LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070723\
Data File : VX036469.D
Acq On : 07 Jul 2023 19:02
Operator : JC/MD
Sample : 03533-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1674

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\82X062323W.M
Title : SW846 8260

Signal : TIC: VX036469.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	83	rBV	1338711	1953781	35.20%	10.844%
2	2.392	208	214	230	rVB	71184	140312	2.53%	0.779%
3	4.391	532	542	563	rBV	64133	214683	3.87%	1.192%
4	4.574	563	572	586	rVB3	19774	66070	1.19%	0.367%
5	5.391	694	706	719	rBV	106577	306728	5.53%	1.702%
6	5.556	723	733	749	rVB	187391	516297	9.30%	2.866%
7	5.958	789	799	811	rBV	120283	318028	5.73%	1.765%
8	6.763	921	931	940	rBV	284500	679736	12.24%	3.773%
9	6.879	940	950	966	rVV	2394273	5551161	100.00%	30.811%
10	7.214	994	1005	1028	rBV	1933688	4166713	75.06%	23.127%
11	7.677	1072	1081	1092	rBV	42820	89177	1.61%	0.495%
12	8.647	1234	1240	1249	rBV	593510	934991	16.84%	5.190%
13	9.000	1291	1298	1313	rBV	52977	86010	1.55%	0.477%
14	9.159	1318	1324	1333	rBV	45998	67074	1.21%	0.372%
15	10.055	1465	1471	1485	rVB	615563	833942	15.02%	4.629%
16	11.079	1634	1639	1647	rBV	493430	637202	11.48%	3.537%
17	12.024	1789	1794	1801	rVB	608802	772104	13.91%	4.285%
18	14.615	2215	2219	2222	rBV	50374	70047	1.26%	0.389%
19	15.213	2314	2317	2321	rVB2	64253	71025	1.28%	0.394%
20	15.420	2346	2351	2356	rVB2	97213	145649	2.62%	0.808%
21	15.487	2357	2362	2368	rBV6	31838	85882	1.55%	0.477%
22	15.743	2399	2404	2409	rVB	106893	173495	3.13%	0.963%
23	15.865	2420	2424	2429	rVB4	43874	80503	1.45%	0.447%
24	16.706	2556	2562	2571	rVB2	27849	56084	1.01%	0.311%

