

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060721\
 Data File : VX022539.D
 Acq On : 07 Jun 2021 17:17
 Operator : JC/MD
 Sample : M2583-19 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 33-34

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\82X060721W.M
 Title : SW846 8260

Signal : TIC: VX022539.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.355	41	44	52	rVB	6068	6868	1.63%	0.239%
2	2.392	206	214	219	rBV	9528	15090	3.57%	0.525%
3	2.550	229	240	253	rVB	11185	22702	5.37%	0.790%
4	4.592	566	575	584	rBV3	3400	11180	2.65%	0.389%
5	5.397	696	707	719	rBV2	42793	123779	29.29%	4.307%
6	5.562	723	734	748	rBV	73083	203960	48.26%	7.098%
7	5.970	790	801	811	rBV2	56814	149662	35.41%	5.208%
8	6.769	923	932	945	rBV	128162	302178	71.50%	10.515%
9	8.580	1222	1229	1234	rBV2	3189	4807	1.14%	0.167%
10	8.653	1234	1241	1250	rBV	274138	422626	100.00%	14.707%
11	8.726	1250	1253	1261	rVB2	5568	9056	2.14%	0.315%
12	10.055	1464	1471	1483	rBV	260797	359316	85.02%	12.504%
13	10.543	1548	1551	1557	rVB	6965	9616	2.28%	0.335%
14	11.085	1635	1640	1652	rBV	208361	259036	61.29%	9.014%
15	11.360	1681	1685	1691	rBV	3946	5248	1.24%	0.183%
16	12.024	1789	1794	1802	rVB	263202	318982	75.48%	11.100%
17	12.103	1802	1807	1813	rBV2	16750	22262	5.27%	0.775%
18	12.219	1821	1826	1834	rBV2	11539	19272	4.56%	0.671%
19	12.768	1912	1916	1918	rBV3	5085	7562	1.79%	0.263%
20	12.792	1918	1920	1926	rVB3	7158	9696	2.29%	0.337%
21	12.865	1927	1932	1945	rBV	56282	99206	23.47%	3.452%
22	12.975	1945	1950	1956	rBV2	18715	37851	8.96%	1.317%
23	13.073	1961	1966	1968	rBV3	21955	31880	7.54%	1.109%
24	13.103	1968	1971	1975	rBV2	49673	74259	17.57%	2.584%
25	13.402	2017	2020	2027	rBV4	7606	15547	3.68%	0.541%
26	13.536	2031	2042	2043	rBV5	13743	33467	7.92%	1.165%
27	13.560	2043	2046	2048	rVV3	6232	7331	1.73%	0.255%
28	13.591	2048	2051	2054	rVV3	14466	18510	4.38%	0.644%
29	13.701	2065	2069	2071	rBV2	18828	29028	6.87%	1.010%
30	13.731	2071	2074	2083	rVV5	41347	97973	23.18%	3.409%
31	13.835	2087	2091	2093	rVV2	24614	41026	9.71%	1.428%
32	13.859	2093	2095	2098	rVV3	22306	35210	8.33%	1.225%
33	13.896	2098	2101	2117	rVB5	26508	69490	16.44%	2.418%

