

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013021\
 Data File : VX020804.D
 Acq On : 29 Jan 2021 15:06
 Operator : JC/SP
 Sample : M1217-17 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1723-1724

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\82X012521W.M
 Title : SW846 8260

Signal : TIC: VX020804.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.471	60	63	70	rVB	21134	24817	1.08%	0.137%
2	2.087	159	164	175	rBV	48031	79896	3.47%	0.442%
3	2.416	213	218	227	rVB	50999	83390	3.63%	0.462%
4	5.458	705	717	731	rBV2	200282	570893	24.83%	3.161%
5	5.623	732	744	760	rVB	314962	873529	37.99%	4.836%
6	6.025	795	810	828	rBV	208205	552542	24.03%	3.059%
7	6.824	931	941	953	rBV	486572	1148955	49.97%	6.361%
8	8.695	1240	1248	1255	rBV	1021718	1620348	70.46%	8.971%
9	10.092	1471	1477	1489	rBV	1111371	1454864	63.27%	8.055%
10	11.122	1640	1646	1658	rBV	846625	1099851	47.83%	6.089%
11	11.963	1780	1784	1788	rBV	35890	40428	1.76%	0.224%
12	12.061	1794	1800	1807	rVB	1172265	1437548	62.52%	7.959%
13	12.140	1807	1813	1823	rBV	411365	548833	23.87%	3.038%
14	12.256	1827	1832	1839	rBV	36635	58602	2.55%	0.324%
15	12.616	1885	1891	1900	rVB7	14341	24254	1.05%	0.134%
16	12.890	1933	1936	1941	rVB	38426	43767	1.90%	0.242%
17	13.006	1950	1955	1964	rBV	122796	173325	7.54%	0.960%
18	13.103	1967	1971	1973	rBV	142537	179165	7.79%	0.992%
19	13.134	1973	1976	1992	rVB	388788	584390	25.41%	3.235%
20	13.304	2000	2004	2013	rVB2	24451	31899	1.39%	0.177%
21	13.457	2024	2029	2040	rBV	1809959	2299513	100.00%	12.731%
22	13.548	2040	2044	2052	rVB	142965	230750	10.03%	1.277%
23	13.743	2070	2076	2080	rBV	252175	412656	17.95%	2.285%
24	13.786	2080	2083	2095	rVV	229744	356525	15.50%	1.974%
