LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060822\
Data File : VX029337.D
Acq On : 08 Jun 2022 21:27
Operator : JC/MD
Sample : N3181-04 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-31702

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\82X060722W.M
Title : SW846 8260

Signal : TIC: VX029337.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.392	206	214	239	rBV	8017458	15065325	100.00%	38.285%
2	5.391	693	706	717	rBV2	226230	653261	4.34%	1.660%
3	5.556	718	733	758	rVB	324522	1000913	6.64%	2.544%
4	5.958	789	799	815	rBV	256952	668238	4.44%	1.698%
5	6.763	920	931	941	rBV	476657	1143935	7.59%	2.907%
6	6.879	941	950	967	rVB	452325	1066568	7.08%	2.710%
7	7.214	996	1005	1022	rBV	291624	623809	4.14%	1.585%
8	7.830	1096	1106	1123	rBV	4949784	9067791	60.19%	23.044%
9	8.653	1234	1241	1247	rBV	1263220	1956019	12.98%	4.971%
10	8.720	1247	1252	1264	rVB	847236	1279751	8.49%	3.252%
11	9.001	1291	1298	1314	rBV	226581	343915	2.28%	0.874%
12	9.165	1319	1325	1333	rBV	130373	191131	1.27%	0.486%
13	10.055	1465	1471	1481	rVB	977535	1286814	8.54%	3.270%
14	11.086	1634	1640	1647	rBV	995885	1293785	8.59%	3.288%
15	12.024	1788	1794	1802	rBV	935044	1171075	7.77%	2.976%
16	12.219	1820	1826	1840	rBV	1706237	2121202	14.08%	5.391%
17	12.469	1862	1867	1872	rVB	213617	249868	1.66%	0.635%
18	15.999	2442	2446	2456	rVB9	58671	166679	1.11%	0.424%

Sum of corrected areas: 39350079

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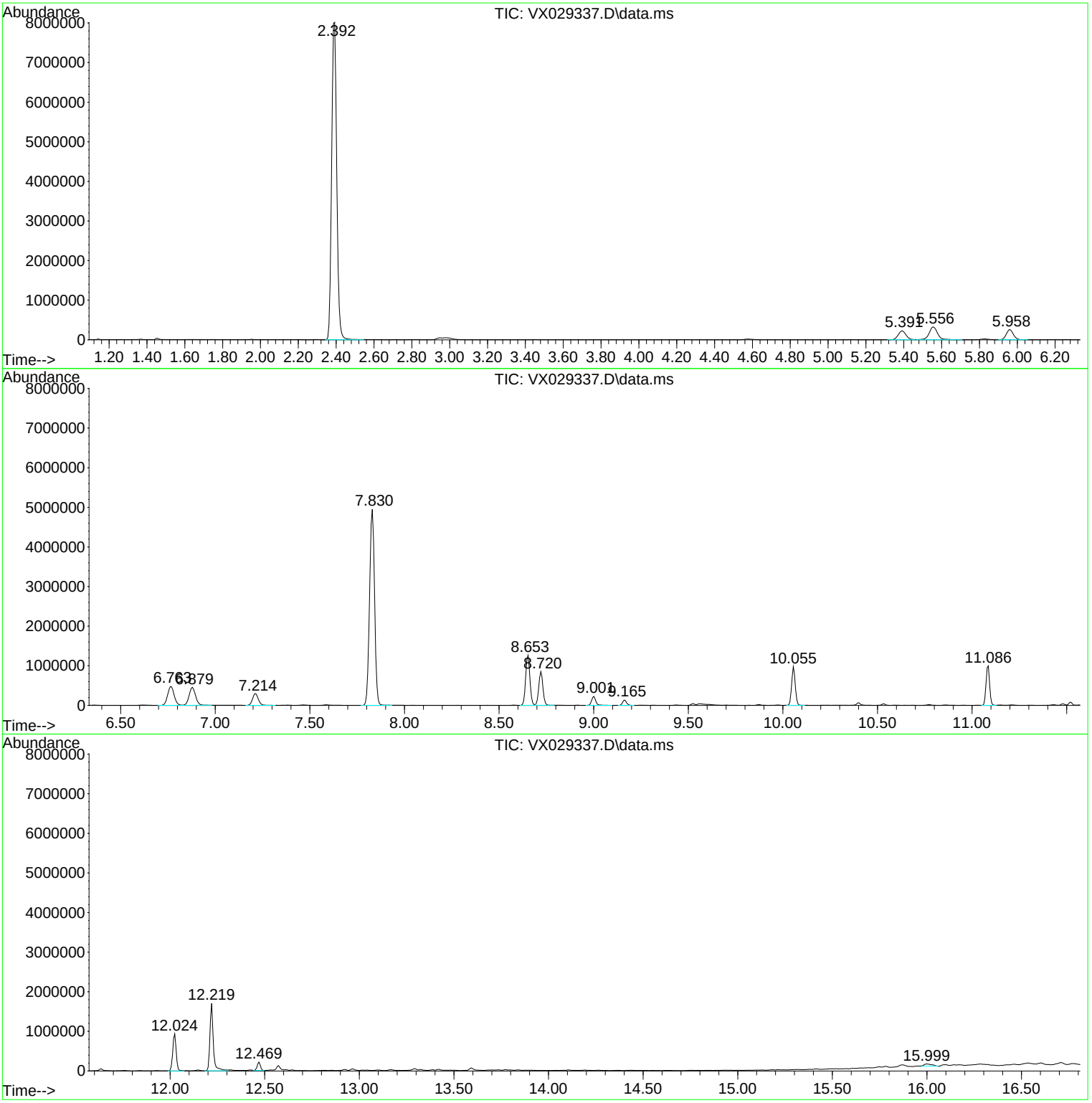
Instrument :
MSVOA_X
ClientSampleId :
TRE-31702

