

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
 Data File : VX035622.D
 Acq On : 11 May 2023 20:56
 Operator : JC/MD
 Sample : 02643-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FSND-PRO-06-79-05042023

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: VX035622.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	7	9	19	rVB	54968	62891	3.70%	0.596%
2	1.355	41	44	50	rBV2	22289	29421	1.73%	0.279%
3	1.453	57	60	65	rBV	20817	28438	1.67%	0.269%
4	2.294	193	198	206	rVB	46696	75776	4.45%	0.718%
5	4.233	508	516	525	rBV4	7537	21842	1.28%	0.207%
6	5.385	692	705	721	rBV	125890	362701	21.31%	3.435%
7	5.549	721	732	747	rVB	217492	611234	35.92%	5.789%
8	5.952	788	798	811	rBV	150771	404011	23.74%	3.827%
9	6.756	921	930	947	rVB	344956	837483	49.21%	7.932%
10	7.122	980	990	1009	rBV	768829	1701729	100.00%	16.118%
11	7.573	1057	1064	1073	rBV	64647	131923	7.75%	1.249%
12	8.646	1233	1240	1249	rBV	724952	1126042	66.17%	10.665%
13	9.518	1376	1383	1396	rBV	867202	1167972	68.63%	11.062%
14	10.055	1465	1471	1484	rVB	736594	994480	58.44%	9.419%
15	10.768	1583	1588	1595	rBV	12655	19024	1.12%	0.180%
16	10.853	1597	1602	1613	rVB	148586	185372	10.89%	1.756%
17	11.079	1634	1639	1647	rBV	617681	773267	45.44%	7.324%
18	11.615	1724	1727	1732	rVB	78486	96612	5.68%	0.915%
19	11.719	1741	1744	1747	rVV3	13419	21091	1.24%	0.200%
20	11.926	1773	1778	1788	rBV	209211	251659	14.79%	2.384%
21	12.024	1788	1794	1800	rVV	707855	910453	53.50%	8.623%
22	12.085	1800	1804	1812	rVB2	13888	19544	1.15%	0.185%
23	12.231	1821	1828	1839	rBV2	20269	44007	2.59%	0.417%
24	12.591	1881	1887	1897	rBV2	39638	70237	4.13%	0.665%
25	12.853	1925	1930	1941	rBV	127722	160837	9.45%	1.523%
26	14.261	2156	2161	2170	rBV2	60338	96619	5.68%	0.915%
27	14.737	2235	2239	2244	rBV	21145	32566	1.91%	0.308%
28	15.182	2303	2312	2318	rBV10	9169	28214	1.66%	0.267%
29	15.541	2361	2371	2379	rBV	99821	162707	9.56%	1.541%
30	16.468	2515	2523	2531	rBV	66919	130003	7.64%	1.231%

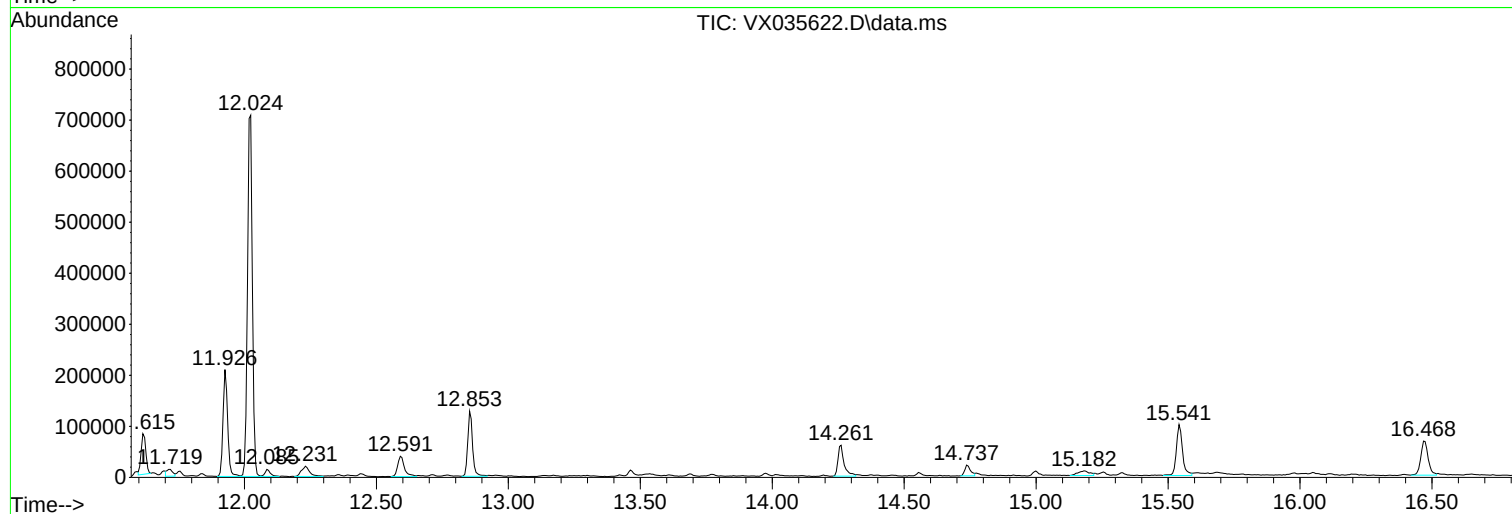
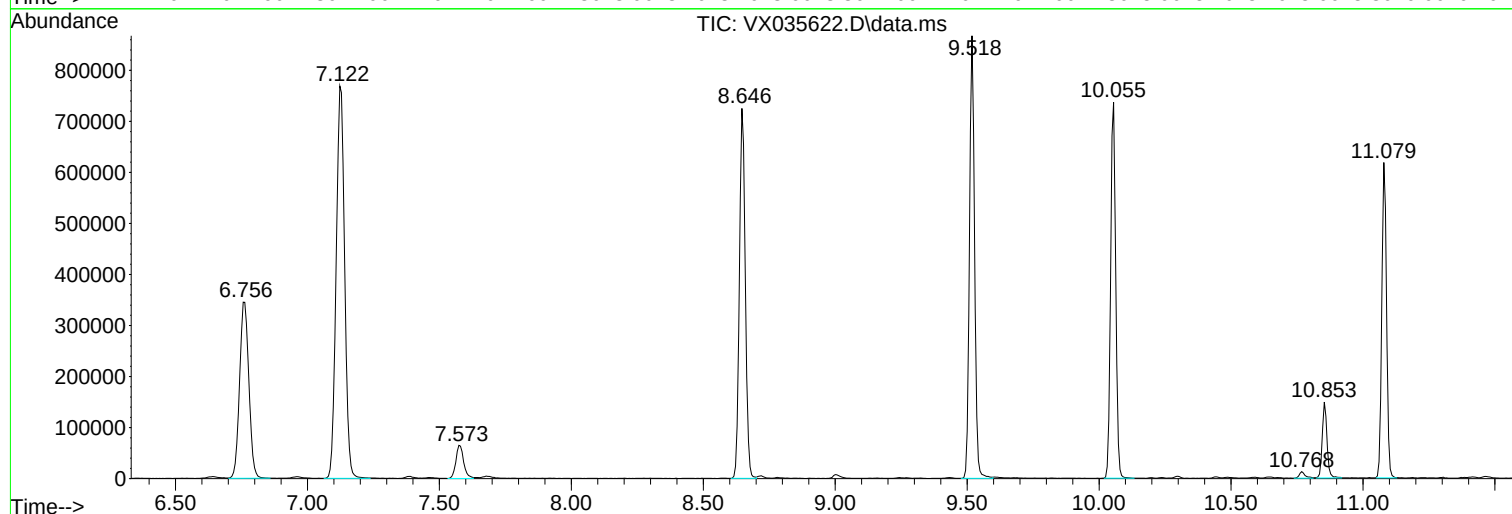
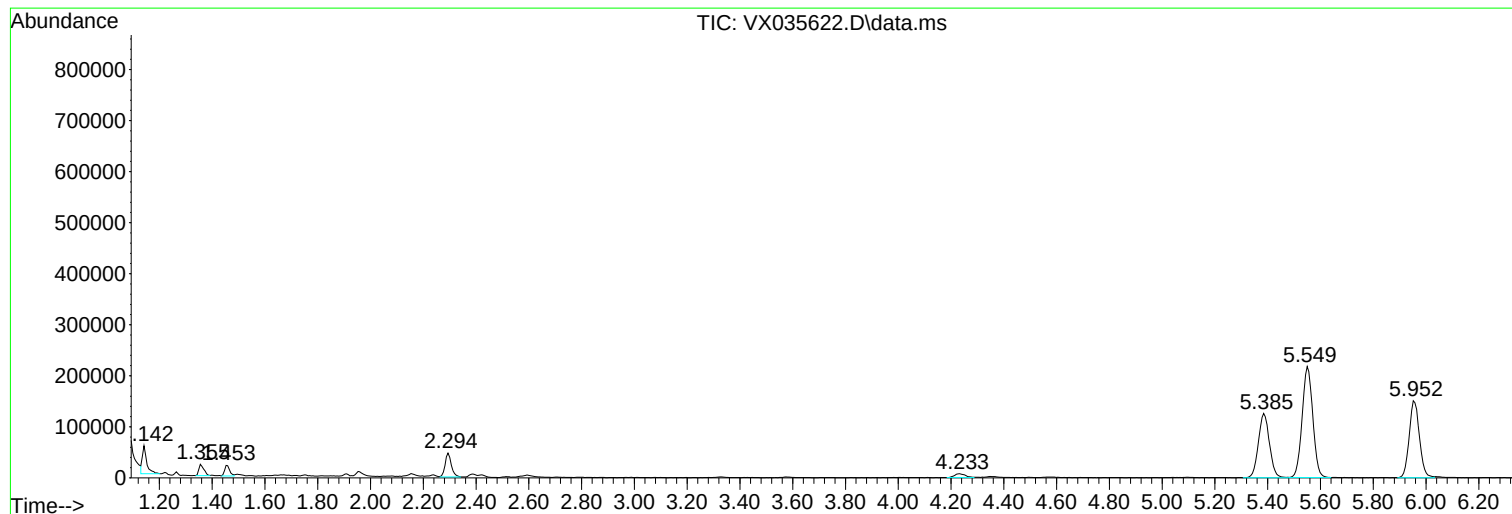
Sum of corrected areas: 10558155

