

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
 Data File : VX043384.D
 Acq On : 14 Oct 2024 16:26
 Operator : JC/MD
 Sample : P4402-02 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 2 - Drum

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: VX043384.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	66	rBV	171861	206159	14.95%	3.834%
2	1.508	66	69	80	rVB	10101	24015	1.74%	0.447%
3	2.392	204	214	225	rBV	77253	141089	10.23%	2.624%
4	2.947	296	305	314	rBV	7215	17522	1.27%	0.326%
5	4.239	506	517	526	rBV4	5795	17928	1.30%	0.333%
6	4.574	564	572	592	rBV2	10512	36155	2.62%	0.672%
7	5.385	695	705	721	rBV	54965	161796	11.74%	3.009%
8	5.550	721	732	745	rBV	91496	261209	18.95%	4.858%
9	5.952	789	798	811	rBV	66017	176620	12.81%	3.285%
10	6.641	896	911	921	rBV4	4752	19237	1.40%	0.358%
11	6.757	921	930	940	rVV	148715	361266	26.20%	6.719%
12	6.873	940	949	970	rVB	571859	1378644	100.00%	25.639%
13	7.208	994	1004	1029	rBV	274320	608083	44.11%	11.309%
14	8.647	1233	1240	1256	rBV	298108	502147	36.42%	9.339%
15	9.000	1292	1298	1312	rBV	42083	66149	4.80%	1.230%
16	9.165	1316	1325	1332	rBV	20173	31991	2.32%	0.595%
17	9.872	1436	1441	1452	rBV2	31601	47927	3.48%	0.891%
18	9.970	1452	1457	1465	rBV	13017	17791	1.29%	0.331%
19	10.055	1465	1471	1487	rVV	282635	410520	29.78%	7.635%
20	10.397	1522	1527	1537	rBV	36972	51599	3.74%	0.960%
21	10.531	1541	1549	1559	rBV	20609	27810	2.02%	0.517%
22	11.079	1634	1639	1647	rBV	238830	307516	22.31%	5.719%
23	11.146	1647	1650	1657	rVV	11217	16022	1.16%	0.298%
24	11.969	1781	1785	1789	rBV	53603	66141	4.80%	1.230%
25	12.018	1789	1793	1803	rVB	276608	366900	26.61%	6.823%
26	12.219	1818	1826	1833	rBV	36605	54838	3.98%	1.020%

