

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
 Data File : VN065430.D
 Acq On : 7 Jan 2021 16:30
 Operator : JC/MD
 Sample : M1022-15
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41095

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: VN065430.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.248	146	158	223	rBV4	13830890	85031681	100.00%	49.327%
2	2.473	224	228	331	rVB	270397	1518406	1.79%	0.881%
3	3.306	450	487	557	rBV	8288626	36263558	42.65%	21.037%
4	3.663	582	598	619	rBV	405111	1040031	1.22%	0.603%
5	3.788	621	637	650	rBV	380745	991265	1.17%	0.575%
6	4.775	922	944	980	rVB	263421	937384	1.10%	0.544%
7	6.502	1457	1481	1503	rBV	2357602	7150109	8.41%	4.148%
8	6.798	1555	1573	1593	rBV	1216649	3476415	4.09%	2.017%
9	7.627	1818	1831	1858	rVB	383281	931749	1.10%	0.541%
10	7.798	1866	1884	1918	rBV	804235	1922118	2.26%	1.115%
11	7.991	1926	1944	1970	rBV3	392396	1005540	1.18%	0.583%
12	8.412	2060	2075	2104	rBV2	465651	1214665	1.43%	0.705%
13	8.550	2105	2118	2140	rVB	652305	1429069	1.68%	0.829%
14	8.766	2168	2185	2212	rBV	1619954	3408830	4.01%	1.977%
15	10.058	2572	2587	2601	rBV	1014013	2021935	2.38%	1.173%
16	10.846	2804	2832	2850	rBV4	392129	1132167	1.33%	0.657%
17	11.380	2986	2998	3020	rVB	1293212	2268555	2.67%	1.316%
18	11.518	3021	3041	3051	rBV	1452036	2601338	3.06%	1.509%
19	11.788	3115	3125	3156	rVB	1473904	2547175	3.00%	1.478%
20	12.373	3296	3307	3330	rVB2	909276	1575495	1.85%	0.914%
21	13.077	3519	3526	3547	rVV	534122	974172	1.15%	0.565%
22	13.315	3589	3600	3619	rBV	937074	1608730	1.89%	0.933%
23	13.421	3622	3633	3650	rBV	3594067	5558750	6.54%	3.225%
24	13.695	3709	3718	3730	rVB	532565	869346	1.02%	0.504%
25	15.100	4140	4155	4168	rBV	1327013	2870849	3.38%	1.665%
26	16.193	4484	4495	4517	rVB	1072905	2033687	2.39%	1.180%

