

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051923\
 Data File : VX035760.D
 Acq On : 19 May 2023 15:08
 Operator : JC/MD
 Sample : 02860-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FSND-PRO-08-71-05112023

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: VX035760.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	19	rVB	96052	106675	2.39%	0.572%
2	1.355	40	44	50	rBV2	50032	74671	1.67%	0.401%
3	1.459	57	61	73	rBV	31559	64365	1.44%	0.345%
4	1.953	138	142	155	rVB	109801	157945	3.54%	0.847%
5	2.300	193	199	210	rBV	135522	260135	5.83%	1.395%
6	4.239	507	517	528	rBV4	23103	70257	1.58%	0.377%
7	5.385	694	705	721	rBV	145988	428195	9.60%	2.297%
8	5.549	721	732	750	rVB	241599	684299	15.35%	3.670%
9	5.958	785	799	822	rBV	198044	527374	11.83%	2.829%
10	6.757	921	930	947	rVB	395917	963944	21.62%	5.170%
11	7.122	981	990	1008	rBV	350609	790015	17.72%	4.237%
12	7.574	1056	1064	1073	rBV	199405	400820	8.99%	2.150%
13	8.646	1233	1240	1248	rBV	810952	1271998	28.53%	6.822%
14	9.274	1334	1343	1356	rVB	81161	128289	2.88%	0.688%
15	9.518	1377	1383	1408	rBV	3244749	4458560	100.00%	23.914%
16	10.055	1462	1471	1485	rBV	844308	1125190	25.24%	6.035%
17	10.853	1597	1602	1616	rVB	544560	687906	15.43%	3.690%
18	11.079	1634	1639	1650	rVB	686188	854540	19.17%	4.583%
19	11.615	1724	1727	1732	rVB	99688	117701	2.64%	0.631%
20	11.926	1773	1778	1788	rBV	736483	873112	19.58%	4.683%
21	12.024	1788	1794	1801	rVB	798848	1031543	23.14%	5.533%
22	12.219	1820	1826	1842	rBV	116974	222940	5.00%	1.196%
23	12.591	1881	1887	1900	rBV	224253	388030	8.70%	2.081%
24	12.853	1925	1930	1945	rBV	1701978	1940953	43.53%	10.411%
25	13.420	2016	2023	2027	rBV	40738	69626	1.56%	0.373%
26	13.463	2027	2030	2043	rVB	70580	115911	2.60%	0.622%
27	14.261	2155	2161	2178	rBV	455283	682043	15.30%	3.658%
28	14.737	2234	2239	2252	rBV2	33679	65757	1.47%	0.353%
29	14.999	2277	2282	2296	rBV2	41497	81380	1.83%	0.436%

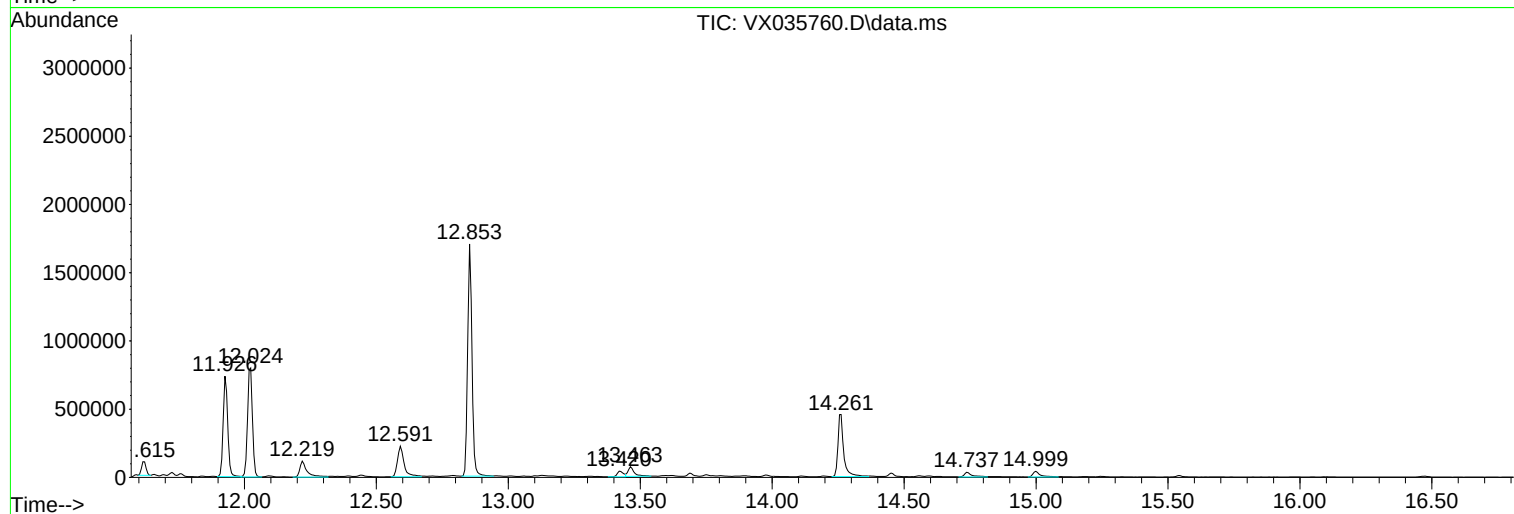
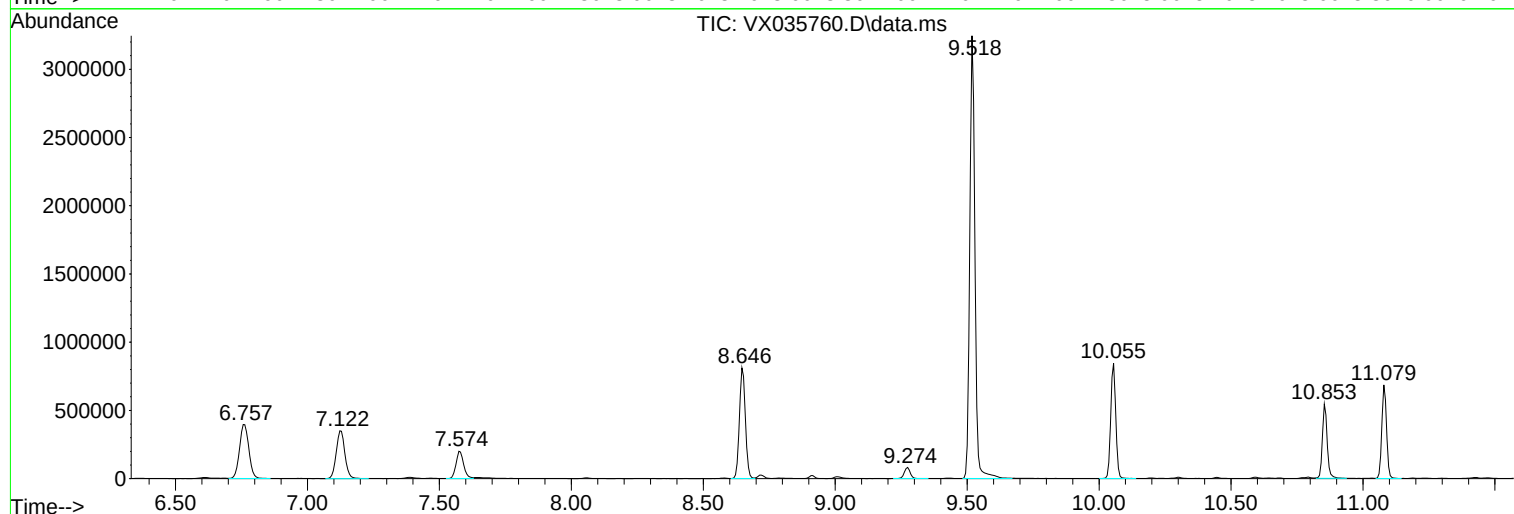
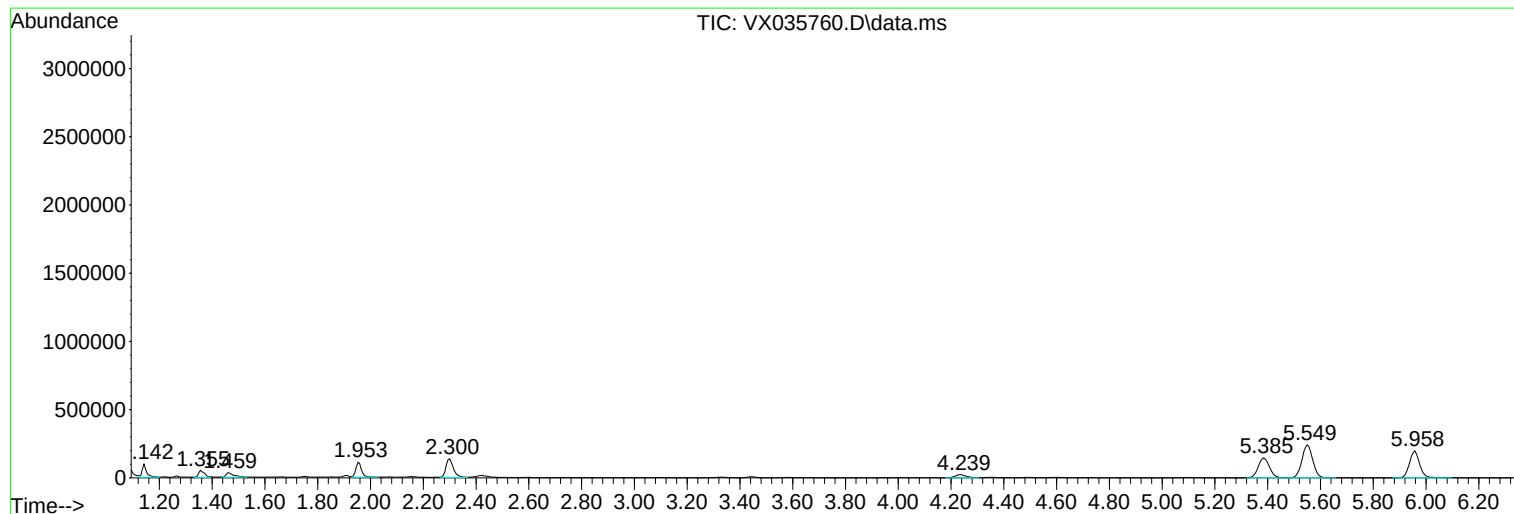
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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



