

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX052820\
 Data File : VX016492.D
 Acq On : 28 May 2020 17:48
 Operator : JC/SP
 Sample : L2777-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SS036MW002-200526

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.470	706	719	732	rBV2	145857	419252	4.73%	1.514%
2	5.629	735	745	758	rVB	277834	774345	8.73%	2.796%
3	6.037	800	812	823	rBV2	166904	443459	5.00%	1.601%
4	6.836	931	943	959	rBV	425346	1023471	11.54%	3.695%
5	8.695	1240	1248	1259	rBV	914977	1439511	16.23%	5.197%
6	10.098	1472	1478	1497	rVB	975792	1313807	14.81%	4.743%
7	11.122	1640	1646	1659	rVB	846433	1064732	12.00%	3.844%
8	12.061	1794	1800	1808	rBV	1073178	1334606	15.04%	4.818%
9	13.463	2025	2030	2066	rBV	7017275	8871271	100.00%	32.028%
10	13.932	2103	2107	2120	rBV5	46103	122054	1.38%	0.441%
11	14.231	2152	2156	2186	rBV	6651777	8608771	97.04%	31.081%
12	14.609	2213	2218	2225	rBV	177288	297131	3.35%	1.073%
13	14.731	2234	2238	2250	rVV	237104	369665	4.17%	1.335%
14	14.834	2251	2255	2271	rVV	585003	985517	11.11%	3.558%
15	14.956	2271	2275	2307	rVB	215781	536439	6.05%	1.937%
16	15.298	2327	2331	2345	rVB	43940	94042	1.06%	0.340%

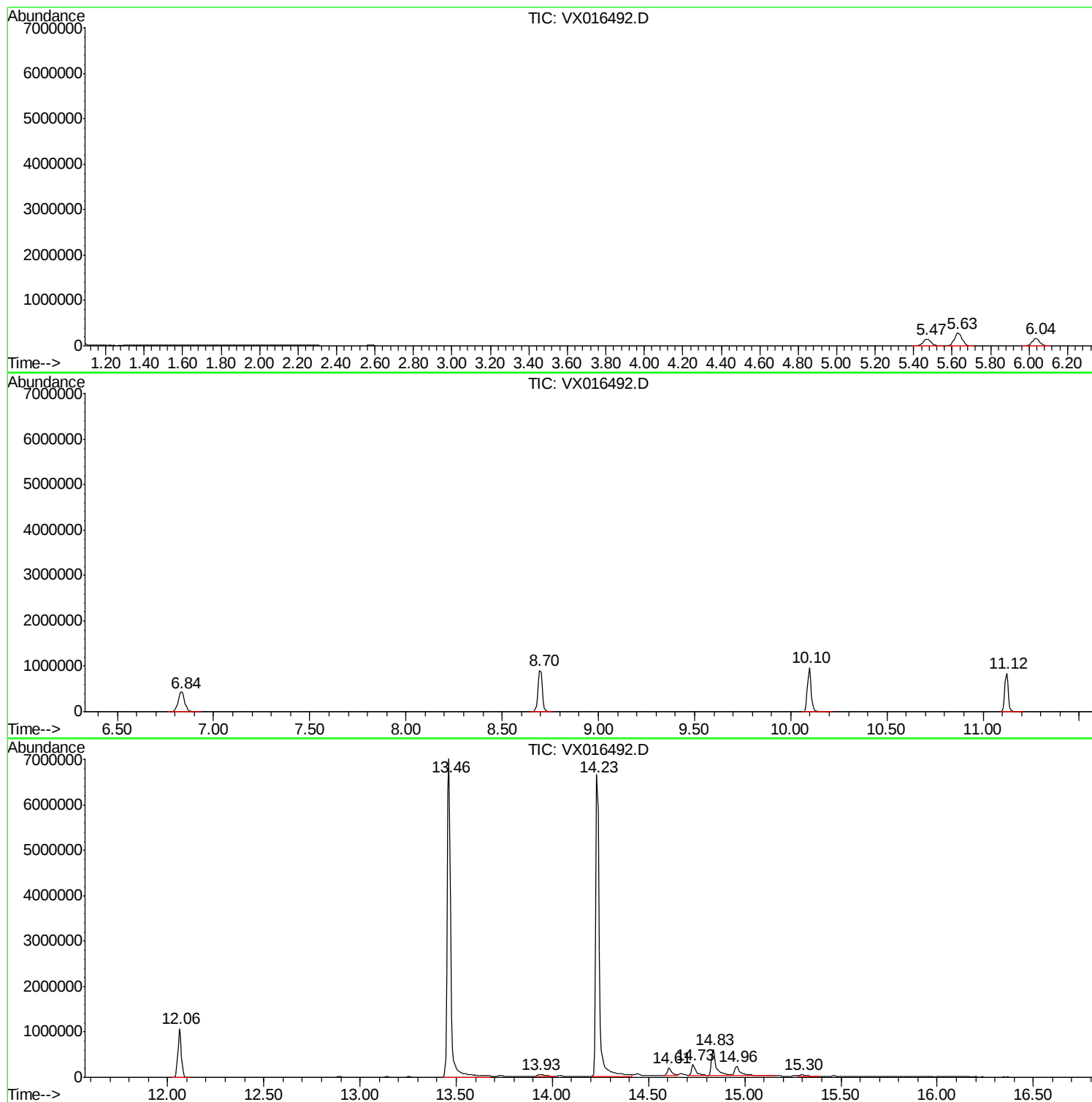
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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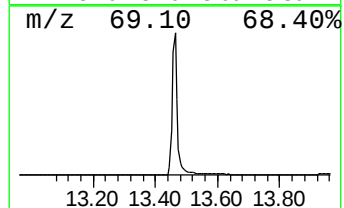
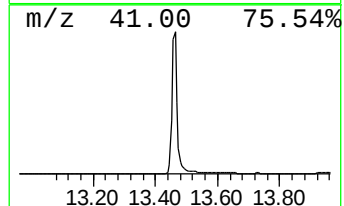
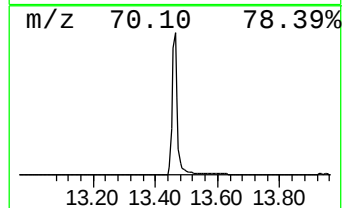
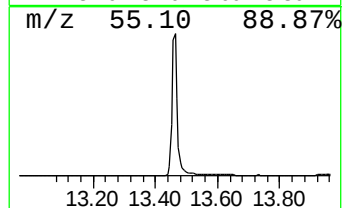
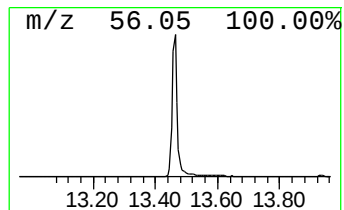
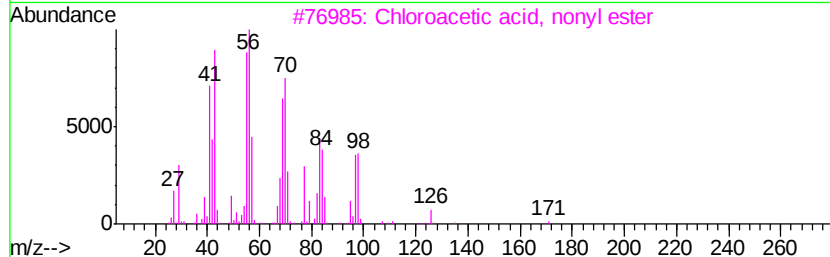
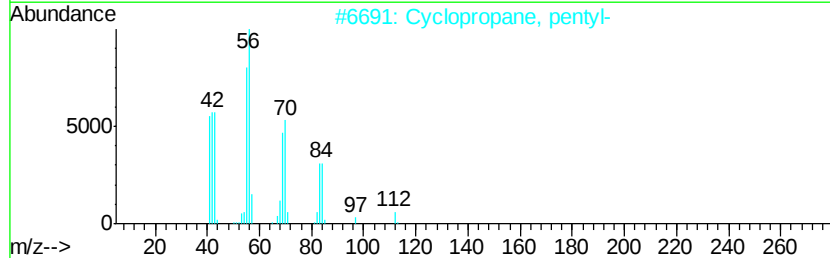
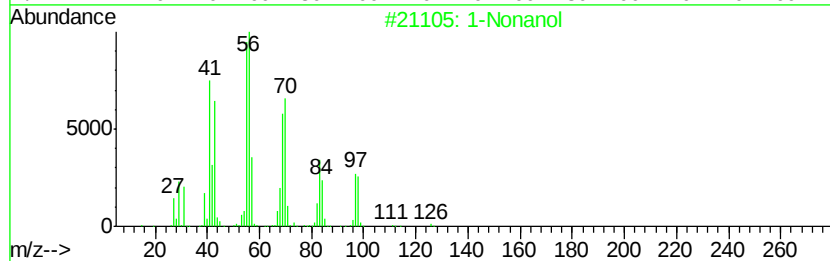
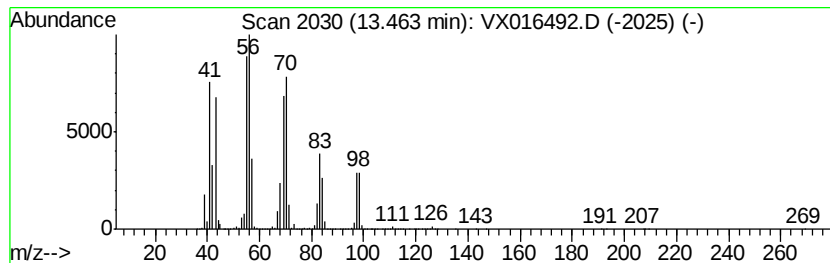
Instrument :
MSVOA_X
ClientSampleId :
SS036MW002-200526

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	332.36 ug/l	8871270	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonanol		144 C9H20O	000143-08-8 91
