

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
 Data File : VN065433.D
 Acq On : 7 Jan 2021 17:44
 Operator : JC/MD
 Sample : M1022-08
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 16790

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_N\methods\82N122220W.M
 Title : SW846 8260

Signal : TIC: VN065433.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.306	163	176	202	rBV	728344	1215663	34.47%	7.308%
2	3.672	583	601	618	rBV	134109	343662	9.74%	2.066%
3	3.791	619	638	673	rVV	1353193	3526678	100.00%	21.200%
4	4.055	705	720	744	rVB	53050	154501	4.38%	0.929%
5	6.023	1318	1332	1363	rBV4	19955	68173	1.93%	0.410%
6	6.614	1499	1516	1539	rBV2	17089	51341	1.46%	0.309%
7	6.807	1559	1576	1602	rBV2	25118	74113	2.10%	0.446%
8	7.364	1733	1749	1780	rBV2	41705	107001	3.03%	0.643%
9	7.553	1790	1808	1819	rBV	196759	490849	13.92%	2.951%
10	7.630	1820	1832	1860	rVB	334216	802233	22.75%	4.822%
11	7.994	1920	1945	1972	rBV2	208928	508951	14.43%	3.059%
12	8.553	2103	2119	2154	rVB2	611553	1339692	37.99%	8.053%
13	8.810	2186	2199	2212	rVB2	63404	126681	3.59%	0.762%
14	9.151	2285	2305	2339	rBV	32851	193492	5.49%	1.163%
15	10.058	2572	2587	2601	rBV	850102	1571751	44.57%	9.448%
16	10.126	2601	2608	2620	rVB	48257	87059	2.47%	0.523%
17	10.318	2657	2668	2683	rVB	44676	80428	2.28%	0.483%
18	10.466	2702	2714	2727	rBV2	34752	60758	1.72%	0.365%
19	11.380	2983	2998	3022	rBV	862301	1529385	43.37%	9.194%
20	11.589	3053	3063	3080	rVB	36458	71253	2.02%	0.428%
21	11.929	3157	3169	3187	rVB4	51013	117582	3.33%	0.707%
22	12.376	3292	3308	3335	rBV	748407	1336612	37.90%	8.035%
23	13.318	3587	3601	3618	rBV	832329	1456411	41.30%	8.755%
24	13.698	3707	3719	3739	rVB	108427	196131	5.56%	1.179%
25	15.103	4139	4156	4176	rBV	549863	1013670	28.74%	6.093%
26	16.312	4518	4532	4550	rBV	16159	42104	1.19%	0.253%
27	16.553	4597	4607	4627	rVB3	31045	69235	1.96%	0.416%

