

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
 Data File : VU050493.D
 Acq On : 29 Aug 2022 18:44
 Operator : SY/MD
 Sample : N4322-08ME
 Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY168ME

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\SFAMULM082422WMA.M
 Title : VOC Analysis

Signal : TIC: VU050493.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	40	44	48	rBV2	3083	2752	0.18%	0.024%
2	1.514	49	54	62	rBV3	4073	5327	0.35%	0.046%
3	1.594	71	79	86	rBV	82734	111083	7.34%	0.967%
4	1.880	164	168	177	rBV	26933	30802	2.03%	0.268%
5	2.520	356	367	387	rVB	285555	463651	30.62%	4.038%
6	2.742	431	436	438	rBV3	768	631	0.04%	0.005%
7	2.960	499	504	505	rBV2	625	562	0.04%	0.005%
8	3.025	514	524	539	rBV3	8229	15874	1.05%	0.138%
9	3.179	557	572	590	rBV	11469	30282	2.00%	0.264%
10	3.330	611	619	627	rVB2	2428	4322	0.29%	0.038%
11	3.362	627	629	633	rBV3	341	241	0.02%	0.002%
12	3.475	657	664	669	rBV2	237	314	0.02%	0.003%
13	3.652	715	719	720	rBV2	787	485	0.03%	0.004%
14	3.845	776	779	787	rVB3	484	645	0.04%	0.006%
15	3.883	787	791	795	rBV3	430	412	0.03%	0.004%
16	4.401	950	952	960	rVB2	214	215	0.01%	0.002%
17	4.491	972	980	985	rBV2	176	296	0.02%	0.003%
18	4.648	1015	1029	1079	rBV	128564	461976	30.51%	4.023%
19	4.896	1103	1106	1111	rVB4	466	349	0.02%	0.003%