2	Cyclopropane, pentyl-		112 C8H16	002511-91-3 81
3	Chloroacetic acid, nonyl ester		220 C11H21ClO2	005451-96-7 80
4	Cyclopropane, 1-methyl-2-octyl-		168 C12H24	037617-26-8 72
5	Cycloheptane		98 C7H14	000291-64-5 72



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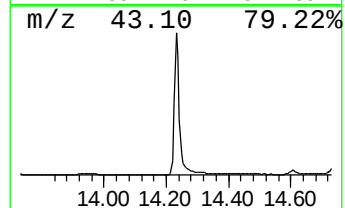
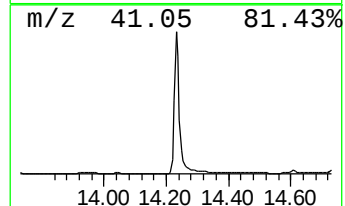
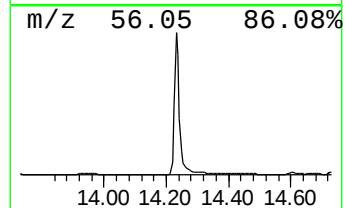
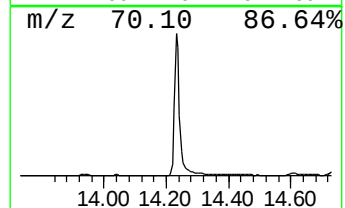
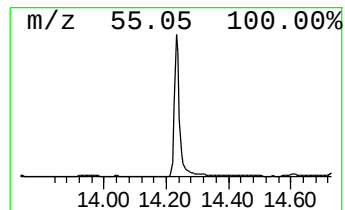
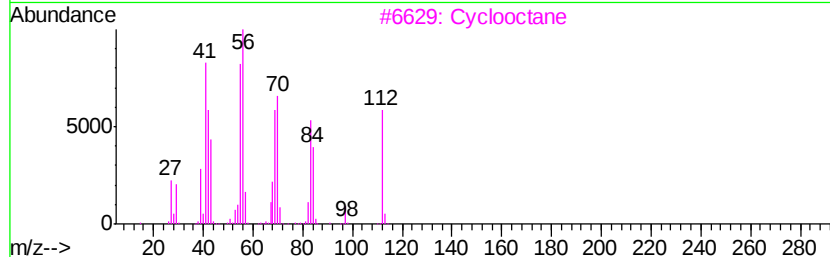
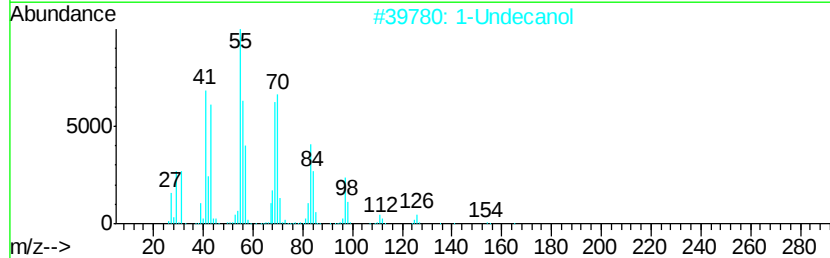
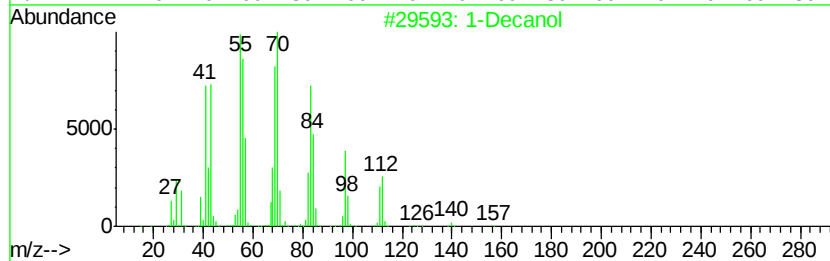
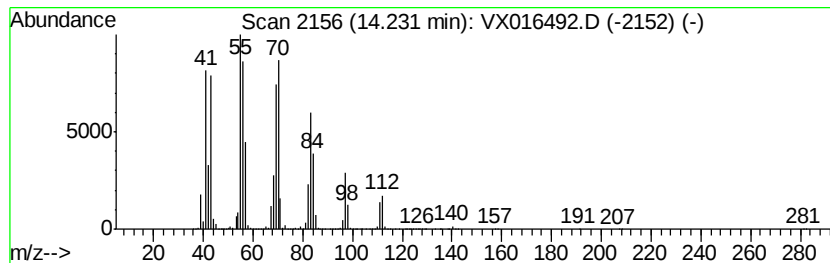
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Decanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	322.52 ug/l	8608770	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decanol	158	C10H22O	000112-30-1	91