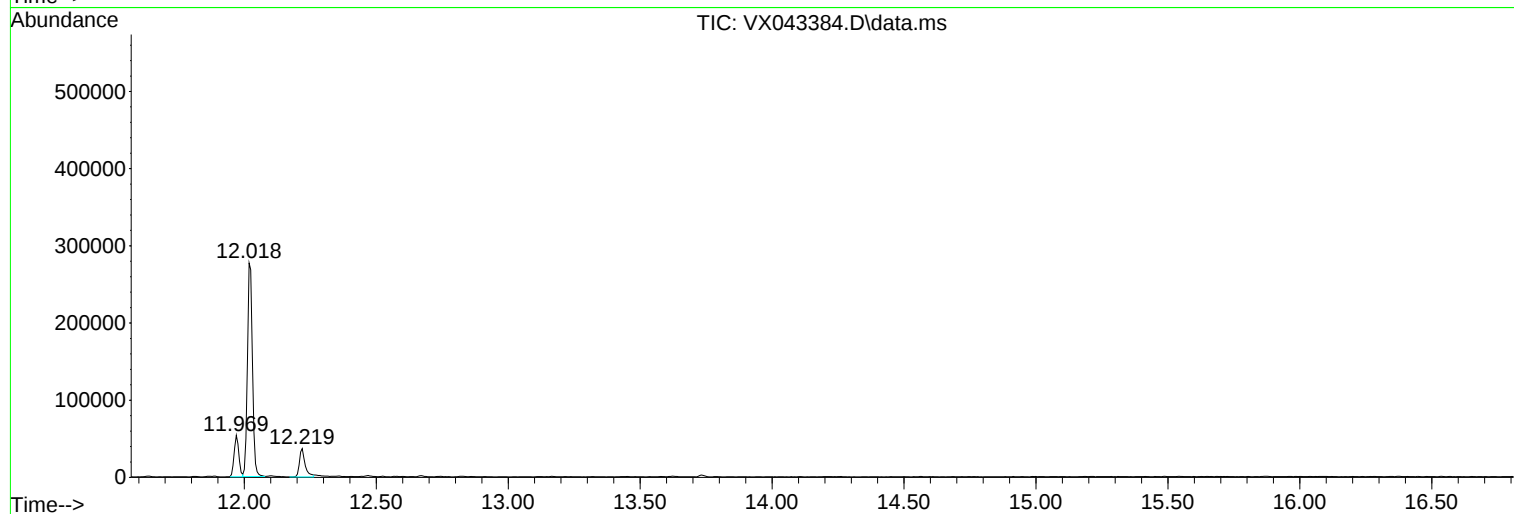
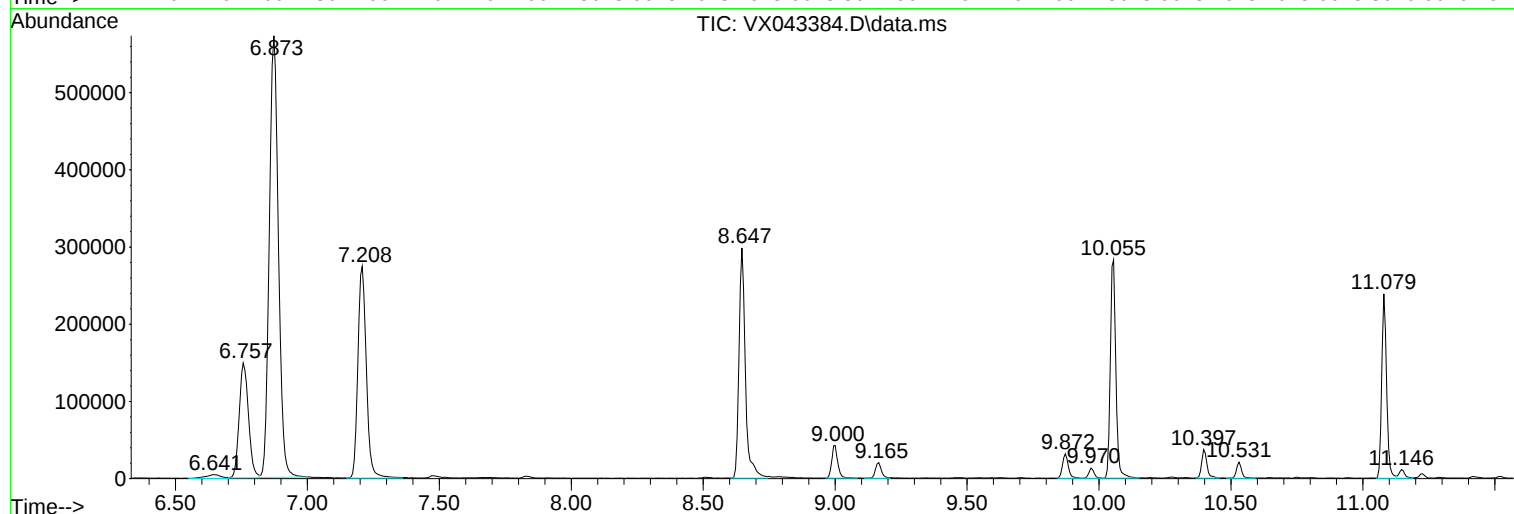
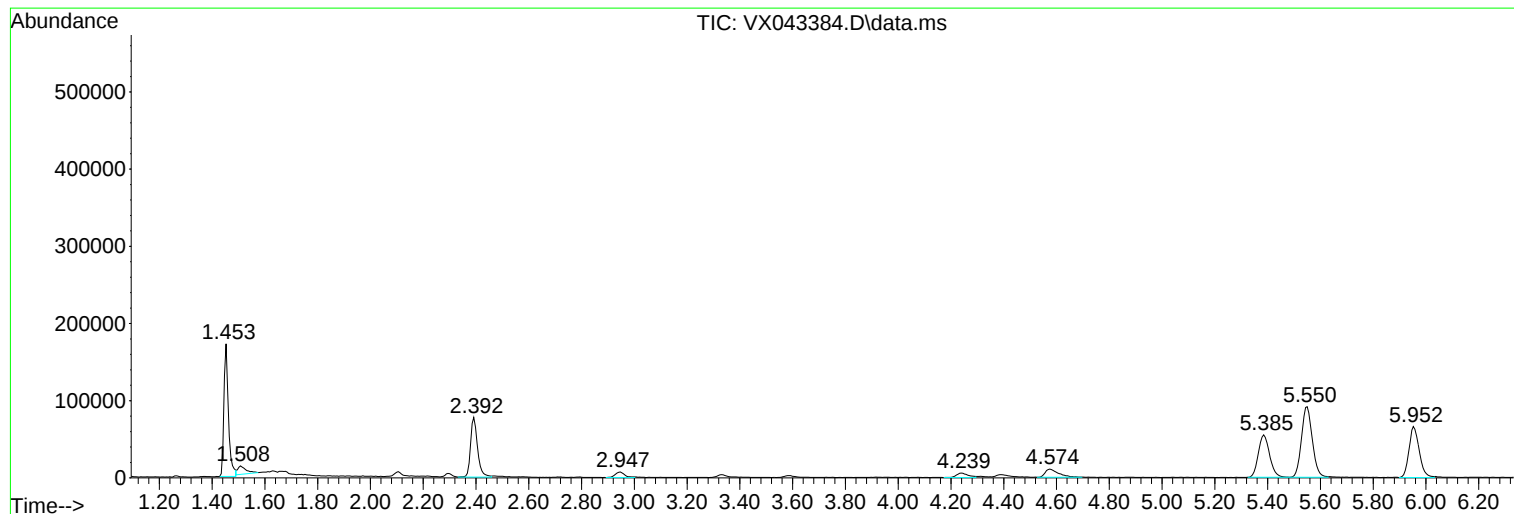
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2 - Drum