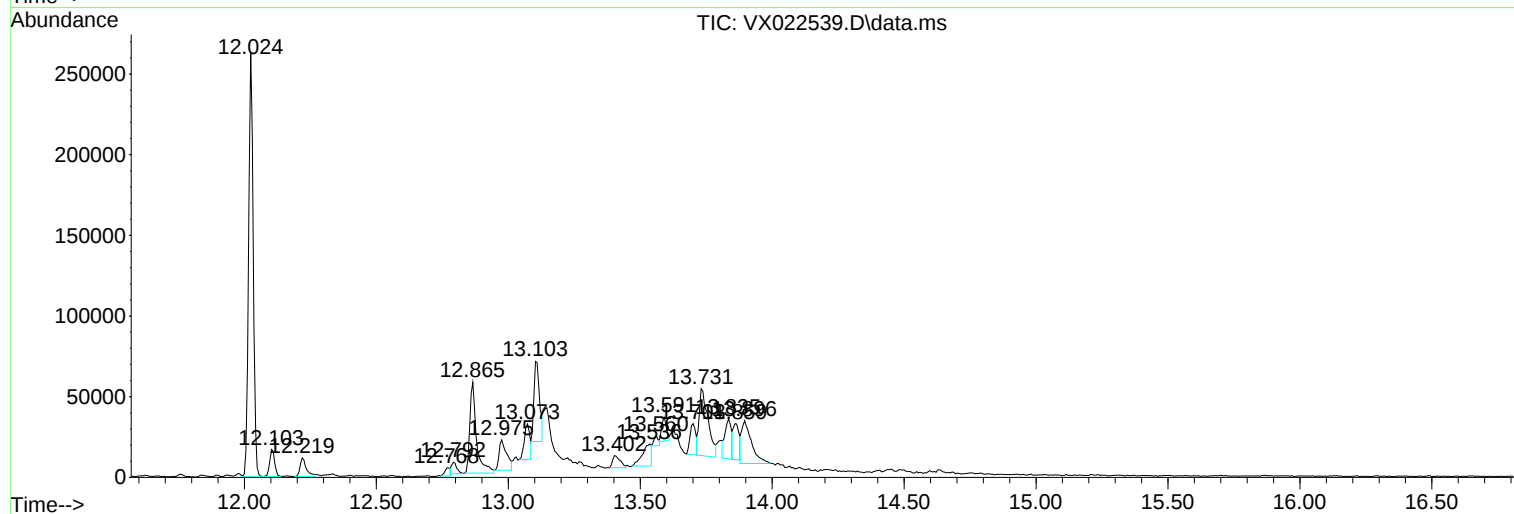
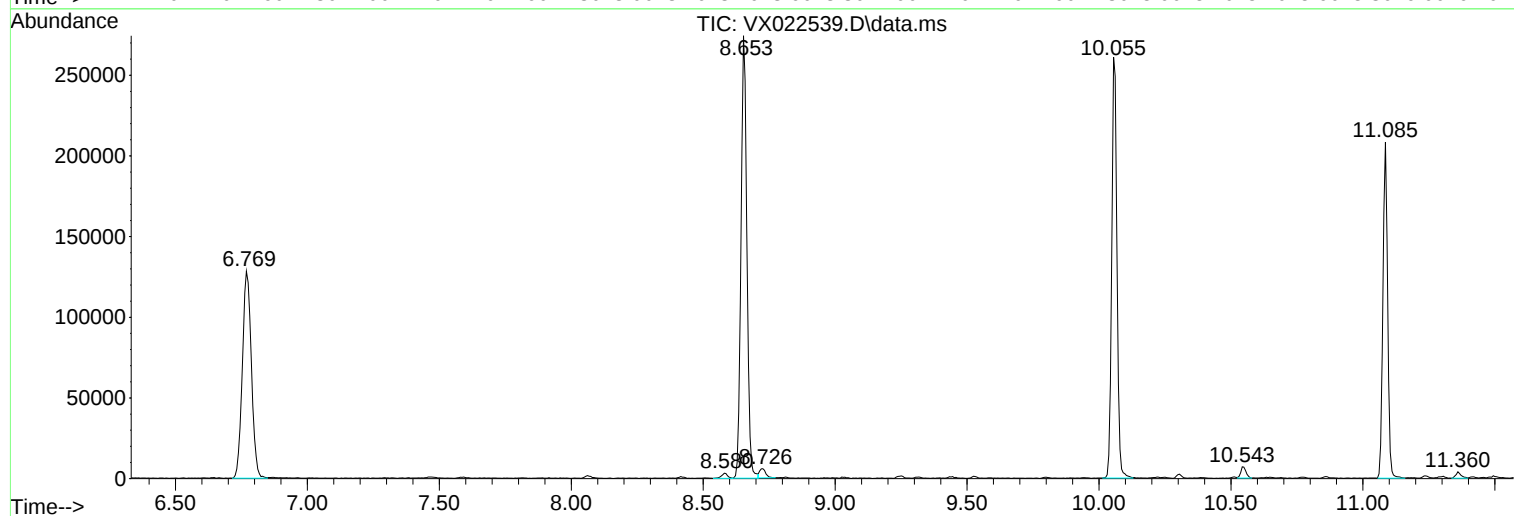
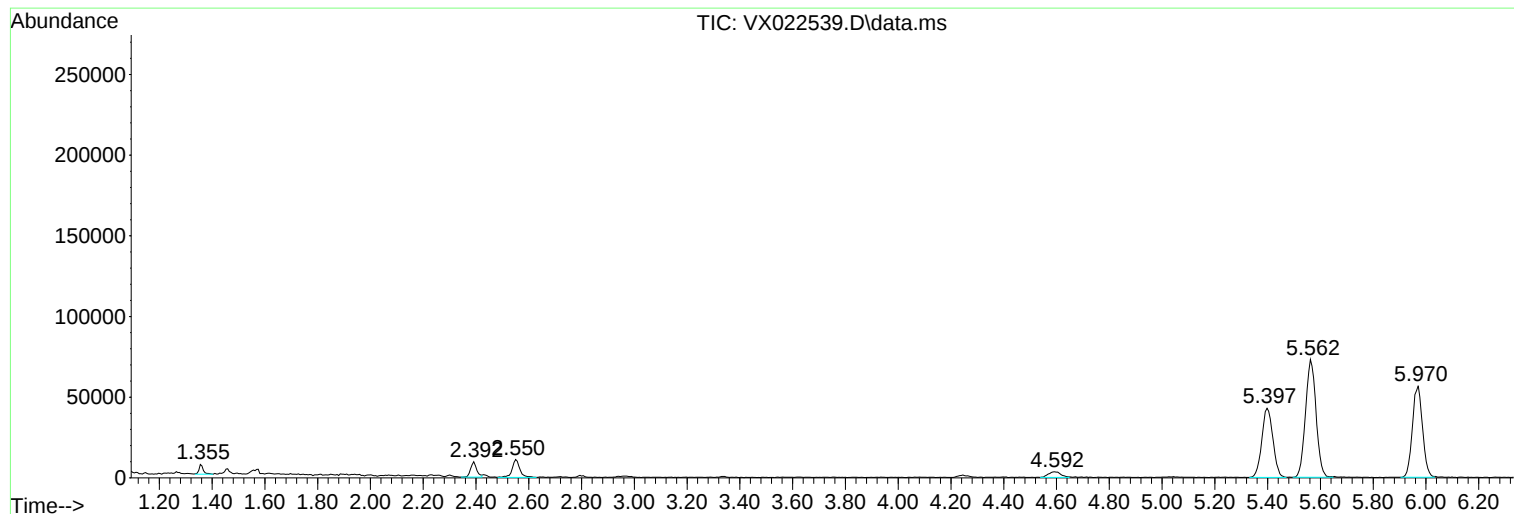
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Quant Title : SW846 8260

