

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
 Data File : VV031741.D
 Acq On : 25 Jul 2023 14:33
 Operator : SY/MD
 Sample : 03712-03
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Y1

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: VV031741.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	89	rBV	214370	234886	16.18%	2.007%
2	1.532	145	153	167	rVB	190929	226565	15.61%	1.936%
3	2.059	308	317	328	rBV	364427	529946	36.51%	4.528%
4	2.114	328	334	352	rVB	67027	112351	7.74%	0.960%
5	2.400	418	423	426	rVB6	1493	1073	0.07%	0.009%
6	2.442	433	436	437	rBV3	1695	919	0.06%	0.008%
7	2.571	465	476	495	rBV	63450	130361	8.98%	1.114%
8	2.686	508	512	514	rBV3	2210	1739	0.12%	0.015%
9	2.815	548	552	555	rVB7	2120	1494	0.10%	0.013%
10	2.841	555	560	567	rBV8	1685	1630	0.11%	0.014%
11	2.998	606	609	613	rVB5	2367	1894	0.13%	0.016%
12	3.082	631	635	637	rBV5	1214	861	0.06%	0.007%
13	3.346	712	717	720	rBV5	1009	932	0.06%	0.008%
14	3.371	720	725	728	rBV3	1136	928	0.06%	0.008%
15	3.442	741	747	750	rVB5	1396	1377	0.09%	0.012%
16	3.494	759	763	766	rBV4	1259	1008	0.07%	0.009%
17	3.796	846	857	886	rBV	124946	390885	26.93%	3.339%
18	4.114	952	956	957	rBV3	1345	970	0.07%	0.008%
19	4.256	984	1000	1025	rBV2	245830	643405	44.33%	5.497%
20	4.635	1115	1118	1122	rBV5	1735	1440	0.10%	0.012%
21	4.657	1122	1125	1127	rVB3	1657	993	0.07%	0.008%
22	4.722	1142	1145	1148	rBV4	1799	1506	0.10%	0.013%
23	4.963	1203	1220	1247	rBV2	544825	1451333	100.00%	12.399%
24	5.284	1318	1320	1323	rVV4	1565	855	0.06%	0.007%
25	5.374	1346	1348	1354	rVB6	1488	994	0.07%	0.008%
26	5.455	1370	1373	1376	rBV3	1220	895	0.06%	0.008%
27	5.497	1381	1386	1387	rBV3	1858	1351	0.09%	0.012%
28	5.542	1388	1400	1421	rBV	323339	674762	46.49%	5.765%
29	5.828	1476	1489	1507	rVV3	43452	96174	6.63%	0.822%
30	5.995	1529	1541	1581	rVB	336950	727909	50.15%	6.219%
31	6.182	1596	1599	1605	rBV8	1560	1538	0.11%	0.013%
32	6.391	1660	1664	1666	rBV4	1521	1470	0.10%	0.013%
33	6.416	1670	1672	1676	rVB2	1254	897	0.06%	0.008%
34	6.445	1678	1681	1684	rBV4	1761	1312	0.09%	0.011%
35	6.513	1689	1702	1718	rBV2	66634	138918	9.57%	1.187%
36	6.760	1773	1779	1781	rBV7	921	857	0.06%	0.007%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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	6.918	1817	1828	1846	rBV	140763	275727	19.00%	2.356%
38	7.075	1875	1877	1881	rBV4	1695	1089	0.08%	0.009%
39	7.249	1919	1931	1952	rBV	537542	965087	66.50%	8.245%
40	7.558	2019	2027	2050	rVV2	107952	198870	13.70%	1.699%
41	7.837	2110	2114	2117	rBV5	1880	1798	0.12%	0.015%
42	7.985	2156	2160	2164	rBV6	1487	1171	0.08%	0.010%
43	8.034	2165	2175	2215	rBV2	345675	783907	54.01%	6.697%
44	8.243	2238	2240	2242	rBV3	2093	1128	0.08%	0.010%
45	8.419	2290	2295	2302	rVB7	2583	3341	0.23%	0.029%
46	8.513	2320	2324	2325	rBV3	1290	882	0.06%	0.008%
47	8.567	2337	2341	2344	rBV5	1735	1210	0.08%	0.010%
48	8.648	2365	2366	2371	rVB5	2152	1318	0.09%	0.011%
49	8.677	2371	2375	2378	rBV5	1298	1048	0.07%	0.009%
50	8.706	2382	2384	2387	rVB3	2306	1119	0.08%	0.010%
51	8.789	2399	2410	2432	rBV	540982	921179	63.47%	7.870%
52	8.953	2456	2461	2462	rBV4	2984	2476	0.17%	0.021%
53	9.033	2482	2486	2489	rBV6	2024	1415	0.10%	0.012%
54	9.471	2618	2622	2624	rBV5	1310	953	0.07%	0.008%
55	9.493	2624	2629	2632	rBV7	2945	3186	0.22%	0.027%
56	9.625	2666	2670	2674	rBV7	1078	1133	0.08%	0.010%
57	9.722	2693	2700	2708	rBV7	3866	6033	0.42%	0.052%
58	9.892	2745	2753	2761	rBV7	5859	10575	0.73%	0.090%
59	10.008	2787	2789	2797	rVB8	1426	1460	0.10%	0.012%
60	10.043	2797	2800	2805	rBV7	1611	1520	0.10%	0.013%
61	10.082	2808	2812	2817	rVB8	1723	1348	0.09%	0.012%
62	10.159	2823	2836	2856	rBV	435354	697708	48.07%	5.961%
63	10.413	2907	2915	2919	rBV8	3352	4015	0.28%	0.034%
64	10.574	2952	2965	2971	rBV8	4880	8262	0.57%	0.071%
65	10.683	2995	2999	3000	rBV4	2247	1199	0.08%	0.010%
66	10.715	3006	3009	3015	rVB6	2103	2199	0.15%	0.019%
67	10.795	3032	3034	3039	rVB5	1650	996	0.07%	0.009%
68	10.908	3066	3069	3075	rVB6	1856	1395	0.10%	0.012%
69	11.001	3091	3098	3100	rBV7	4860	5277	0.36%	0.045%
70	11.133	3127	3139	3146	rBV8	18636	29842	2.06%	0.255%
71	11.191	3146	3157	3175	rVB	529633	837099	57.68%	7.152%
72	11.377	3210	3215	3219	rBV5	1697	1947	0.13%	0.017%
73	11.496	3239	3252	3260	rBV9	13163	28307	1.95%	0.242%
74	11.567	3263	3274	3297	rVB	565775	891175	61.40%	7.614%
75	11.750	3327	3331	3333	rBV5	2284	1914	0.13%	0.016%
76	11.812	3346	3350	3354	rVB6	1388	1324	0.09%	0.011%

