

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051523\
 Data File : VX035657.D
 Acq On : 15 May 2023 12:07
 Operator : JC/MD
 Sample : 02643-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FSND-PRO-07-99-05032023

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\82X051123W.M
 Title : SW846 8260

Signal : TIC: VX035657.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	693	705	721	rBV	143488	412058	3.84%	1.523%
2	5.550	721	732	750	rVB	239539	682522	6.37%	2.523%
3	5.958	786	799	812	rBV	171976	457288	4.27%	1.691%
4	6.757	920	930	943	rBV	392076	940340	8.77%	3.476%
5	7.129	980	991	1007	rBV	4854542	10717932	100.00%	39.624%
6	7.452	1037	1044	1057	rBV	432209	856836	7.99%	3.168%
7	7.574	1057	1064	1073	rBV	61011	118563	1.11%	0.438%
8	8.647	1233	1240	1249	rBV	815828	1263402	11.79%	4.671%
9	9.427	1362	1368	1377	rBV	541734	757927	7.07%	2.802%
10	9.519	1377	1383	1402	rVB	416634	583937	5.45%	2.159%
11	10.055	1465	1471	1484	rVB	829391	1130737	10.55%	4.180%
12	10.768	1582	1588	1597	rBV	2758748	3416029	31.87%	12.629%
13	10.854	1597	1602	1616	rVB	120911	166000	1.55%	0.614%
14	11.079	1634	1639	1647	rVB	731930	899914	8.40%	3.327%
15	11.835	1758	1763	1774	rBV	2777378	3278588	30.59%	12.121%
16	11.927	1774	1778	1784	rVV	135098	163289	1.52%	0.604%
17	12.018	1788	1793	1802	rVB	863421	1094415	10.21%	4.046%
18	12.219	1820	1826	1841	rBV	59040	109195	1.02%	0.404%