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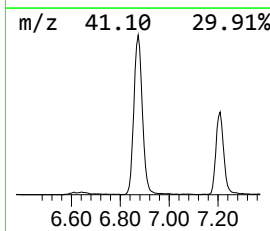
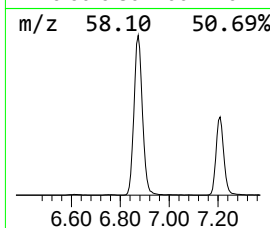
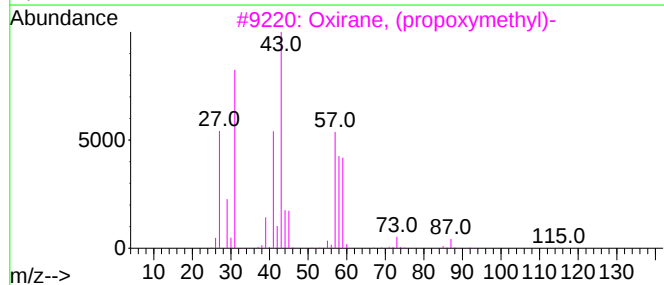
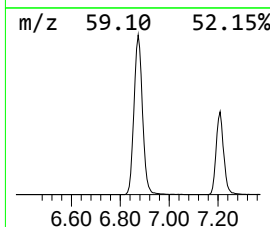
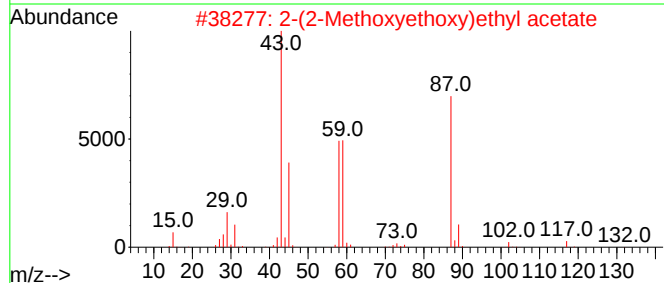
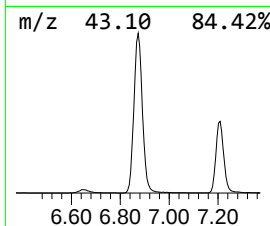
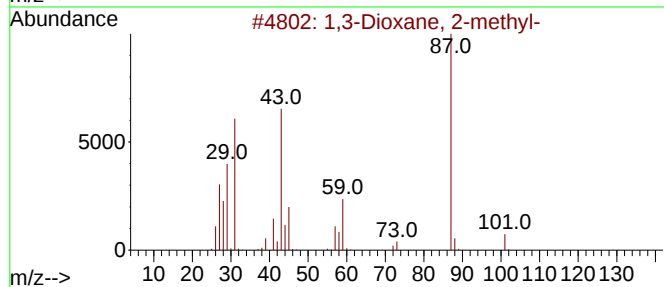
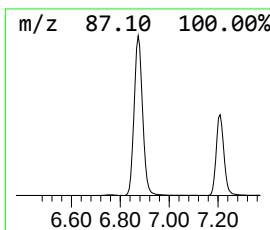
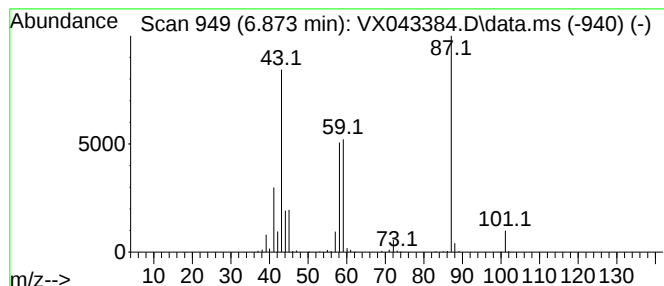
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.873	190.81 ug/l	1378640	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	38
3	Oxirane, (propoxymethyl)-			116	C6H12O2	003126-95-2	37
4	1,3-Dioxolane, 4-methyl-2-propyl-			130	C7H14O2	004352-99-2	37
5	Methyl 4-O-methyl-d-arabinopyran...			178	C7H14O5	1000129-79-9	36



