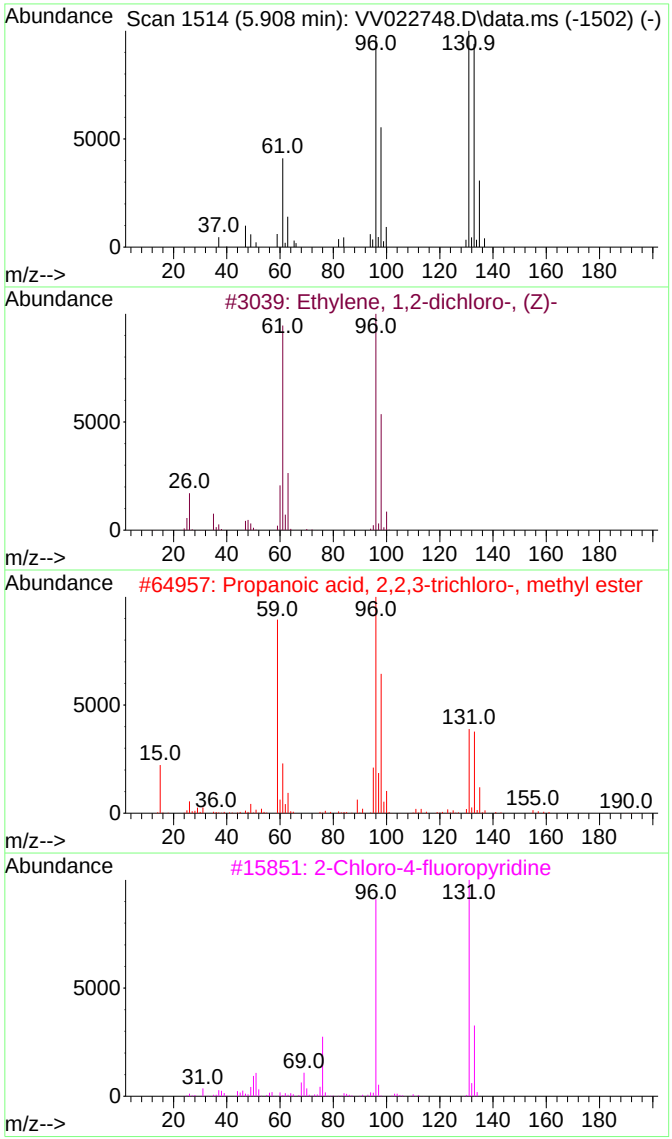
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

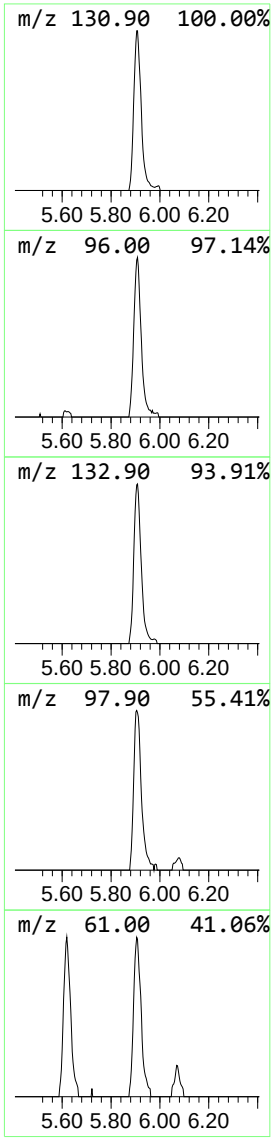
****

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	7.60 ug/L	58228	1,4-Difluorobenzene	5.619

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
2	Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	37
3	2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	32
4	4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
5	Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101221\
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Sample : M4126-18
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AD0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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

