

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
 Data File : VX043380.D
 Acq On : 14 Oct 2024 14:53
 Operator : JC/MD
 Sample : P4402-03 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 3 - Tote

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_X\Method\82X100124W.M
 Title : SW846 8260

Signal : TIC: VX043380.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	67	rBV	349365	457491	16.89%	5.809%
2	1.520	67	71	81	rVB	24844	61057	2.25%	0.775%
3	2.111	161	168	174	rBV	14169	28502	1.05%	0.362%
4	2.392	204	214	229	rBV	159227	305278	11.27%	3.876%
5	4.568	562	571	595	rBV	16553	60564	2.24%	0.769%
6	5.379	693	704	720	rBV	57958	170701	6.30%	2.167%
7	5.538	720	730	751	rVB	94433	272551	10.06%	3.461%
8	5.946	788	797	816	rBV	69043	183143	6.76%	2.325%
9	6.751	921	929	939	rVV	156330	375970	13.88%	4.774%
10	6.867	939	948	973	rVB	1101762	2709265	100.00%	34.399%
11	7.202	995	1003	1030	rBV	488223	1105466	40.80%	14.036%
12	8.641	1233	1239	1257	rBV	295112	516095	19.05%	6.553%
13	8.994	1291	1297	1304	rBV	45931	69382	2.56%	0.881%
14	9.159	1318	1324	1333	rBV	20756	32626	1.20%	0.414%
15	10.049	1465	1470	1488	rBV	299764	428741	15.82%	5.444%
16	10.397	1520	1527	1539	rBV	21610	33718	1.24%	0.428%
17	11.079	1634	1639	1647	rBV	248740	324008	11.96%	4.114%
18	12.018	1788	1793	1802	rBV	300577	390232	14.40%	4.955%
19	12.219	1820	1826	1842	rBV	249704	351232	12.96%	4.460%

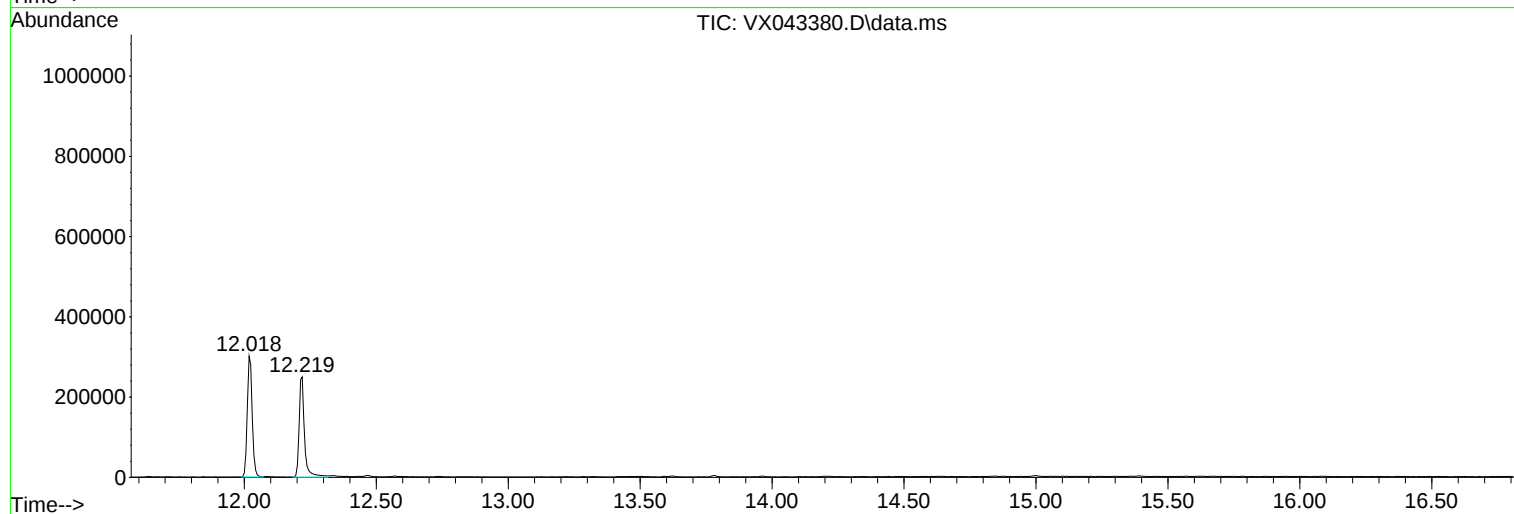
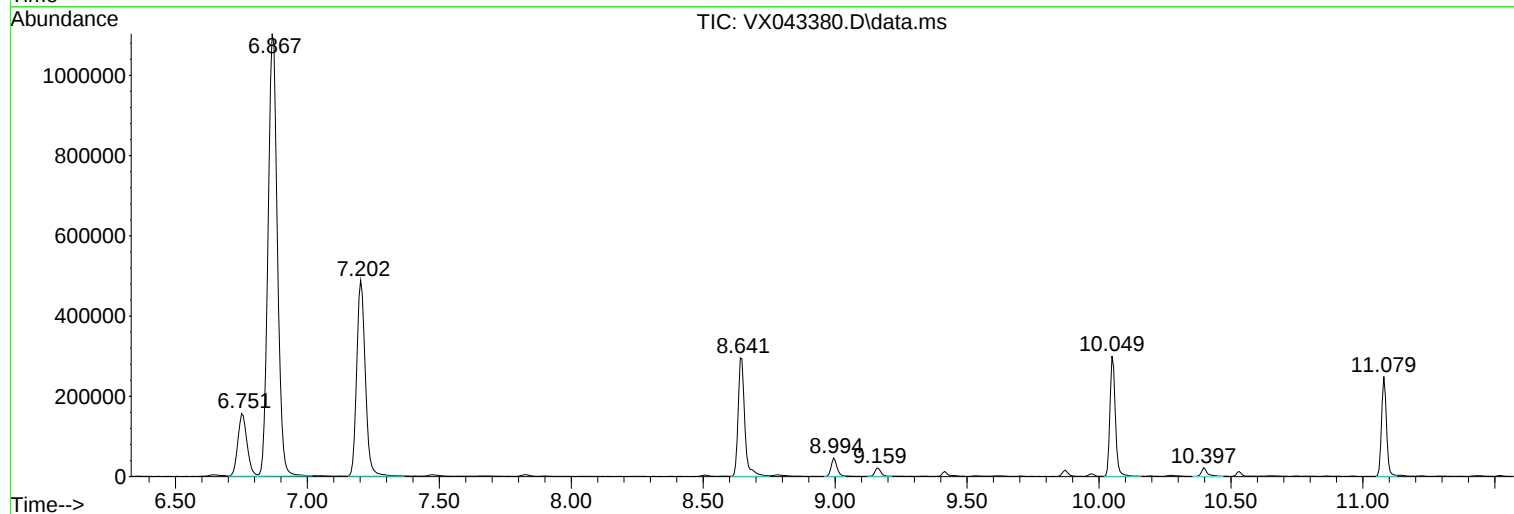
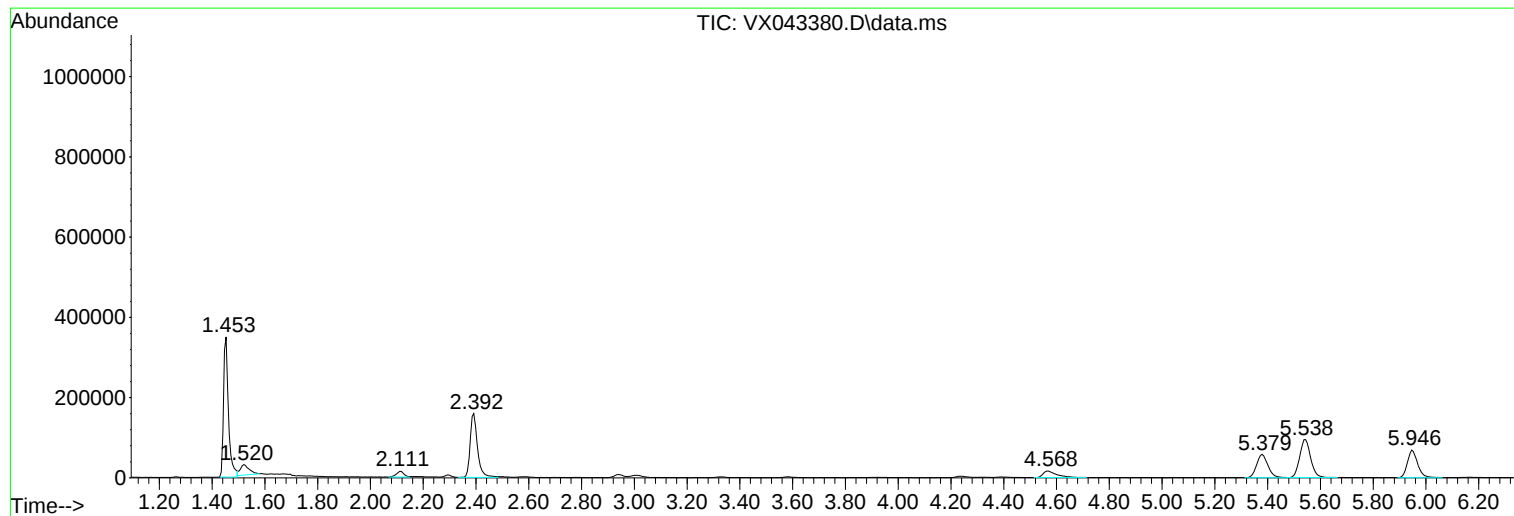
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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



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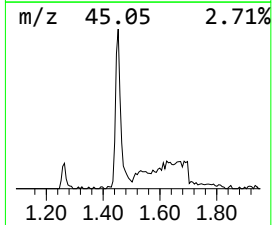
