

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
 Data File : VU045011.D
 Acq On : 29 Sep 2021 22:21
 Operator : SY/MD
 Sample : VSTDCCC050
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 LabSampleId :
 VSTDCCC050

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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\82U092821W.M
 Title : SW846 8260

Signal : TIC: VU045011.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.385	7	14	29	rBV	163222	174894	5.83%	0.227%
2	1.520	50	56	67	rVB	169460	189753	6.33%	0.246%
3	1.604	75	82	89	rBV	202771	226479	7.55%	0.294%
4	1.684	99	107	122	rVB	122126	138549	4.62%	0.180%
5	1.832	146	153	170	rVB	188188	221643	7.39%	0.288%
6	1.922	171	181	202	rVB	126105	179018	5.97%	0.232%
7	2.131	236	246	265	rVB	269691	415760	13.86%	0.539%
8	2.379	312	323	342	rVB	234334	346156	11.54%	0.449%
9	2.488	345	357	371	rVB	50989	80946	2.70%	0.105%
10	2.578	371	385	394	rBV	529105	924252	30.82%	1.199%
11	2.629	394	401	419	rVV	301355	509800	17.00%	0.661%
12	2.723	419	430	441	rVV	103078	182227	6.08%	0.236%
13	2.793	441	452	471	rVB	205369	355381	11.85%	0.461%
14	2.928	472	494	517	rVV2	274828	845269	28.19%	1.097%
15	3.047	517	531	558	rVB	251182	491160	16.38%	0.637%
16	3.189	558	575	597	rBV	125731	306731	10.23%	0.398%
17	3.314	600	614	621	rBV	461421	939881	31.34%	1.219%
18	3.359	622	628	657	rVB2	552083	1237505	41.27%	1.606%
19	3.874	770	788	800	rBV	184676	435947	14.54%	0.566%
20	3.961	800	815	873	rVB2	780112	2673383	89.15%	3.468%
21	4.671	1009	1036	1041	rBV2	472205	1055662	35.20%	1.370%
22	4.774	1058	1068	1084	rBV2	251454	734613	24.50%	0.953%
23	4.977	1116	1131	1143	rBV2	361316	783350	26.12%	1.016%
24	5.054	1143	1155	1163	rBV	485824	1087298	36.26%	1.411%
25	5.317	1214	1237	1247	rBV2	276966	865783	28.87%	1.123%
26	5.385	1247	1258	1272	rVV2	539550	1322145	44.09%	1.715%
27	5.462	1272	1282	1291	rVV	273820	556323	18.55%	0.722%
28	5.530	1291	1303	1327	rVB	508823	1074801	35.84%	1.394%
29	5.706	1342	1358	1368	rBV	176208	373856	12.47%	0.485%
30	5.780	1368	1381	1407	rVV2	576089	1448666	48.31%	1.879%
31	5.915	1407	1423	1451	rVB	293514	579122	19.31%	0.751%
32	6.253	1513	1528	1547	rBV	391070	734395	24.49%	0.953%
33	6.546	1604	1619	1639	rBV	347520	645533	21.53%	0.837%
34	6.768	1672	1688	1718	rBV4	481625	1515736	50.55%	1.966%
35	6.922	1722	1736	1741	rBV	216253	375998	12.54%	0.488%
36	6.964	1741	1749	1762	rVV	419335	753961	25.14%	0.978%

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Integrator: RTE

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Min Area: 1 % 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

