

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
 Data File : VX043382.D
 Acq On : 14 Oct 2024 15:39
 Operator : JC/MD
 Sample : P4402-05 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 5 - 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: VX043382.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	68	rBV	418390	532283	14.76%	5.474%
2	1.526	68	72	82	rVB	22833	55273	1.53%	0.568%
3	2.398	208	215	229	rBV	164019	313675	8.70%	3.226%
4	4.574	564	572	595	rBV	14312	53374	1.48%	0.549%
5	5.385	694	705	720	rBV	57383	168389	4.67%	1.732%
6	5.550	722	732	747	rVV	93072	267943	7.43%	2.756%
7	5.952	789	798	817	rVB	65695	179854	4.99%	1.850%
8	6.757	921	930	940	rBV	151890	365457	10.13%	3.758%
9	6.879	940	950	978	rVB	1427467	3606892	100.00%	37.094%
10	7.208	995	1004	1030	rBV	638051	1444683	40.05%	14.858%
11	8.647	1233	1240	1245	rBV	306135	492853	13.66%	5.069%
12	9.000	1292	1298	1309	rBV	88593	140299	3.89%	1.443%
13	9.165	1318	1325	1341	rBV	39012	63758	1.77%	0.656%
14	9.872	1432	1441	1452	rBV	89066	130936	3.63%	1.347%
15	9.970	1452	1457	1465	rBV	34936	48316	1.34%	0.497%
16	10.055	1465	1471	1485	rBV	303880	435642	12.08%	4.480%
17	10.396	1518	1527	1539	rBV	66667	93368	2.59%	0.960%
18	10.530	1544	1549	1558	rVV	34086	43193	1.20%	0.444%
19	11.079	1634	1639	1646	rBV	258006	336186	9.32%	3.457%
20	11.146	1646	1650	1658	rVV	33176	45679	1.27%	0.470%
21	12.018	1788	1793	1803	rBV	309569	410411	11.38%	4.221%
22	12.213	1821	1825	1842	rBV	362162	495064	13.73%	5.091%