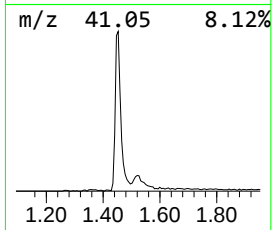
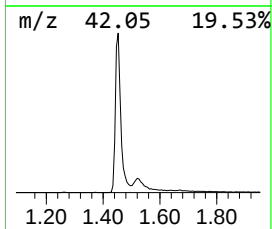
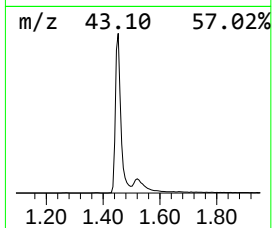
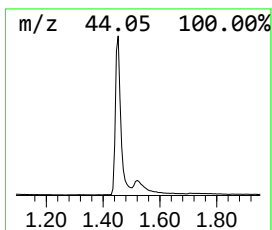
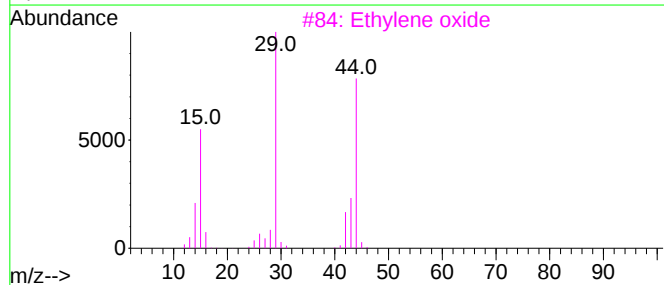
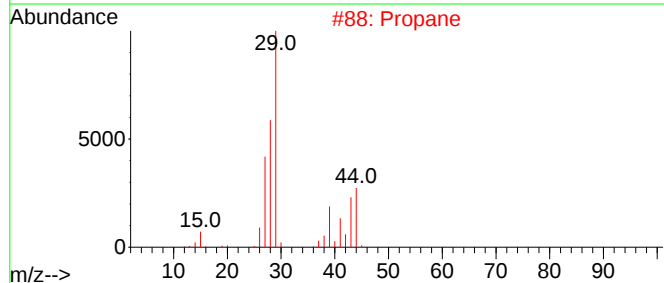
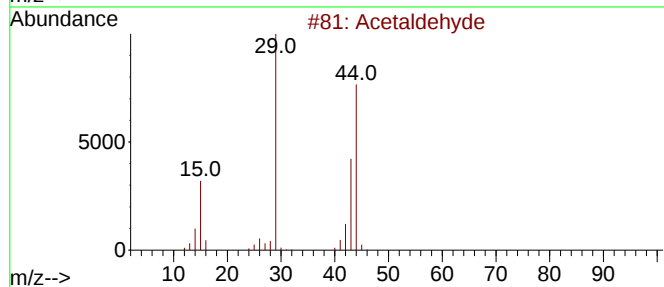
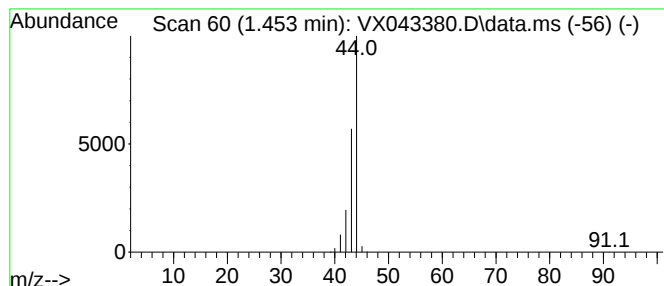
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	83.93 ug/l	457491	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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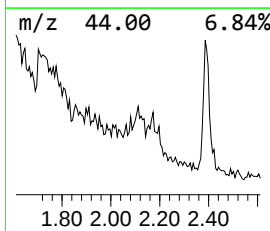
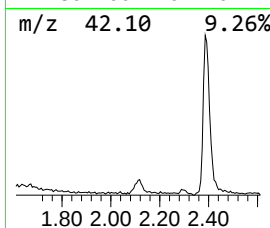
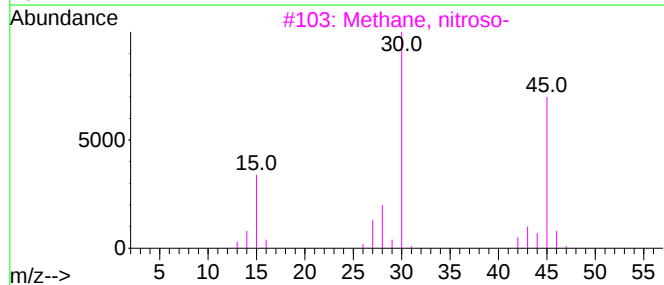
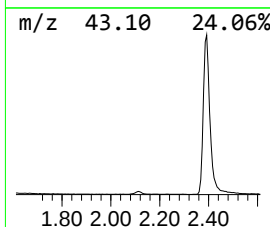
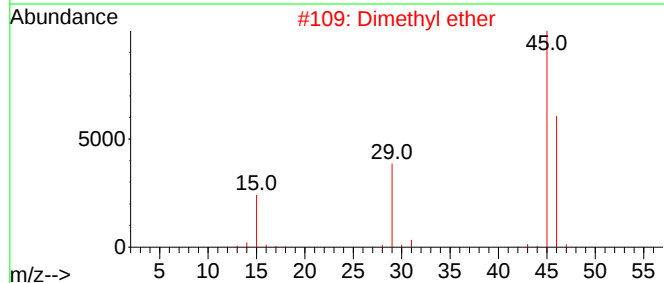
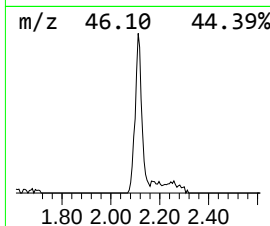
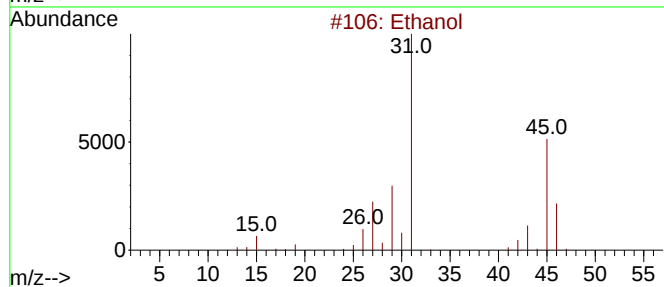
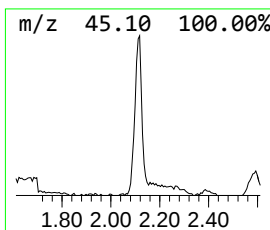
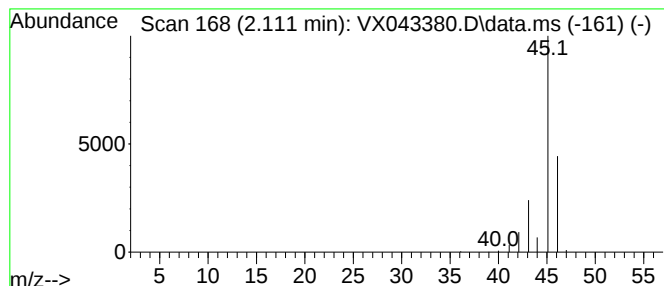