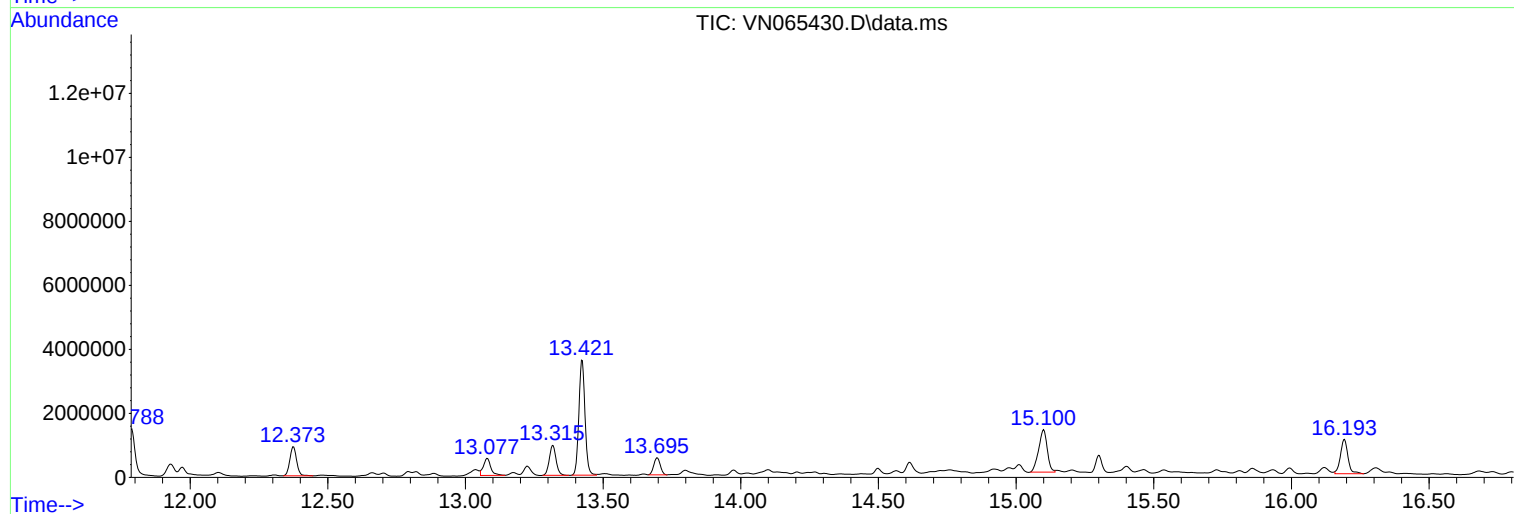
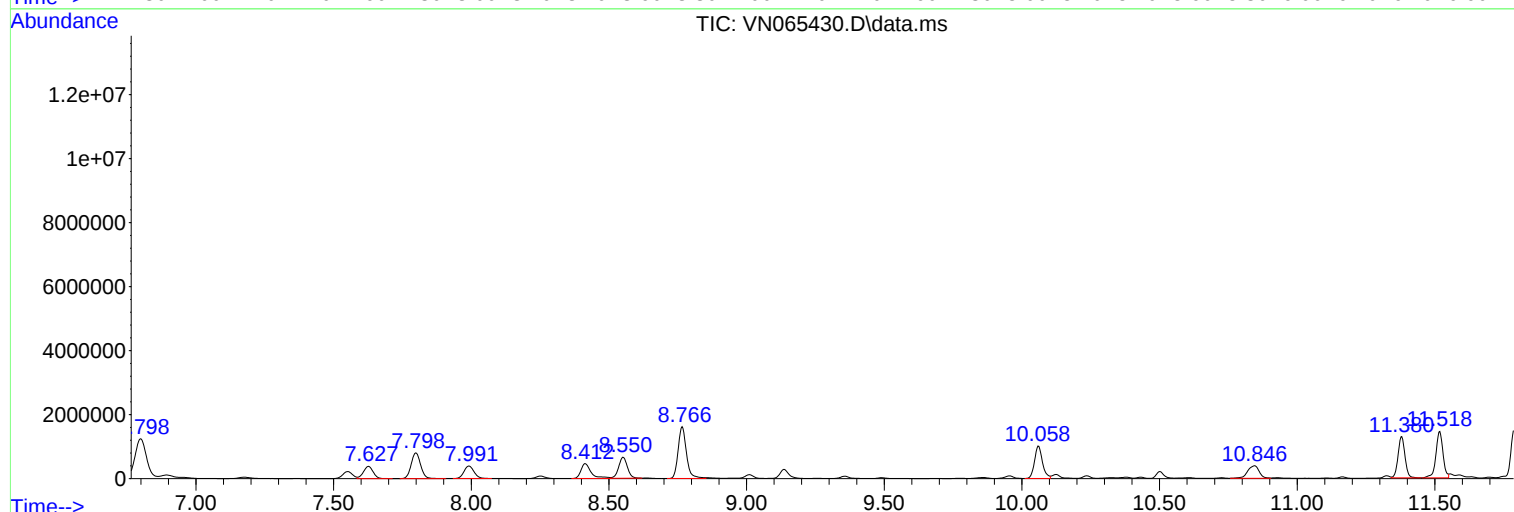
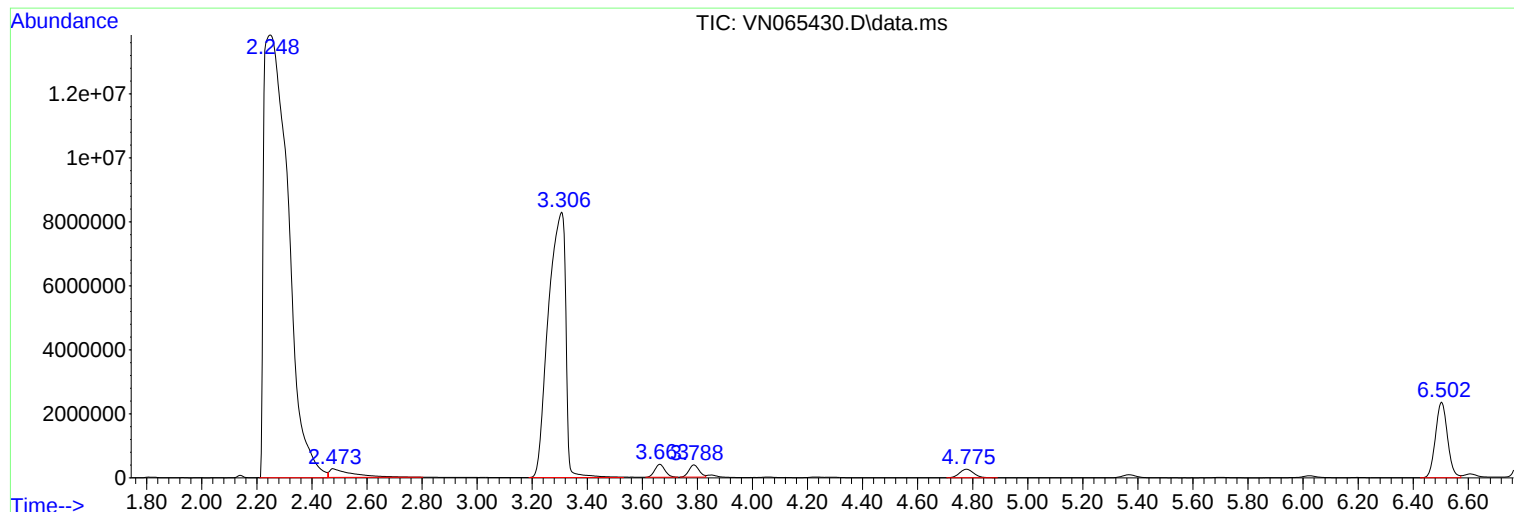
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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