2		1-Undecanol	172	C11H24O	000112-42-5	90
3		Cyclooctane	112	C8H16	000292-64-8	87
4		Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	86
5		Cyclopropane, 1-heptyl-2-methyl-	154	C11H22	074663-91-5	86



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Instrument :
MSVOA_X
ClientSampleId :
SS036MW002-200526

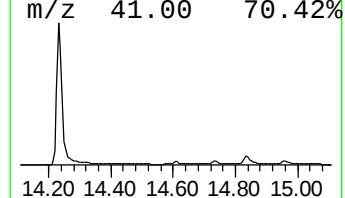
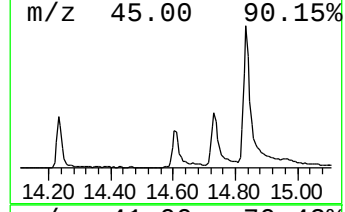
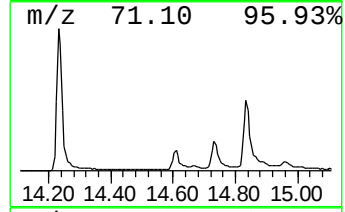
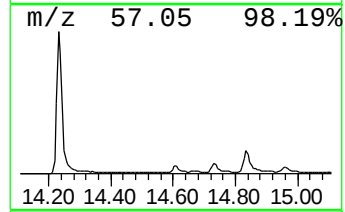
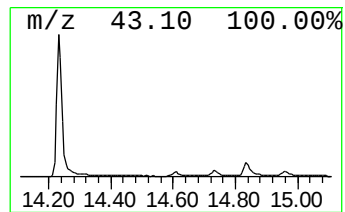
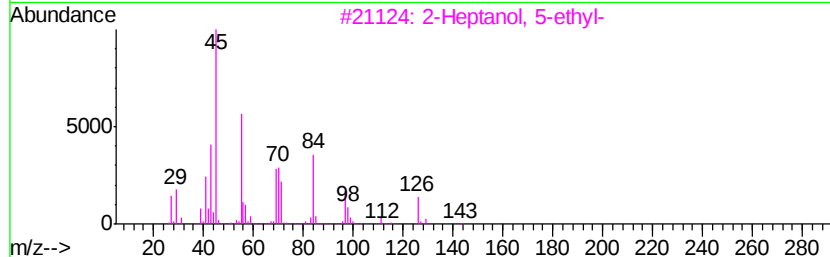
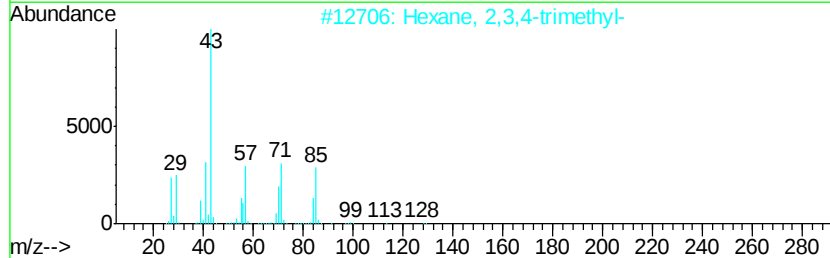
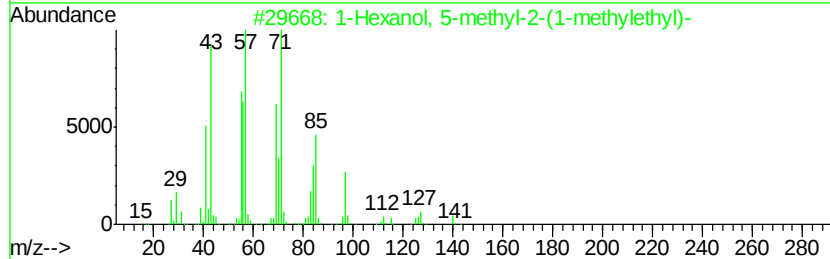
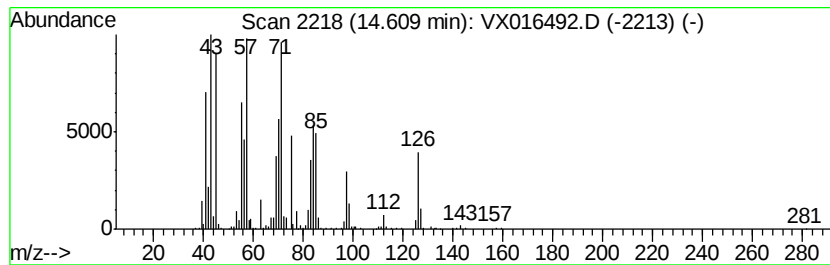
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Peak Number 3 unknown14.61 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	11.13 ug/l	297131	1,4-Dichlorobenzene-d4	12.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 5-methyl-2-(1-methyle...	158	C10H22O	002051-33-4	43	