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 Title : SW846 8260

37	7.041	1762	1773	1783	rVV	299965	534895	17.84%	0.694%
38	7.108	1784	1794	1822	rVB	286933	584052	19.48%	0.758%
39	7.366	1860	1874	1892	rBV	92284	177197	5.91%	0.230%
40	7.465	1892	1905	1928	rVB	772422	1277939	42.62%	1.658%
41	7.610	1937	1950	1967	rBV	358027	612753	20.43%	0.795%
42	7.793	1990	2007	2028	rBV	1723254	2998778	100.00%	3.891%
43	7.903	2028	2041	2052	rVV	579598	981859	32.74%	1.274%
44	7.973	2052	2063	2086	rVB	722111	1220327	40.69%	1.583%
45	8.214	2122	2138	2155	rBV	361700	587675	19.60%	0.762%
46	8.337	2162	2176	2186	rBV	433670	681777	22.74%	0.885%
47	8.404	2186	2197	2214	rVB	407759	683801	22.80%	0.887%
48	8.558	2231	2245	2263	rBV2	534061	1428816	47.65%	1.854%
49	8.687	2272	2285	2312	rBV	1421276	2275353	75.88%	2.952%
50	8.835	2312	2331	2348	rVV2	485799	1101928	36.75%	1.430%
51	8.928	2348	2360	2380	rVB	197635	336903	11.23%	0.437%
52	9.420	2499	2513	2517	rBV	588919	929814	31.01%	1.206%
53	9.449	2518	2522	2537	rVV	627581	904367	30.16%	1.173%
54	9.539	2537	2550	2554	rVV	427213	696583	23.23%	0.904%
55	9.571	2554	2560	2584	rVV	835294	1327003	44.25%	1.722%
56	9.697	2585	2599	2629	rVB	1591079	2624860	87.53%	3.405%
57	10.108	2711	2727	2744	rBV4	1311338	2546208	84.91%	3.303%
58	10.295	2773	2785	2787	rBV	216517	284967	9.50%	0.370%
59	10.324	2788	2794	2832	rVV	541990	858804	28.64%	1.114%
60	10.488	2832	2845	2855	rVV	901969	1407002	46.92%	1.825%
61	10.549	2855	2864	2880	rVV	312664	498187	16.61%	0.646%
62	10.636	2880	2891	2909	rVB	427557	672855	22.44%	0.873%
63	10.787	2923	2938	2945	rBV	976894	1603639	53.48%	2.081%
64	10.828	2945	2951	2966	rVV2	510588	1124028	37.48%	1.458%
65	10.909	2966	2976	2989	rVV	923150	1413373	47.13%	1.834%
66	10.989	2989	3001	3020	rVV	755766	1192049	39.75%	1.547%
67	11.095	3020	3034	3053	rVB3	1532487	2564483	85.52%	3.327%
68	11.423	3118	3136	3144	rBV2	1161596	2039623	68.02%	2.646%
69	11.472	3144	3151	3167	rVB	1001159	1523679	50.81%	1.977%
70	11.645	3185	3205	3219	rBV	918993	1420102	47.36%	1.842%
71	11.748	3224	3237	3244	rBV	660442	1017526	33.93%	1.320%
72	11.799	3244	3253	3261	rBV3	969372	2004403	66.84%	2.600%
73	11.896	3277	3283	3294	rVB	22285	33478	1.12%	0.043%
74	12.099	3333	3346	3363	rVB3	21875	37139	1.24%	0.048%
75	12.214	3363	3382	3399	rBV2	1468196	2305811	76.89%	2.992%
76	12.478	3445	3464	3480	rBV	414355	692201	23.08%	0.898%

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LabSampleId :
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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Title : SW846 8260

77	12.999	3604	3626	3645	rBV2	217835	408192	13.61%	0.530%
78	13.211	3680	3692	3703	rBV	23363	39501	1.32%	0.051%
79	13.449	3744	3766	3785	rBV	885573	1363495	45.47%	1.769%
80	13.844	3877	3889	3905	rBV	501069	802682	26.77%	1.041%
81	14.024	3933	3945	3954	rBV	335932	517442	17.26%	0.671%
82	14.089	3954	3965	3989	rVB	737975	1155550	38.53%	1.499%
83	14.333	4028	4041	4056	rBV	504612	803496	26.79%	1.042%

