LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031765.D
Acq On : 26 Jul 2023 13:39
Operator : SY/MD
Sample : 03712-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y2

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\SFAMVLM072523WMA.M
Title : VOC Analysis

Signal : TIC: VV031765.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	67	74	90	rVV	181635	205223	13.13%	1.596%
2	1.352	92	97	109	rVB	15369	19422	1.24%	0.151%
3	1.532	146	153	164	rBV	189788	221763	14.19%	1.725%
4	2.063	308	318	327	rBV	314485	460924	29.49%	3.585%
5	2.114	328	334	352	rVB	71280	118631	7.59%	0.923%
6	2.214	362	365	366	rBV3	2206	1255	0.08%	0.010%
7	2.356	406	409	411	rBV3	1313	860	0.06%	0.007%
8	2.497	450	453	457	rVB5	1268	769	0.05%	0.006%
9	2.568	460	475	493	rBV2	59116	125695	8.04%	0.978%
10	2.696	512	515	517	rBV3	1326	795	0.05%	0.006%
11	2.754	530	533	534	rBV2	1536	843	0.05%	0.007%
12	2.851	561	563	566	rBV4	1338	870	0.06%	0.007%
13	2.995	603	608	610	rBV5	1464	1322	0.08%	0.010%
14	3.092	635	638	640	rBV3	984	748	0.05%	0.006%
15	3.114	642	645	649	rBV5	1513	1480	0.09%	0.012%
16	3.310	701	706	708	rBV6	1131	1020	0.07%	0.008%
17	3.349	715	718	720	rBV3	1586	895	0.06%	0.007%
18	3.384	727	729	732	rBV4	1022	679	0.04%	0.005%
19	3.474	753	757	760	rBV5	1114	1103	0.07%	0.009%
20	3.526	772	773	777	rVB3	1073	662	0.04%	0.005%
21	3.590	782	793	794	rBV8	4557	6434	0.41%	0.050%
22	3.790	846	855	884	rBV	135658	380548	24.35%	2.959%
23	4.256	985	1000	1028	rVV	279424	731732	46.81%	5.691%
24	4.478	1067	1069	1071	rVB3	2231	928	0.06%	0.007%
25	4.590	1101	1104	1113	rBV8	2276	2895	0.19%	0.023%
26	4.648	1120	1122	1126	rBV5	907	702	0.04%	0.005%
27	4.735	1146	1149	1152	rVB5	1501	1131	0.07%	0.009%
28	4.793	1163	1167	1169	rBV5	1543	969	0.06%	0.008%
29	4.902	1199	1201	1203	rBV3	1596	665	0.04%	0.005%
30	4.963	1203	1220	1244	rBV3	577743	1563137	100.00%	12.156%
31	5.542	1387	1400	1423	rBV	378362	802708	51.35%	6.243%
32	5.828	1479	1489	1504	rBV2	61271	126276	8.08%	0.982%
33	5.995	1528	1541	1560	rBV	385555	795947	50.92%	6.190%
34	6.381	1656	1661	1664	rVB6	1612	1230	0.08%	0.010%
35	6.513	1690	1702	1718	rBV2	70706	144082	9.22%	1.120%
36	6.703	1758	1761	1767	rVB7	1595	1301	0.08%	0.010%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031765.D
Acq On : 26 Jul 2023 13:39
Operator : SY/MD
Sample : 03712-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y2

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\SFAMVLM072523WMA.M
Title : VOC Analysis