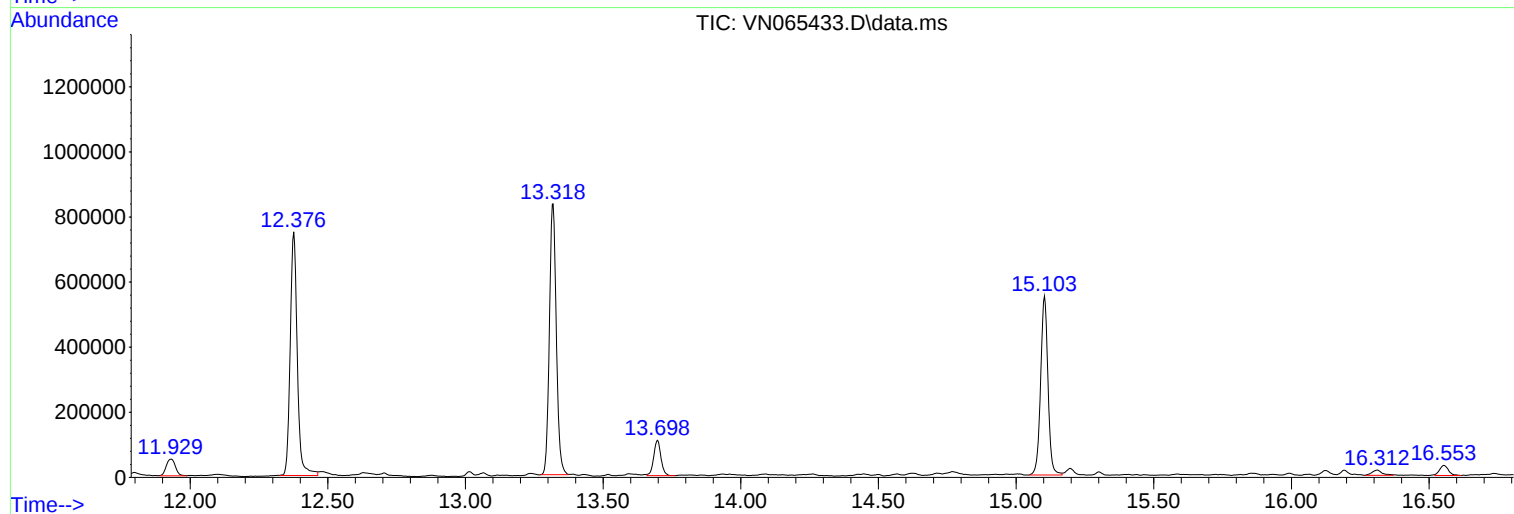
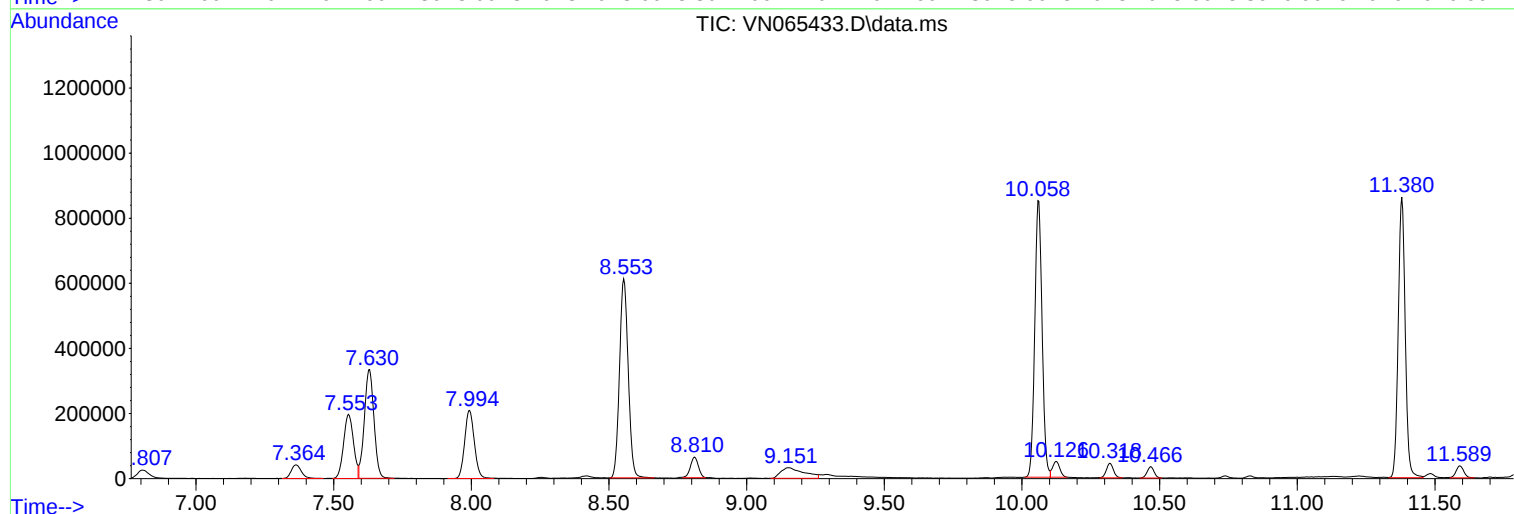
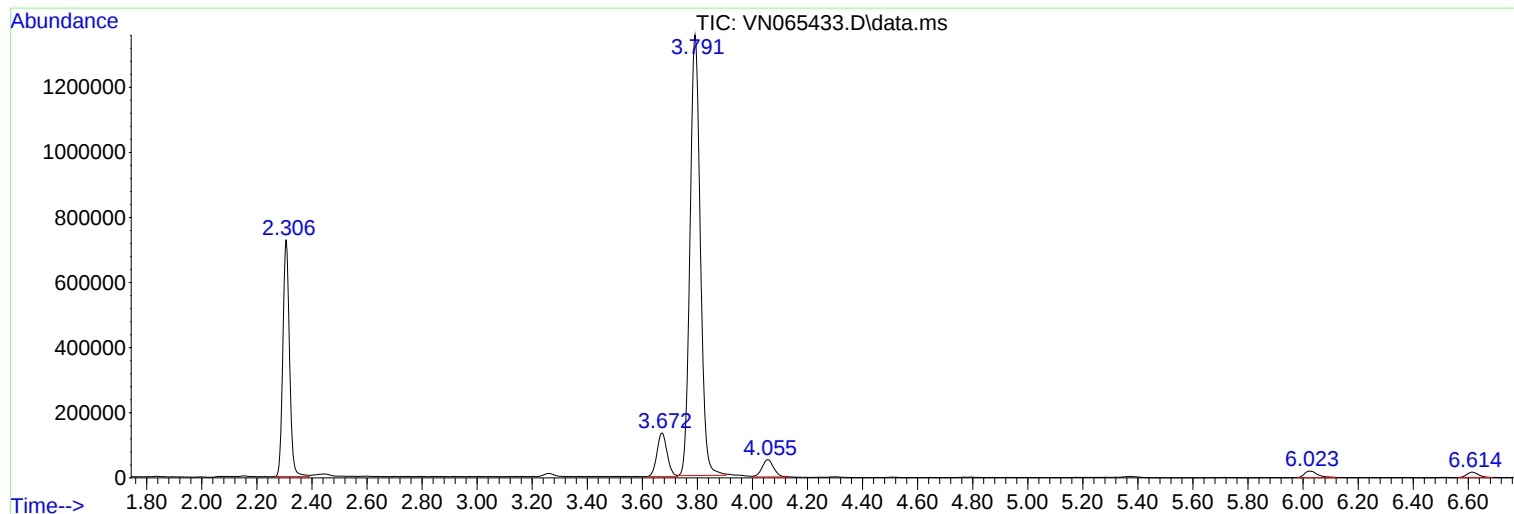
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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