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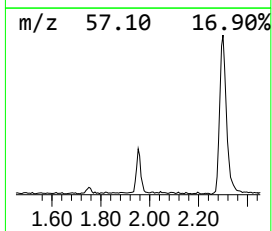
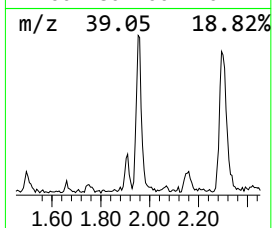
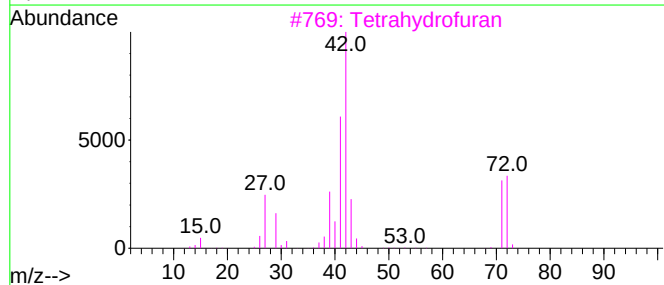
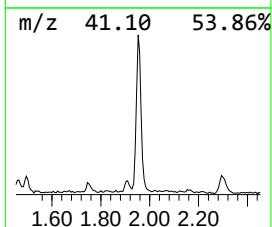
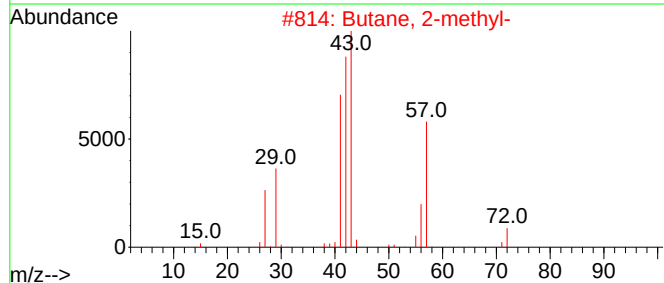
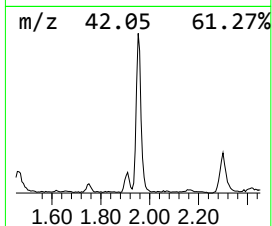
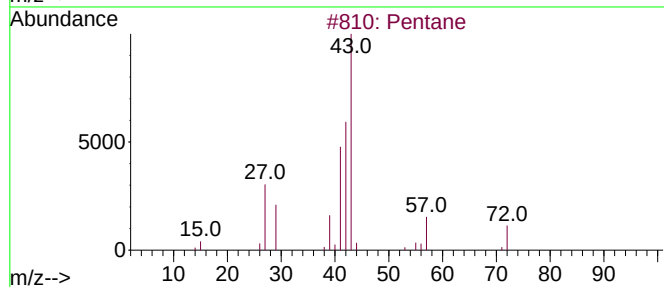
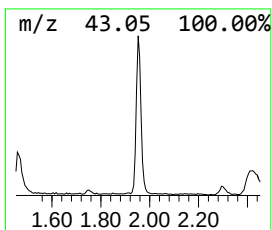
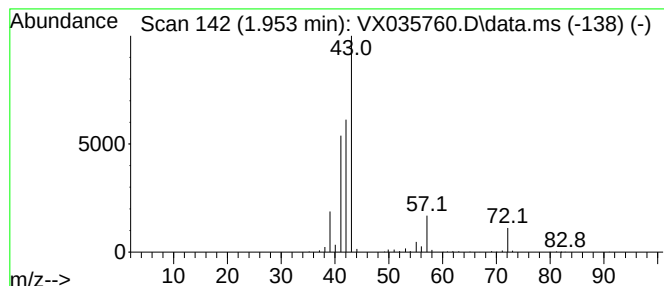
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	11.54 ug/l	157945	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	86
2			Butane, 2-methyl-	72	C5H12	000078-78-4	50
3			Tetrahydrofuran	72	C4H8O	000109-99-9	9
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5			Propanal, 2-methyl-	72	C4H8O	000078-84-2	9