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ClientSampleId :
2 - Drum

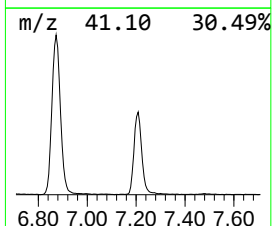
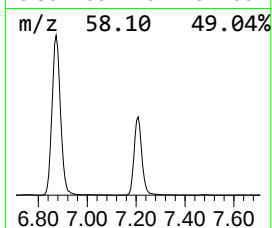
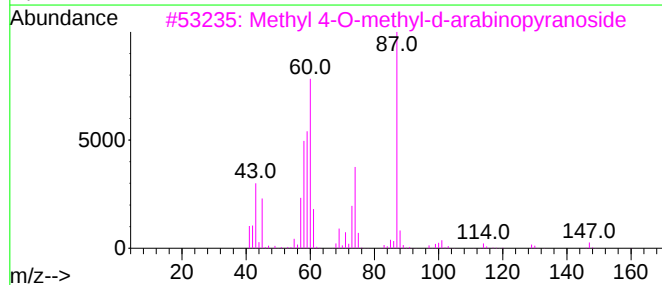
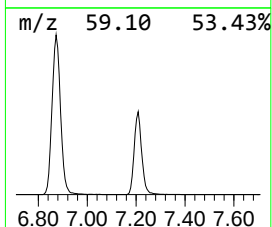
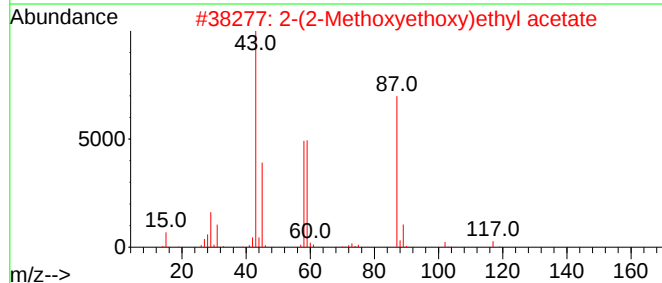
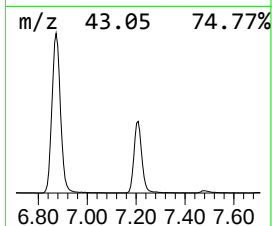
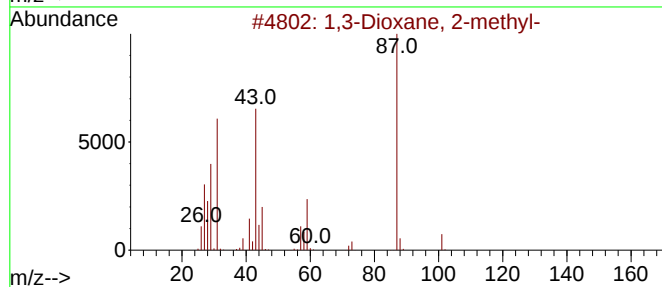
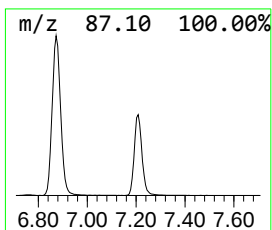
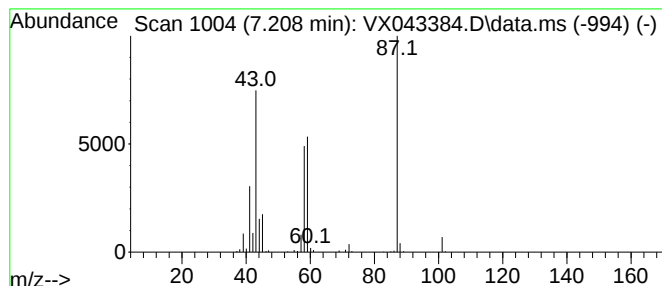
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown7.208 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	84.16 ug/l	608083	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	47
2			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	40
3			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	39
4			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38
5			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	38