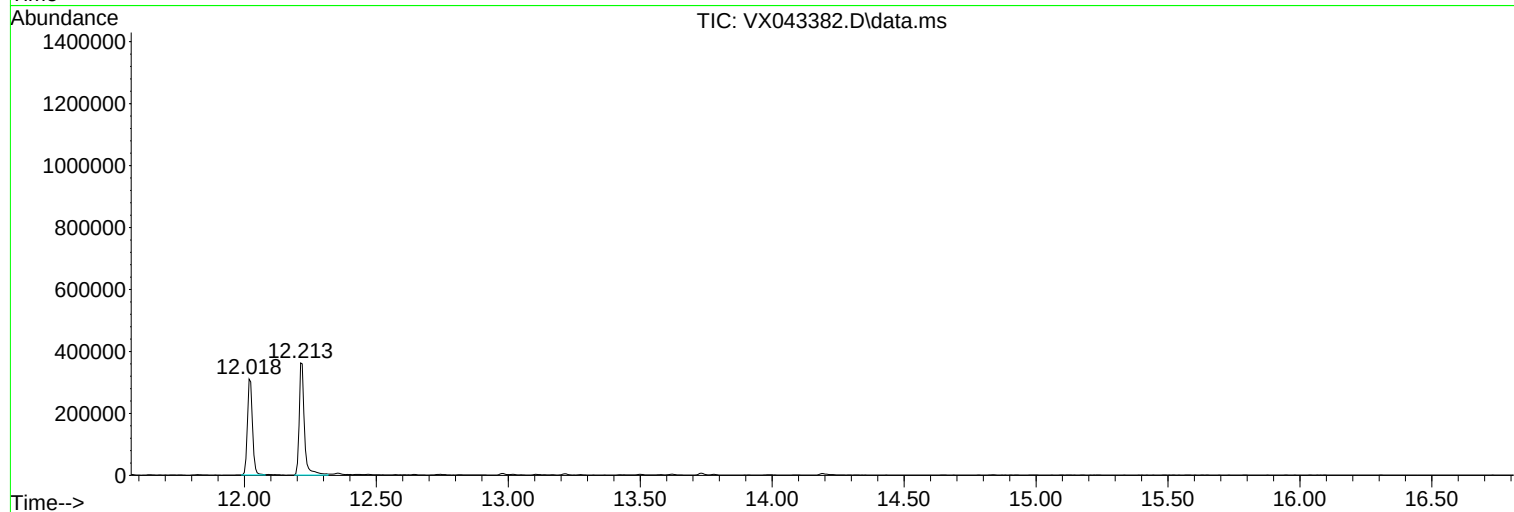
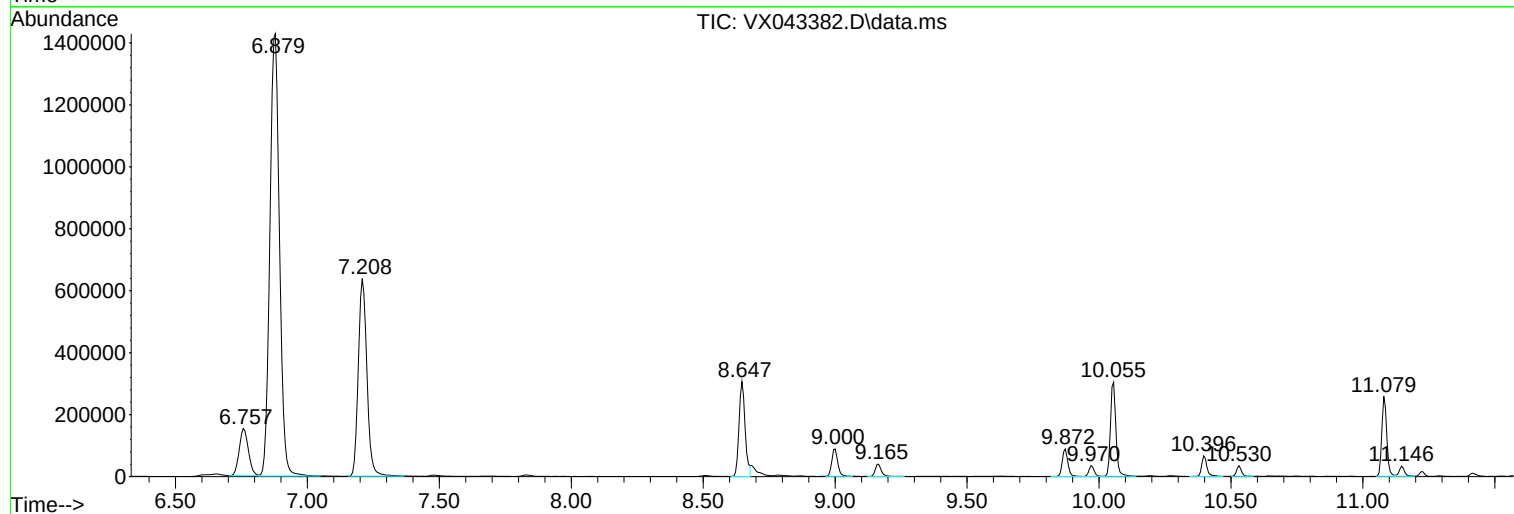
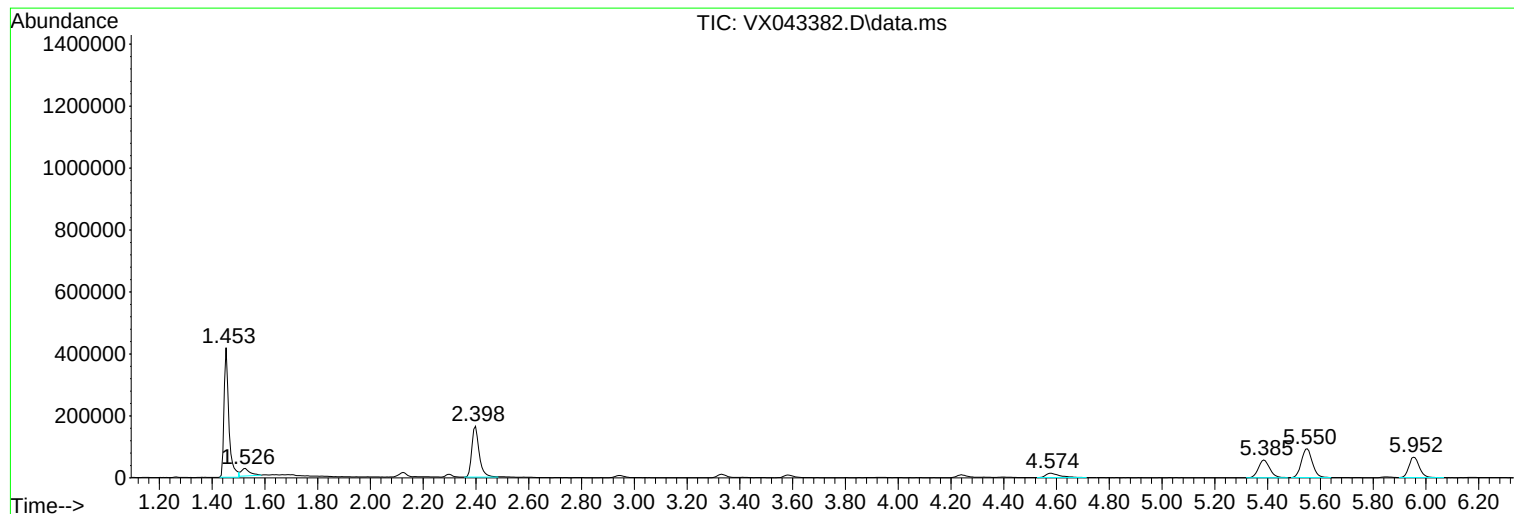
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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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



