

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071124\
 Data File : VN082881.D
 Acq On : 11 Jul 2024 17:09
 Operator : JC\MD
 Sample : P3206-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 626-A

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\82N070824W.M
 Title : SW846 8260

Signal : TIC: VN082881.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.660	112	120	134	rBV	1088820	1960746	16.03%	4.740%
2	3.795	304	313	330	rBV	60687	160571	1.31%	0.388%
3	4.289	385	397	413	rBV	2331510	6663196	54.49%	16.107%
4	4.430	413	421	434	rVB2	85341	270514	2.21%	0.654%
5	6.736	799	813	834	rBV	725298	2163459	17.69%	5.230%
6	7.306	901	910	924	rVB	77340	207664	1.70%	0.502%
7	8.171	1046	1057	1061	rBV	97421	232854	1.90%	0.563%
8	8.224	1061	1066	1078	rVB	165982	366385	3.00%	0.886%
9	8.583	1112	1127	1138	rBV	102117	248884	2.04%	0.602%
10	9.106	1206	1216	1237	rBV	1588227	3172572	25.94%	7.669%
11	9.341	1248	1256	1265	rBV	822039	1590228	13.00%	3.844%
12	10.571	1457	1465	1472	rBV	389708	725651	5.93%	1.754%
13	10.806	1495	1505	1521	rBV	7203959	12228366	100.00%	29.560%
14	10.947	1521	1529	1545	rVB	4643004	7681787	62.82%	18.569%
15	11.212	1564	1574	1595	rBV	709158	1763201	14.42%	4.262%
16	11.865	1675	1685	1695	rVB	413402	737734	6.03%	1.783%
17	12.847	1846	1852	1860	rVB	300824	523812	4.28%	1.266%
18	13.794	2005	2013	2020	rBV	394220	670769	5.49%	1.621%

