

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072022\
 Data File : VU049807.D
 Acq On : 20 Jul 2022 16:49
 Operator : SY/MD
 Sample : N3709-07ME
 Misc : 6.52g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 H0B23ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

Signal : TIC: VU049807.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	39	44	48	rBV3	2577	2725	0.42%	0.046%
2	1.594	71	79	85	rBV	39934	52305	8.11%	0.885%
3	1.848	124	158	160	rBV3	39405	106645	16.54%	1.805%
4	2.517	355	366	385	rVB	111271	180596	28.02%	3.056%
5	2.652	400	408	413	rBV3	1774	2585	0.40%	0.044%
6	2.742	428	436	444	rBV2	1582	2348	0.36%	0.040%
7	2.906	482	487	489	rBV3	303	327	0.05%	0.006%
8	2.957	489	503	518	rBV	13322	27377	4.25%	0.463%
9	3.018	518	522	523	rBV2	850	625	0.10%	0.011%
10	3.092	536	545	553	rVB3	1798	2970	0.46%	0.050%
11	3.176	561	571	582	rVB2	1705	3499	0.54%	0.059%
12	3.440	647	653	656	rVB2	195	208	0.03%	0.004%
13	3.652	717	719	722	rBV	402	291	0.05%	0.005%
14	3.832	772	775	777	rBV2	326	230	0.04%	0.004%
15	3.899	793	796	800	rVV	193	191	0.03%	0.003%
16	3.922	800	803	812	rVV2	154	245	0.04%	0.004%
17	4.247	897	904	907	rBV2	281	327	0.05%	0.006%
18	4.639	1011	1026	1063	rBV	65842	202804	31.46%	3.432%
19	4.877	1097	1100	1101	rBV	310	176	0.03%	0.003%
20	5.060	1138	1157	1181	rBV	111977	254357	39.46%	4.304%
21	5.218	1199	1206	1211	rBV3	413	619	0.10%	0.010%
22	5.282	1220	1226	1227	rBV	608	550	0.09%	0.009%
23	5.333	1238	1242	1243	rBV2	402	291	0.05%	0.005%
24	5.465	1278	1283	1287	rBV2	361	498	0.08%	0.008%
25	5.713	1342	1360	1381	rBV2	255376	644600	100.00%	10.908%
26	5.874	1407	1410	1415	rVB	244	193	0.03%	0.003%
27	5.903	1415	1419	1421	rBV2	230	183	0.03%	0.003%
28	5.973	1438	1441	1442	rBV	574	338	0.05%	0.006%
29	6.121	1482	1487	1488	rBV2	278	210	0.03%	0.004%
30	6.137	1489	1492	1495	rVB3	326	233	0.04%	0.004%
31	6.243	1512	1525	1548	rBV	232700	450148	69.83%	7.617%
32	6.382	1565	1568	1571	rBV3	391	204	0.03%	0.003%
33	6.446	1585	1588	1595	rBV2	214	250	0.04%	0.004%
34	6.520	1604	1611	1623	rBV3	1767	2871	0.45%	0.049%
35	6.597	1630	1635	1639	rBV3	560	607	0.09%	0.010%
36	6.687	1649	1663	1685	rBV	151345	302981	47.00%	5.127%

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 ClientSampleId :
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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

