LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043381.D
Acq On : 14 Oct 2024 15:16
Operator : JC/MD
Sample : P4402-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4 - 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: VX043381.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	503988	636770	19.65%	6.762%
2	1.514	67	70	84	rVB	44336	113491	3.50%	1.205%
3	2.111	161	168	174	rBV	18330	34025	1.05%	0.361%
4	2.392	205	214	235	rVB	177325	337925	10.43%	3.589%
5	3.331	359	368	376	rBV	14207	34186	1.06%	0.363%
6	4.233	509	516	526	rBV2	11794	33162	1.02%	0.352%
7	4.568	563	571	589	rBV3	15245	55024	1.70%	0.584%
8	5.385	694	705	721	rBV2	56117	168299	5.19%	1.787%
9	5.544	721	731	747	rVV2	91688	266780	8.23%	2.833%
10	5.952	788	798	813	rBV	68820	182385	5.63%	1.937%
11	6.757	920	930	940	rBV	150811	366587	11.31%	3.893%
12	6.873	940	949	973	rVB	1335003	3240370	100.00%	34.412%
13	7.208	995	1004	1025	rBV	618297	1391802	42.95%	14.781%
14	8.647	1233	1240	1245	rBV	303157	490830	15.15%	5.213%
15	8.994	1291	1297	1309	rBV	78814	122118	3.77%	1.297%
16	9.159	1318	1324	1335	rBV	38731	58632	1.81%	0.623%
17	9.872	1435	1441	1450	rBV	81568	119651	3.69%	1.271%
18	9.970	1452	1457	1465	rVV	34674	48167	1.49%	0.512%
19	10.055	1465	1471	1486	rVB	294428	423006	13.05%	4.492%
20	10.396	1522	1527	1539	rBV	58094	76475	2.36%	0.812%
21	10.531	1544	1549	1557	rVB	30888	38744	1.20%	0.411%
22	11.079	1634	1639	1646	rBV	244445	315864	9.75%	3.354%
23	11.146	1646	1650	1658	rVV	29181	40935	1.26%	0.435%
24	12.018	1788	1793	1806	rBV	289767	371165	11.45%	3.942%
25	12.213	1820	1825	1842	rBV	331740	450001	13.89%	4.779%

Sum of corrected areas: 9416394

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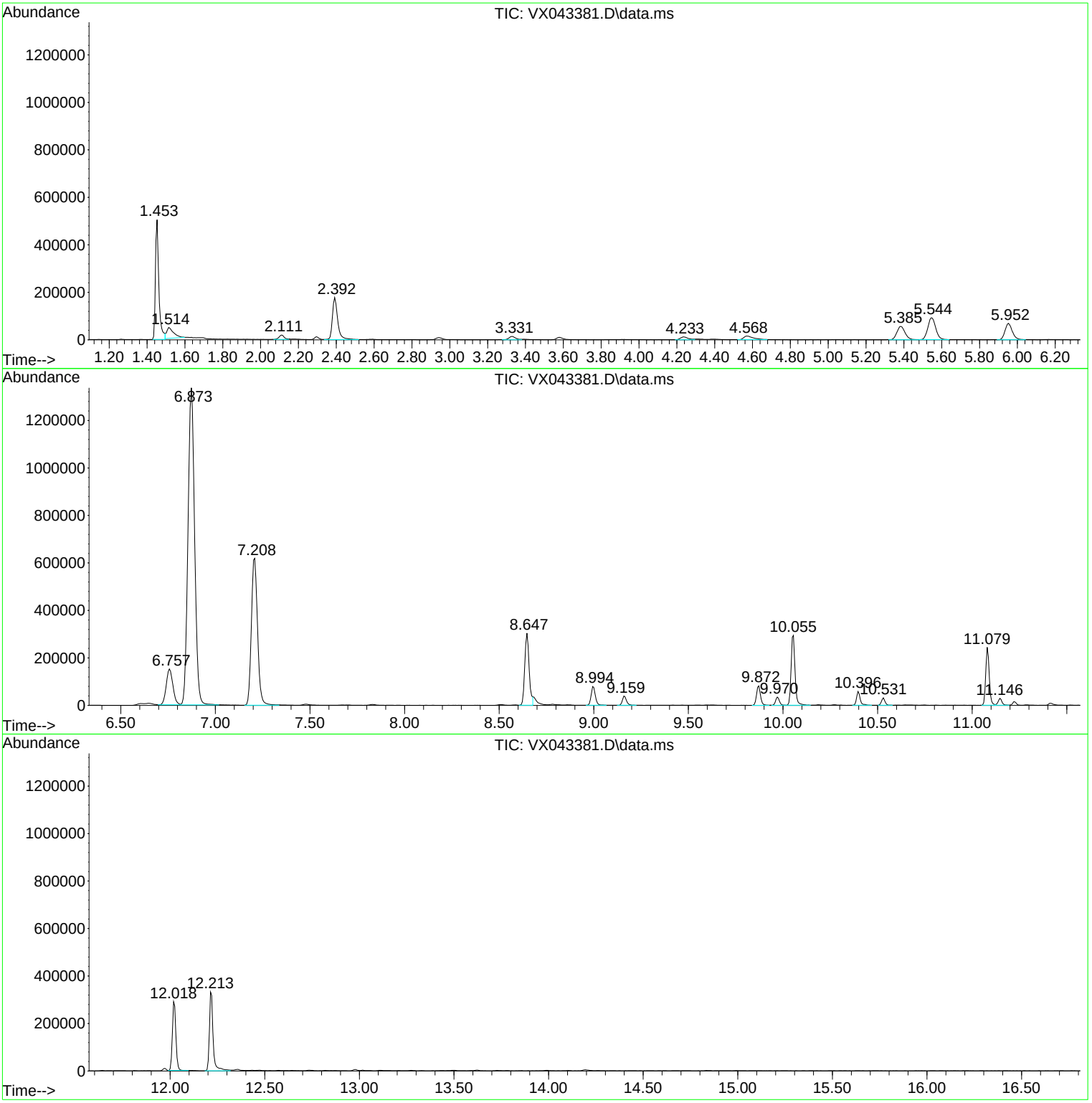
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4 - 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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043381.D
Acq On : 14 Oct 2024 15:16
Operator : JC/MD
Sample : P4402-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4 - Tote