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



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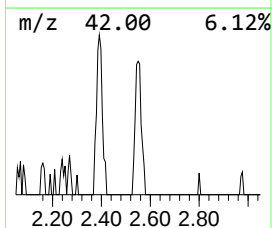
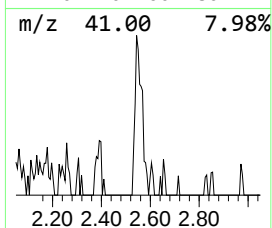
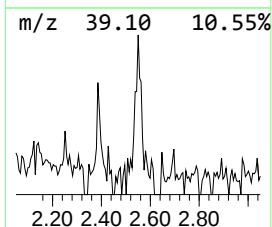
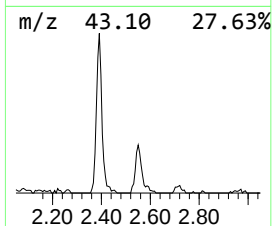
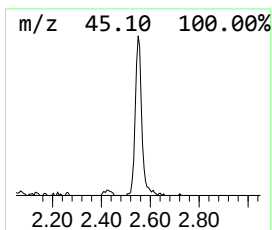
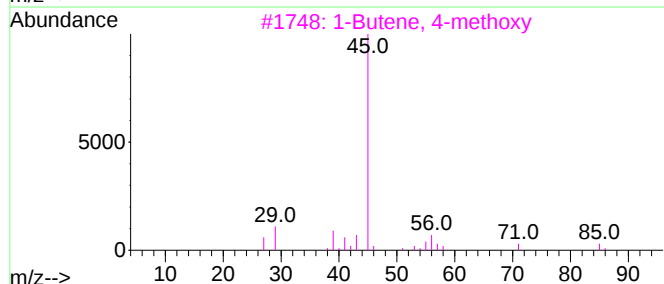
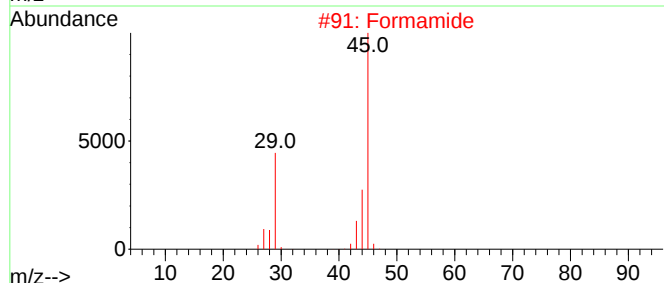
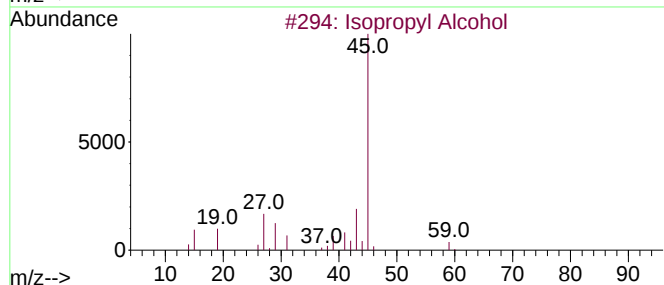
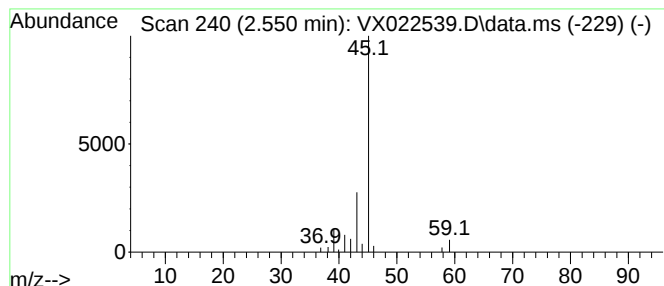
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.550 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.550	5.57 ug/l	22702	Pentafluorobenzene	5.568

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	43
2		Formamide	45	CH3NO	000075-12-7	4
3		1-Butene, 4-methoxy	86	C5H10O	004696-30-4	4
4		2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4
5		Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4



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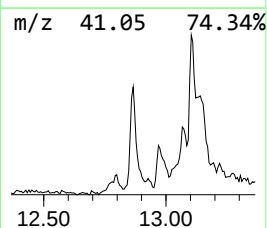
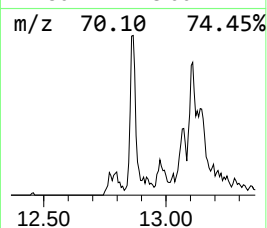
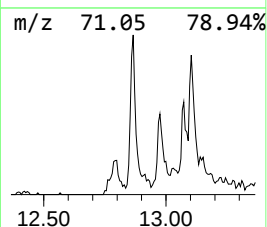
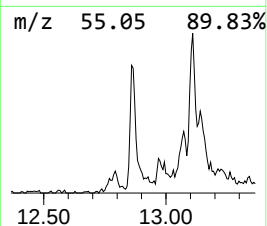
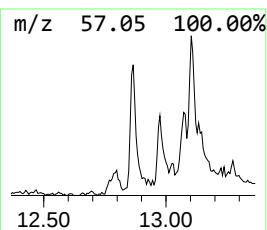
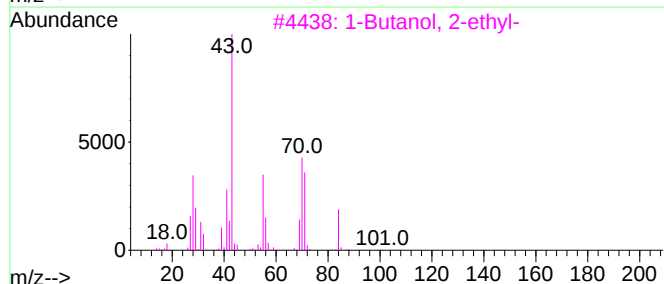
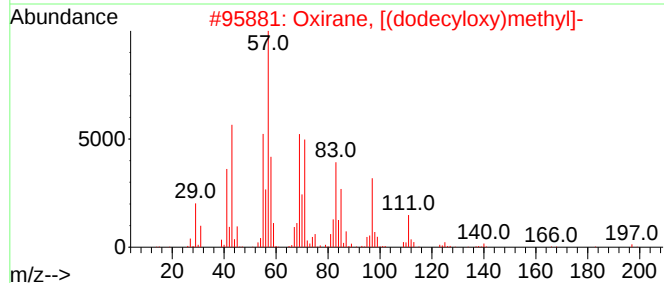
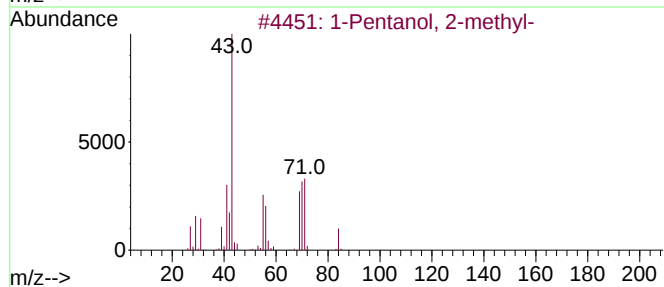
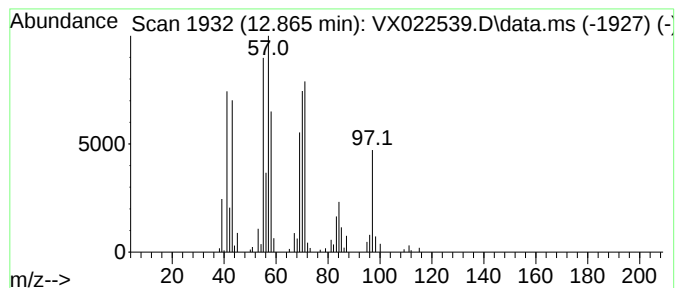
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Pentanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.865	15.55 ug/l	99206	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	50
2			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	47
3			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	47
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	47
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	43



