

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042822\
 Data File : VU048343.D
 Acq On : 28 Apr 2022 16:01
 Operator : SY/MD
 Sample : N2587-03DL 40X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXET1DL

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\SFAMULM042522WMA.M

Title : VOC Analysis

Signal : TIC: VU048343.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	24	rVB	1015702	1009471	59.27%	7.086%
2	1.600	73	81	103	rBV	175367	229537	13.48%	1.611%
3	1.903	169	175	200	rVB	155755	235106	13.80%	1.650%
4	2.481	352	355	357	rBV2	644	477	0.03%	0.003%
5	2.568	369	382	398	rBV	325384	542354	31.84%	3.807%
6	2.684	411	418	430	rVB4	4519	7673	0.45%	0.054%
7	2.797	443	453	459	rBV4	1597	2720	0.16%	0.019%
8	3.047	521	531	542	rVV3	3184	6280	0.37%	0.044%
9	3.115	548	552	555	rBV3	392	299	0.02%	0.002%
10	3.134	555	558	561	rVB	659	471	0.03%	0.003%
11	3.153	561	564	565	rBV2	807	490	0.03%	0.003%
12	3.192	565	576	587	rBV2	5890	13711	0.81%	0.096%
13	3.366	624	630	635	rVB4	617	576	0.03%	0.004%
14	3.449	650	656	663	rVB3	1352	1933	0.11%	0.014%
15	3.854	779	782	786	rBV4	346	288	0.02%	0.002%
16	3.989	819	824	826	rBV2	376	334	0.02%	0.002%
17	4.533	987	993	996	rBV2	514	498	0.03%	0.003%
18	4.571	999	1005	1009	rBV4	1110	1498	0.09%	0.011%
19	4.629	1010	1023	1047	rBV	177676	461118	27.07%	3.237%
20	5.063	1141	1158	1185	rVV	299005	661308	38.83%	4.642%
21	5.250	1213	1216	1220	rVB2	435	303	0.02%	0.002%
22	5.295	1220	1230	1235	rBV4	701	1065	0.06%	0.007%
23	5.378	1252	1256	1269	rVB5	922	1567	0.09%	0.011%
24	5.530	1300	1303	1307	rVB2	461	310	0.02%	0.002%
25	5.726	1341	1364	1373	rBV2	634758	1703148	100.00%	11.955%
26	5.973	1435	1441	1448	rVB8	1021	1473	0.09%	0.010%
27	6.028	1449	1458	1459	rBV4	1205	1803	0.11%	0.013%
28	6.250	1511	1527	1554	rBV	390203	752623	44.19%	5.283%
29	6.481	1589	1599	1603	rBV5	3736	6108	0.36%	0.043%
30	6.529	1607	1614	1632	rVB5	5226	12821	0.75%	0.090%
31	6.690	1649	1664	1682	rBV	392314	766717	45.02%	5.382%
32	6.861	1713	1717	1723	rBV4	402	492	0.03%	0.003%
33	6.928	1732	1738	1739	rBV2	468	353	0.02%	0.002%
34	6.938	1739	1741	1746	rVV3	446	333	0.02%	0.002%
35	7.002	1750	1761	1769	rBV4	3198	5964	0.35%	0.042%
36	7.185	1809	1818	1830	rBV5	3228	6607	0.39%	0.046%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
 Title : VOC Analysis