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

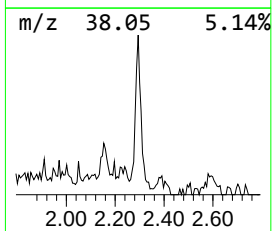
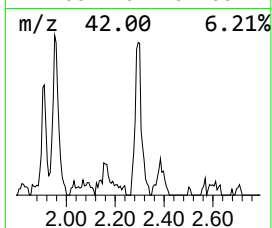
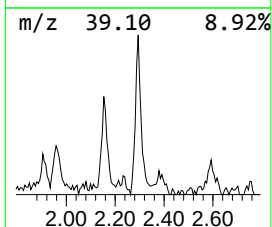
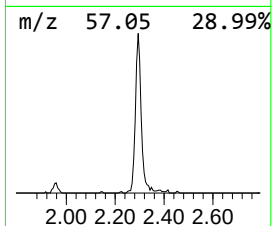
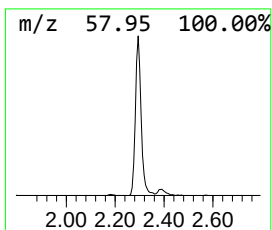
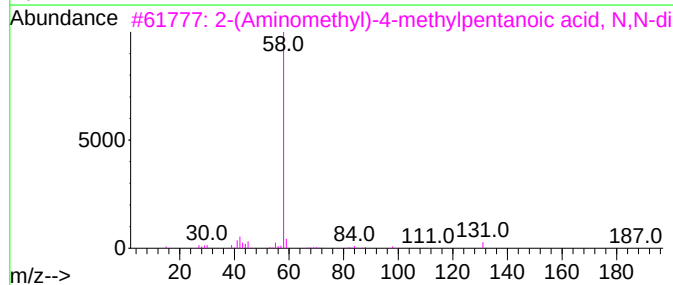
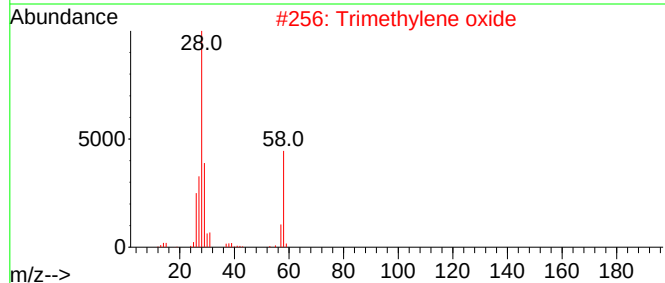
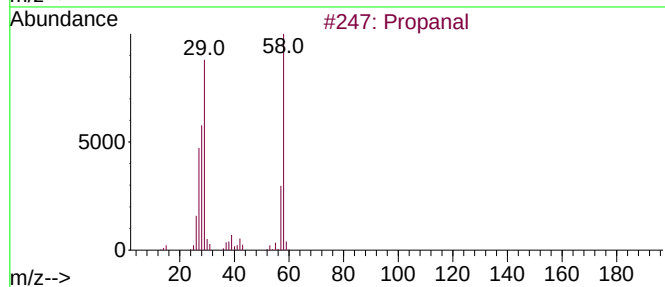
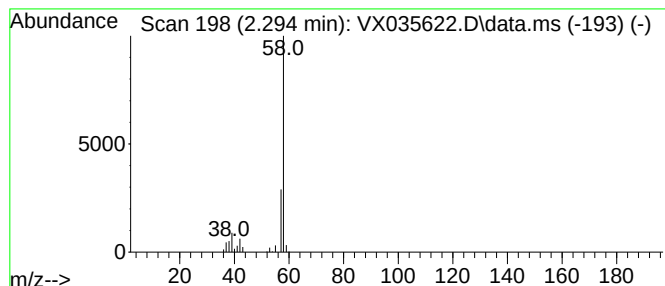
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	6.20 ug/l	75776	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			2-(Aminomethyl)-4-methylpentanoic...	187	C10H21NO2	1891211-54-3	9
4			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