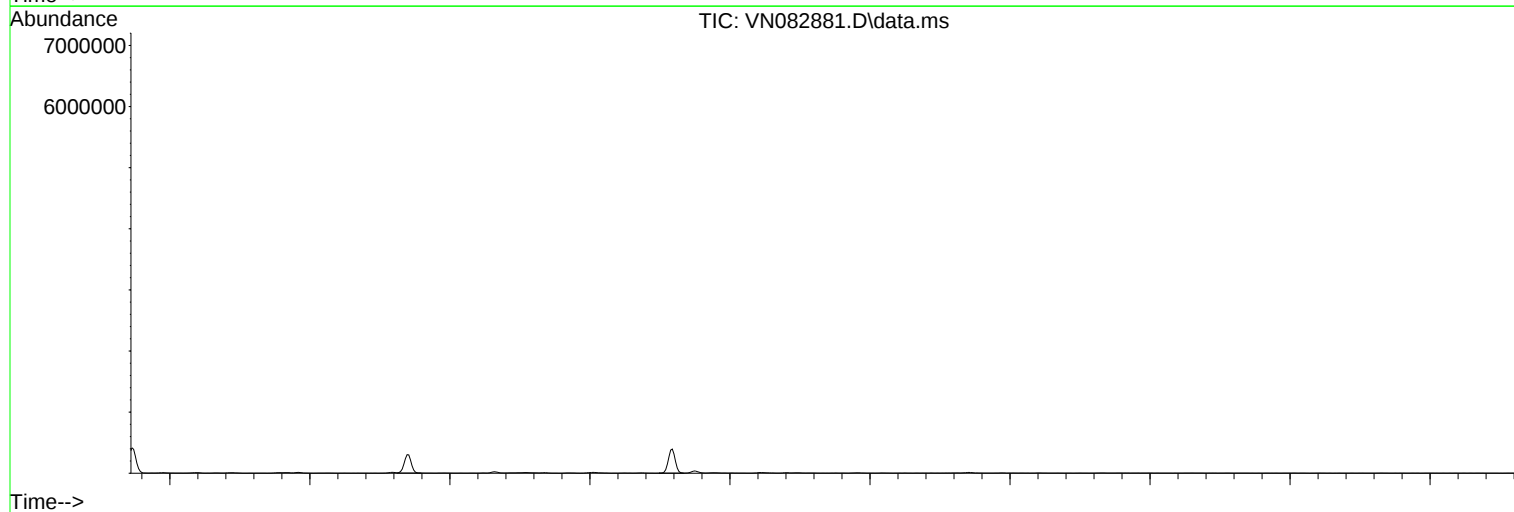
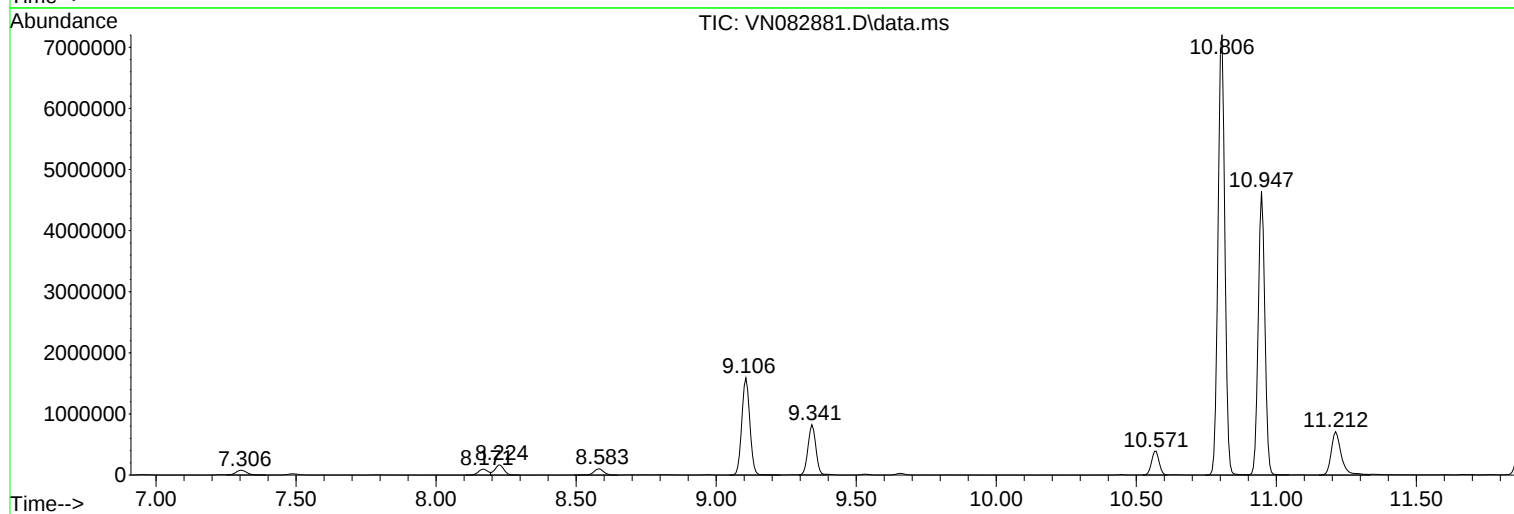
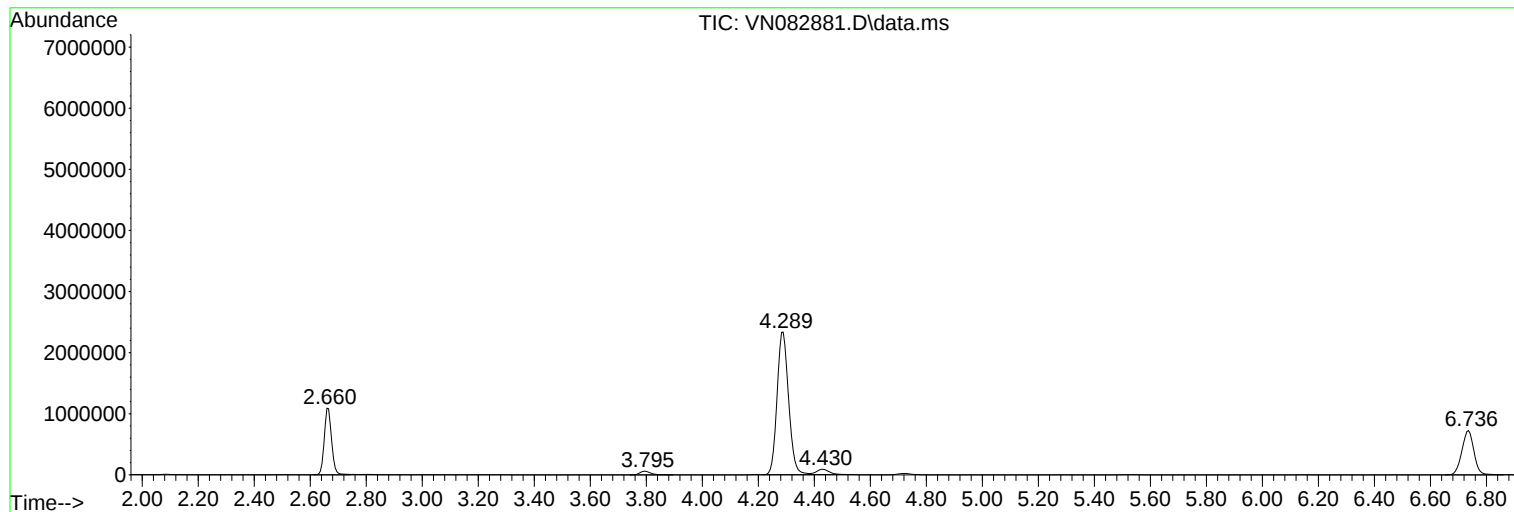
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