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.111	5.23 ug/l	28502	Pentafluorobenzene	5.544

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	7
4	Formic acid			46	CH2O2	000064-18-6	5
5	Oxalic acid			90	C2H2O4	000144-62-7	4



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
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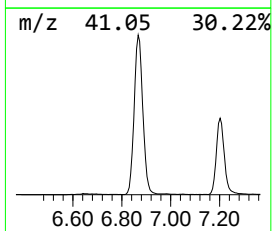
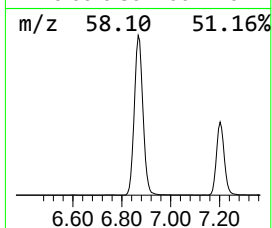
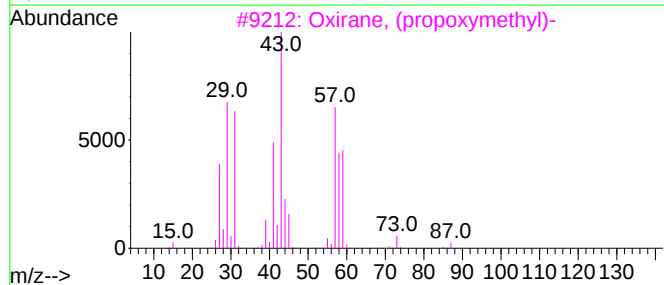
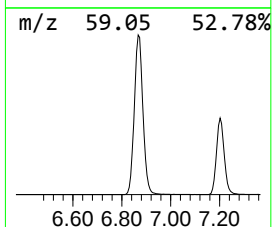
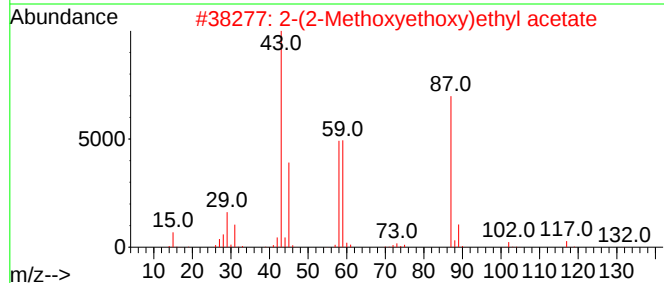
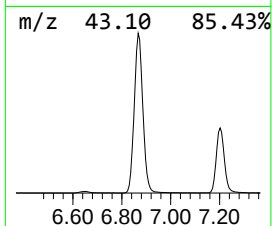
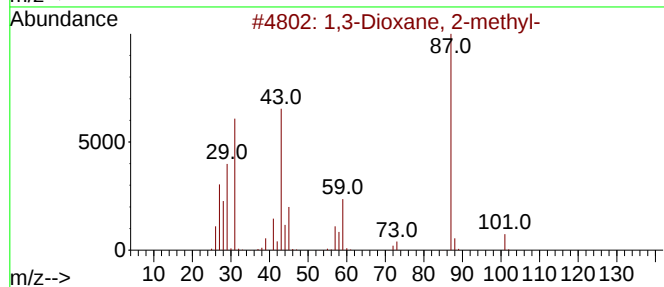
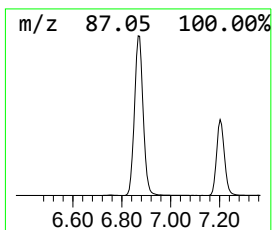
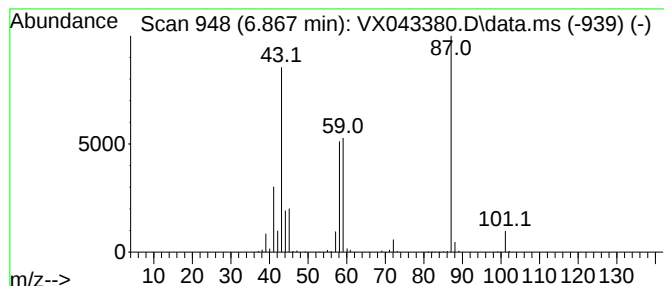
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Quant Title : SW846 8260

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