20	4.948	1120	1122	1125	rVB2	457	221	0.01%	0.002%
21	5.060	1139	1157	1182	rBV	253693	590615	39.00%	5.144%
22	5.288	1218	1228	1231	rBV4	1656	2314	0.15%	0.020%
23	5.378	1244	1256	1259	rBV4	1239	2070	0.14%	0.018%
24	5.513	1296	1298	1302	rVB	381	287	0.02%	0.002%
25	5.716	1341	1361	1394	rBV2	600348	1514392	100.00%	13.189%
26	5.980	1430	1443	1467	rBV3	11525	29807	1.97%	0.260%
27	6.246	1510	1526	1552	rBV	420964	850013	56.13%	7.403%
28	6.529	1606	1614	1626	rBV7	6827	13456	0.89%	0.117%
29	6.603	1626	1637	1649	rBV3	5102	10651	0.70%	0.093%
30	6.690	1649	1664	1685	rVV	336788	690464	45.59%	6.013%
31	6.800	1692	1698	1702	rBV8	749	833	0.06%	0.007%
32	7.028	1764	1769	1774	rBV	218	220	0.01%	0.002%
33	7.105	1789	1793	1797	rVB2	258	244	0.02%	0.002%
34	7.224	1813	1830	1831	rBV4	5010	7840	0.52%	0.068%
35	7.314	1853	1858	1863	rVV3	682	925	0.06%	0.008%
36	7.497	1909	1915	1921	rBV6	1180	1534	0.10%	0.013%

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Instrument :
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 ClientSampleId :
 EY168ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Sampling : 1

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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\SFAMULM082422WMA.M
 Title : VOC Analysis