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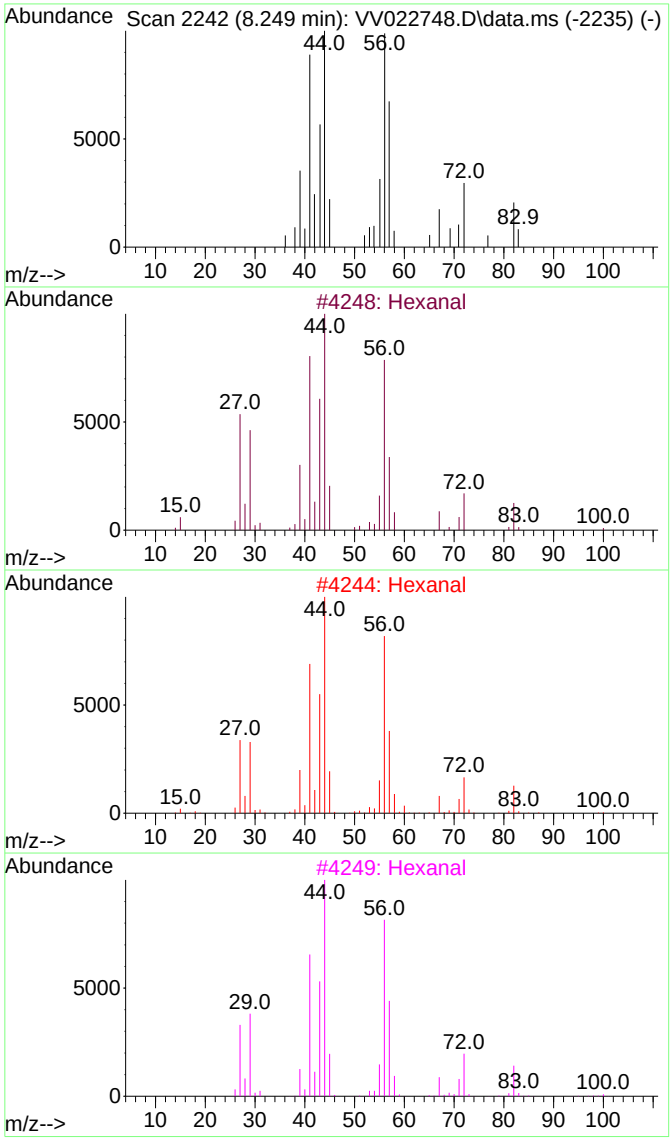
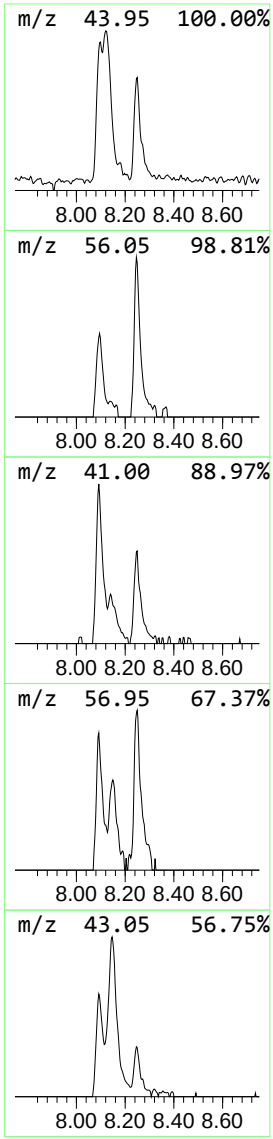
Peak Number 3 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.249	2.80 ug/L	26536	Chlorobenzene-d5	8.853

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	64
2	Hexanal	100	C6H12O	000066-25-1	64
3	Hexanal	100	C6H12O	000066-25-1	64
4	Hexanal	100	C6H12O	000066-25-1	64
5	Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101221\
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Acq On : 12 Oct 2021 12:59
Operator : SY/MD
Sample : M4126-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AD0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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