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
 Title : VOC Analysis

37	6.793	1692	1696	1698	rBV3	275	223	0.03%	0.004%
38	7.041	1768	1773	1777	rVB	172	176	0.03%	0.003%
39	7.195	1812	1821	1822	rBV3	2125	2530	0.39%	0.043%
40	7.565	1924	1936	1957	rVB2	72057	136500	21.18%	2.310%
41	7.687	1971	1974	1975	rBV	296	162	0.03%	0.003%
42	7.896	2025	2039	2056	rBV	260937	456563	70.83%	7.726%
43	8.182	2117	2128	2144	rBV	47601	90085	13.98%	1.524%
44	8.369	2184	2186	2190	rVB3	313	181	0.03%	0.003%
45	8.475	2207	2219	2231	rBV3	3084	5606	0.87%	0.095%
46	8.533	2231	2237	2244	rVV4	720	923	0.14%	0.016%
47	8.652	2258	2274	2299	rBV2	190932	451311	70.01%	7.637%
48	8.790	2311	2317	2318	rBV3	1725	1200	0.19%	0.020%
49	8.861	2336	2339	2345	rVB3	728	578	0.09%	0.010%
50	8.893	2345	2349	2351	rBV	212	196	0.03%	0.003%
51	8.925	2353	2359	2364	rVB5	975	1087	0.17%	0.018%
52	9.166	2429	2434	2437	rVB4	583	522	0.08%	0.009%
53	9.208	2437	2447	2452	rBV6	1723	2244	0.35%	0.038%
54	9.333	2479	2486	2494	rVB4	952	1247	0.19%	0.021%
55	9.420	2500	2513	2535	rBV	314094	578800	89.79%	9.795%
56	9.568	2552	2559	2561	rBV6	797	882	0.14%	0.015%
57	9.700	2590	2600	2612	rVB2	11530	20456	3.17%	0.346%
58	9.873	2648	2654	2656	rBV2	640	576	0.09%	0.010%
59	9.963	2676	2682	2690	rVB4	558	691	0.11%	0.012%
60	10.015	2690	2698	2715	rBV7	2258	5336	0.83%	0.090%
61	10.111	2721	2728	2729	rBV4	1787	1385	0.21%	0.023%
62	10.172	2744	2747	2751	rVB3	864	707	0.11%	0.012%
63	10.253	2760	2772	2786	rBV7	7152	13154	2.04%	0.223%
64	10.314	2786	2791	2794	rBV4	820	951	0.15%	0.016%
65	10.356	2796	2804	2810	rBV7	4611	7678	1.19%	0.130%
66	10.462	2829	2837	2838	rBV3	1657	1520	0.24%	0.026%
67	10.478	2838	2842	2845	rBV3	1639	1603	0.25%	0.027%
68	10.558	2854	2867	2875	rBV9	4477	9764	1.51%	0.165%
69	10.623	2882	2887	2893	rVB4	4720	5569	0.86%	0.094%
70	10.761	2915	2930	2944	rBV	238023	403919	62.66%	6.835%
71	10.896	2961	2972	2984	rBV3	57896	103150	16.00%	1.746%
72	11.012	2998	3008	3018	rBV2	36523	58129	9.02%	0.984%
73	11.063	3018	3024	3029	rBV5	4911	5983	0.93%	0.101%
74	11.279	3086	3091	3093	rBV3	1472	1490	0.23%	0.025%
75	11.417	3127	3134	3140	rBV3	10296	13304	2.06%	0.225%
76	11.468	3141	3150	3173	rVB4	19251	45972	7.13%	0.778%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
 Title : VOC Analysis

77	11.578	3173	3184	3192	rBV4	6178	12027	1.87%	0.204%
78	11.700	3214	3222	3233	rBV6	19623	32294	5.01%	0.546%
79	11.815	3246	3258	3281	rBV	362482	621270	96.38%	10.513%
80	11.944	3290	3298	3303	rBV4	13833	22247	3.45%	0.376%
81	12.102	3338	3347	3349	rBV6	7313	10202	1.58%	0.173%
82	12.195	3359	3376	3391	rBV	285929	484224	75.12%	8.194%
83	12.381	3429	3434	3438	rBV5	5206	6779	1.05%	0.115%
84	12.770	3549	3555	3567	rVB5	3957	5824	0.90%	0.099%
85	13.024	3627	3634	3651	rVB7	4314	10247	1.59%	0.173%
86	13.227	3692	3697	3701	rBV5	1010	770	0.12%	0.013%
87	13.346	3727	3734	3739	rVB5	1042	1423	0.22%	0.024%
88	13.397	3748	3750	3751	rBV	493	230	0.04%	0.004%
89	13.458	3759	3769	3780	rVB	5120	9220	1.43%	0.156%
90	13.584	3805	3808	3813	rBV6	624	527	0.08%	0.009%
91	13.632	3820	3823	3825	rBV3	559	257	0.04%	0.004%
92	13.777	3863	3868	3871	rVB2	477	379	0.06%	0.006%
93	13.822	3878	3882	3884	rBV3	670	498	0.08%	0.008%
94	13.835	3884	3886	3890	rVB4	499	420	0.07%	0.007%
95	13.957	3922	3924	3925	rBV	338	161	0.02%	0.003%
96	14.092	3959	3966	3973	rBV2	2111	3079	0.48%	0.052%
97	14.192	3990	3997	4003	rBV5	965	1686	0.26%	0.029%
98	14.577	4109	4117	4127	rVB3	3832	6894	1.07%	0.117%
99	15.696	4463	4465	4467	rBV2	503	306	0.05%	0.005%
100	16.098	4588	4590	4594	rBV2	602	496	0.08%	0.008%