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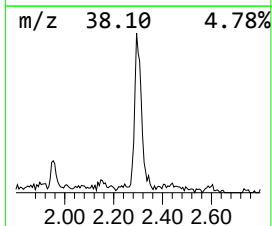
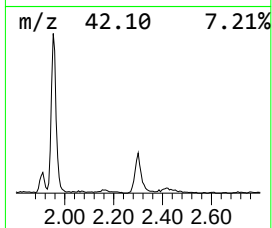
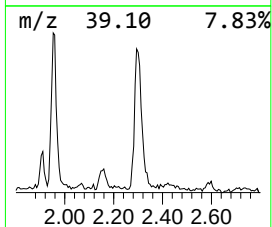
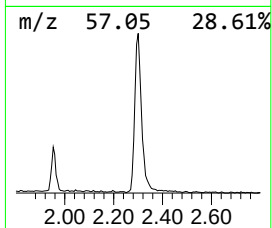
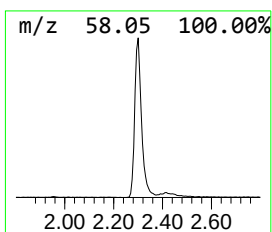
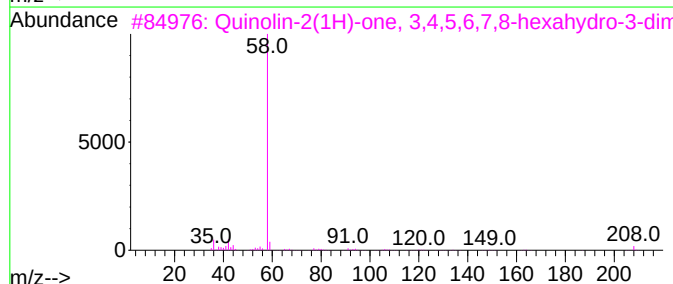
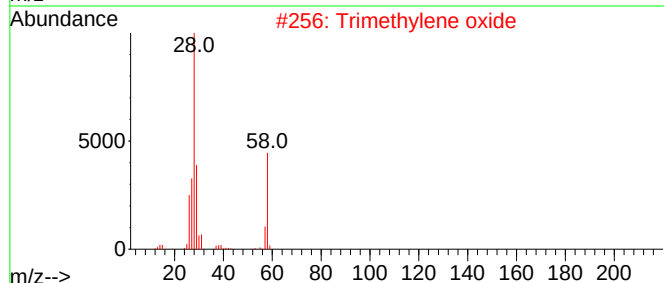
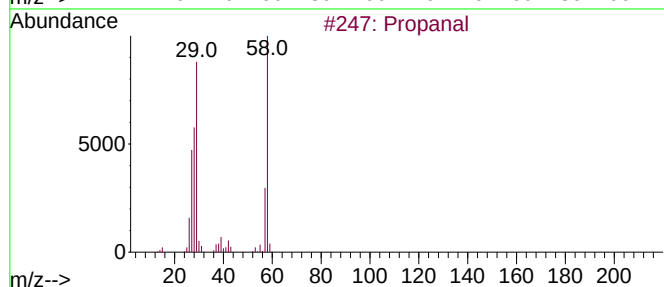
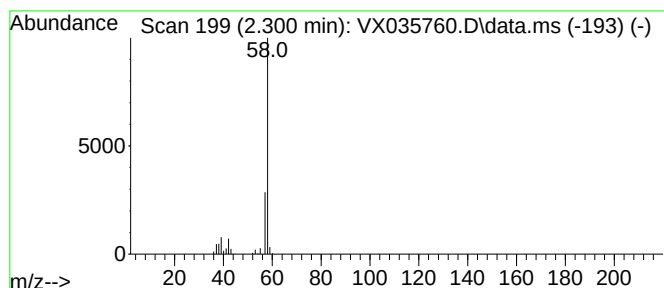
Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-71-05112023

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 Propanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.300	19.01 ug/l	260135	Pentafluorobenzene	5.549	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4	2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9
5	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-71-05112023