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

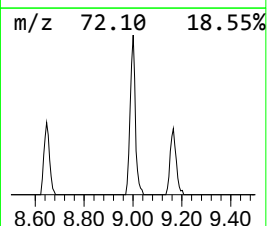
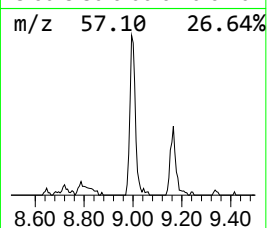
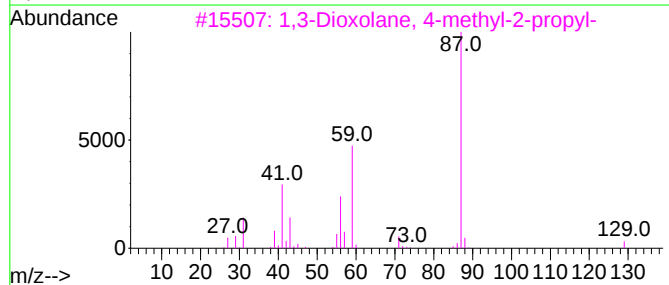
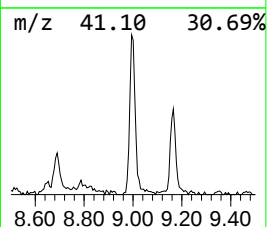
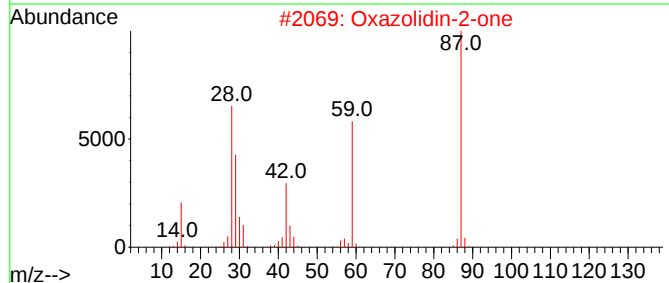
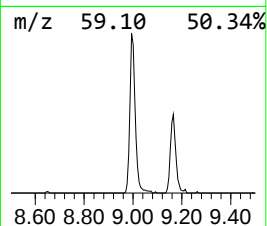
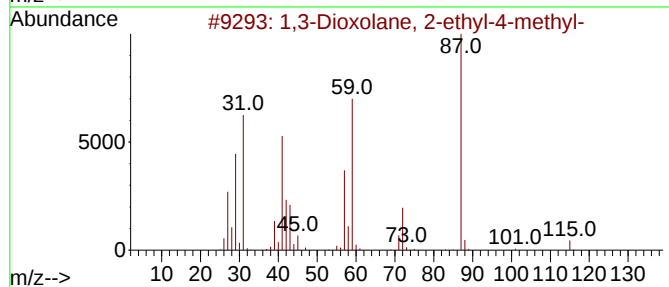
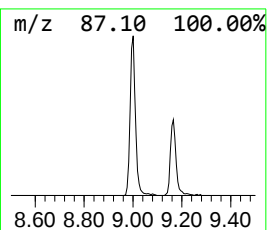
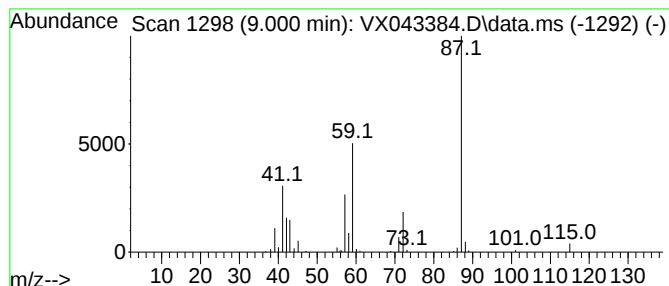
Instrument :
MSVOA_X
ClientSampleId :
2 - Drum

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-Dioxolane, 2-ethyl-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.000	8.06 ug/l	66149	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	83
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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
5	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2 - Drum

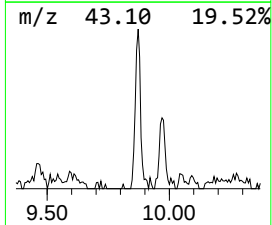
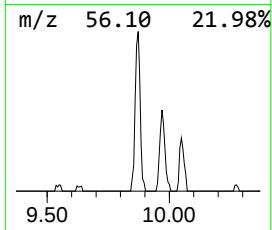
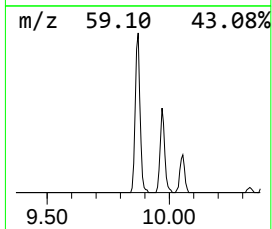
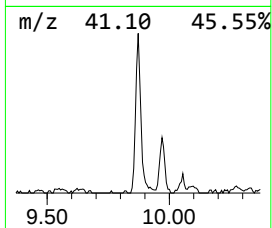
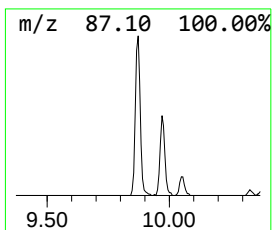
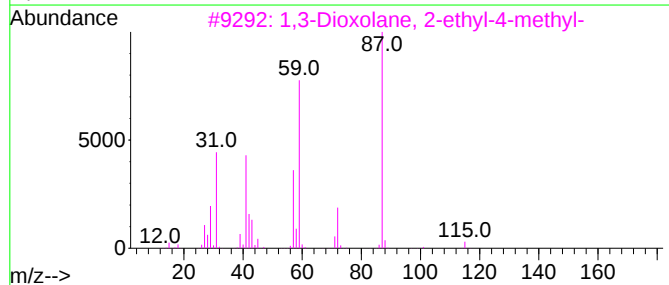
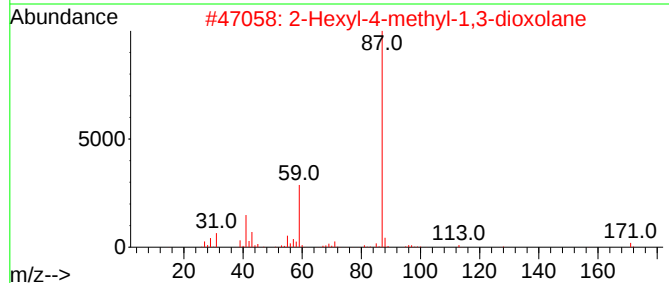
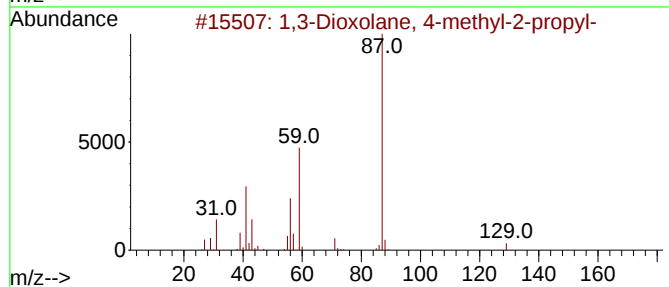
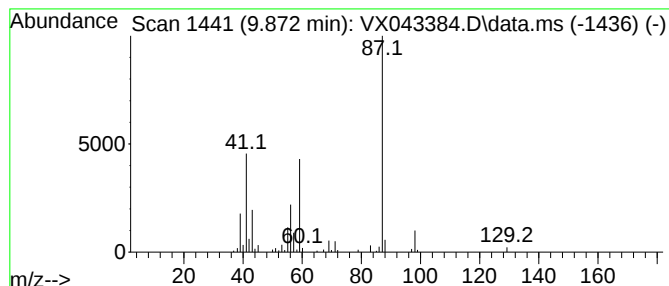
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Quant Title : SW846 8260