37	7.266	1841	1843	1852	rVB2	271	294	0.02%	0.002%
38	7.494	1900	1914	1925	rBV2	44521	80388	4.72%	0.564%
39	7.565	1925	1936	1953	rVV	212949	374712	22.00%	2.630%
40	7.687	1970	1974	1984	rVB5	1227	1994	0.12%	0.014%
41	7.796	2001	2008	2009	rBV3	1591	1276	0.07%	0.009%
42	7.899	2025	2040	2053	rBV	776592	1351831	79.37%	9.489%
43	7.976	2054	2064	2080	rVB2	91855	196642	11.55%	1.380%
44	8.179	2114	2127	2143	rBV	148761	251400	14.76%	1.765%
45	8.359	2172	2183	2194	rBV4	21101	36902	2.17%	0.259%
46	8.574	2239	2250	2259	rBV	29864	52091	3.06%	0.366%
47	8.639	2259	2270	2306	rVB	590687	1054459	61.91%	7.401%
48	8.893	2346	2349	2353	rVB2	553	389	0.02%	0.003%
49	8.918	2353	2357	2360	rBV3	334	299	0.02%	0.002%
50	9.018	2378	2388	2400	rVB5	13343	23883	1.40%	0.168%
51	9.092	2410	2411	2415	rBV	472	305	0.02%	0.002%
52	9.121	2415	2420	2424	rVB3	389	332	0.02%	0.002%
53	9.166	2430	2434	2436	rBV3	1174	966	0.06%	0.007%
54	9.359	2489	2494	2499	rBV4	1744	1880	0.11%	0.013%
55	9.420	2500	2513	2517	rBV	565380	945270	55.50%	6.635%
56	9.642	2577	2582	2583	rBV3	563	526	0.03%	0.004%
57	9.655	2583	2586	2591	rVV4	956	1023	0.06%	0.007%
58	9.697	2591	2599	2610	rVB2	5184	7864	0.46%	0.055%
59	9.934	2666	2673	2675	rBV5	1431	1728	0.10%	0.012%
60	10.102	2717	2725	2738	rVB5	3753	6234	0.37%	0.044%
61	10.298	2783	2786	2788	rBV2	466	291	0.02%	0.002%
62	10.330	2791	2796	2797	rBV	379	317	0.02%	0.002%
63	10.491	2838	2846	2851	rVB4	819	1166	0.07%	0.008%
64	10.542	2859	2862	2868	rBV5	719	620	0.04%	0.004%
65	10.655	2887	2897	2910	rVB7	6292	11242	0.66%	0.079%
66	10.758	2915	2929	2950	rVV	617401	1003661	58.93%	7.045%
67	10.896	2964	2972	2978	rBV6	1281	1914	0.11%	0.013%
68	10.983	2987	2999	3011	rBV7	3733	7764	0.46%	0.054%
69	11.098	3027	3035	3042	rBV3	2046	3697	0.22%	0.026%
70	11.253	3076	3083	3090	rBV4	1104	1381	0.08%	0.010%
71	11.295	3090	3096	3097	rBV3	635	516	0.03%	0.004%
72	11.375	3119	3121	3127	rVV2	609	495	0.03%	0.003%
73	11.414	3130	3133	3137	rBV2	392	321	0.02%	0.002%
74	11.465	3140	3149	3159	rVB9	2777	4782	0.28%	0.034%
75	11.507	3159	3162	3168	rBV3	587	598	0.04%	0.004%
76	11.587	3179	3187	3193	rBV5	2017	2676	0.16%	0.019%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
 Title : VOC Analysis

77	11.671	3207	3213	3214	rBV2	419	409	0.02%	0.003%
78	11.690	3217	3219	3227	rVV4	981	1004	0.06%	0.007%
79	11.748	3230	3237	3245	rBV5	3700	5654	0.33%	0.040%
80	11.812	3245	3257	3272	rVV	562181	893715	52.47%	6.273%
81	11.880	3272	3278	3287	rVB8	4646	7502	0.44%	0.053%
82	11.950	3295	3300	3305	rBV6	1362	1852	0.11%	0.013%
83	12.063	3331	3335	3336	rBV2	722	481	0.03%	0.003%
84	12.195	3358	3376	3394	rBV	735733	1207728	70.91%	8.477%
85	12.323	3414	3416	3421	rVB2	792	579	0.03%	0.004%
86	12.388	3433	3436	3441	rBV3	537	393	0.02%	0.003%
87	12.529	3471	3480	3484	rBV2	443	678	0.04%	0.005%
88	12.684	3523	3528	3535	rBV2	1113	1211	0.07%	0.009%
89	12.777	3547	3557	3562	rBV4	2379	3632	0.21%	0.025%
90	12.970	3605	3617	3628	rVB9	3827	7869	0.46%	0.055%
91	13.221	3687	3695	3696	rBV3	496	537	0.03%	0.004%
92	13.333	3723	3730	3735	rBV2	2413	3190	0.19%	0.022%
93	13.378	3735	3744	3754	rVB4	13450	21284	1.25%	0.149%
94	13.497	3778	3781	3785	rVV2	629	506	0.03%	0.004%
95	14.044	3949	3951	3959	rVB3	581	576	0.03%	0.004%
96	14.362	4044	4050	4057	rVB6	3617	4329	0.25%	0.030%
97	14.494	4079	4091	4105	rBV3	25635	41587	2.44%	0.292%
98	14.593	4110	4122	4134	rBV7	3173	5658	0.33%	0.040%
99	15.545	4408	4418	4430	rBV2	39407	59290	3.48%	0.416%
100	16.388	4671	4680	4694	rBV2	62581	105003	6.17%	0.737%