37	6.738	1770	1772	1775	rVB3	1303	651	0.04%	0.005%
38	6.777	1782	1784	1787	rVB3	1250	729	0.05%	0.006%
39	6.796	1787	1790	1793	rBV3	1209	869	0.06%	0.007%
40	6.918	1816	1828	1857	rVV	170756	327129	20.93%	2.544%
41	7.108	1884	1887	1890	rVV4	1463	862	0.06%	0.007%
42	7.127	1890	1893	1898	rVV7	1724	1475	0.09%	0.011%
43	7.150	1898	1900	1906	rVB7	1373	963	0.06%	0.007%
44	7.249	1919	1931	1953	rBV	551486	992913	63.52%	7.722%
45	7.400	1976	1978	1982	rBV4	1491	1018	0.07%	0.008%
46	7.503	2008	2010	2016	rVB6	1181	844	0.05%	0.007%
47	7.558	2017	2027	2043	rBV2	129989	235314	15.05%	1.830%
48	7.732	2078	2081	2086	rVB7	1884	1760	0.11%	0.014%
49	7.834	2109	2113	2114	rBV3	1014	742	0.05%	0.006%
50	7.876	2116	2126	2128	rBV9	8102	10510	0.67%	0.082%
51	8.031	2164	2174	2188	rBV2	410589	778404	49.80%	6.053%
52	8.359	2274	2276	2283	rVB8	1925	1625	0.10%	0.013%
53	8.442	2300	2302	2307	rBV5	1742	1428	0.09%	0.011%
54	8.481	2311	2314	2315	rBV3	1549	952	0.06%	0.007%
55	8.622	2356	2358	2362	rVB4	1376	889	0.06%	0.007%
56	8.670	2370	2373	2374	rBV2	1313	747	0.05%	0.006%
57	8.699	2380	2382	2385	rVB4	1489	859	0.05%	0.007%
58	8.715	2385	2387	2390	rBV4	1553	1129	0.07%	0.009%
59	8.789	2399	2410	2439	rBV	641969	1081015	69.16%	8.407%
60	9.326	2575	2577	2580	rBV4	1459	906	0.06%	0.007%
61	9.432	2608	2610	2613	rVB4	1790	1069	0.07%	0.008%
62	9.474	2621	2623	2624	rBV2	1431	792	0.05%	0.006%
63	9.497	2628	2630	2632	rVV3	2370	1351	0.09%	0.011%
64	9.510	2632	2634	2637	rVB4	1960	977	0.06%	0.008%
65	9.641	2673	2675	2678	rVB3	1494	743	0.05%	0.006%
66	9.773	2713	2716	2718	rBV3	1327	992	0.06%	0.008%
67	9.895	2745	2754	2761	rBV3	6763	12247	0.78%	0.095%
68	10.159	2824	2836	2858	rBV	487524	786898	50.34%	6.120%
69	10.317	2881	2885	2887	rBV4	3689	3001	0.19%	0.023%
70	10.394	2903	2909	2911	rBV6	2786	3067	0.20%	0.024%
71	10.574	2957	2965	2970	rBV8	6165	8782	0.56%	0.068%
72	10.635	2980	2984	2988	rVB7	2293	1932	0.12%	0.015%
73	10.661	2988	2992	2993	rBV4	1323	920	0.06%	0.007%
74	10.709	3005	3007	3011	rBV4	3168	2423	0.16%	0.019%
75	10.796	3029	3034	3037	rBV6	2278	2584	0.17%	0.020%
76	10.812	3037	3039	3041	rVB3	1445	681	0.04%	0.005%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031765.D
Acq On : 26 Jul 2023 13:39
Operator : SY/MD
Sample : 03712-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y2

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\SFAMVLM072523WMA.M
Title : VOC Analysis

77	10.956	3080	3084	3086	rBV4	2336	1889	0.12%	0.015%
78	11.082	3120	3123	3126	rBV6	1212	1101	0.07%	0.009%
79	11.133	3132	3139	3146	rBV6	20027	28032	1.79%	0.218%
80	11.191	3146	3157	3176	rVB	660141	1011320	64.70%	7.865%
81	11.346	3202	3205	3208	rBV4	1432	1114	0.07%	0.009%
82	11.436	3230	3233	3234	rBV3	1334	805	0.05%	0.006%
83	11.500	3243	3253	3255	rBV7	11151	16630	1.06%	0.129%
84	11.567	3263	3274	3292	rVB	683064	1075404	68.80%	8.363%
85	11.850	3353	3362	3370	rBV	6397	11619	0.74%	0.090%
86	11.944	3381	3391	3413	rBV	169280	275767	17.64%	2.145%
87	12.252	3476	3487	3503	rBV3	115869	187998	12.03%	1.462%
88	12.529	3568	3573	3577	rVB8	4326	4694	0.30%	0.037%
89	12.673	3615	3618	3621	rBV4	2714	2056	0.13%	0.016%
90	12.722	3631	3633	3634	rBV2	1671	649	0.04%	0.005%
91	12.837	3666	3669	3670	rBV3	1998	1181	0.08%	0.009%
92	12.860	3674	3676	3677	rBV2	1666	766	0.05%	0.006%
93	12.937	3698	3700	3702	rBV3	1607	779	0.05%	0.006%
94	12.979	3711	3713	3715	rBV4	2255	1252	0.08%	0.010%
95	13.426	3842	3852	3865	rBV4	8443	18808	1.20%	0.146%
96	13.873	3982	3991	4012	rVB	132678	204477	13.08%	1.590%
97	13.985	4024	4026	4038	rVB	6369	8416	0.54%	0.065%
98	14.834	4288	4290	4297	rBV7	1770	2327	0.15%	0.018%
99	14.892	4303	4308	4311	rBV7	2492	2329	0.15%	0.018%
100	15.406	4466	4468	4472	rBV4	1688	1501	0.10%	0.012%