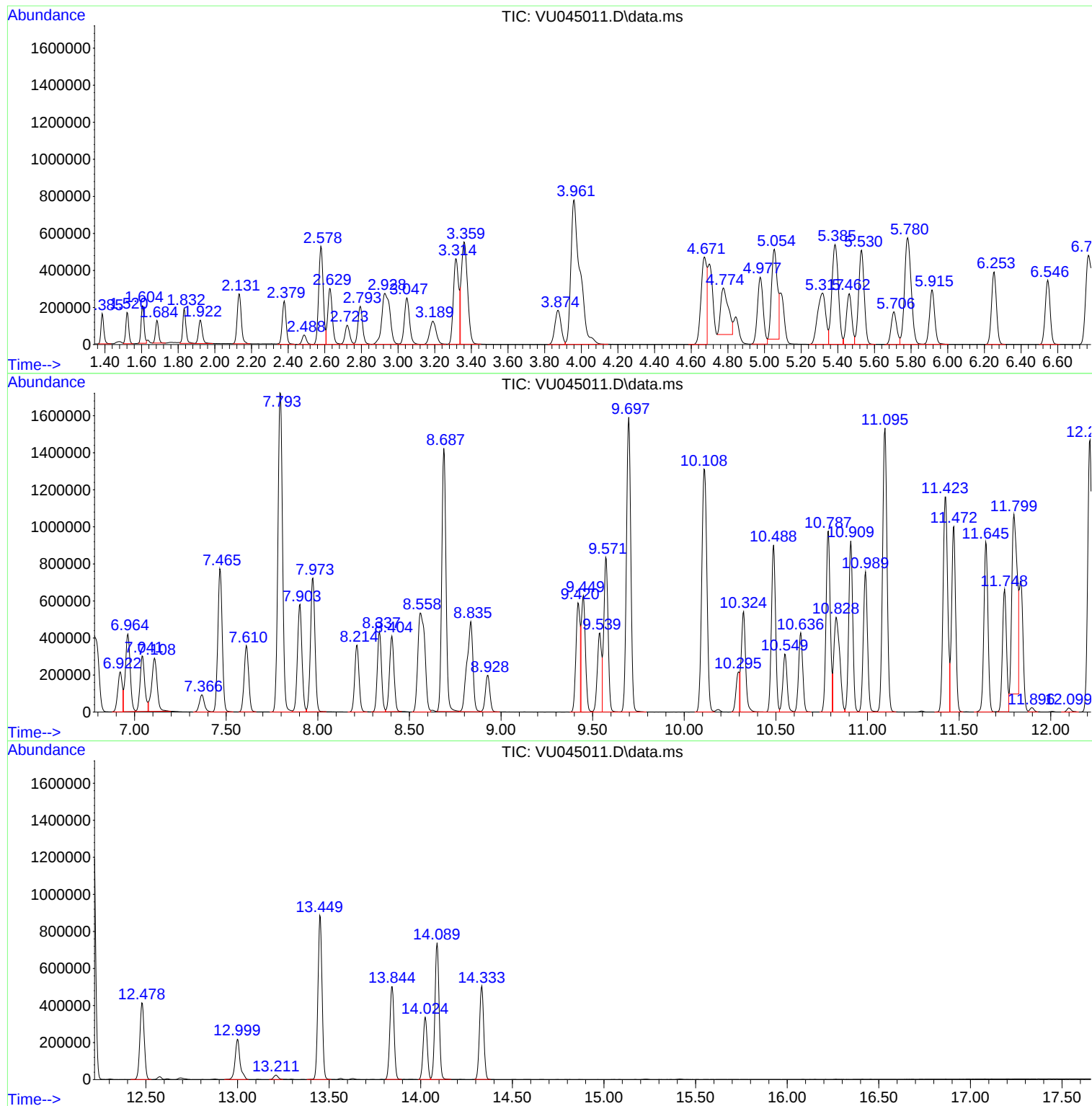
Sum of corrected areas: 77078571

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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



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Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
LabSampleId :
VSTDCCC050