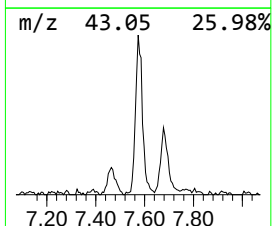
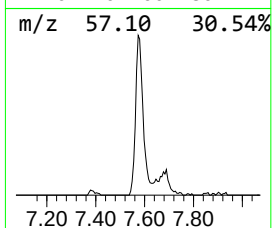
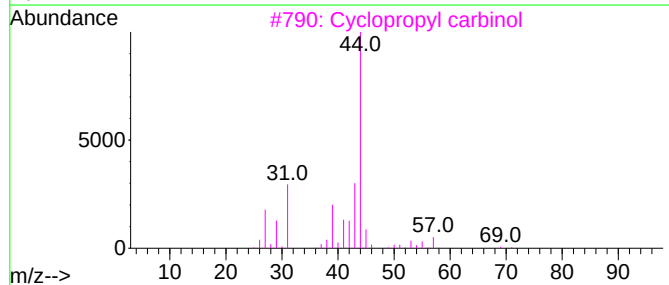
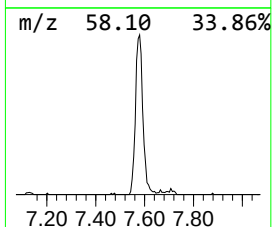
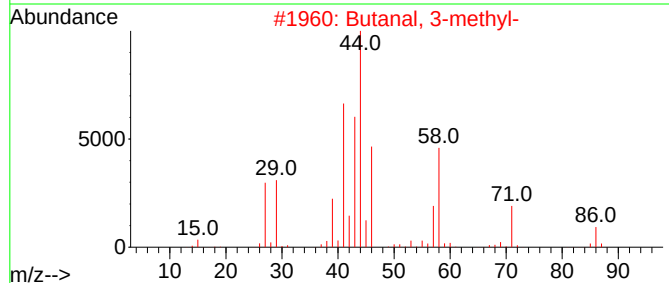
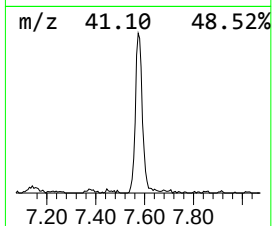
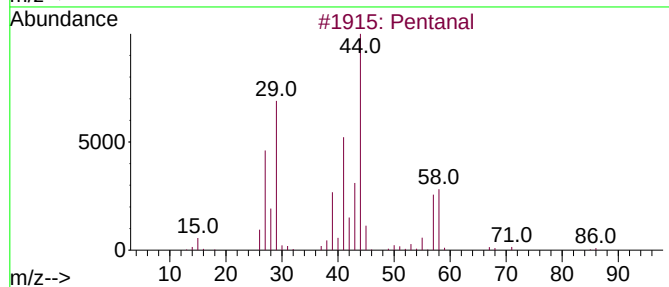
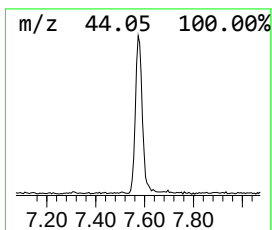
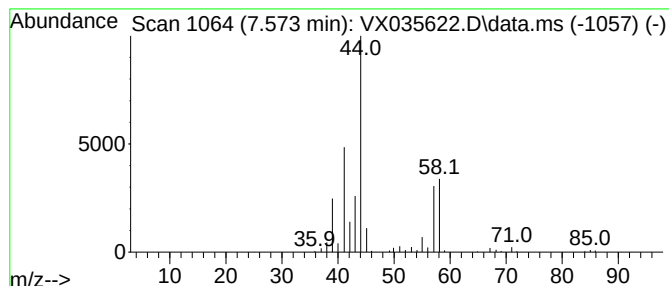
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.573	7.88 ug/l	131923	1,4-Difluorobenzene	6.763

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	43
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	38
4			Cyclobutanol	72	C4H8O	002919-23-5	9
5			Glycidol	74	C3H6O2	000556-52-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