Sum of corrected areas: 18016694

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Instrument :
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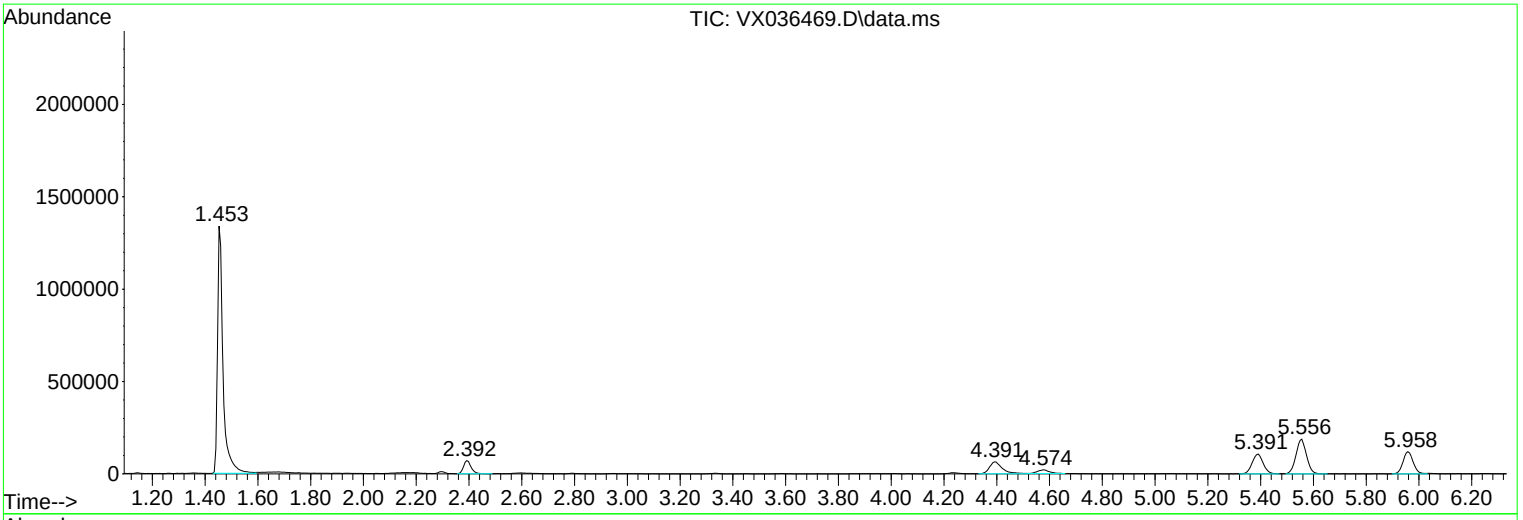
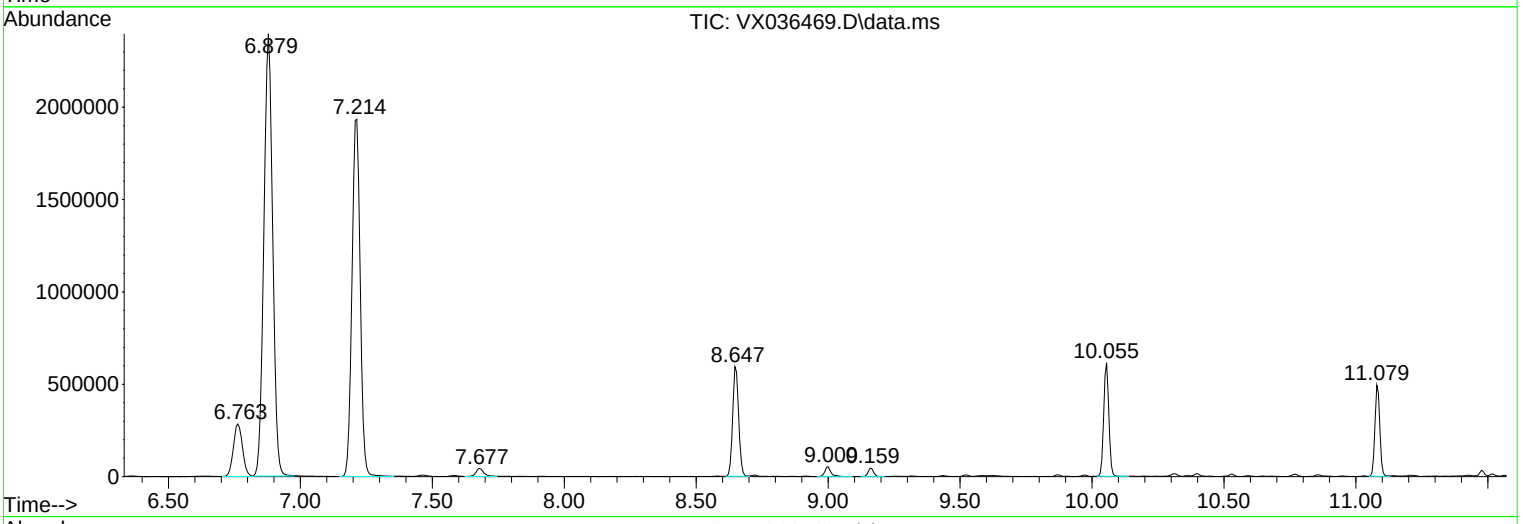
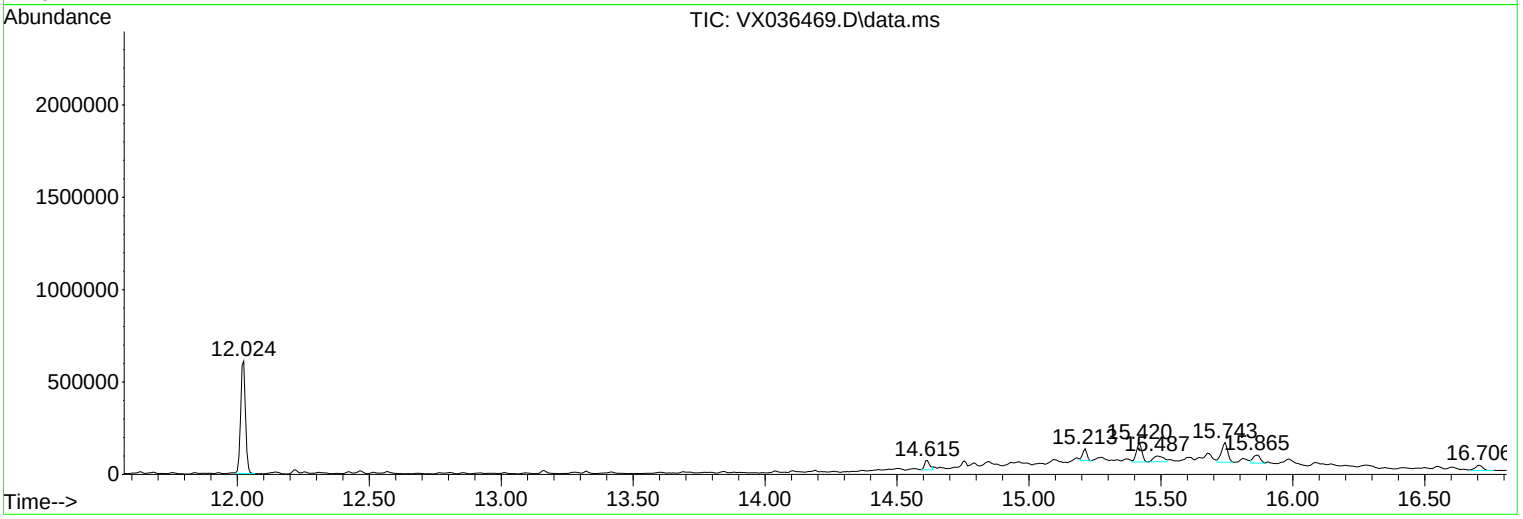
ClientSampleId :
1674

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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