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	38	
3	2-Heptanol, 5-ethyl-	144	C9H20O	019780-40-6	38	
4	Octane, 4-methyl-	128	C9H20	002216-34-4	27	
5	Propanal, 2-methyl-, 2-propenylh...	126	C7H14N2	066075-08-9	25	



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Instrument :
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SS036MW002-200526

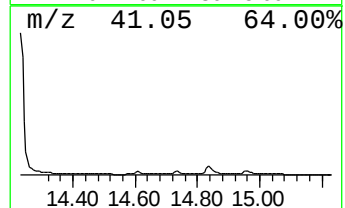
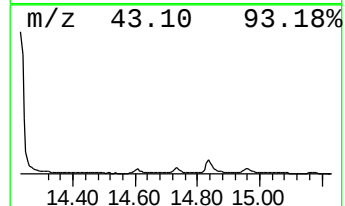
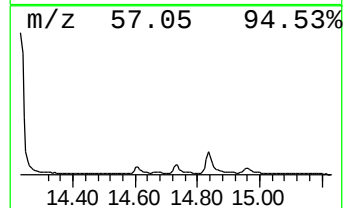
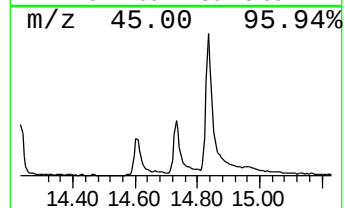
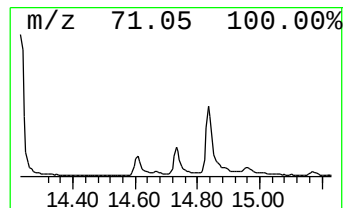
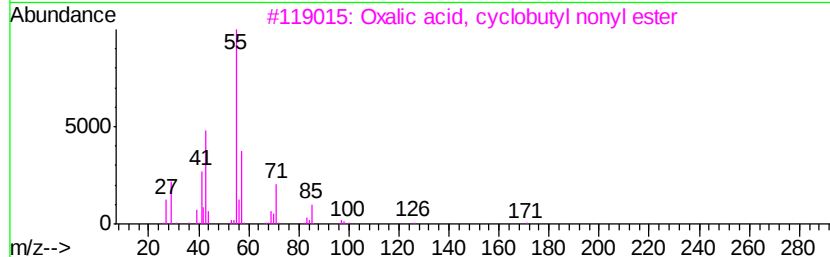
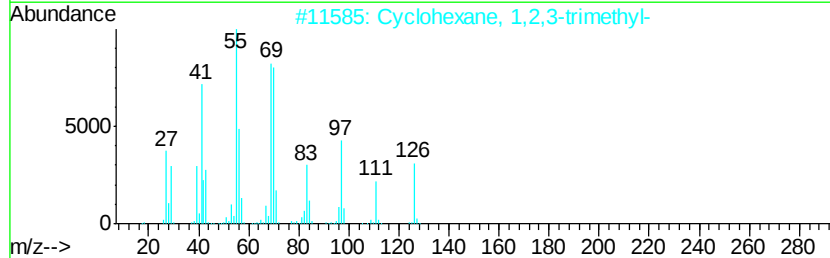
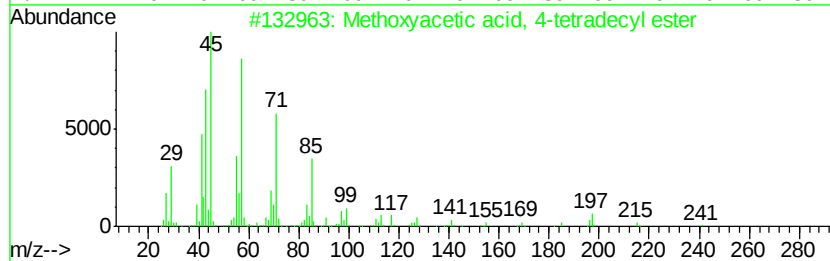
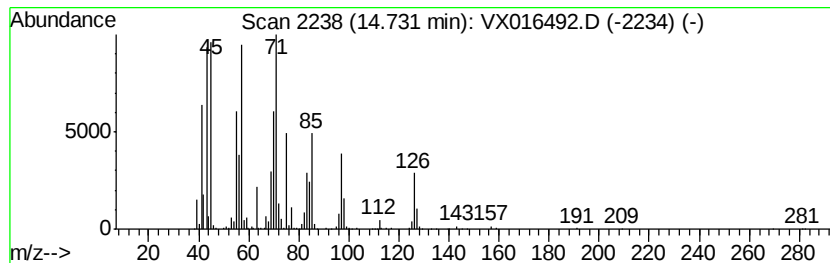
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TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.73 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	13.85 ug/l	369665	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methoxyvacetic acid, 4-tetradecyl...	