LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
Data File : VX041404.D
Acq On : 07 May 2024 14:17
Operator : JC/MD
Sample : P2389-01 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

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\82X043024W.M
Title : SW846 8260

Signal : TIC: VX041404.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	36	rBV2	6565	13652	1.91%	0.239%
2	1.453	56	60	69	rBV	200238	284563	39.84%	4.985%
3	1.532	69	73	82	rVB2	11830	33743	4.72%	0.591%
4	2.294	193	198	205	rBV	18702	33828	4.74%	0.593%
5	2.392	208	214	231	rVB	17796	40850	5.72%	0.716%
6	2.947	295	305	320	rBV	23426	59502	8.33%	1.042%
7	4.391	532	542	555	rBV	15283	51849	7.26%	0.908%
8	4.629	570	581	595	rBV3	4248	18227	2.55%	0.319%
9	5.385	695	705	721	rVB	87163	256632	35.93%	4.496%
10	5.550	721	732	748	rBV	162415	468727	65.63%	8.211%
11	5.952	789	798	814	rBV	92614	250630	35.09%	4.391%
12	6.757	921	930	941	rBV	237212	579863	81.19%	10.158%
13	6.879	941	950	967	rVB	204079	532694	74.58%	9.332%
14	7.214	998	1005	1018	rBV2	29486	71967	10.08%	1.261%
15	8.647	1233	1240	1254	rBV	422984	677078	94.80%	11.861%
16	9.000	1293	1298	1305	rBV	13747	23264	3.26%	0.408%
17	10.055	1465	1471	1490	rBV	512385	714218	100.00%	12.512%
18	10.988	1619	1624	1634	rBV3	6926	11486	1.61%	0.201%
19	11.079	1634	1639	1653	rVV	434026	566809	79.36%	9.930%
20	11.195	1653	1658	1669	rVB	8917	12762	1.79%	0.224%
21	12.018	1788	1793	1811	rVB	472932	633444	88.69%	11.097%
22	12.219	1822	1826	1834	rBV	7218	11366	1.59%	0.199%
23	12.768	1911	1916	1928	rBV	293379	361121	50.56%	6.326%