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



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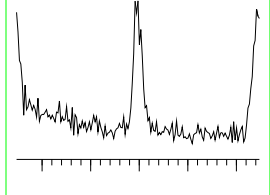
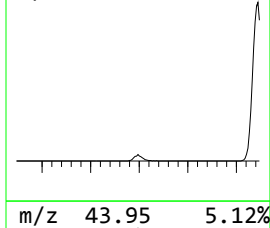
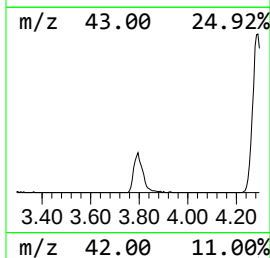
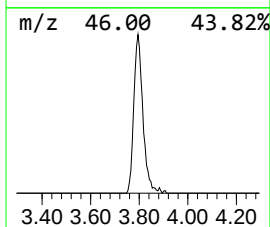
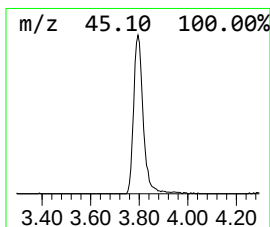
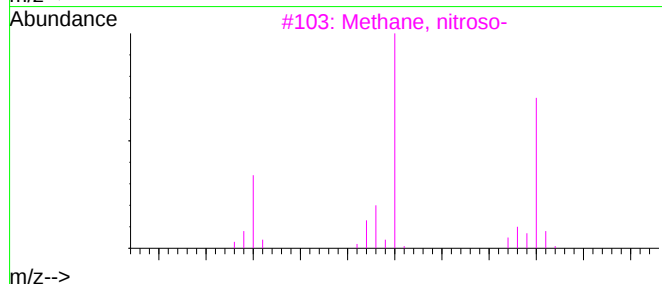
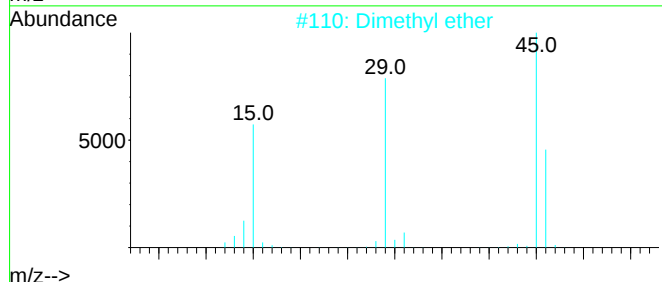
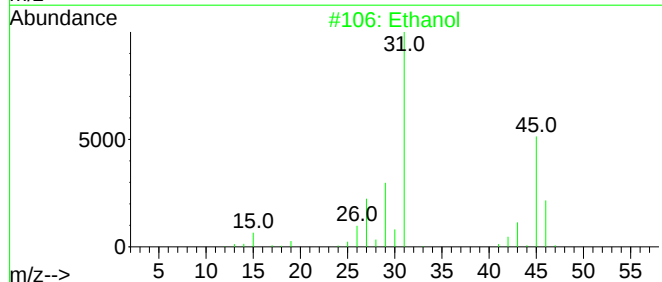
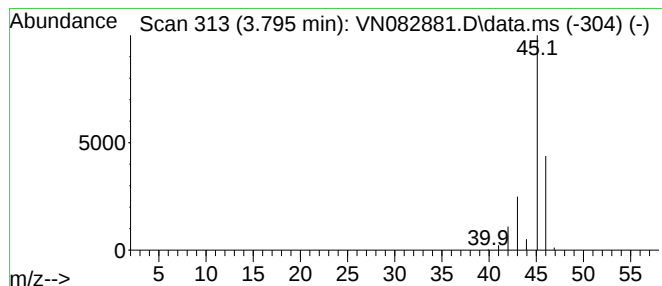
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.795	21.91 ug/l	160571	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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626-A

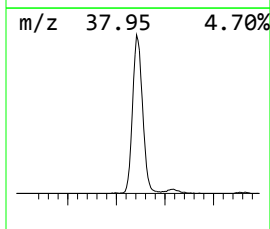
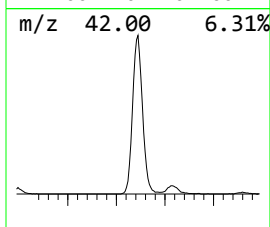
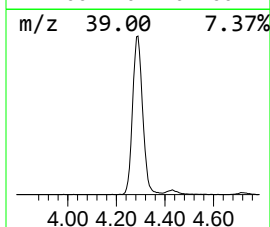
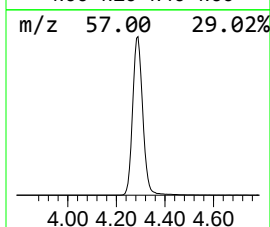
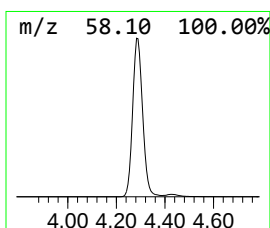
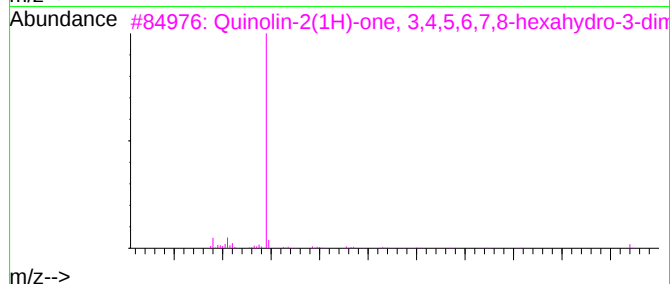
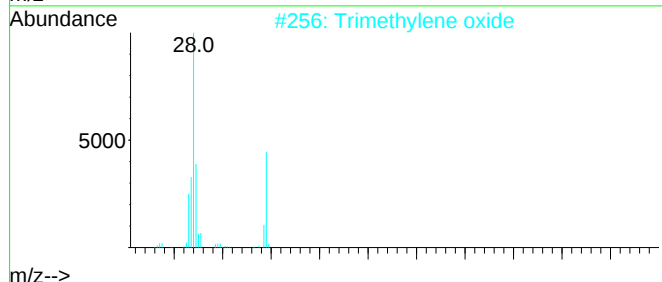
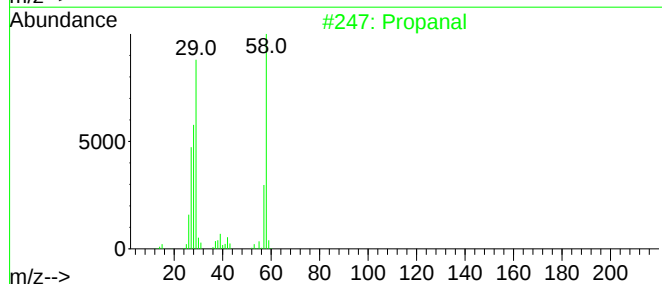
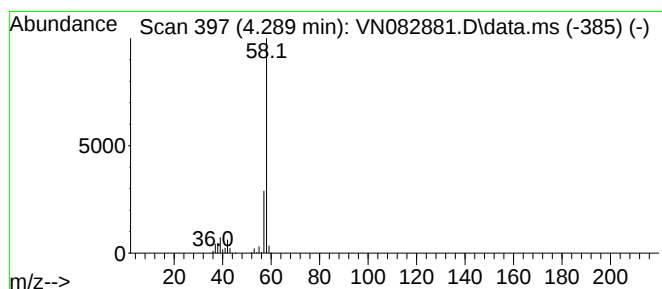
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.289	909.32 ug/l	6663200	Pentafluorobenzene	8.224