37	7.568	1924	1937	1960	rVB	144334	282257	18.64%	2.458%
38	7.674	1968	1970	1973	rVV2	496	314	0.02%	0.003%
39	7.726	1982	1986	1989	rVB4	331	276	0.02%	0.002%
40	7.780	2000	2003	2004	rBV	441	241	0.02%	0.002%
41	7.796	2006	2008	2013	rVB3	351	242	0.02%	0.002%
42	7.899	2025	2040	2059	rBV	597322	1081926	71.44%	9.423%
43	8.124	2105	2110	2116	rBV5	993	1325	0.09%	0.012%
44	8.182	2116	2128	2154	rVB	94332	188836	12.47%	1.645%
45	8.356	2175	2182	2185	rBV5	1579	1948	0.13%	0.017%
46	8.398	2193	2195	2201	rVB4	561	383	0.03%	0.003%
47	8.552	2233	2243	2256	rBV2	17006	30243	2.00%	0.263%
48	8.661	2256	2277	2307	rBV2	338062	898741	59.35%	7.827%
49	8.861	2337	2339	2344	rVB2	416	272	0.02%	0.002%
50	8.925	2352	2359	2365	rBV6	2874	4046	0.27%	0.035%
51	8.983	2373	2377	2379	rBV2	376	309	0.02%	0.003%
52	9.121	2412	2420	2423	rBV3	824	793	0.05%	0.007%
53	9.166	2429	2434	2437	rBV4	1500	1722	0.11%	0.015%
54	9.214	2442	2449	2460	rVB5	2725	4384	0.29%	0.038%
55	9.336	2477	2487	2495	rVB6	2043	3481	0.23%	0.030%
56	9.420	2498	2513	2538	rBV	563626	1060184	70.01%	9.233%
57	9.565	2551	2558	2559	rBV5	1033	940	0.06%	0.008%
58	9.574	2559	2561	2563	rVB2	837	415	0.03%	0.004%
59	9.648	2580	2584	2585	rBV2	300	216	0.01%	0.002%
60	9.693	2595	2598	2599	rBV	783	362	0.02%	0.003%