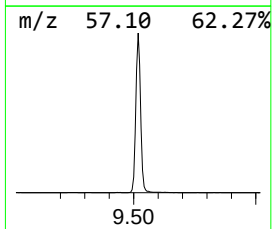
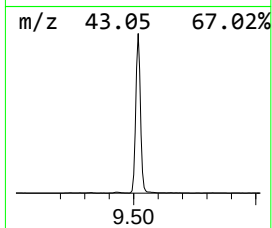
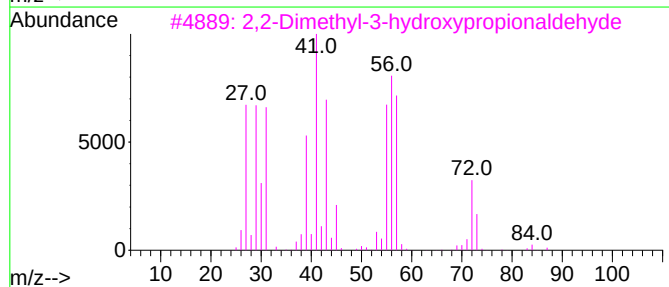
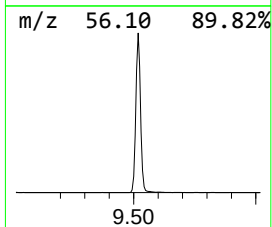
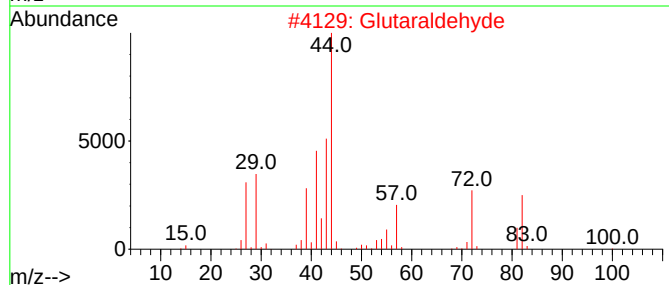
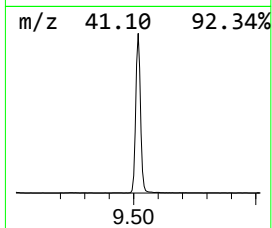
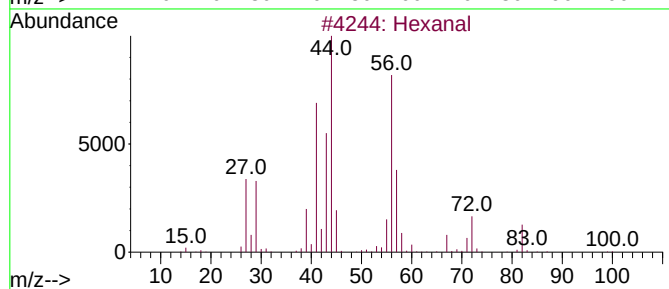
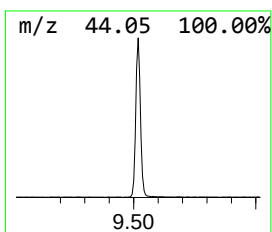
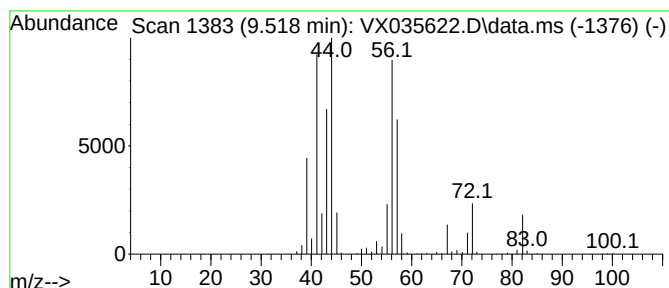
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 3 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.518	58.72 ug/l	1167970	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	87
2			Glutaraldehyde	100	C5H8O2	000111-30-8	30
3			2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	25
4			Butanal	72	C4H8O	000123-72-8	22
5			1-Hexene	84	C6H12	000592-41-6	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

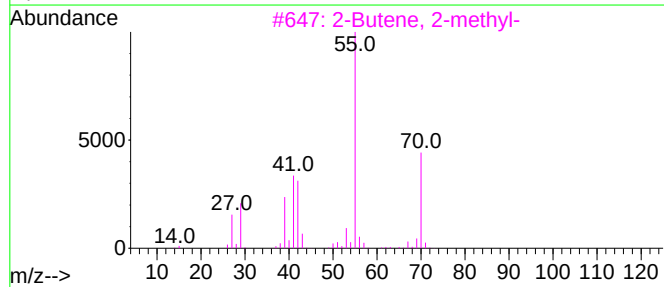
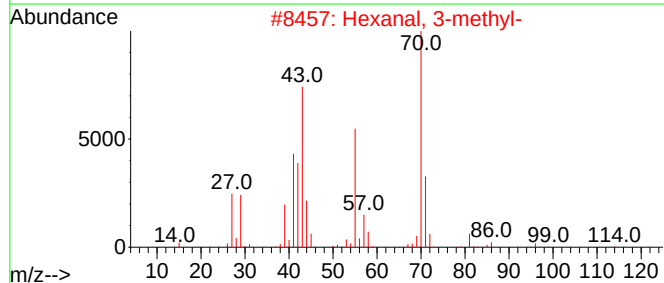
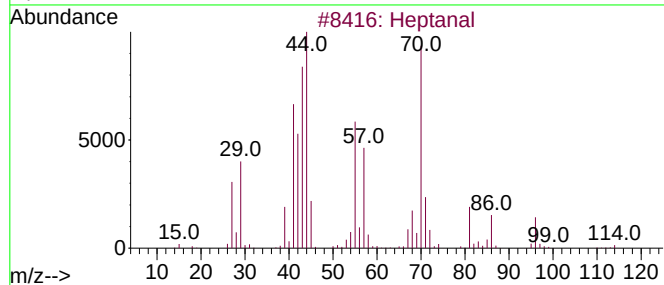
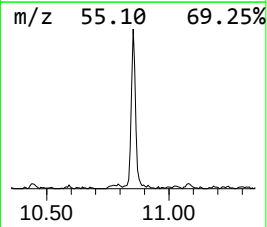
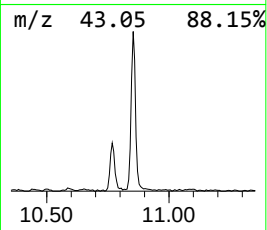
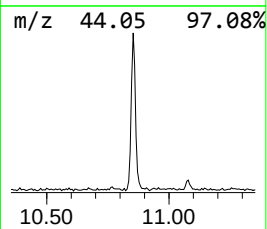
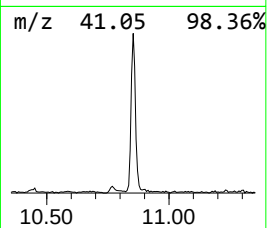
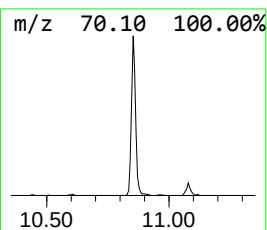
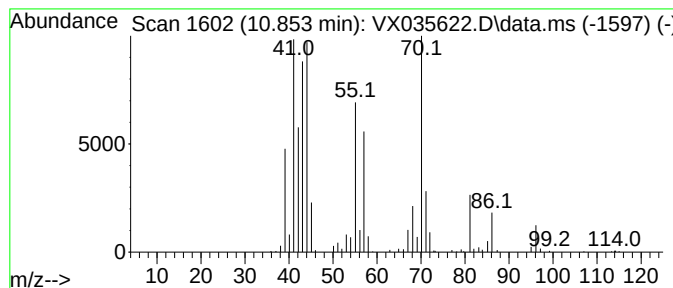
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 4 Heptanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.853	9.32 ug/l	185372	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	97
2			Hexanal, 3-methyl-	114	C7H14O	019269-28-4	38
3			2-Butene, 2-methyl-	70	C5H10	000513-35-9	38
4			2-Methyl-1-butene	70	C5H10	000563-46-2	38
5			Oxirane, 2-(1,1-dimethylethyl)-3...	114	C7H14O	053897-30-6	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