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Integrator: RTE

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

77	11.844	3354	3360	3366	rBV10	4824	6538	0.45%	0.056%
78	11.943	3377	3391	3407	rBV2	160720	257881	17.77%	2.203%
79	12.037	3416	3420	3428	rVB2	4025	4723	0.33%	0.040%
80	12.252	3477	3487	3504	rBV2	101478	161258	11.11%	1.378%
81	12.377	3524	3526	3529	rBV4	1869	1141	0.08%	0.010%
82	12.529	3570	3573	3577	rVB5	2644	1800	0.12%	0.015%
83	12.577	3586	3588	3589	rBV2	2243	1063	0.07%	0.009%
84	12.657	3609	3613	3616	rBV5	1575	1310	0.09%	0.011%
85	12.911	3689	3692	3695	rBV4	2306	1377	0.09%	0.012%
86	13.085	3744	3746	3749	rBV3	1490	1060	0.07%	0.009%
87	13.207	3776	3784	3795	rVV8	11710	19933	1.37%	0.170%
88	13.252	3795	3798	3805	rVB9	3037	3105	0.21%	0.027%
89	13.342	3822	3826	3834	rVB10	2982	3254	0.22%	0.028%
90	13.429	3847	3853	3855	rBV5	4809	5557	0.38%	0.047%
91	13.660	3921	3925	3926	rBV4	2208	1455	0.10%	0.012%
92	13.689	3931	3934	3943	rVB10	5541	7624	0.53%	0.065%
93	13.757	3953	3955	3959	rVV5	2195	1377	0.09%	0.012%
94	13.873	3983	3991	4001	rVB	88401	126649	8.73%	1.082%
95	14.123	4067	4069	4073	rBV4	1677	1055	0.07%	0.009%
96	14.245	4105	4107	4111	rVB5	1848	1321	0.09%	0.011%
97	14.554	4200	4203	4212	rVB8	1916	1914	0.13%	0.016%
98	15.126	4376	4381	4384	rBV7	3303	3303	0.23%	0.028%
99	15.426	4472	4474	4477	rBV4	1980	989	0.07%	0.008%
100	15.721	4563	4566	4569	rBV6	1642	1237	0.09%	0.011%