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

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



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Data File : VX029337.D
Acq On : 08 Jun 2022 21:27
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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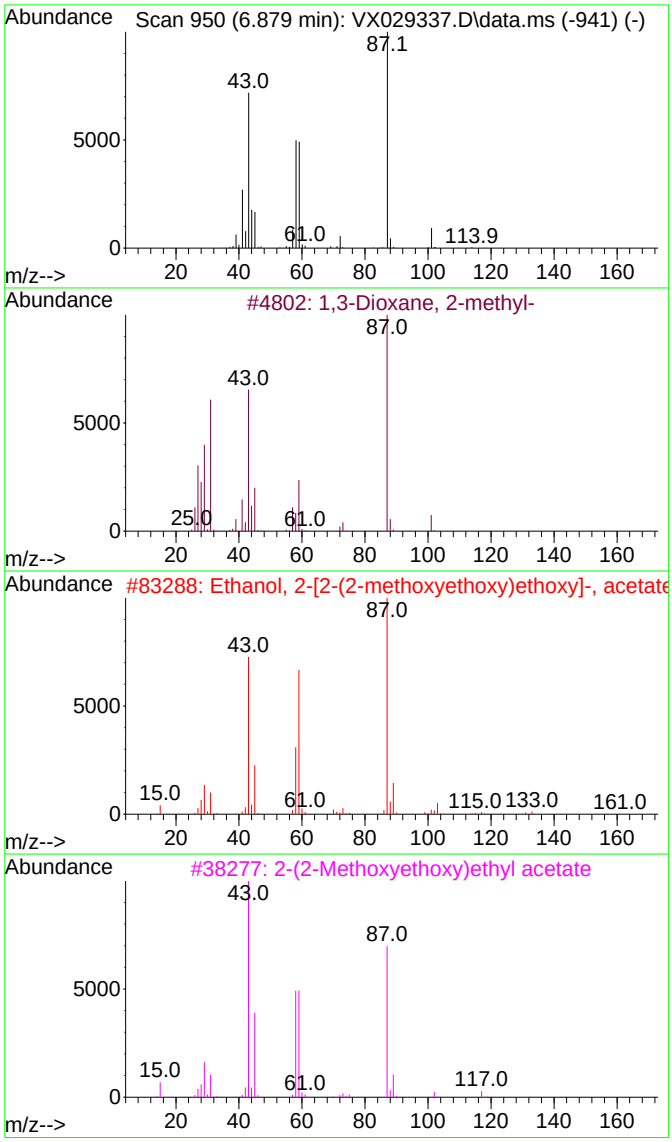
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