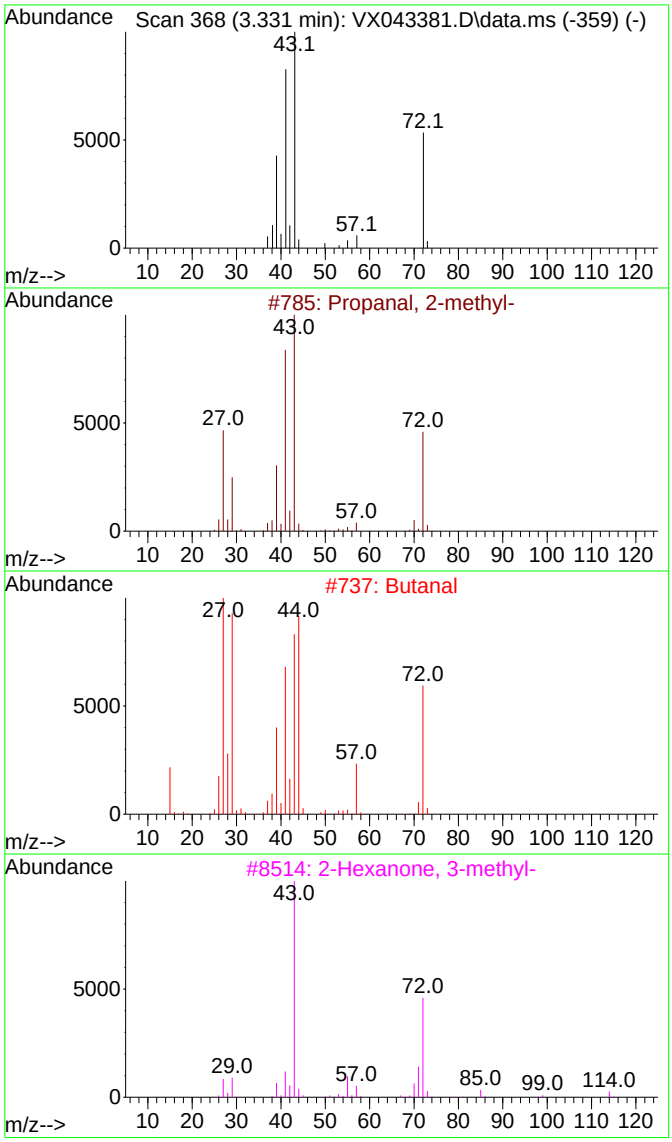
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