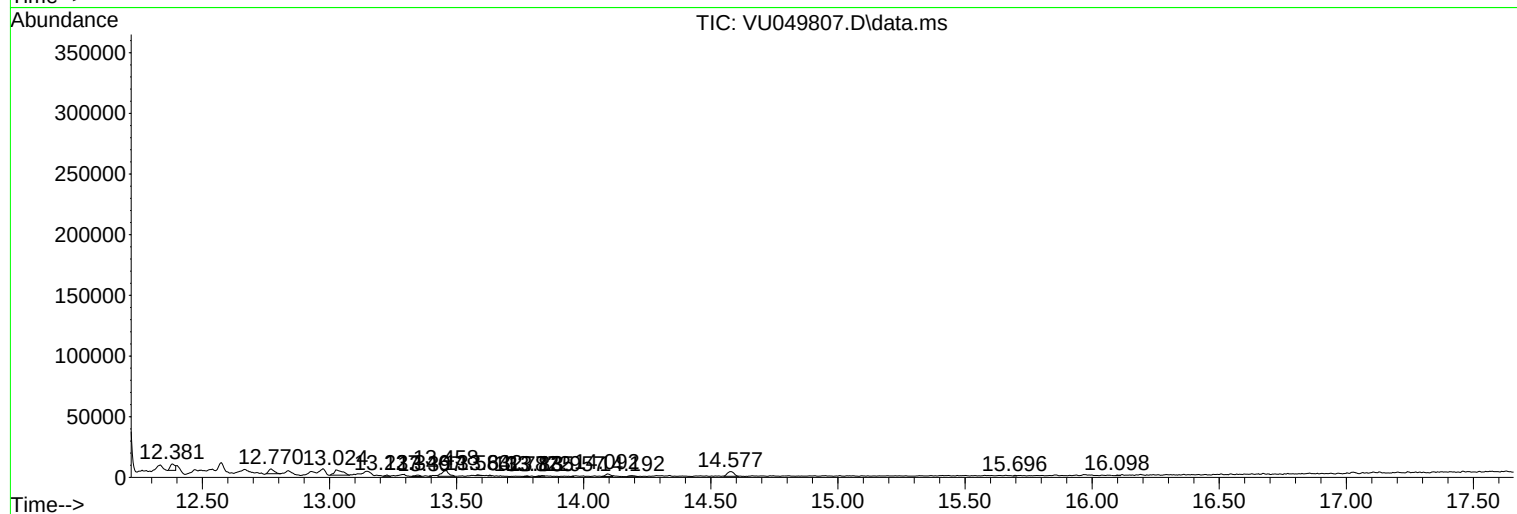
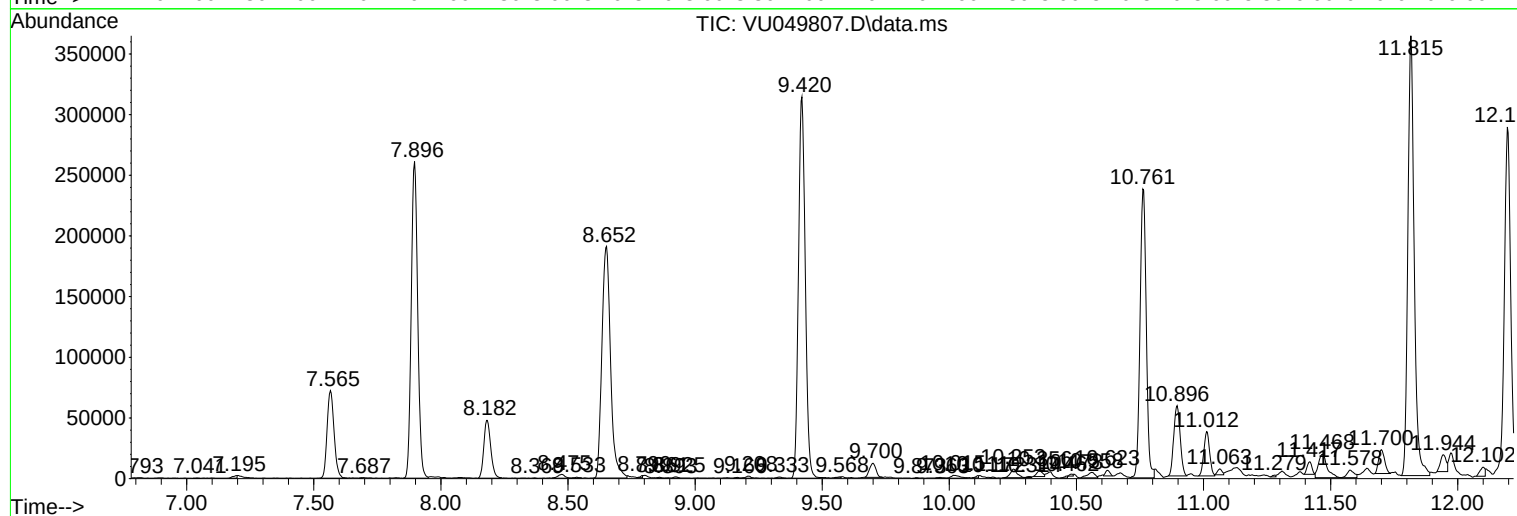