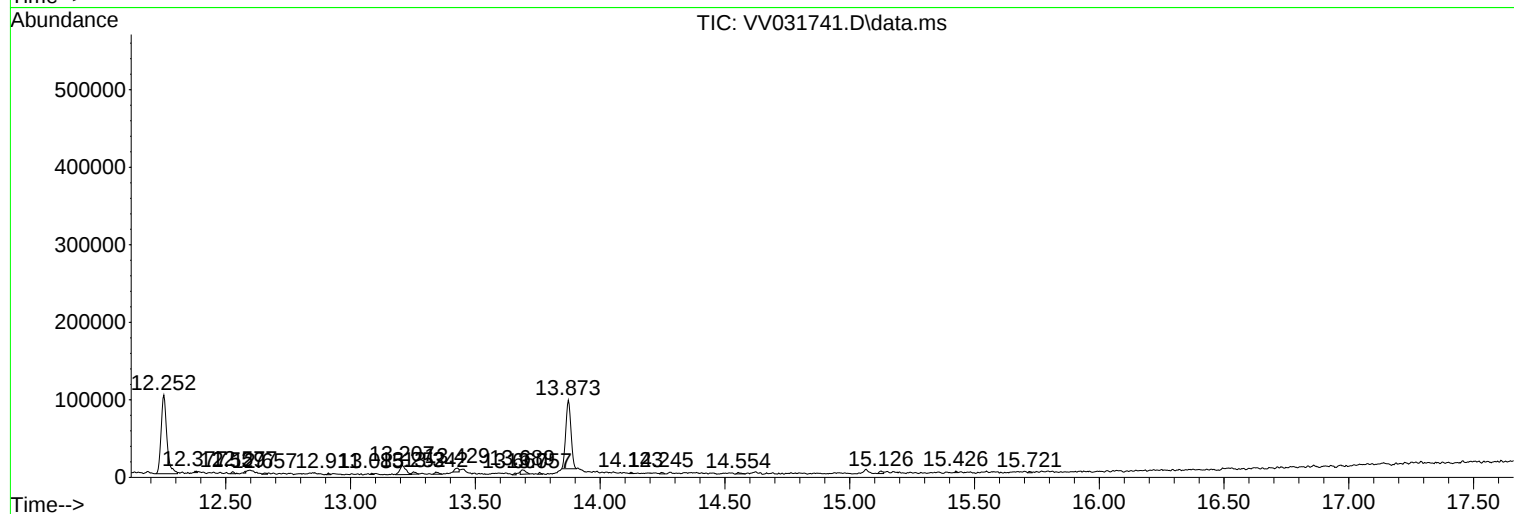
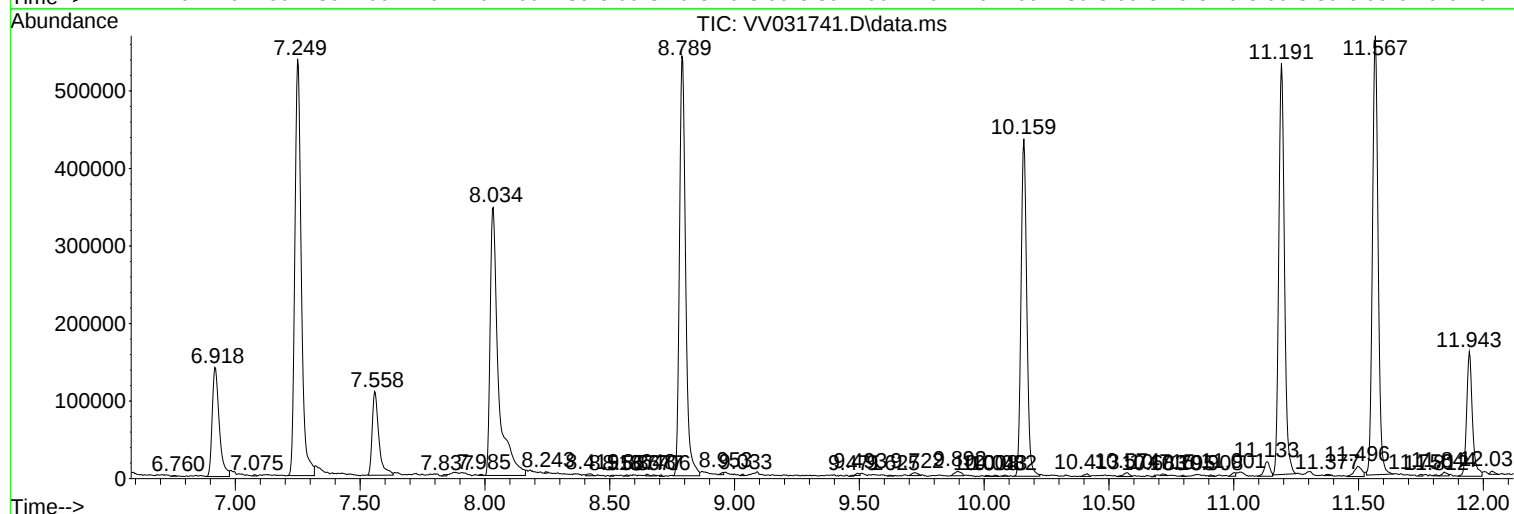
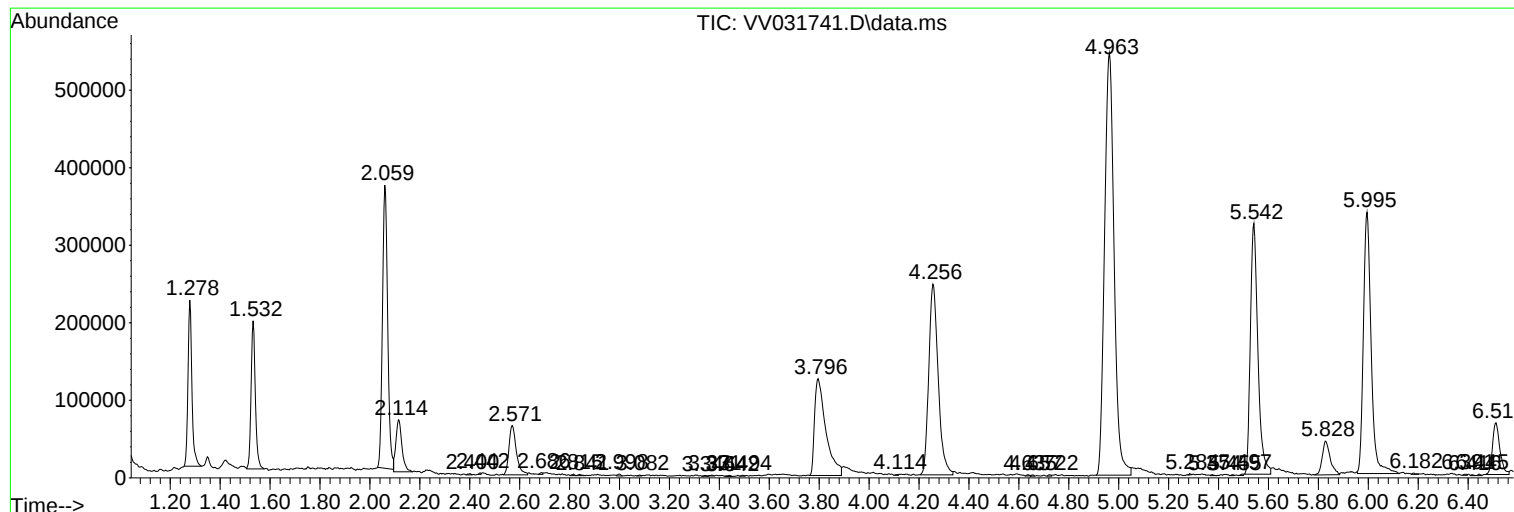
Sum of corrected areas: 11704984