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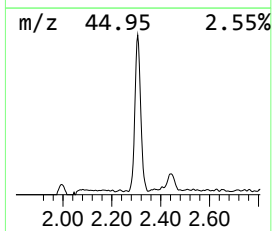
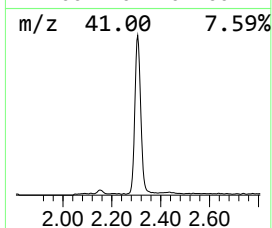
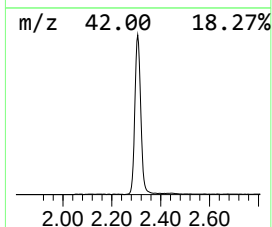
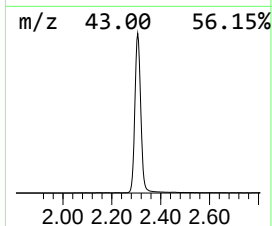
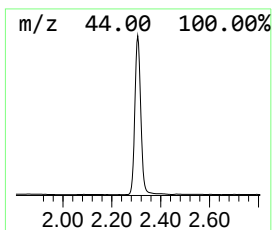
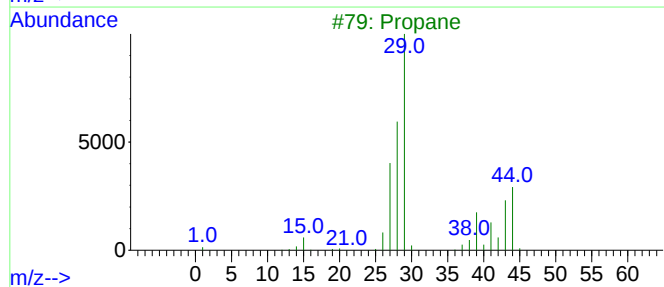
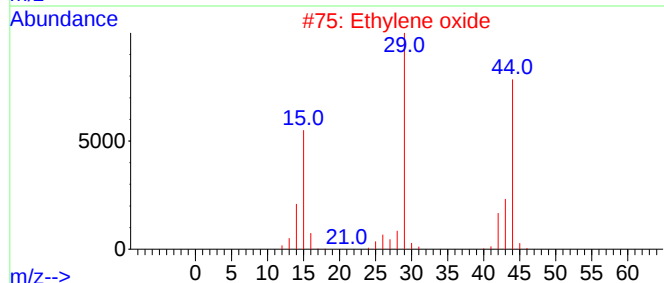
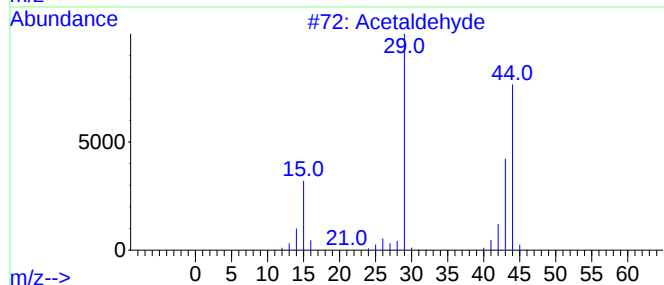
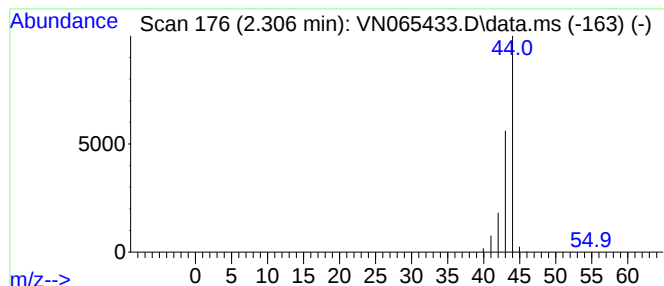
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.306	75.77 ug/l	1215660	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Ethyne, fluoro-	44	C2HF	002713-09-9	3