286	C17H34O3	1000282-05-0	47
2		Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	38
3		Oxalic acid, cyclobutyl nonyl ester	270	C15H26O4	1000309-70-0	35
4		Propanoic acid, nonyl ester	200	C12H24O2	053184-67-1	27
5		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	22



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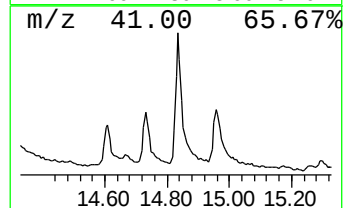
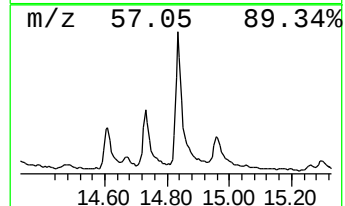
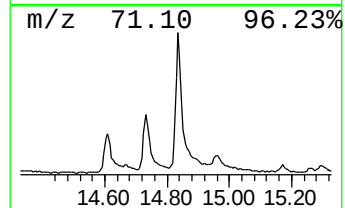
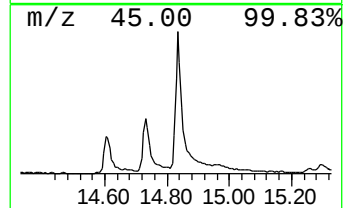
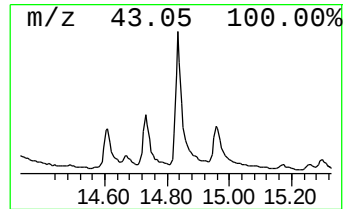
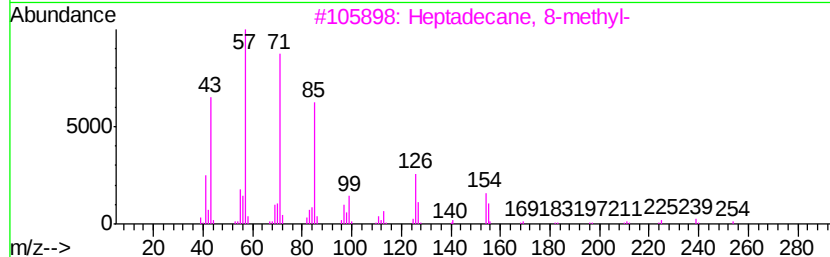
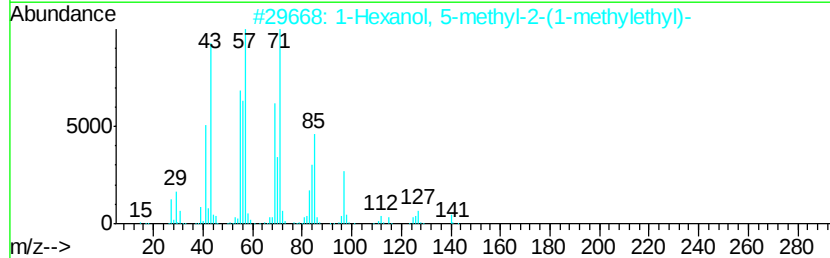
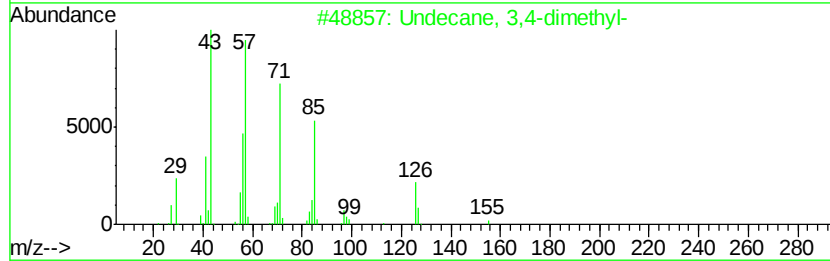
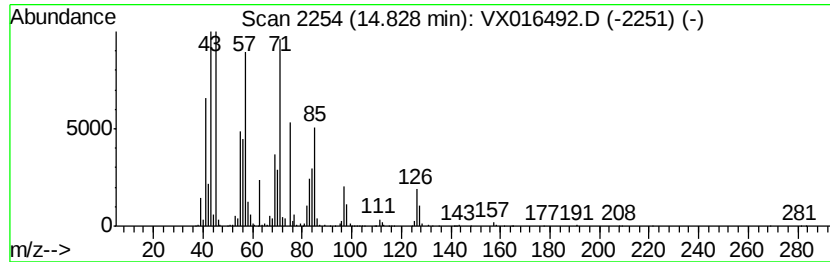