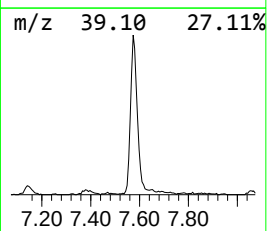
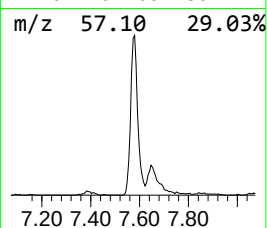
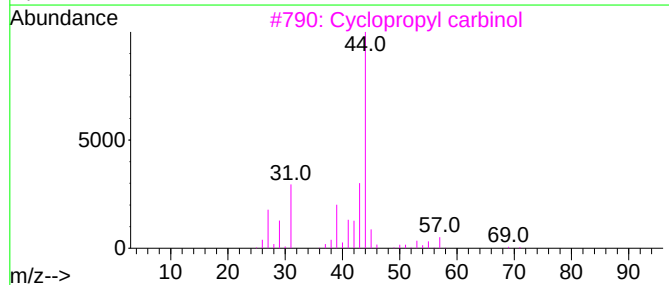
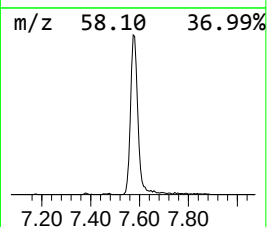
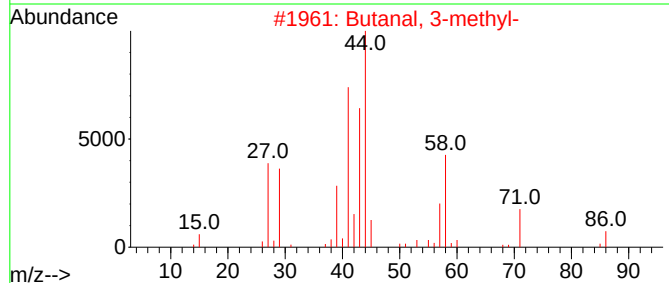
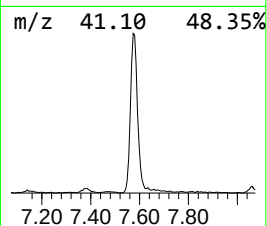
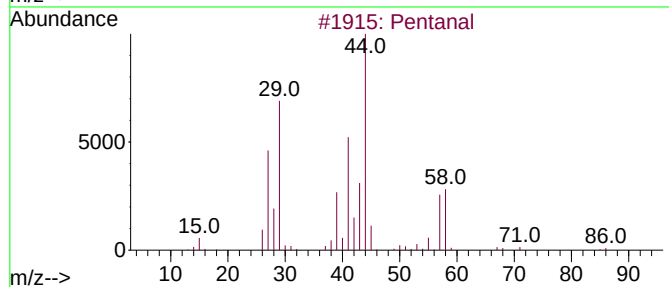
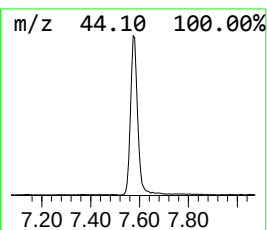
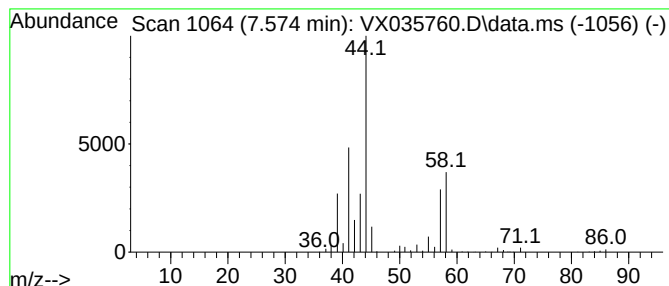
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.574	20.79 ug/l	400820	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	90
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	64
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	64
4			Piperazine	86	C4H10N2	000110-85-0	9
5			1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	9



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-71-05112023

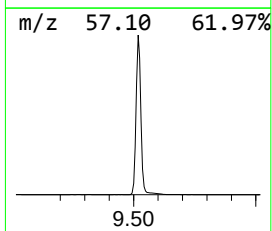
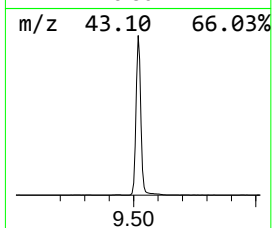
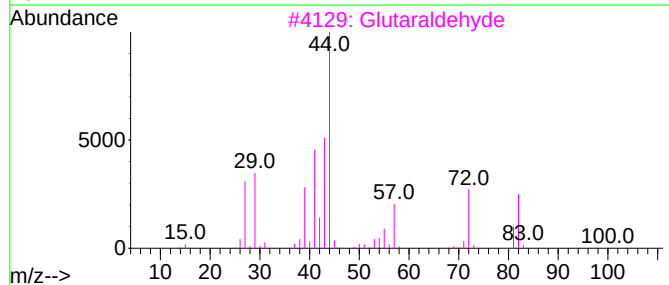
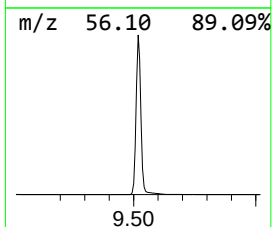
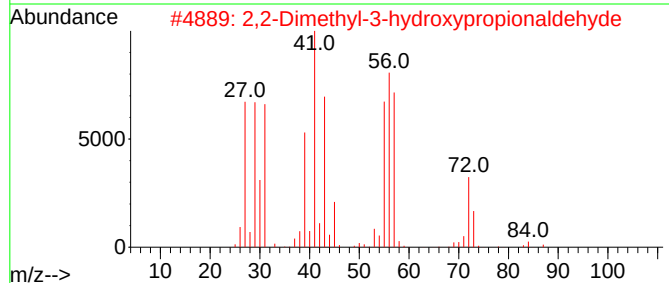
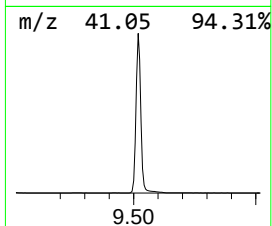
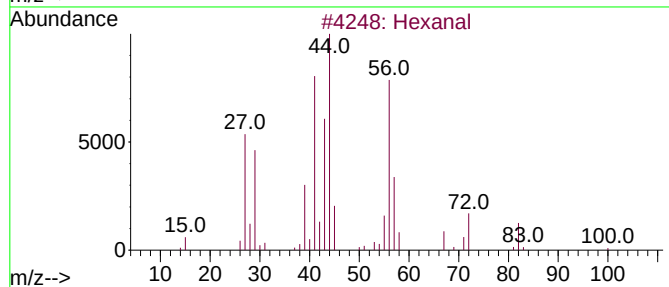
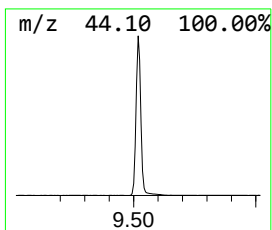
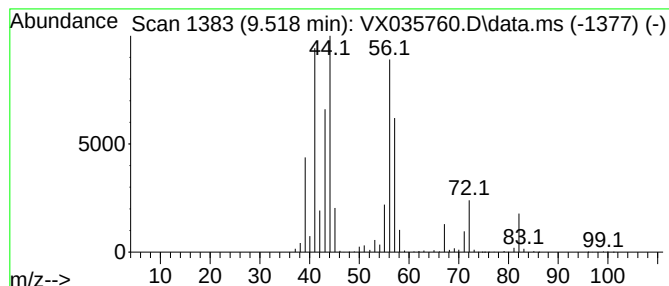
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Peak Number 4 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.518	198.13 ug/l	4458560	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	80
2			2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	37
3			Glutaraldehyde	100	C5H8O2	000111-30-8	30
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	27
5			Butanal	72	C4H8O	000123-72-8	16