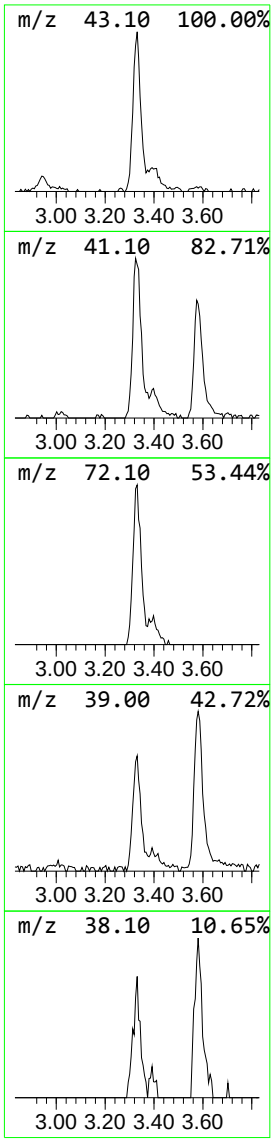
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanal, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.331	6.41 ug/l	34186	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-	72	C4H8O	000078-84-2	91
2	Butanal	72	C4H8O	000123-72-8	38
3	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	37
4	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	33
5	Isobutylene epoxide	72	C4H8O	000558-30-5	32





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043381.D
Acq On : 14 Oct 2024 15:16
Operator : JC/MD
Sample : P4402-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4 - Tote

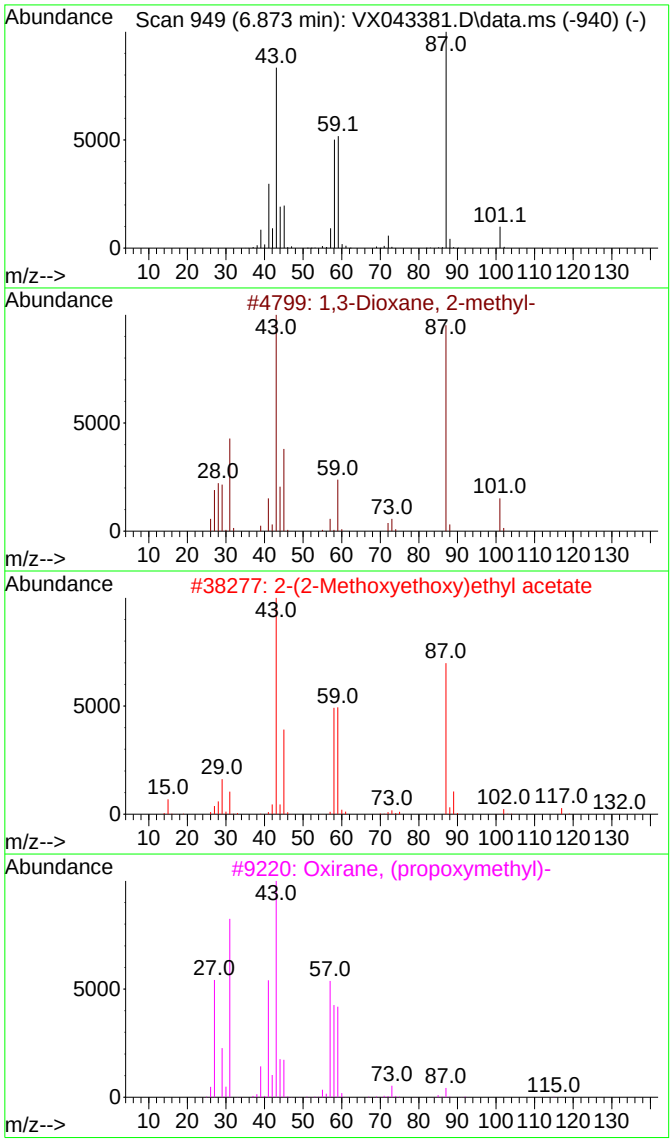
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

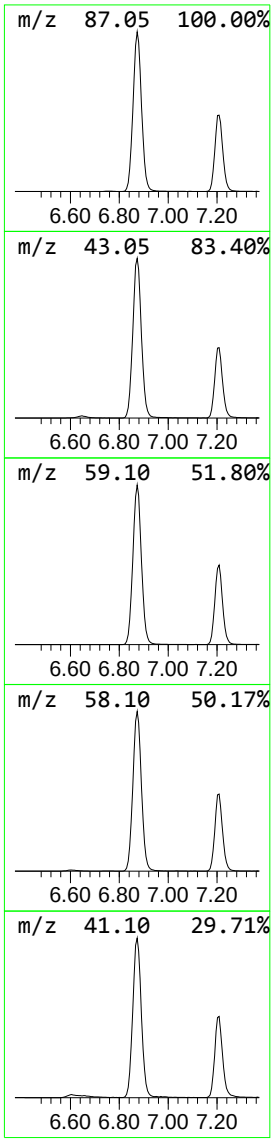
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown6.873 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.873	441.96 ug/l	3240370	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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043381.D
Acq On : 14 Oct 2024 15:16
Operator : JC/MD
Sample : P4402-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4 - Tote