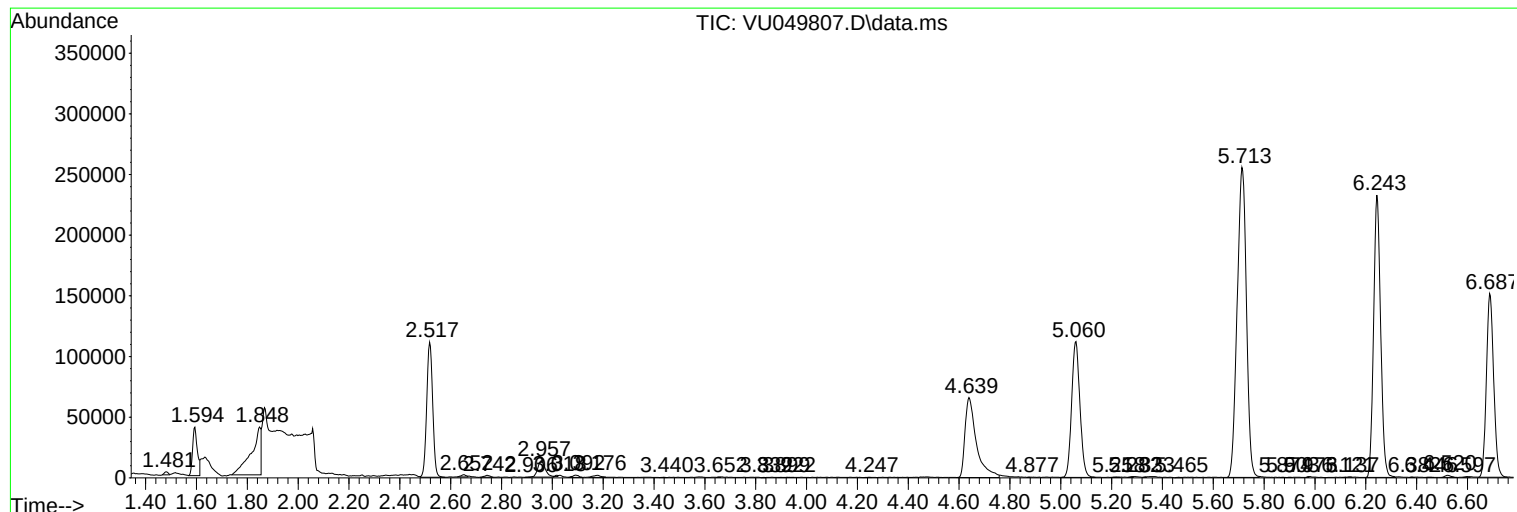
Sum of corrected areas: 5909420