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Data File : VX036469.D
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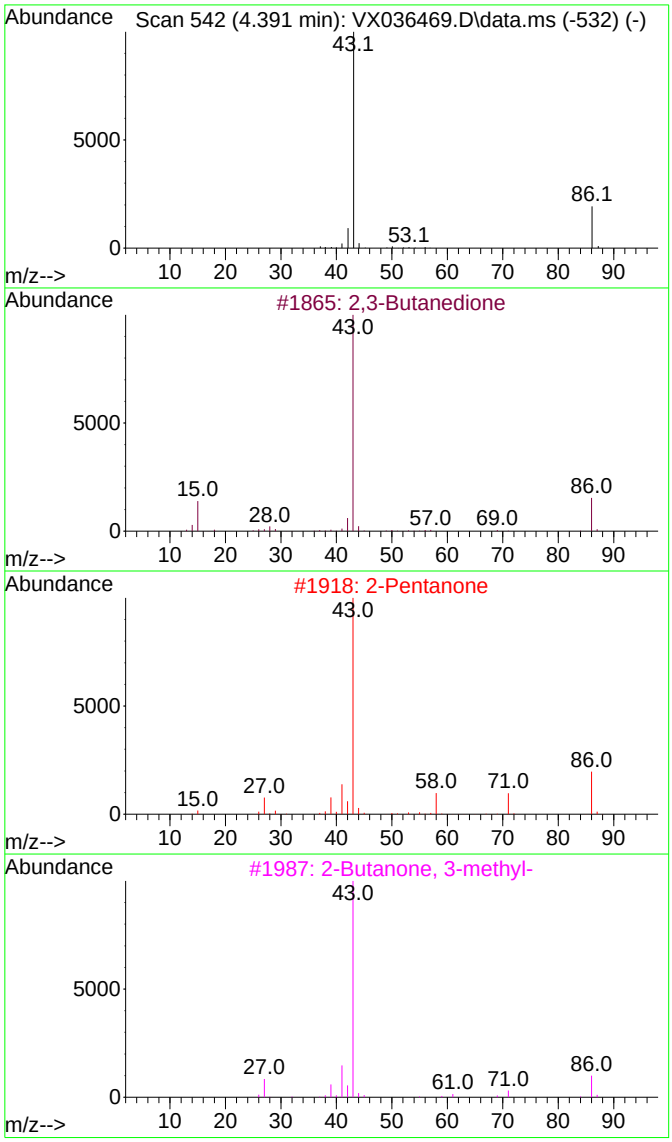
Quant Title : SW846 8260

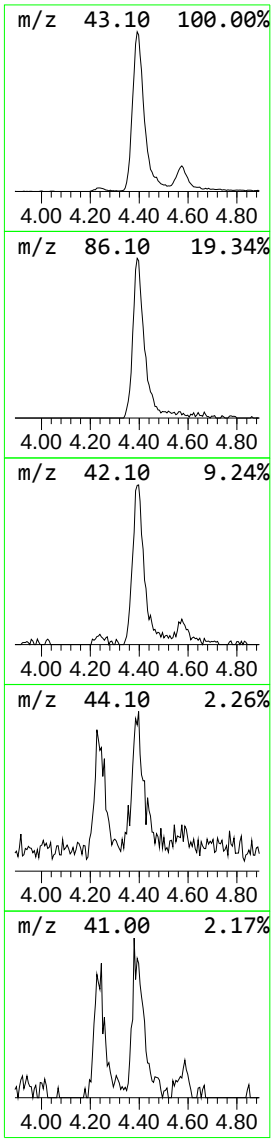
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,3-Butanedione Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.391	20.79 ug/l	214683	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione	86	C4H6O2	000431-03-8	72
2	2-Pentanone	86	C5H10O	000107-87-9	56
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
4	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	9
5	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7





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Instrument :
MSVOA_X
ClientSampleId :
1674

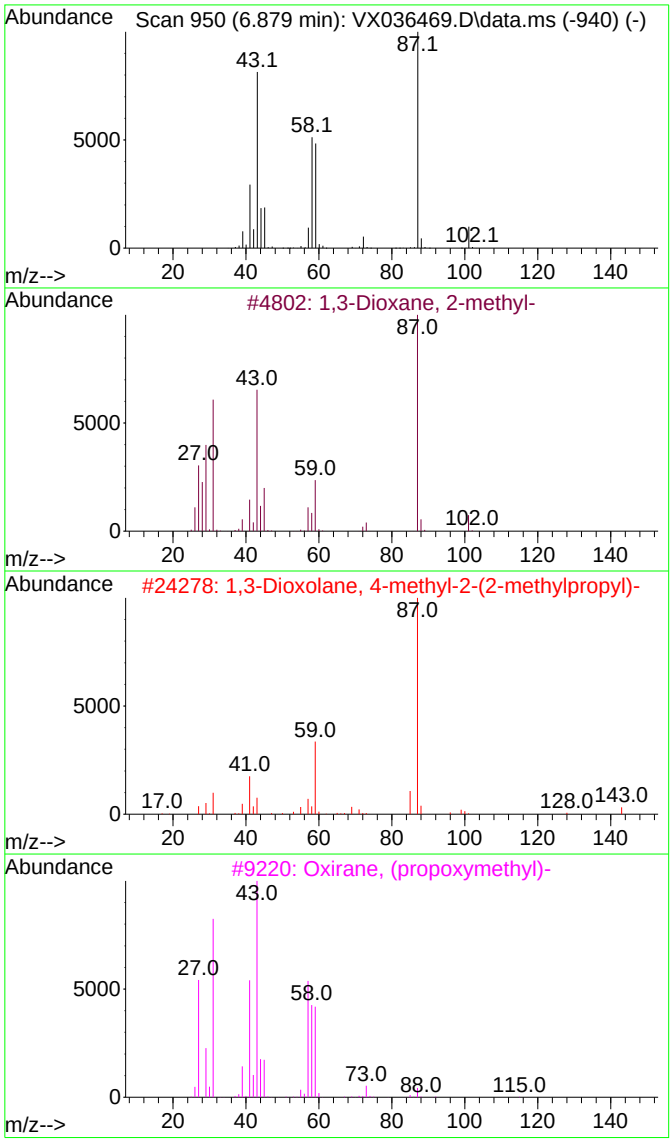
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