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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y1

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



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Data File : VV031741.D
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Instrument :
MSVOA_V
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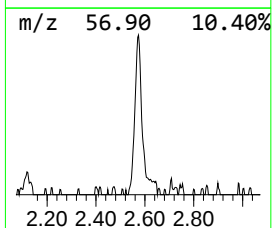
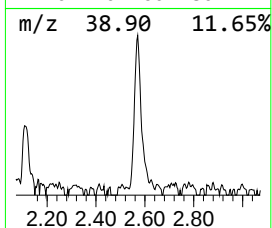
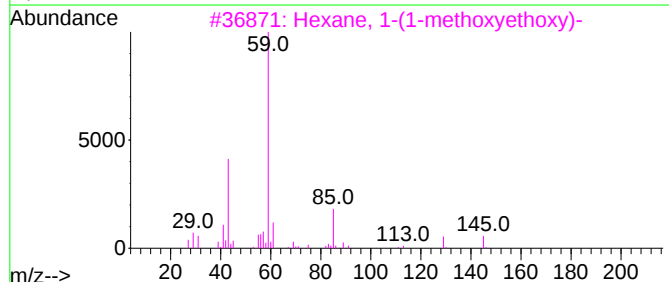
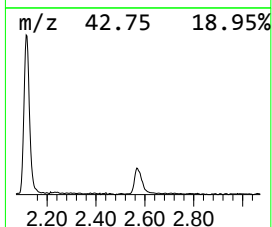
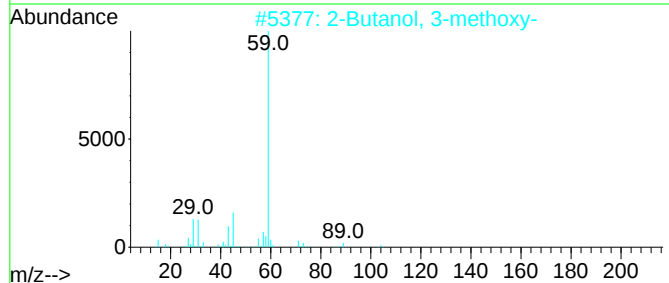
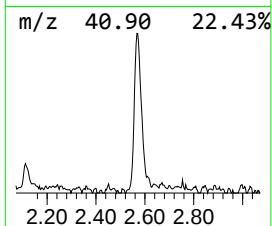
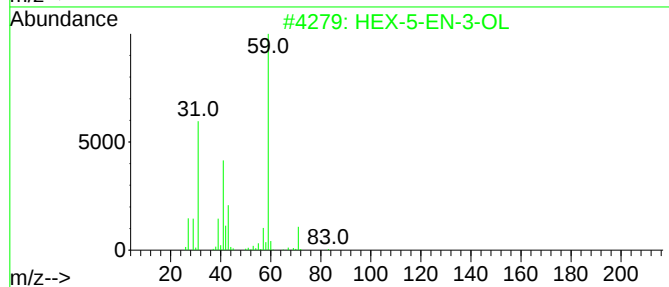
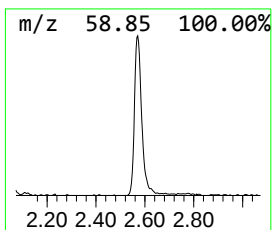
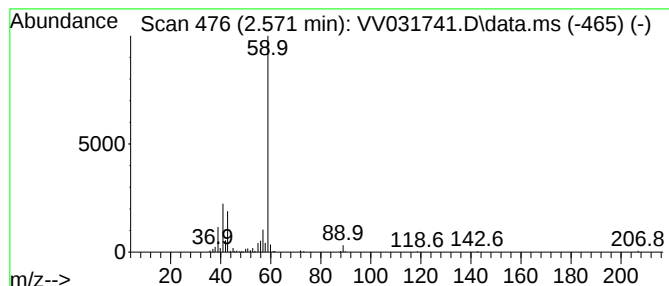
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 HEX-5-EN-3-OL Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.571	9.66 ug/L	130361	1,4-Difluorobenzene	5.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	HEX-5-EN-3-OL			100	C6H12O	000688-99-3	72
2	2-Butanol, 3-methoxy-			104	C5H12O2	053778-72-6	64
3	Hexane, 1-(1-methoxyethoxy)-			160	C9H20O2	054340-90-8	64
4	2-Pentanol, 2,4-dimethyl-			116	C7H16O	000625-06-9	64
5	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	56



