

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV042921\
 Data File : VV021223.D
 Acq On : 29 Apr 2021 16:17
 Operator : SY/MD
 Sample : M2177-05ME
 Misc : 5.49g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG582ME

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\SFAMVLM042121WMA.M

Title : VOC Analysis

Signal : TIC: VV021223.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.163	36	38	42	rBV5	6895	4779	0.22%	0.027%
2	1.272	69	72	74	rBV3	11925	8587	0.39%	0.049%
3	1.304	77	82	89	rBV	159253	174517	7.89%	0.993%
4	1.391	107	109	112	rBV4	9062	6277	0.28%	0.036%
5	1.568	158	164	171	rBV	92314	113888	5.15%	0.648%
6	2.095	320	328	339	rVB	441367	620698	28.07%	3.531%
7	2.275	382	384	387	rBV4	7592	4978	0.23%	0.028%
8	2.333	398	402	403	rBV4	8663	5448	0.25%	0.031%
9	2.365	407	412	413	rBV5	11088	9653	0.44%	0.055%
10	2.446	434	437	439	rBV4	7016	5127	0.23%	0.029%
11	2.610	485	488	490	rBV4	10424	8956	0.41%	0.051%
12	2.719	517	522	524	rVB6	6248	5349	0.24%	0.030%
13	2.751	528	532	537	rBV8	6960	8587	0.39%	0.049%
14	2.851	559	563	564	rBV4	6059	4789	0.22%	0.027%
15	2.870	567	569	571	rVV3	8340	4442	0.20%	0.025%
16	2.905	577	580	584	rVV6	7015	5449	0.25%	0.031%
17	2.989	603	606	608	rBV4	7177	4777	0.22%	0.027%
18	3.011	609	613	615	rBV5	6358	5168	0.23%	0.029%
19	3.121	644	647	650	rBV5	10978	5898	0.27%	0.034%
20	3.172	661	663	667	rVB5	10281	5761	0.26%	0.033%
21	3.243	683	685	689	rVB5	7534	6075	0.27%	0.035%
22	3.346	713	717	719	rBV4	10175	8035	0.36%	0.046%
23	3.417	735	739	742	rBV5	6784	5265	0.24%	0.030%
24	3.606	792	798	799	rBV6	8880	7504	0.34%	0.043%
25	3.696	822	826	828	rVB5	6584	4588	0.21%	0.026%
26	3.722	832	834	835	rBV2	8835	4411	0.20%	0.025%
27	3.847	870	873	874	rBV3	10064	5060	0.23%	0.029%
28	3.857	874	876	879	rVB4	9268	4566	0.21%	0.026%
29	3.921	888	896	899	rBV	51291	75660	3.42%	0.430%
30	4.105	951	953	957	rVB5	13514	8634	0.39%	0.049%
31	4.288	1007	1010	1015	rBV6	5355	5733	0.26%	0.033%
32	4.349	1015	1029	1051	rVV	323191	825227	37.33%	4.694%
33	4.632	1115	1117	1120	rBV3	7440	5907	0.27%	0.034%
34	4.796	1166	1168	1170	rBV3	9026	4311	0.19%	0.025%
35	4.876	1189	1193	1196	rBV6	5690	4516	0.20%	0.026%
36	4.947	1212	1215	1221	rVB8	8784	8127	0.37%	0.046%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042121WMA.M
 Title : VOC Analysis