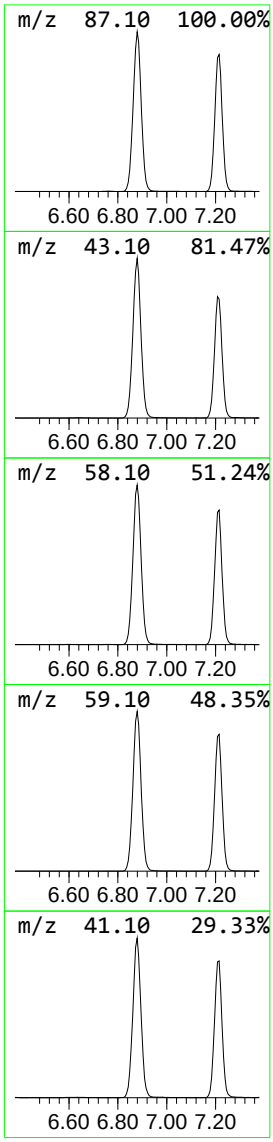
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	408.33 ug/l	5551160	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	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	38
3	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37
4	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	37
5	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	33





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Instrument :
MSVOA_X
ClientSampleId :
1674

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

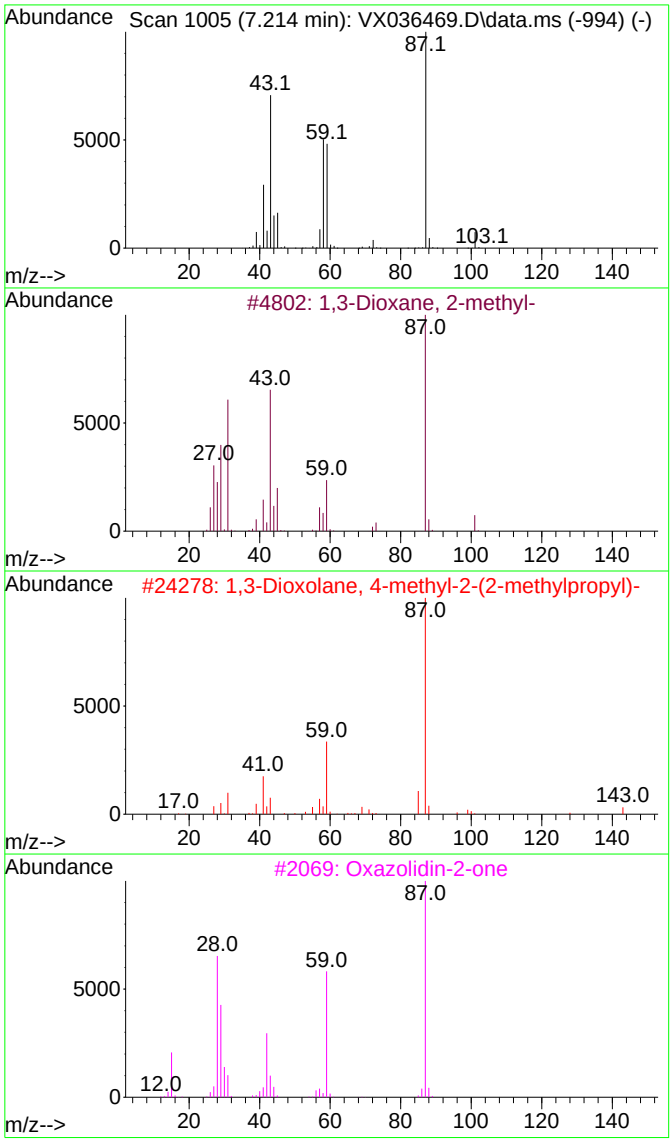
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

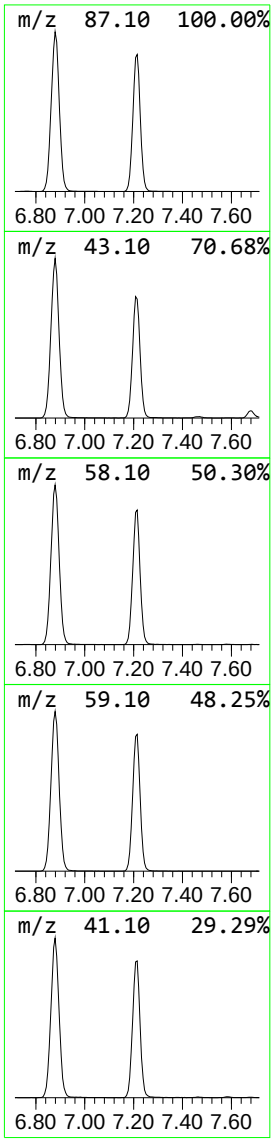
****

Peak Number 5 unknown7.214 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	306.50 ug/l	4166710	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	49
2	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	40
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
4	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
5	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	33