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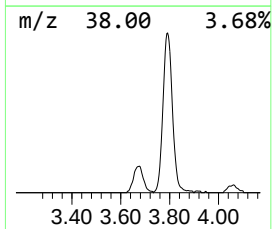
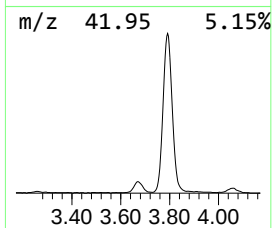
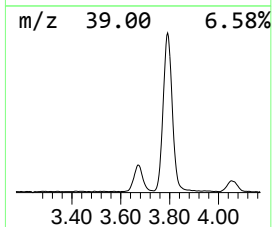
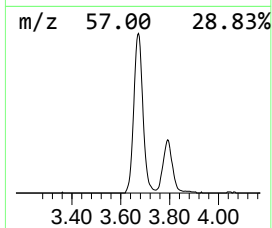
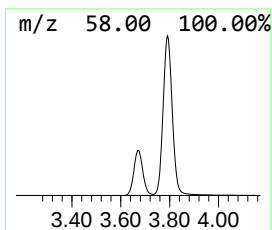
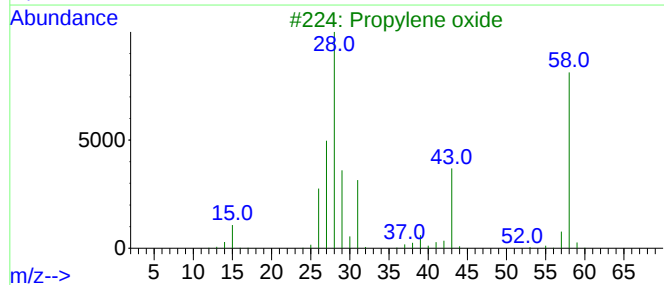
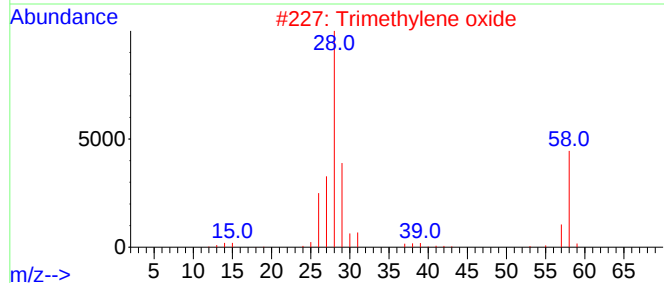
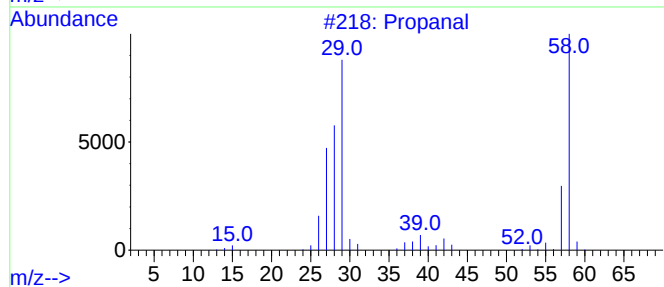
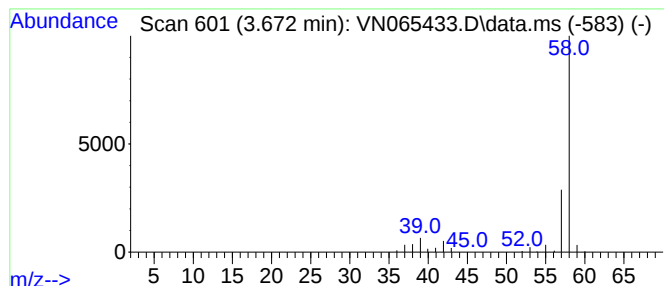
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 2 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.672	21.42 ug/l	343662	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	9
3			Propylene oxide	58	C3H6O	000075-56-9	5
4			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	4
5			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	4