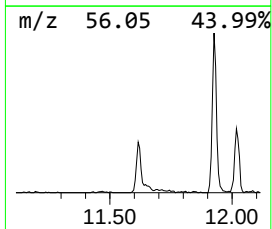
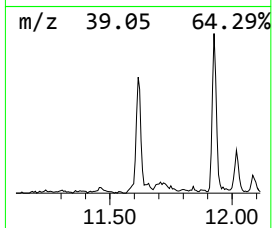
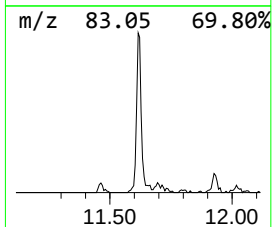
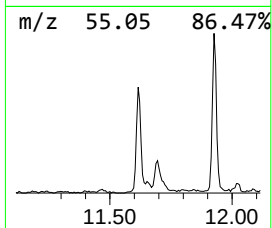
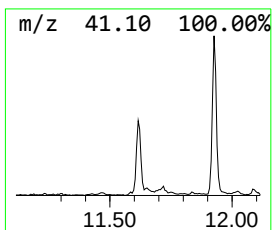
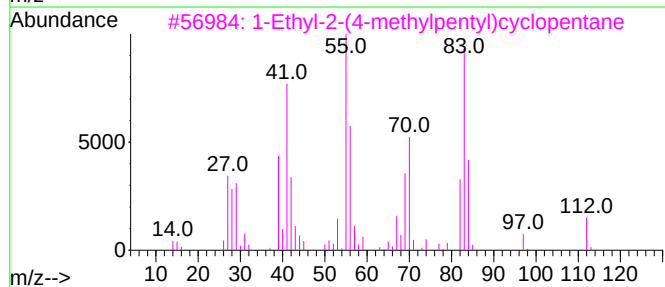
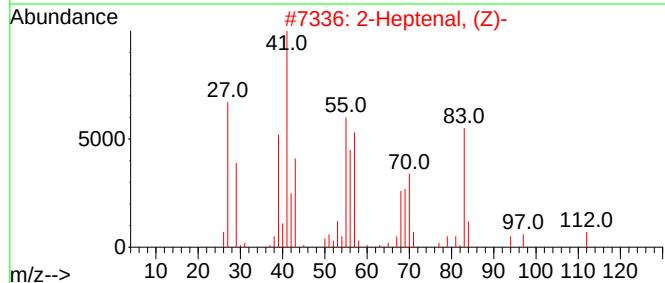
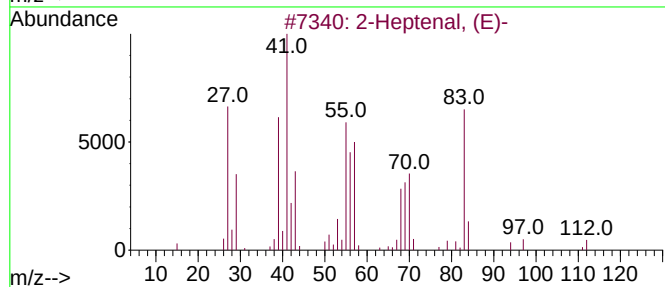
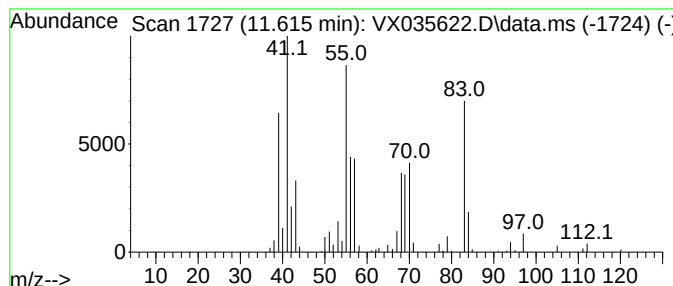
Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

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 5 2-Heptenal, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.615	5.31 ug/l	96612	1,4-Dichlorobenzene-d4			12.024
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Heptenal, (E)-		112	C7H12O	018829-55-5	94
2	2-Heptenal, (Z)-		112	C7H12O	057266-86-1	59
3	1-Ethyl-2-(4-methylpentyl)cyclop...		182	C13H26	219726-60-0	53
4	Cyclopentane, 1-ethyl-2-methyl-,...		112	C8H16	000930-89-2	47
5	Cyclopentane, 1-ethyl-3-methyl-,...		112	C8H16	002613-65-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