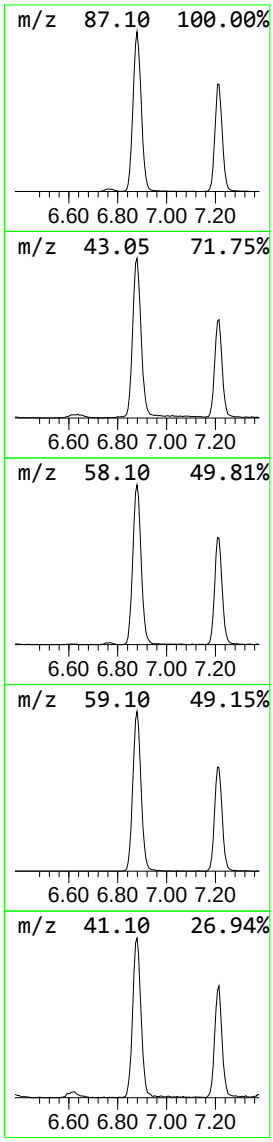
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	46.62 ug/l	1066570	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	53
2	Ethanol, 2-[2-(2-methoxyethoxy)e...	206	C9H18O5	003610-27-3	45
3	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
4	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	38
5	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38





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Operator : JC/MD
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-31702

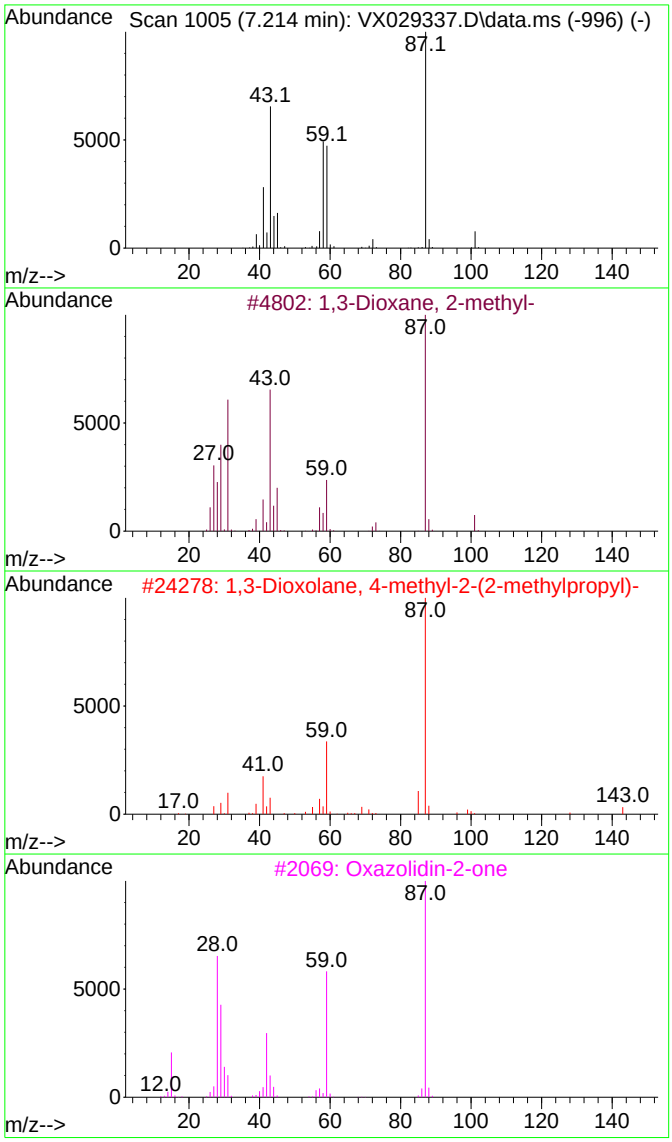
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