37	5.043	1225	1245	1269	rBV2	791173	1976345	89.39%	11.242%
38	5.224	1299	1301	1305	rBV4	5121	4278	0.19%	0.024%
39	5.304	1321	1326	1327	rBV4	6340	5293	0.24%	0.030%
40	5.355	1339	1342	1344	rBV4	6820	4298	0.19%	0.024%
41	5.471	1374	1378	1380	rBV5	6263	4832	0.22%	0.027%
42	5.619	1412	1424	1442	rBV	649795	1345505	60.86%	7.654%
43	5.722	1453	1456	1460	rVB6	8420	6368	0.29%	0.036%
44	5.812	1480	1484	1488	rBV7	10725	8726	0.39%	0.050%
45	5.915	1511	1516	1518	rBV6	9907	9991	0.45%	0.057%
46	6.076	1553	1566	1582	rBV2	413344	866009	39.17%	4.926%
47	6.519	1702	1704	1707	rBV4	7113	4574	0.21%	0.026%
48	6.539	1707	1710	1714	rBV5	7049	5775	0.26%	0.033%
49	6.577	1717	1722	1723	rBV5	8580	6113	0.28%	0.035%
50	6.632	1734	1739	1740	rBV4	6832	5764	0.26%	0.033%
51	6.641	1740	1742	1747	rVV6	8515	7057	0.32%	0.040%
52	6.664	1747	1749	1751	rVV3	9075	4653	0.21%	0.026%
53	6.712	1759	1764	1767	rVB6	8151	7355	0.33%	0.042%
54	6.818	1794	1797	1802	rVV6	7483	6298	0.28%	0.036%
55	6.857	1806	1809	1814	rVB6	7404	6355	0.29%	0.036%
56	6.883	1814	1817	1820	rVB4	6182	4945	0.22%	0.028%
57	6.992	1841	1851	1863	rBV2	228067	437599	19.79%	2.489%
58	7.111	1886	1888	1894	rBV7	8515	7353	0.33%	0.042%
59	7.185	1908	1911	1913	rBV4	7517	4317	0.20%	0.025%
60	7.211	1915	1919	1920	rBV4	6034	4744	0.21%	0.027%
61	7.256	1930	1933	1935	rBV4	9382	6986	0.32%	0.040%
62	7.320	1942	1953	1970	rBV	908777	1624444	73.47%	9.240%
63	7.481	1999	2003	2005	rBV4	8516	4875	0.22%	0.028%
64	7.629	2038	2049	2071	rBV	151017	322270	14.58%	1.833%
65	7.754	2086	2088	2092	rVB5	6359	4525	0.20%	0.026%
66	7.793	2097	2100	2104	rBV5	6694	4966	0.22%	0.028%
67	7.908	2133	2136	2138	rBV4	9404	5361	0.24%	0.030%
68	7.928	2138	2142	2145	rVB6	5582	4718	0.21%	0.027%
69	7.998	2159	2164	2166	rBV5	8130	5569	0.25%	0.032%
70	8.130	2187	2205	2226	rBV2	225444	779816	35.27%	4.436%
71	8.365	2276	2278	2281	rVB3	10781	4655	0.21%	0.026%
72	8.407	2287	2291	2294	rBV6	9955	7470	0.34%	0.042%
73	8.436	2298	2300	2303	rVV4	7640	4236	0.19%	0.024%
74	8.535	2327	2331	2334	rVB6	7191	5039	0.23%	0.029%
75	8.551	2334	2336	2340	rBV5	10064	7191	0.33%	0.041%
76	8.616	2354	2356	2360	rVB4	15158	10001	0.45%	0.057%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042121WMA.M
 Title : VOC Analysis

77	8.645	2360	2365	2366	rBV4	9780	8099	0.37%	0.046%
78	8.760	2396	2401	2402	rVB5	6125	4695	0.21%	0.027%
79	8.770	2402	2404	2407	rBV3	9122	4827	0.22%	0.027%
80	8.796	2409	2412	2415	rVB5	9747	6345	0.29%	0.036%
81	8.818	2415	2419	2421	rBV5	7010	5117	0.23%	0.029%
82	8.860	2421	2432	2452	rVV	905179	1713846	77.52%	9.749%
83	9.056	2492	2493	2497	rBV4	8131	5142	0.23%	0.029%
84	9.075	2497	2499	2502	rBV4	10122	5365	0.24%	0.031%
85	9.114	2502	2511	2518	rVV4	20006	33126	1.50%	0.188%
86	9.230	2544	2547	2548	rBV3	9112	5211	0.24%	0.030%
87	9.262	2555	2557	2562	rVB6	7494	4976	0.23%	0.028%
88	9.323	2571	2576	2580	rBV7	15640	19167	0.87%	0.109%
89	9.368	2586	2590	2593	rBV6	5395	5686	0.26%	0.032%
90	9.448	2609	2615	2625	rVV6	26112	43828	1.98%	0.249%
91	9.754	2705	2710	2717	rBV9	15363	24700	1.12%	0.141%
92	9.985	2773	2782	2789	rBV9	29202	45889	2.08%	0.261%
93	10.133	2820	2828	2836	rVB4	67680	105849	4.79%	0.602%
94	10.233	2849	2859	2871	rVB2	579105	964265	43.61%	5.485%
95	11.037	3104	3109	3116	rBV4	99011	126475	5.72%	0.719%
96	11.198	3154	3159	3168	rVB7	232226	341894	15.46%	1.945%
97	11.259	3169	3178	3195	rBV	1270570	2115296	95.68%	12.032%
98	11.635	3285	3295	3308	rBV	1304383	2210881	100.00%	12.576%
99	11.792	3337	3344	3348	rBV5	145204	230607	10.43%	1.312%
100	17.422	5093	5095	5097	rBV3	10208	5288	0.24%	0.030%