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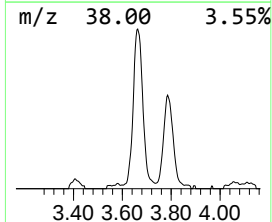
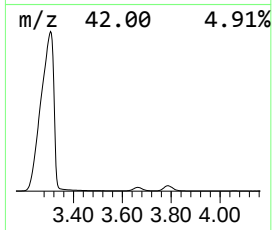
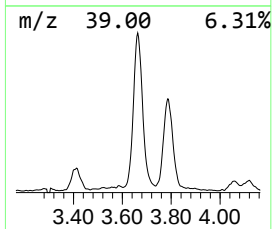
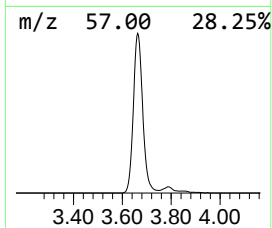
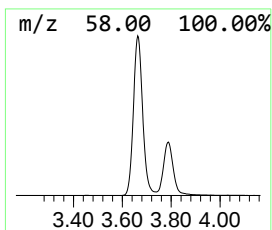
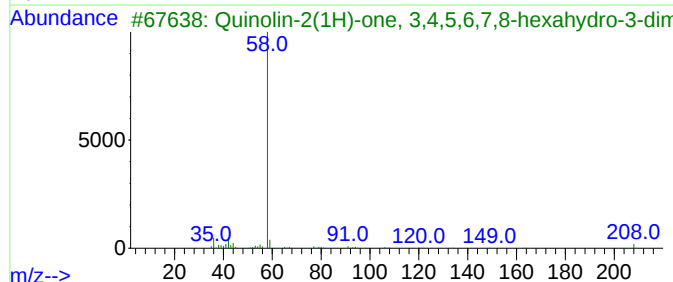
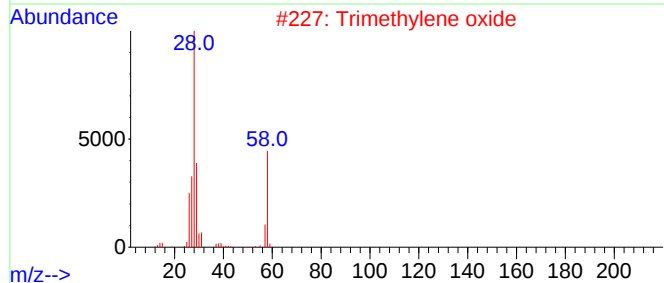
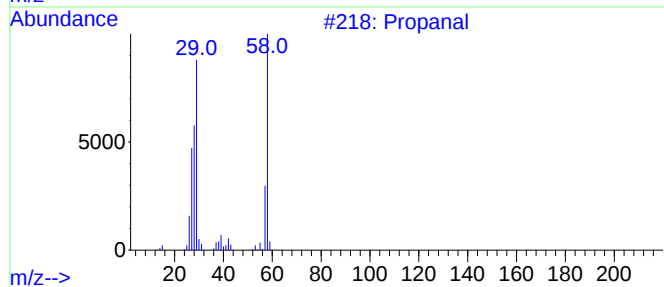
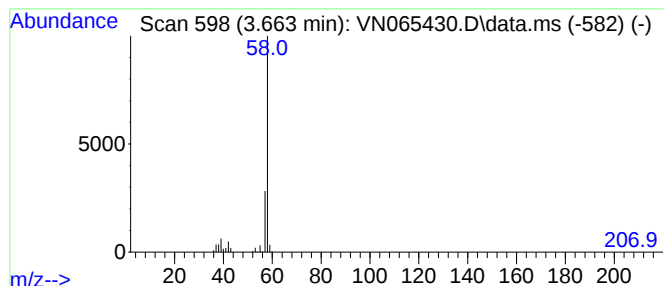
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 4 Propanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.663	55.81 ug/l	1040030	Pentafluorobenzene	7.627

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	56
3			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4			Propylene oxide	58	C3H6O	000075-56-9	7
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	4