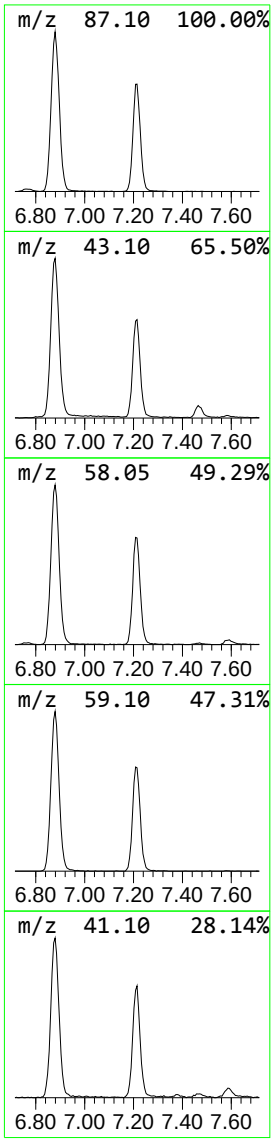
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	27.27 ug/l	623809	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	52
2	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	50
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
4	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	36
5	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	33





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Data File : VX029337.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-31702

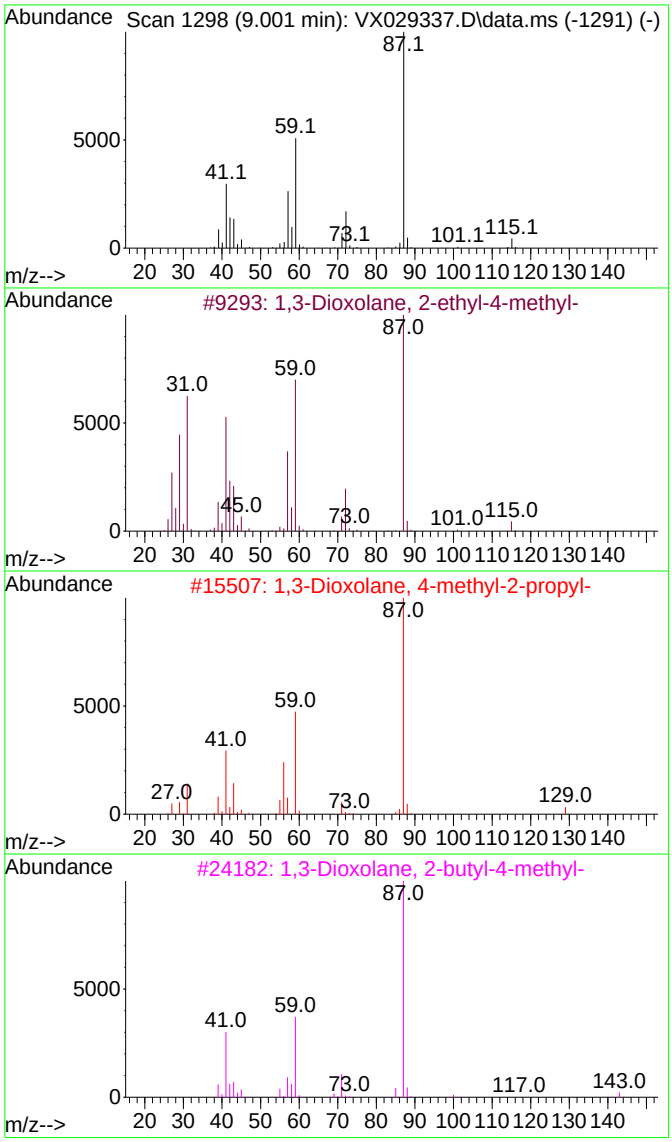
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

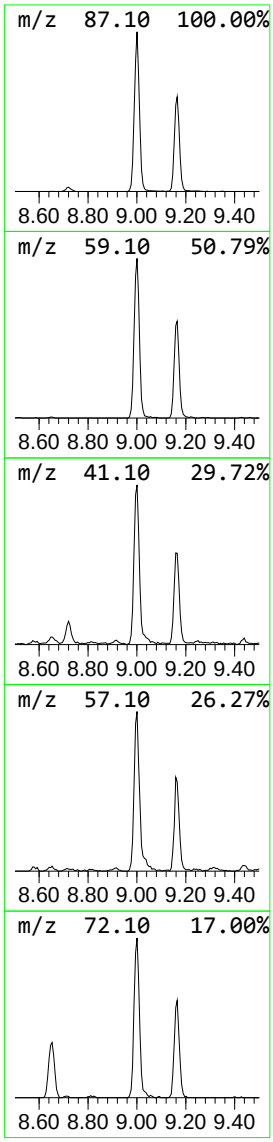
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.001	13.36 ug/l	343915	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	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	59
3	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	56
4	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	50