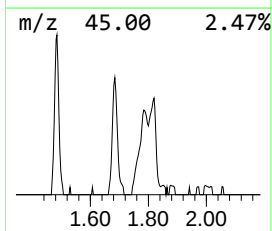
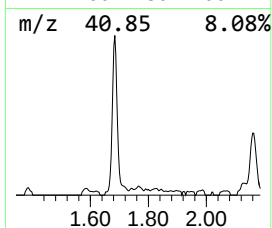
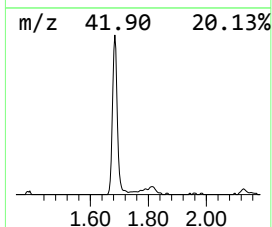
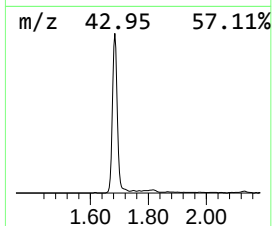
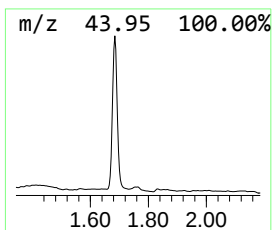
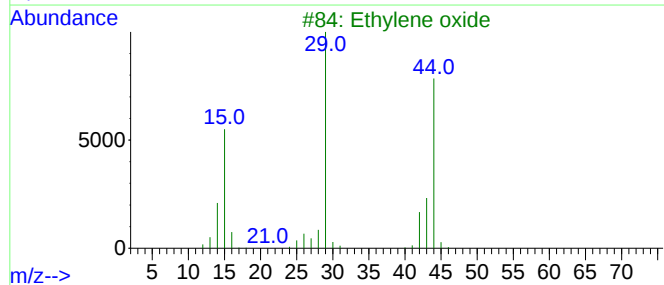
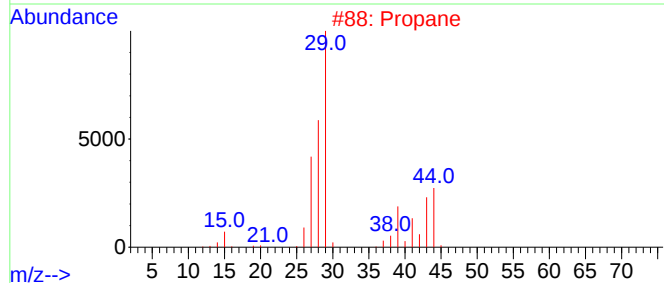
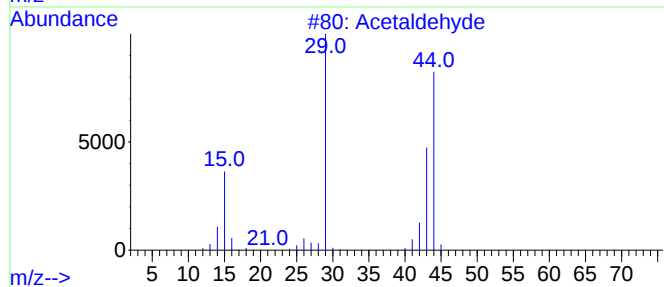
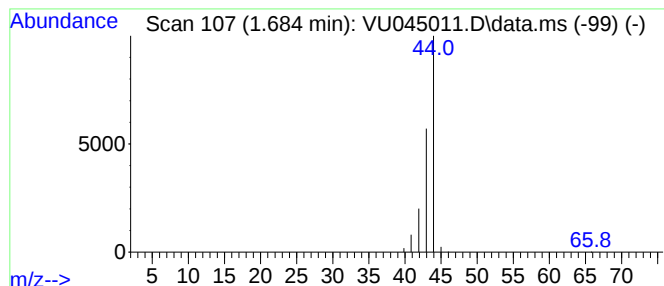
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.684	5.24 ug/l	138549	Pentafluorobenzene	5.379

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Hydrogen isocyanate	43	CHNO	000075-13-8	3
5			Ethyne, fluoro-	44	C2HF	002713-09-9	3



