LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047999.D
Acq On : 13 Apr 2022 13:30
Operator : SY/MD
Sample : N2345-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J86

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\SFAMULM032422WMA.M
Title : VOC Analysis

Signal : TIC: VU047999.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	39	45	51	rBV	30330	32488	0.48%	0.166%
2	1.601	74	81	99	rVB	156625	182342	2.71%	0.932%
3	1.916	172	179	197	rVB	126352	169916	2.52%	0.869%
4	2.572	370	383	399	rBV	265911	440168	6.53%	2.250%
5	2.777	434	447	473	rBV	112127	298721	4.43%	1.527%
6	3.276	600	602	604	rBV	337	193	0.00%	0.001%
7	3.298	604	609	615	rVV3	537	663	0.01%	0.003%
8	3.363	621	629	642	rVB3	4450	9328	0.14%	0.048%
9	3.465	659	661	665	rVB3	287	146	0.00%	0.001%
10	3.494	665	670	671	rBV2	353	266	0.00%	0.001%
11	3.607	703	705	707	rBV	259	141	0.00%	0.001%
12	3.649	713	718	725	rBV2	551	615	0.01%	0.003%
13	3.710	735	737	740	rBV3	251	156	0.00%	0.001%
14	3.954	811	813	815	rBV2	316	174	0.00%	0.001%
15	4.002	824	828	832	rBV3	283	261	0.00%	0.001%
16	4.025	833	835	836	rBV3	379	160	0.00%	0.001%
17	4.166	876	879	883	rBV3	466	486	0.01%	0.002%
18	4.199	887	889	891	rVB2	299	143	0.00%	0.001%
19	4.211	891	893	896	rBV2	255	136	0.00%	0.001%
20	4.273	910	912	915	rVB3	388	159	0.00%	0.001%
21	4.301	918	921	924	rBV2	398	288	0.00%	0.001%
22	4.340	931	933	938	rVB3	373	256	0.00%	0.001%
23	4.369	938	942	944	rVB2	286	207	0.00%	0.001%
24	4.401	949	952	955	rBV2	326	225	0.00%	0.001%
25	4.462	968	971	972	rBV	304	169	0.00%	0.001%
26	4.562	999	1002	1006	rBV3	536	456	0.01%	0.002%
27	4.626	1008	1022	1050	rBV	131038	329868	4.89%	1.686%
28	4.896	1104	1106	1109	rBV3	401	199	0.00%	0.001%
29	5.067	1141	1159	1181	rBV	233366	545437	8.09%	2.788%
30	5.617	1327	1330	1333	rBV2	338	235	0.00%	0.001%
31	5.729	1339	1365	1391	rBV2	466221	1278976	18.98%	6.538%
32	5.973	1437	1441	1444	rVB3	501	382	0.01%	0.002%
33	5.993	1444	1447	1451	rBV3	666	440	0.01%	0.002%
34	6.018	1451	1455	1458	rBV2	529	466	0.01%	0.002%
35	6.141	1491	1493	1496	rBV	247	172	0.00%	0.001%
36	6.250	1512	1527	1545	rBV	425376	809837	12.02%	4.140%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047999.D
Acq On : 13 Apr 2022 13:30
Operator : SY/MD
Sample : N2345-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J86

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\SFAMULM032422WMA.M
Title : VOC Analysis