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	2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9
5	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9



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ClientSampleId :
626-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

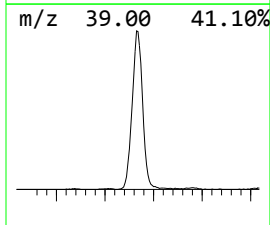
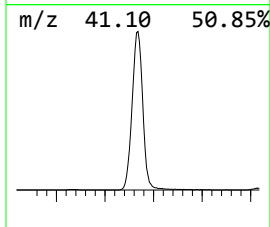
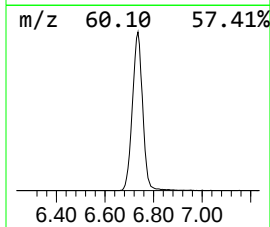
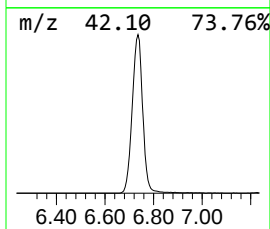
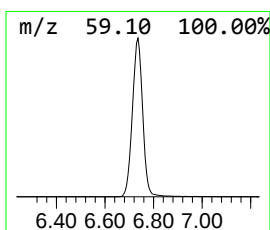
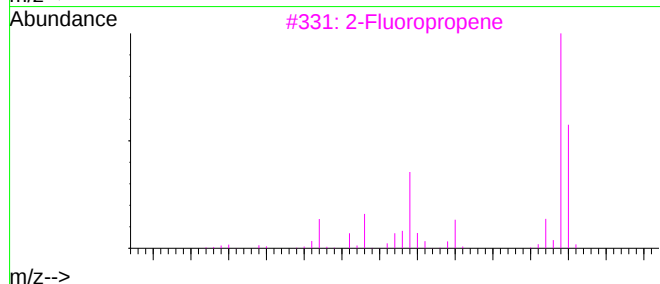
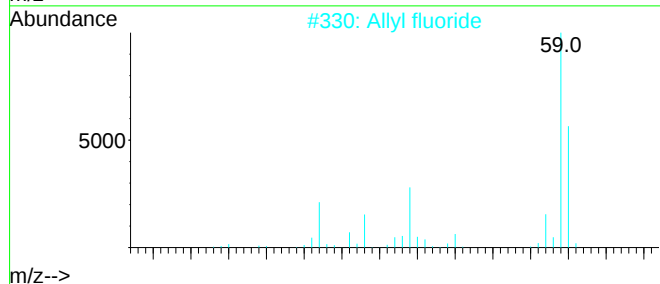
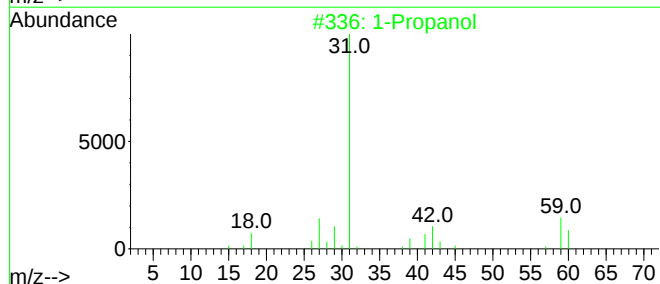
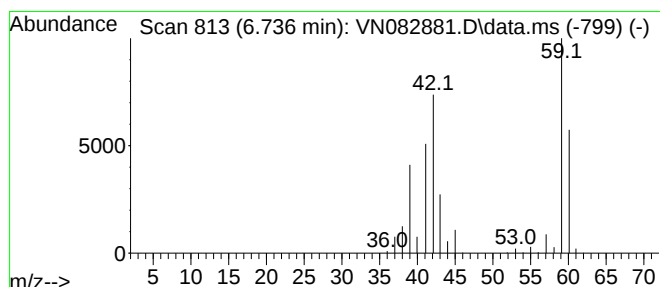
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.736	295.24 ug/l	2163460	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	59
2	Allyl fluoride	60	C3H5F	000818-92-8	38
3	2-Fluoropropene	60	C3H5F	001184-60-7	38
4	Propene	42	C3H6	000115-07-1	25
5	Cyclopropane	42	C3H6	000075-19-4	25