25	13.896	2096	2101	2103	rVV	232768	286985	12.48%	1.589%
26	13.926	2103	2106	2122	rVB	474687	731039	31.79%	4.047%
27	14.146	2138	2142	2150	rVB	73947	90271	3.93%	0.500%
28	14.231	2151	2156	2175	rBV	1124527	1582951	68.84%	8.764%
29	14.444	2186	2191	2194	rBV	214901	246013	10.70%	1.362%
30	14.481	2194	2197	2201	rVV	110035	155702	6.77%	0.862%
31	14.524	2201	2204	2214	rVV	96872	159811	6.95%	0.885%
32	14.603	2214	2217	2219	rVV3	23096	29098	1.27%	0.161%
33	14.633	2219	2222	2224	rVV	89012	109163	4.75%	0.604%
34	14.664	2224	2227	2235	rVV2	139605	217466	9.46%	1.204%
35	14.725	2235	2237	2243	rVB4	21826	31442	1.37%	0.174%
36	14.835	2251	2255	2270	rVB	40816	66254	2.88%	0.367%

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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

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37	14.957	2270	2275	2286	rBV	138866	222891	9.69%	1.234%
38	15.292	2326	2330	2338	rVB	102148	143853	6.26%	0.796%
39	15.456	2353	2357	2365	rVB7	18245	32827	1.43%	0.182%
40	15.597	2375	2380	2385	rBV4	15518	26168	1.14%	0.145%

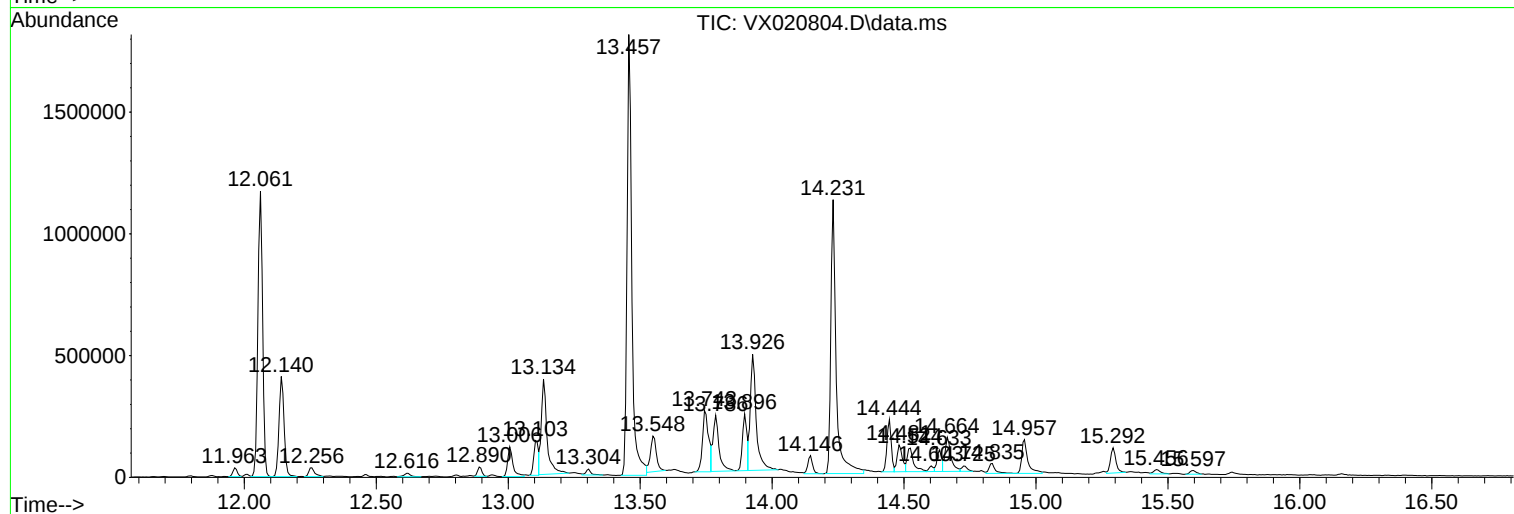
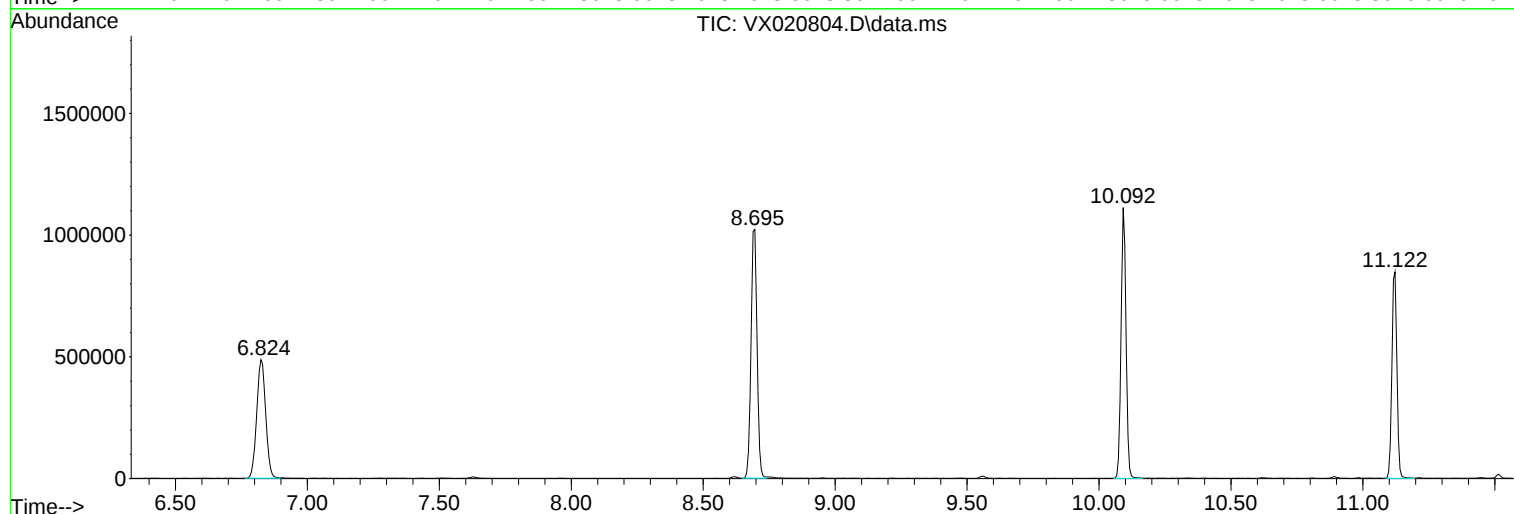
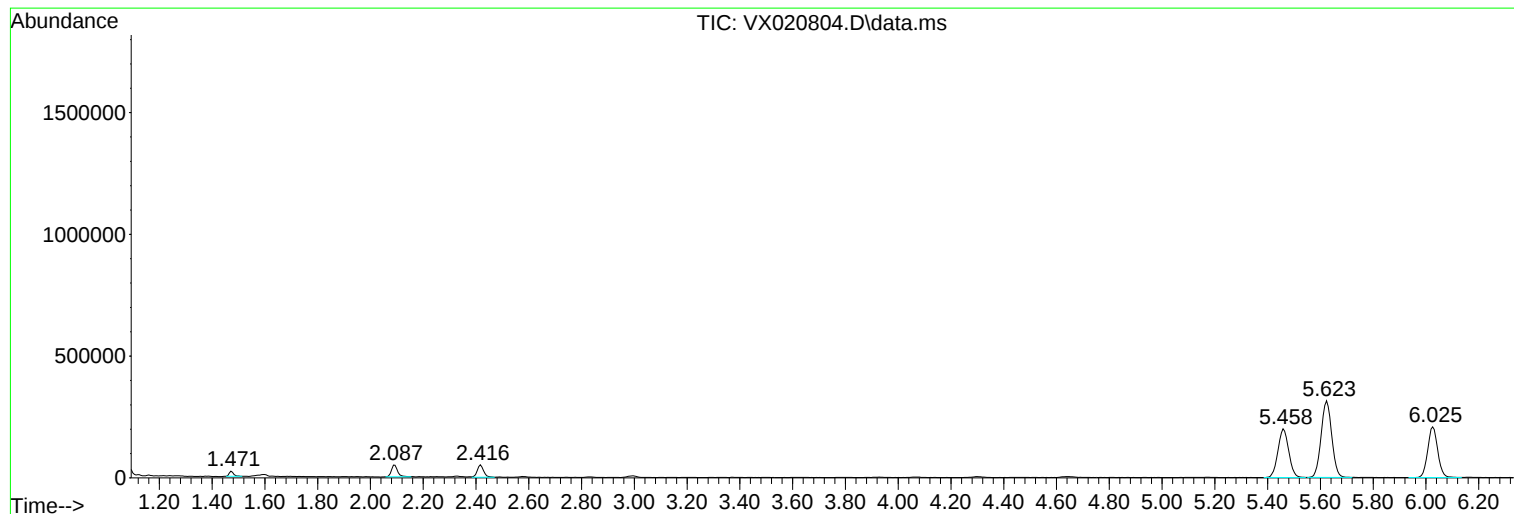
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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



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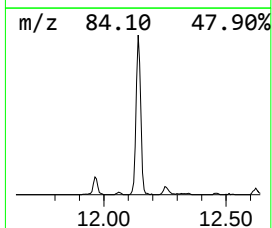
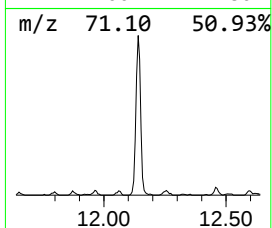
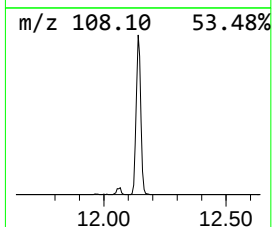
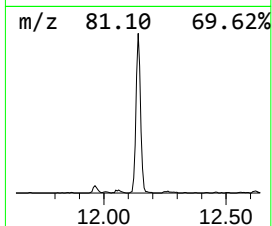
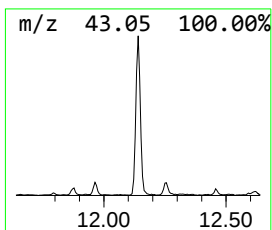
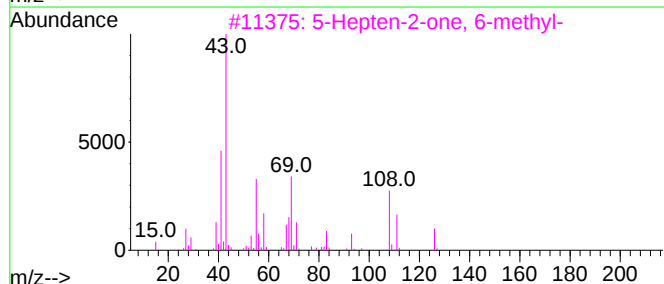
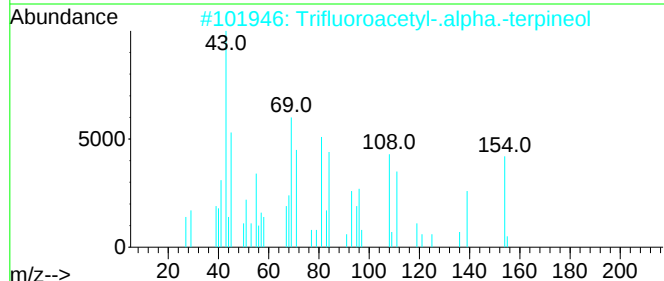
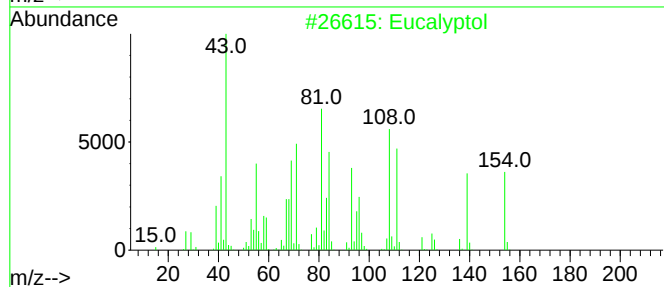