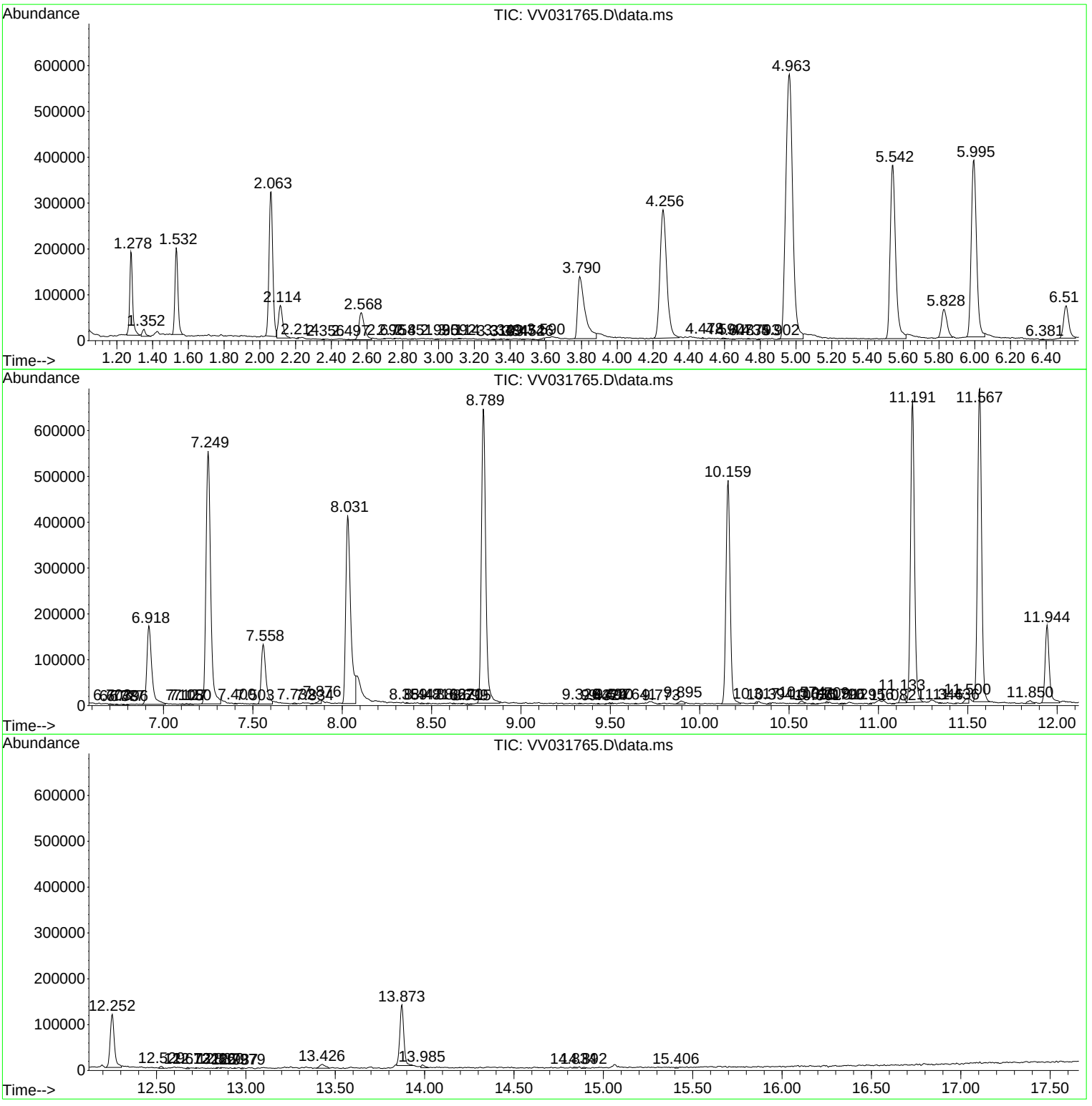
Sum of corrected areas: 12858750

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031765.D
Acq On : 26 Jul 2023 13:39
Operator : SY/MD
Sample : 03712-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031765.D
Acq On : 26 Jul 2023 13:39
Operator : SY/MD
Sample : 03712-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y2