61	9.745	2608	2614	2624	rVB6	5117	7918	0.52%	0.069%
62	9.864	2648	2651	2653	rBV2	319	220	0.01%	0.002%
63	9.877	2653	2655	2658	rVB2	462	254	0.02%	0.002%
64	10.015	2693	2698	2699	rBV3	908	650	0.04%	0.006%
65	10.121	2718	2731	2736	rBV7	1582	2643	0.17%	0.023%
66	10.253	2763	2772	2782	rVB5	4658	7154	0.47%	0.062%
67	10.307	2784	2789	2790	rBV4	431	314	0.02%	0.003%
68	10.359	2796	2805	2809	rBV7	1527	1871	0.12%	0.016%
69	10.394	2809	2816	2825	rVB7	4284	7388	0.49%	0.064%
70	10.442	2829	2831	2834	rVB	391	234	0.02%	0.002%
71	10.462	2834	2837	2844	rBV6	834	1134	0.07%	0.010%
72	10.555	2851	2866	2874	rBV8	2693	5345	0.35%	0.047%
73	10.623	2878	2887	2893	rBV5	3905	6228	0.41%	0.054%
74	10.764	2912	2931	2960	rBV	524574	904500	59.73%	7.877%
75	10.873	2963	2965	2968	rBV	424	255	0.02%	0.002%
76	10.950	2981	2989	2990	rBV4	926	936	0.06%	0.008%

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Instrument :
 MSVOA_U
 ClientSampleId :
 EY168ME

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_U\Method\SFAMULM082422WMA.M
 Title : VOC Analysis

77	10.979	2995	2998	3001	rVB3	557	400	0.03%	0.003%
78	11.024	3008	3012	3013	rBV2	505	373	0.02%	0.003%
79	11.063	3017	3024	3030	rVV7	2528	3856	0.25%	0.034%
80	11.114	3031	3040	3057	rVB2	19543	33588	2.22%	0.293%
81	11.192	3059	3064	3065	rBV5	727	646	0.04%	0.006%