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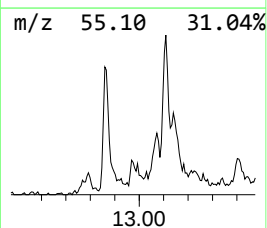
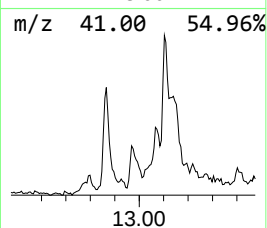
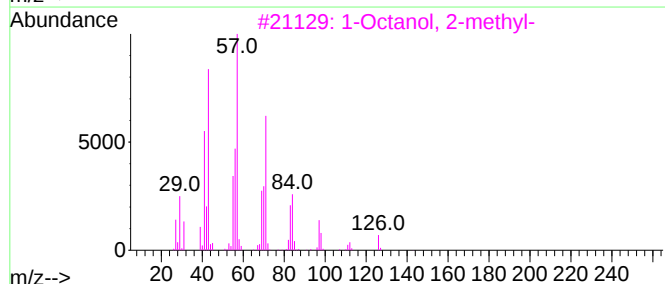
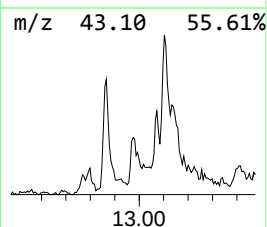
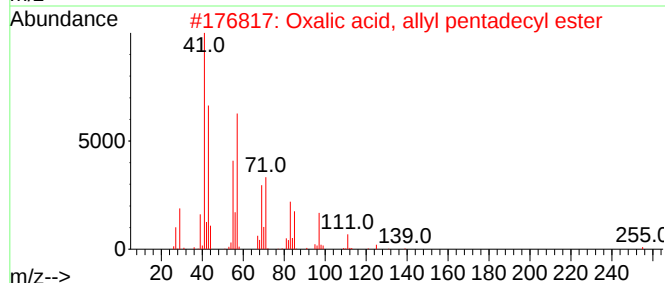
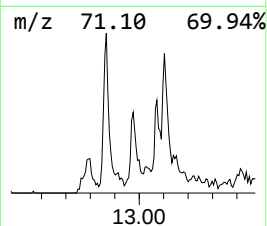
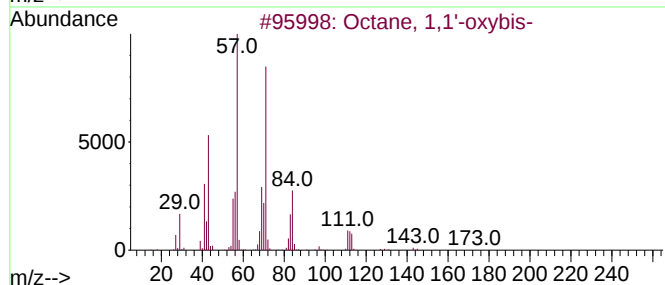
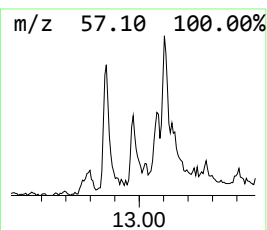
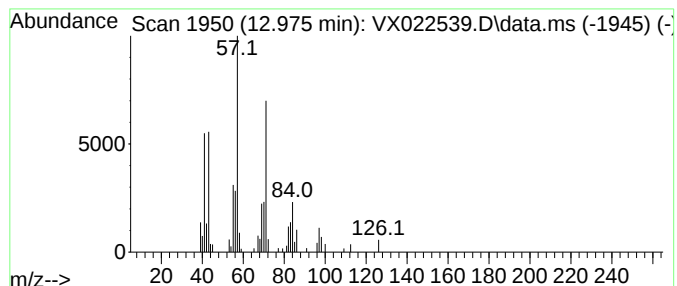
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octane, 1,1'-oxybis- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.975	5.93 ug/l	37851	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
2			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	59
3			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	58
4			Tetradecane	198	C14H30	000629-59-4	50
5			Nonane, 2,3-dimethyl-	156	C11H24	002884-06-2	43