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Data File : VX029337.D
Acq On : 08 Jun 2022 21:27
Operator : JC/MD
Sample : N3181-04 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-31702

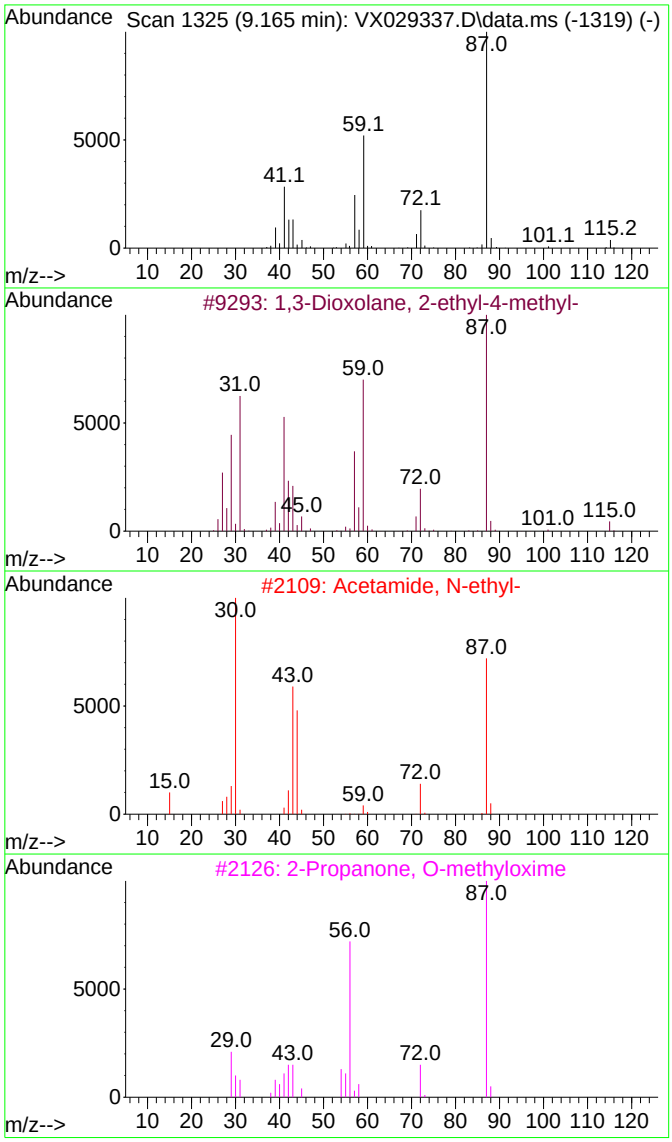
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

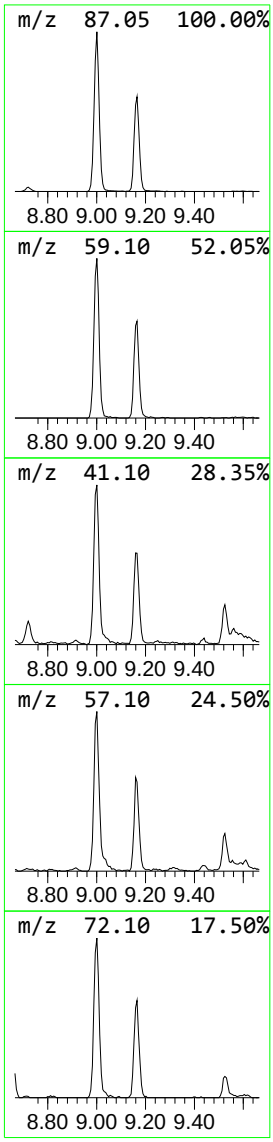
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Acetamide, N-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.165	7.43 ug/l	191131	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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
3	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
4	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	50
5	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	50





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Data File : VX029337.D
Acq On : 08 Jun 2022 21:27
Operator : JC/MD
Sample : N3181-04 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-31702