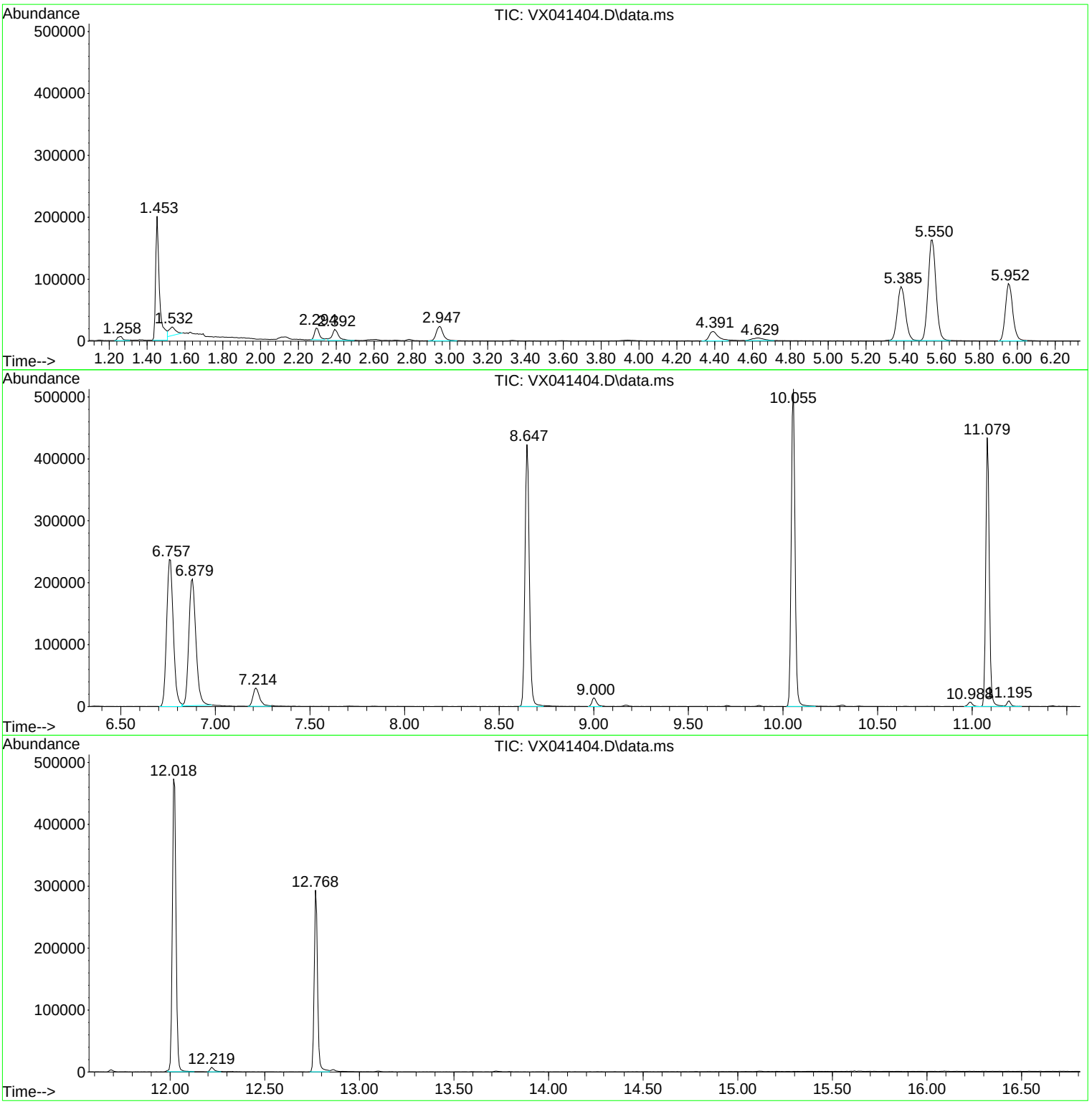
Sum of corrected areas: 5708275

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
Data File : VX041404.D
Acq On : 07 May 2024 14:17
Operator : JC/MD
Sample : P2389-01 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
Data File : VX041404.D
Acq On : 07 May 2024 14:17
Operator : JC/MD
Sample : P2389-01 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

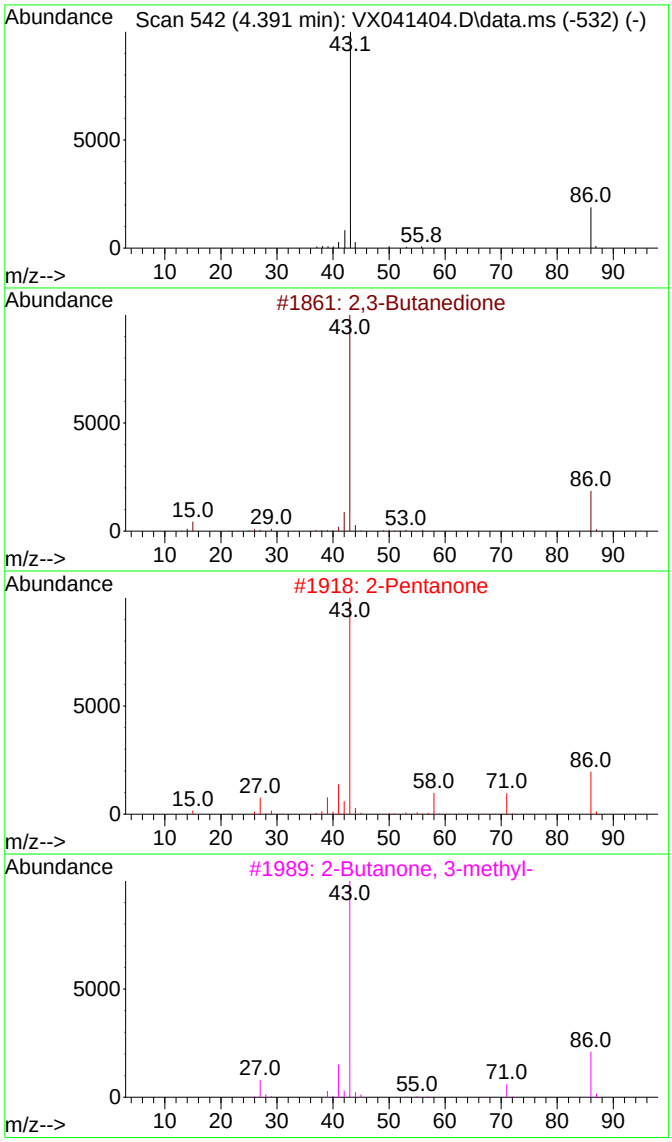
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