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
LabSampleId :
VSTDCCC050

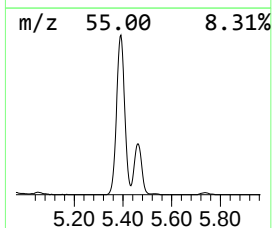
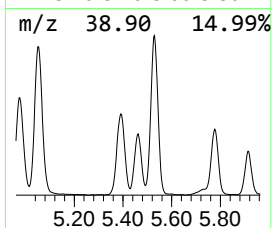
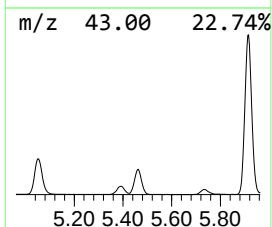
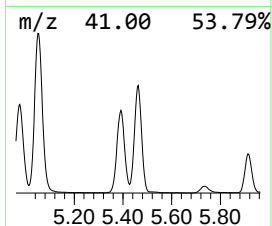
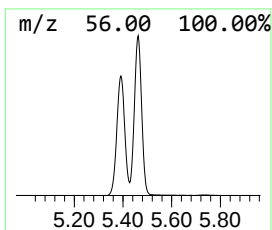
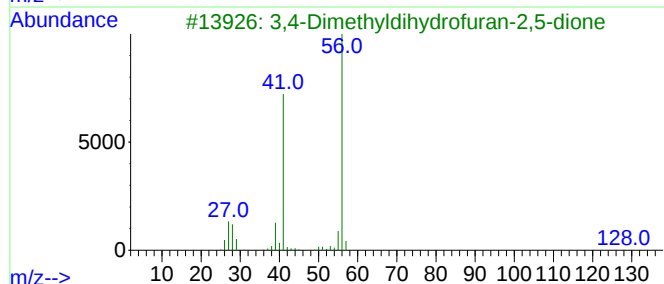
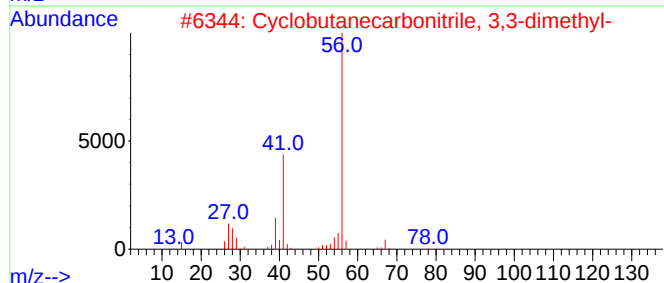
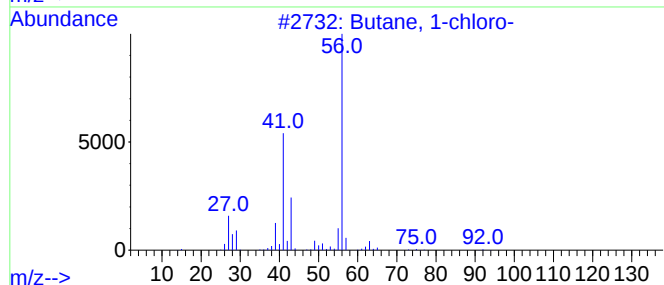
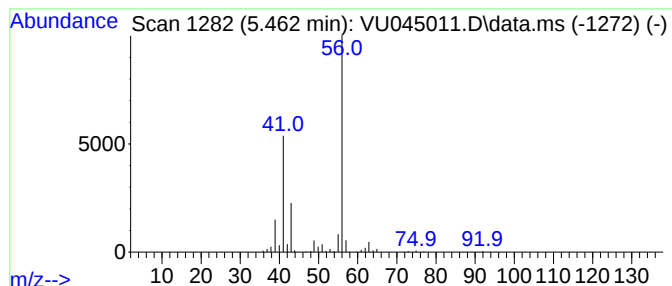
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 1-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.462	21.04 ug/l	556323	Pentafluorobenzene	5.379

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	91
2			Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	64
3			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	39
4			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	38
5			2-Propenal	56	C3H4O	000107-02-8	9