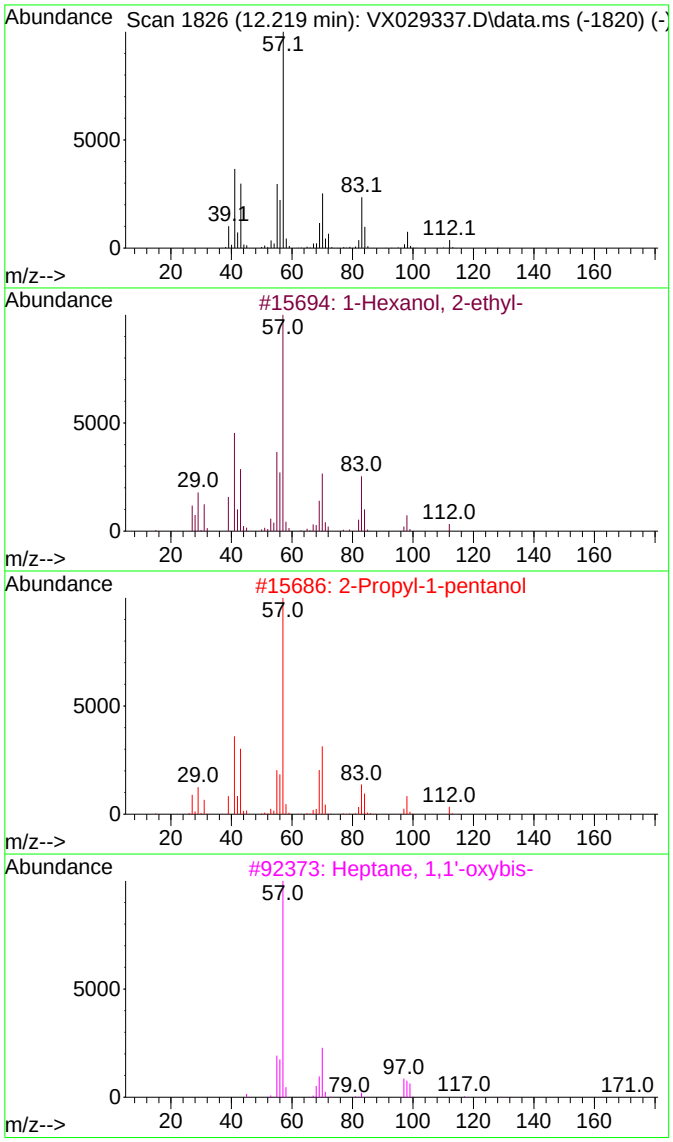
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

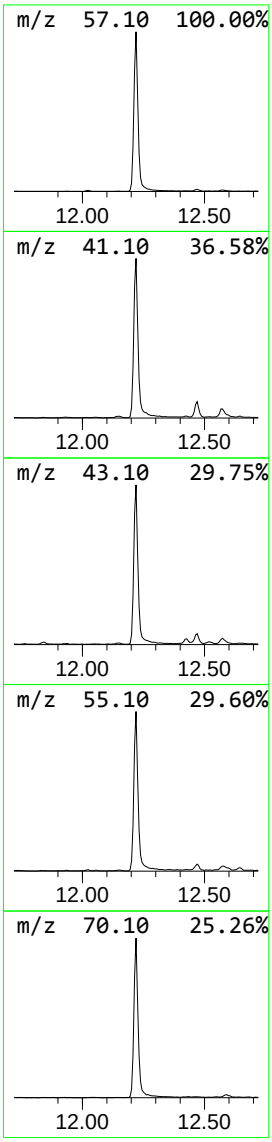
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.220	90.57 ug/l	2121200	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	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	47
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	43





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Instrument :
MSVOA_X
ClientSampleId :
TRE-31702