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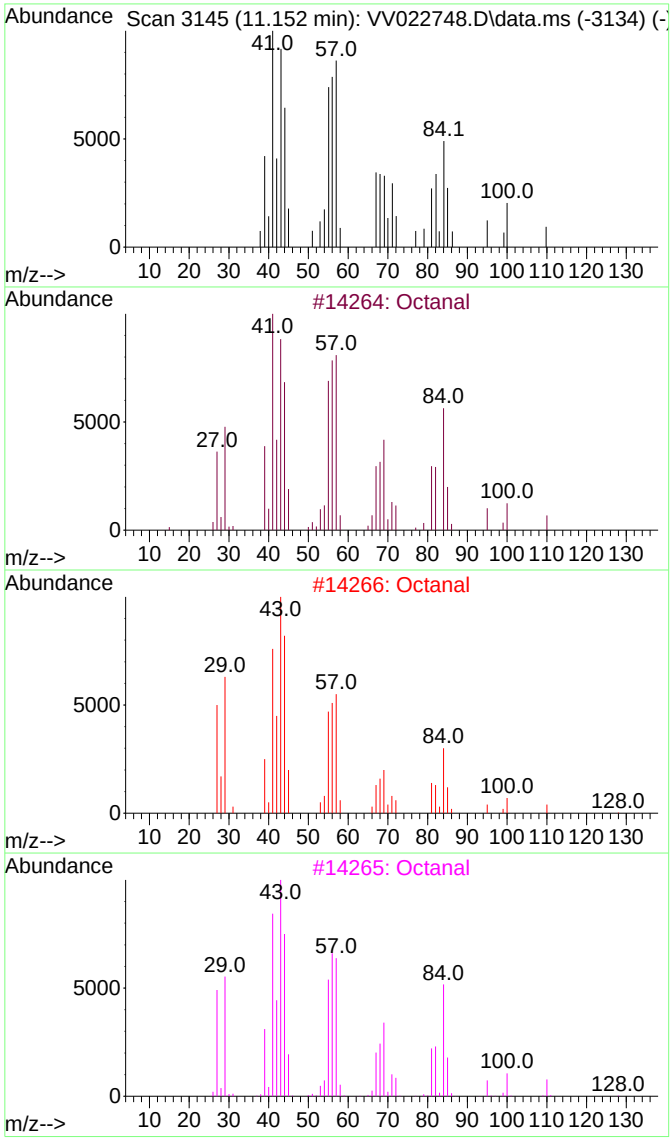
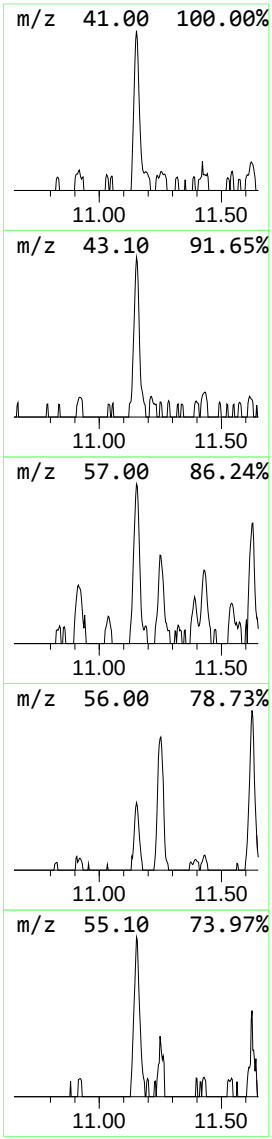
Peak Number 4 Octanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.152	2.91 ug/L	24495	1,4-Dichlorobenzene-d4	11.252

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	87
2	Octanal	128	C8H16O	000124-13-0	83
3	Octanal	128	C8H16O	000124-13-0	78
4	Octanal	128	C8H16O	000124-13-0	53
5	Piperazine, 2-methyl-	100	C5H12N2	000109-07-9	46





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ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AD0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