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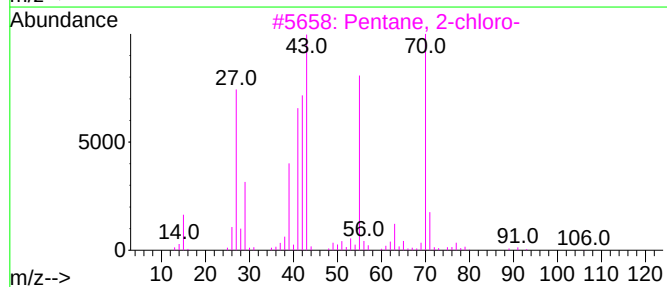
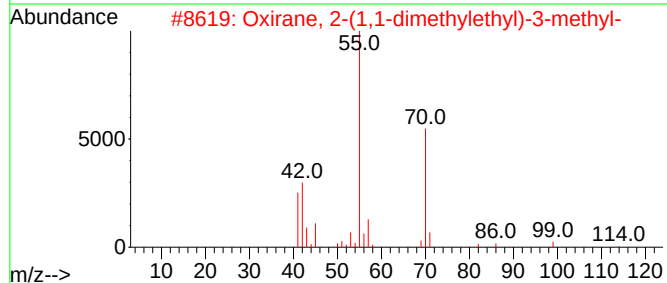
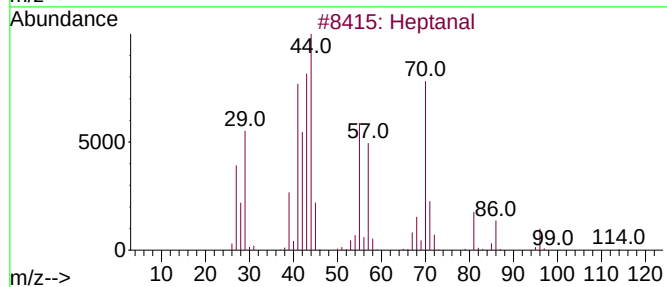
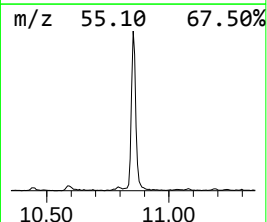
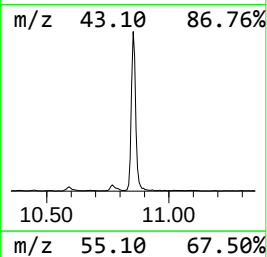
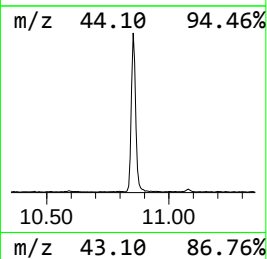
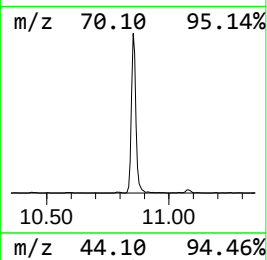
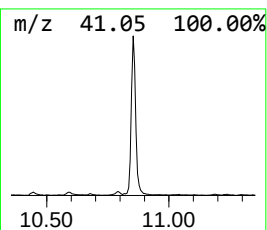
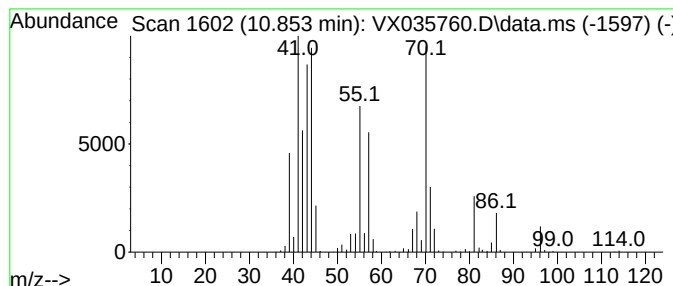
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.853	30.57 ug/l	687906	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	96
2			Oxirane, 2-(1,1-dimethylethyl)-3...	114	C7H14O	053897-30-6	43
3			Pentane, 2-chloro-	106	C5H11Cl	000625-29-6	32
4			2-Pentene, (Z)-	70	C5H10	000627-20-3	32
5			Hexanal, 3-methyl-	114	C7H14O	019269-28-4	32



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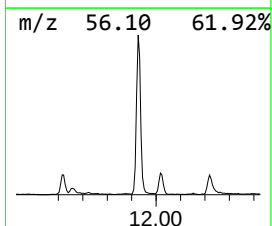
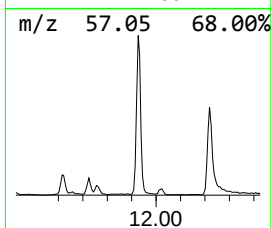
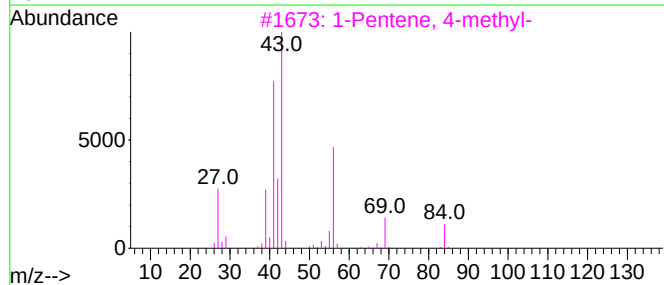
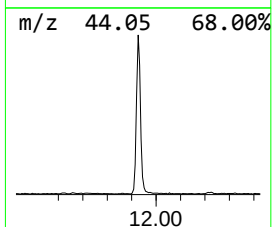
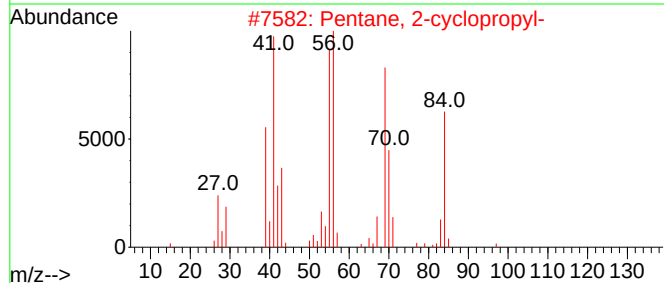
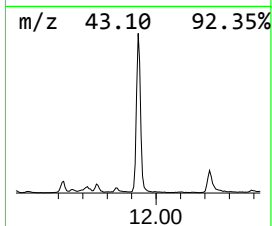
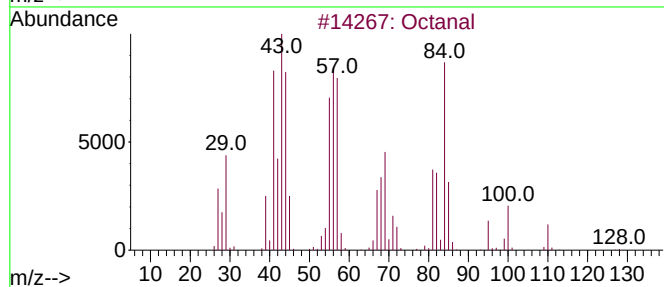
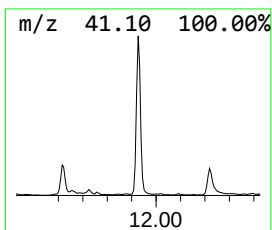
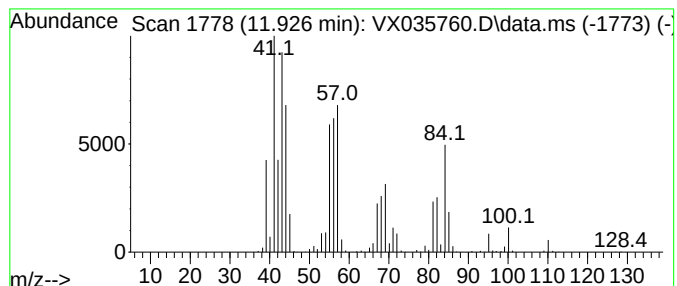
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Quant Title : SW846 8260