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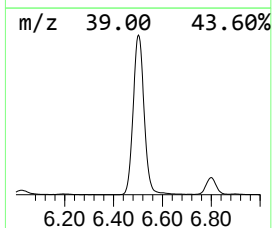
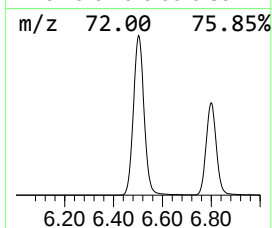
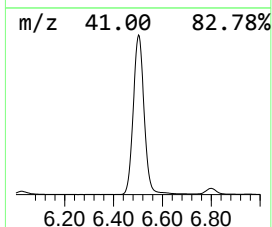
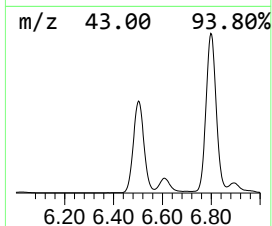
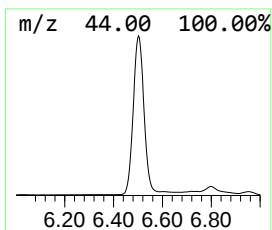
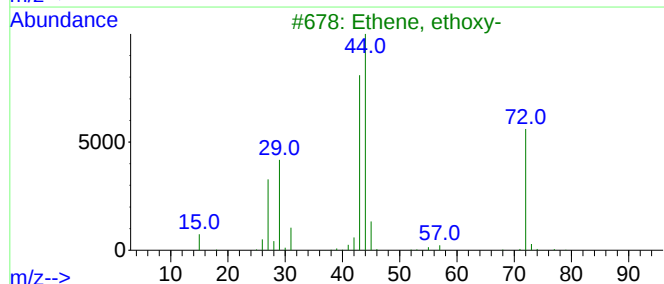
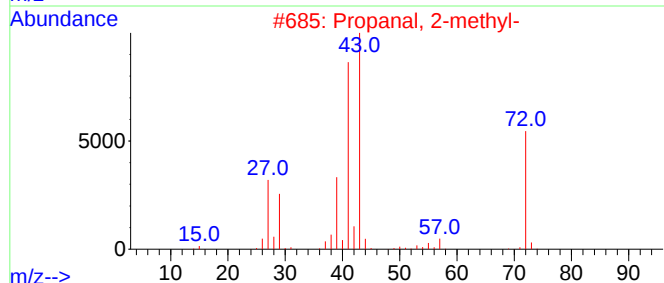
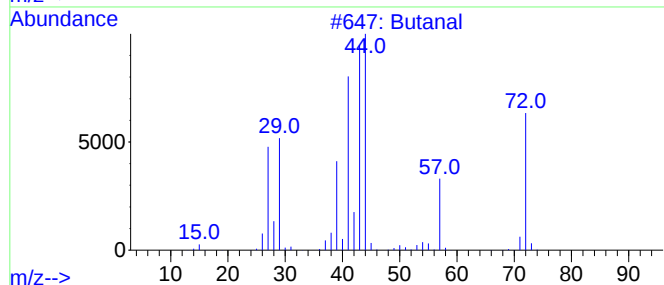
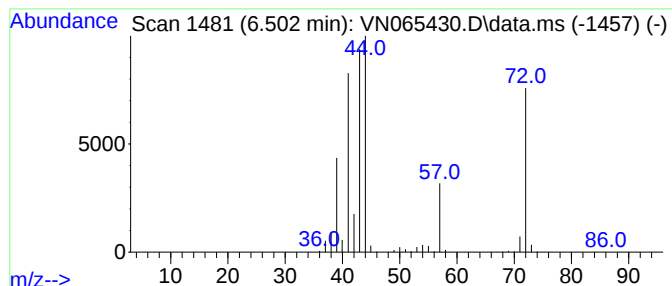
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 5 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.502	383.69 ug/l	7150110	Pentafluorobenzene	7.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	58
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	52
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5			Isobutylene epoxide	72	C4H8O	000558-30-5	35