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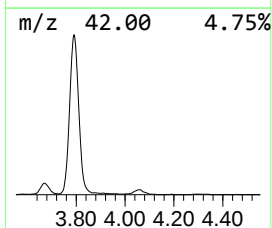
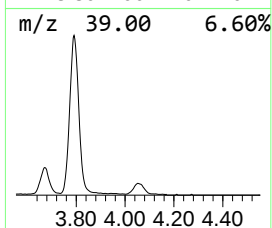
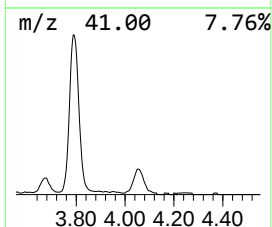
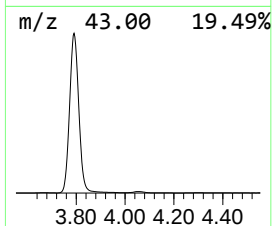
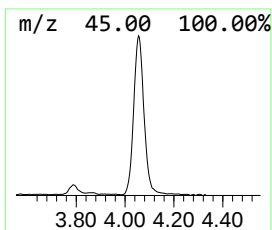
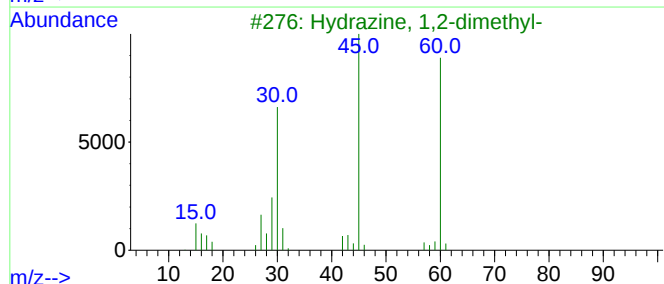
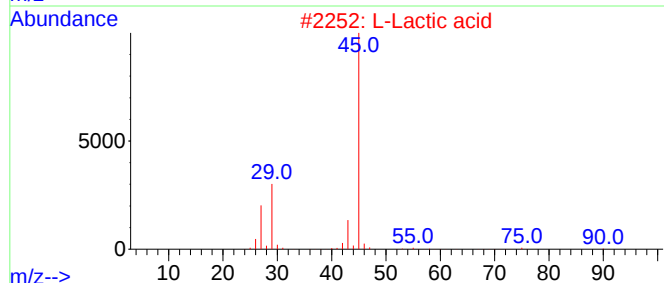
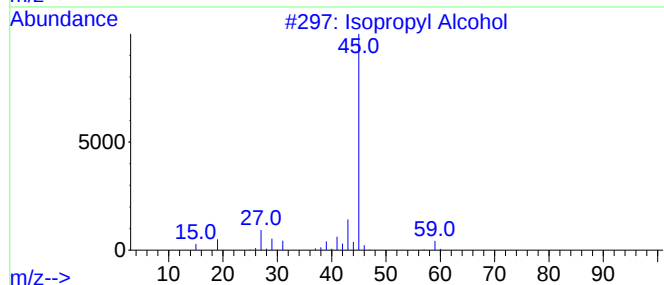
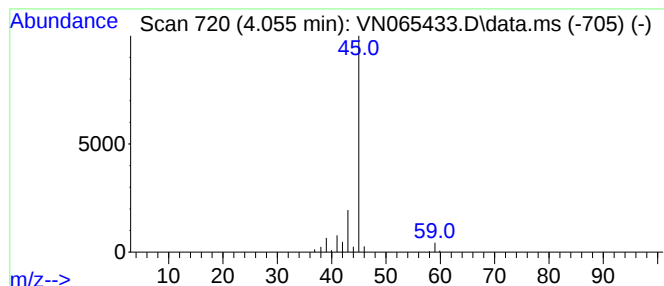
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.055	9.63 ug/l	154501	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2			L-Lactic acid	90	C3H6O3	000079-33-4	9
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			4-Penten-2-ol	86	C5H10O	000625-31-0	9
5			Formamide	45	CH3NO	000075-12-7	7