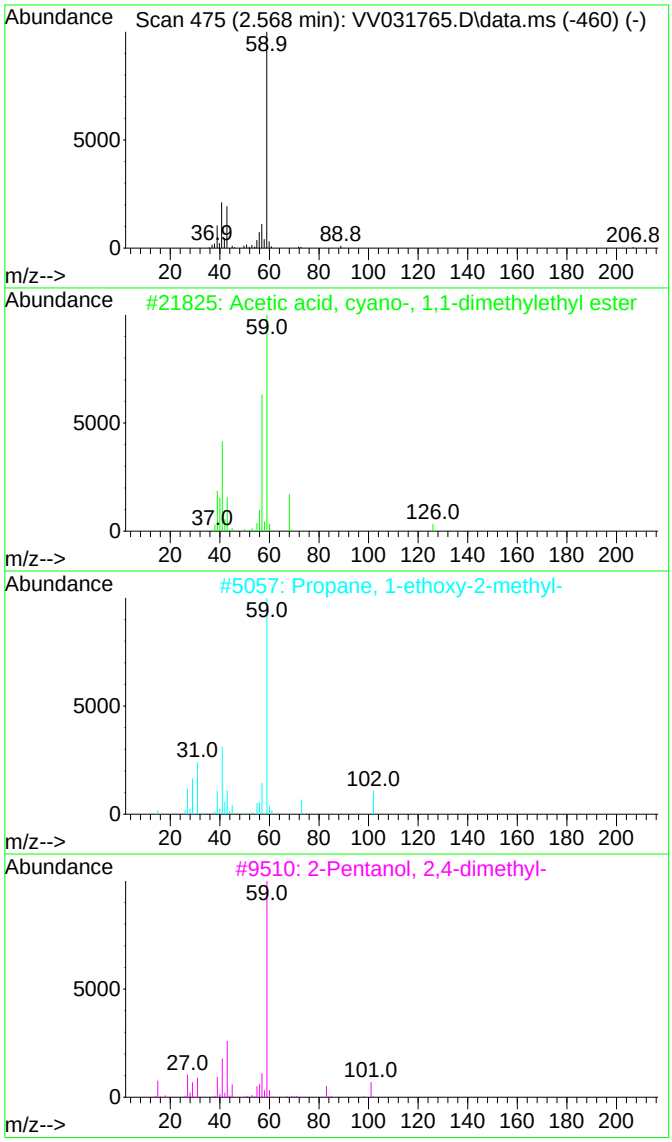
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

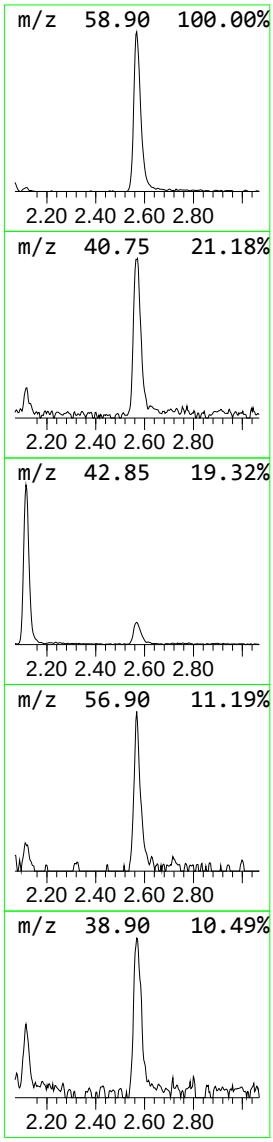
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Acetic acid, cyano-, 1,1-di... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.568	7.83 ug/L	125695	1,4-Difluorobenzene	5.542