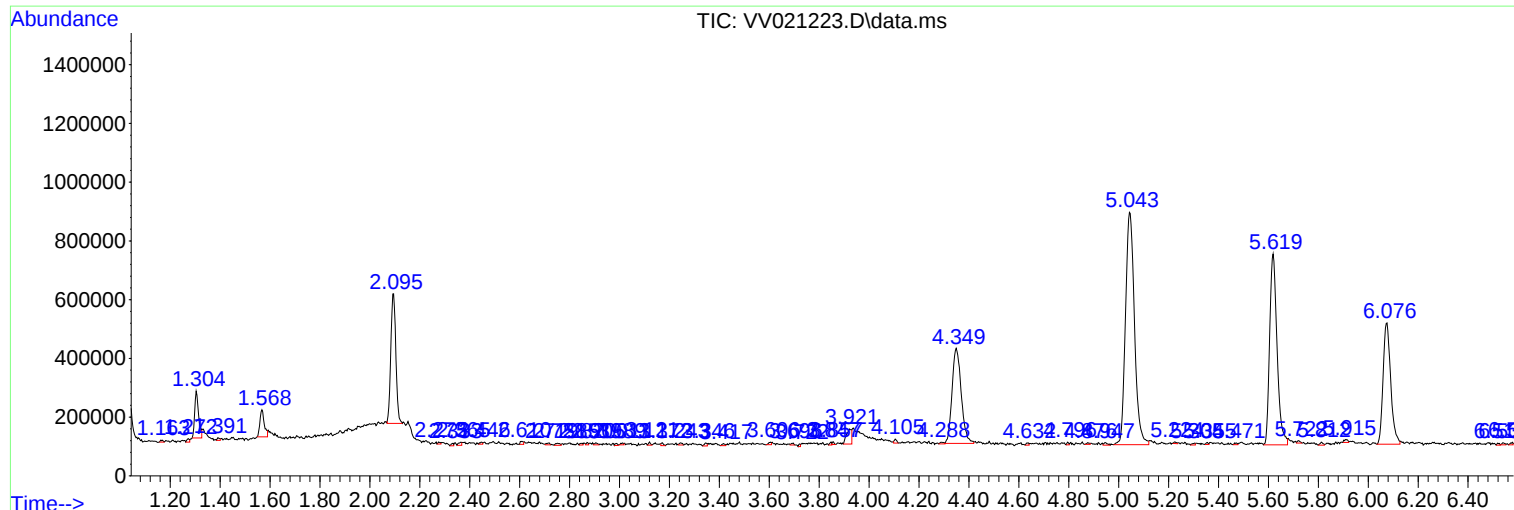
Sum of corrected areas: 17579990

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG582ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042121WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV042921\
Data File : VV021223.D
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Instrument :
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ClientSampleId :
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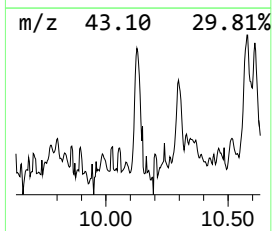
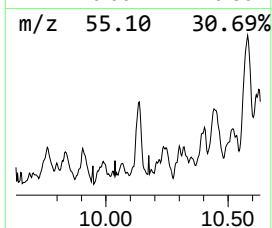
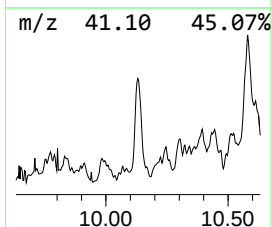
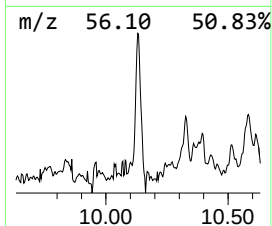