82	11.311	3095	3101	3113	rBV7	2106	3643	0.24%	0.032%
83	11.375	3114	3121	3126	rBV6	2162	2941	0.19%	0.026%
84	11.417	3126	3134	3141	rVV3	12532	16563	1.09%	0.144%
85	11.574	3174	3183	3189	rBV7	1716	2912	0.19%	0.025%
86	11.645	3189	3205	3209	rBV8	3323	6805	0.45%	0.059%
87	11.815	3246	3258	3272	rBV	517607	829949	54.80%	7.228%
88	11.999	3306	3315	3324	rVB8	5040	9146	0.60%	0.080%
89	12.198	3364	3377	3391	rBV	556454	901104	59.50%	7.848%
90	12.327	3409	3417	3429	rBV	41568	59828	3.95%	0.521%
91	12.667	3514	3523	3531	rBV8	6495	10141	0.67%	0.088%
92	12.947	3593	3610	3622	rBV8	8999	29479	1.95%	0.257%
93	13.008	3623	3629	3634	rBV6	3848	4898	0.32%	0.043%
94	13.092	3653	3655	3662	rVB8	1335	1221	0.08%	0.011%
95	13.134	3662	3668	3679	rBV7	5207	7407	0.49%	0.065%
96	13.433	3752	3761	3770	rBV2	47629	72762	4.80%	0.634%
97	13.587	3801	3809	3827	rBV2	28945	51315	3.39%	0.447%
98	14.452	4070	4078	4086	rBV	36016	47536	3.14%	0.414%
99	15.208	4309	4313	4322	rVB8	7486	9982	0.66%	0.087%
100	15.400	4368	4373	4380	rVB3	14445	18658	1.23%	0.162%

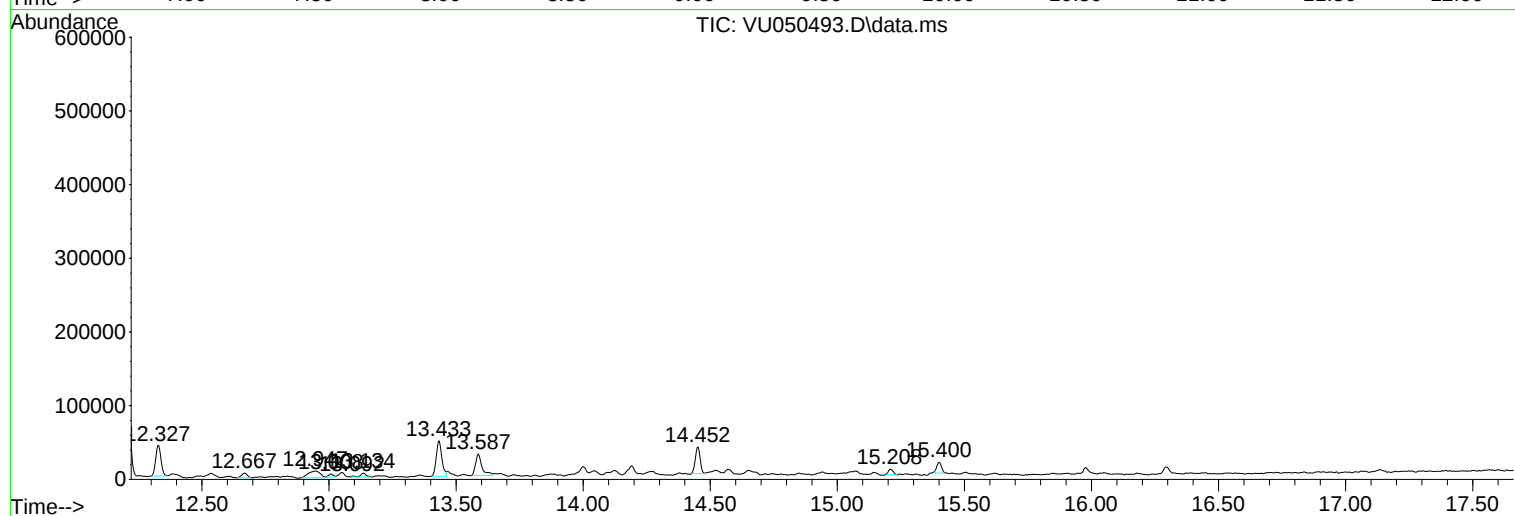
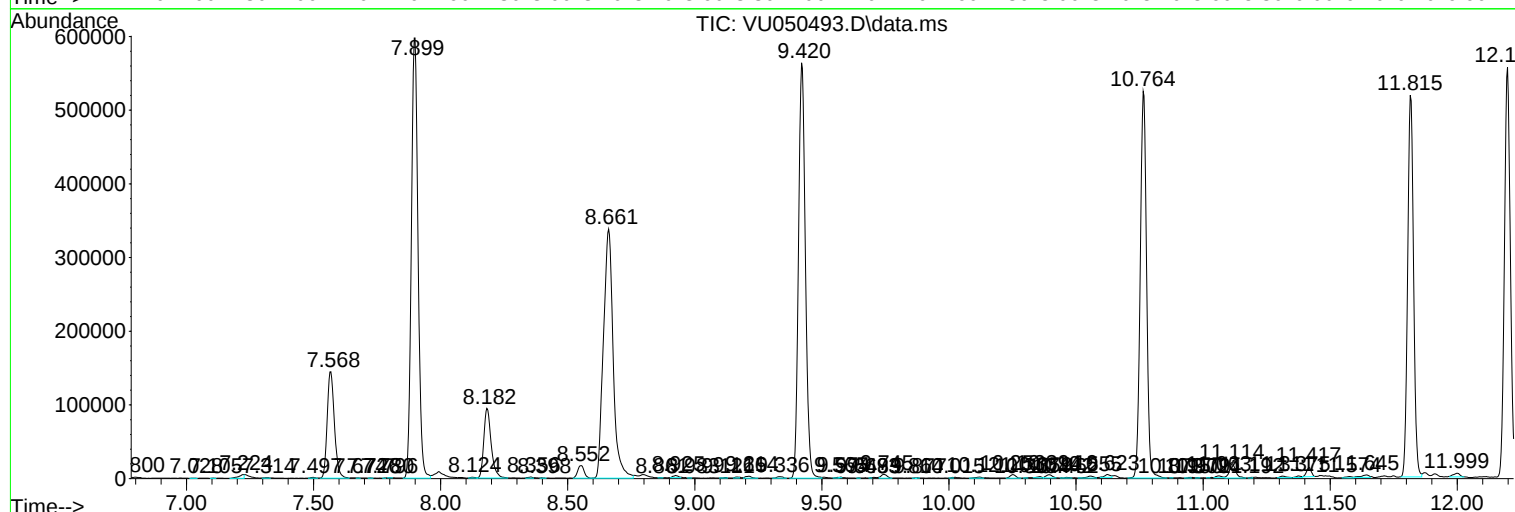
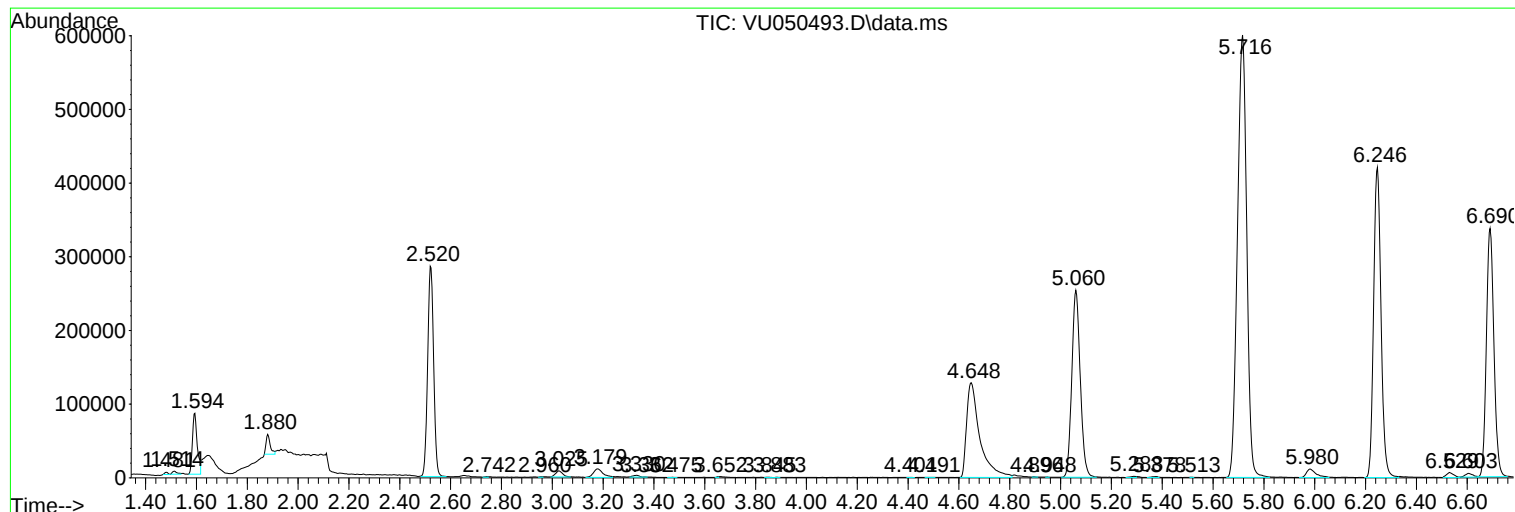
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY168ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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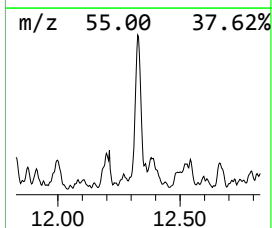