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Sample : P3206-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
626-A

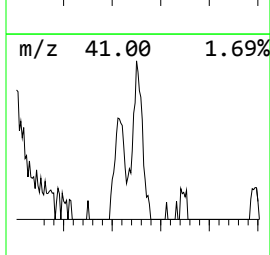
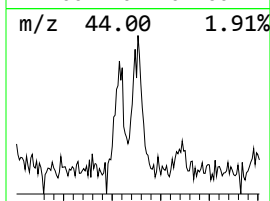
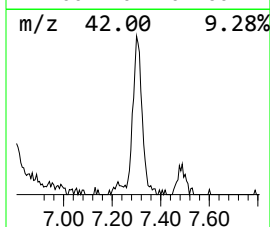
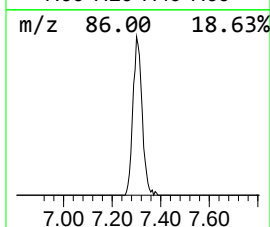
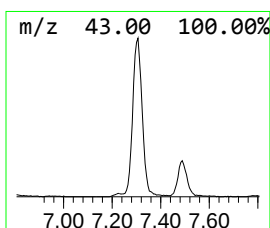
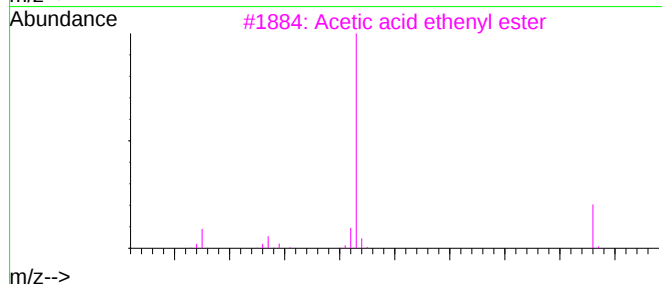
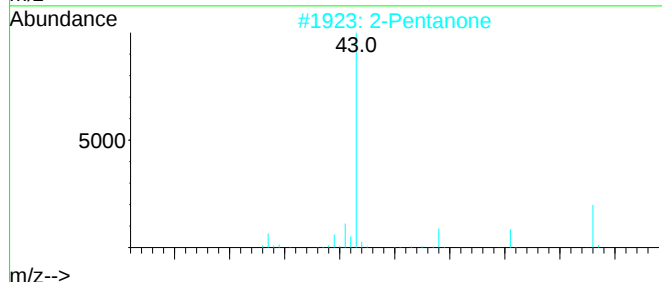
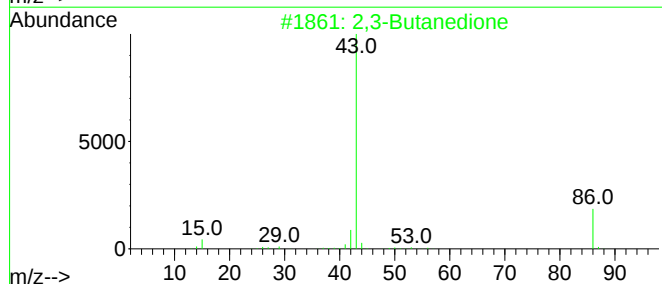
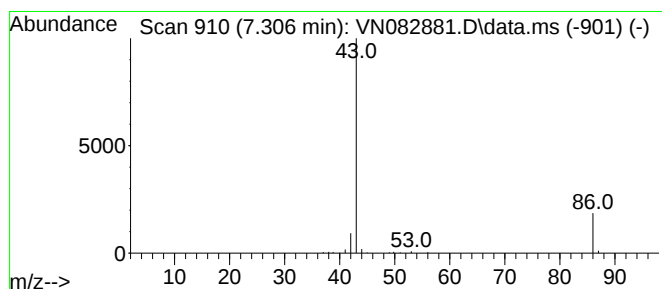
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

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

Peak Number 5 2,3-Butanedione Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.306	28.34 ug/l	207664	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,3-Butanedione	86	C4H6O2	000431-03-8	72
2			2-Pentanone	86	C5H10O	000107-87-9	50
3			Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	9
4			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	7
5			Propane, 2-(ethenyloxy)-	86	C5H10O	000926-65-8	5