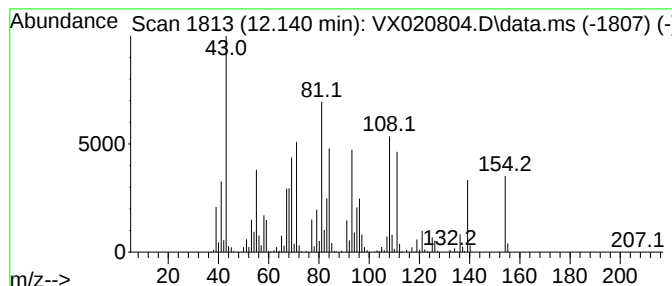
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 1 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.140	19.09 ug/l	548833	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	72
3			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	22
4			Sulfurous acid, 2-pentyl propyl ...	194	C8H18O3S	1000309-15-1	22
5			.alpha.-Campholenal	152	C10H16O	004501-58-0	22



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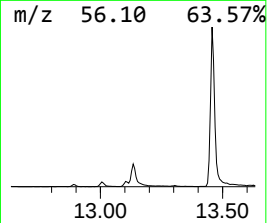
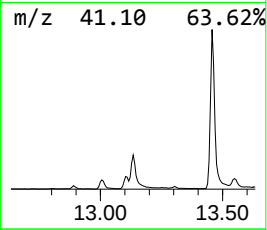
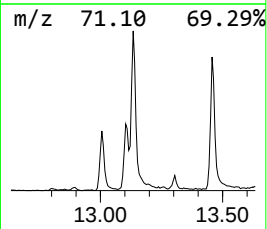
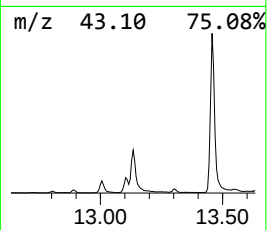
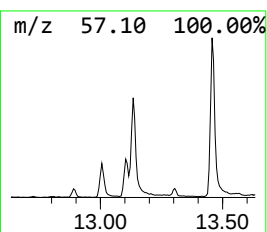
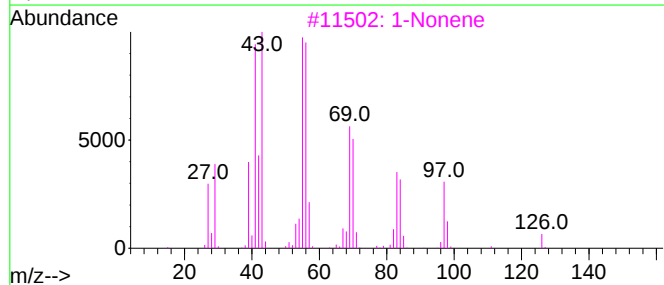
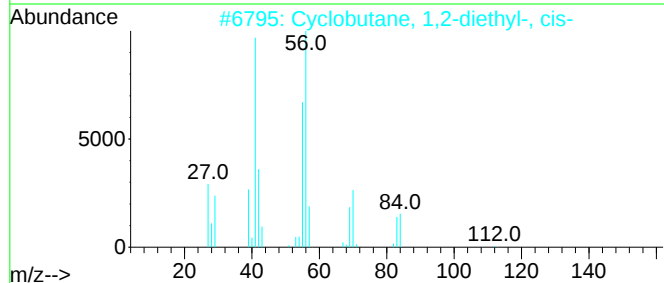
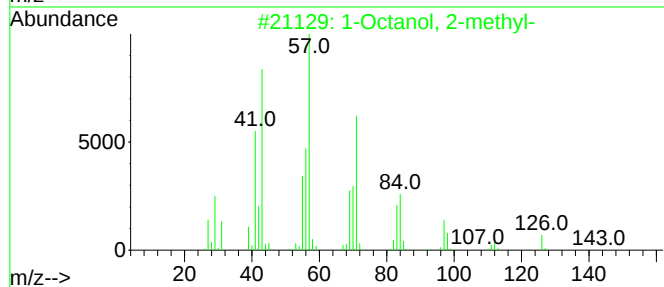
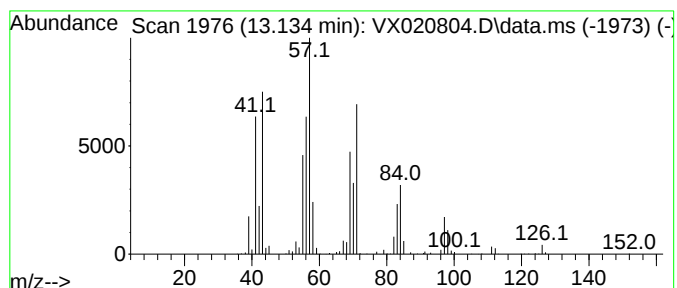