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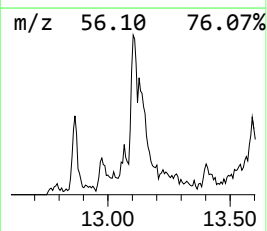
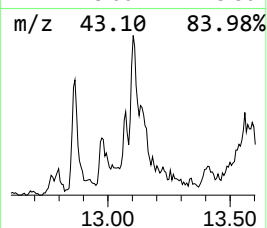
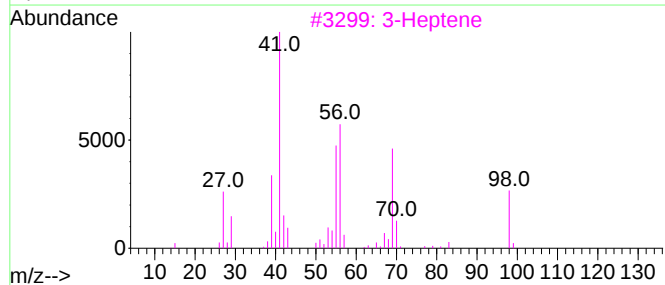
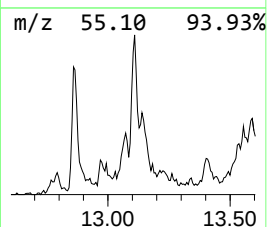
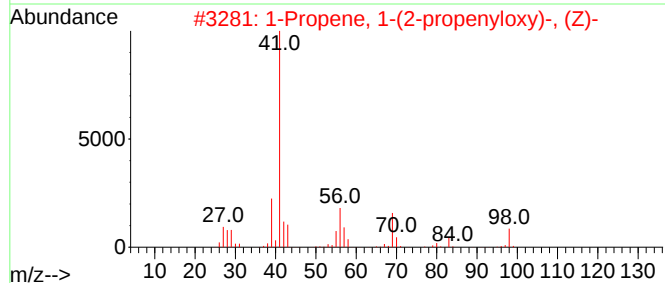
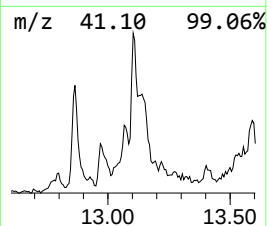
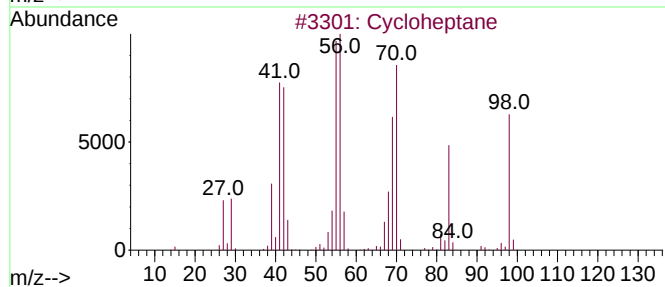
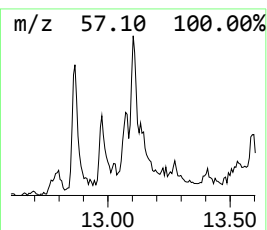
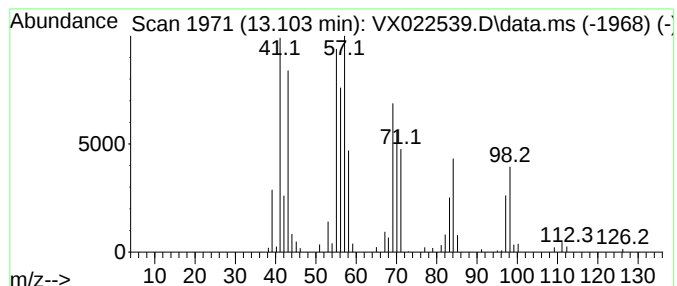
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown13.103 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.103	11.64 ug/l	74259	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloheptane	98	C7H14	000291-64-5	46
2			1-Propene, 1-(2-propenyloxy)-, (Z)-	98	C6H10O	061142-12-9	43
3			3-Heptene	98	C7H14	000592-78-9	38
4			Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	38
5			(Z)-3-Heptene	98	C7H14	007642-10-6	30



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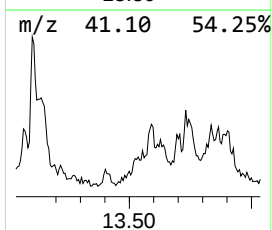
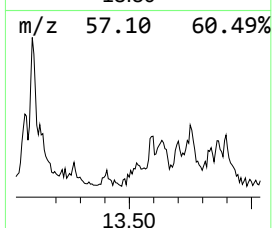
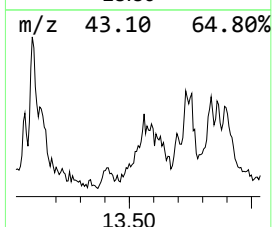
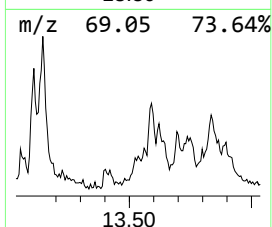
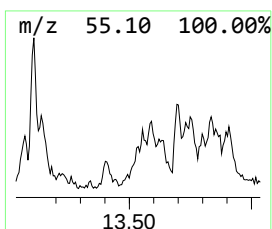
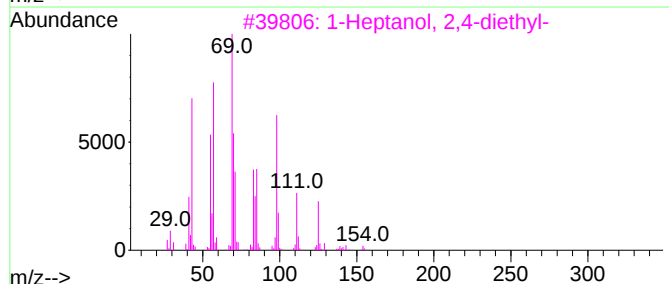
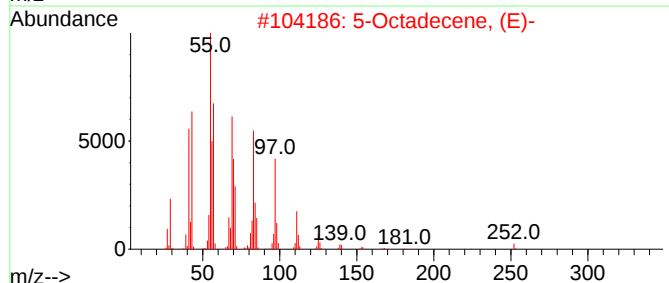
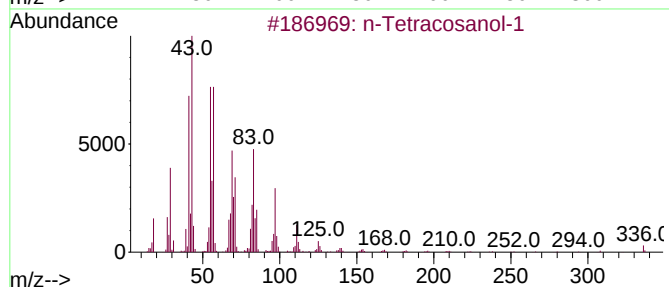
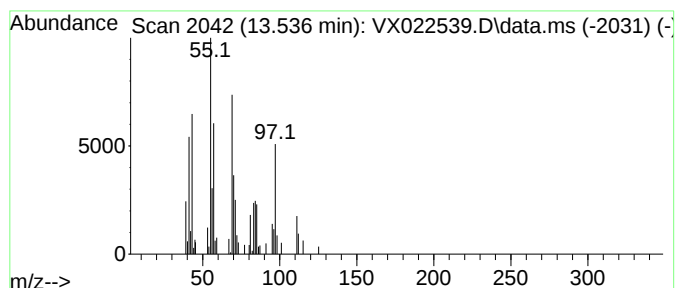
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Quant Title : SW846 8260

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

Peak Number 5 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.536	5.25 ug/l	33467	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	72
2		5-Octadecene, (E)-	252	C18H36	007206-21-5	64
3		1-Heptanol, 2,4-diethyl-	172	C11H24O	080192-55-8	50
4		n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	38
5		1-Pentene, 3-methyl-	84	C6H12	000760-20-3	38