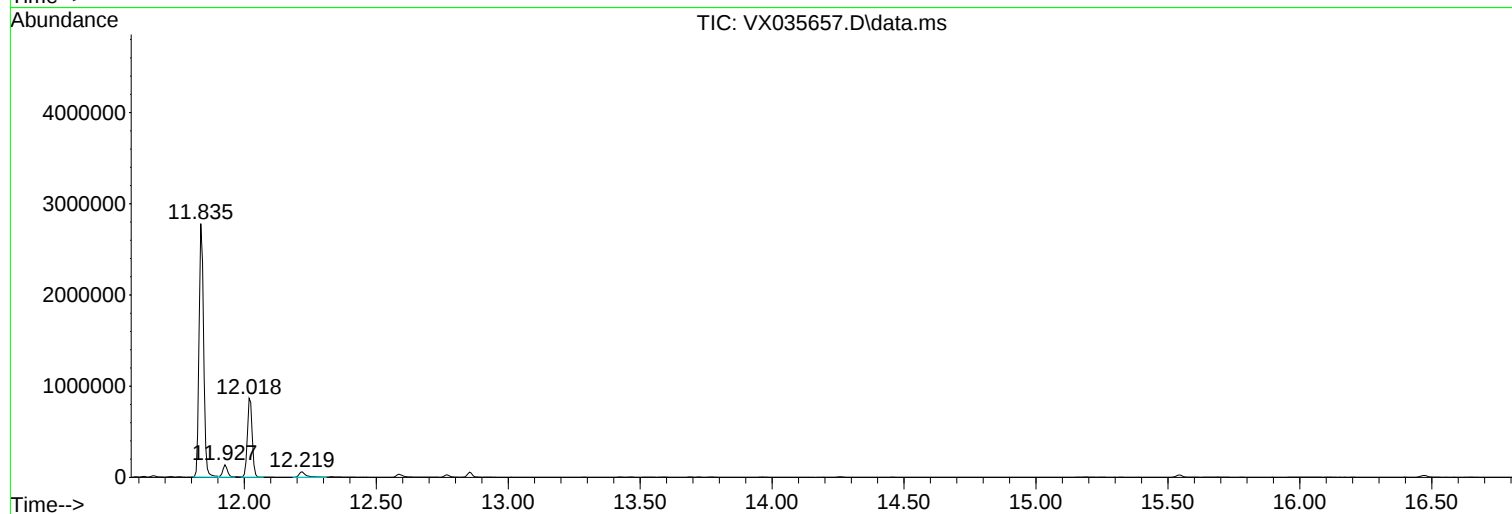
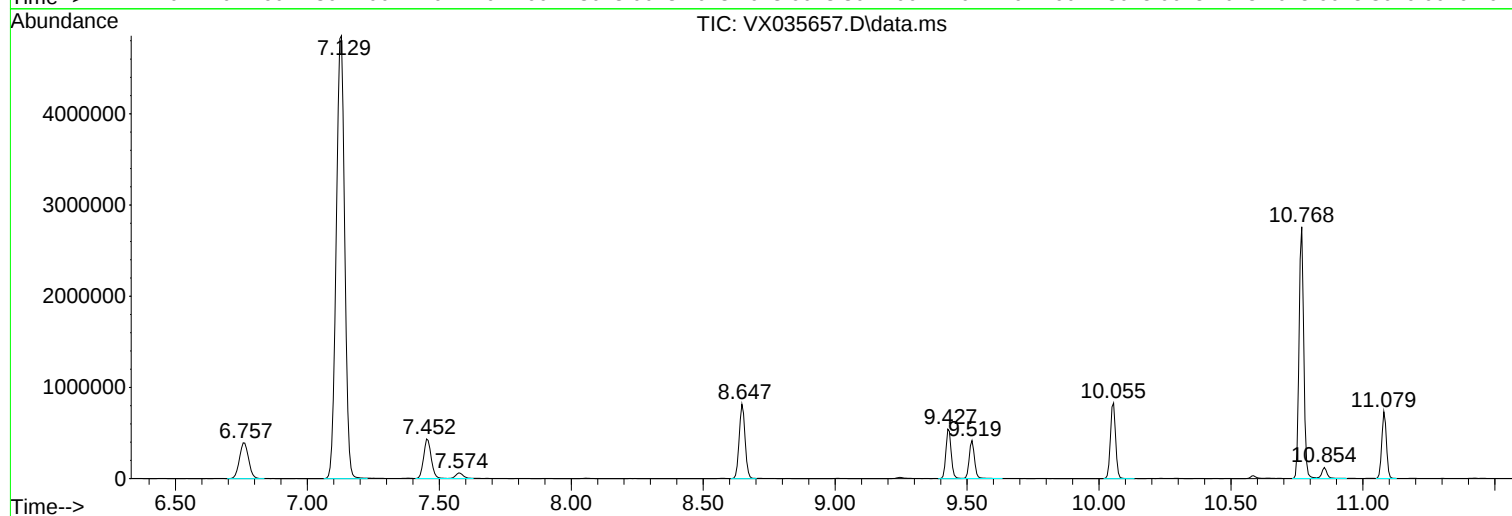
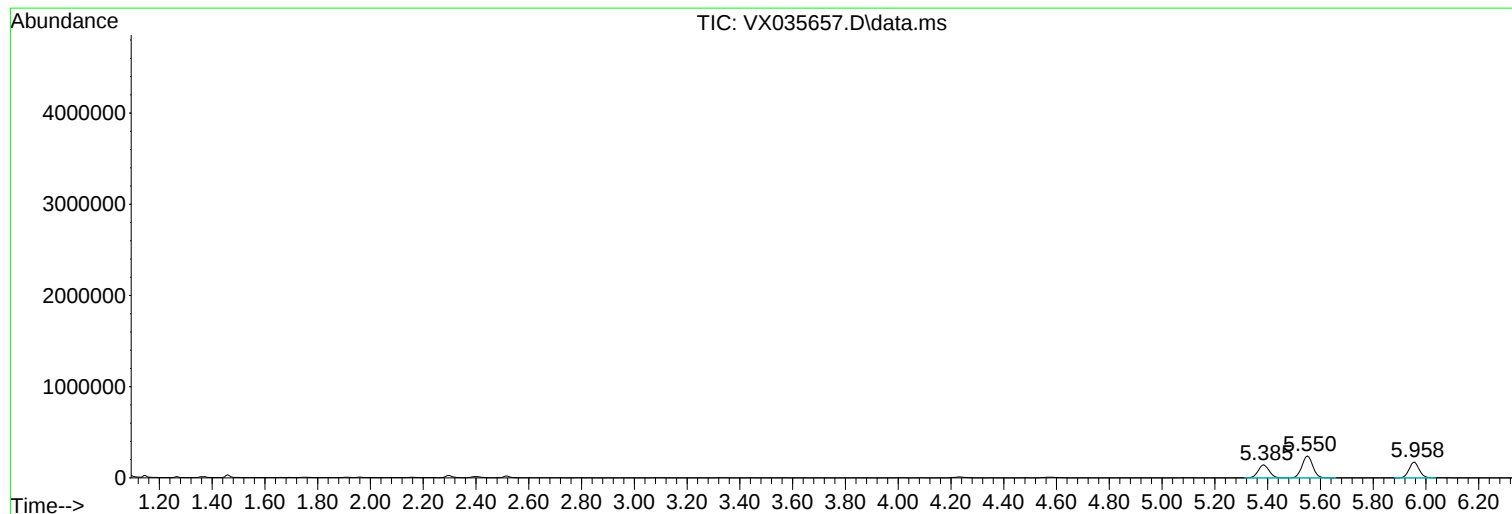
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Quant Title : SW846 8260