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

Peak Number 5 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.872	5.84 ug/l	47927	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	78
2			2-Hexyl-4-methyl-1,3-dioxolane	172	C10H20O2	004351-10-4	45
3			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	45
4			2-[2-[2-(2-Methoxyethoxy)etho...	294	C13H26O7	1000351-91-3	45
5			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	45



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ClientSampleId :
2 - Drum

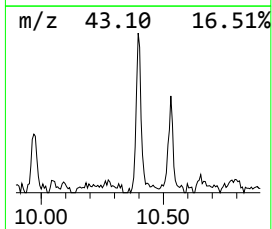
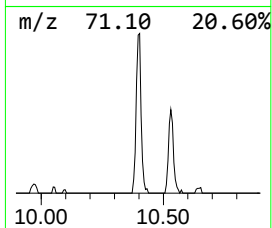
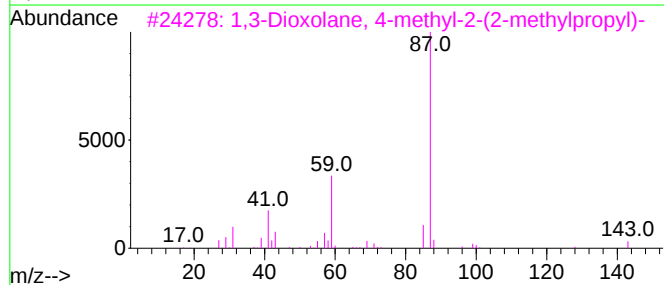
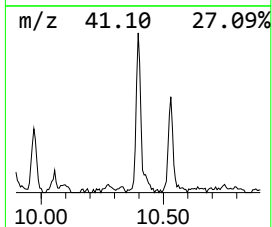
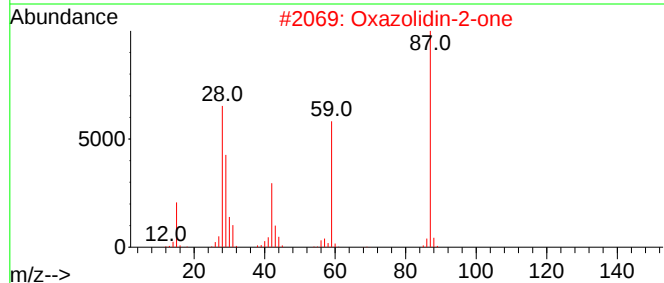
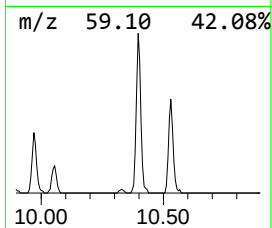
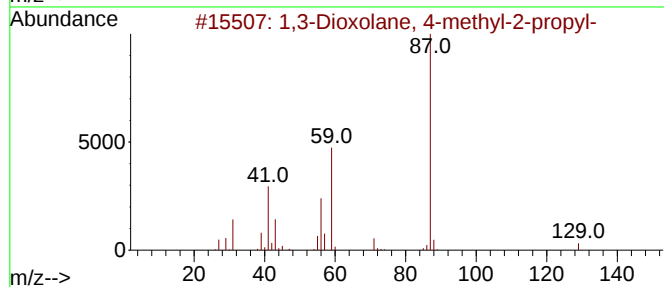
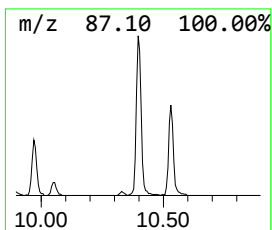
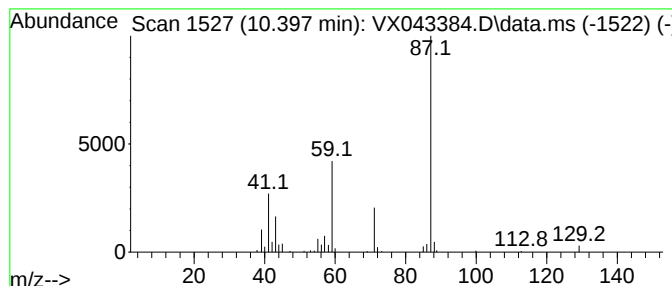
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 6 Oxazolidin-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.397	6.28 ug/l	51599	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			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	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	64