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

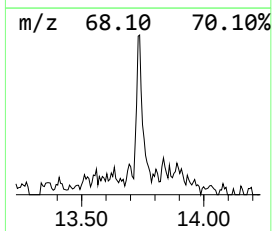
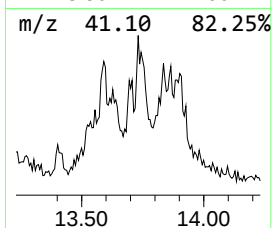
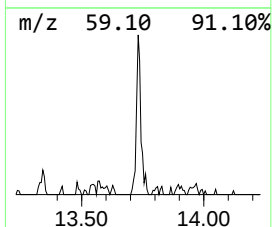
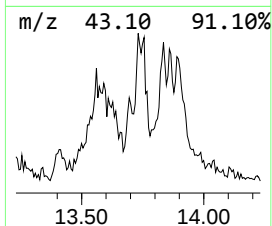
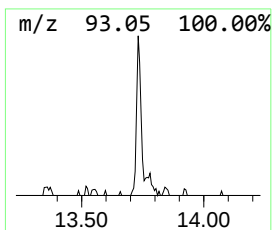
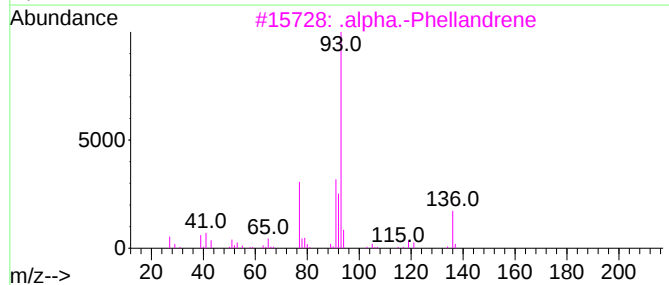
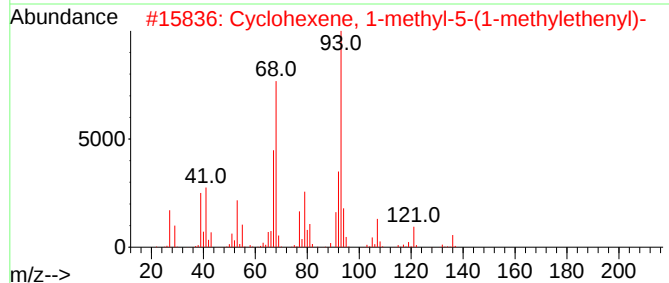
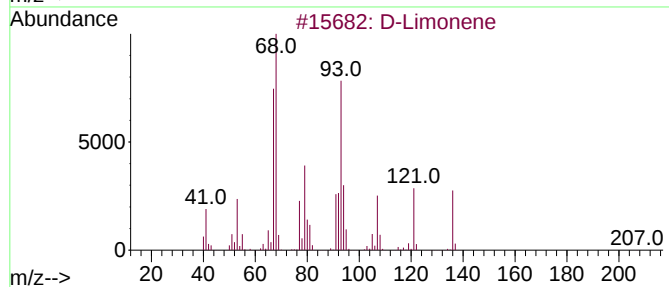
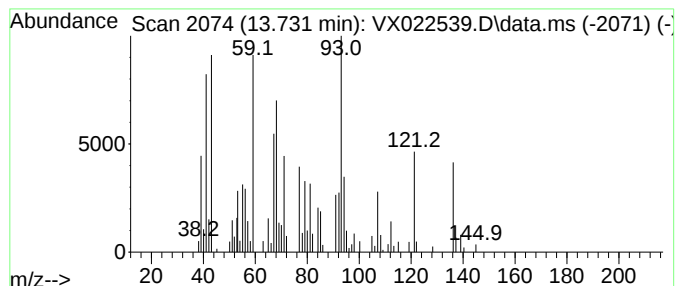
Instrument :
MSVOA_X
ClientSampleId :
33-34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

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

Peak Number 6 D-Limonene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.731	15.36 ug/l	97973	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	74
2	Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	013898-73-2	49
3	.alpha.-Phellandrene	136	C10H16	000099-83-2	38
4	Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	38
5	Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060721\
Data File : VX022539.D
Acq On : 07 Jun 2021 17:17
Operator : JC/MD
Sample : M2583-19 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
33-34