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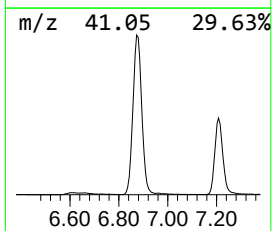
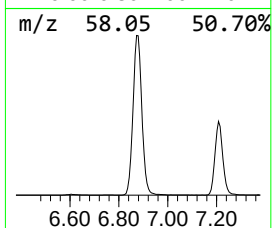
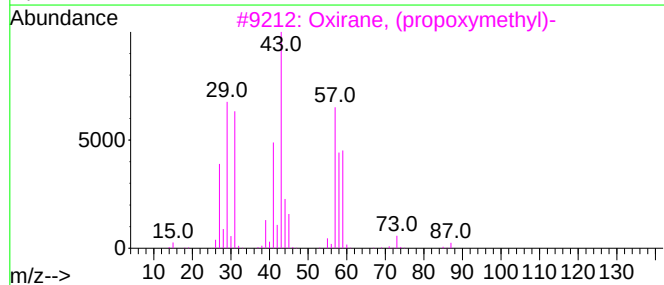
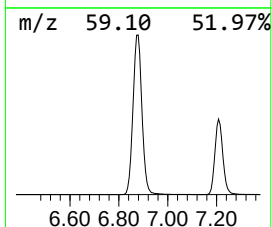
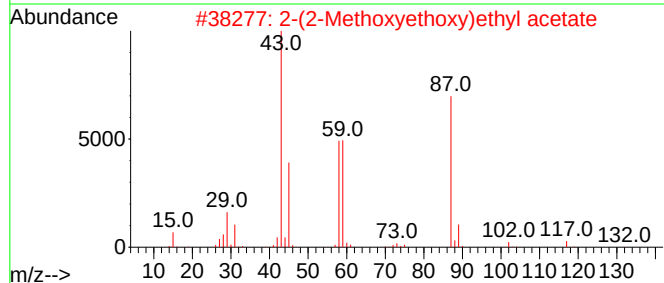
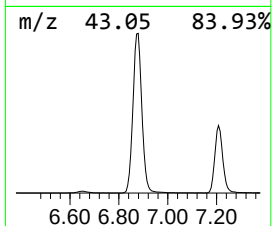
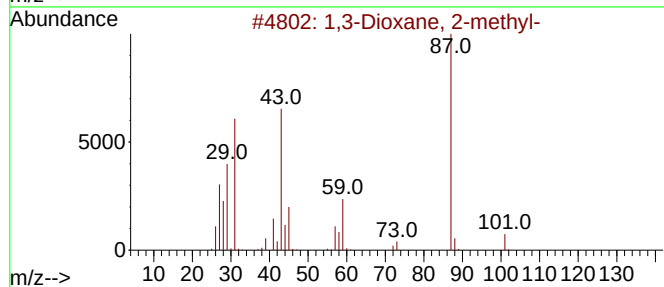
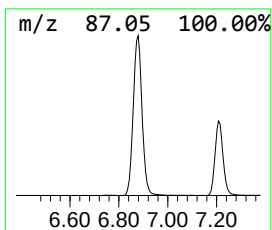
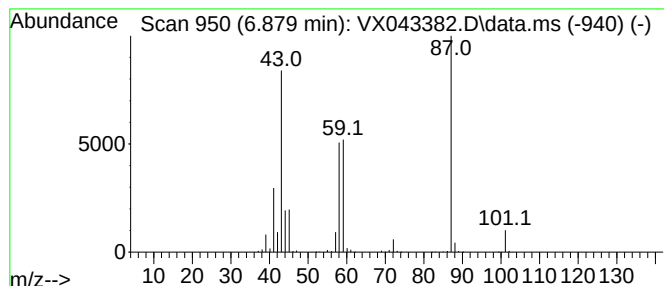
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown6.879 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	493.48 ug/l	3606890	1,4-Difluorobenzene	6.757

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	40
2		2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	38
3		Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37
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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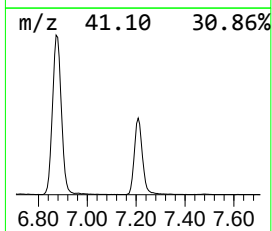
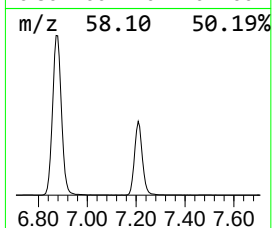
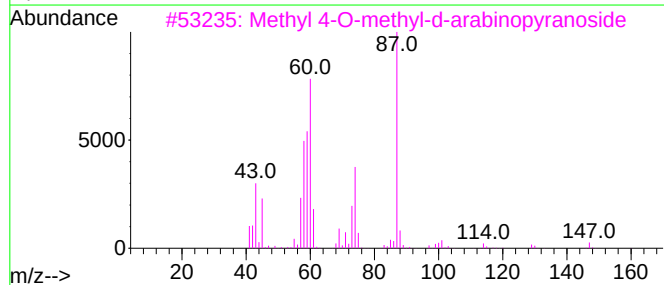
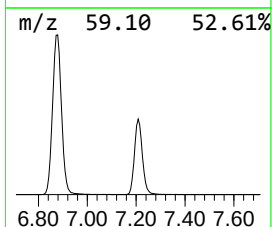
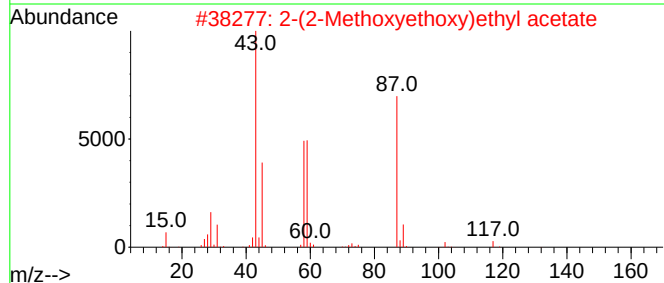
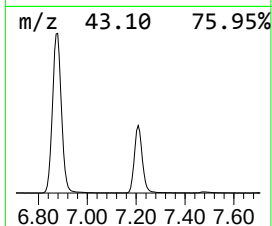
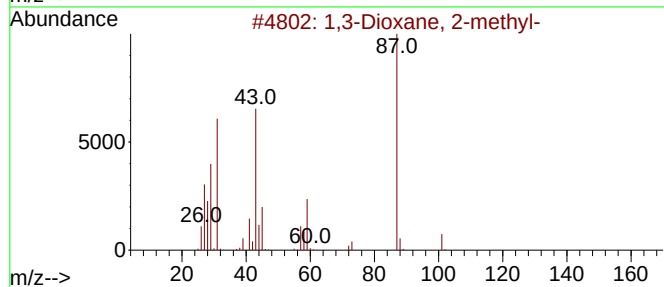
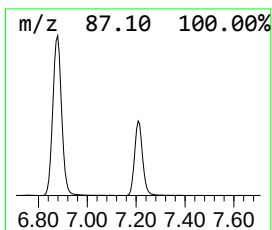
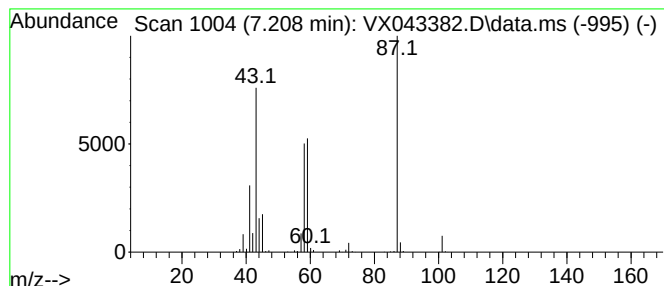
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	197.65 ug/l	1444680	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	50
2			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	40
3			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
4			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38
5			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	28