37	6.523	1607	1612	1617	rBV4	1007	1269	0.02%	0.006%
38	6.620	1639	1642	1647	rVB3	426	288	0.00%	0.001%
39	6.690	1647	1664	1693	rBV	292679	575512	8.54%	2.942%
40	6.877	1719	1722	1725	rVV	346	228	0.00%	0.001%
41	6.941	1739	1742	1745	rBV2	273	183	0.00%	0.001%
42	7.015	1760	1765	1768	rBV3	360	298	0.00%	0.002%
43	7.038	1768	1772	1773	rBV2	491	347	0.01%	0.002%
44	7.089	1785	1788	1791	rBV2	384	242	0.00%	0.001%
45	7.102	1791	1792	1795	rVV2	342	173	0.00%	0.001%
46	7.137	1799	1803	1806	rVV2	412	308	0.00%	0.002%
47	7.182	1810	1817	1834	rVB3	4676	8202	0.12%	0.042%
48	7.247	1834	1837	1841	rVB2	234	151	0.00%	0.001%
49	7.301	1850	1854	1856	rBV2	318	259	0.00%	0.001%
50	7.398	1879	1884	1887	rBV2	324	335	0.00%	0.002%
51	7.452	1896	1901	1902	rBV2	317	208	0.00%	0.001%
52	7.488	1907	1912	1915	rBV4	478	446	0.01%	0.002%
53	7.568	1924	1937	1957	rBV	155587	277036	4.11%	1.416%
54	7.690	1968	1975	1986	rVB7	2750	4740	0.07%	0.024%
55	7.780	2000	2003	2005	rBV3	335	267	0.00%	0.001%
56	7.825	2013	2017	2018	rBV	264	149	0.00%	0.001%
57	7.899	2026	2040	2055	rBV	591122	1023065	15.18%	5.230%
58	8.118	2106	2108	2112	rVB2	352	232	0.00%	0.001%
59	8.179	2115	2127	2142	rBV	109402	187885	2.79%	0.960%
60	8.475	2212	2219	2232	rVB2	3749	7049	0.10%	0.036%
61	8.539	2232	2239	2240	rBV2	1139	1159	0.02%	0.006%
62	8.632	2256	2268	2298	rBV	425495	767308	11.38%	3.922%
63	8.861	2337	2339	2342	rBV	389	233	0.00%	0.001%
64	9.018	2381	2388	2392	rBV4	1155	1416	0.02%	0.007%
65	9.054	2397	2399	2403	rBV2	444	304	0.00%	0.002%
66	9.108	2413	2416	2417	rBV3	304	155	0.00%	0.001%
67	9.166	2427	2434	2438	rBV5	958	1256	0.02%	0.006%
68	9.198	2442	2444	2448	rVB2	334	195	0.00%	0.001%
69	9.359	2490	2494	2499	rBV5	1526	1874	0.03%	0.010%
70	9.417	2500	2512	2547	rVB	645986	1102541	16.36%	5.636%
71	9.578	2556	2562	2569	rBV6	2632	3839	0.06%	0.020%
72	9.748	2611	2615	2619	rBV	400	426	0.01%	0.002%
73	9.851	2643	2647	2649	rBV3	877	712	0.01%	0.004%
74	10.214	2752	2760	2772	rVB6	3566	7269	0.11%	0.037%
75	10.401	2807	2818	2821	rBV5	3117	4220	0.06%	0.022%
76	10.703	2894	2912	2918	rBV3	23050	44930	0.67%	0.230%

LSC Area Percent Report

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Data File : VU047999.D
Acq On : 13 Apr 2022 13:30
Operator : SY/MD
Sample : N2345-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J86

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\SFAMULM032422WMA.M
Title : VOC Analysis

77	10.758	2919	2929	2947	rVB	435304	709887	10.53%	3.629%
78	11.034	3010	3015	3017	rBV3	433	317	0.00%	0.002%
79	11.050	3018	3020	3023	rVB	512	270	0.00%	0.001%
80	11.070	3023	3026	3028	rBV2	240	165	0.00%	0.001%
81	11.086	3028	3031	3033	rBV	459	231	0.00%	0.001%
82	11.147	3048	3050	3059	rVB5	811	645	0.01%	0.003%
83	11.185	3059	3062	3065	rBV3	458	378	0.01%	0.002%
84	11.375	3117	3121	3126	rBV4	941	1161	0.02%	0.006%
85	11.430	3136	3138	3139	rBV4	339	167	0.00%	0.001%
86	11.626	3193	3199	3203	rBV4	410	420	0.01%	0.002%
87	11.693	3215	3220	3223	rBV4	1649	1547	0.02%	0.008%
88	11.742	3232	3235	3239	rVB3	722	502	0.01%	0.003%
89	11.812	3244	3257	3279	rBV	758224	1207680	17.92%	6.173%
90	11.951	3293	3300	3315	rVB5	18253	30459	0.45%	0.156%
91	12.063	3323	3335	3348	rBV2	18223	34143	0.51%	0.175%
92	12.192	3360	3375	3402	rBV	637833	1079024	16.01%	5.516%
93	12.835	3567	3575	3587	rBV6	6130	9904	0.15%	0.051%
94	12.964	3603	3615	3633	rVB4	26704	64360	0.95%	0.329%
95	13.330	3722	3729	3736	rBV2	15479	22911	0.34%	0.117%
96	13.375	3737	3743	3755	rVB3	30648	45825	0.68%	0.234%
97	14.359	4041	4049	4060	rVB2	22221	32269	0.48%	0.165%
98	15.542	4406	4417	4433	rBV	704930	1081934	16.05%	5.530%
99	16.388	4669	4680	4691	rBV	4530490	6739877	100.00%	34.452%
100	17.259	4944	4951	4965	rVB	231301	368099	5.46%	1.882%