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	72
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	64
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	64
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	56
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031765.D
Acq On : 26 Jul 2023 13:39
Operator : SY/MD
Sample : 03712-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y2

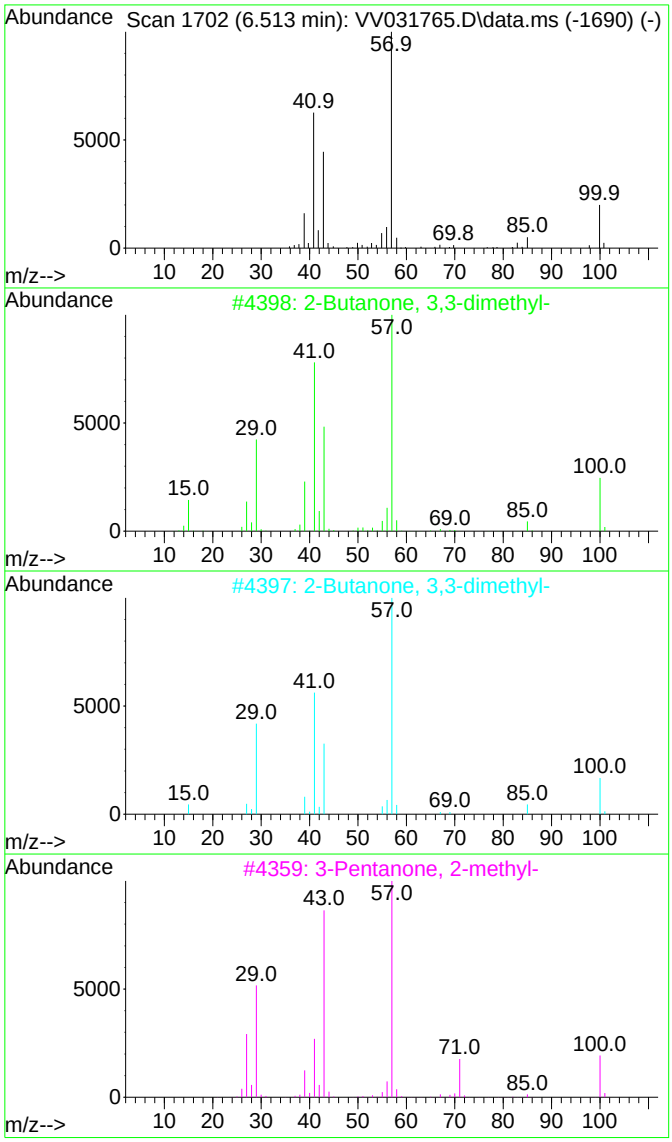
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

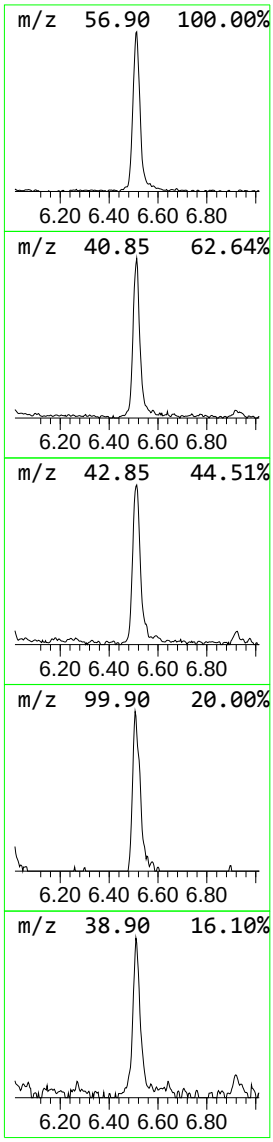
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.513	8.97 ug/L	144082	1,4-Difluorobenzene	5.542