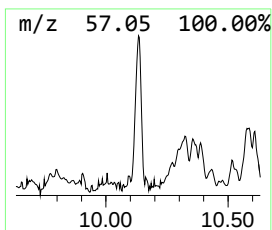
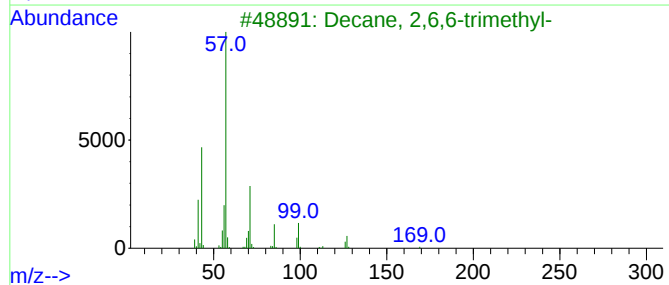
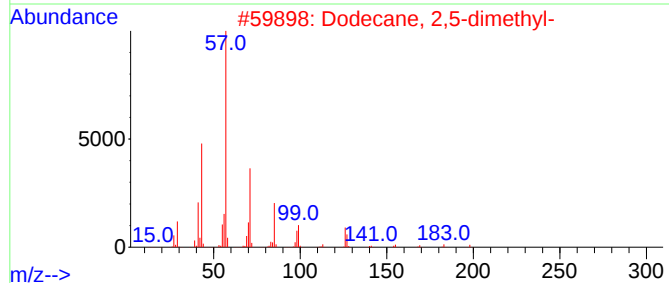
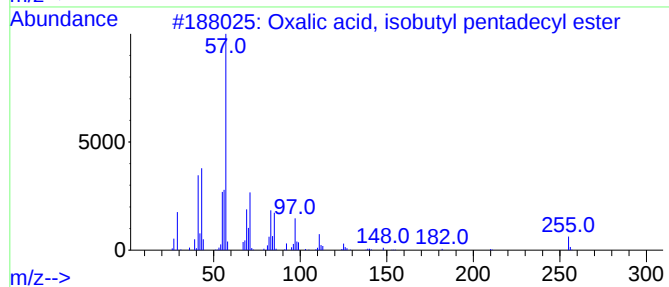
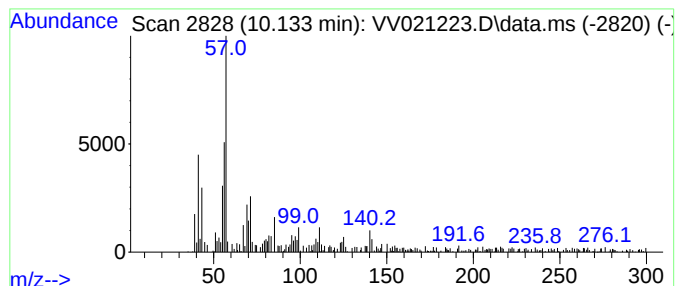
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042121WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.133	2.50 ug/L	105849	1,4-Dichlorobenzene-d4	11.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	47
2			Dodecane, 2,5-dimethyl-	198	C14H30	056292-65-0	43
3			Decane, 2,6,6-trimethyl-	184	C13H28	062108-24-1	38
4			5-Ethyldecane	170	C12H26	017302-36-2	38
5			Nonane, 4-methylene-	140	C10H20	033717-91-8	35