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



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FSND-PRO-07-99-05032023

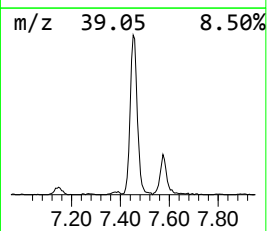
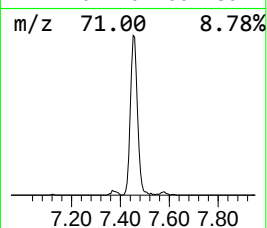
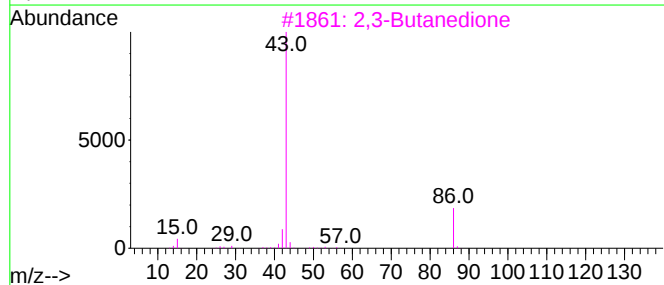
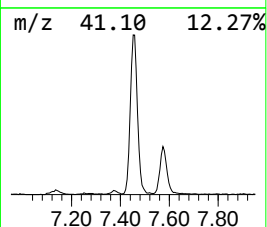
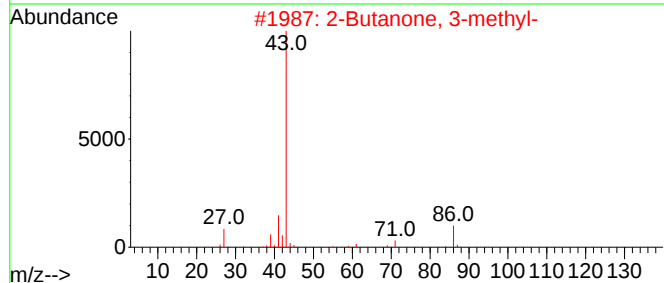
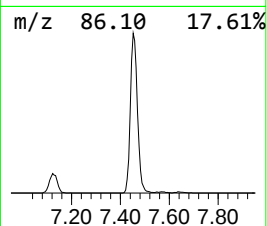
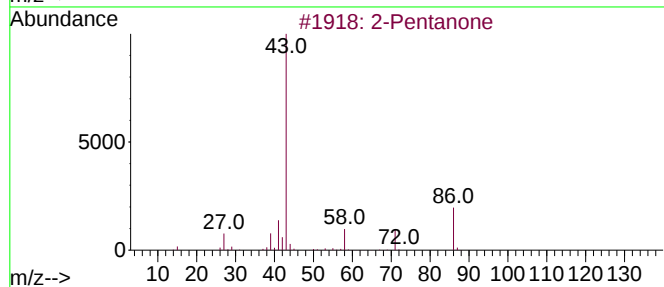
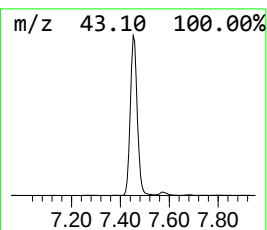
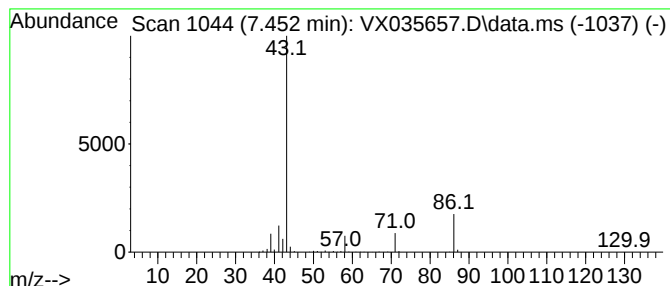
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Pentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.452	45.56 ug/l	856836	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone	86	C5H10O	000107-87-9	91
2		2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3		2,3-Butanedione	86	C4H6O2	000431-03-8	50
4		Butane	58	C4H10	000106-97-8	9
5		Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	9



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MSVOA_X
ClientSampleId :
FSND-PRO-07-99-05032023