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ALS Vial : 15 Sample Multiplier: 1

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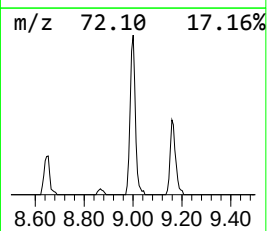
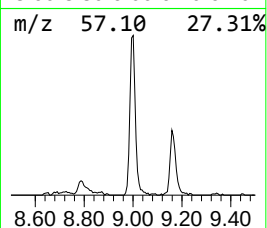
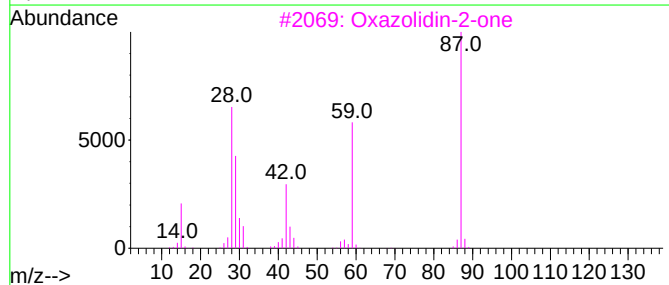
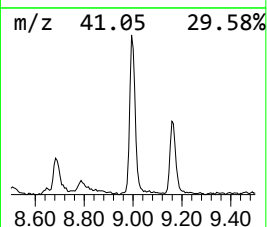
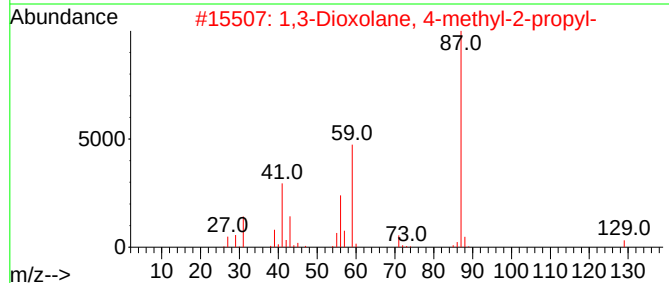
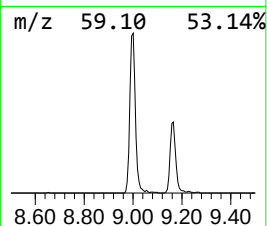
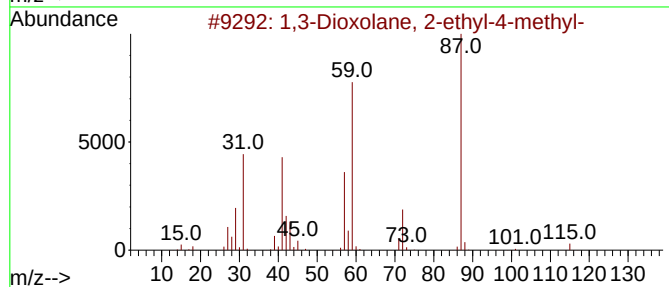
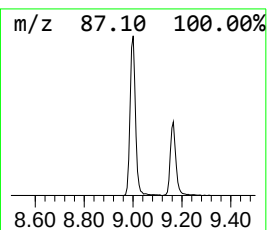
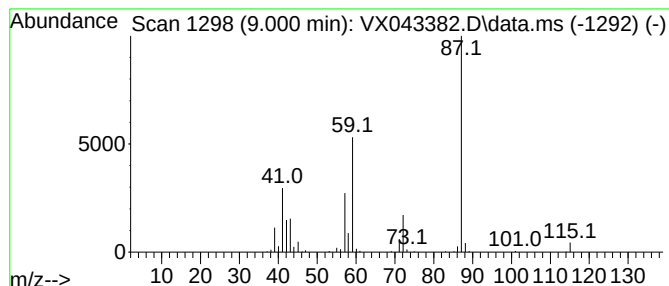
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 5 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.000	16.10 ug/l	140299	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	90
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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