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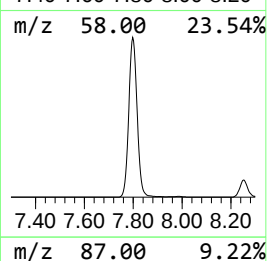
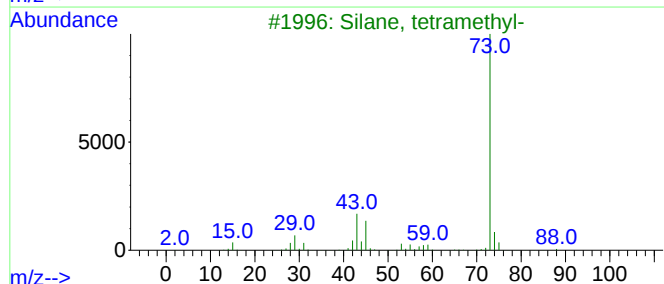
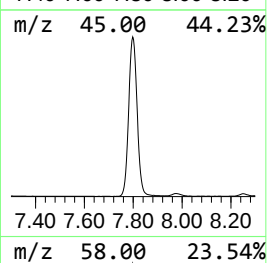
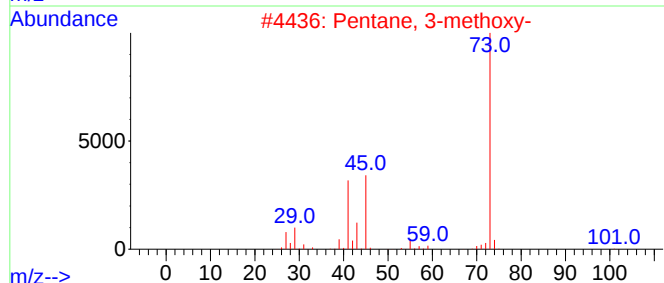
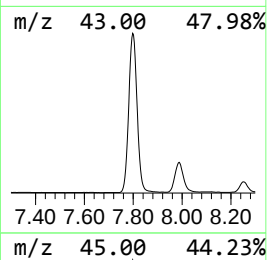
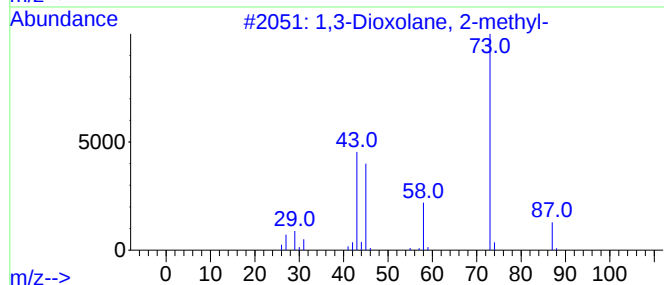
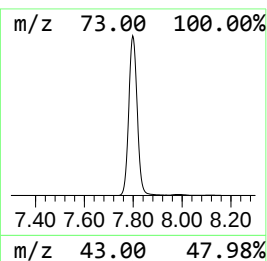
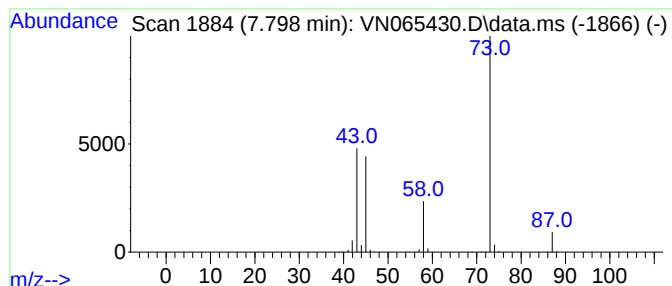
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 6 1,3-Dioxolane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.798	103.15 ug/l	1922120	Pentafluorobenzene	7.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
5			1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9



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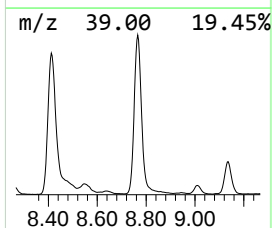
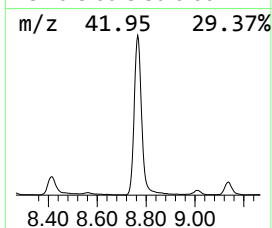
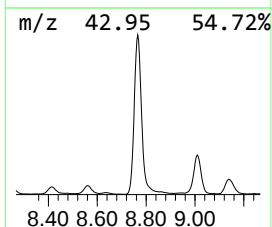
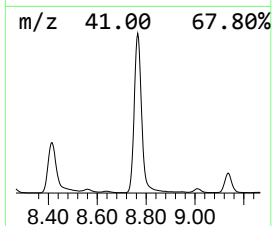
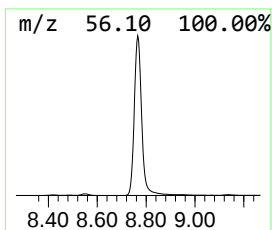
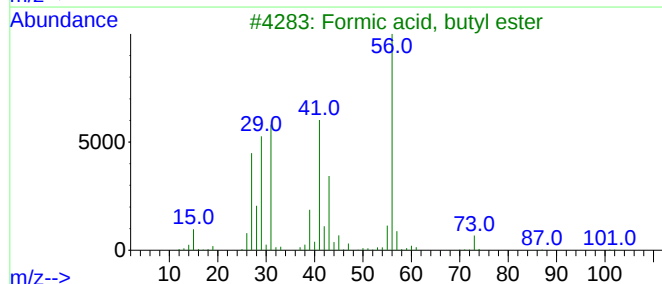
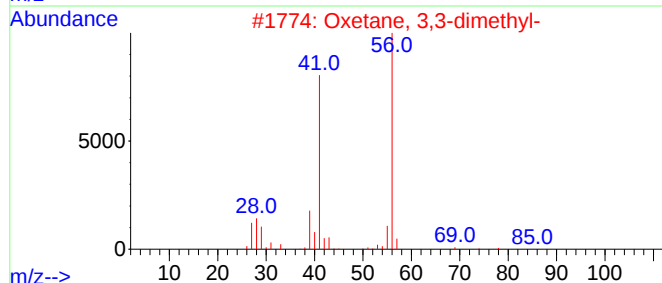
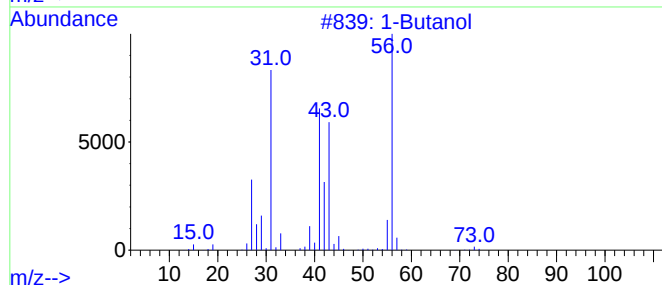
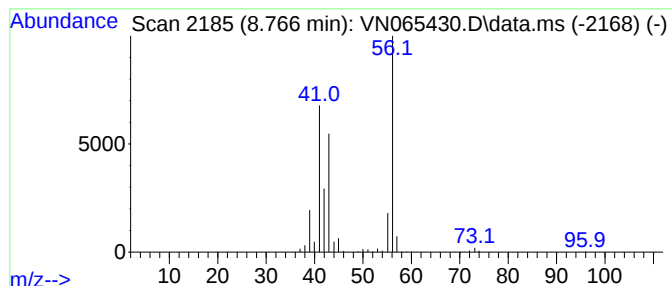
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.766	119.27 ug/l	3408830	1,4-Difluorobenzene	8.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9
3			Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
4			3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
5			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	9