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Instrument :
MSVOA_X
ClientSampleId :
1674

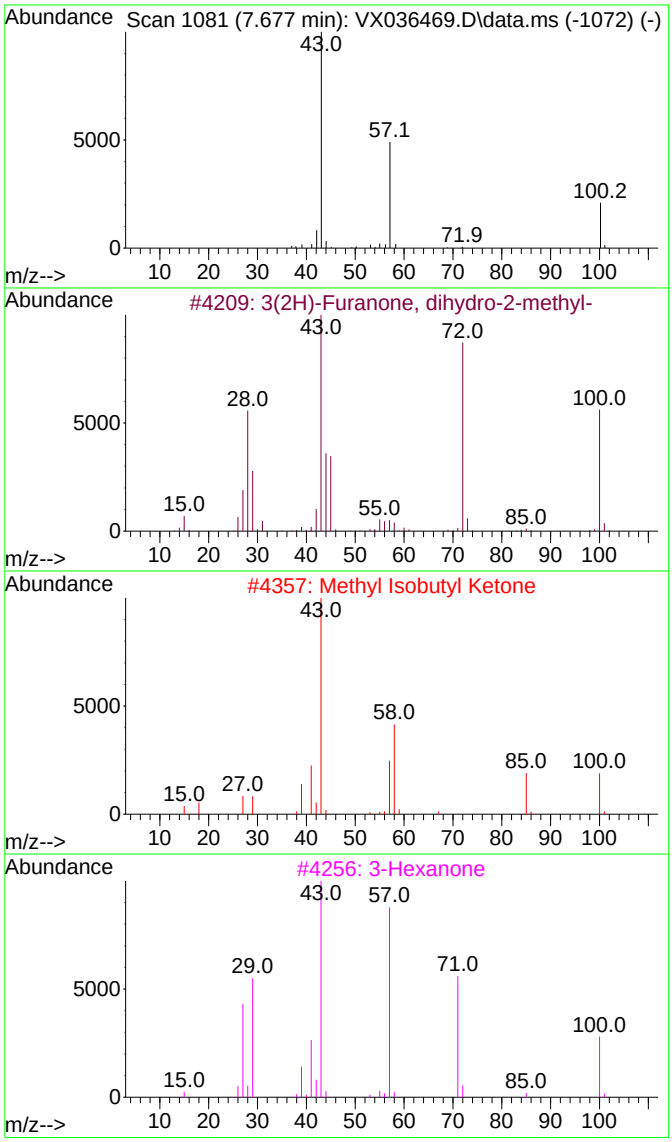
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

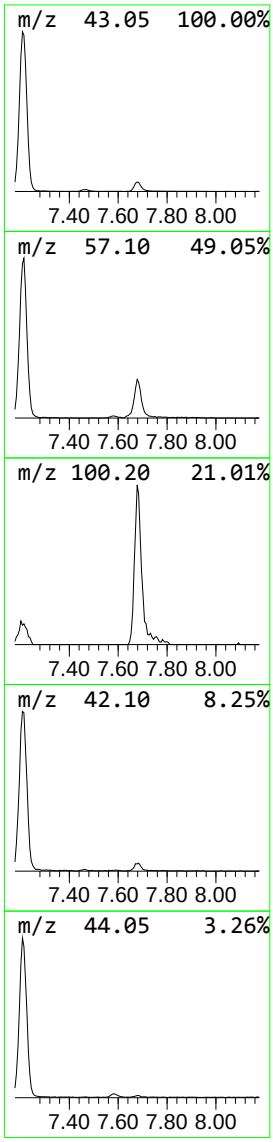
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3(2H)-Furanone, dihydro-2-m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.677	6.56 ug/l	89177	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3(2H)-Furanone, dihydro-2-methyl-	100	C5H8O2	003188-00-9	64
2	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	59
3	3-Hexanone	100	C6H12O	000589-38-8	59
4	Acetylacetone	100	C5H8O2	000123-54-6	53
5	2-Hexanone	100	C6H12O	000591-78-6	45





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Instrument :
MSVOA_X
ClientSampleId :
1674