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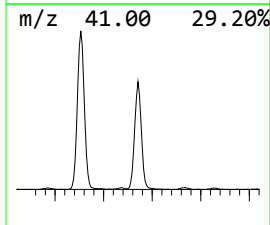
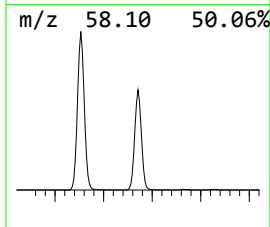
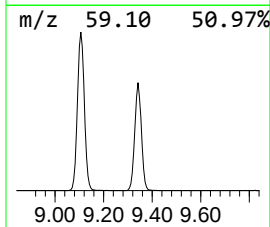
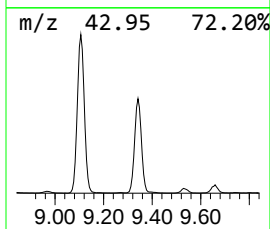
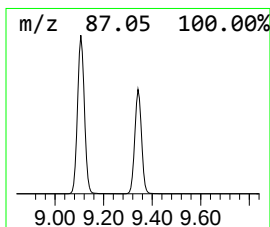
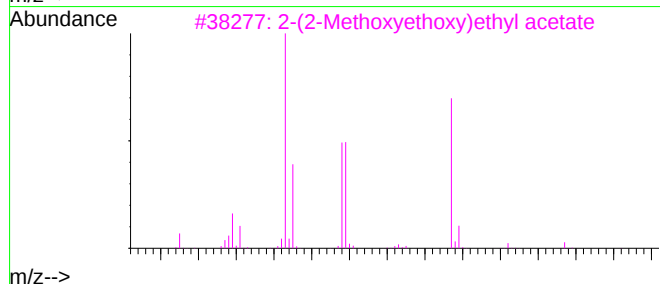
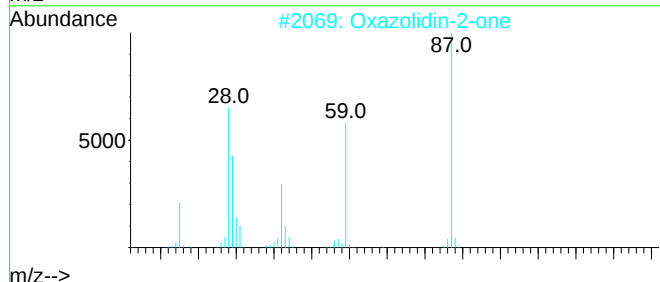
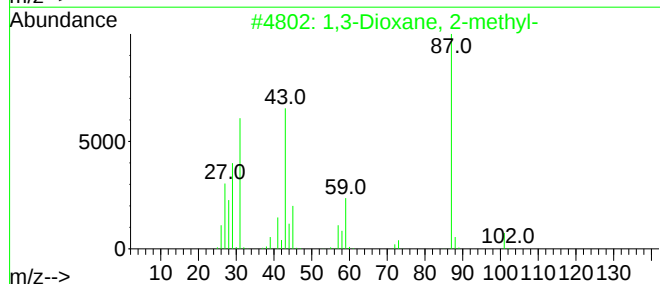
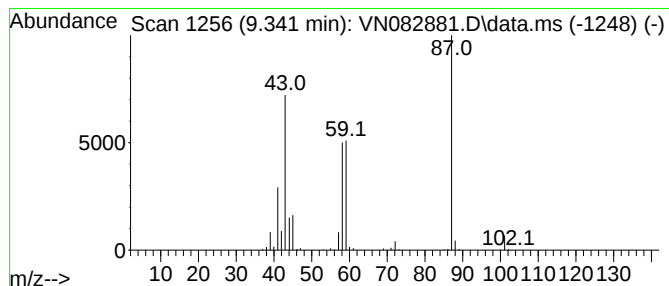
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 1,3-Dioxane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.341	25.06 ug/l	1590230	1,4-Difluorobenzene	9.100	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	52
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
3	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
4	Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	39
5	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	38



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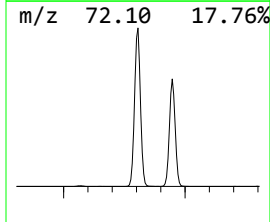
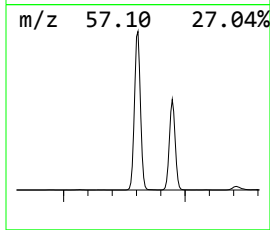
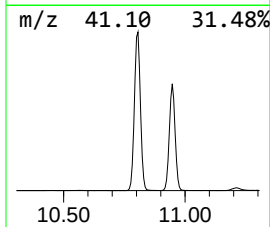
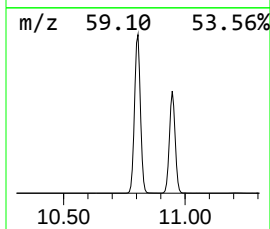
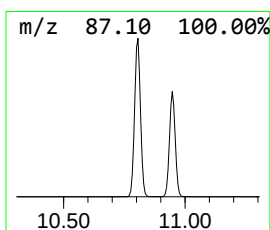
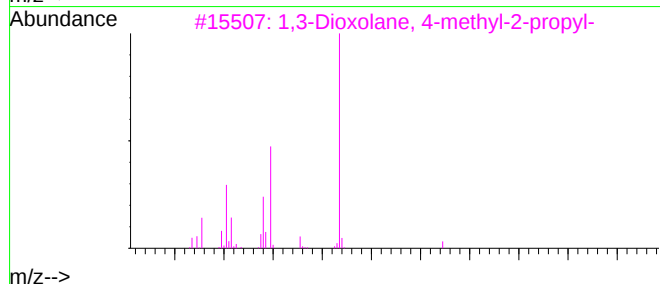
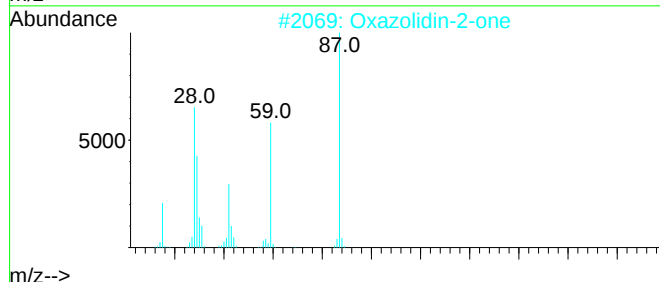
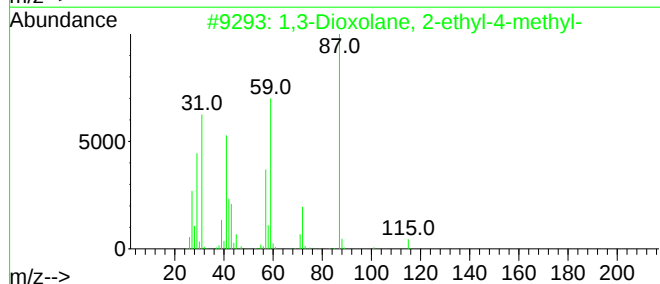
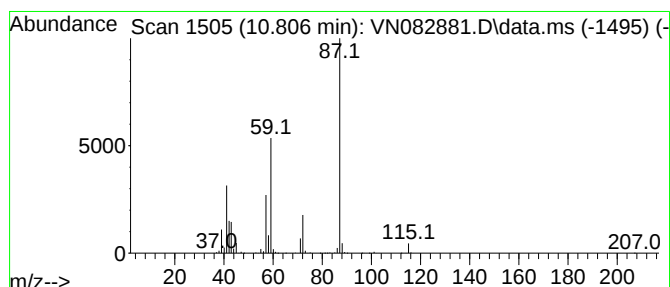
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MSVOA_N
ClientSampleId :
626-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