Sum of corrected areas: 19563159

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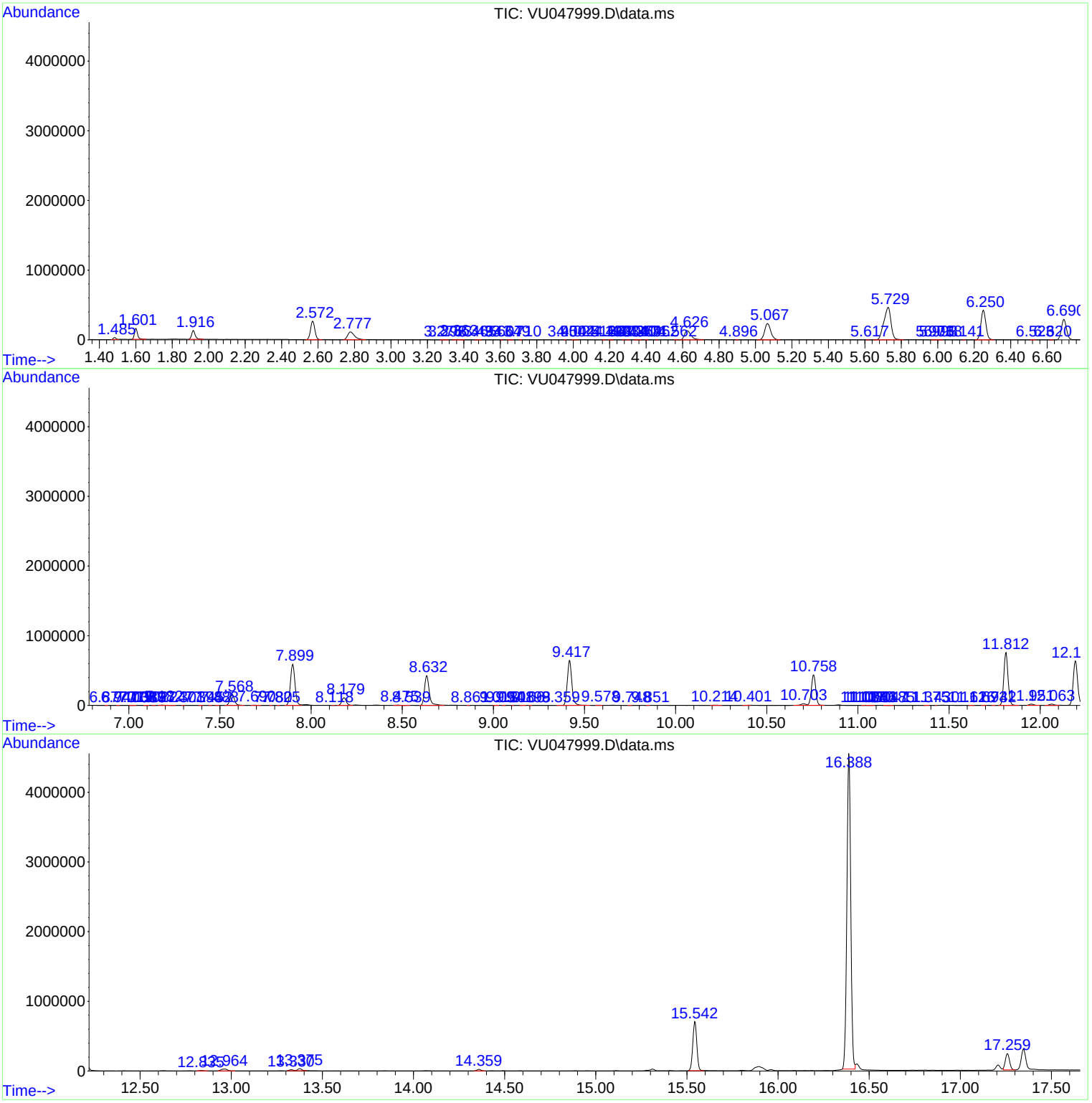
Acq On : 13 Apr 2022 13:30
Operator : SY/MD
Sample : N2345-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J86