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ALS Vial : 20 Sample Multiplier: 1

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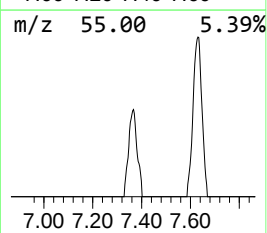
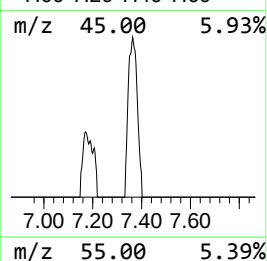
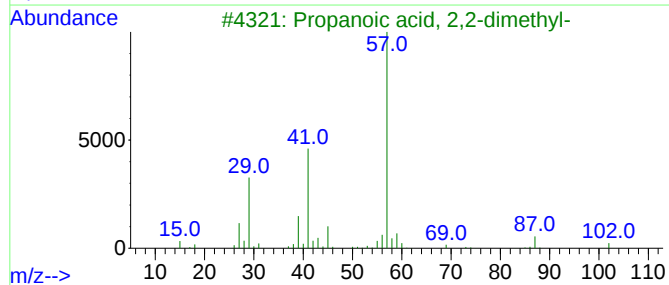
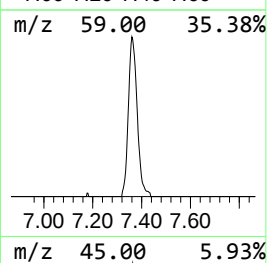
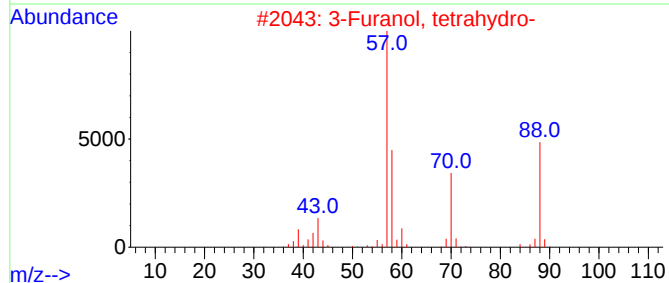
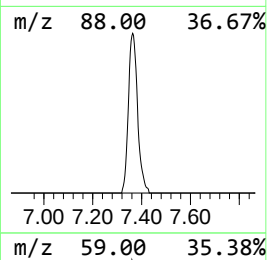
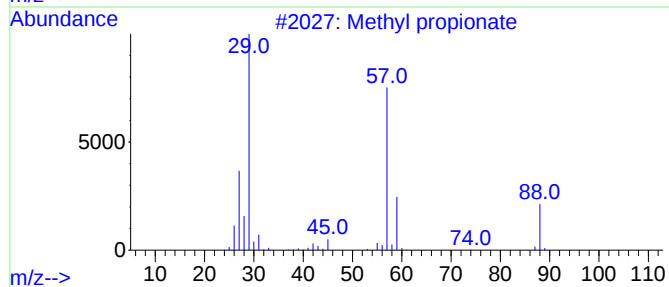
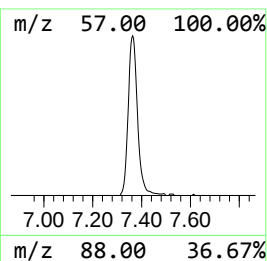
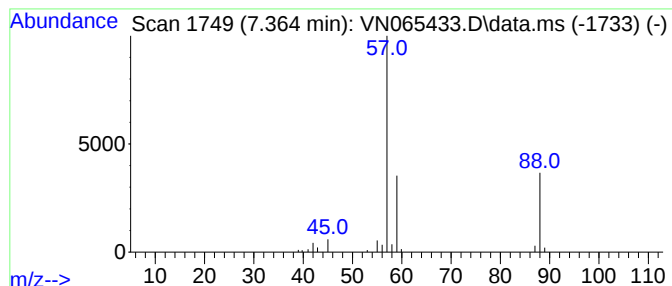
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Quant Title : SW846 8260

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

Peak Number 4 Methyl propionate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.364	6.67 ug/l	107001	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl propionate	88	C4H8O2	000554-12-1	90
2			3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	9
3			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9
4			Hydrazinecarboxylic acid, 1,1-di...	132	C5H12N2O2	000870-46-2	9
5			tert-Butyl isopropyl carbonate	160	C8H16O3	030221-21-7	9