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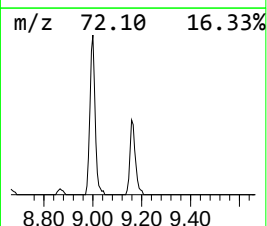
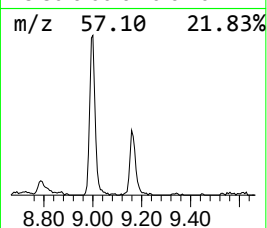
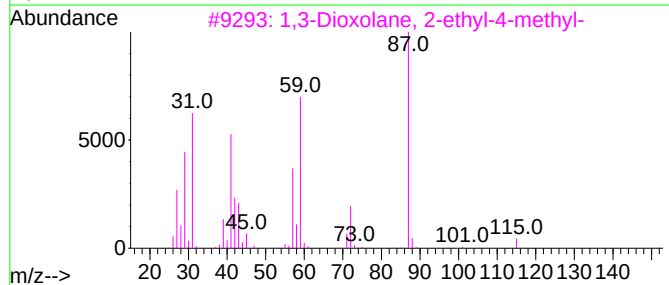
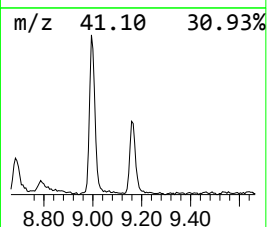
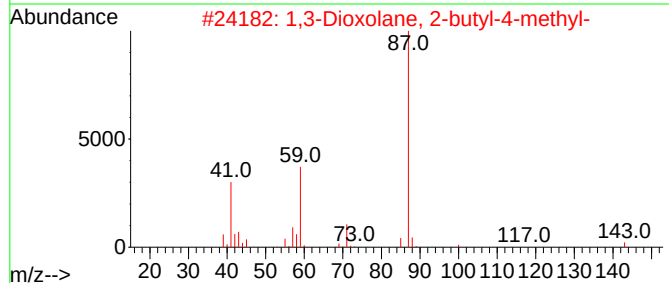
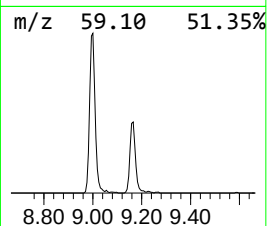
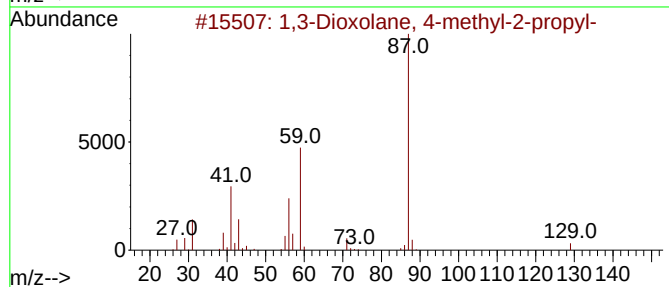
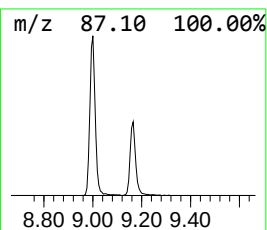
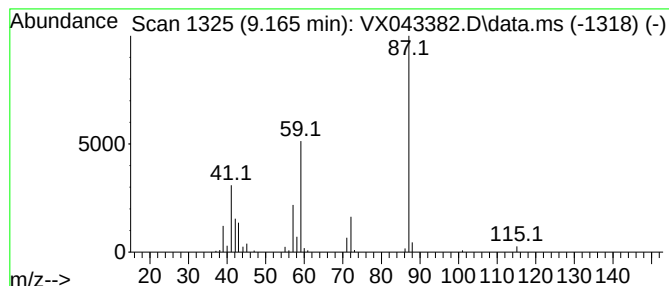
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 6 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.165	7.32 ug/l	63758	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	72
2			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	64
3			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	59
4			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	56
5			2-Propanone, 0-methyloxime	87	C4H9NO	003376-35-0	52