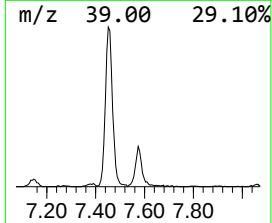
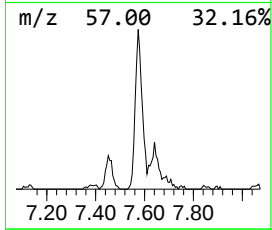
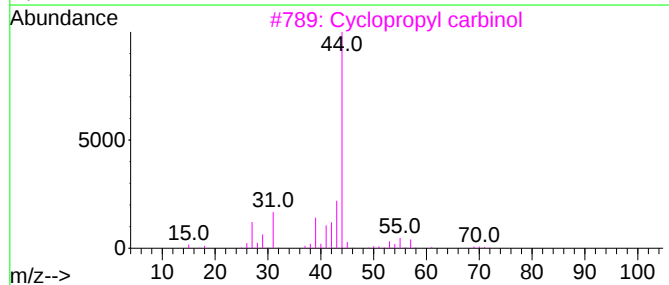
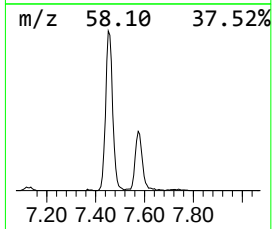
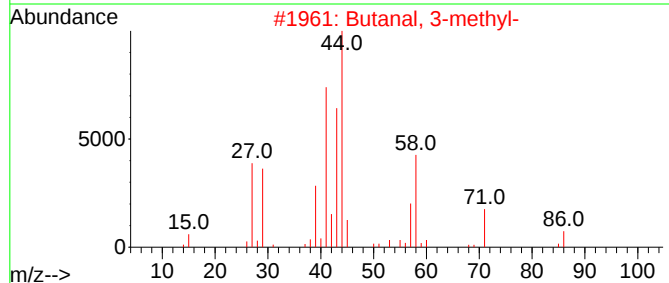
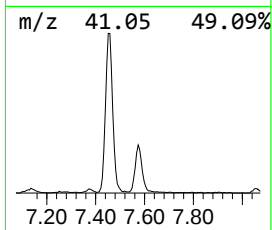
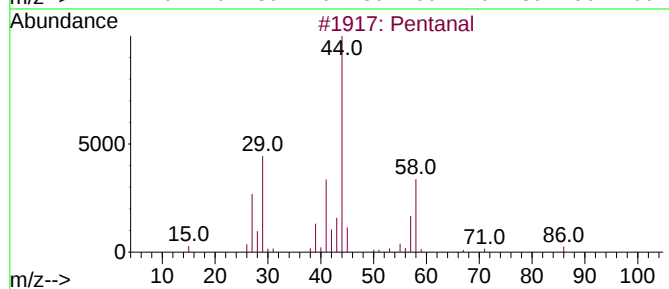
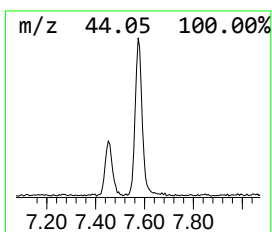
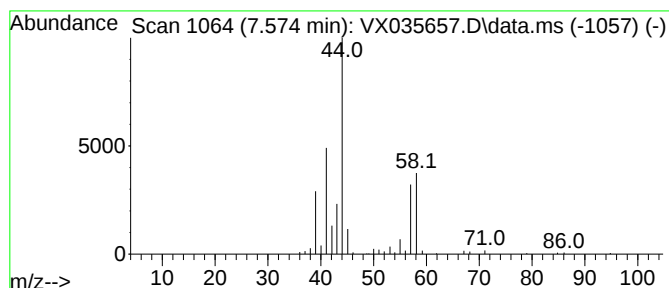
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.574	6.30 ug/l	118563	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	83
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	78
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	38
4			2-Formylhistamine	139	C6H9N3O	1000132-95-8	33
5			Butane, 2-nitro-	103	C4H9NO2	000600-24-8	9



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Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-07-99-05032023