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	90
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	86
3	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	72
4	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
5	3-Hexanone	100	C6H12O	000589-38-8	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031765.D
Acq On : 26 Jul 2023 13:39
Operator : SY/MD
Sample : 03712-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y2

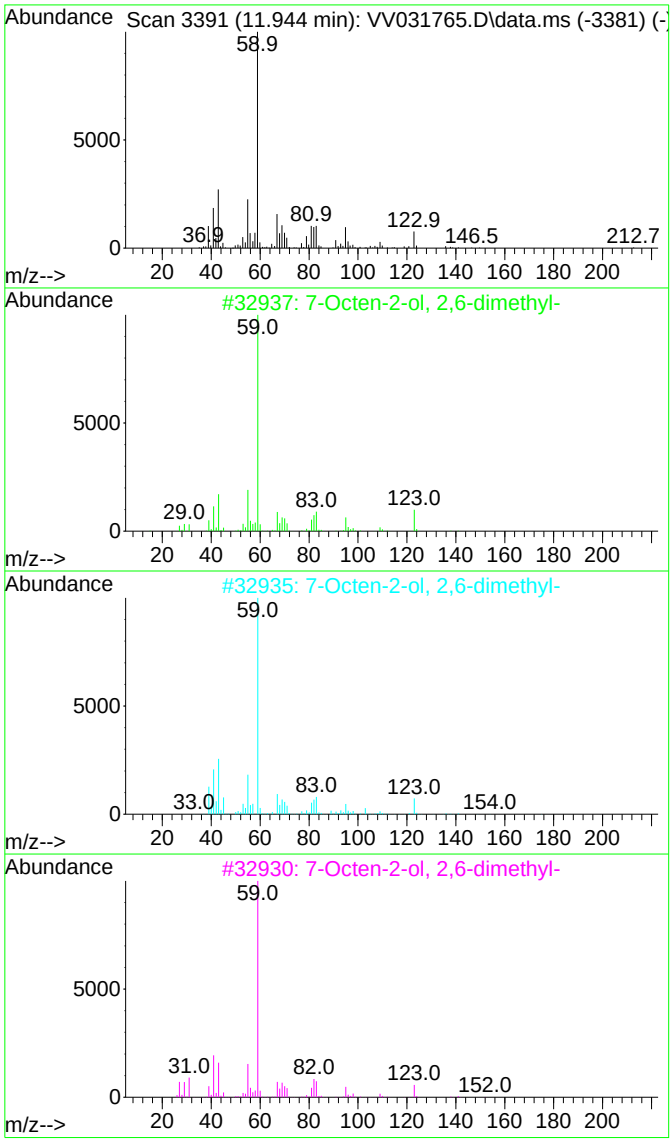
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

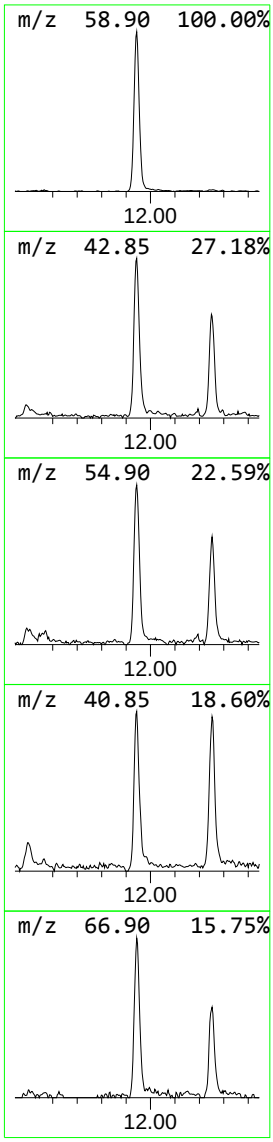
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.944	13.63 ug/L	275767	1,4-Dichlorobenzene-d4	11.191

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	83
2	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
3	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	64
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	59
5	Succinic acid, dodec-2-en-1-yl 2...	342	C19H34O5	1000390-75-0	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031765.D
Acq On : 26 Jul 2023 13:39
Operator : SY/MD
Sample : 03712-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y2