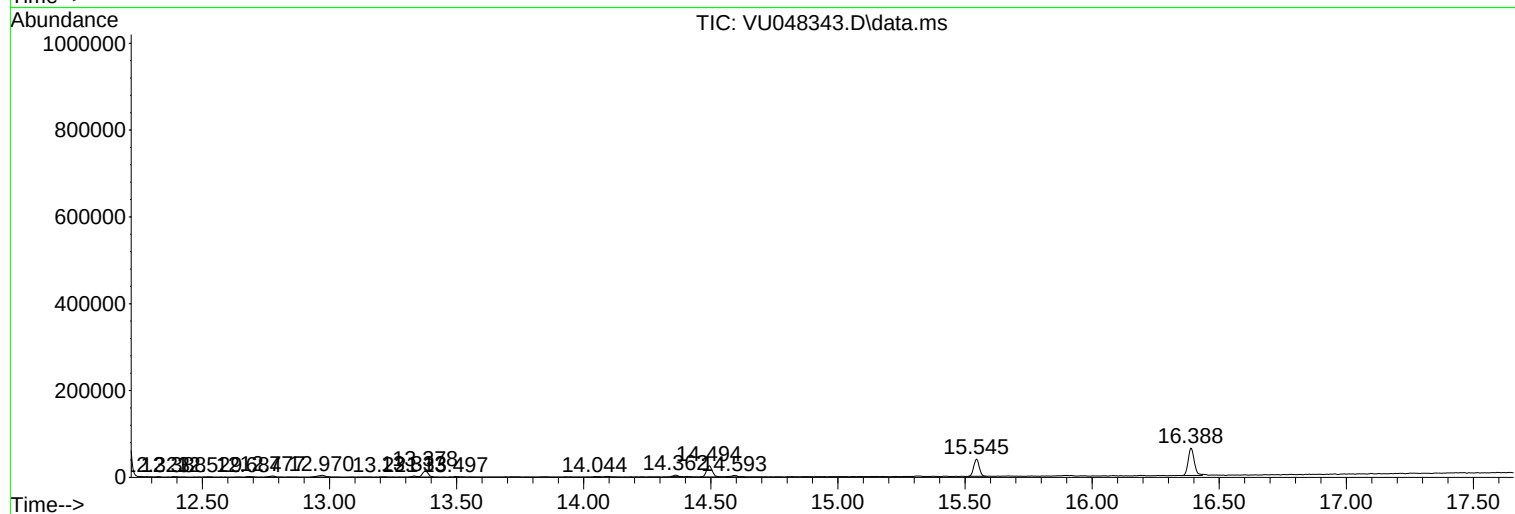
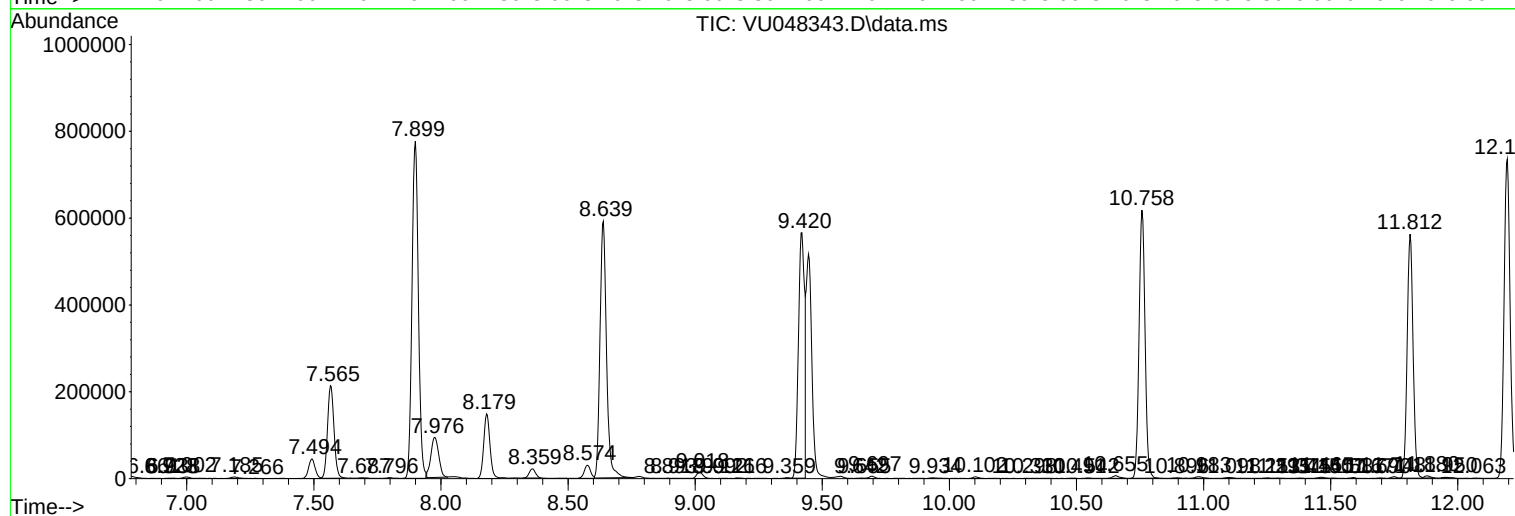
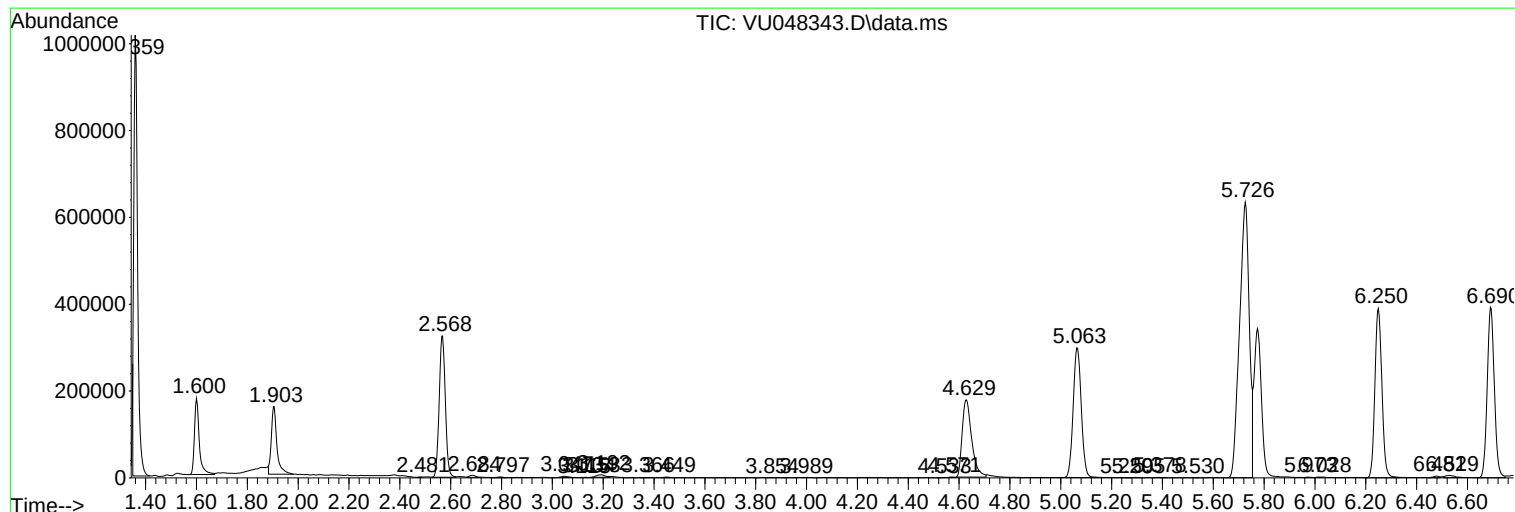
Sum of corrected areas: 14246625