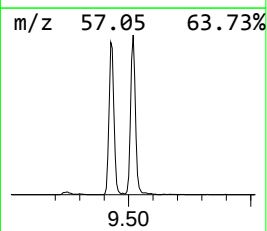
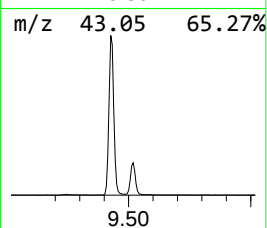
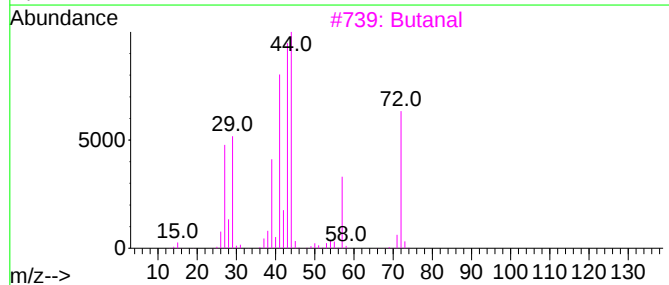
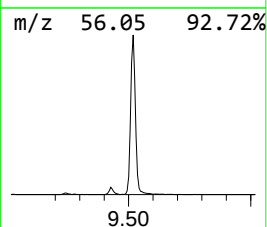
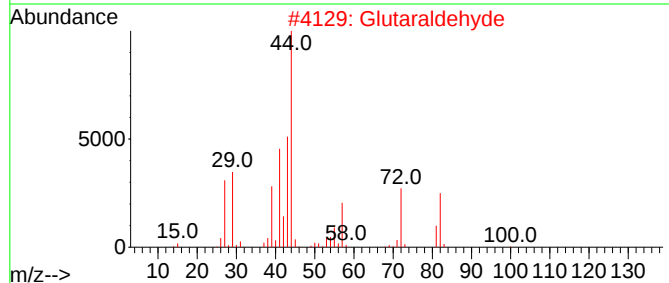
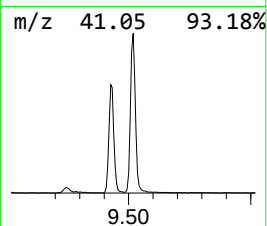
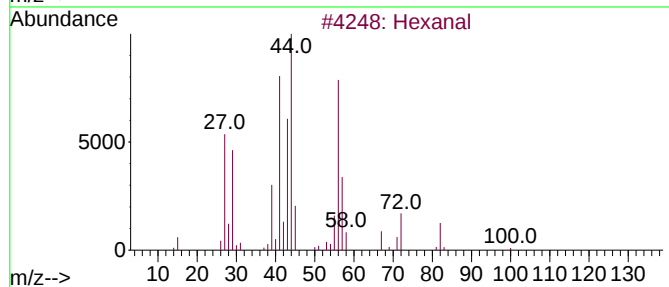
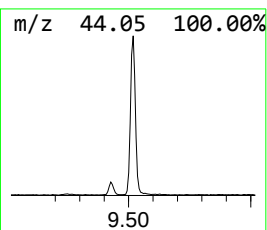
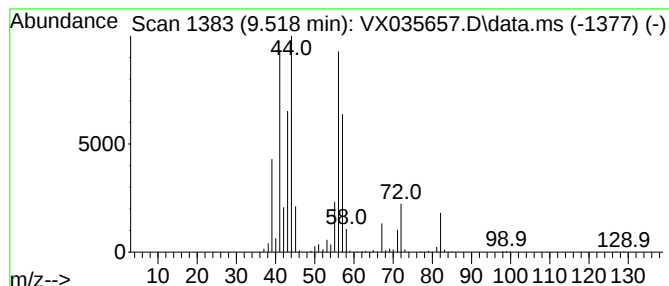
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.518	25.82 ug/l	583937	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	72
2			Glutaraldehyde	100	C5H8O2	000111-30-8	30
3			Butanal	72	C4H8O	000123-72-8	16
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	16
5			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	12



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-07-99-05032023

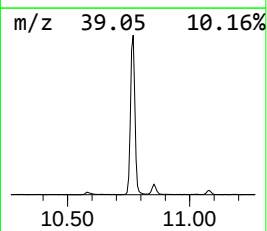
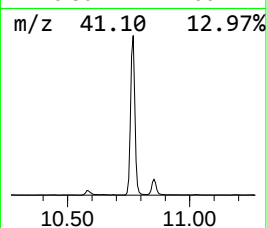
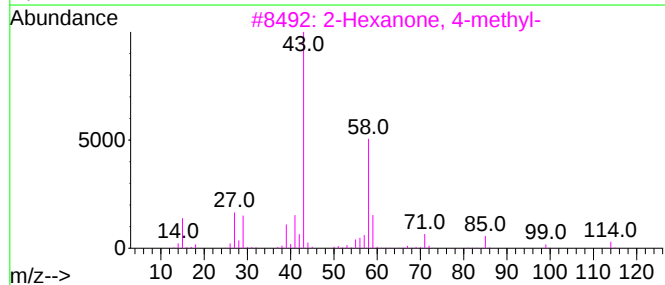
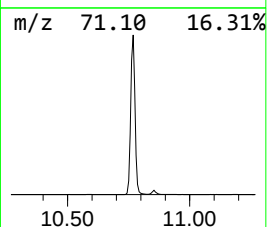
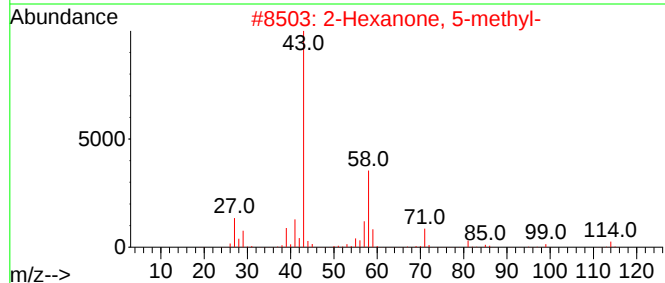
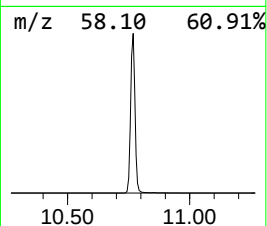
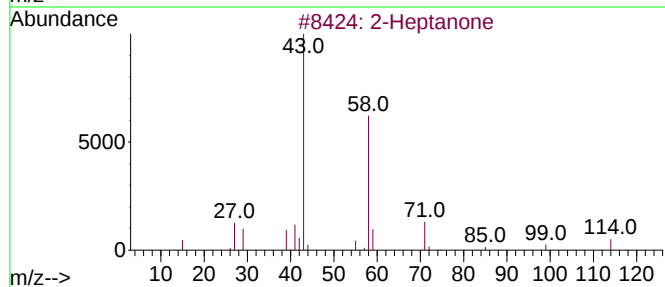
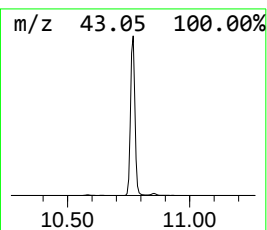
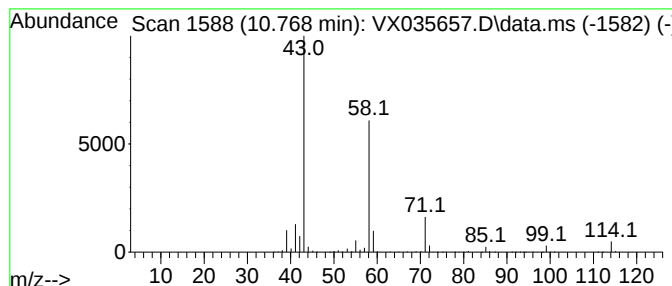
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Quant Title : SW846 8260