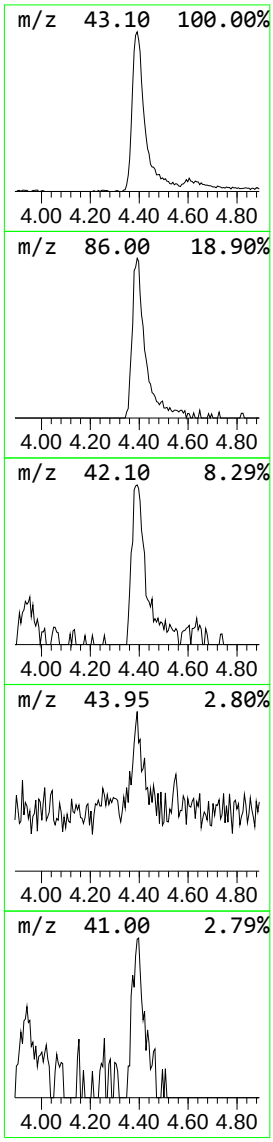
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,3-Butanedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.391	5.53 ug/l	51849	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione	86	C4H6O2	000431-03-8	90
2	2-Pentanone	86	C5H10O	000107-87-9	86
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	7
4	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	7
5	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
Data File : VX041404.D
Acq On : 07 May 2024 14:17
Operator : JC/MD
Sample : P2389-01 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

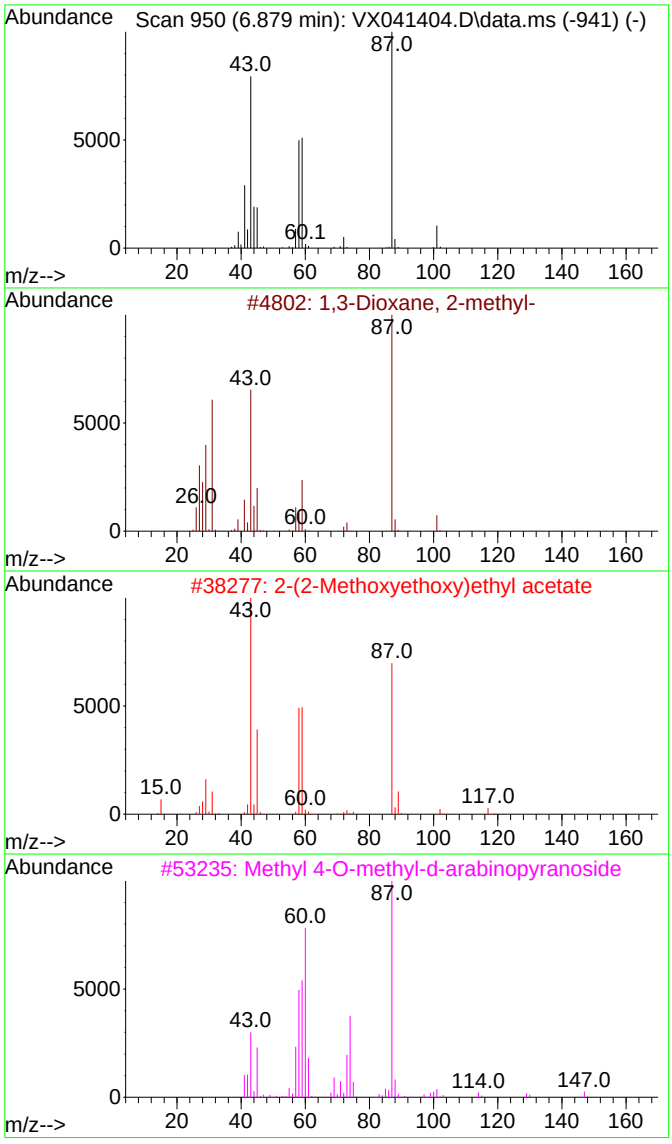
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

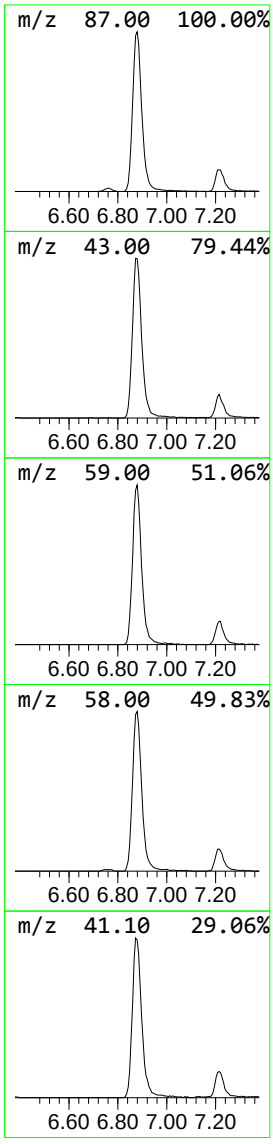
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	45.93 ug/l	532694	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	50
2	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
3	Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
4	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	37
5	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
Data File : VX041404.D
Acq On : 07 May 2024 14:17
Operator : JC/MD
Sample : P2389-01 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