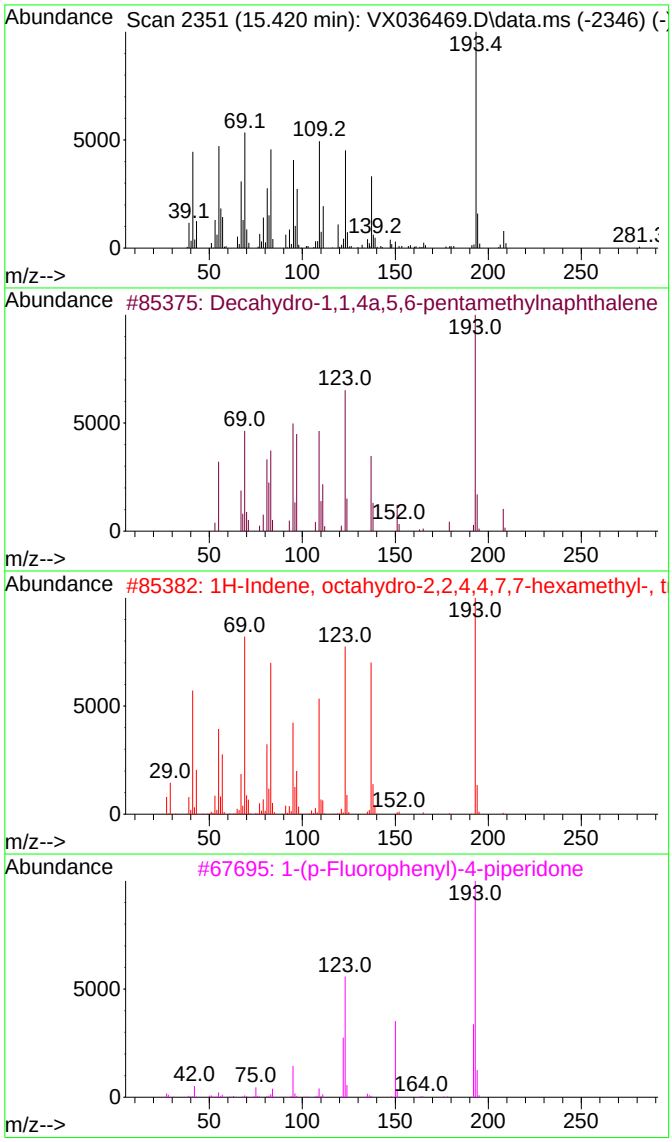
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

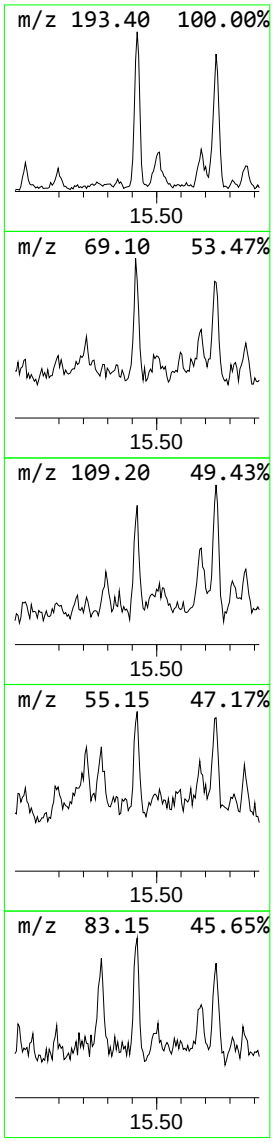
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.420	9.43 ug/l	145649	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	55
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	43
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
4	2-Anthracenamine	193	C14H11N	000613-13-8	22
5	Iminostilbene	193	C14H11N	000256-96-2	14





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Instrument :
MSVOA_X
ClientSampleId :
1674

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

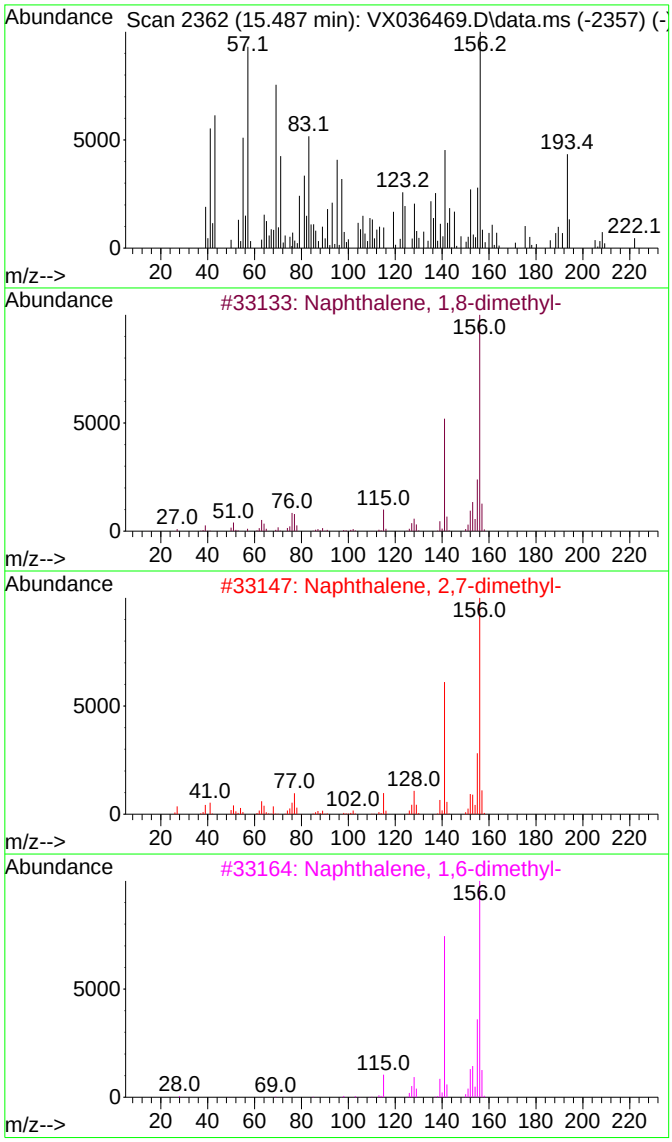
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