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

Peak Number 4 2-Heptanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.768	151.05 ug/l	3416030	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone	114	C7H14O	000110-43-0	91
2			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	90
3			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	64
4			2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	52
5			2-Hexanone	100	C6H12O	000591-78-6	40



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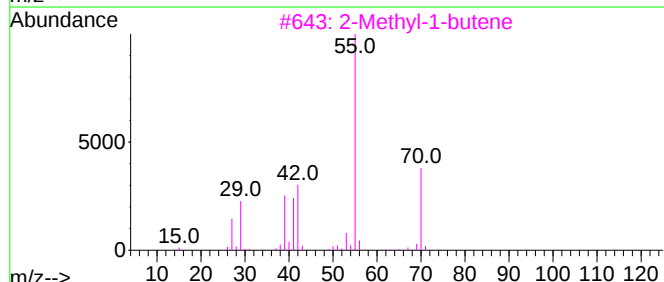
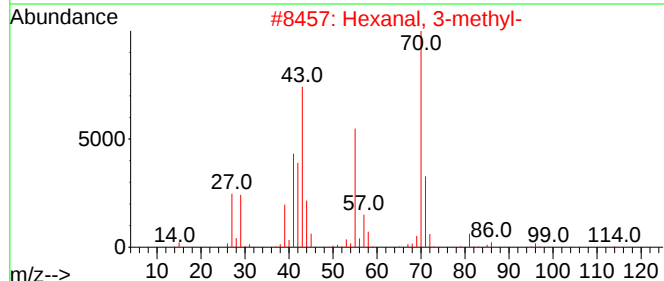
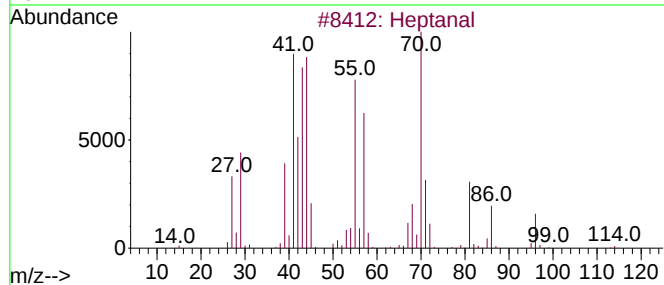
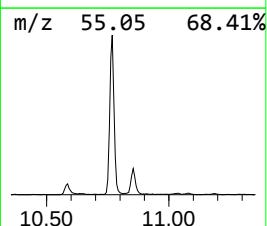
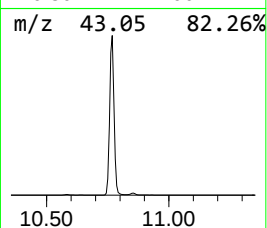
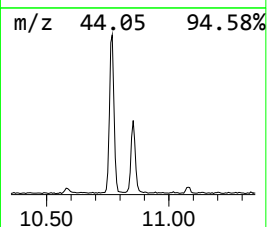
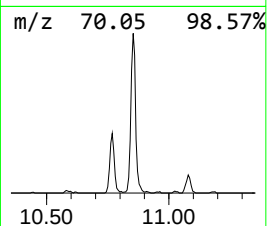
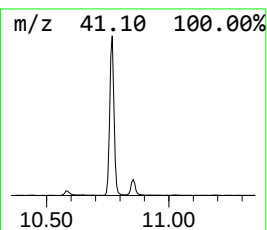
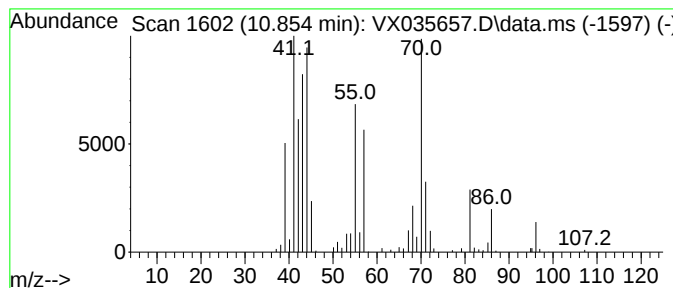
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Quant Title : SW846 8260