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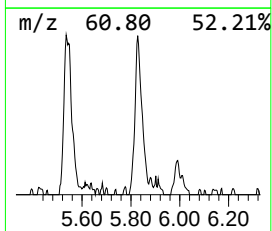
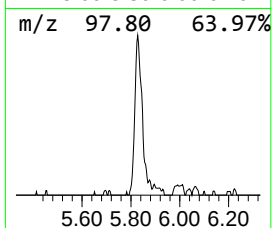
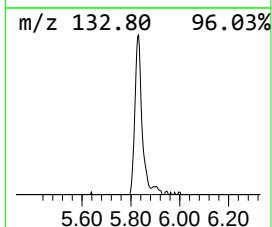
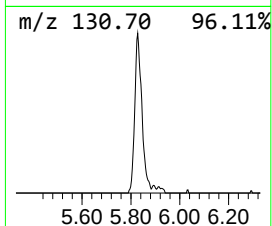
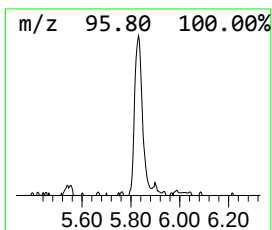
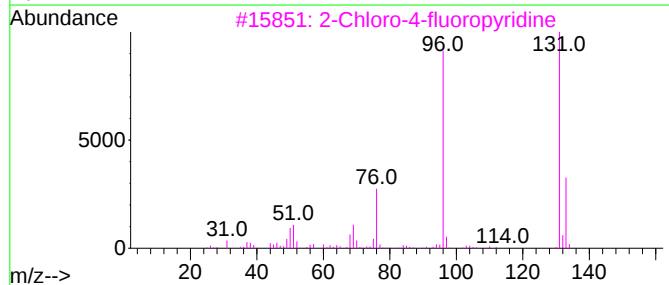
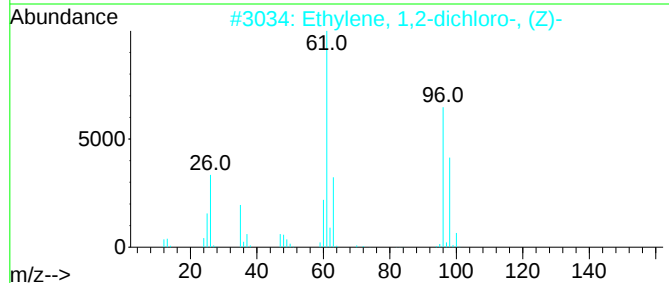
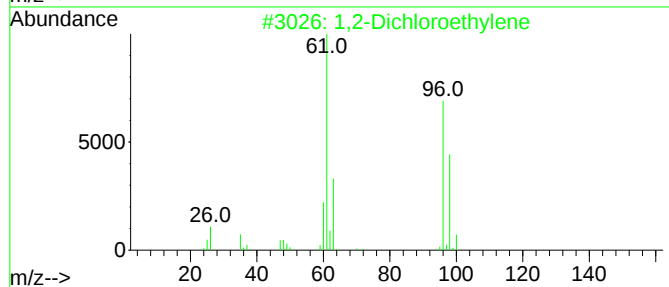
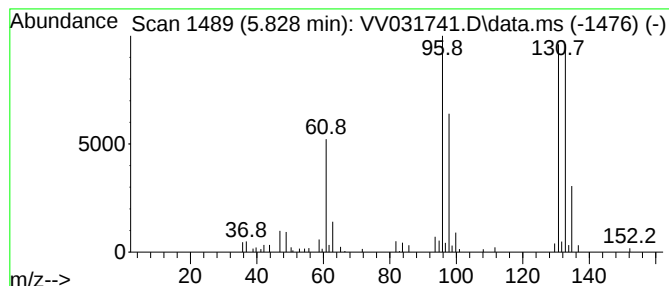
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	7.13 ug/L	96174	1,4-Difluorobenzene	5.542

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2-Dichloroethylene	96	C2H2Cl2	000540-59-0	38
2		Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3		2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
4		Ethene, 1,1-dichloro-	96	C2H2Cl2	000075-35-4	38
5		Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38