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H0B23ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H0B23ME

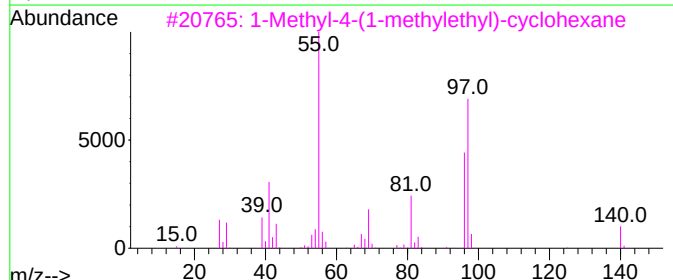
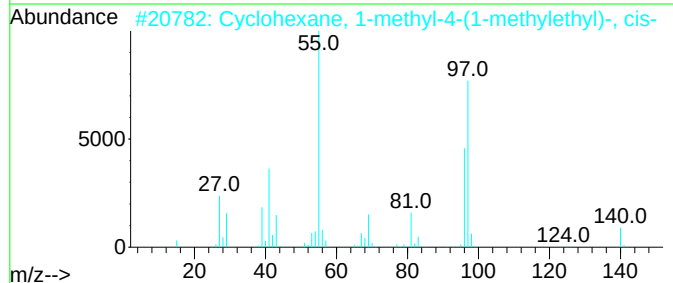
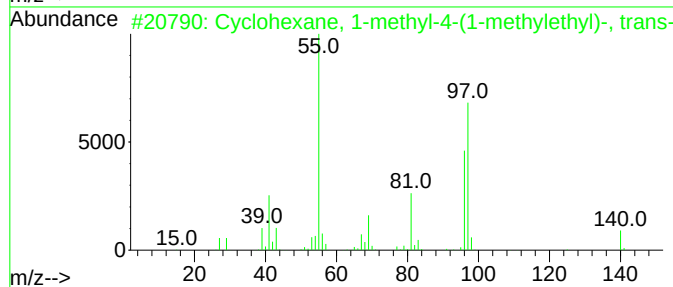
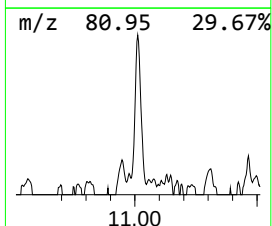
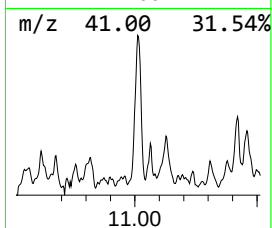
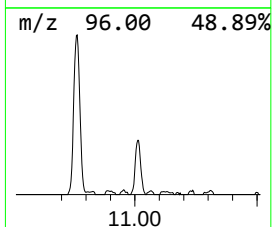
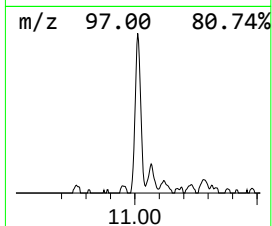
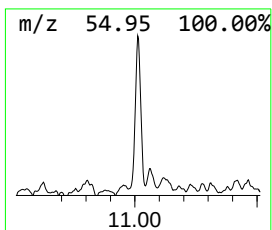
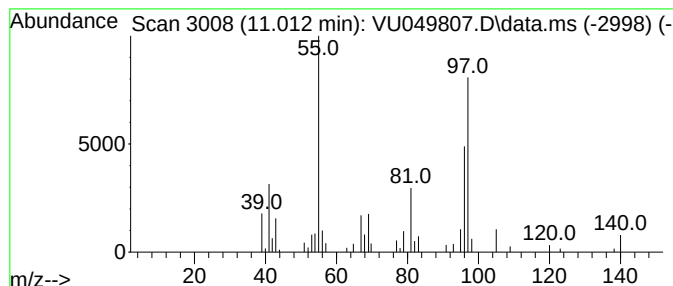
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Cyclic11.012 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.012	4.68 ug/L	58129	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	81
2			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	81
3			1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	81
4			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	74
5			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	74