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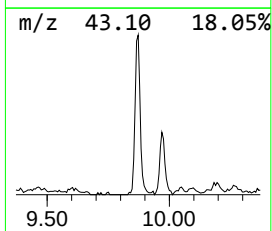
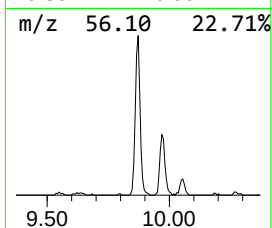
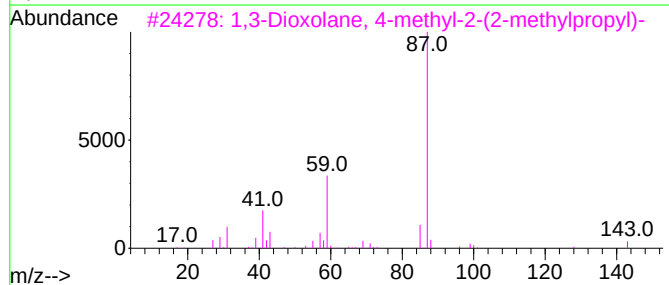
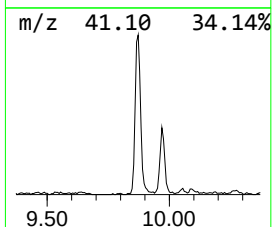
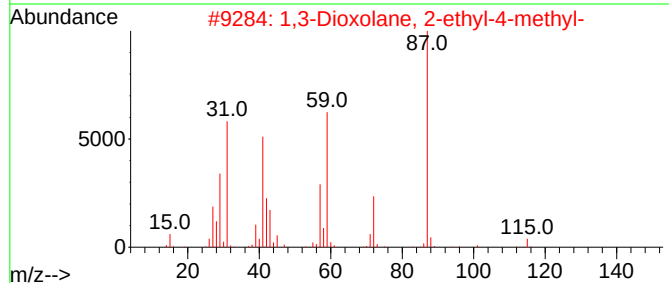
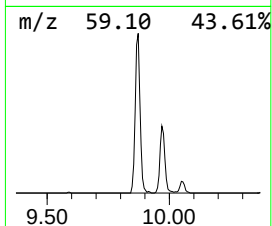
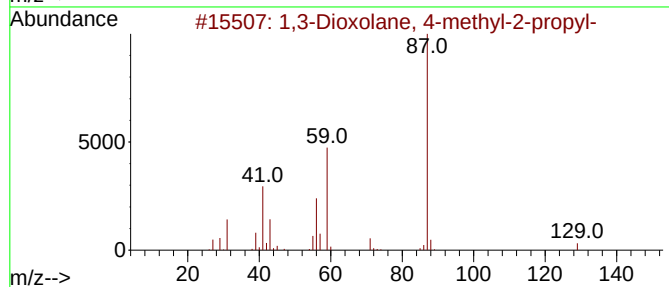
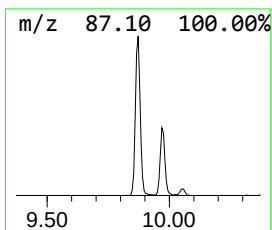
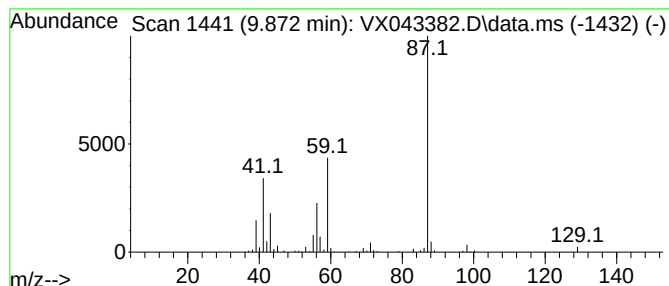
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 7 1,3-Dioxolane, 4-methyl-2-(... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.872	15.03 ug/l	130936	Chlorobenzene-d5	10.055

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	90	
2	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	64	
3	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	64	
4	2-Hexyl-4-methyl-1,3-dioxolane	172	C10H20O2	004351-10-4	64	
5	Ethoxycitronellal	198	C12H22O2	1000132-02-6	59	



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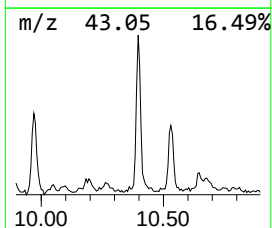
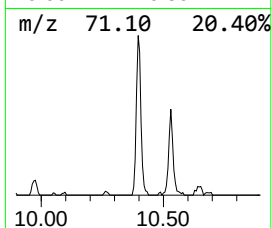
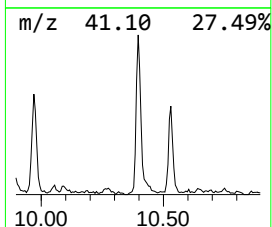
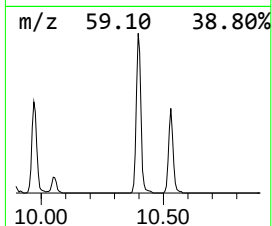
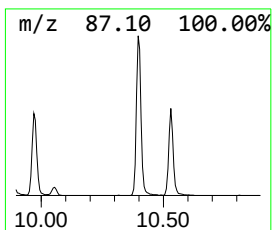
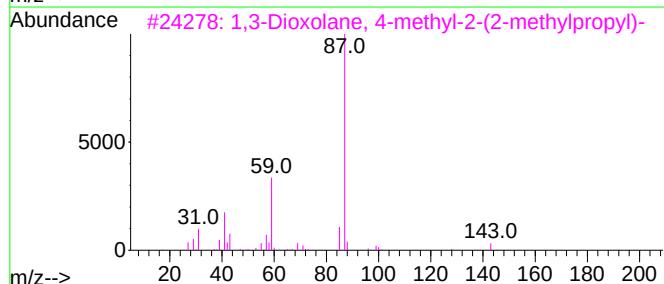
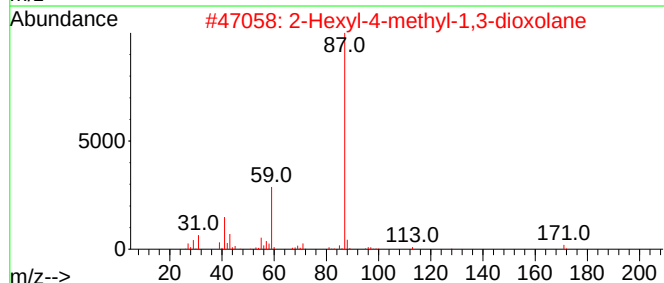
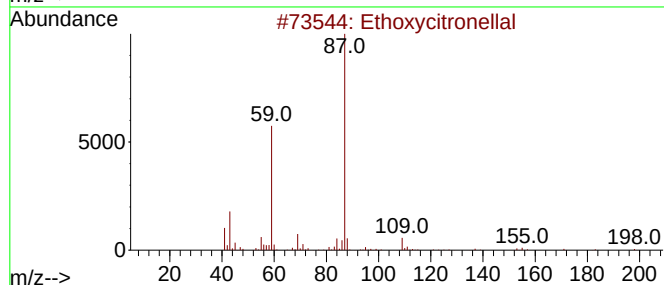
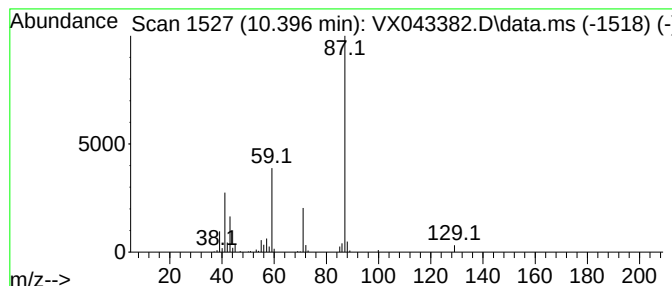
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Quant Title : SW846 8260