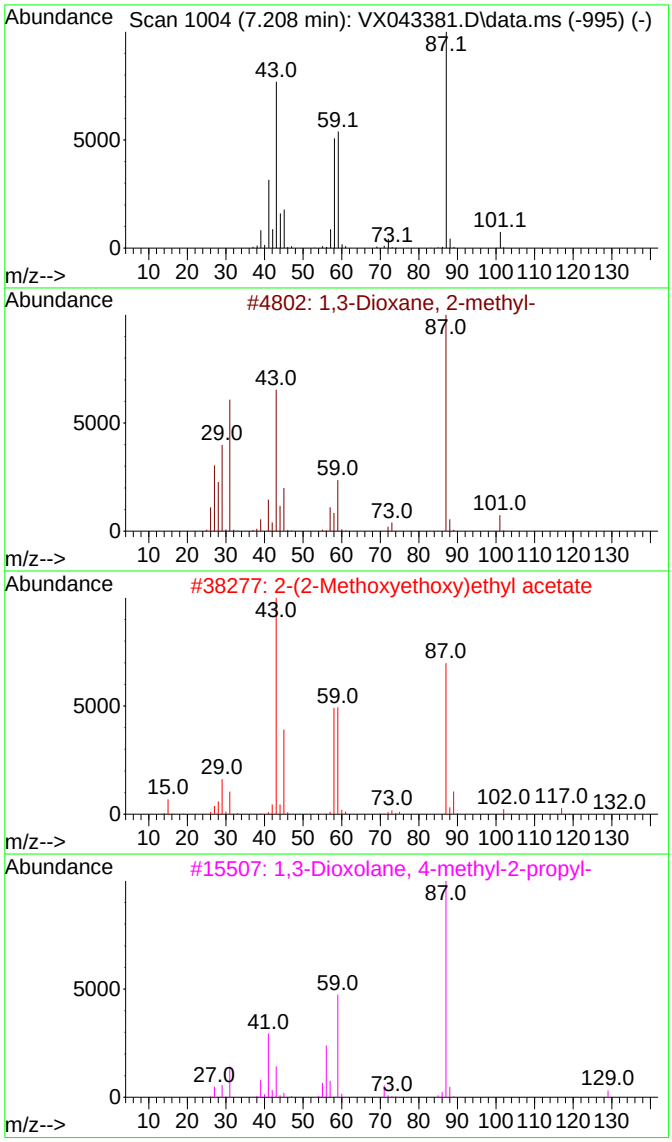
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

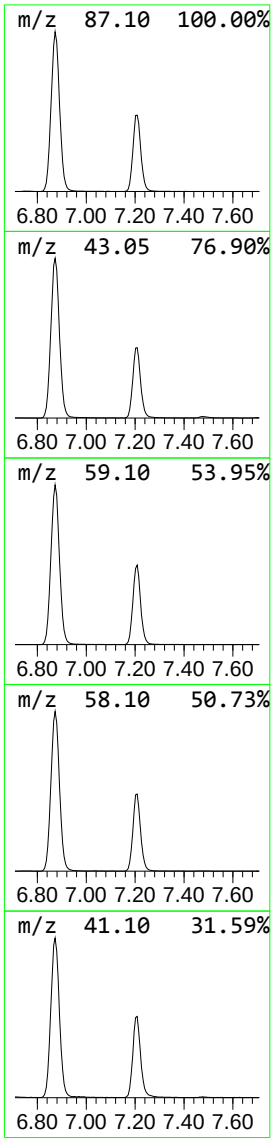
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,3-Dioxane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	189.83 ug/l	1391800	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	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	38
4	Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
5	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043381.D
Acq On : 14 Oct 2024 15:16
Operator : JC/MD
Sample : P4402-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4 - Tote