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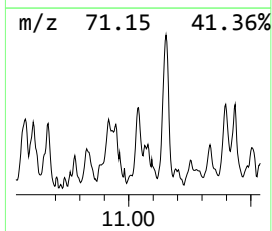
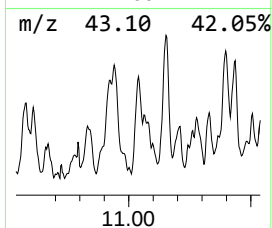
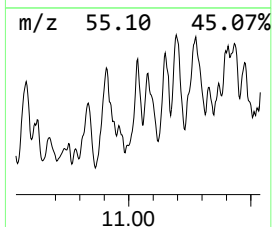
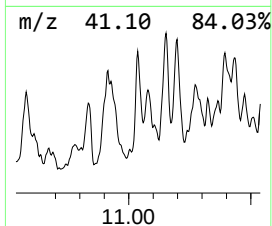
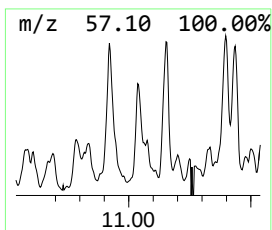
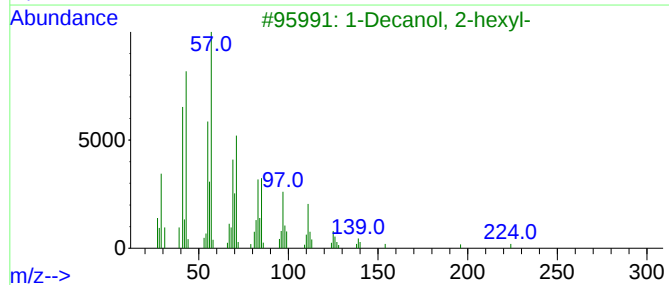
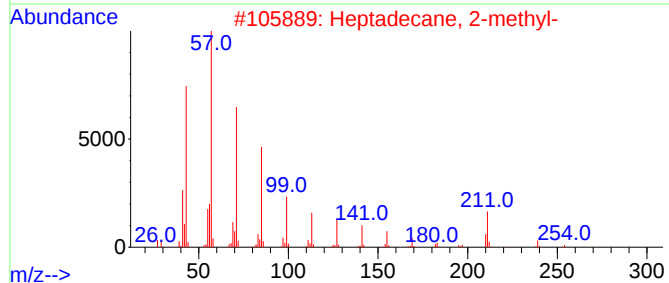
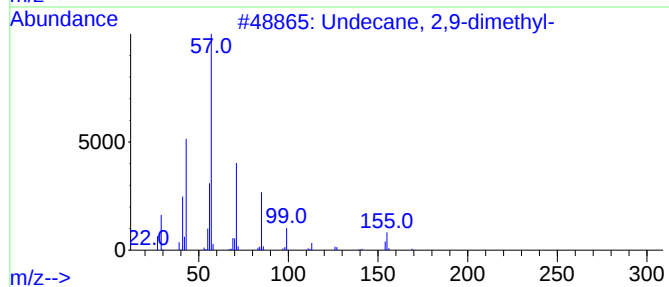
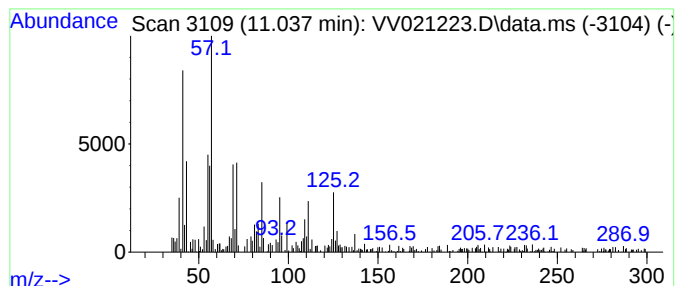
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042121WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.037	2.99 ug/L	126475	1,4-Dichlorobenzene-d4	11.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	43
2			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	38
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	35
4			Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	35
5			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	35