Peak Number 4 1,3-Dioxane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.867	360.30 ug/l	2709270	1,4-Difluorobenzene	6.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-			102	C5H10O2	000626-68-6	53
2	2-(2-Methoxyethoxy)ethyl acetate			162	C7H14O4	1000351-95-4	38
3	Oxirane, (propoxymethyl)-			116	C6H12O2	003126-95-2	38
4	Methyl 4-O-methyl-d-arabinopyran...			178	C7H14O5	1000129-79-9	36
5	Oxazolidin-2-one			87	C3H5NO2	000497-25-6	32



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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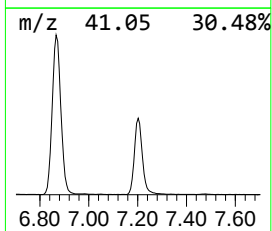
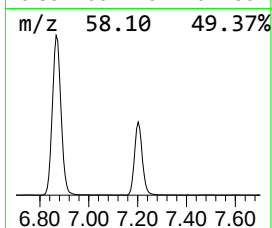
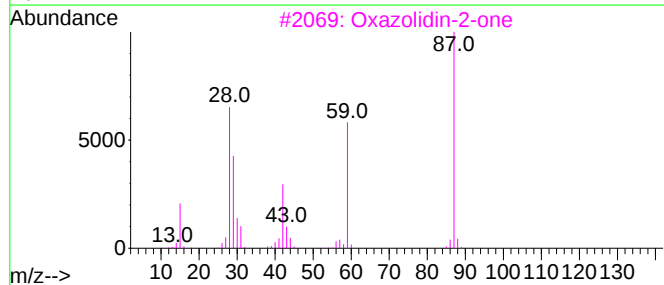
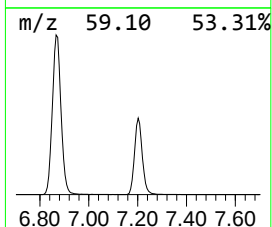
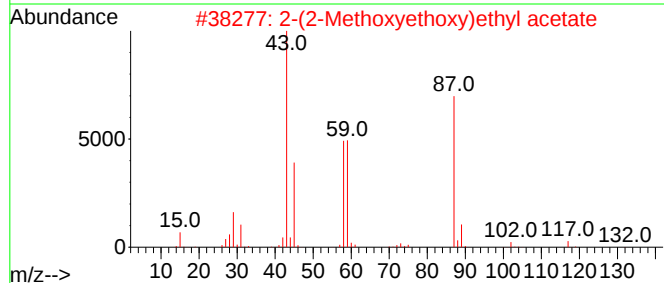
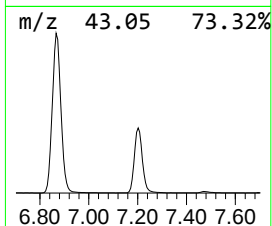
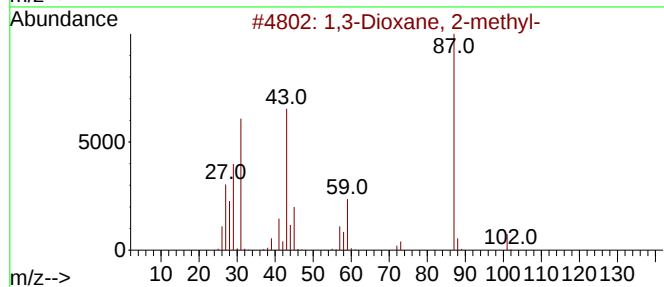
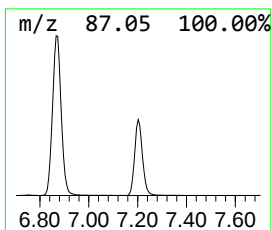