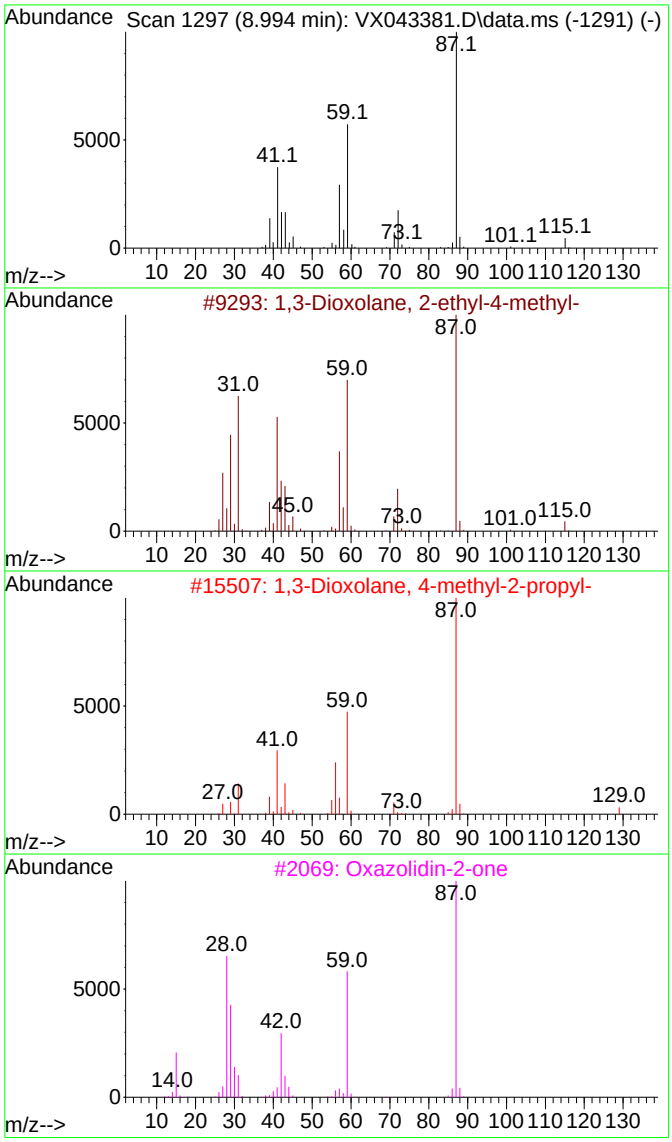
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

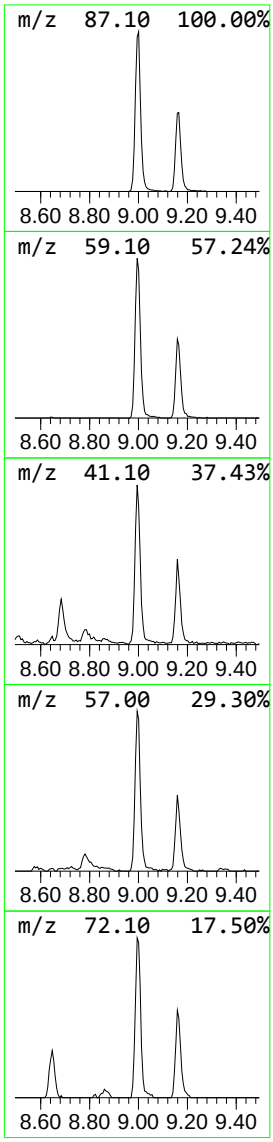
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.994	14.43 ug/l	122118	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	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	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043381.D
Acq On : 14 Oct 2024 15:16
Operator : JC/MD
Sample : P4402-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4 - Tote

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

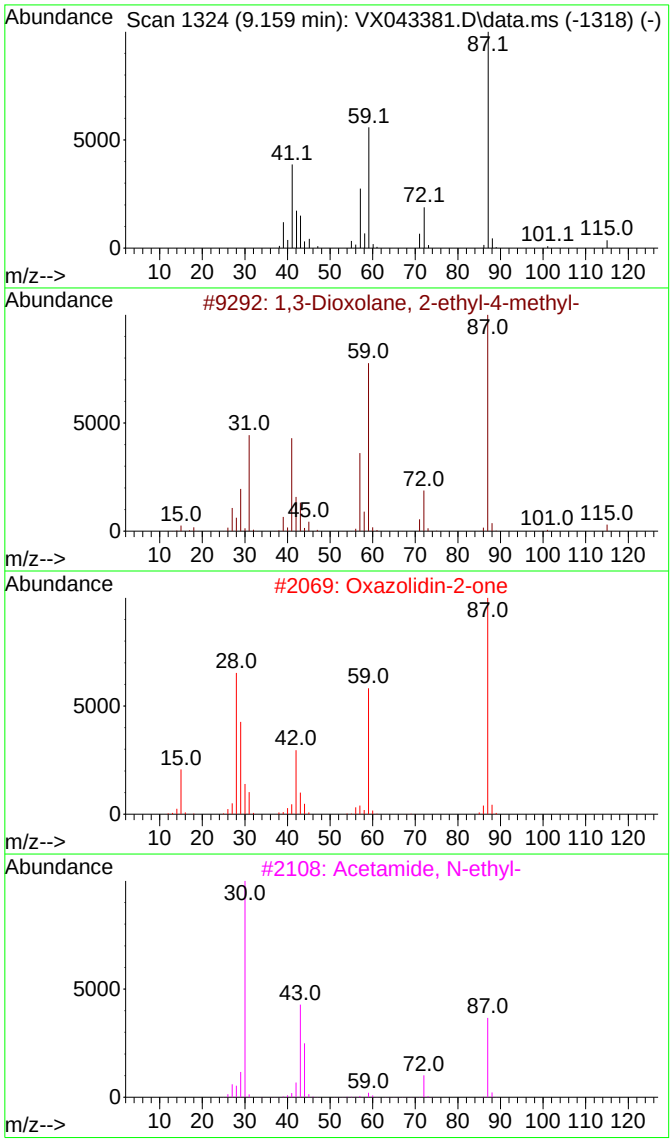
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