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H0B23ME

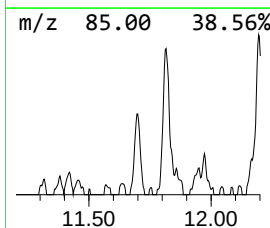
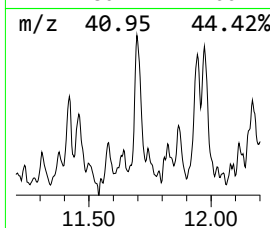
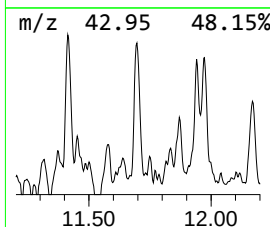
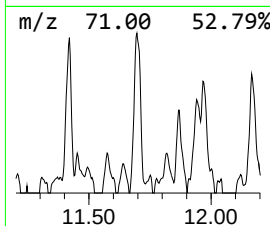
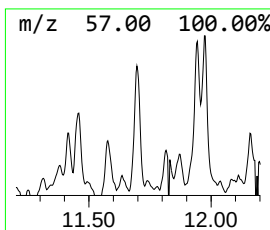
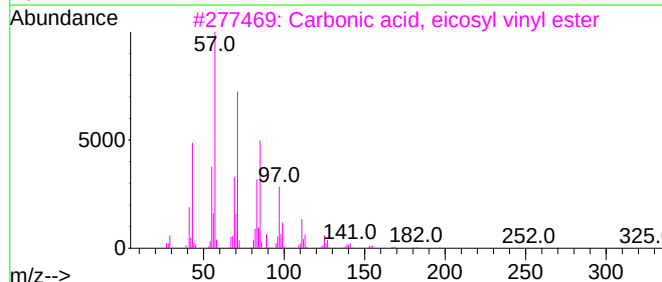
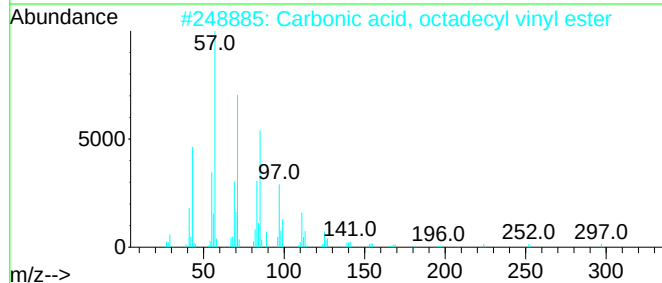
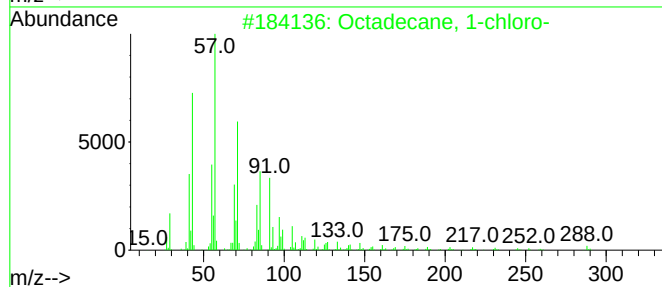
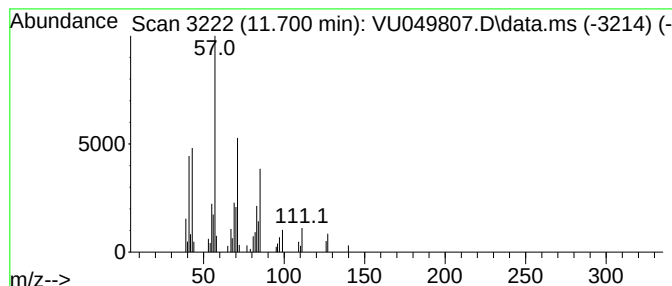
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Octadecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.700	2.60 ug/L	32294	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	78
2			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	78
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	72
4			Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	72
5			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	64



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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	11.012	4.7	ug/L	58129	3	11.816	621270	50.0
Octadecane, 1-C...	11.700	2.6	ug/L	32294	3	11.816	621270	50.0