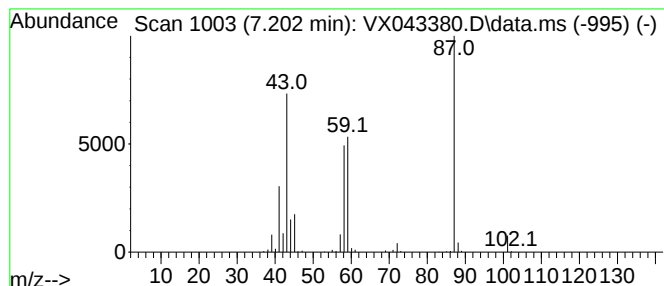
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown7.202 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.202	147.01 ug/l	1105470	1,4-Difluorobenzene	6.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	47
2			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	40
3			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38
4			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
5			Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	33



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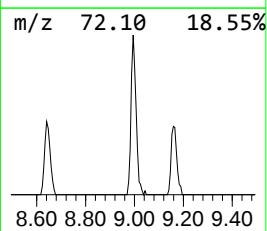
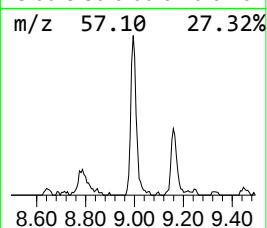
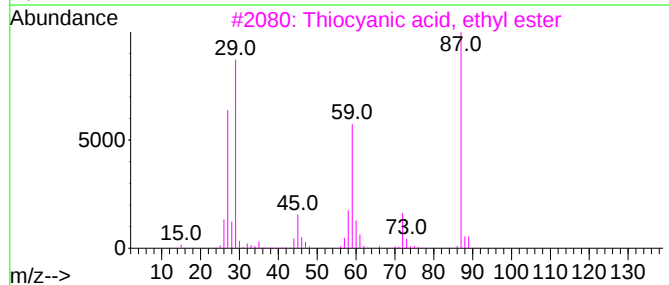
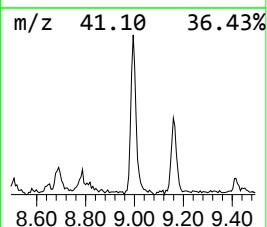
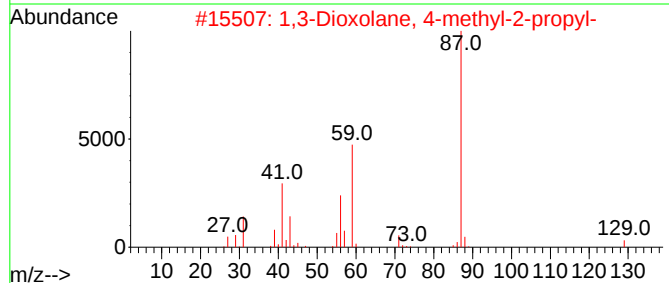
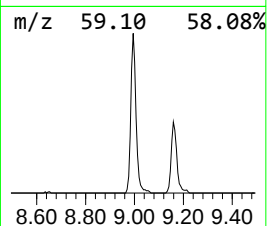
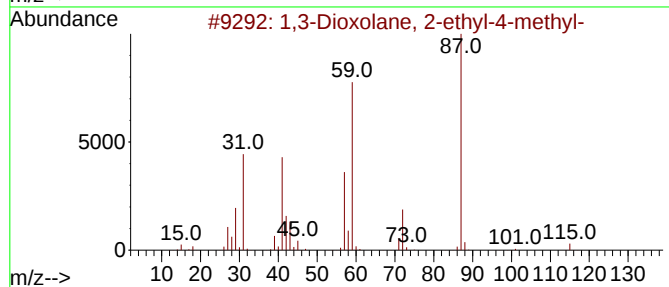