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXET1DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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



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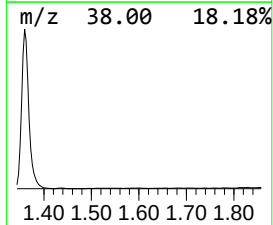
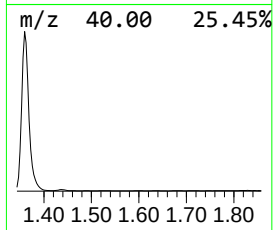
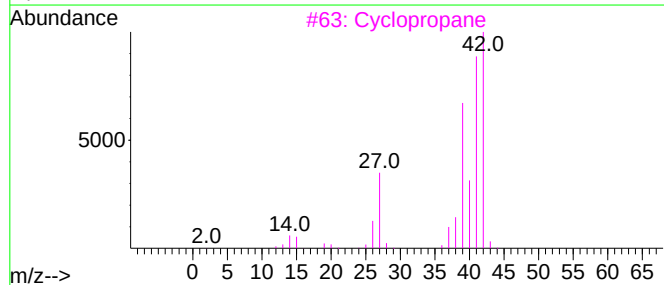
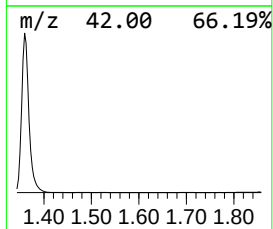
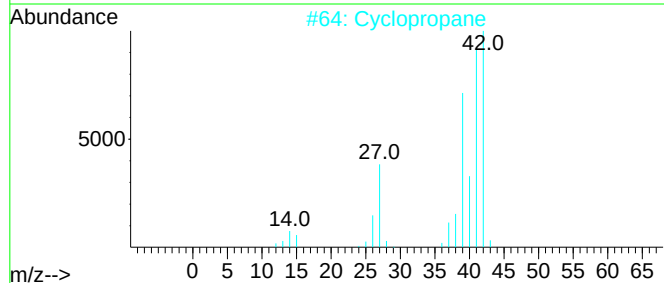
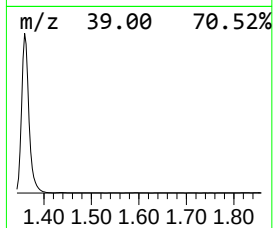
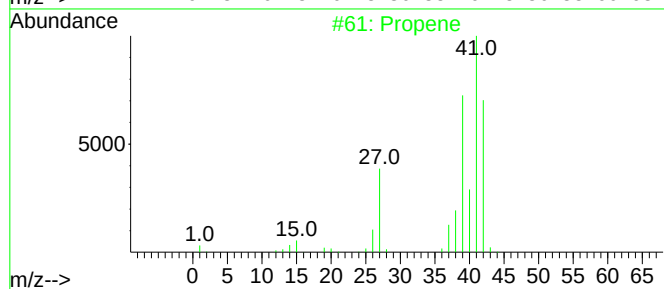
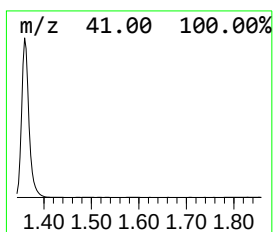
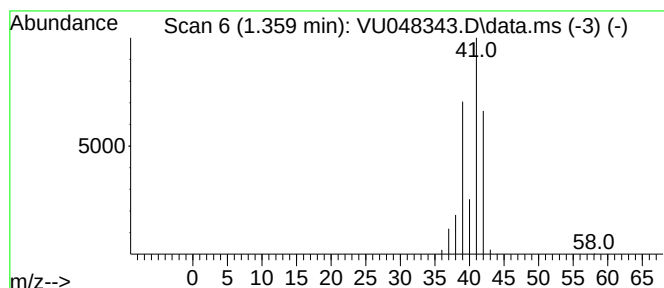
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	67.06 ug/L	1009470	1,4-Difluorobenzene	6.250