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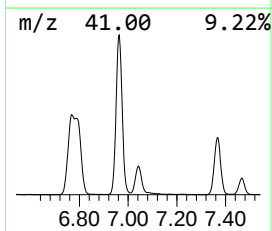
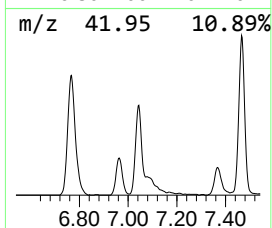
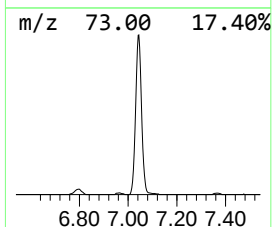
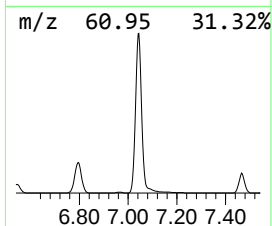
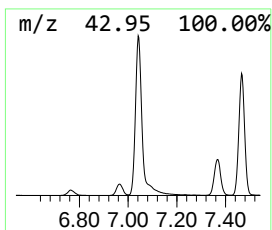
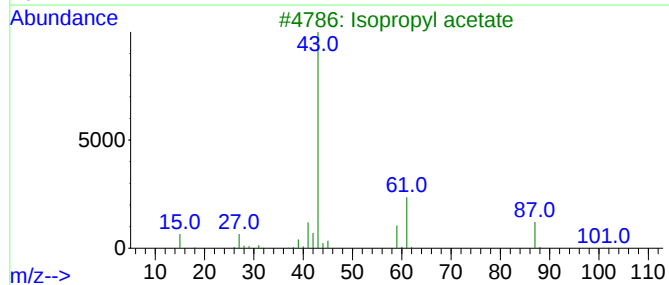
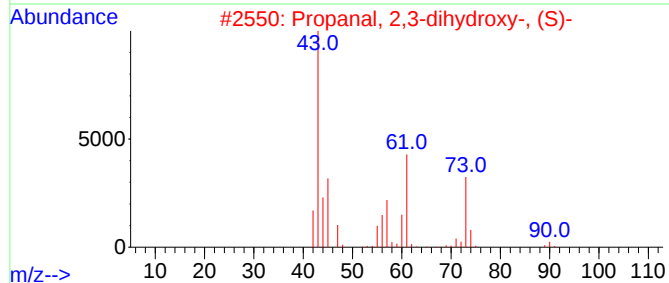
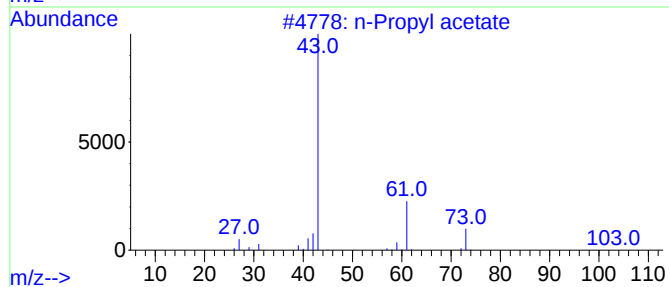
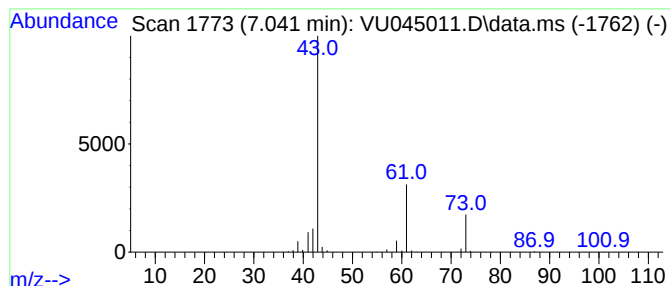
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	36.42 ug/l	534895	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	83
2			Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
3			Isopropyl acetate	102	C5H10O2	000108-21-4	36
4			Isobutyl acetate	116	C6H12O2	000110-19-0	9
5			1-Butanamine	73	C4H11N	000109-73-9	5