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown14.83 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	36.92 ug/l	985517	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane, 3,4-dimethyl-	184	C13H28	017312-78-6	43
2		1-Hexanol, 5-methyl-2-(1-methyle...	158	C10H22O	002051-33-4	38
3		Heptadecane, 8-methyl-	254	C18H38	013287-23-5	35
4		Nonane, 5-butyl-	184	C13H28	017312-63-9	35
5		Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	30



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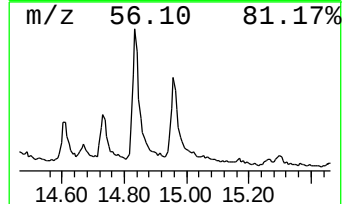
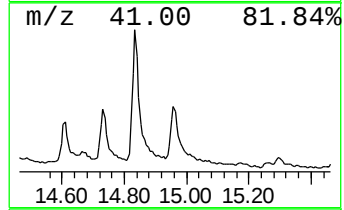
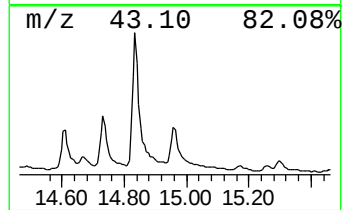
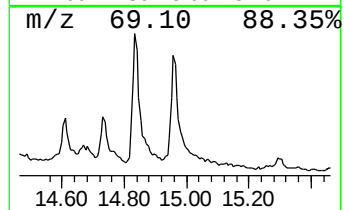
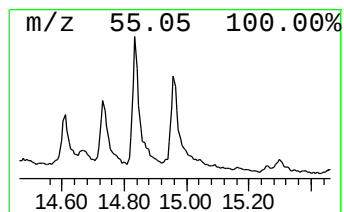
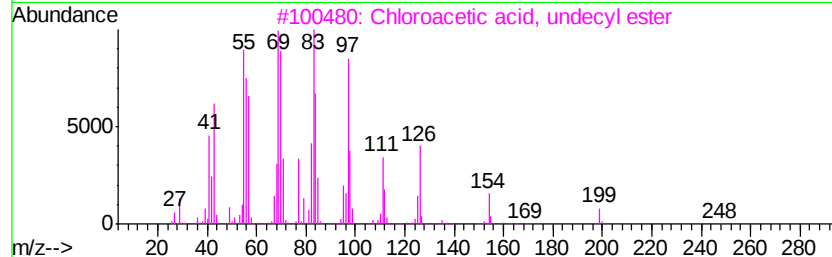
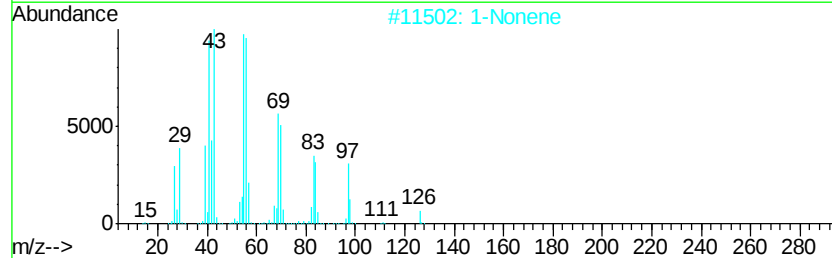
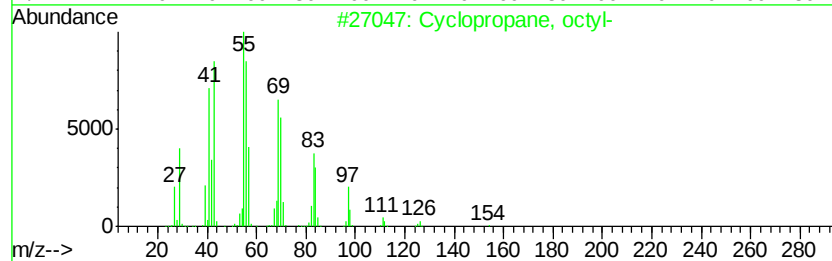
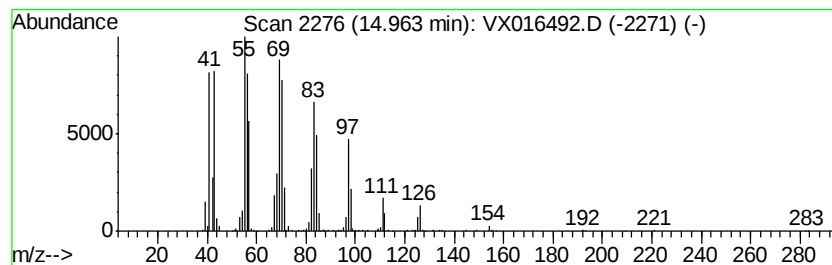
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclopropane, octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	20.10 ug/l	536439	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropane, octyl-	154	C11H22	001472-09-9	94
2		1-Nonene	126	C9H18	000124-11-8	93
3		Chloroacetic acid, undecyl ester	248	C13H25ClO2	005458-29-7	90
4		Carbonochloridic acid, decyl ester	220	C11H21ClO2	055488-51-2	90
5		1-Decanol	158	C10H22O	000112-30-1	87



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX052820\
Data File : VX016492.D
Acq On : 28 May 2020 17:48
Operator : JC/SP
Sample : L2777-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SS036MW002-200526

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Nonanol	13.46	332.4	ug/l	8871270	4	12.06	1334610	50.0
1-Decanol	14.23	322.5	ug/l	8608770	4	12.06	1334610	50.0
unknown14.61	14.61	11.1	ug/l	297131	4	12.06	1334610	50.0
unknown14.73	14.73	13.9	ug/l	369665	4	12.06	1334610	50.0
unknown14.83	14.83	36.9	ug/l	985517	4	12.06	1334610	50.0
Cyclopropane, octyl-	14.96	20.1	ug/l	536439	4	12.06	1334610	50.0