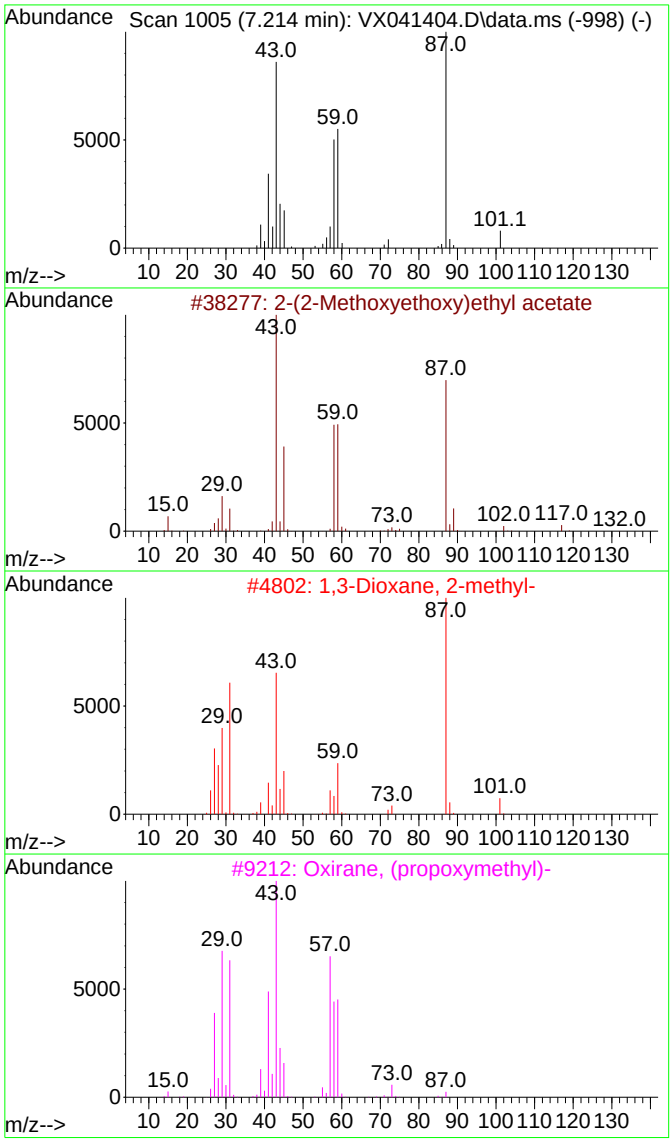
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

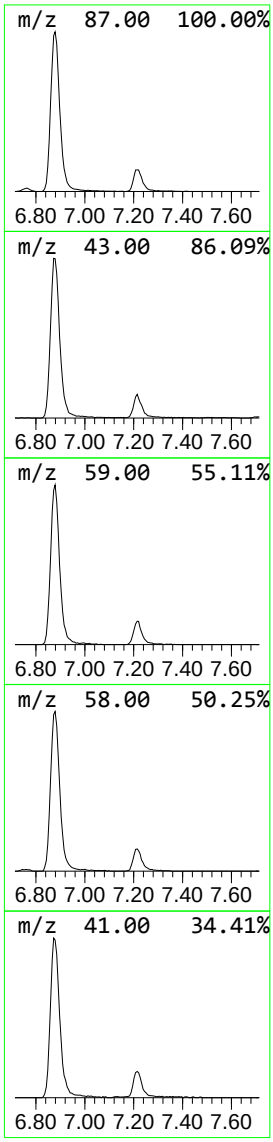
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-(2-Methoxyethoxy)ethyl ac... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	6.21 ug/l	71967	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	64
2	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	45
3	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	43
4	trans-1-Nitro-1-propene	87	C3H5NO2	017082-05-2	38
5	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
Data File : VX041404.D
Acq On : 07 May 2024 14:17
Operator : JC/MD
Sample : P2389-01 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