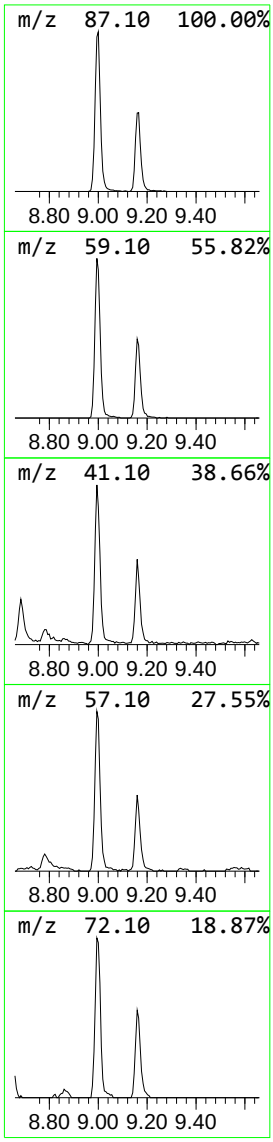
****

Peak Number 7 Oxazolidin-2-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.159	6.93 ug/l	58632	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	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	72
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
4	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
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 : VX043381.D
Acq On : 14 Oct 2024 15:16
Operator : JC/MD
Sample : P4402-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4 - Tote

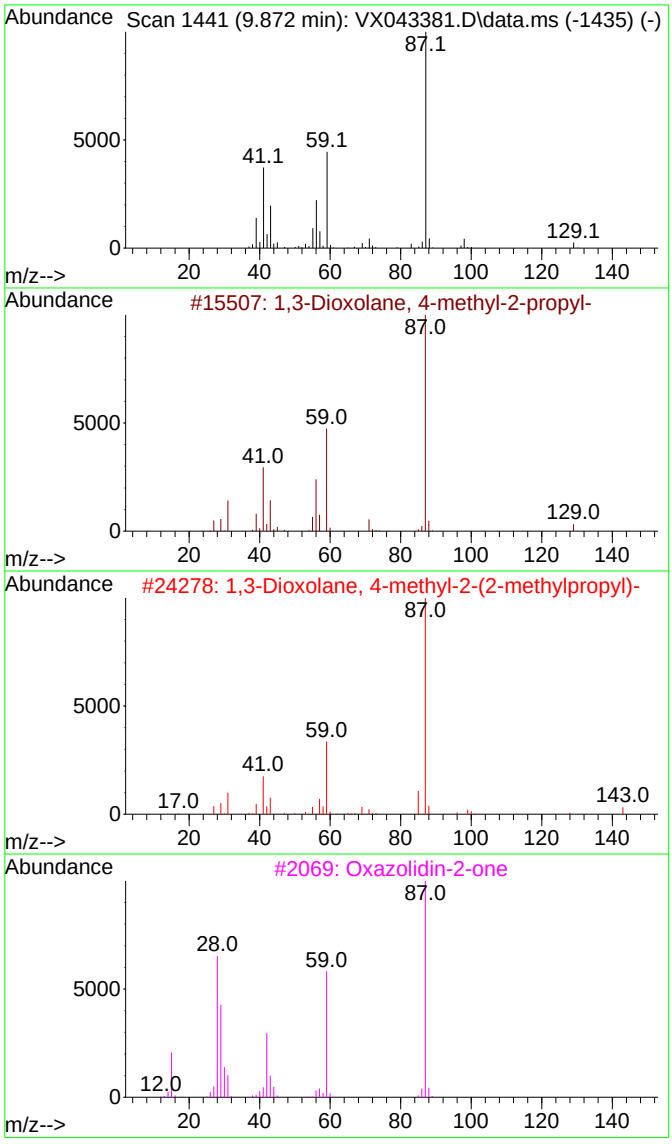
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