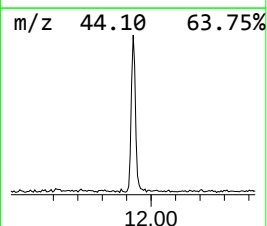
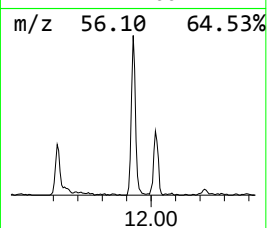
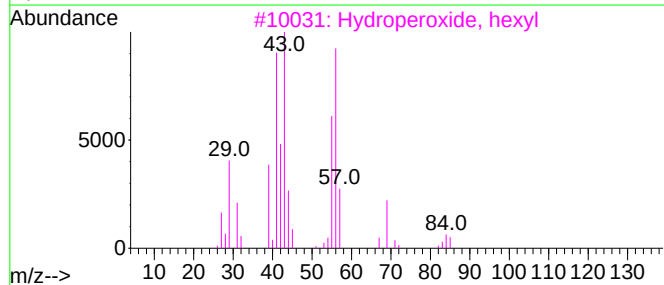
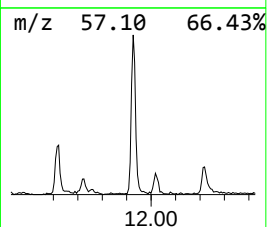
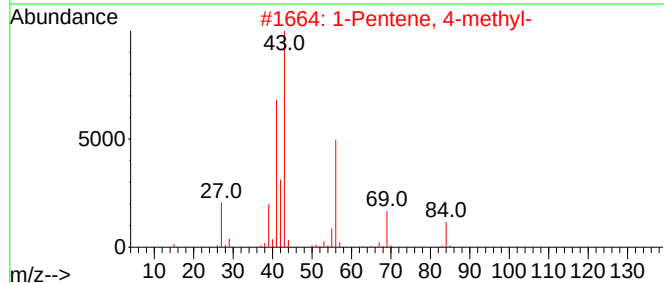
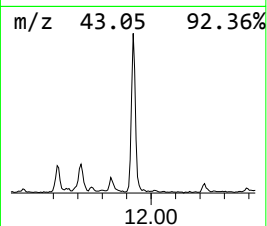
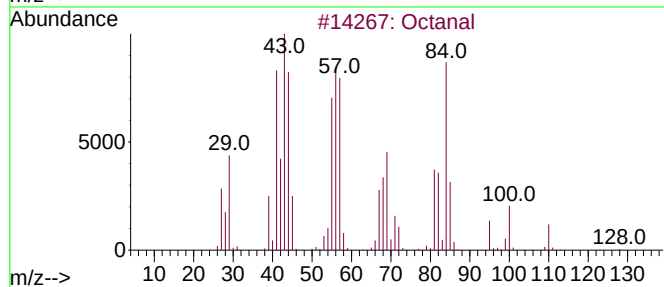
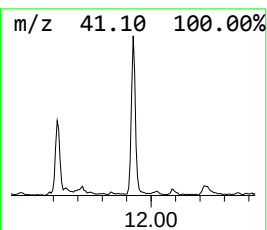
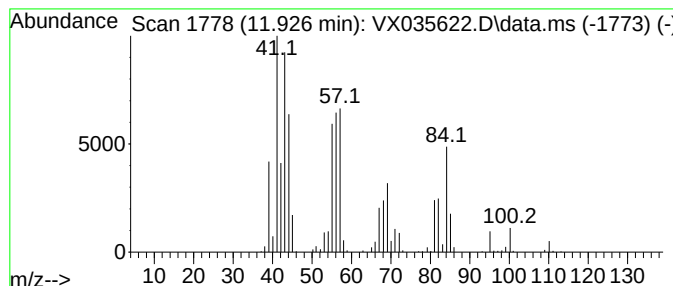
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 6 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.926	13.82 ug/l	251659	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanal	128	C8H16O	000124-13-0	91
2			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	38
3			Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	35
4			Piperazine, 2-methyl-	100	C5H12N2	000109-07-9	27
5			1-Pentene, 3-methyl-	84	C6H12	000760-20-3	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

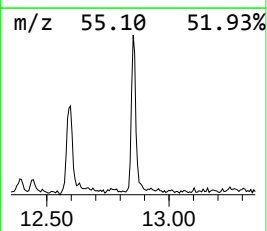
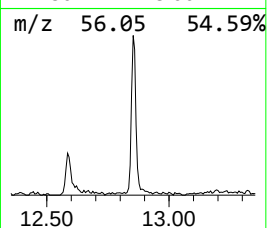
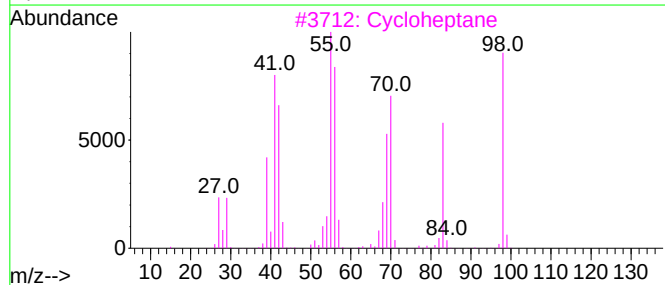
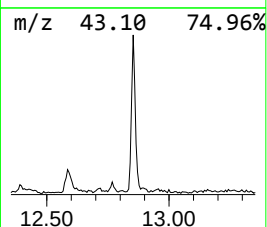
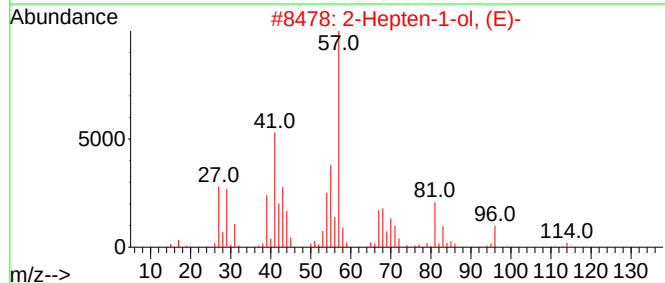
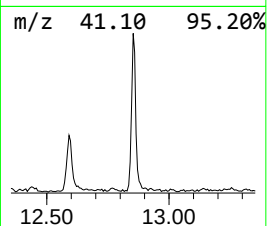
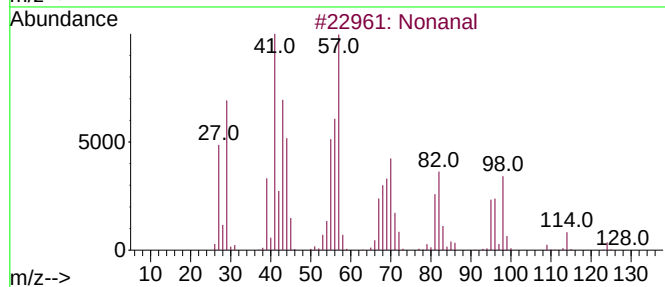
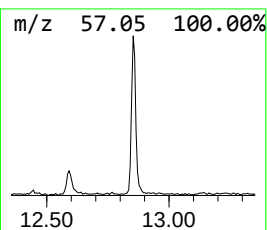
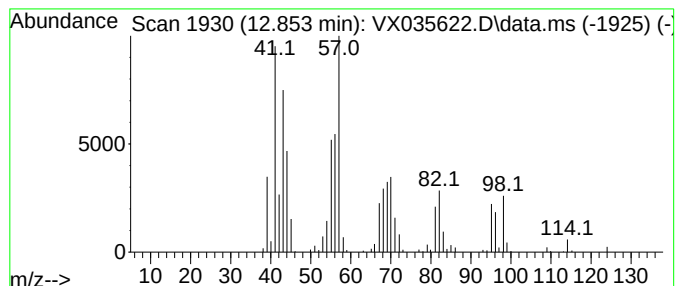
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 7 Nonanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.853	8.83 ug/l	160837	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	91
2			2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	38
3			Cycloheptane	98	C7H14	000291-64-5	30
4			5-Methyl-2-hexene,c&t	98	C7H14	003404-62-4	27
5			(Z)-2-Heptene	98	C7H14	006443-92-1	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