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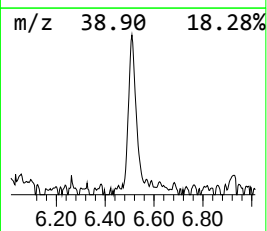
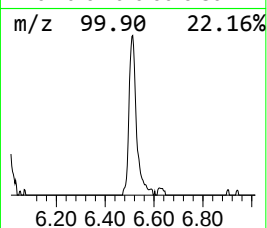
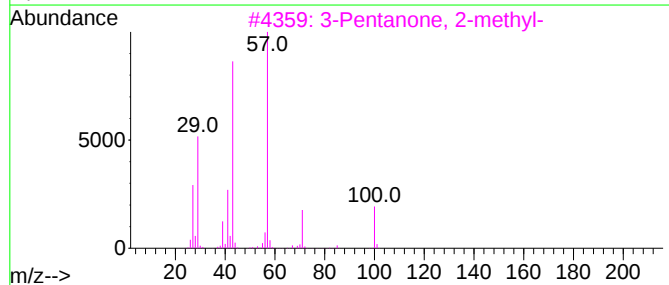
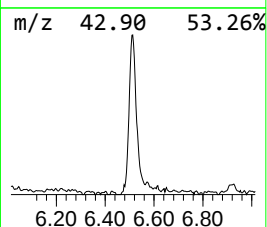
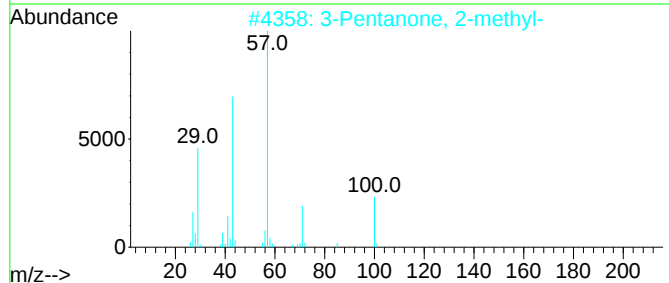
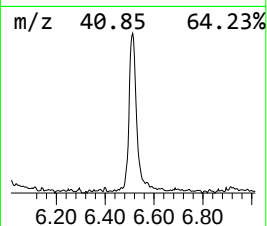
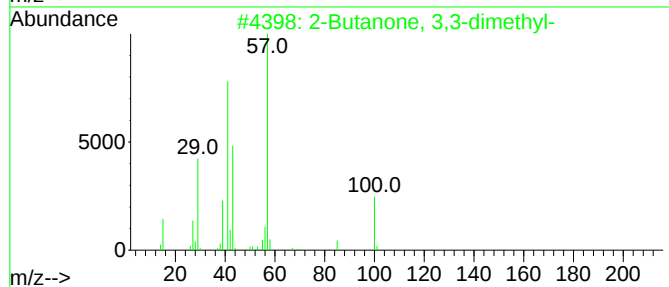
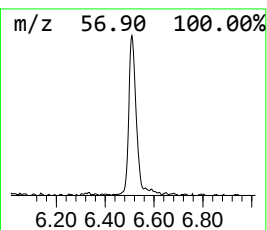
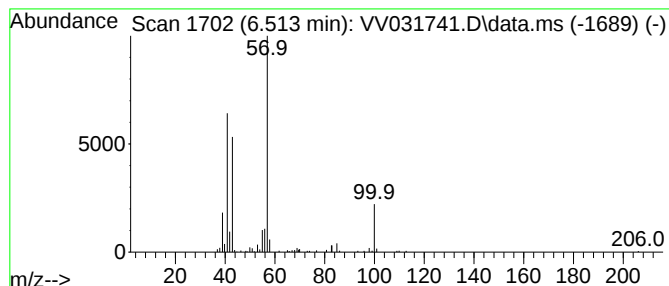
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.513	10.29 ug/L	138918	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	83
2	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	59
3	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	58
4	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	50
5	Butane, 2,3-dimethyl-2,3-dinitro-			176	C6H12N2O4	003964-18-9	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031741.D
Acq On : 25 Jul 2023 14:33
Operator : SY/MD
Sample : 03712-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y1

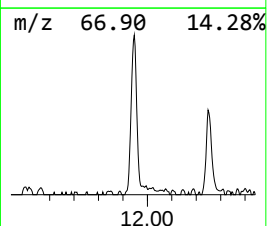
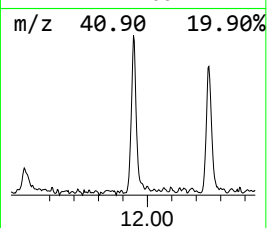
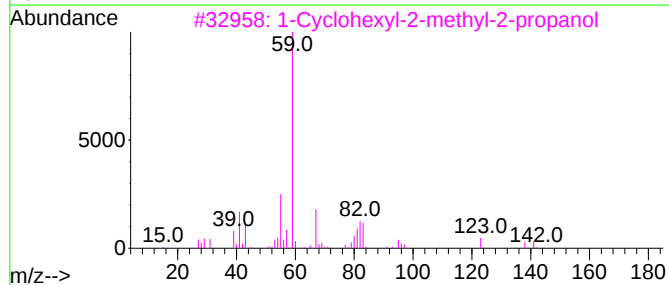
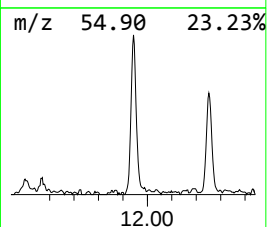
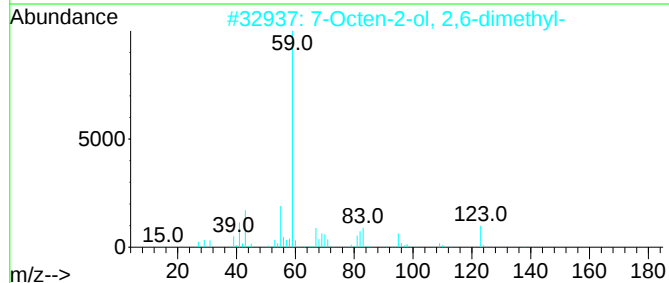
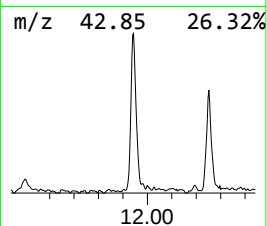
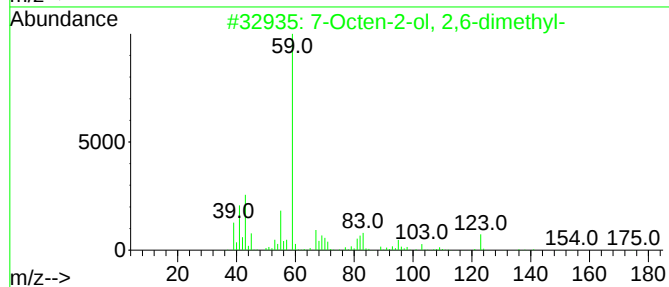
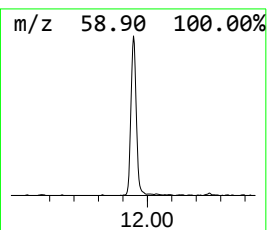
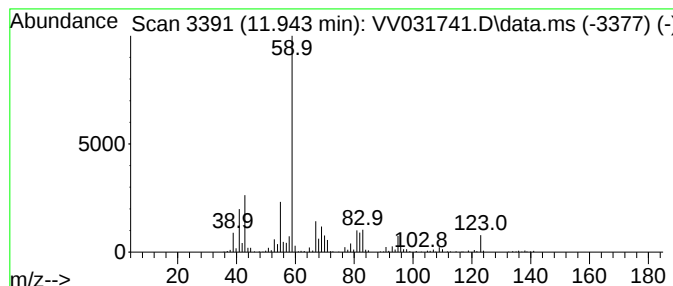
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Quant Title : VOC Analysis