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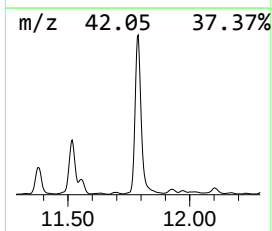
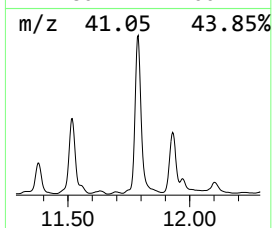
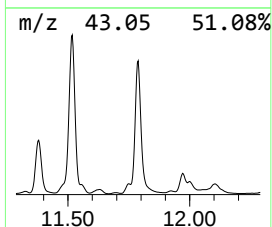
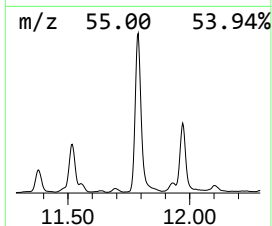
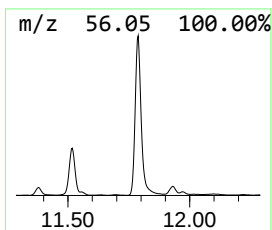
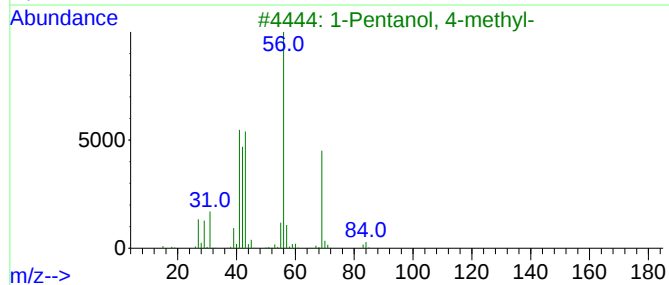
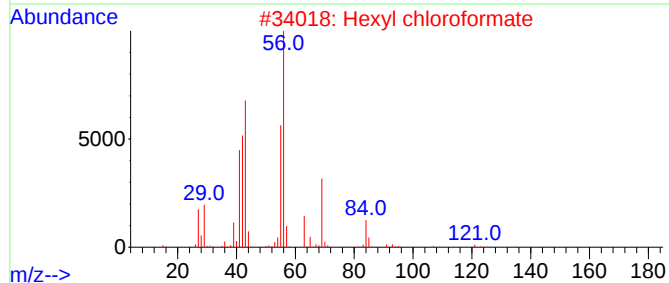
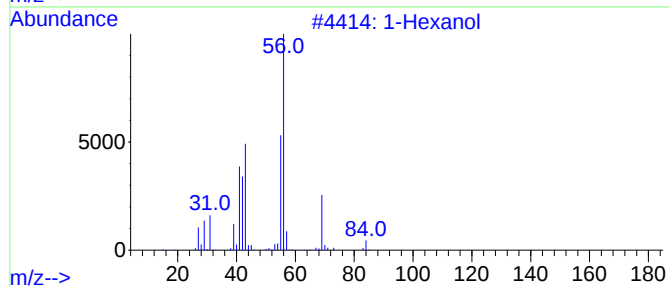
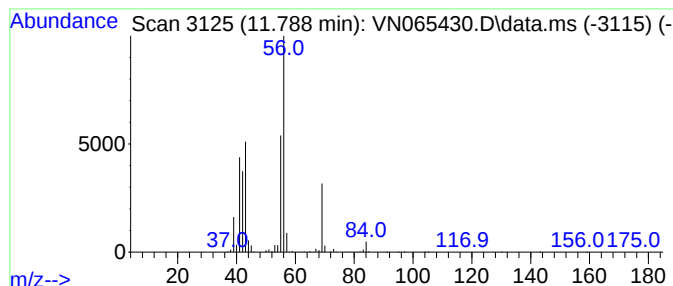
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Quant Title : SW846 8260