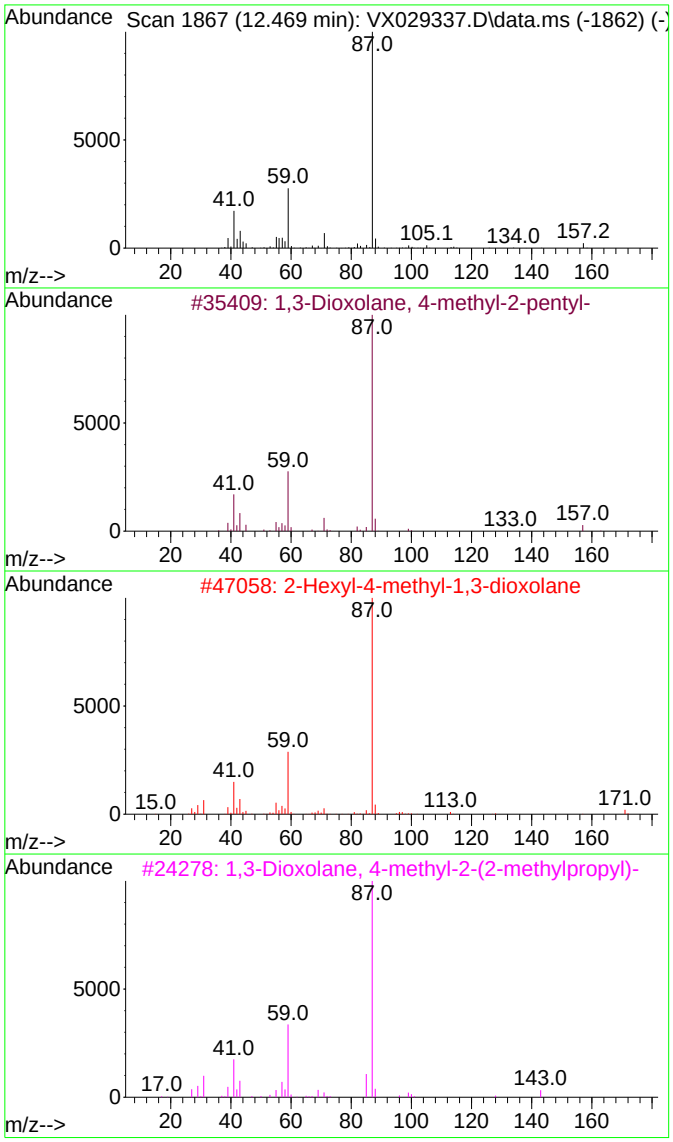
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

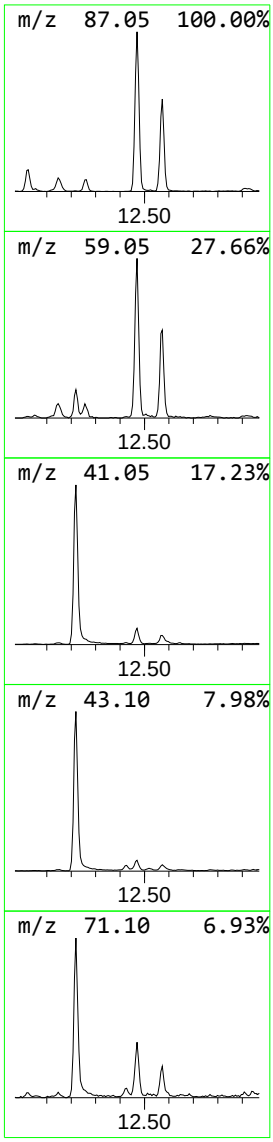
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	10.67 ug/l	249868	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	83
2	2-Hexyl-4-methyl-1,3-dioxolane	172	C10H20O2	004351-10-4	72
3	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	56
4	1,3-Dioxolane, 2-heptyl-4-methyl-	186	C11H22O2	074094-61-4	56
5	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	56