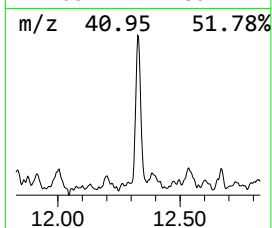
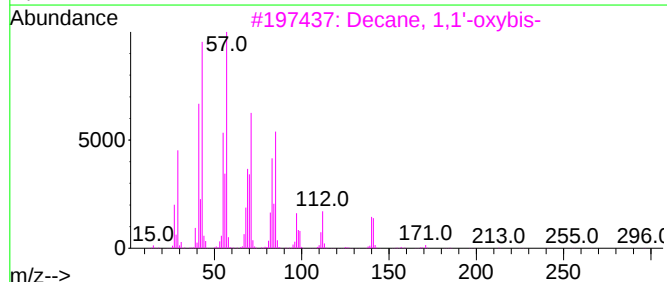
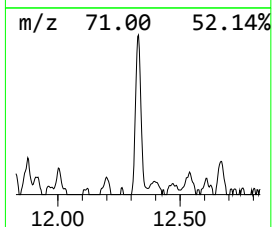
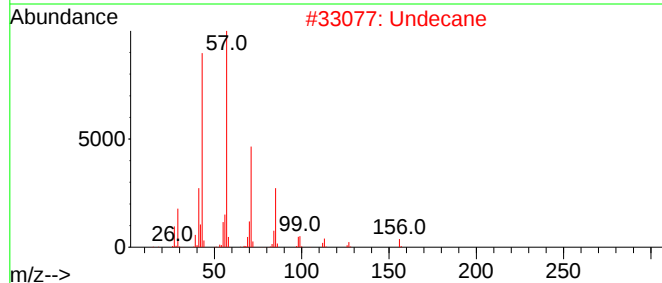
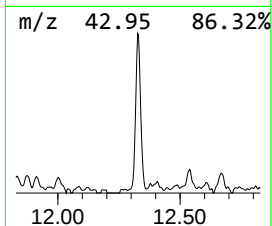
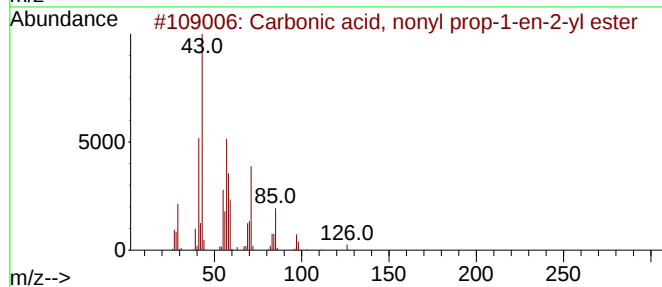
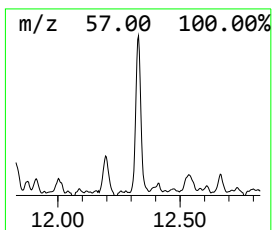
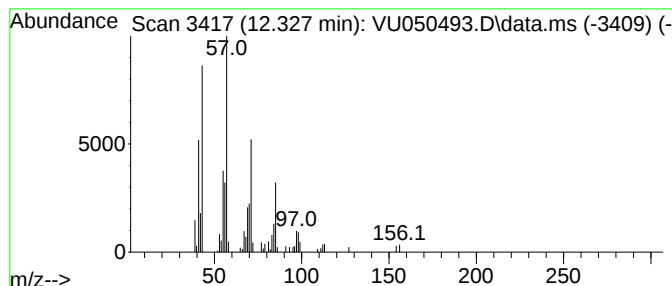
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Carbonic acid, nonyl prop-1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	3.60 ug/L	59828	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	86
2			Undecane	156	C11H24	001120-21-4	81
3			Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	78
4			Decane	142	C10H22	000124-18-5	72
5			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	59



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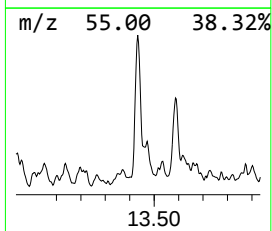
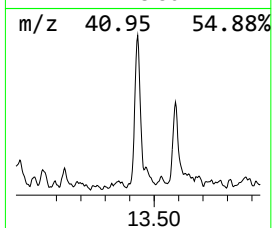
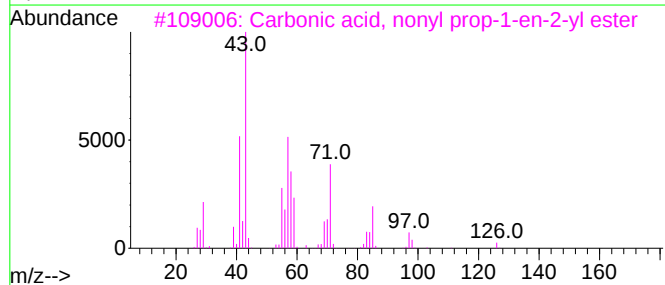
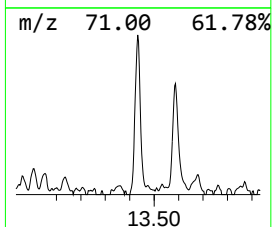
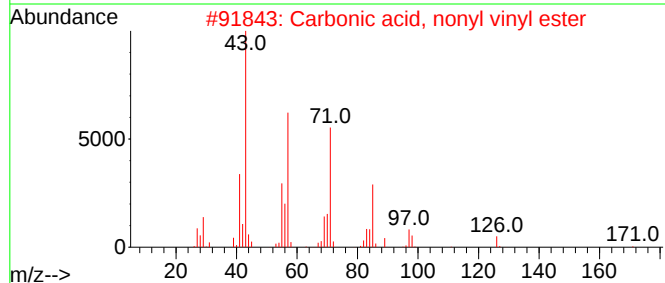
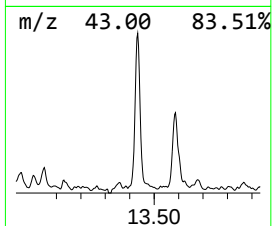
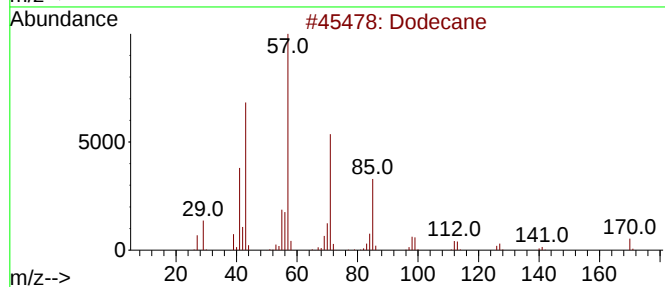
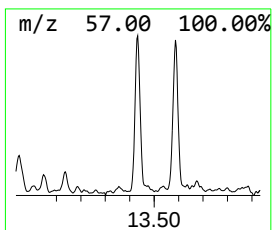
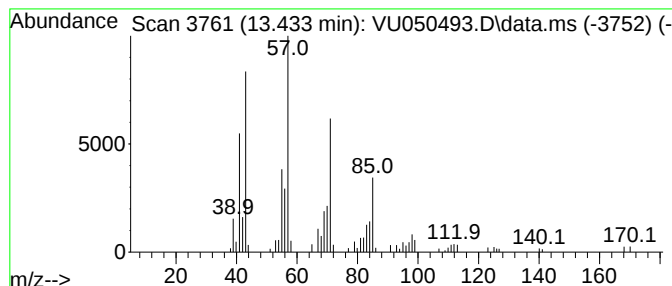