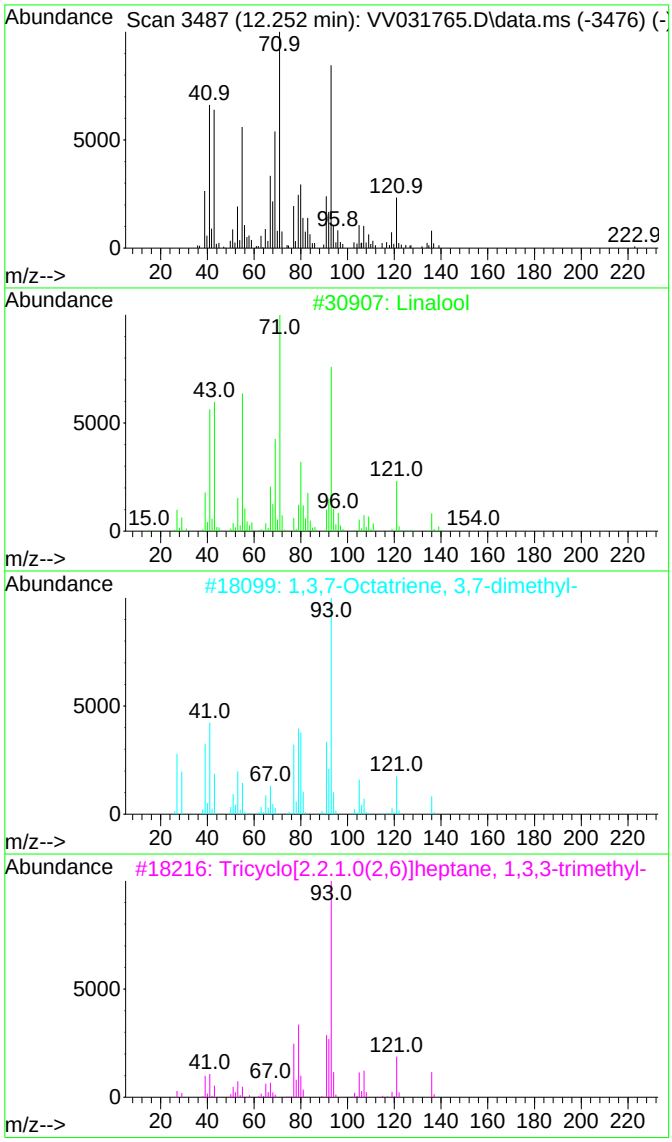
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

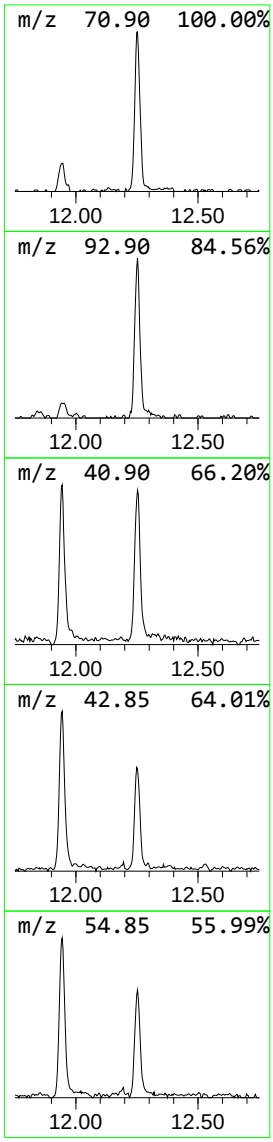
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Linalool Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.252	9.29 ug/L	187998	1,4-Dichlorobenzene-d4	11.191

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Linalool	154	C10H18O	000078-70-6	64
2	1,3,7-Octatriene, 3,7-dimethyl-	136	C10H16	000502-99-8	55
3	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	50
4	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	50
5	Linalool	154	C10H18O	000078-70-6	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031765.D
Acq On : 26 Jul 2023 13:39
Operator : SY/MD
Sample : 03712-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y2