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

Peak Number 7 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.806	828.78 ug/l	12228400	Chlorobenzene-d5	11.865	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	72
3	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	72
4	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071124\
Data File : VN082881.D
Acq On : 11 Jul 2024 17:09
Operator : JC\MD
Sample : P3206-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
626-A

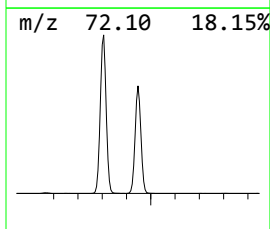
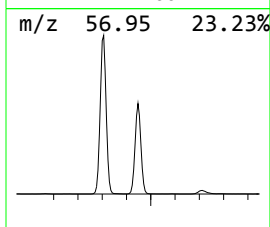
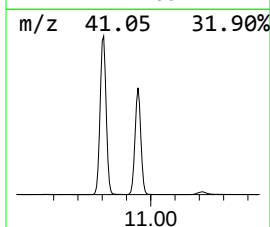
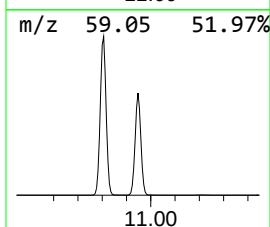
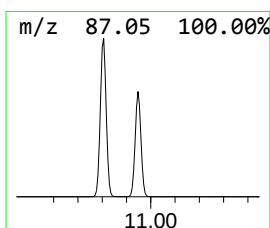
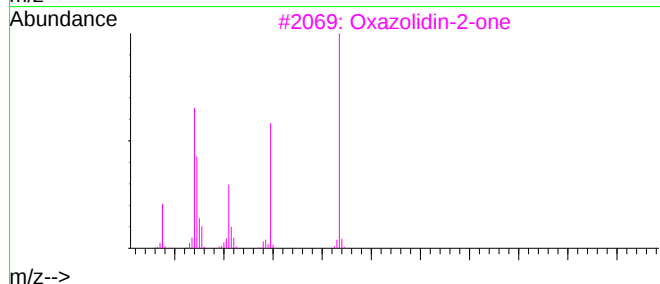
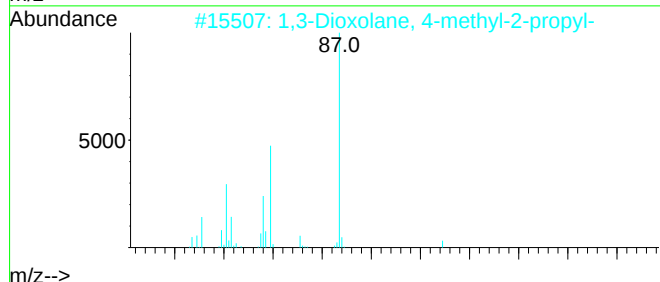
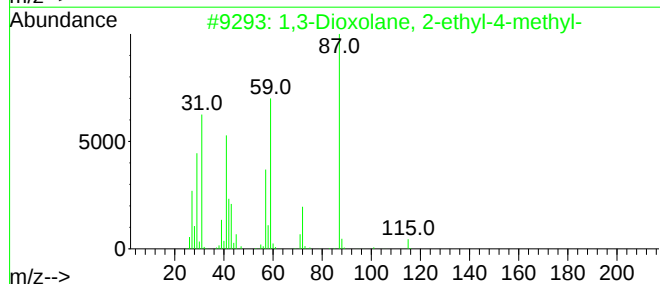
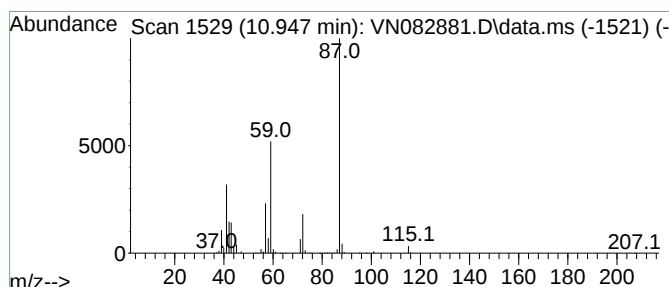
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Quant Title : SW846 8260