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

Peak Number 6 Octanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.926	42.32 ug/l	873112	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanal	128	C8H16O	000124-13-0	97
2			Pentane, 2-cyclopropyl-	112	C8H16	005458-16-2	35
3			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	35
4			Cyclopentanol, 2-methyl-	100	C6H12O	024070-77-7	27
5			Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051923\
Data File : VX035760.D
Acq On : 19 May 2023 15:08
Operator : JC/MD
Sample : 02860-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-71-05112023

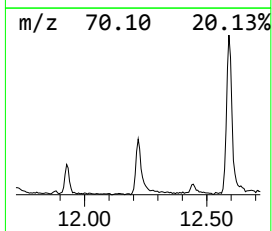
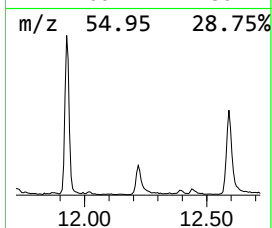
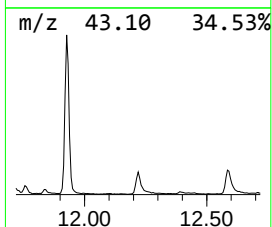
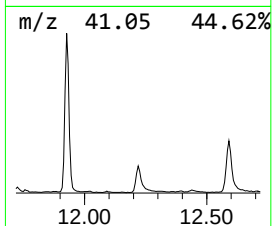
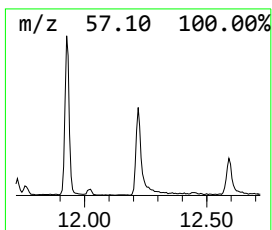
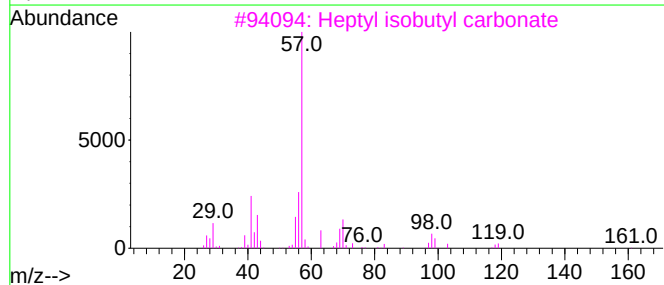
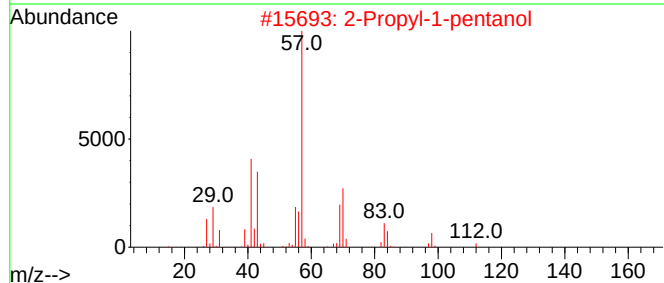
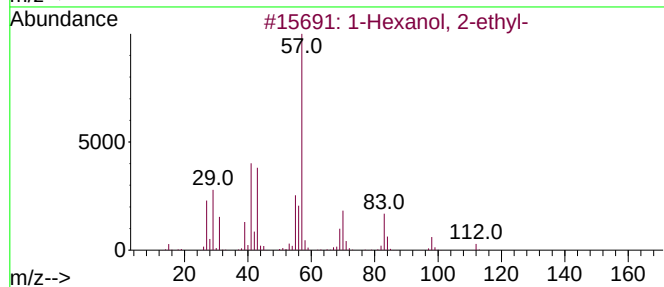
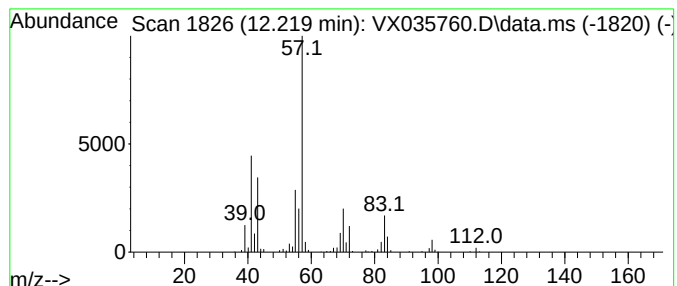
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	10.81 ug/l	222940	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	72
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47
4			2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	42
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051923\
Data File : VX035760.D
Acq On : 19 May 2023 15:08
Operator : JC/MD
Sample : 02860-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-71-05112023