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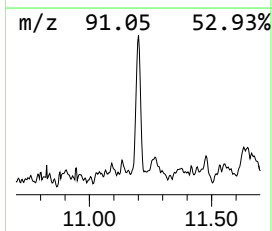
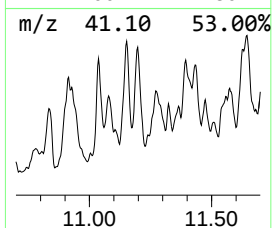
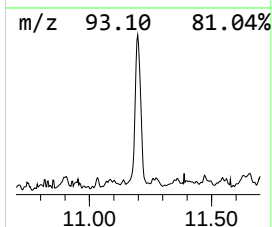
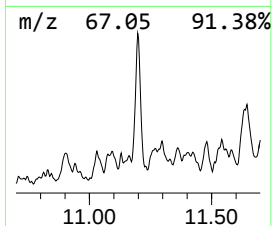
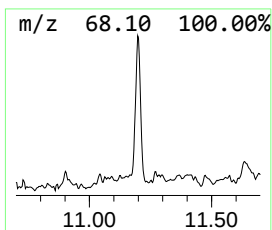
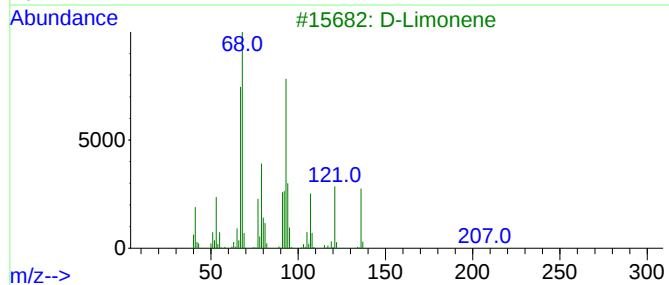
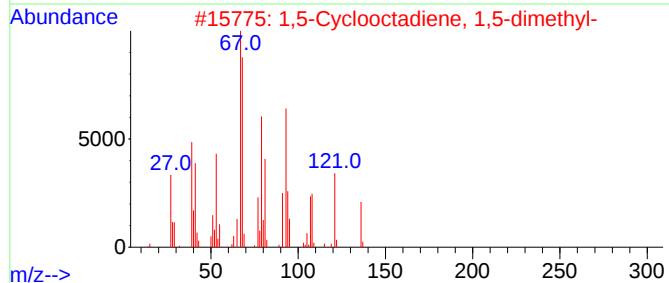
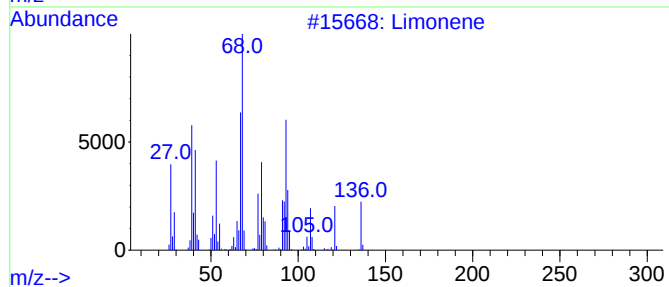
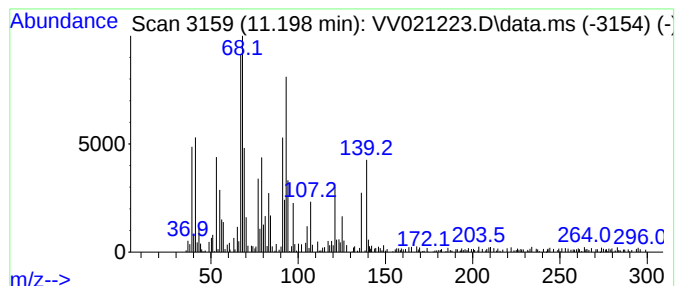
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Quant Title : VOC Analysis

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

Peak Number 4 Limonene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.198	8.08 ug/L	341894	1,4-Dichlorobenzene-d4	11.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Limonene	136	C10H16	000138-86-3	93
2			1,5-Cyclooctadiene, 1,5-dimethyl-	136	C10H16	003760-14-3	91
3			D-Limonene	136	C10H16	005989-27-5	78
4			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	76
5			Limonene	136	C10H16	000138-86-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV042921\
Data File : VV021223.D
Acq On : 29 Apr 2021 16:17
Operator : SY/MD
Sample : M2177-05ME
Misc : 5.49g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG582ME