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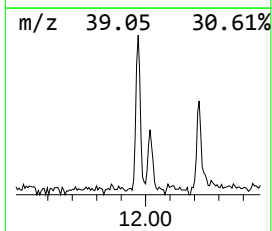
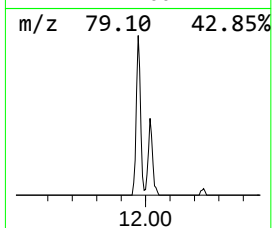
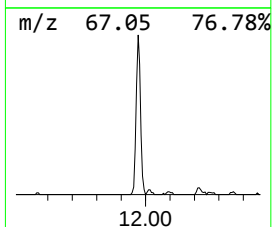
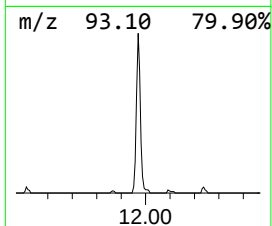
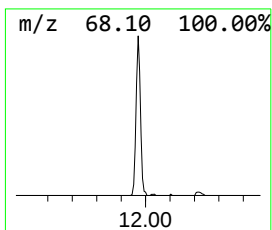
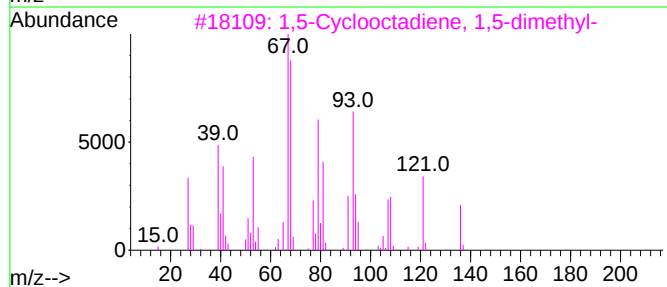
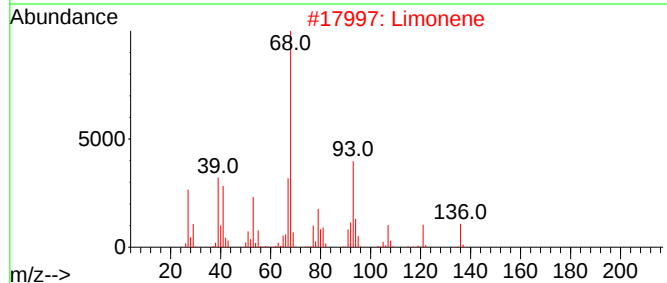
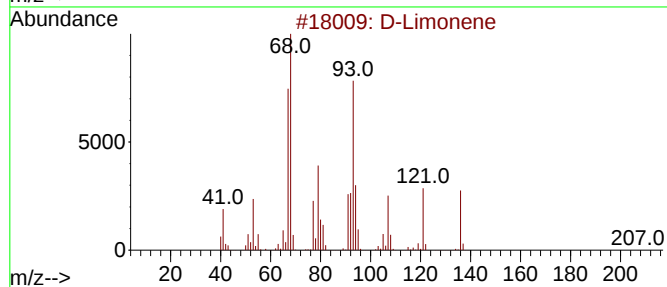
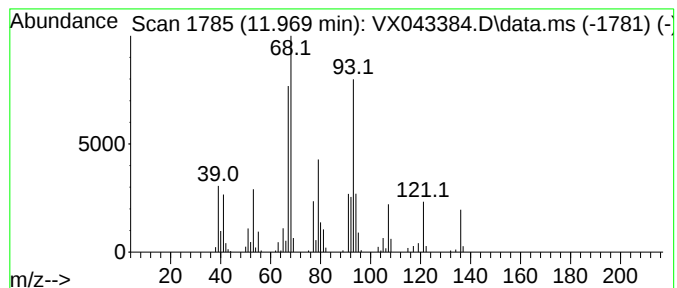
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Quant Title : SW846 8260

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

Peak Number 7 D-Limonene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	9.01 ug/l	66141	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	98
2			Limonene	136	C10H16	000138-86-3	89
3			1,5-Cyclooctadiene, 1,5-dimethyl-	136	C10H16	003760-14-3	70
4			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	64
5			Cyclohexene, 1-methyl-4-(1-methyl...	136	C10H16	005989-54-8	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043384.D
Acq On : 14 Oct 2024 16:26
Operator : JC/MD
Sample : P4402-02 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2 - Drum