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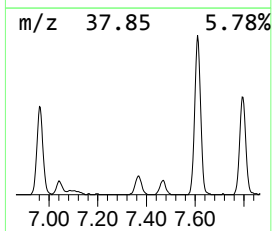
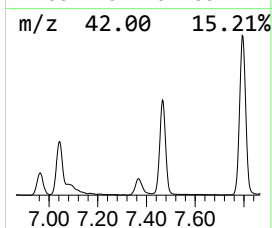
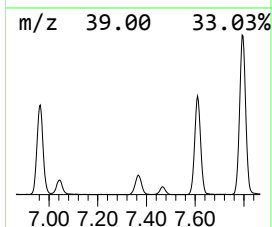
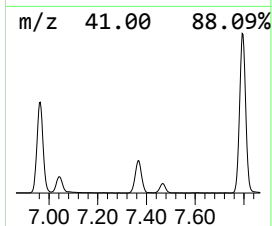
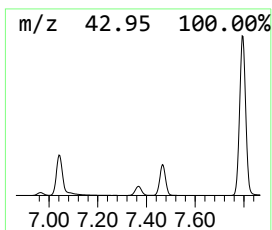
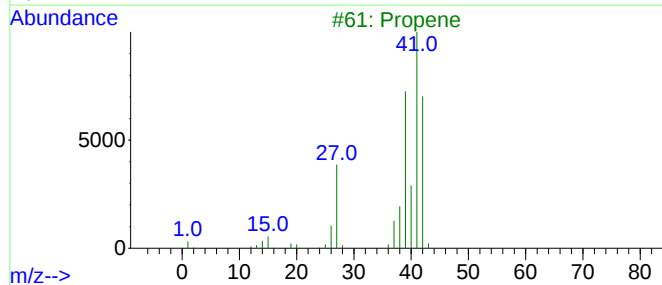
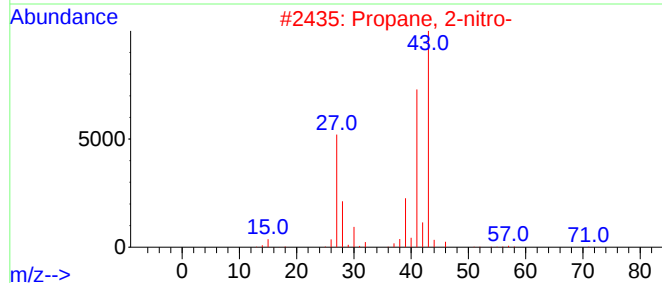
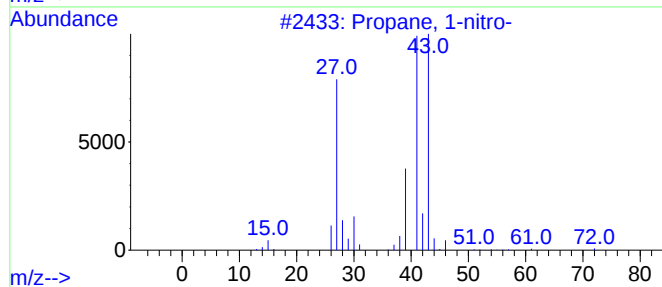
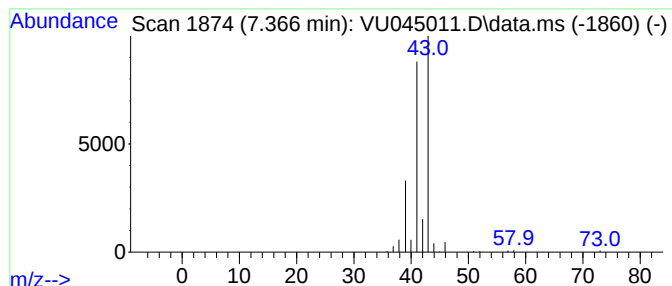
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Quant Title : SW846 8260

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

Peak Number 4 Propane, 1-nitro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.366	12.06 ug/l	177197	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	78
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	64
3			Propene	42	C3H6	000115-07-1	9
4			Isobutyl nitrite	103	C4H9NO2	000542-56-3	9
5			Oxirane, ethyl-	72	C4H8O	000106-88-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045011.D
Acq On : 29 Sep 2021 22:21
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
LabSampleId :
VSTDCCC050