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

Peak Number 8 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	520.63 ug/l	7681790	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	72
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	56
4	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5	Ethanol, 2-[2-(2-methoxyethoxy)e...	206	C9H18O5	003610-27-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071124\
Data File : VN082881.D
Acq On : 11 Jul 2024 17:09
Operator : JC\MD
Sample : P3206-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
626-A

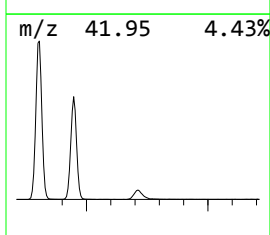
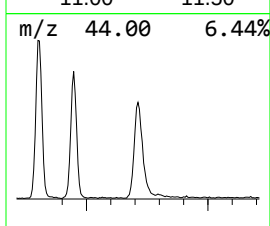
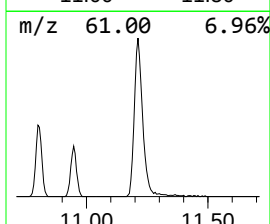
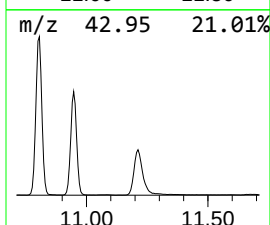
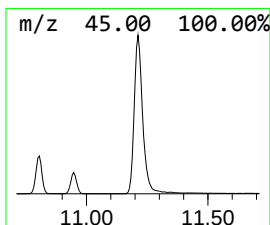
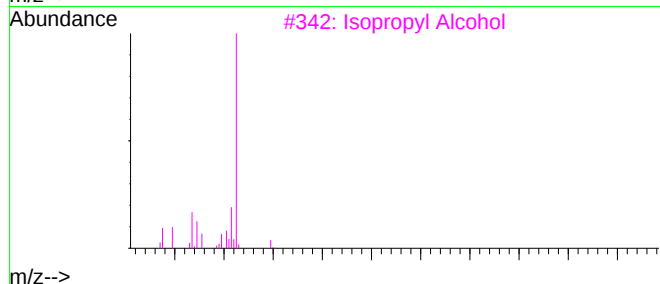
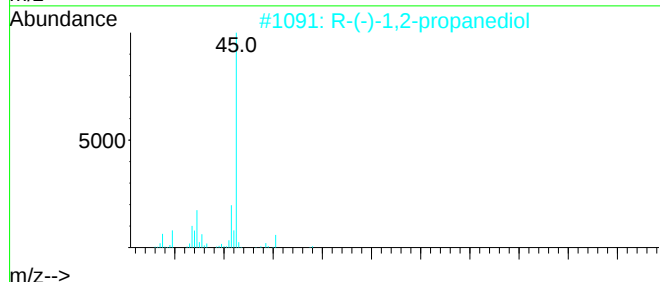
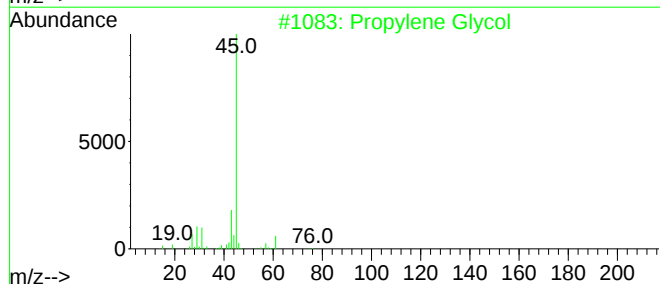
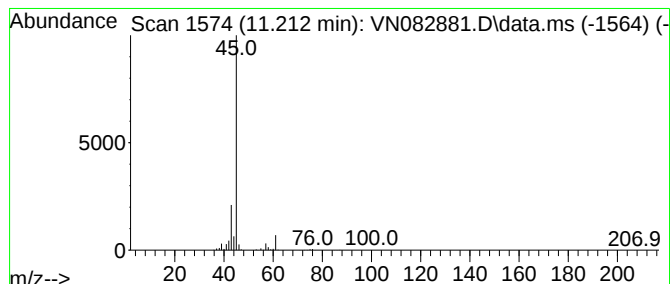
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Quant Title : SW846 8260

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

Peak Number 9 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.212	119.50 ug/l	1763200	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	2-Pentanol	88	C5H12O	006032-29-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071124\
Data File : VN082881.D
Acq On : 11 Jul 2024 17:09
Operator : JC\MD
Sample : P3206-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
626-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.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
Ethanol	3.795	21.9	ug/l	160571	1	8.224	366385	50.0
Propanal	4.289	909.3	ug/l	6663200	1	8.224	366385	50.0
1-Propanol	6.736	295.2	ug/l	2163460	1	8.224	366385	50.0
2,3-Butanedione	7.306	28.3	ug/l	207664	1	8.224	366385	50.0
1,3-Dioxane, 2-...	9.341	25.1	ug/l	1590230	2	9.100	3172570	50.0
1,3-Dioxolane, ...	10.806	828.8	ug/l	12228400	3	11.865	737734	50.0
1,3-Dioxolane, ...	10.947	520.6	ug/l	7681790	3	11.865	737734	50.0
Propylene Glycol	11.212	119.5	ug/l	1763200	3	11.865	737734	50.0