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.
11.943	15.40 ug/L	257881	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	72
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	64
3			1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	64
4			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	64
5			1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031741.D
Acq On : 25 Jul 2023 14:33
Operator : SY/MD
Sample : 03712-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y1

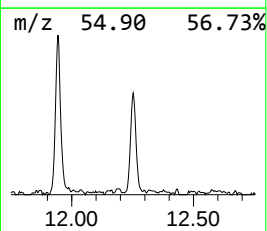
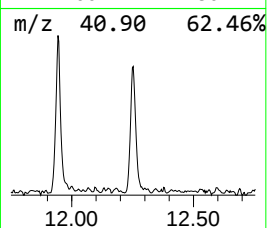
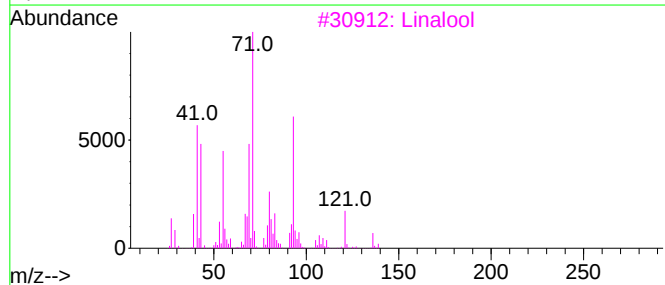
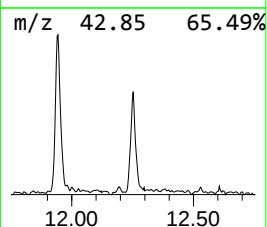
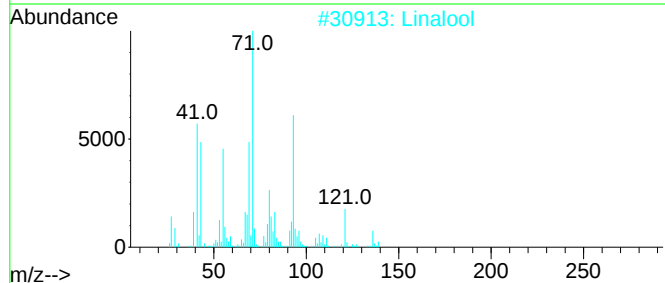
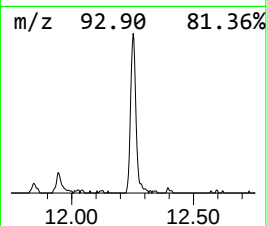
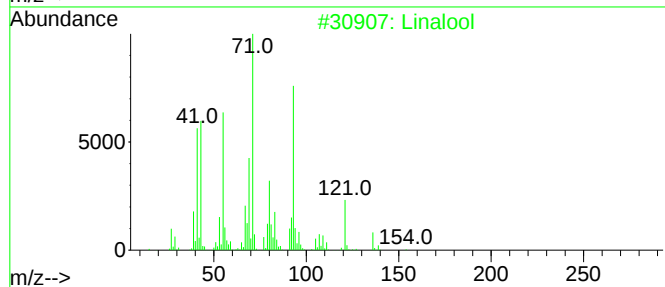
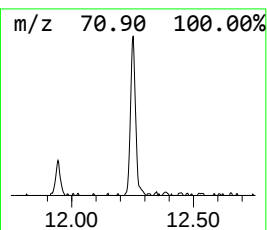
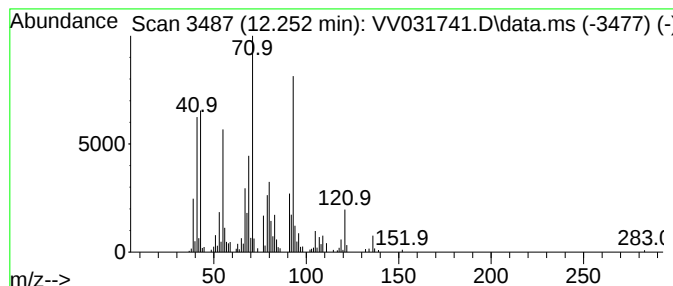
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Quant Title : VOC Analysis

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

Peak Number 6 Linalool Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.252	9.63 ug/L	161258	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Linalool	154	C10H18O	000078-70-6	80
2			Linalool	154	C10H18O	000078-70-6	74
3			Linalool	154	C10H18O	000078-70-6	74
4			Linalool	154	C10H18O	000078-70-6	72
5			4-Carene, (1S,3R,6R)-(-)-	136	C10H16	005208-49-1	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031741.D
Acq On : 25 Jul 2023 14:33
Operator : SY/MD
Sample : 03712-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y1