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propene	42	C3H6	000115-07-1	90
2		Cyclopropane	42	C3H6	000075-19-4	86
3		Cyclopropane	42	C3H6	000075-19-4	78
4		Propene	42	C3H6	000115-07-1	50
5		Cyclopropene	40	C3H4	002781-85-3	16



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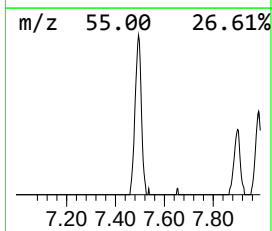
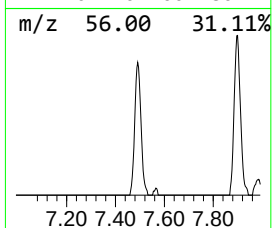
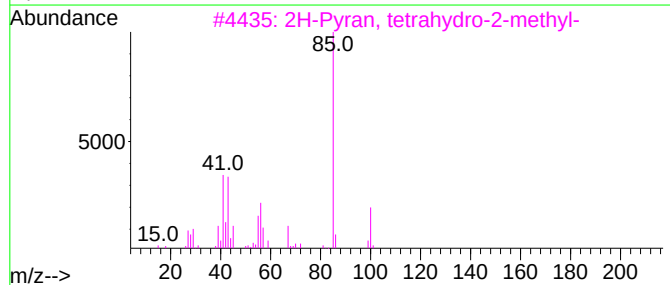
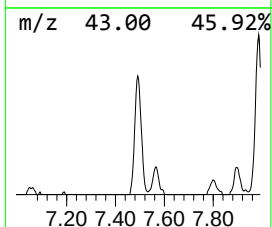
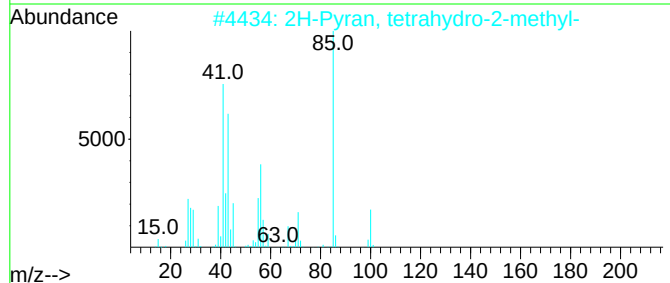
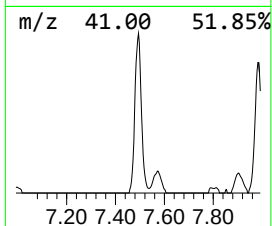
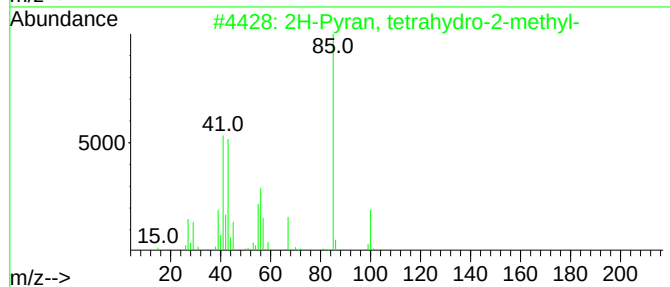
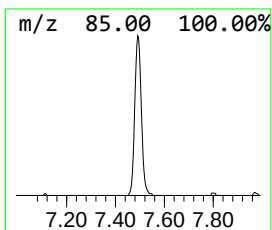
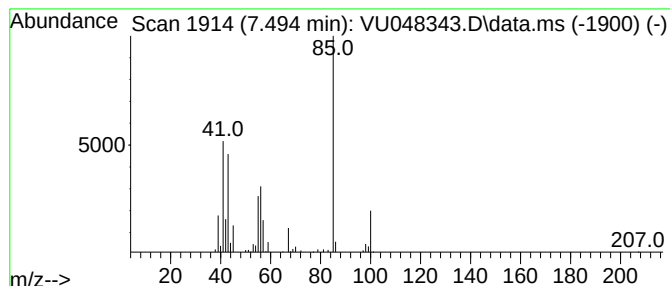
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2H-Pyran, tetrahydro-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.494	5.34 ug/L	80388	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	93		
2	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	91		
3	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	90		
4	Furan, tetrahydro-2,4-dimethyl-,...	100	C6H12O	039168-01-9	64		
5	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	53		