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047999.D
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Operator : SY/MD
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J86

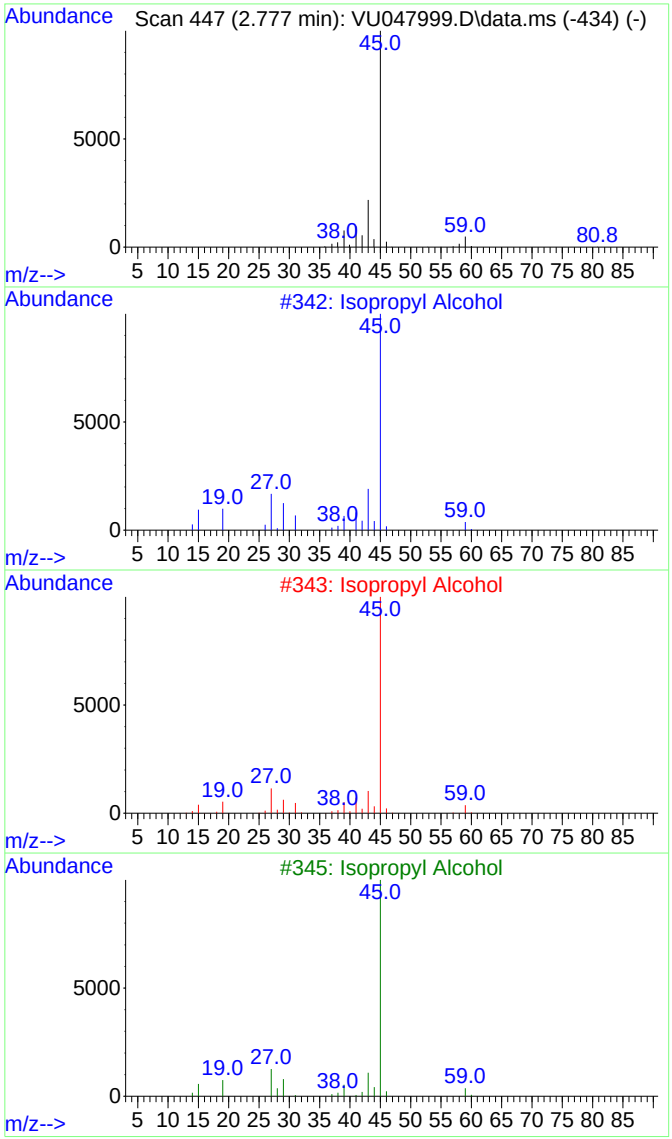
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

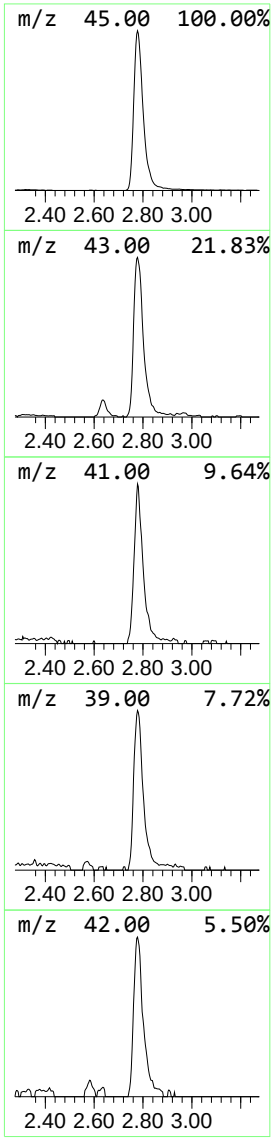
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.777	18.44 ug/L	298721	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047999.D
Acq On : 13 Apr 2022 13:30
Operator : SY/MD
Sample : N2345-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J86