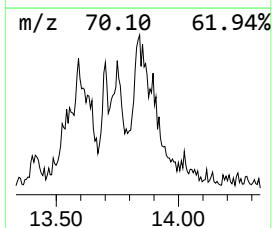
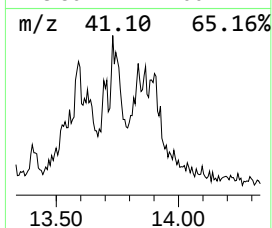
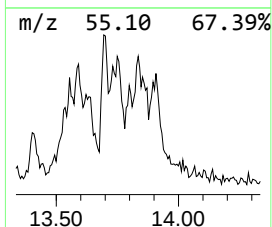
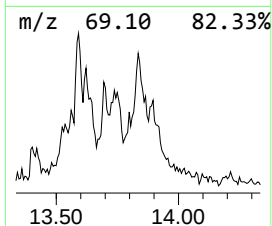
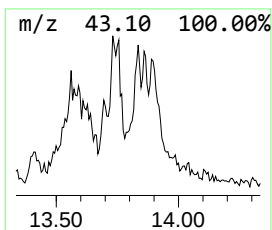
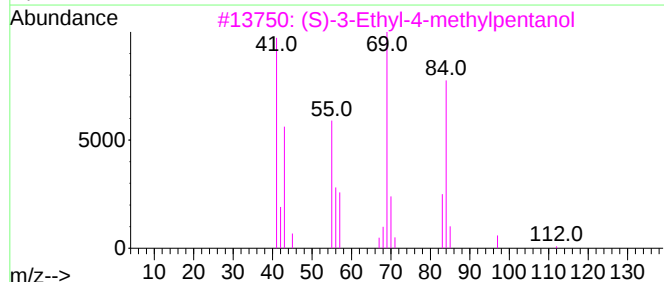
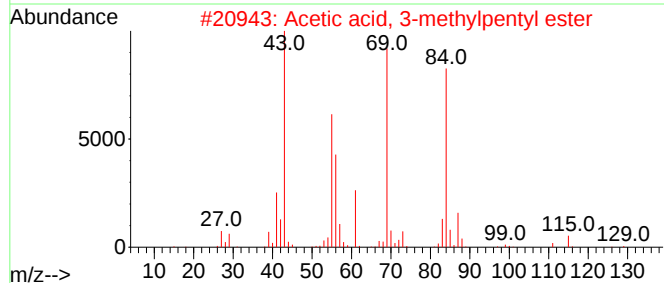
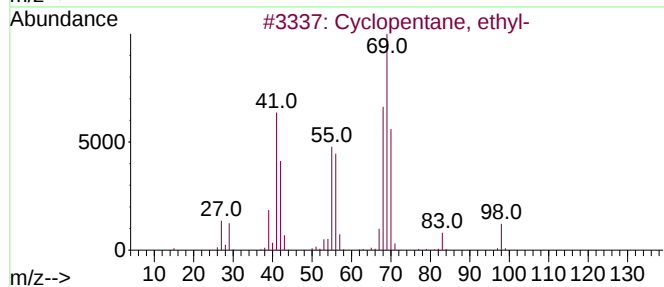
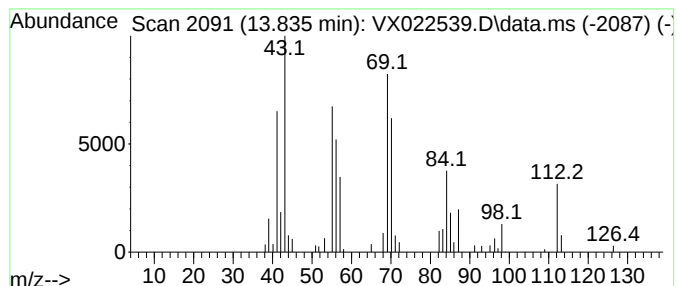
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.835	6.43 ug/l	41026	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, ethyl-	98	C7H14	001640-89-7	52
2			Acetic acid, 3-methylpentyl ester	144	C8H16O2	1000368-21-4	47
3			(S)-3-Ethyl-4-methylpentanol	130	C8H18O	1000144-07-1	43
4			1-Acetyl-4,5-dihydro-1H-pyrazole	112	C5H8N2O	1000373-42-6	43
5			Pentane, 3-methylene-	84	C6H12	000760-21-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060721\
Data File : VX022539.D
Acq On : 07 Jun 2021 17:17
Operator : JC/MD
Sample : M2583-19 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
33-34

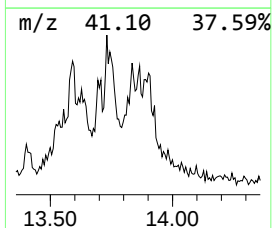
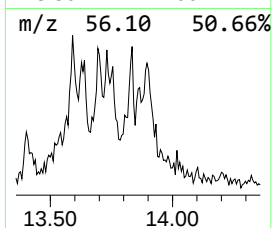
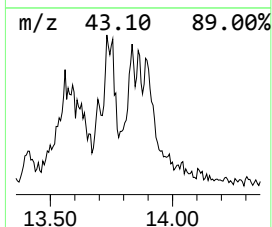
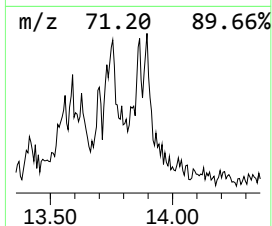
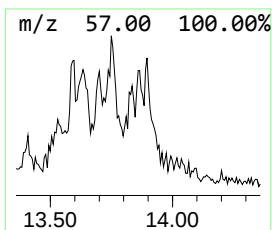
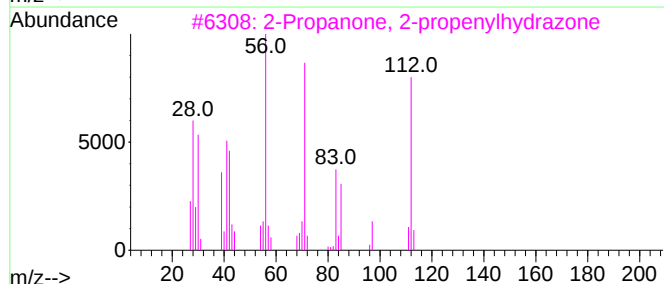
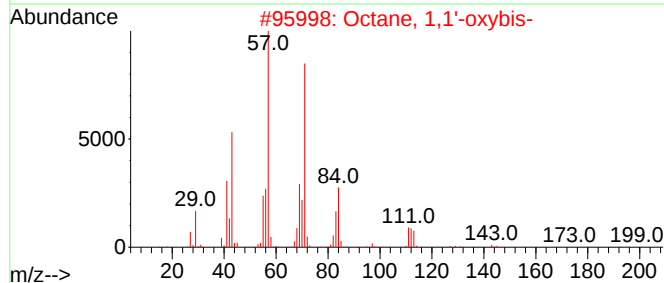
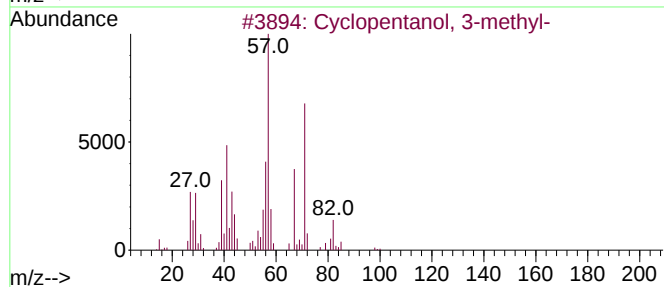
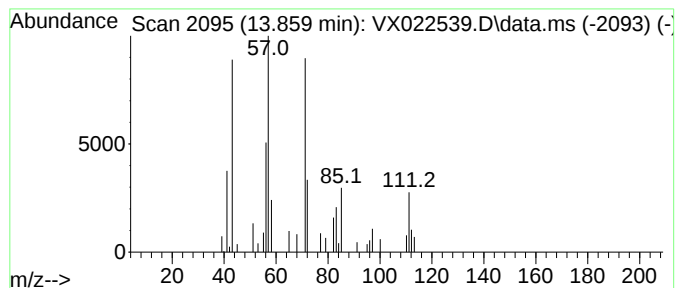
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