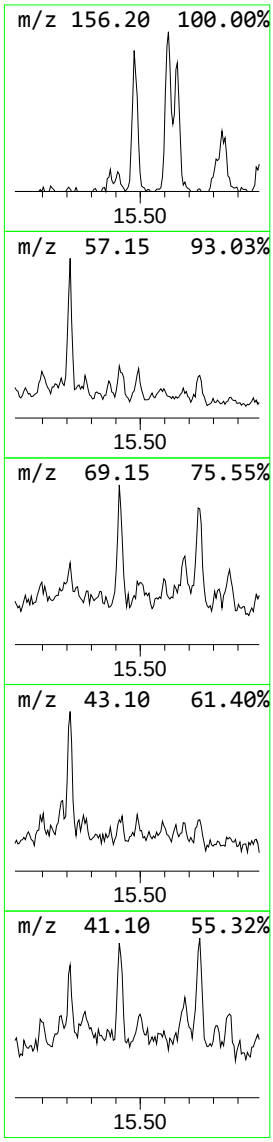
****

Peak Number 8 unknown15.487 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.487	5.56 ug/l	85882	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	38
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	30
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	27
4	4-(Methylthio)thiophenol	156	C7H8S2	001122-97-0	25
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	25





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1674

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

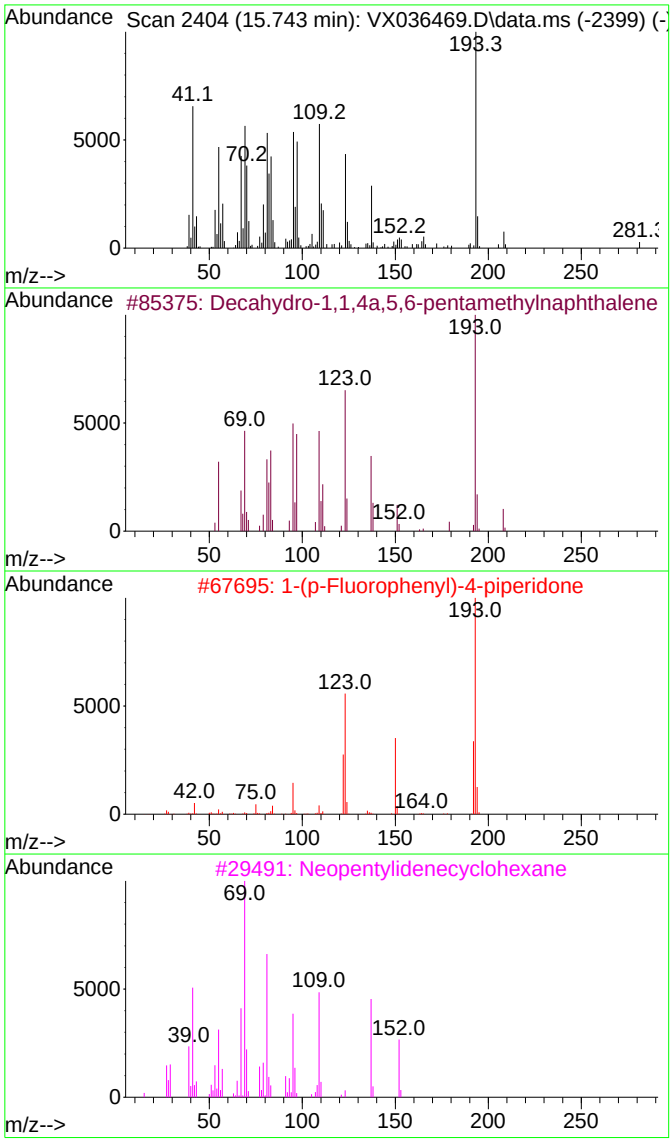
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

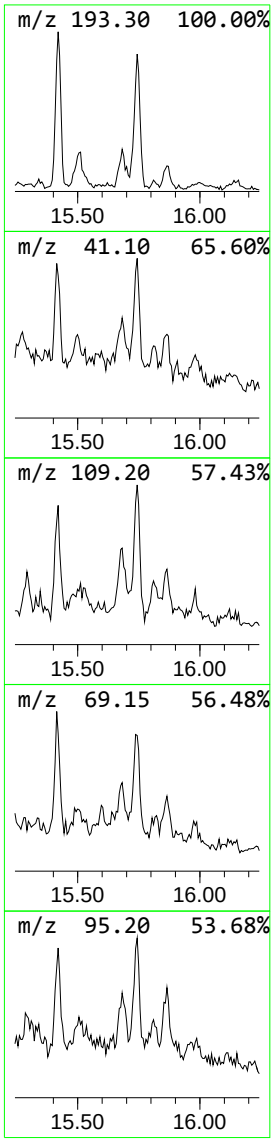
****

Peak Number 9 unknown15.743 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.743	11.24 ug/l	173495	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	76
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
3	Neopentylidenecyclohexane	152	C11H20	039546-80-0	30
4	6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	27
5	2(1H)-Naphthalenone, octahydro-4...	208	C14H24O	054594-42-2	22