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

Peak Number 5 Heptanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.854	7.34 ug/l	166000	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	91
2			Hexanal, 3-methyl-	114	C7H14O	019269-28-4	38
3			2-Methyl-1-butene	70	C5H10	000563-46-2	35
4			2-Butene, 2-methyl-	70	C5H10	000513-35-9	35
5			Acetic acid, trifluoro-, 3-methy...	184	C7H11F3O2	000327-69-5	27



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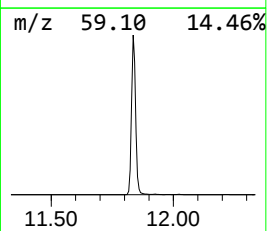
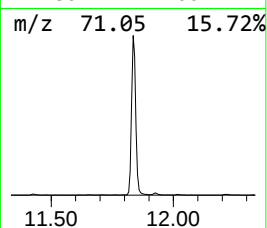
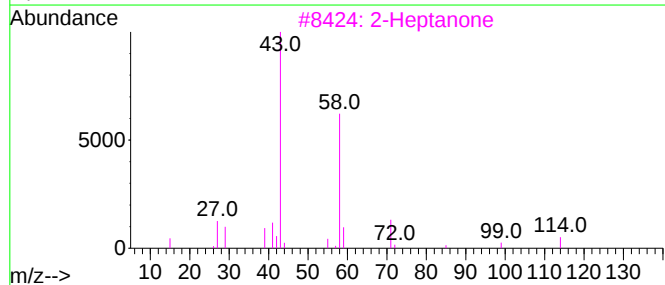
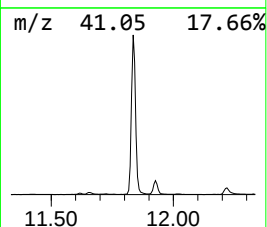
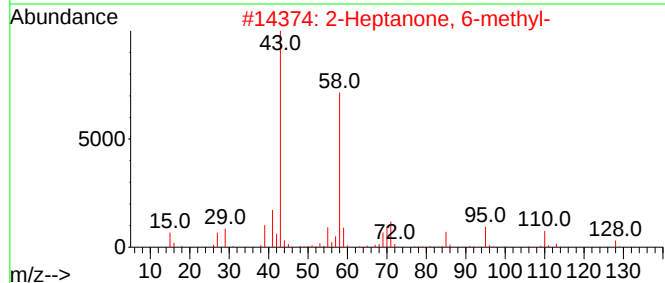
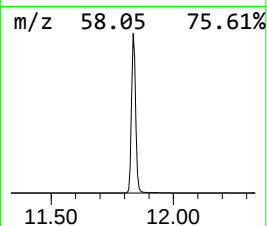
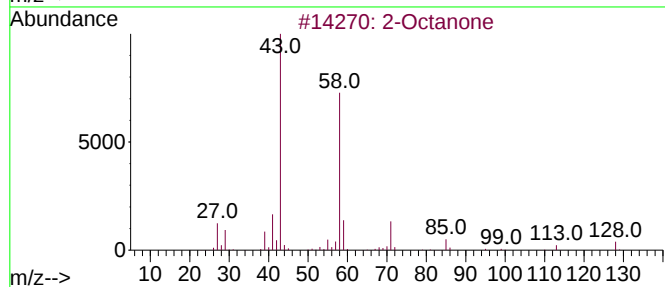
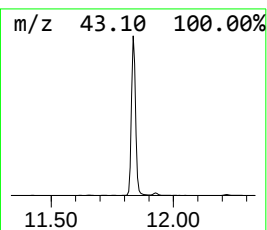
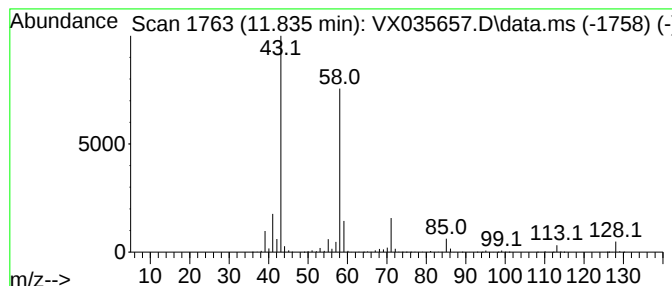
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Quant Title : SW846 8260

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

Peak Number 6 2-Octanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.835	149.79 ug/l	3278590	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octanone	128	C8H16O	000111-13-7	94
2			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	83
3			2-Heptanone	114	C7H14O	000110-43-0	78
4			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78
5			2-Hexanone	100	C6H12O	000591-78-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051523\
Data File : VX035657.D
Acq On : 15 May 2023 12:07
Operator : JC/MD
Sample : 02643-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-07-99-05032023