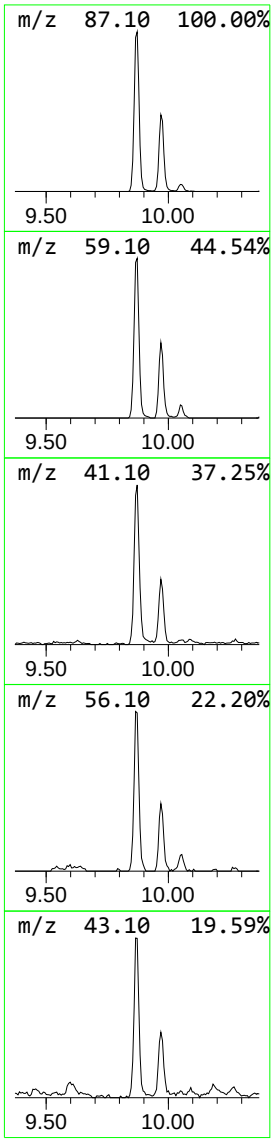
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.872	14.14 ug/l	119651	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	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	59
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	59
4	2-Hexyl-4-methyl-1,3-dioxolane	172	C10H20O2	004351-10-4	50
5	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	45





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Instrument :
MSVOA_X
ClientSampleId :
4 - Tote

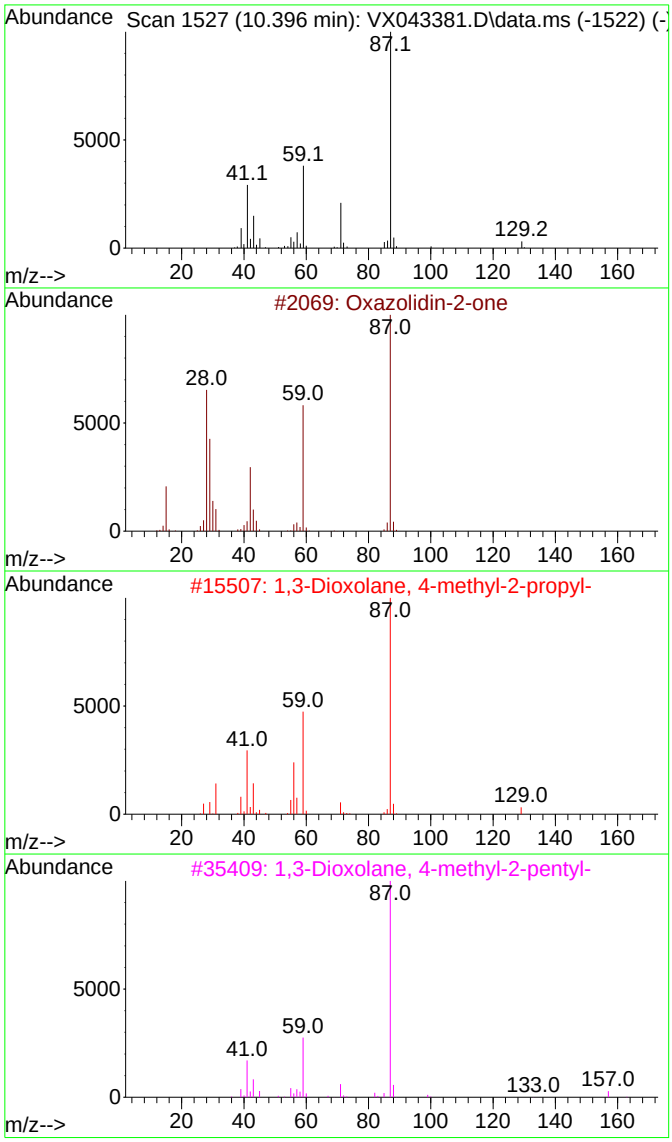
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

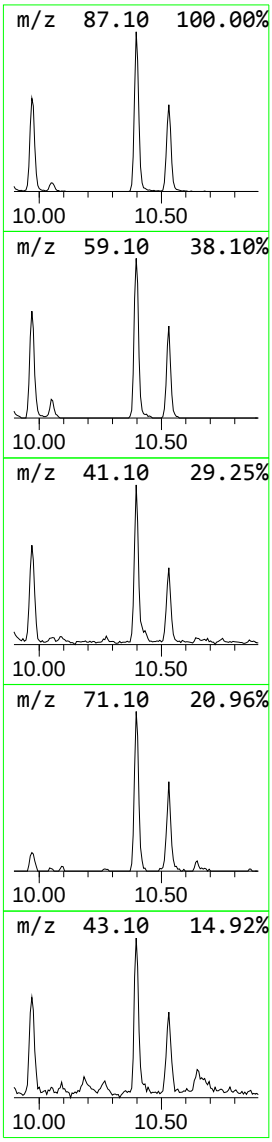
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.397	9.04 ug/l	76475	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
2	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	56
3	1,3-Dioxolane, 4-methyl-2-pentyl-	158	C9H18O2	001599-49-1	50
4	1,3-Dioxolane, 2-heptyl-4-methyl-	186	C11H22O2	074094-61-4	39
5	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	39