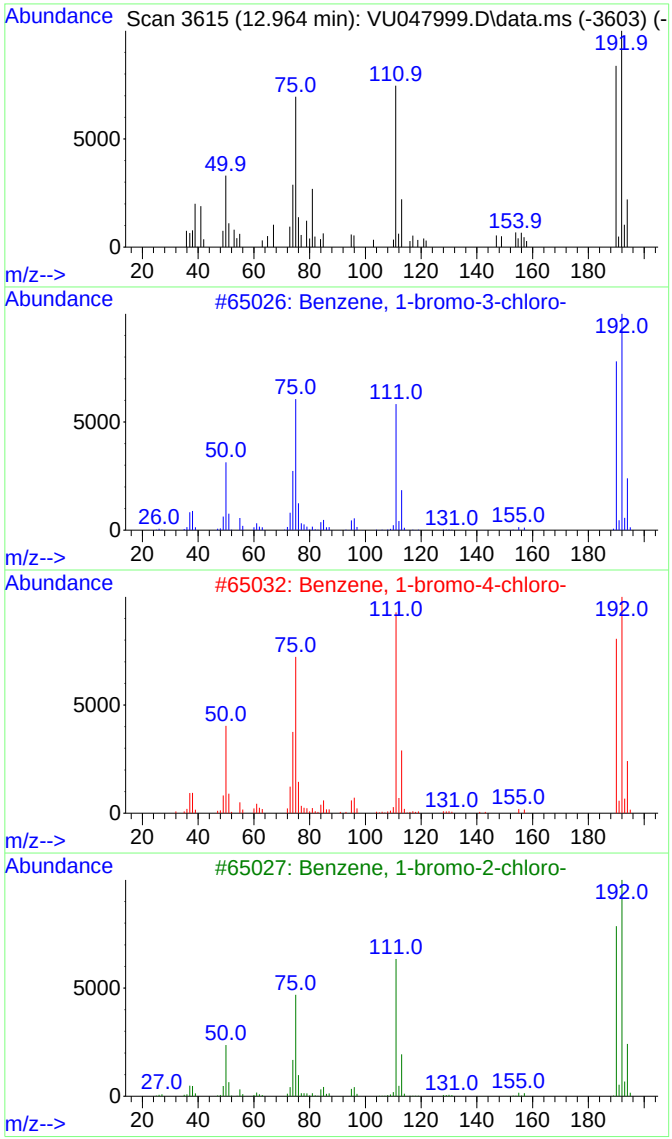
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

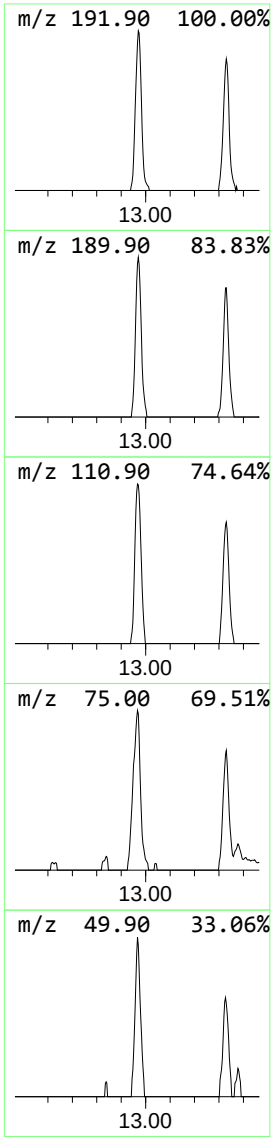
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-bromo-3-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.964	2.66 ug/L	64360	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	98
2	Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98
3	Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	97
4	Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	96
5	Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	96





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Data File : VU047999.D
Acq On : 13 Apr 2022 13:30
Operator : SY/MD
Sample : N2345-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J86

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

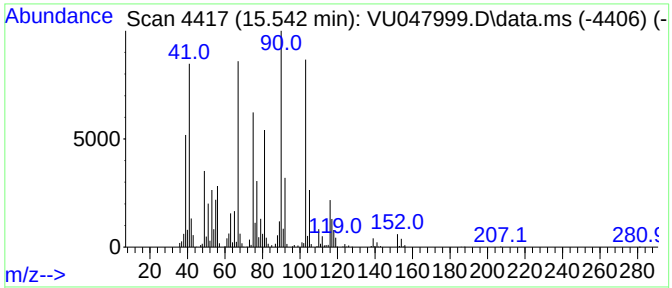
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