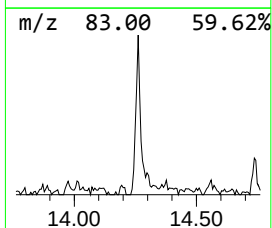
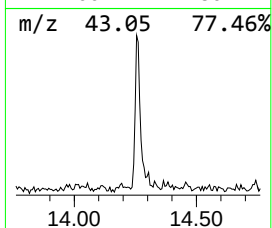
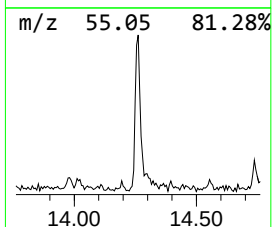
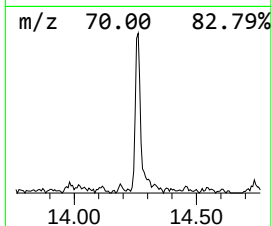
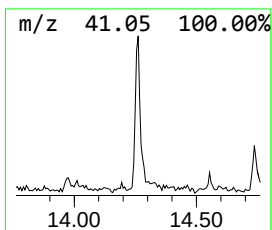
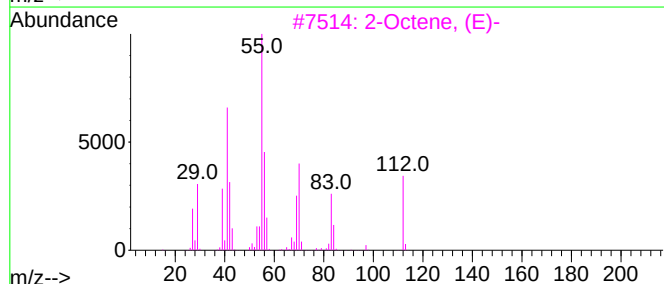
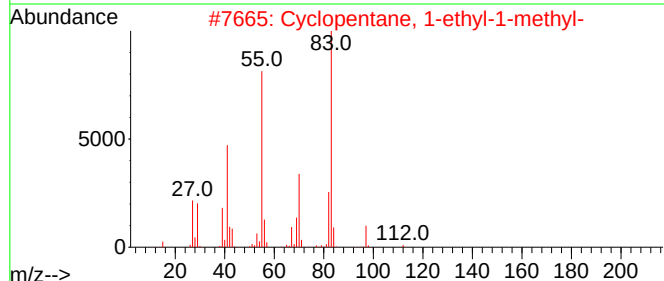
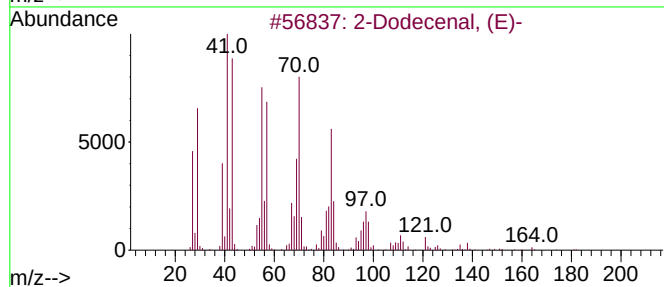
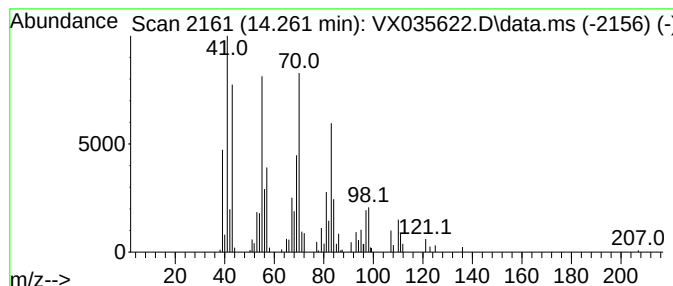
Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

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 8 2-Dodecenal, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.261	5.31 ug/l	96619	1,4-Dichlorobenzene-d4		12.024	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Dodecenal, (E)-		182	C12H22O	020407-84-5	80
2	Cyclopentane, 1-ethyl-1-methyl-		112	C8H16	016747-50-5	53
3	2-Octene, (E)-		112	C8H16	013389-42-9	43
4	Cyclopentane, 1,2,3-trimethyl-, ...		112	C8H16	002613-69-6	38
5	2-Propen-1-amine, N-2-propenyl-		97	C6H11N	000124-02-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

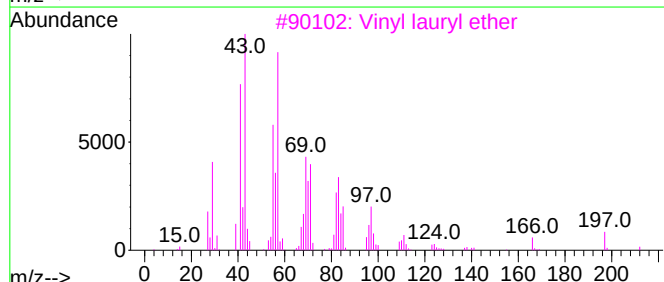
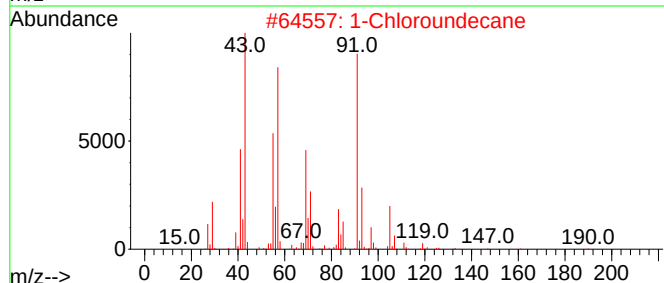
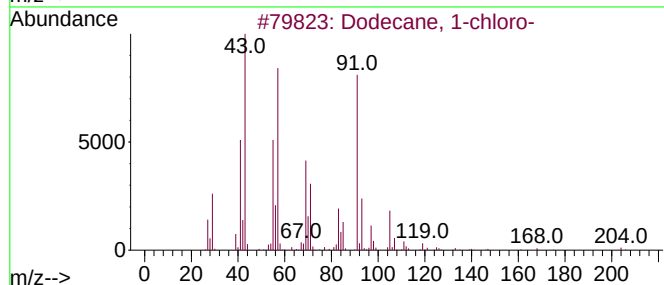
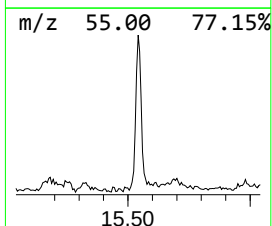
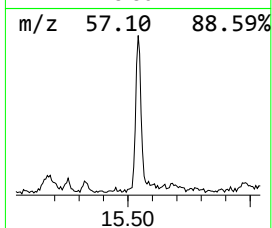
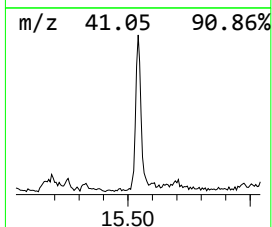
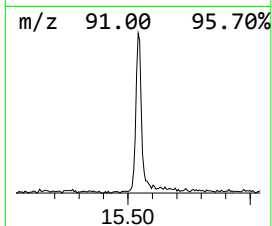
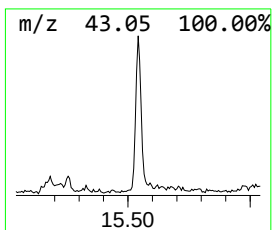
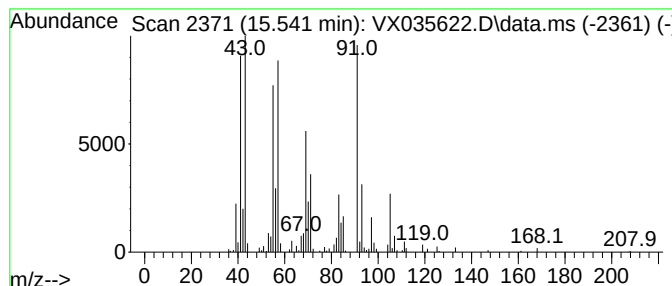
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 9 Dodecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.541	8.94 ug/l	162707	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	91
2			1-Chloroundecane	190	C11H23Cl	002473-03-2	90
3			Vinyl lauryl ether	212	C14H28O	000765-14-0	52
4			Nonane, 1-chloro-	162	C9H19Cl	002473-01-0	47
5			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