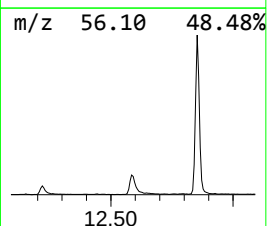
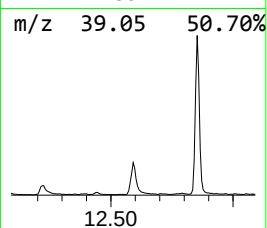
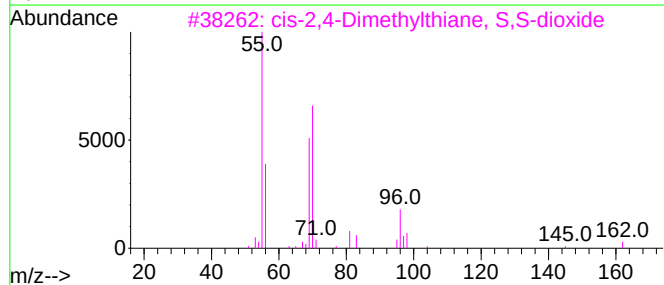
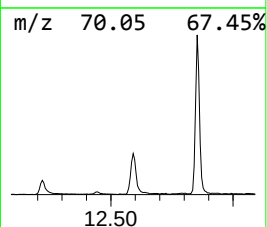
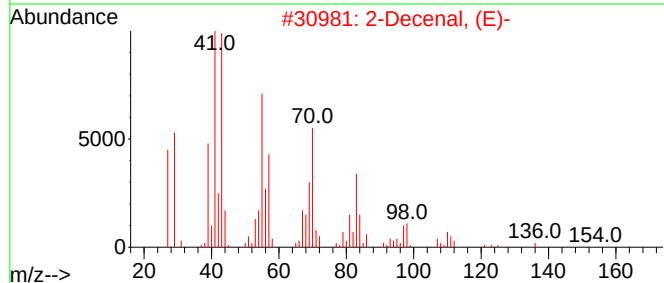
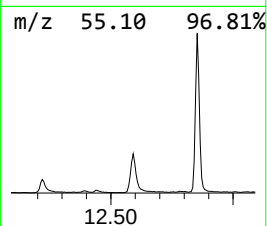
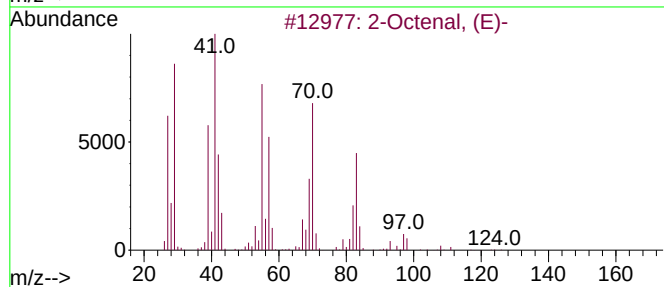
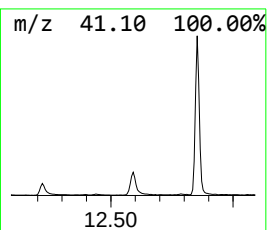
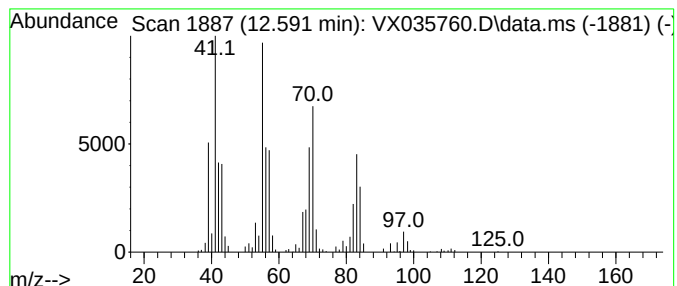
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Quant Title : SW846 8260

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

Peak Number 8 2-Octenal, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.591	18.81 ug/l	388030	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octenal, (E)-	126	C8H14O	002548-87-0	64
2			2-Decenal, (E)-	154	C10H18O	003913-81-3	47
3			cis-2,4-Dimethylthiane, S,S-dioxide	162	C7H14O2S	1000215-67-5	38
4			2-Methyl-1-butene	70	C5H10	000563-46-2	38
5			1-Pentene, 3-methyl-	84	C6H12	000760-20-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051923\
Data File : VX035760.D
Acq On : 19 May 2023 15:08
Operator : JC/MD
Sample : 02860-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-71-05112023

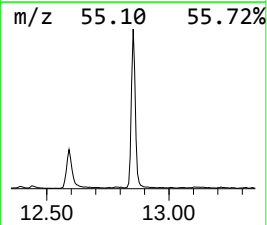
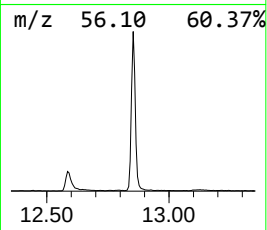
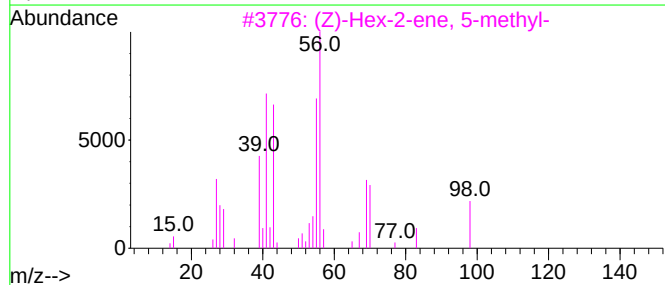
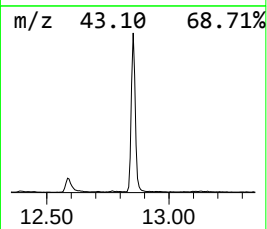
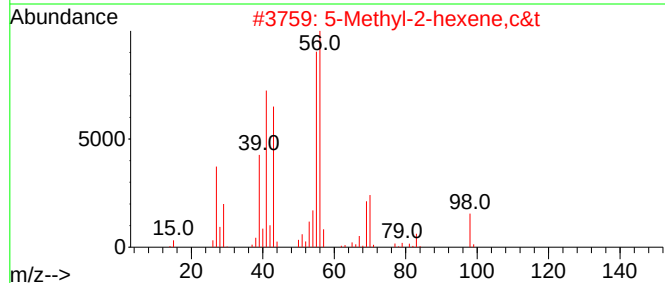
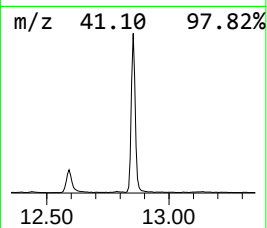
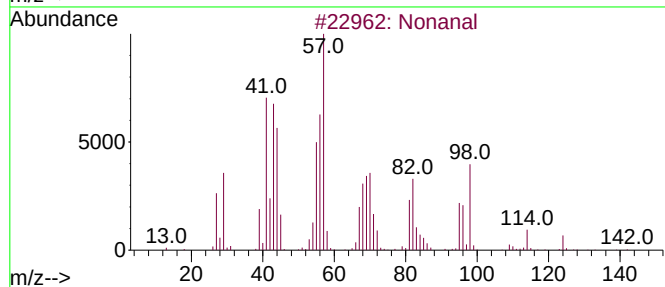
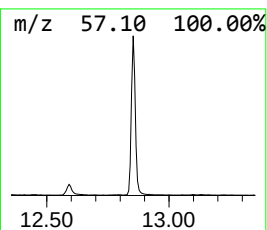
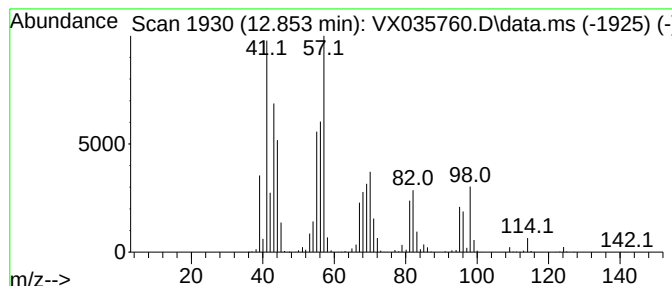
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Quant Title : SW846 8260