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

Peak Number 8 1-Hexanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.788	56.14 ug/l	2547180	Chlorobenzene-d5	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol	102	C6H14O	000111-27-3	83
2			Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
3			1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	72
4			Cyclopropane, propyl-	84	C6H12	002415-72-7	72
5			Formic acid, hexyl ester	130	C7H14O2	000629-33-4	64



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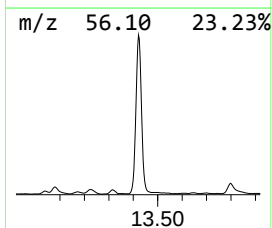
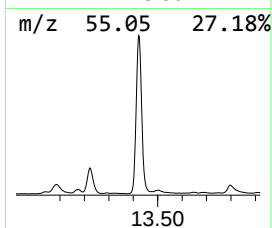
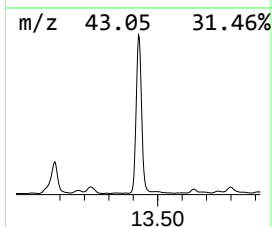
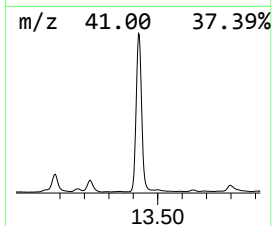
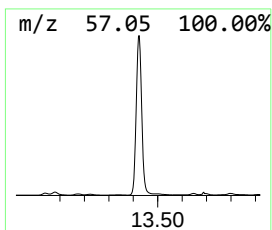
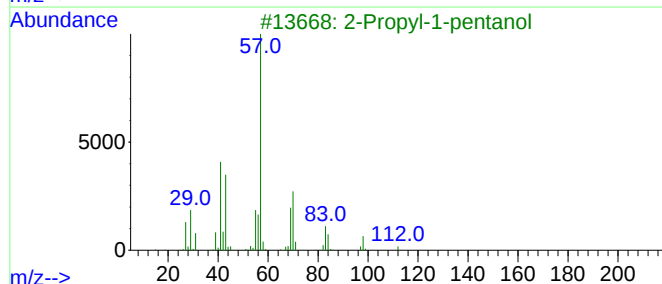
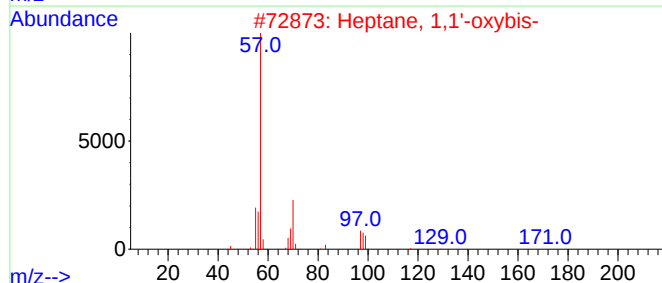
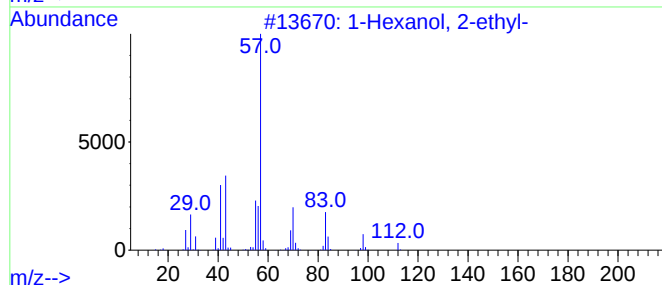
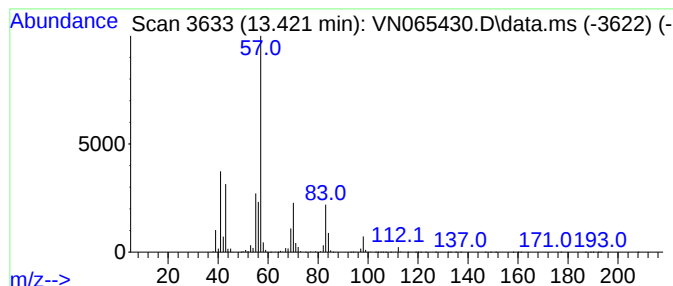
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Quant Title : SW846 8260

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.421	172.77 ug/l	5558750	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50
5			3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065430.D
Acq On : 7 Jan 2021 16:30
Operator : JC/MD
Sample : M1022-15
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41095