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Octanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.134	20.33 ug/l	584390	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	86
2			Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	53
3			1-Nonene	126	C9H18	000124-11-8	53
4			1-Fluorononane	146	C9H19F	000463-18-3	50
5			Formic acid, 2-methylpentyl ester	130	C7H14O2	381670-34-4	47



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

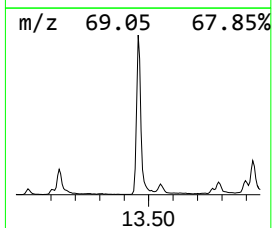
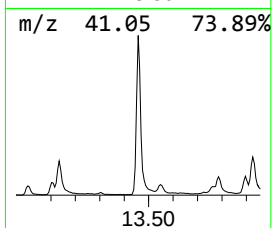
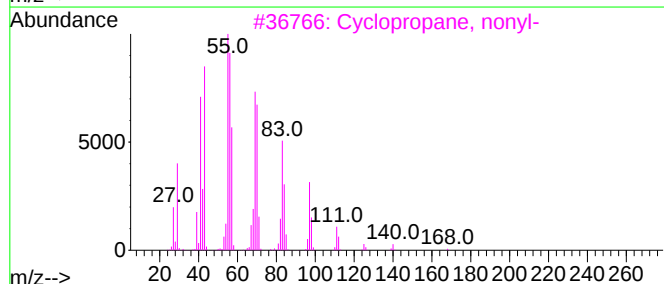
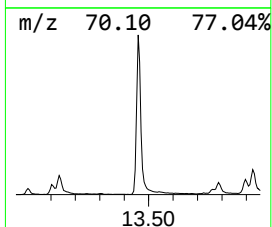
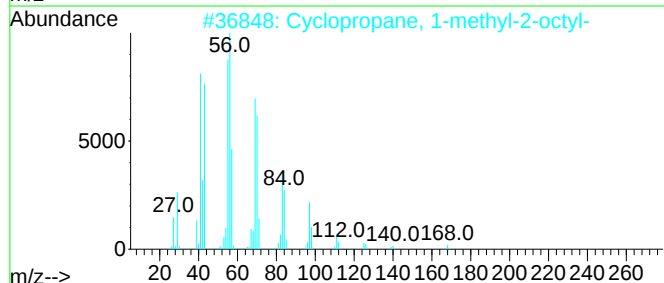
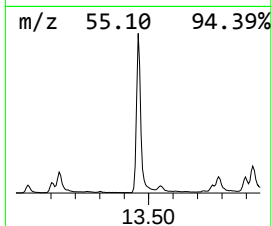
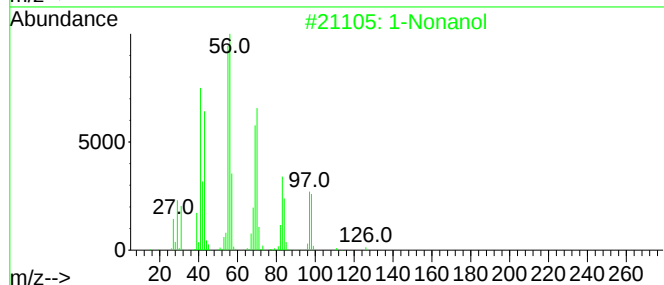
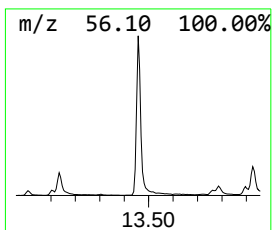
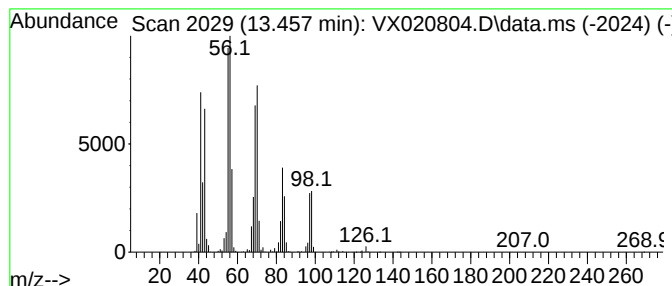
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Quant Title : SW846 8260