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

Peak Number 8 Ethoxycitronellal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.396	10.72 ug/l	93368	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethoxycitronellal	198	C12H22O2	1000132-02-6	64
2			2-Hexyl-4-methyl-1,3-dioxolane	172	C10H20O2	004351-10-4	64
3			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	64
4			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	56
5			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043382.D
Acq On : 14 Oct 2024 15:39
Operator : JC/MD
Sample : P4402-05 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

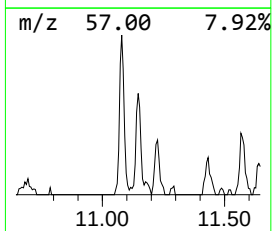
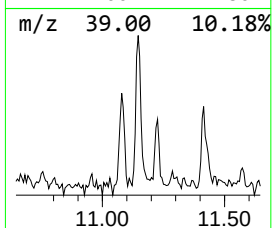
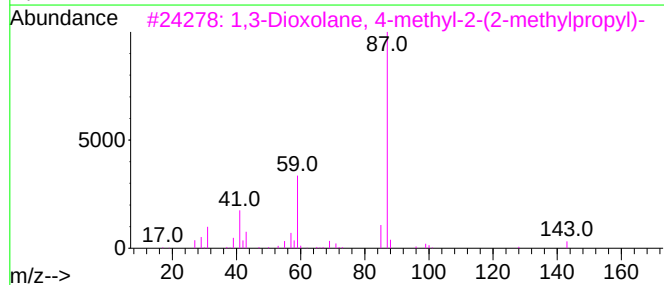
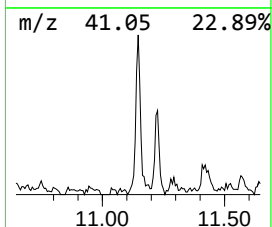
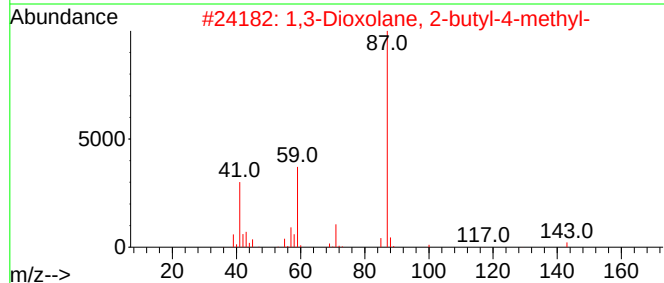
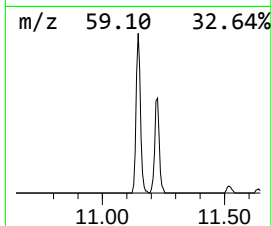
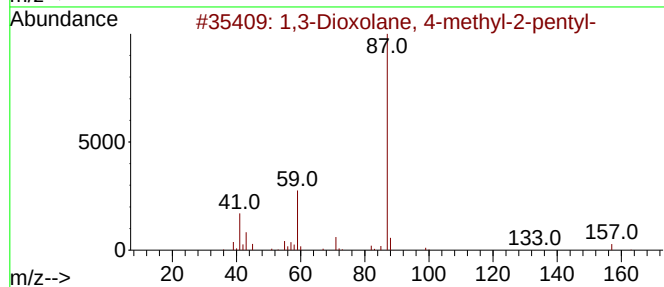
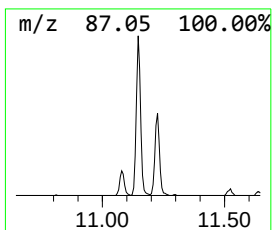
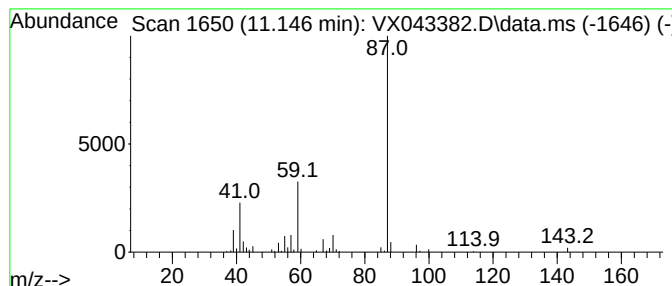
Instrument :
MSVOA_X
ClientSampleId :
5 - Tote