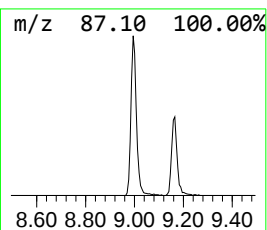
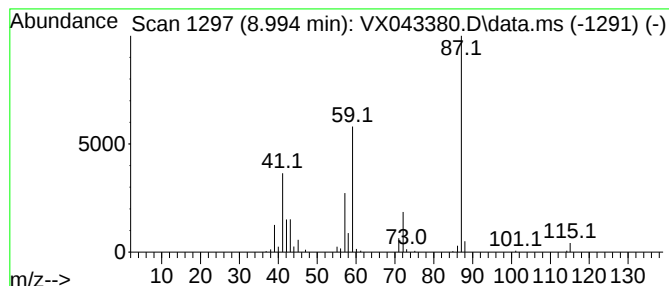
Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 6 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.994	8.09 ug/l	69382	Chlorobenzene-d5	10.049	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	86
2	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64
3	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	56
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
5	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52



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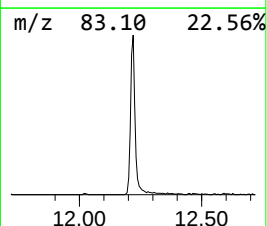
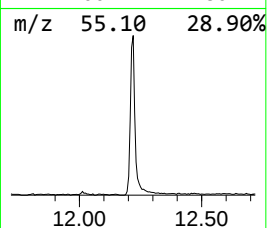
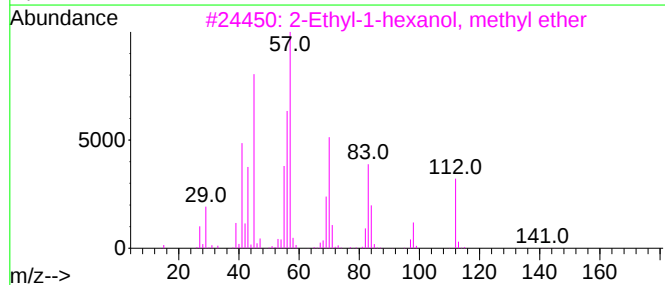
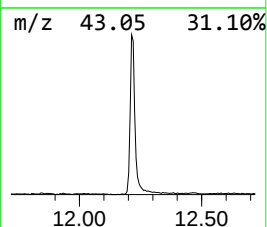
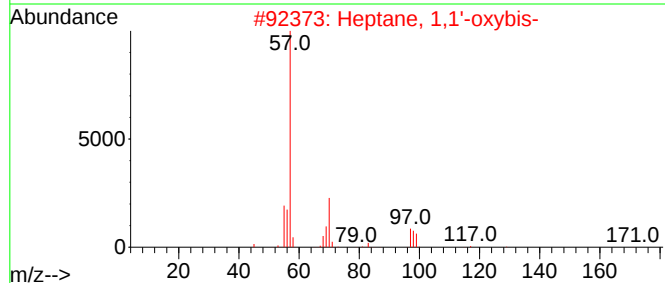
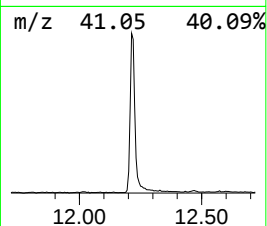
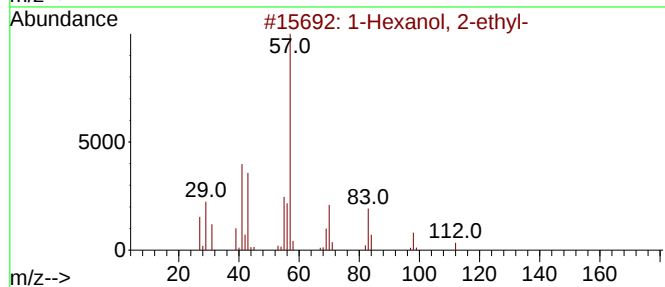