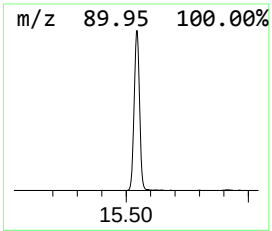
****

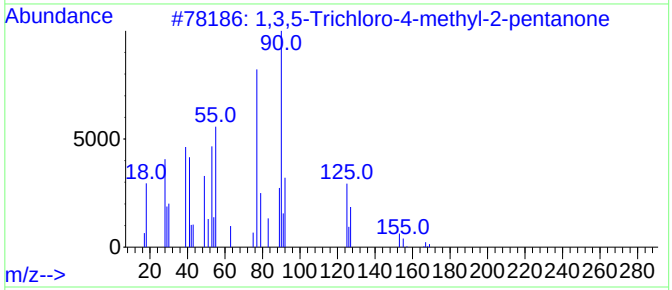
Peak Number 4 unknown-01 Concentration Rank 2

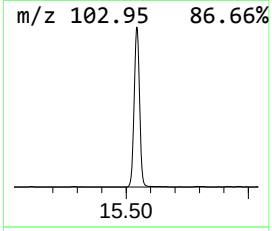
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.542	44.79 ug/L	1081930	1,4-Dichlorobenzene-d4	11.812

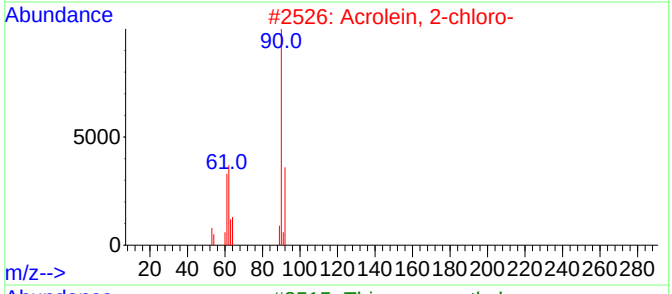
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	38
2	Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	37
3	Thiourea, methyl-	90	C2H6N2S	000598-52-7	35
4	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	35
5	Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	28

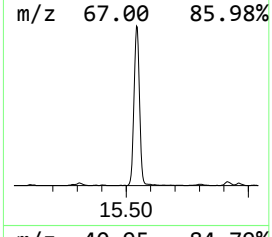


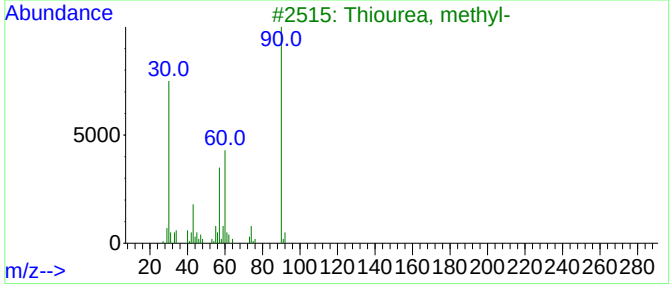


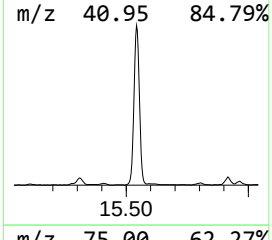


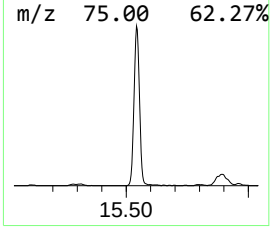












Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047999.D
Acq On : 13 Apr 2022 13:30
Operator : SY/MD
Sample : N2345-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J86