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 9 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.146	5.57 ug/l	45679	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 4-methyl-2-pentyl-	158	C9H18O2	001599-49-1	72
2	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	56
3	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	56
4	2-Hexyl-4-methyl-1,3-dioxolane	172	C10H20O2	004351-10-4	56
5	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043382.D
Acq On : 14 Oct 2024 15:39
Operator : JC/MD
Sample : P4402-05 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
5 - Tote

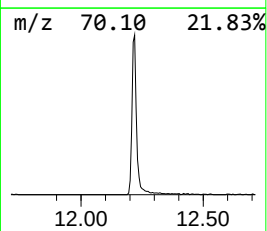
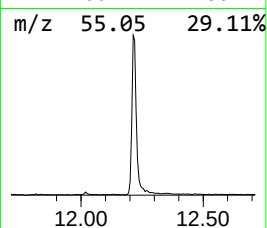
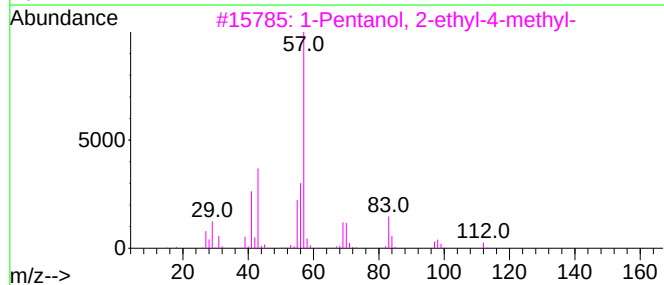
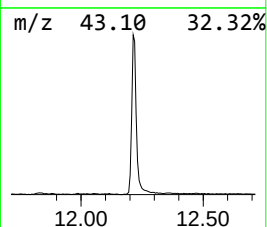
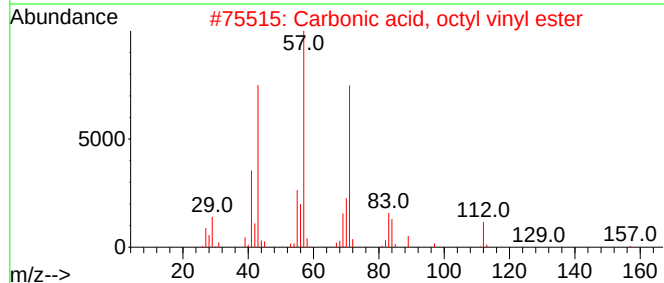
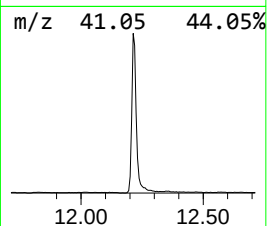
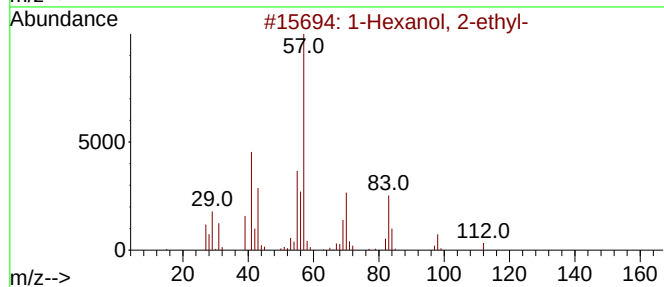
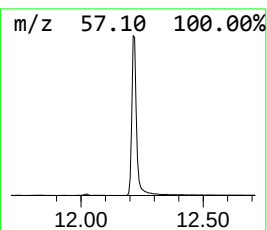
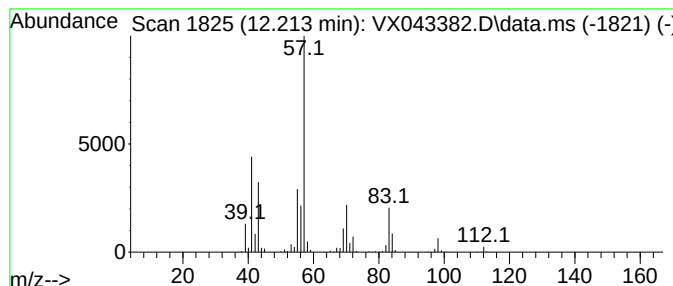
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Quant Title : SW846 8260

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	60.31 ug/l	495064	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	59
3		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5		Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043382.D
Acq On : 14 Oct 2024 15:39
Operator : JC/MD
Sample : P4402-05 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
5 - 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
unknown6.879	6.879	493.5	ug/l	3606890	2	6.757	365457	50.0
1,3-Dioxane, 2-...	7.208	197.7	ug/l	1444680	2	6.757	365457	50.0
1,3-Dioxolane, ...	9.000	16.1	ug/l	140299	3	10.055	435642	50.0
1,3-Dioxolane, ...	9.165	7.3	ug/l	63758	3	10.055	435642	50.0
1,3-Dioxolane, ...	9.872	15.0	ug/l	130936	3	10.055	435642	50.0
Ethoxycitronellal	10.396	10.7	ug/l	93368	3	10.055	435642	50.0
1,3-Dioxolane, ...	11.146	5.6	ug/l	45679	4	12.024	410411	50.0
1-Hexanol, 2-et...	12.213	60.3	ug/l	495064	4	12.024	410411	50.0