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MSVOA_U
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EXET1DL

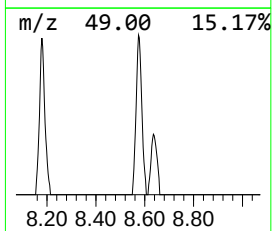
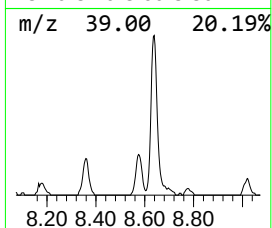
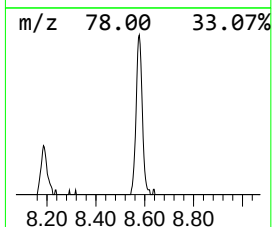
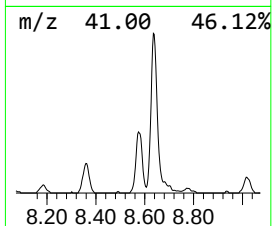
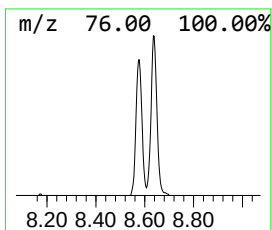
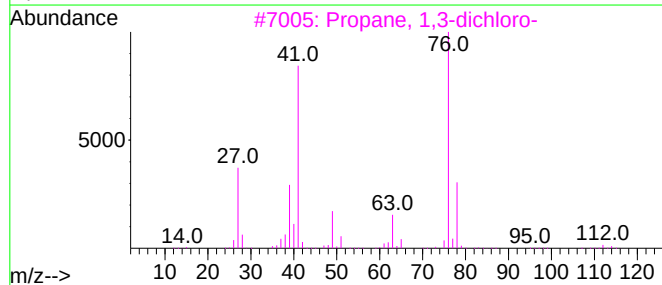
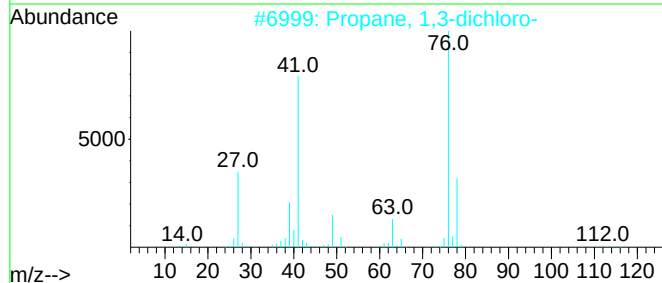
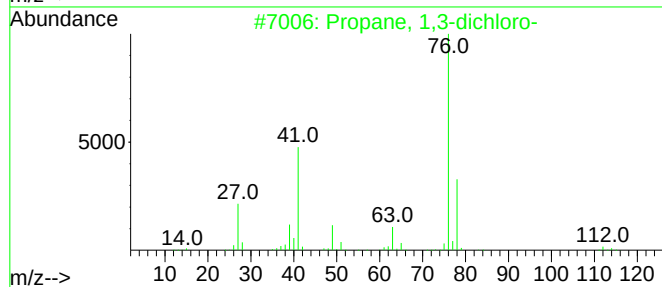
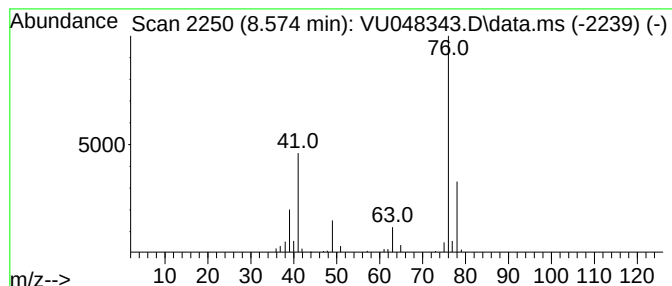
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propane, 1,3-dichloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.574	2.76 ug/L	52091	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,3-dichloro-		112	C3H6Cl2	000142-28-9	83	
2	Propane, 1,3-dichloro-		112	C3H6Cl2	000142-28-9	83	
3	Propane, 1,3-dichloro-		112	C3H6Cl2	000142-28-9	74	
4	Thiourea		76	CH4N2S	000062-56-6	9	
5	Thiourea		76	CH4N2S	000062-56-6	4	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042822\
Data File : VU048343.D
Acq On : 28 Apr 2022 16:01
Operator : SY/MD
Sample : N2587-03DL 40X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXET1DL