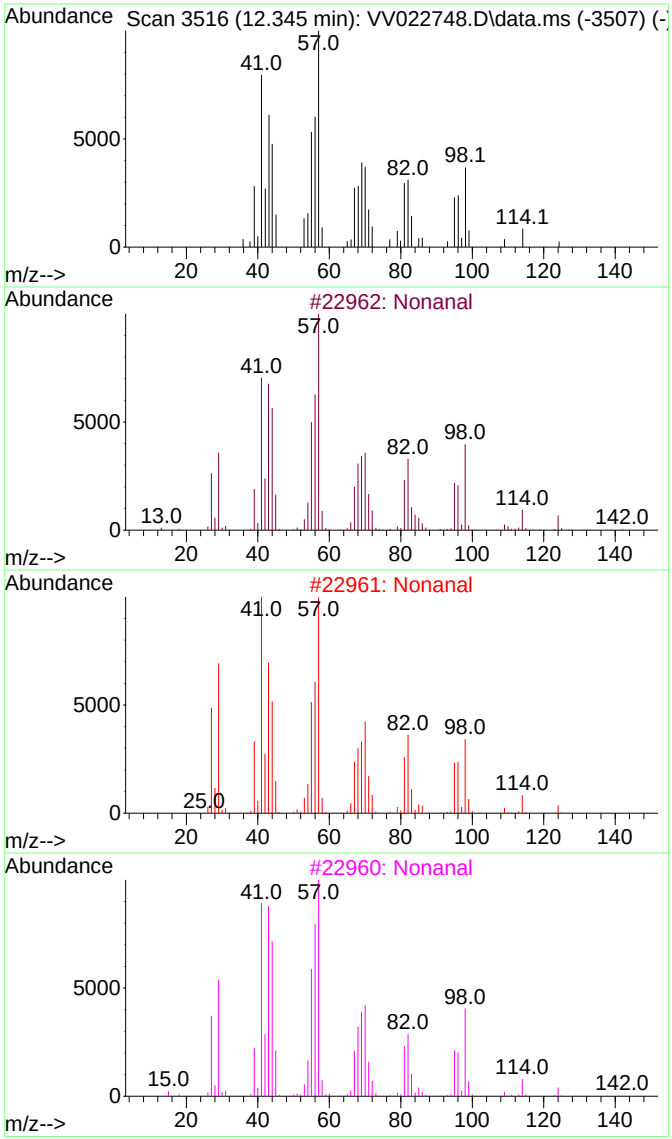
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

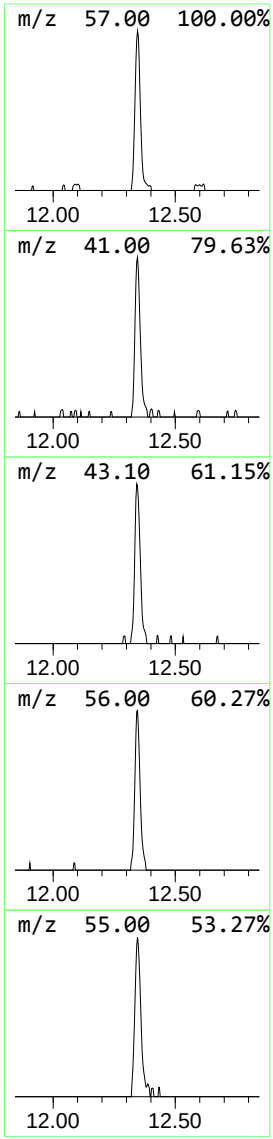
****

Peak Number 5 Nonanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.345	6.15 ug/L	51784	1,4-Dichlorobenzene-d4	11.252

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	91
2	Nonanal	142	C9H18O	000124-19-6	91
3	Nonanal	142	C9H18O	000124-19-6	90
4	Nonanal	142	C9H18O	000124-19-6	90
5	Cyclohexanol, 2-methyl-, trans-	114	C7H14O	007443-52-9	30





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.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	5.908	7.6	ug/L	58228	1	5.619	382909	50.0
Hexanal	8.249	2.8	ug/L	26536	2	8.853	474309	50.0
Octanal	11.152	2.9	ug/L	24495	3	11.252	420698	50.0
Nonanal	12.345	6.2	ug/L	51784	3	11.252	420698	50.0