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

Peak Number 3 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.457	79.98 ug/l	2299510	1,4-Dichlorobenzene-d4	12.061	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	91
2	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	86
3	Cyclopropane, nonyl-	168	C12H24	074663-85-7	78
4	Cycloheptane	98	C7H14	000291-64-5	74
5	Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	72



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Instrument :
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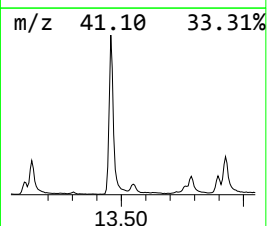
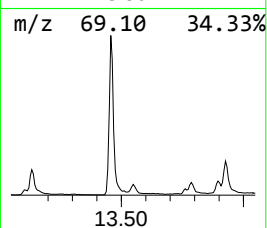
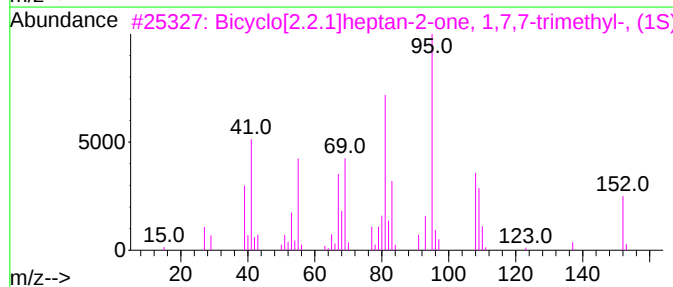
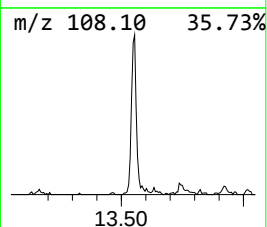
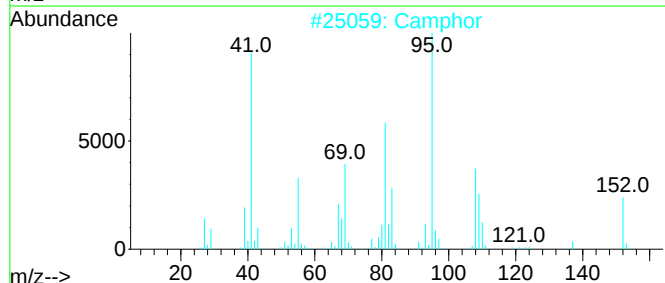
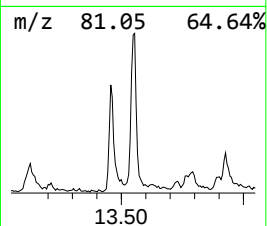