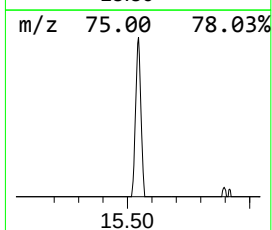
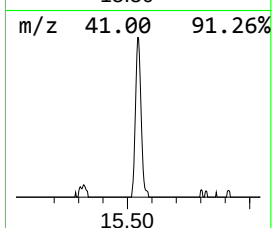
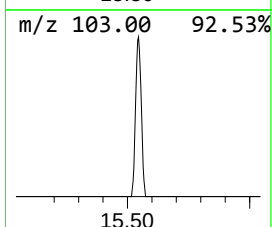
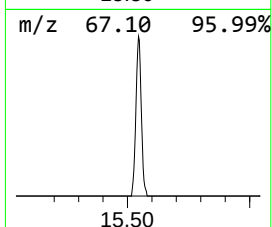
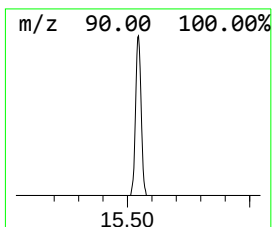
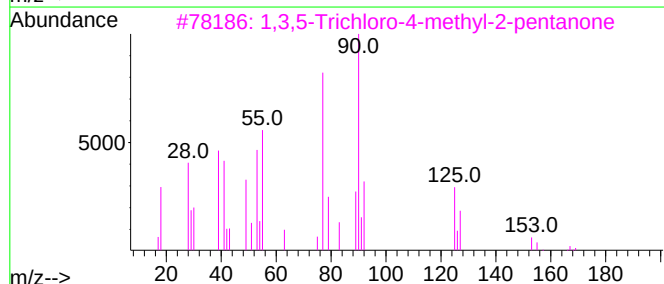
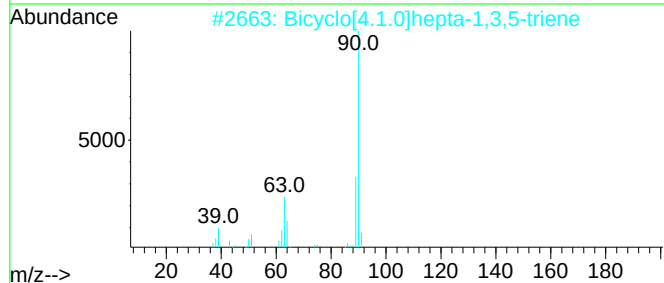
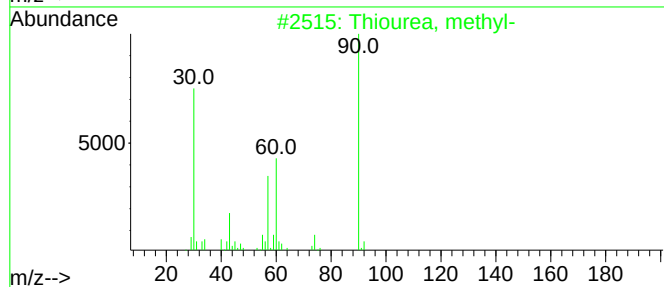
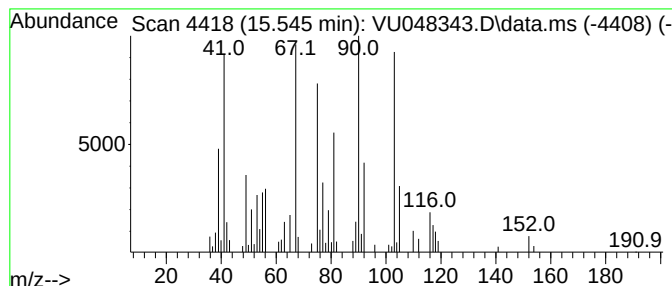
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	3.32 ug/L	59290	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiourea, methyl-	90	C2H6N2S	000598-52-7	35
2			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	35
3			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	28
4			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	25
5			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042822\
Data File : VU048343.D
Acq On : 28 Apr 2022 16:01
Operator : SY/MD
Sample : N2587-03DL 40X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXET1DL