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

Peak Number 8 unknown13.859 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.859	5.52 ug/l	35210	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanol, 3-methyl-	100	C6H12O	018729-48-1	40
2			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	40
3			2-Propanone, 2-propenylhydrazone	112	C6H12N2	019031-79-9	38
4			Decane, 4-methyl-	156	C11H24	002847-72-5	32
5			Octane, 2,3,6-trimethyl-	156	C11H24	062016-33-5	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060721\
Data File : VX022539.D
Acq On : 07 Jun 2021 17:17
Operator : JC/MD
Sample : M2583-19 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

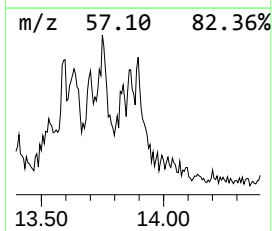
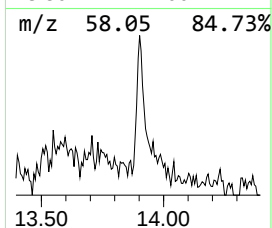
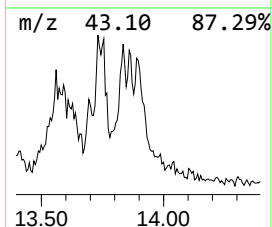
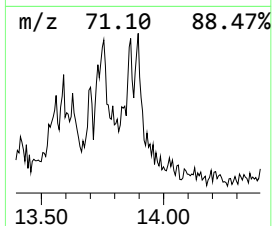
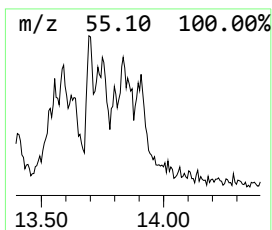
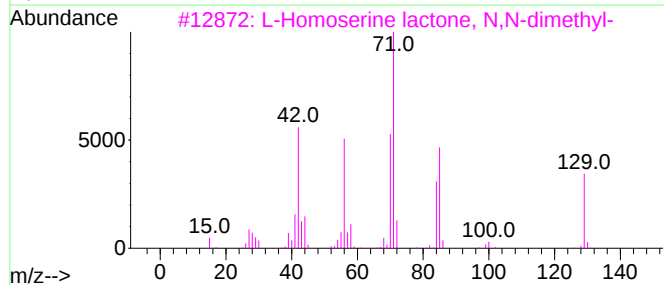
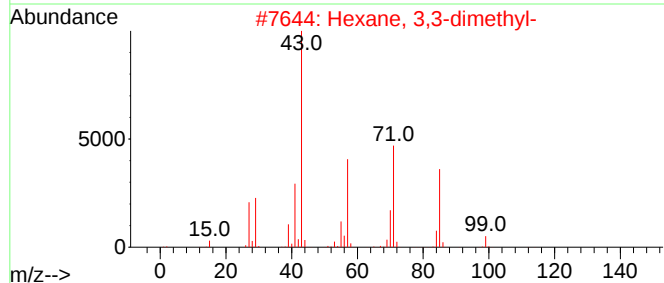
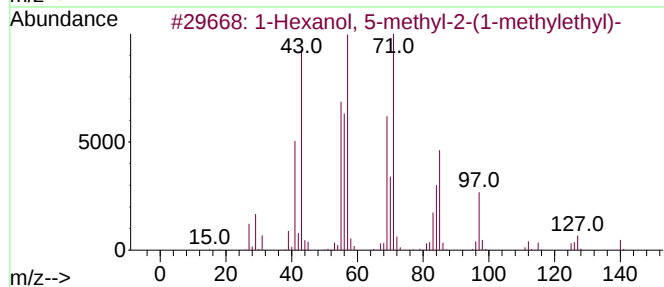
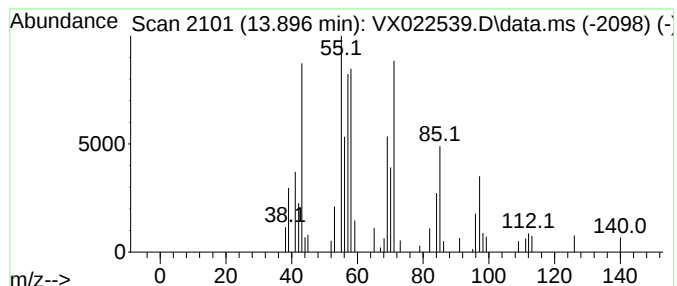
Instrument :
MSVOA_X
ClientSampleId :
33-34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

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

Peak Number 9 1-Hexanol, 5-methyl-2-(1-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.896	10.89 ug/l	69490	1,4-Dichlorobenzene-d4		12.024	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Hexanol, 5-methyl-2-(1-methyle...		158	C10H22O	002051-33-4	53
2	Hexane, 3,3-dimethyl-		114	C8H18	000563-16-6	43
3	L-Homoserine lactone, N,N-dimethyl-		129	C6H11NO2	1000374-45-7	38
4	2,3-Dimethyldecane		170	C12H26	017312-44-6	38
5	Decane, 4-methyl-		156	C11H24	002847-72-5	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060721\
Data File : VX022539.D
Acq On : 07 Jun 2021 17:17
Operator : JC/MD
Sample : M2583-19 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
33-34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.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
unknown2.550	2.550	5.6	ug/l	22702	1	5.568	203960	50.0
1-Pentanol, 2-m...	12.865	15.6	ug/l	99206	4	12.024	318982	50.0
Octane, 1,1'-ox...	12.975	5.9	ug/l	37851	4	12.024	318982	50.0
unknown13.103	13.103	11.6	ug/l	74259	4	12.024	318982	50.0
n-Tetracosanol-1	13.536	5.3	ug/l	33467	4	12.024	318982	50.0
D-Limonene	13.731	15.4	ug/l	97973	4	12.024	318982	50.0
Cyclopentane, e...	13.835	6.4	ug/l	41026	4	12.024	318982	50.0
unknown13.859	13.859	5.5	ug/l	35210	4	12.024	318982	50.0
1-Hexanol, 5-me...	13.896	10.9	ug/l	69490	4	12.024	318982	50.0