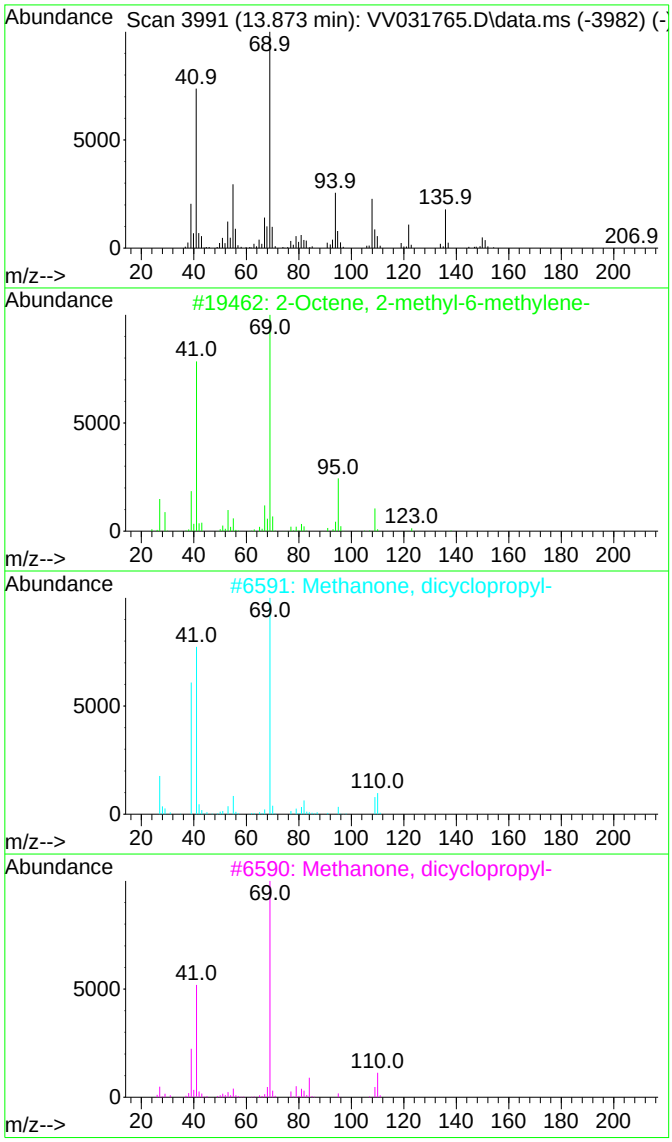
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

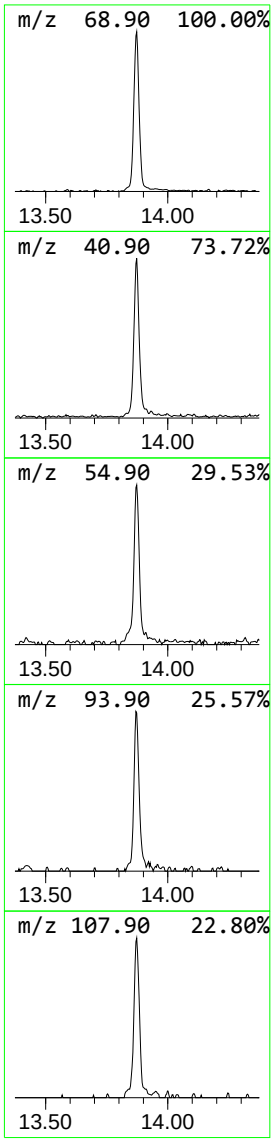
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	10.11 ug/L	204477	1,4-Dichlorobenzene-d4	11.191

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	43
2	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	43
3	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	43
4	Pentane, 1,5-dibromo-	228	C5H10Br2	000111-24-0	43
5	Geranyl formate	182	C11H18O2	000105-86-2	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031765.D
Acq On : 26 Jul 2023 13:39
Operator : SY/MD
Sample : 03712-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.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
Acetic acid, cy...	2.568	7.8	ug/L	125695	1	5.542	802708	50.0
2-Butanone, 3,3...	6.513	9.0	ug/L	144082	1	5.542	802708	50.0
7-Octen-2-ol, 2...	11.944	13.6	ug/L	275767	3	11.191	1011320	50.0
Linalool	12.252	9.3	ug/L	187998	3	11.191	1011320	50.0
unknown-01	13.873	10.1	ug/L	204477	3	11.191	1011320	50.0