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

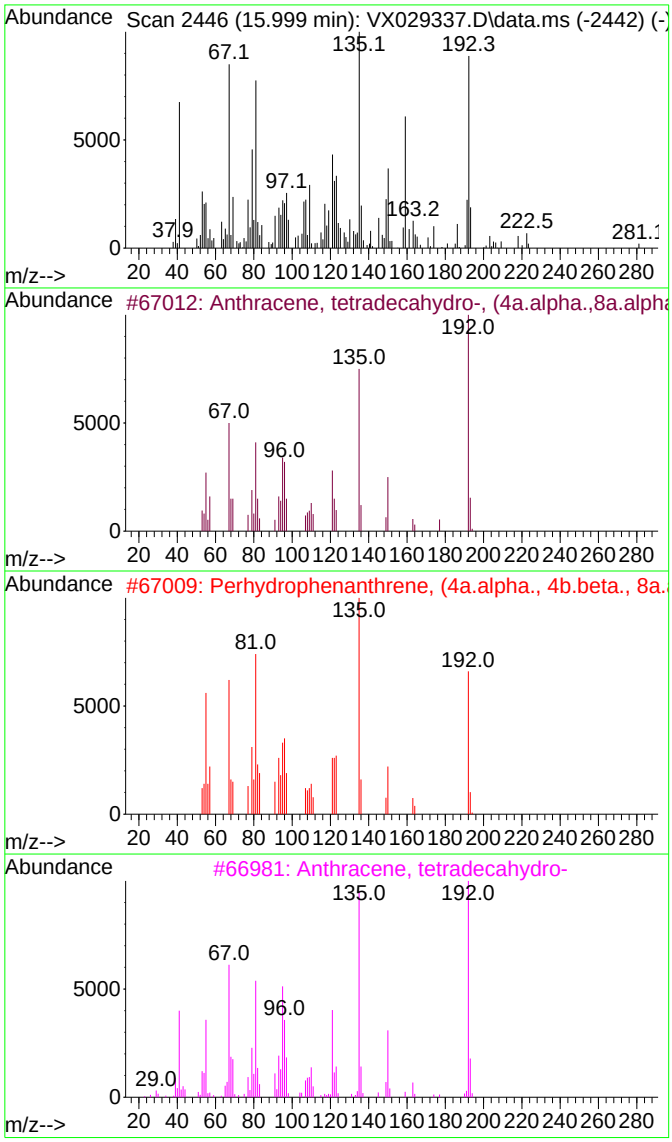
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

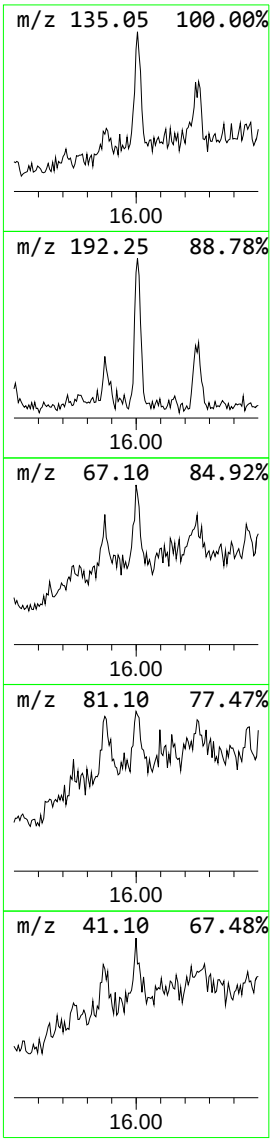
****

Peak Number 7 unknown15.999 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.999	7.12 ug/l	166679	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, tetradecahydro-, (4a...	192	C14H24	001755-19-7	53
2	Perhydrophenanthrene, (4a.alpha....	192	C14H24	002108-89-6	49
3	Anthracene, tetradecahydro-	192	C14H24	006596-35-6	45
4	Cyclopropane, (2-methylenebutyl)-	110	C8H14	074685-56-6	25
5	4-Hydroxy-3,5-dimethylcinnamic acid	192	C11H12O3	1000132-15-8	11





Tentatively Identified Compound (LSC) summary

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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
1,3-Dioxane, 2-...	6.879	46.6	ug/l	1066570	2	6.763	1143940	50.0
1,3-Dioxolane, ...	7.214	27.3	ug/l	623809	2	6.763	1143940	50.0
1,3-Dioxolane, ...	9.001	13.4	ug/l	343915	3	10.055	1286810	50.0
Acetamide, N-et...	9.165	7.4	ug/l	191131	3	10.055	1286810	50.0
1-Hexanol, 2-et...	12.220	90.6	ug/l	2121200	4	12.024	1171080	50.0
1,3-Dioxolane, ...	12.469	10.7	ug/l	249868	4	12.024	1171080	50.0
unknown15.999	15.999	7.1	ug/l	166679	4	12.024	1171080	50.0