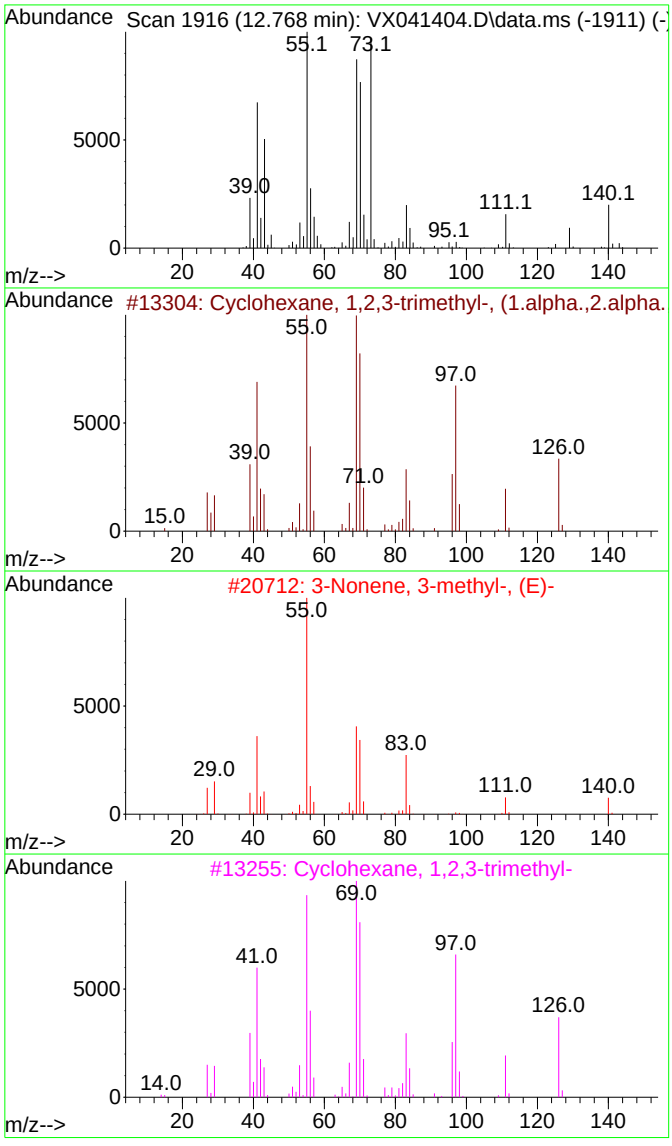
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

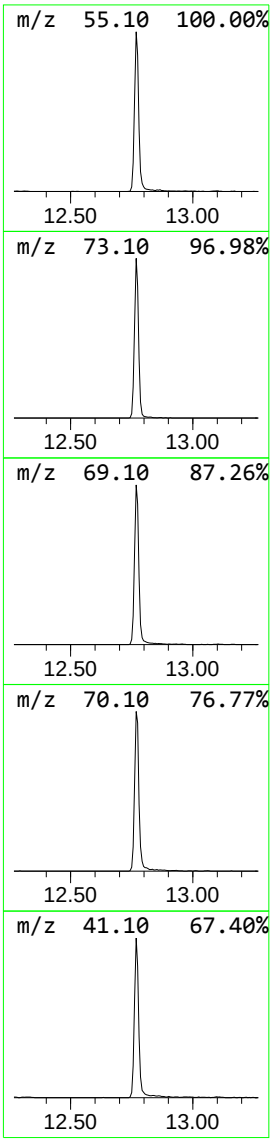
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclohexane, 1,2,3-trimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.768	28.50 ug/l	361121	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,3-trimethyl-, (...	126	C9H18	001839-88-9	72
2	3-Nonene, 3-methyl-, (E)-	140	C10H20	069405-42-1	68
3	Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	64
4	4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	64
5	3-Octene, 4-ethyl-	140	C10H20	053966-51-1	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
Data File : VX041404.D
Acq On : 07 May 2024 14:17
Operator : JC/MD
Sample : P2389-01 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.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
2,3-Butanedione	4.391	5.5	ug/l	51849	1	5.550	468727	50.0
1,3-Dioxane, 2-...	6.879	45.9	ug/l	532694	2	6.763	579863	50.0
2-(2-Methoxyeth...	7.214	6.2	ug/l	71967	2	6.763	579863	50.0
Cyclohexane, 1,...	12.768	28.5	ug/l	361121	4	12.024	633444	50.0