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	4.38 ug/L	72762	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	74
2			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	72
3			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	64
4			2,6-Dimethyldecane	170	C12H26	013150-81-7	62
5			Hexadecane	226	C16H34	000544-76-3	53



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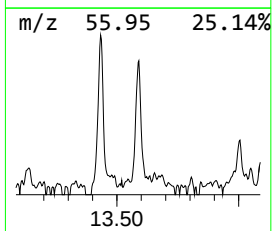
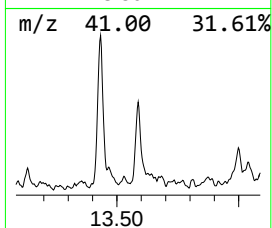
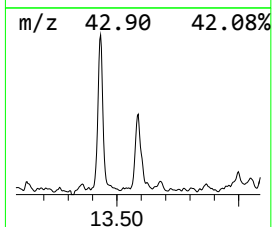
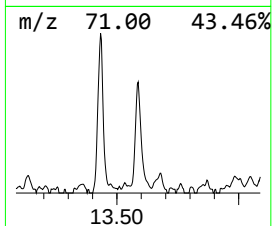
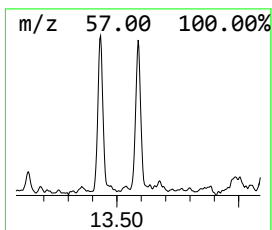
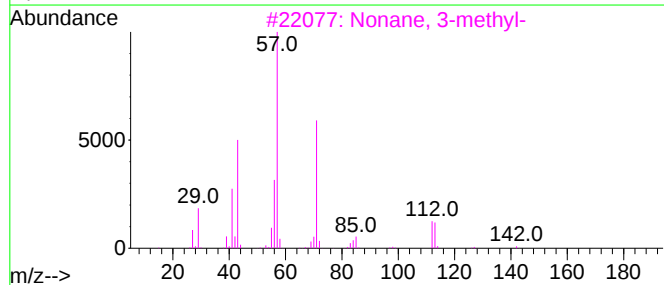
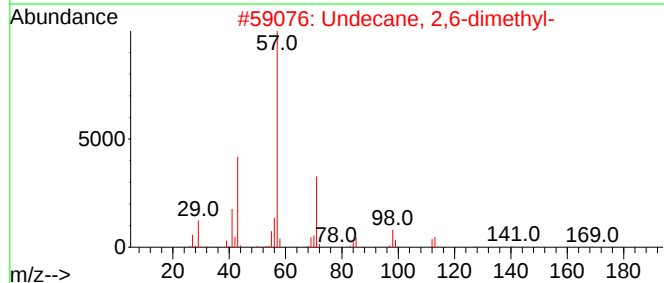
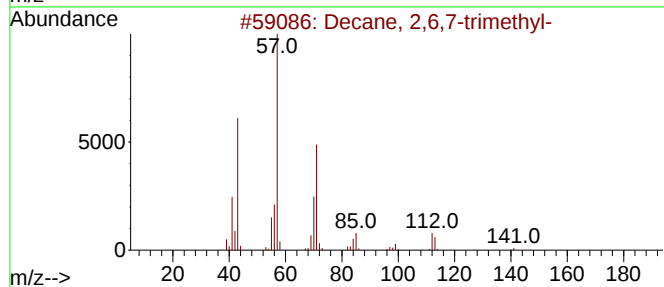
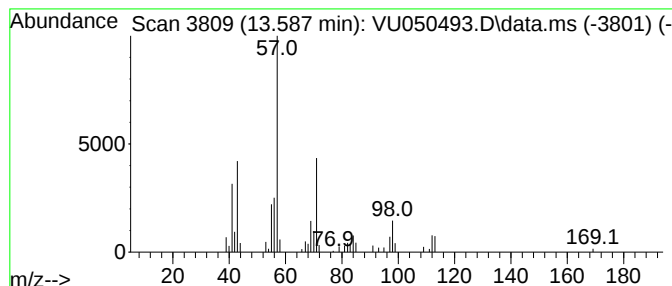
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.587	3.09 ug/L	51315	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	72
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	72
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	64
4			Octane, 4-ethyl-	142	C10H22	015869-86-0	64
5			Carbonic acid, 2-ethylhexyl unde...	328	C20H40O3	1000383-13-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050493.D
Acq On : 29 Aug 2022 18:44
Operator : SY/MD
Sample : N4322-08ME
Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY168ME