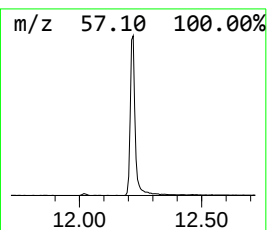
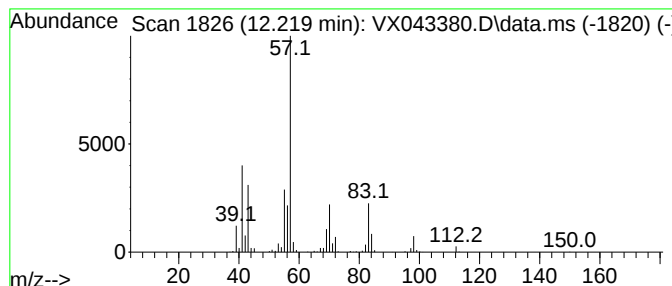
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	45.00 ug/l	351232	1,4-Dichlorobenzene-d4	12.018

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-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
4			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043380.D
Acq On : 14 Oct 2024 14:53
Operator : JC/MD
Sample : P4402-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3 - Tote

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	83.9	ug/l	457491	1	5.544	272551	50.0
Ethanol	2.111	5.2	ug/l	28502	1	5.544	272551	50.0
1,3-Dioxane, 2-...	6.867	360.3	ug/l	2709270	2	6.751	375970	50.0
unknown7.202	7.202	147.0	ug/l	1105470	2	6.751	375970	50.0
1,3-Dioxolane, ...	8.994	8.1	ug/l	69382	3	10.049	428741	50.0
1-Hexanol, 2-et...	12.219	45.0	ug/l	351232	4	12.018	390232	50.0