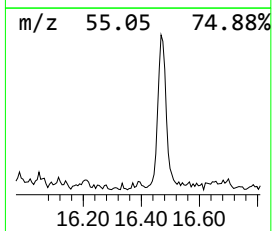
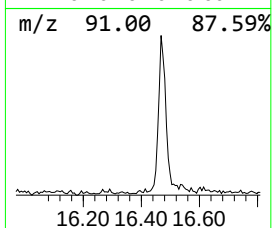
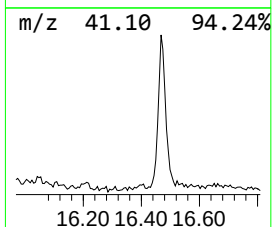
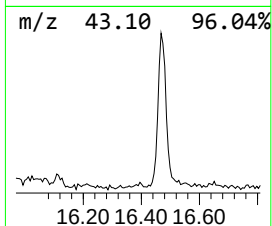
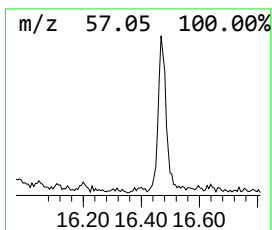
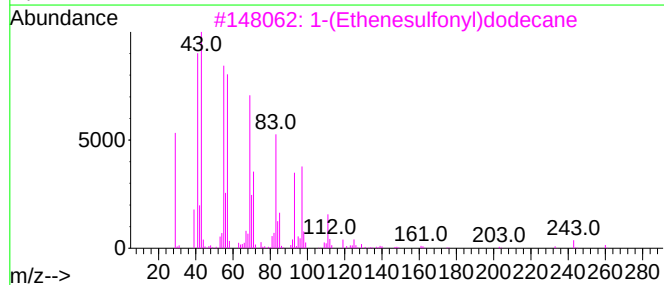
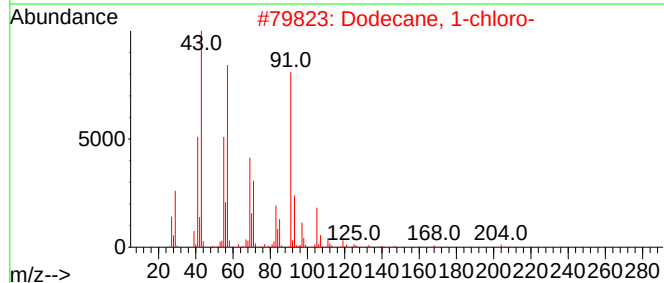
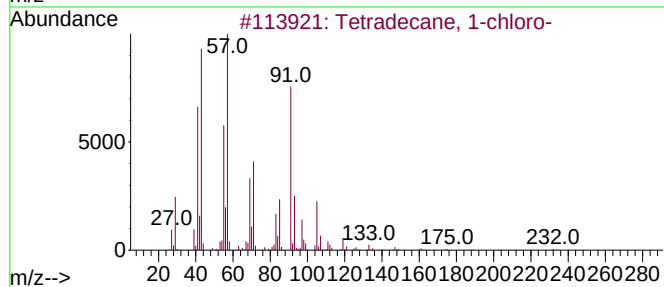
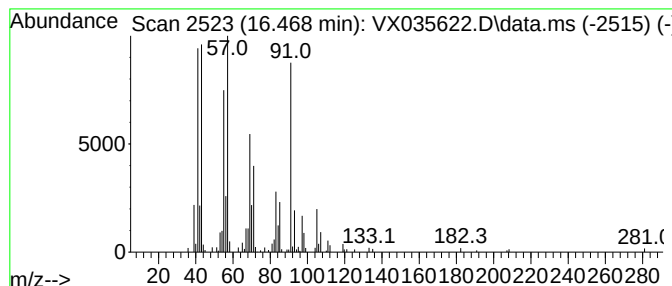
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 10 Tetradecane, 1-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.468	7.14 ug/l	130003	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	64
2			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	64
3			1-(Ethenesulfonyl)dodecane	260	C14H28O2S	030719-66-5	46
4			Oxalic acid, allyl undecyl ester	284	C16H28O4	1000309-23-9	38
5			Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051123\
Data File : VX035622.D
Acq On : 11 May 2023 20:56
Operator : JC/MD
Sample : 02643-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-06-79-05042023

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
Propanal	2.294	6.2	ug/l	75776	1	5.549	611234	50.0
Pentanal	7.573	7.9	ug/l	131923	2	6.763	837483	50.0
Hexanal	9.518	58.7	ug/l	1167970	3	10.055	994480	50.0
Heptanal	10.853	9.3	ug/l	185372	3	10.055	994480	50.0
2-Heptenal, (E)-	11.615	5.3	ug/l	96612	4	12.024	910453	50.0
Octanal	11.926	13.8	ug/l	251659	4	12.024	910453	50.0
Nonanal	12.853	8.8	ug/l	160837	4	12.024	910453	50.0
2-Dodecenal, (E)-	14.261	5.3	ug/l	96619	4	12.024	910453	50.0
Dodecane, 1-chl...	15.541	8.9	ug/l	162707	4	12.024	910453	50.0
Tetradecane, 1-...	16.468	7.1	ug/l	130003	4	12.024	910453	50.0