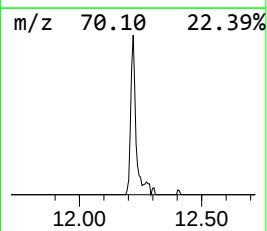
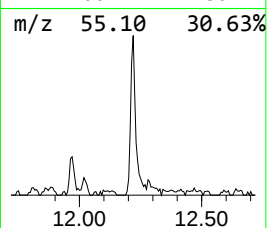
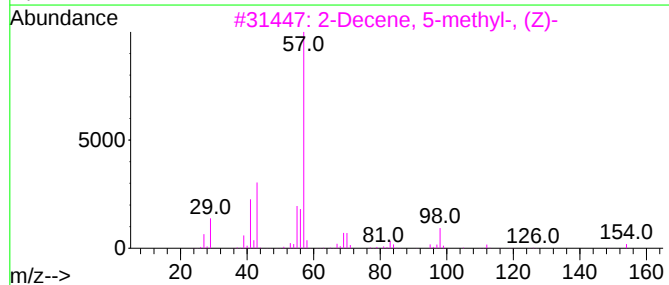
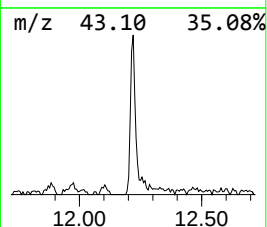
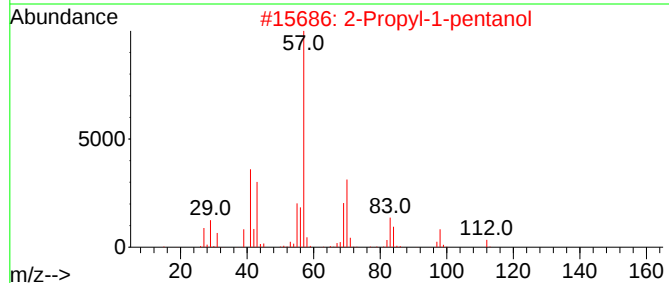
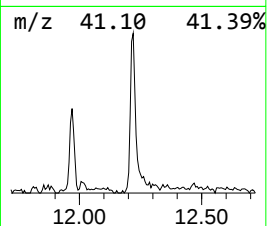
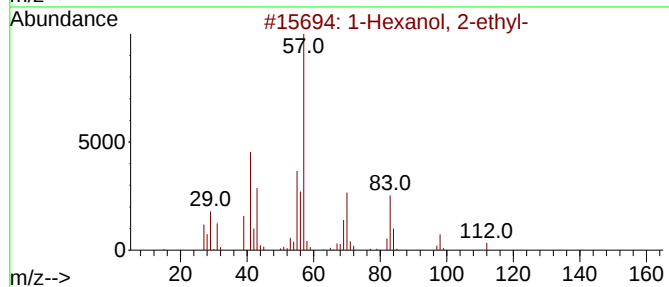
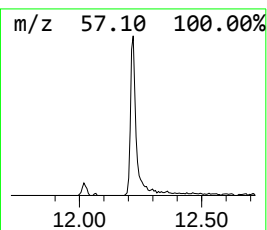
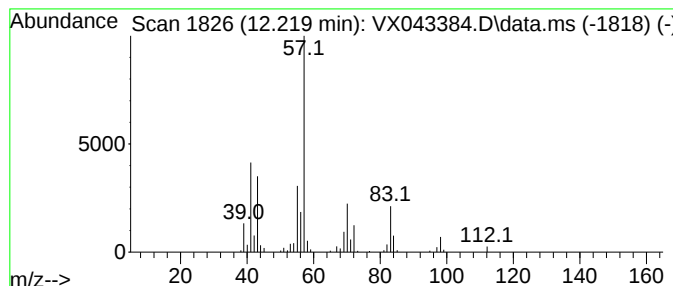
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Quant Title : SW846 8260

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

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	7.47 ug/l	54838	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	86
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3			2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	43
4			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	42
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043384.D
Acq On : 14 Oct 2024 16:26
Operator : JC/MD
Sample : P4402-02 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2 - Drum

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
1,3-Dioxane, 2-...	6.873	190.8	ug/l	1378640	2	6.757	361266	50.0
unknown7.208	7.208	84.2	ug/l	608083	2	6.757	361266	50.0
1,3-Dioxolane, ...	9.000	8.1	ug/l	66149	3	10.055	410520	50.0
1,3-Dioxolane, ...	9.872	5.8	ug/l	47927	3	10.055	410520	50.0
Oxazolidin-2-one	10.397	6.3	ug/l	51599	3	10.055	410520	50.0
D-Limonene	11.969	9.0	ug/l	66141	4	12.024	366900	50.0
1-Hexanol, 2-et...	12.219	7.5	ug/l	54838	4	12.024	366900	50.0