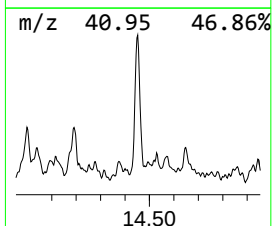
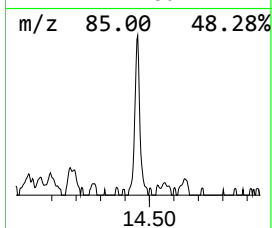
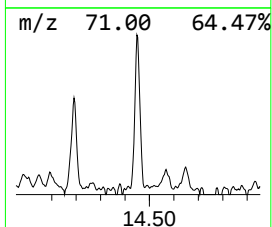
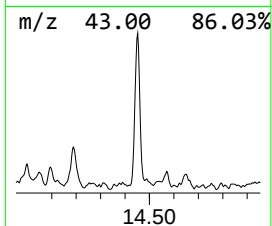
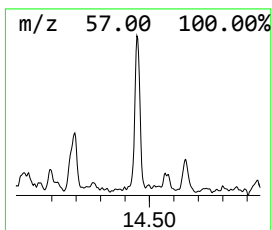
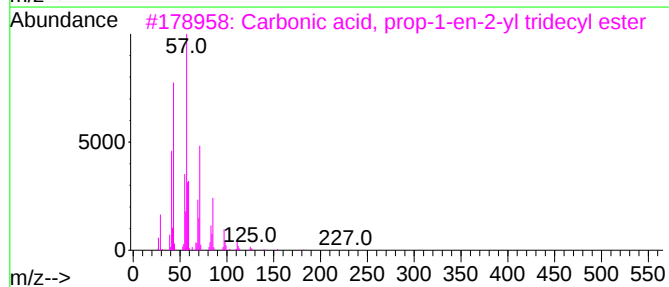
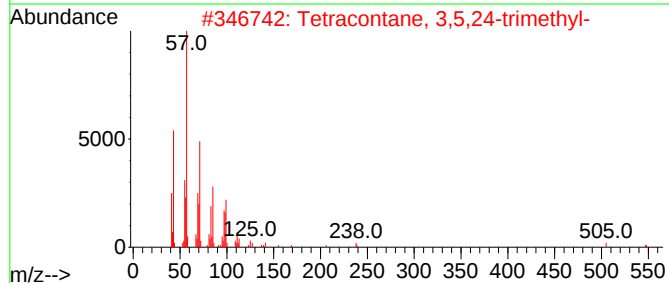
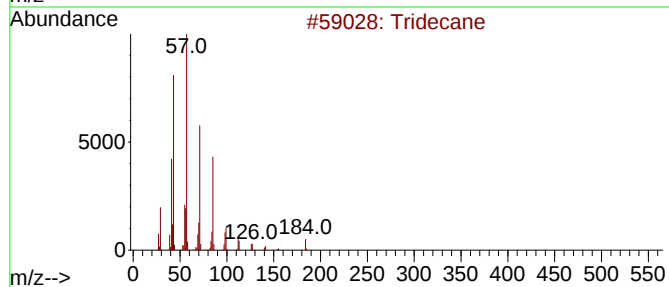
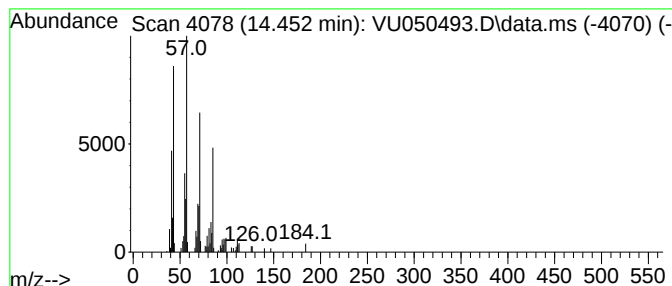
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.452	2.86 ug/L	47536	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	83
2			Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	72
3			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	72
4			Hydroxylamine, 0-decyl-	173	C10H23NO	029812-79-1	72
5			Tetradecane	198	C14H30	000629-59-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050493.D
Acq On : 29 Aug 2022 18:44
Operator : SY/MD
Sample : N4322-08ME
Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY168ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.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
Carbonic acid, ...	12.327	3.6	ug/L	59828	3	11.815	829949	50.0
(DEL) Alkane: S...	13.433	4.4	ug/L	72762	3	11.815	829949	50.0
(DEL) Alkane: S...	13.587	3.1	ug/L	51315	3	11.815	829949	50.0
(DEL) Alkane: S...	14.452	2.9	ug/L	47536	3	11.815	829949	50.0