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

Peak Number 9 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.853	94.08 ug/l	1940950	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	90
2			5-Methyl-2-hexene,c&t	98	C7H14	003404-62-4	27
3			(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	27
4			2-Heptene	98	C7H14	000592-77-8	25
5			(Z)-2-Heptene	98	C7H14	006443-92-1	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051923\
Data File : VX035760.D
Acq On : 19 May 2023 15:08
Operator : JC/MD
Sample : 02860-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-71-05112023

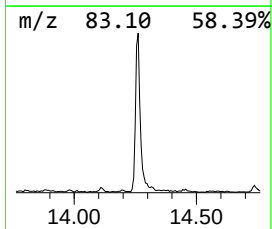
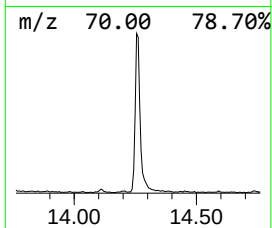
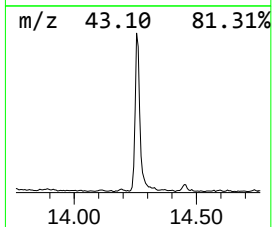
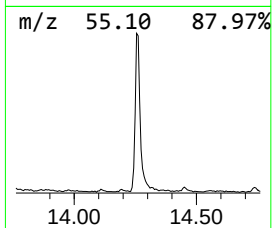
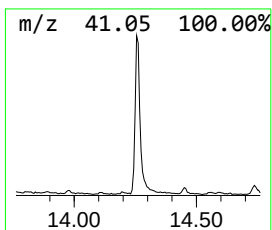
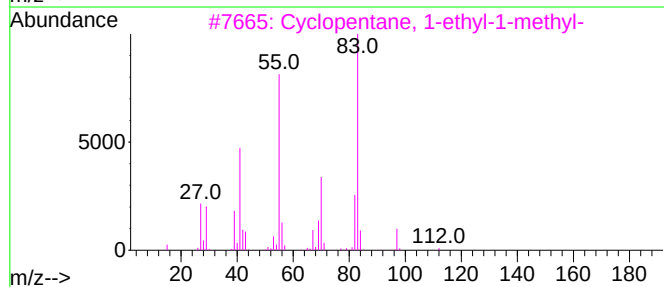
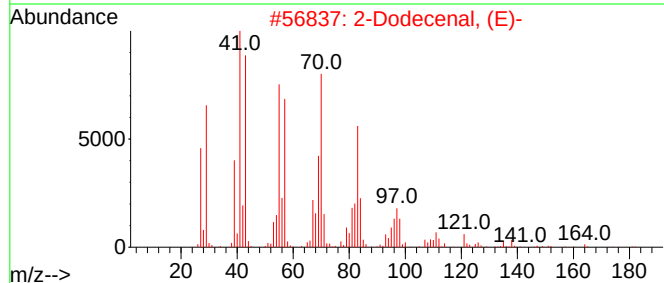
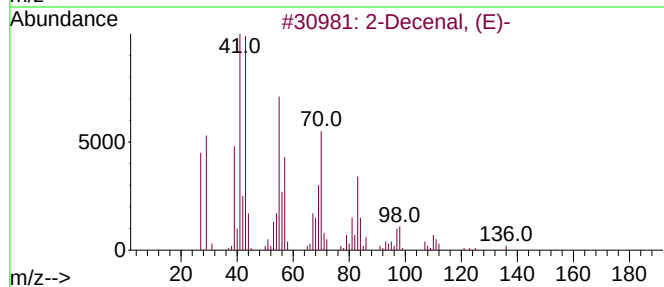
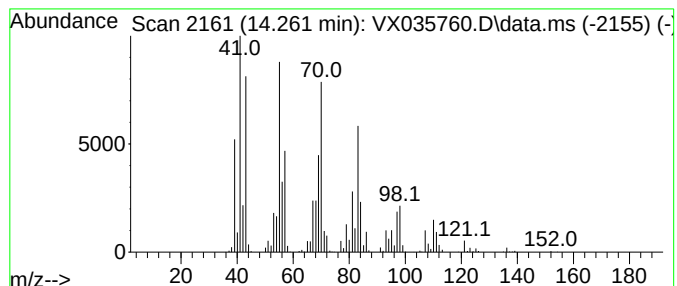
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 10 2-Decenal, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.261	33.06 ug/l	682043	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Decenal, (E)-	154	C10H18O	003913-81-3	90
2		2-Dodecenal, (E)-	182	C12H22O	020407-84-5	64
3		Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	45
4		2-Undecanethiol, 2-methyl-	202	C12H26S	010059-13-9	38
5		Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051923\
Data File : VX035760.D
Acq On : 19 May 2023 15:08
Operator : JC/MD
Sample : 02860-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-08-71-05112023

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
Pentane	1.953	11.5	ug/l	157945	1	5.549	684299	50.0
Propanal	2.300	19.0	ug/l	260135	1	5.549	684299	50.0
Pentanal	7.574	20.8	ug/l	400820	2	6.757	963944	50.0
Hexanal	9.518	198.1	ug/l	4458560	3	10.055	1125190	50.0
Heptanal	10.853	30.6	ug/l	687906	3	10.055	1125190	50.0
Octanal	11.926	42.3	ug/l	873112	4	12.024	1031540	50.0
1-Hexanol, 2-et...	12.219	10.8	ug/l	222940	4	12.024	1031540	50.0
2-Octenal, (E)-	12.591	18.8	ug/l	388030	4	12.024	1031540	50.0
Nonanal	12.853	94.1	ug/l	1940950	4	12.024	1031540	50.0
2-Decenal, (E)-	14.261	33.1	ug/l	682043	4	12.024	1031540	50.0