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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

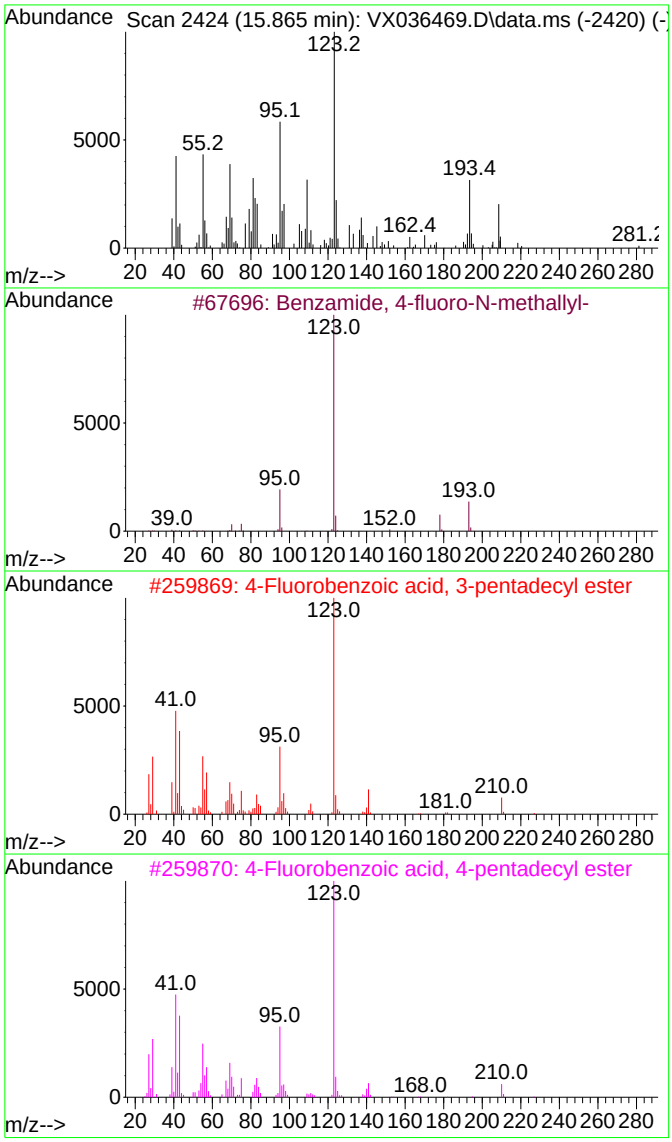
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

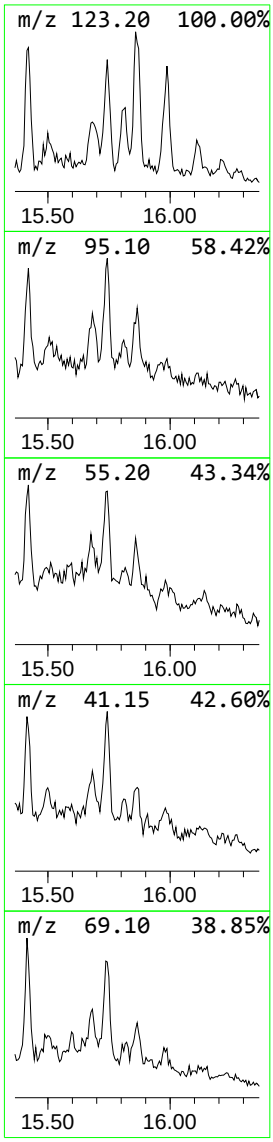
****

Peak Number 10 unknown15.865 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.865	5.21 ug/l	80503	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, 4-fluoro-N-methallyl-	193	C11H12FNO	1000340-31-9	47
2	4-Fluorobenzoic acid, 3-pentadec...	350	C22H35FO2	1000280-68-4	43
3	4-Fluorobenzoic acid, 4-pentadec...	350	C22H35FO2	1000280-68-5	43
4	4-Fluorobenzoic acid, 3-tridecyl...	322	C20H31FO2	1000280-67-9	38
5	2-Cyclopenten-1-one, 3,4,5,5-tet...	138	C9H14O	090611-02-2	38





Tentatively Identified Compound (LSC) summary

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Instrument :
MSVOA_X
ClientSampleId :
1674

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.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	20.8	ug/l	214683	1	5.556	516297	50.0
1,3-Dioxane, 2-...	6.879	408.3	ug/l	5551160	2	6.763	679736	50.0
unknown7.214	7.214	306.5	ug/l	4166710	2	6.763	679736	50.0
3(2H)-Furanone,...	7.677	6.6	ug/l	89177	2	6.763	679736	50.0
Decahydro-1,1,4...	15.420	9.4	ug/l	145649	4	12.024	772104	50.0
unknown15.487	15.487	5.6	ug/l	85882	4	12.024	772104	50.0
unknown15.743	15.743	11.2	ug/l	173495	4	12.024	772104	50.0
unknown15.865	15.865	5.2	ug/l	80503	4	12.024	772104	50.0