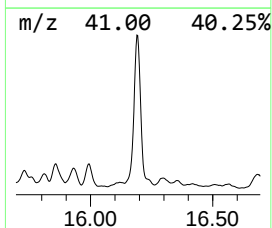
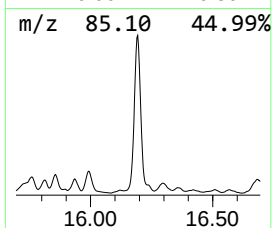
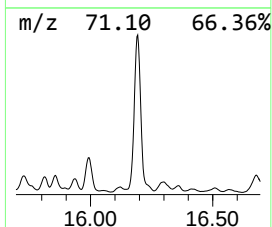
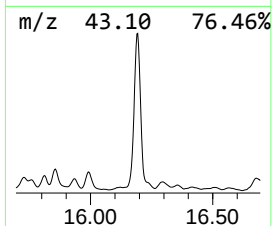
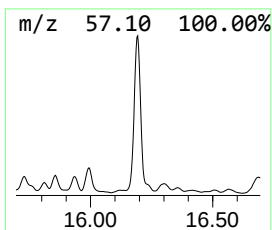
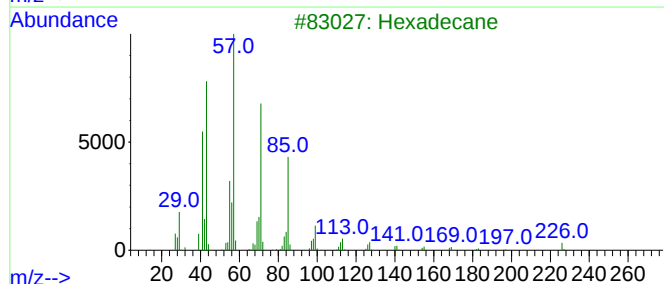
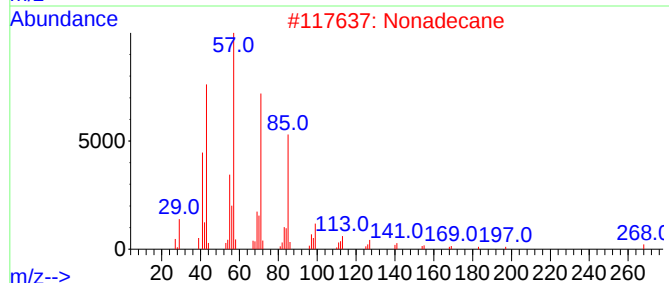
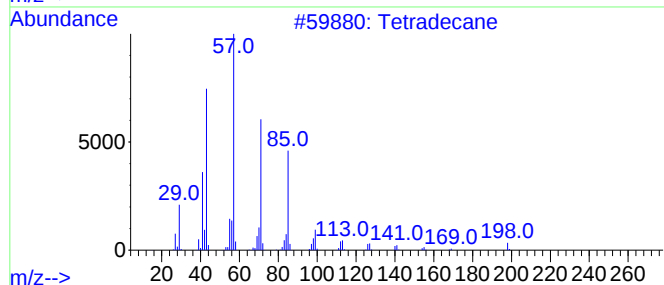
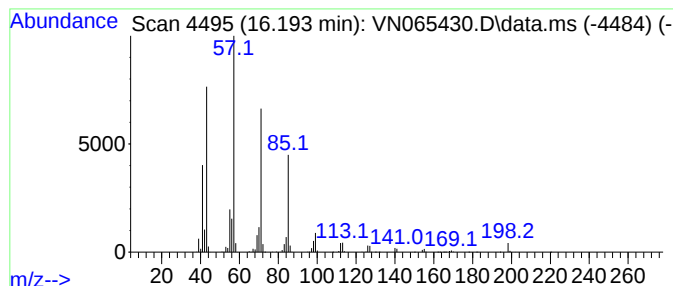
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Quant Title : SW846 8260

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

Peak Number 10 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.193	63.21 ug/l	2033690	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	97
2			Nonadecane	268	C19H40	000629-92-5	91
3			Hexadecane	226	C16H34	000544-76-3	90
4			Pentadecane	212	C15H32	000629-62-9	86
5			Dodecane	170	C12H26	000112-40-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065430.D
Acq On : 7 Jan 2021 16:30
Operator : JC/MD
Sample : M1022-15
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41095

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	3.663	55.8	ug/l	1040030	1	7.627	931749	50.0
Butanal	6.502	383.7	ug/l	7150110	1	7.627	931749	50.0
1,3-Dioxolane, ...	7.798	103.2	ug/l	1922120	1	7.627	931749	50.0
1-Butanol	8.766	119.3	ug/l	3408830	2	8.550	1429070	50.0
1-Hexanol	11.788	56.1	ug/l	2547180	3	11.380	2268560	50.0
1-Hexanol, 2-et...	13.421	172.8	ug/l	5558750	4	13.315	1608730	50.0
Tetradecane	16.193	63.2	ug/l	2033690	4	13.315	1608730	50.0