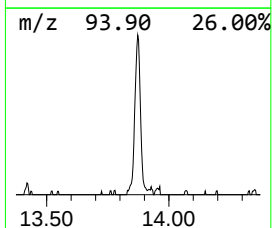
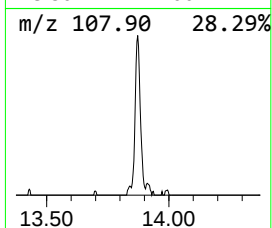
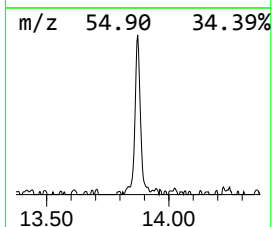
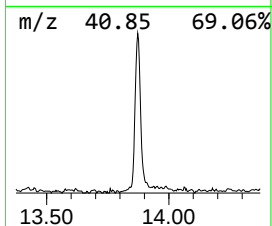
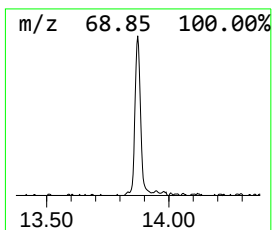
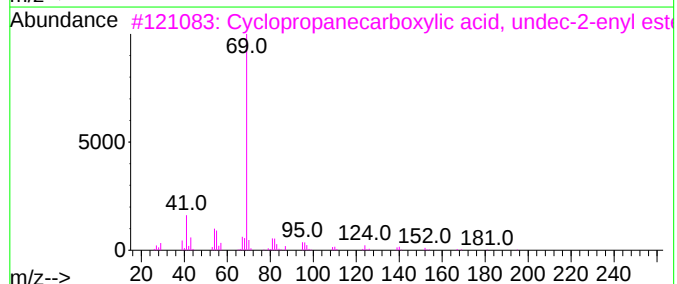
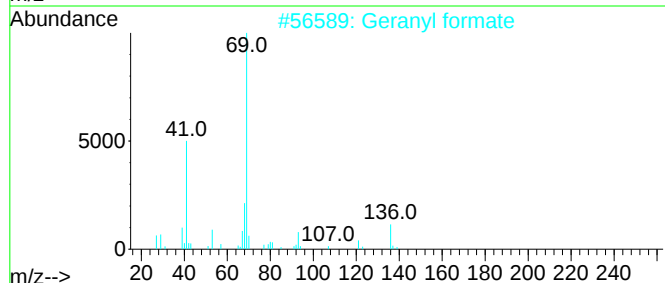
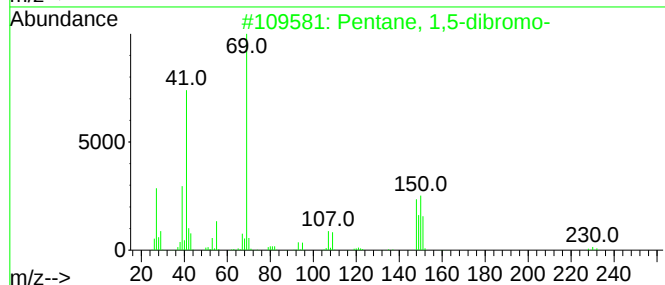
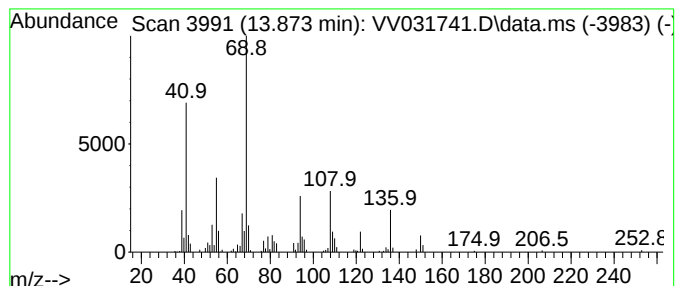
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Quant Title : VOC Analysis

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

Peak Number 7 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	7.56 ug/L	126649	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 1,5-dibromo-	228	C5H10Br2	000111-24-0	43
2			Geranyl formate	182	C11H18O2	000105-86-2	43
3			Cyclopropanecarboxylic acid, und...	238	C15H26O2	1000299-38-1	38
4			(.+/-)-Lavandulol, chlorodifluo...	266	C12H17ClF2O2	1000376-22-9	38
5			Cyclopropanecarboxaldehyde, 2-me...	166	C11H18O	097231-35-1	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031741.D
Acq On : 25 Jul 2023 14:33
Operator : SY/MD
Sample : 03712-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y1

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
HEX-5-EN-3-OL	2.571	9.7	ug/L	130361	1	5.542	674762	50.0
unknown-01	5.828	7.1	ug/L	96174	1	5.542	674762	50.0
2-Butanone, 3,3...	6.513	10.3	ug/L	138918	1	5.542	674762	50.0
7-Octen-2-ol, 2...	11.943	15.4	ug/L	257881	3	11.191	837099	50.0
Linalool	12.252	9.6	ug/L	161258	3	11.191	837099	50.0
unknown-02	13.873	7.6	ug/L	126649	3	11.191	837099	50.0