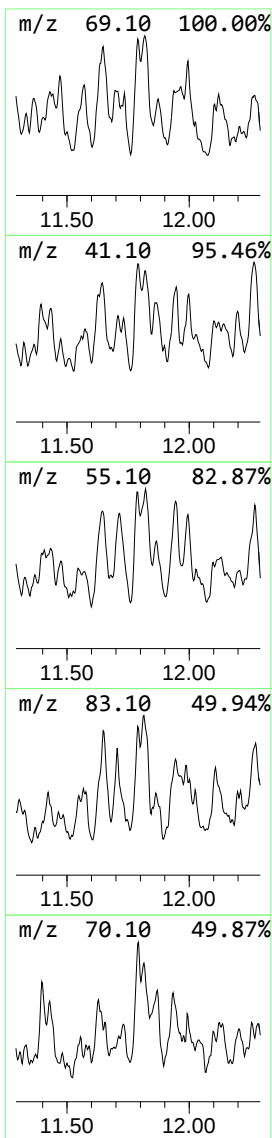
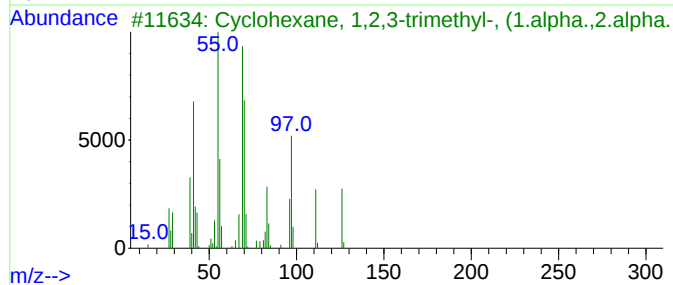
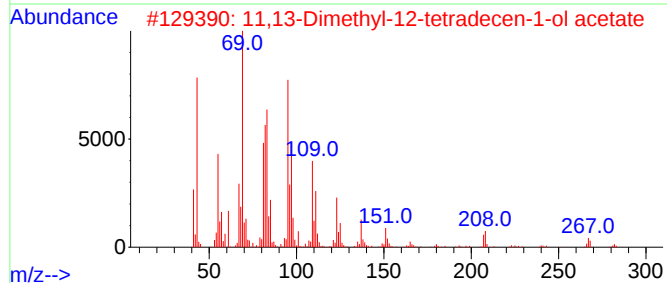
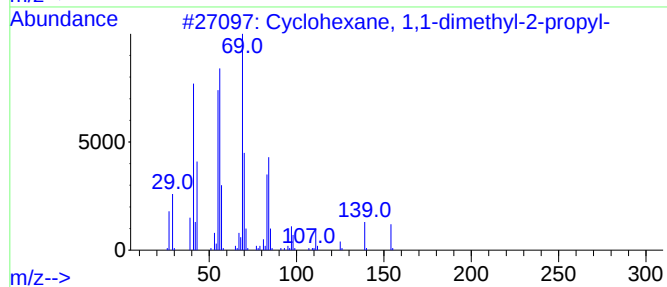
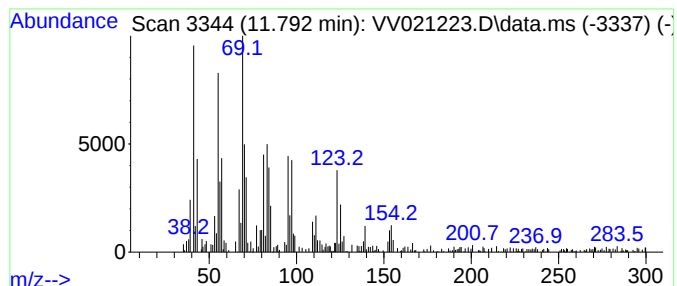
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042121WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Cyclic11.792 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	5.45 ug/L	230607	1,4-Dichlorobenzene-d4	11.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1-dimethyl-2-propyl-	154	C11H22	081983-71-3	53
2			11,13-Dimethyl-12-tetradecen-1-ol...	282	C18H34O2	1000130-81-0	53
3			Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	007667-55-2	50
4			6-Octen-1-ol, 3,7-dimethyl-, for...	184	C11H20O2	000105-85-1	42
5			6-Octen-1-ol, 3,7-dimethyl-, for...	184	C11H20O2	000105-85-1	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV042921\
Data File : VV021223.D
Acq On : 29 Apr 2021 16:17
Operator : SY/MD
Sample : M2177-05ME
Misc : 5.49g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG582ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042121WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	10.133	2.5	ug/L	105849	3	11.259	2115300	50.0
(DEL) Alkane: S...	11.037	3.0	ug/L	126475	3	11.259	2115300	50.0
Limonene	11.198	8.1	ug/L	341894	3	11.259	2115300	50.0
(DEL) Alkane: C...	11.792	5.5	ug/L	230607	3	11.259	2115300	50.0