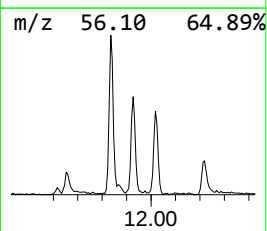
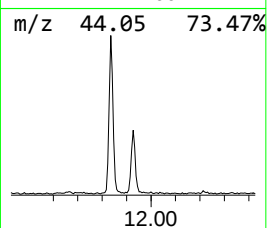
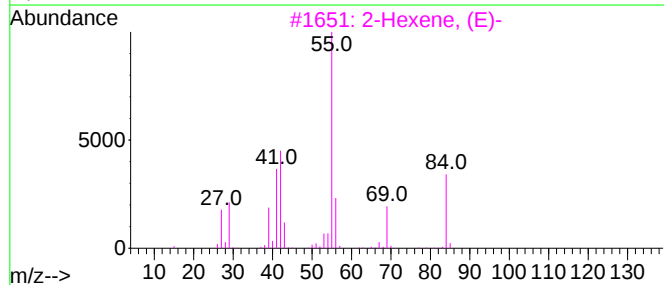
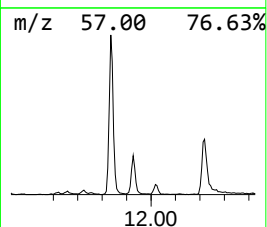
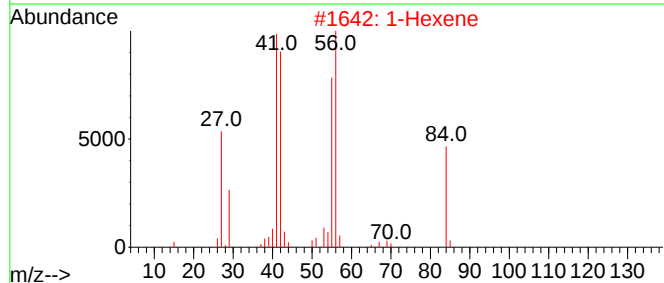
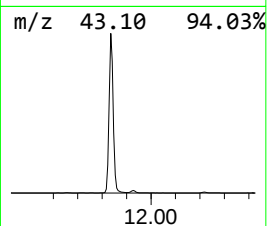
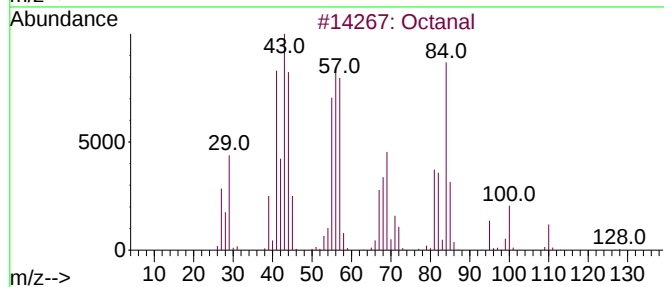
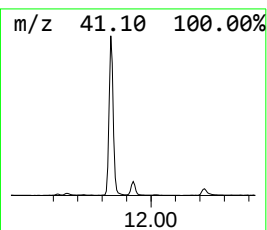
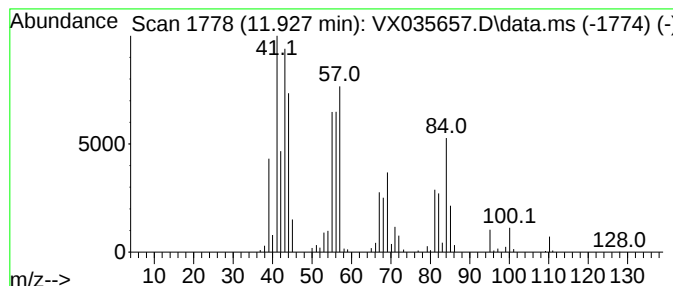
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Quant Title : SW846 8260

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

Peak Number 7 Octanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	7.46 ug/l	163289	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanal	128	C8H16O	000124-13-0	97
2			1-Hexene	84	C6H12	000592-41-6	27
3			2-Hexene, (E)-	84	C6H12	004050-45-7	22
4			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	18
5			Cyanoic acid, propyl ester	85	C4H7NO	001768-36-1	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051523\
Data File : VX035657.D
Acq On : 15 May 2023 12:07
Operator : JC/MD
Sample : 02643-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-07-99-05032023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.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
2-Pentanone	7.452	45.6	ug/l	856836	2	6.763	940340	50.0
Pentanal	7.574	6.3	ug/l	118563	2	6.763	940340	50.0
Hexanal	9.518	25.8	ug/l	583937	3	10.055	1130740	50.0
2-Heptanone	10.768	151.1	ug/l	3416030	3	10.055	1130740	50.0
Heptanal	10.854	7.3	ug/l	166000	3	10.055	1130740	50.0
2-Octanone	11.835	149.8	ug/l	3278590	4	12.024	1094420	50.0
Octanal	11.927	7.5	ug/l	163289	4	12.024	1094420	50.0