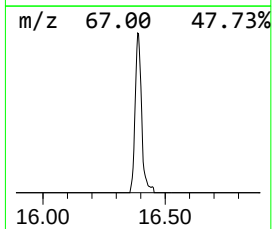
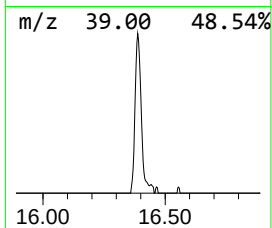
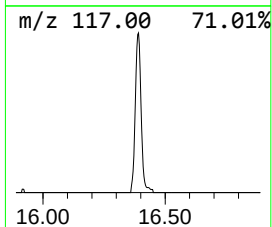
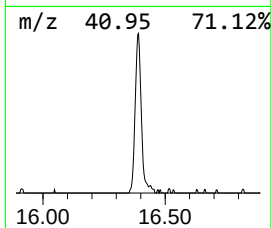
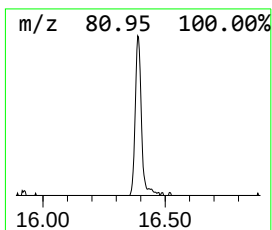
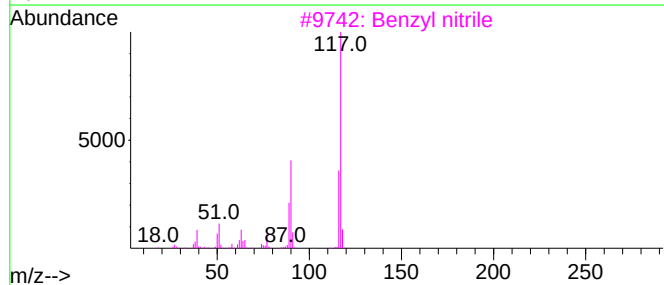
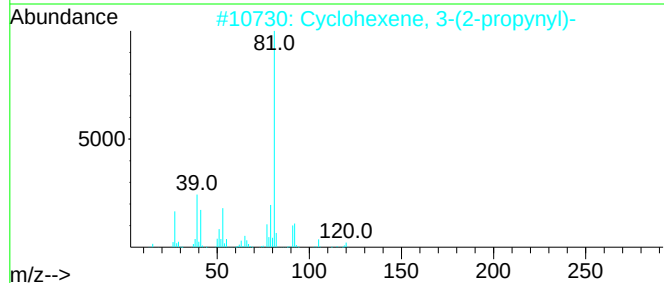
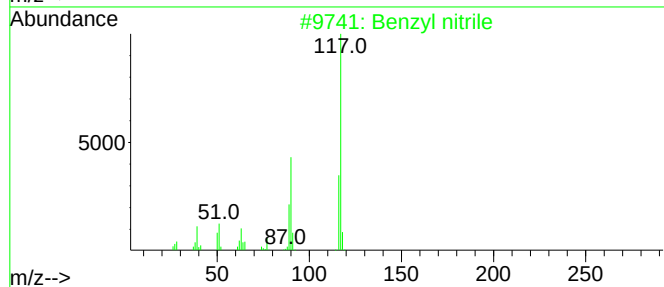
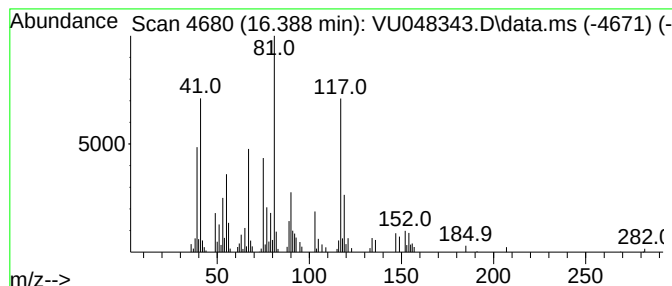
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Quant Title : VOC Analysis

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

Peak Number 6 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	5.87 ug/L	105003	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl nitrile	117	C8H7N	000140-29-4	25
2			Cyclohexene, 3-(2-propynyl)-	120	C9H12	055956-43-9	18
3			Benzyl nitrile	117	C8H7N	000140-29-4	15
4			Benzonitrile, 3-methyl-	117	C8H7N	000620-22-4	15
5			Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	15



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042822\
Data File : VU048343.D
Acq On : 28 Apr 2022 16:01
Operator : SY/MD
Sample : N2587-03DL 40X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXET1DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.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: S...	1.359	67.1	ug/L	1009470	1	6.250	752623	50.0
2H-Pyran, tetra...	7.494	5.3	ug/L	80388	1	6.250	752623	50.0
Propane, 1,3-di...	8.574	2.8	ug/L	52091	2	9.417	945270	50.0
unknown-01	15.545	3.3	ug/L	59290	3	11.812	893715	50.0
unknown-02	16.388	5.9	ug/L	105003	3	11.812	893715	50.0