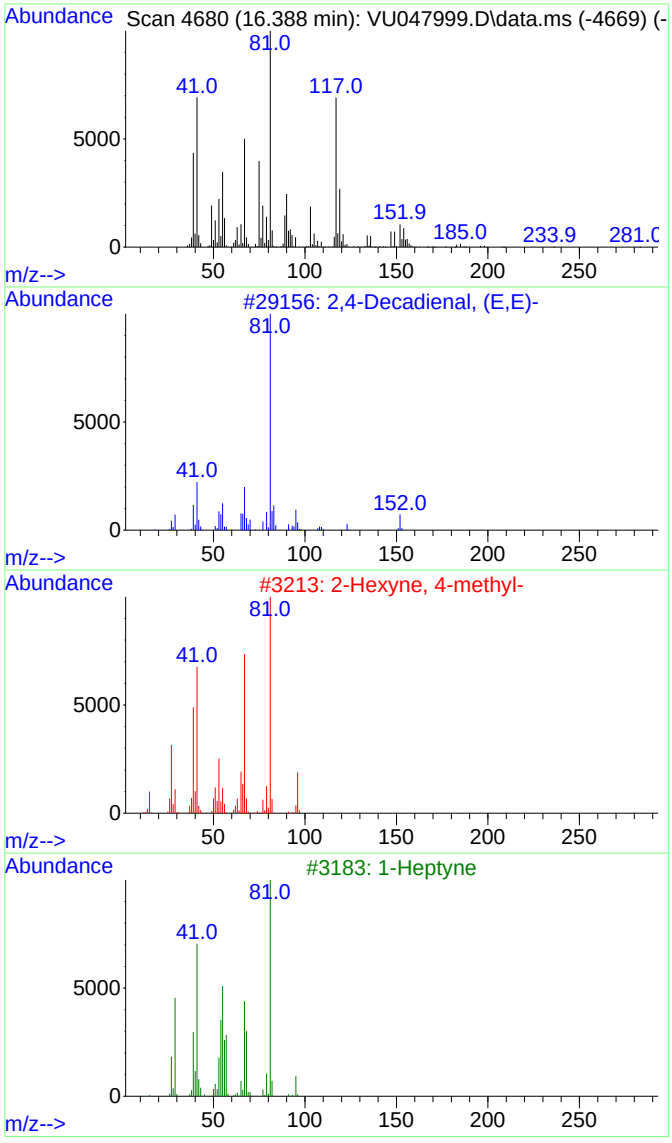
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

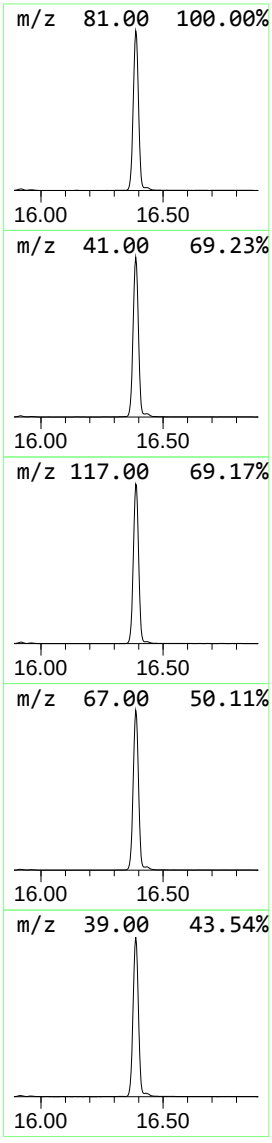
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	279.04 ug/L	6739880	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	22
2	2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	12
3	1-Heptyne	96	C7H12	000628-71-7	12
4	Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	12
5	Acetamide, N-(1-furan-2-ylmethyl...	372	C14H11F3N4O5	1000303-51-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047999.D
Acq On : 13 Apr 2022 13:30
Operator : SY/MD
Sample : N2345-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J86

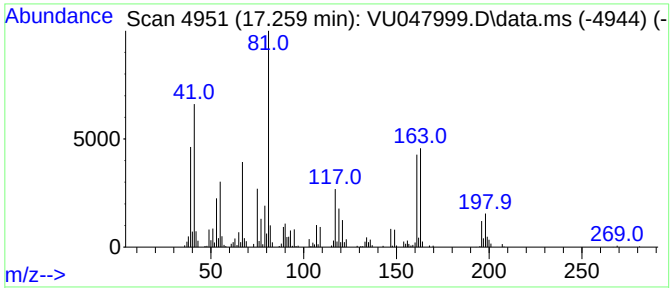
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

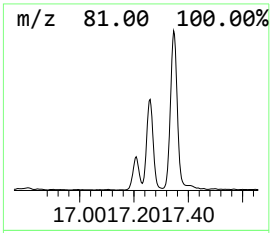
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