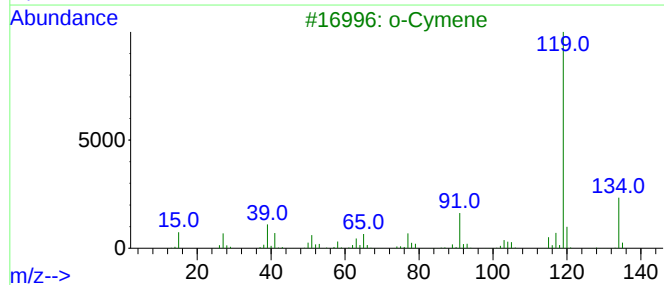
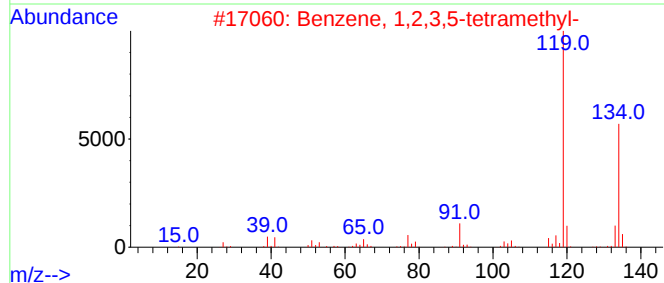
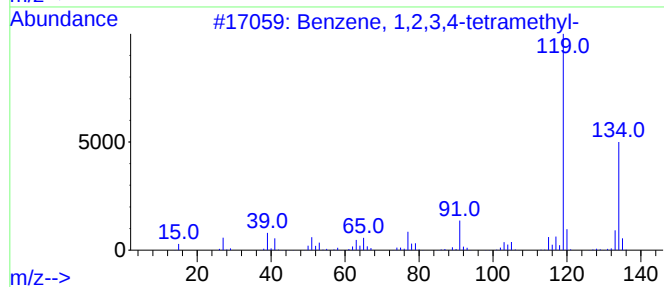
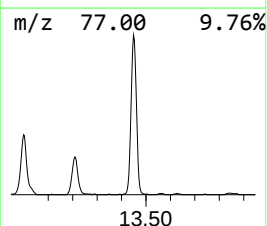
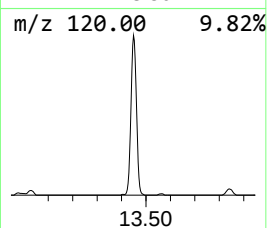
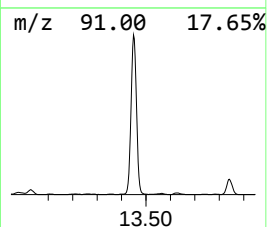
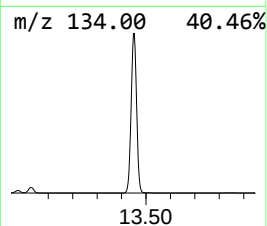
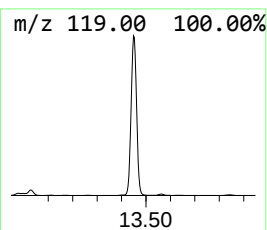
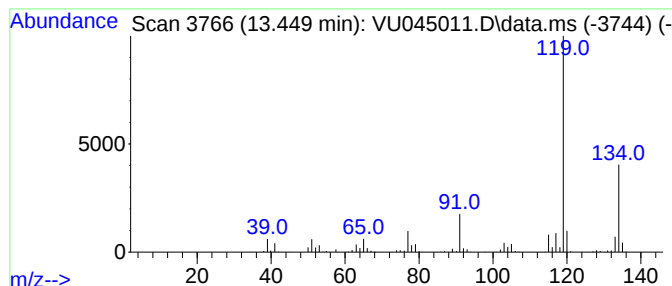
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.449	34.01 ug/l	1363500	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045011.D
Acq On : 29 Sep 2021 22:21
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
LabSampleId :
VSTDCCC050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.684	5.2	ug/l	138549	1	5.379	1322150	50.0
Butane, 1-chloro-	5.462	21.0	ug/l	556323	1	5.379	1322150	50.0
n-Propyl acetate	7.041	36.4	ug/l	534895	2	6.253	734395	50.0
Propane, 1-nitro-	7.366	12.1	ug/l	177197	2	6.253	734395	50.0
Benzene, 1,2,3,...	13.449	34.0	ug/l	1363500	4	11.816	2004400	50.0