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MSVOA_X
ClientSampleId :
4 - Tote

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

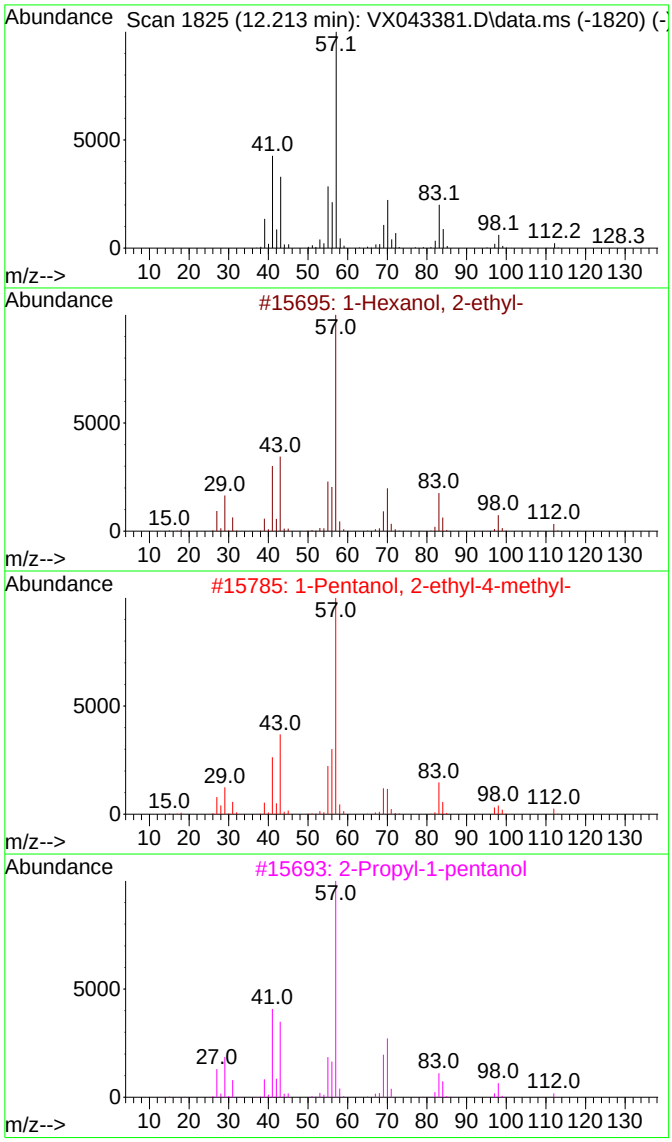
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

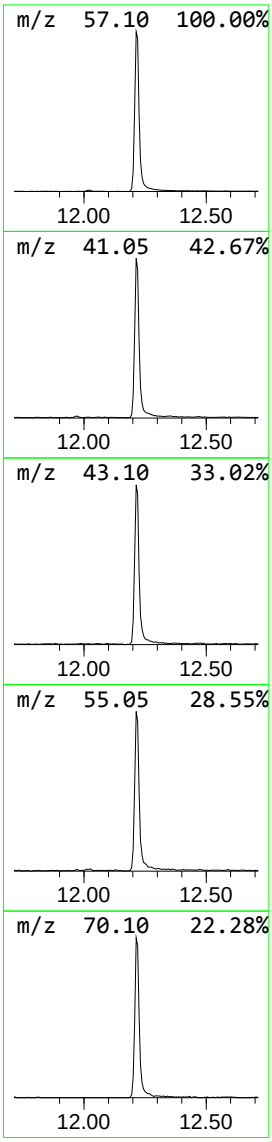
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	60.62 ug/l	450001	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	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	42
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
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Instrument :
MSVOA_X
ClientSampleId :
4 - 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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanal, 2-met...	3.331	6.4	ug/l	34186	1	5.544	266780	50.0
unknown6.873	6.873	442.0	ug/l	3240370	2	6.757	366587	50.0
1,3-Dioxane, 2-...	7.208	189.8	ug/l	1391800	2	6.757	366587	50.0
1,3-Dioxolane, ...	8.994	14.4	ug/l	122118	3	10.055	423006	50.0
Oxazolidin-2-one	9.159	6.9	ug/l	58632	3	10.055	423006	50.0
1,3-Dioxolane, ...	9.872	14.1	ug/l	119651	3	10.055	423006	50.0
1,3-Dioxolane, ...	10.397	9.0	ug/l	76475	3	10.055	423006	50.0
1-Hexanol, 2-et...	12.213	60.6	ug/l	450001	4	12.024	371165	50.0