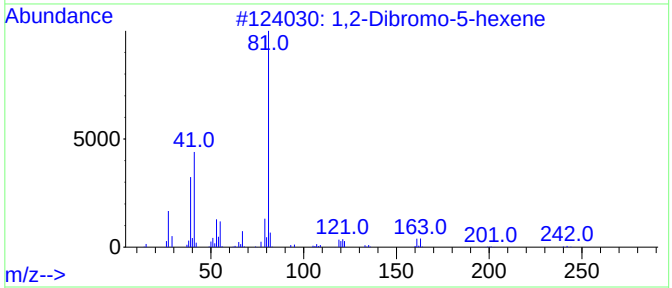
****
Peak Number 6 unknown-03 Concentration Rank 5

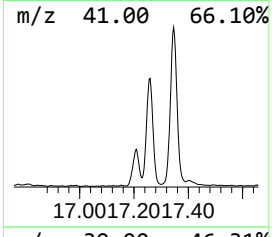
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.259	15.24 ug/L	368099	1,4-Dichlorobenzene-d4	11.812

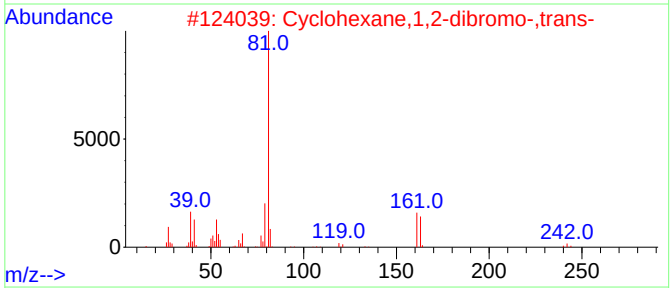
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Dibromo-5-hexene	240	C6H10Br2	004285-48-7	40
2	Cyclohexane,1,2-dibromo-,trans-	240	C6H10Br2	007429-37-0	38
3	Cyclohexane, 1,2-dibromo-	240	C6H10Br2	005401-62-7	38
4	Cyclohexane, 1,4-dibromo-	240	C6H10Br2	035076-92-7	38
5	Fenchol, exo-	154	C10H18O	022627-95-8	25

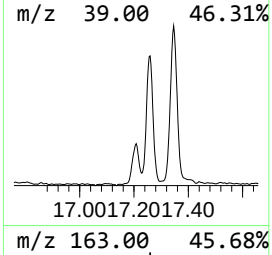


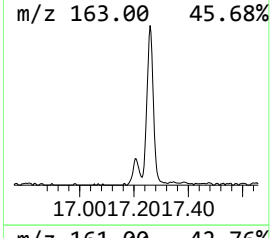


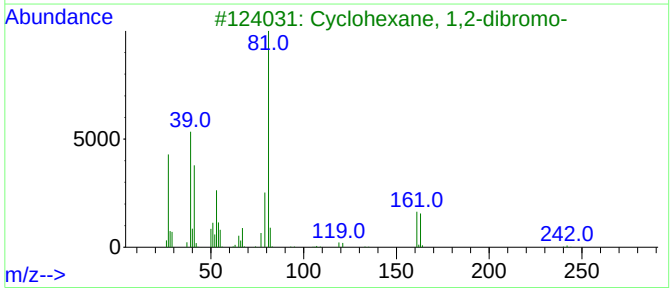


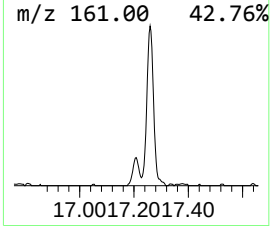












Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047999.D
Acq On : 13 Apr 2022 13:30
Operator : SY/MD
Sample : N2345-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J86

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.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
Isopropyl Alcohol	2.777	18.4	ug/L	298721	1	6.250	809837	50.0
Benzene, 1-brom...	12.964	2.7	ug/L	64360	3	11.812	1207680	50.0
unknown-01	15.542	44.8	ug/L	1081930	3	11.812	1207680	50.0
unknown-02	16.388	279.0	ug/L	6739880	3	11.812	1207680	50.0
unknown-03	17.259	15.2	ug/L	368099	3	11.812	1207680	50.0