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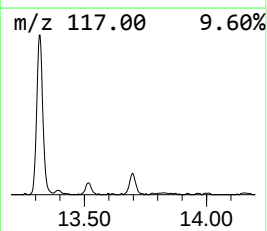
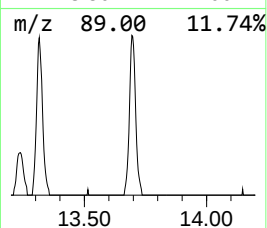
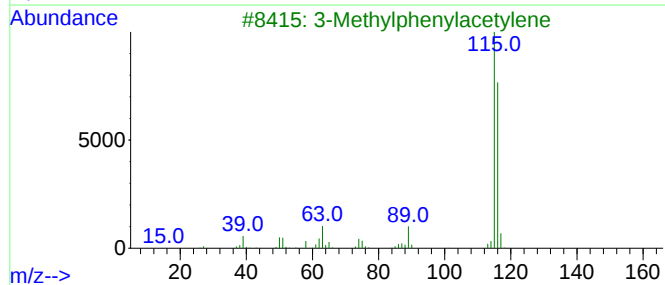
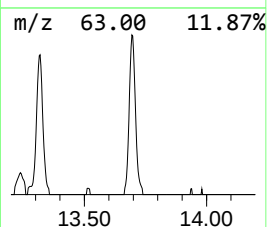
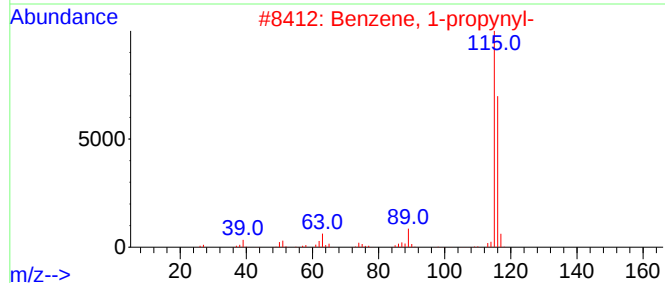
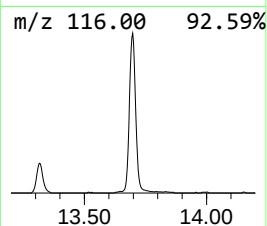
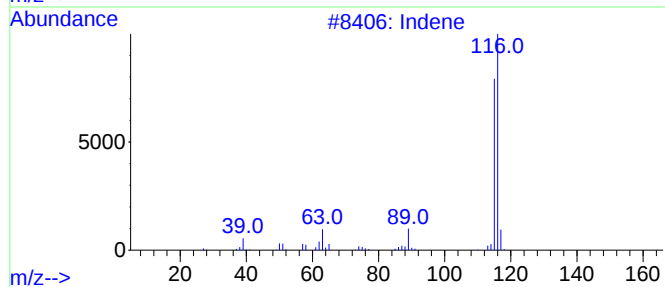
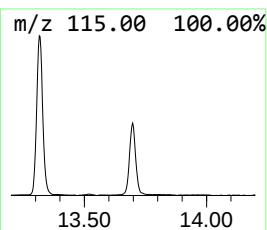
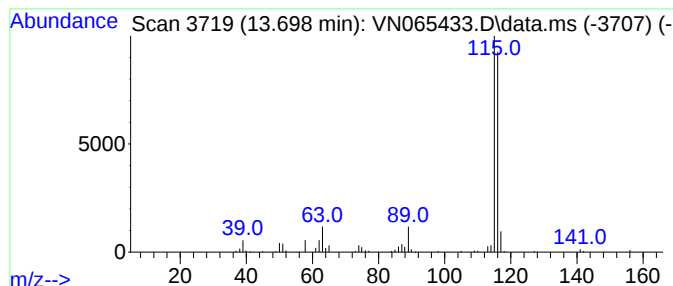
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Quant Title : SW846 8260

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

Peak Number 6 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.698	6.73 ug/l	196131	1,4-Dichlorobenzene-d4	13.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	95
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	94
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	90



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.306	75.8	ug/l	1215660	1	7.630	802233	50.0
Propanal	3.672	21.4	ug/l	343662	1	7.630	802233	50.0
Isopropyl Alcohol	4.055	9.6	ug/l	154501	1	7.630	802233	50.0
Methyl propionate	7.364	6.7	ug/l	107001	1	7.630	802233	50.0
Indene	13.698	6.7	ug/l	196131	4	13.318	1456410	50.0