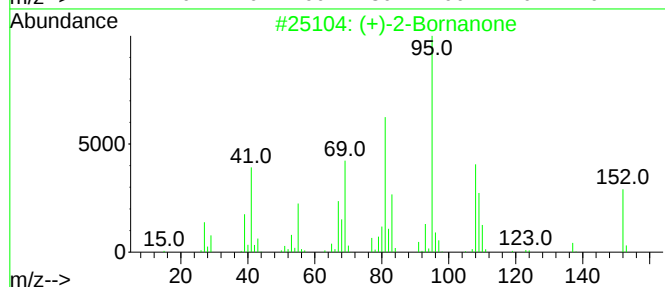
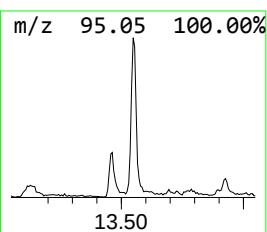
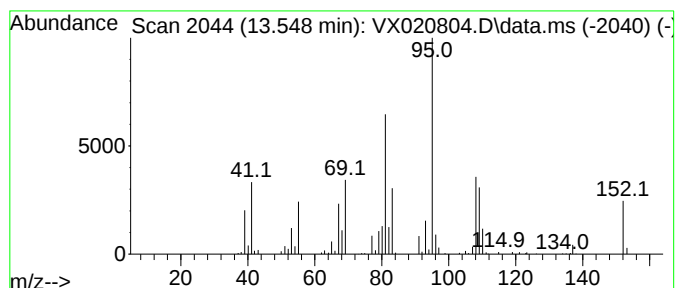
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Peak Number 4 (+)-2-Bornanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.548	8.03 ug/l	230750	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	95
2			Camphor	152	C10H16O	000076-22-2	95
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49
5			Isoborneol	154	C10H18O	000124-76-5	43



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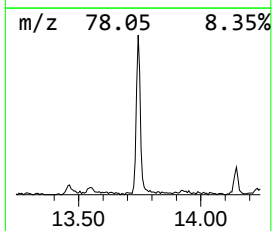
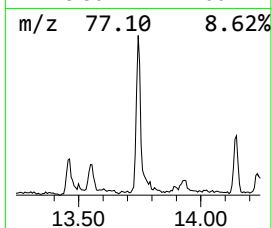
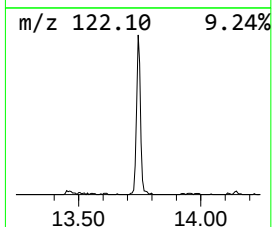
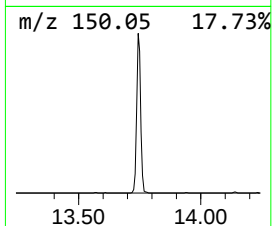
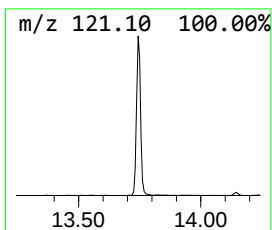
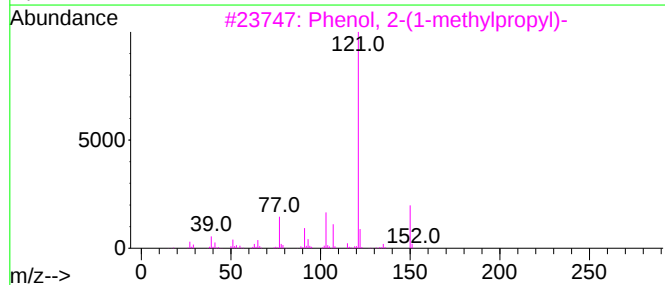
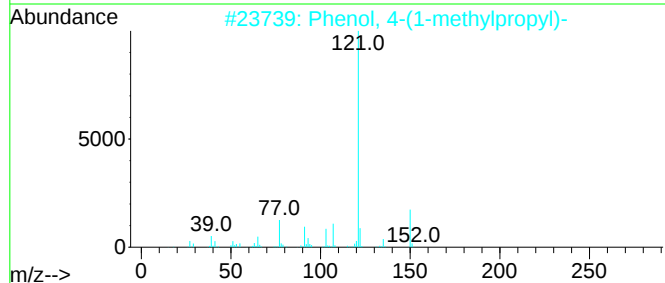
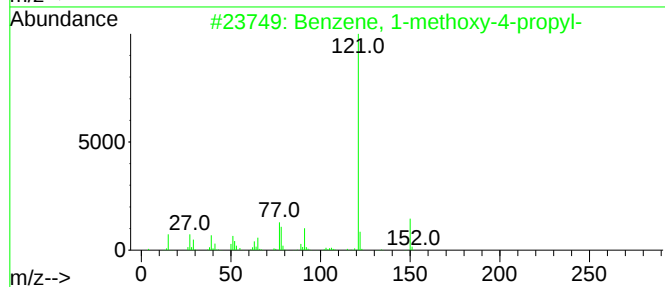
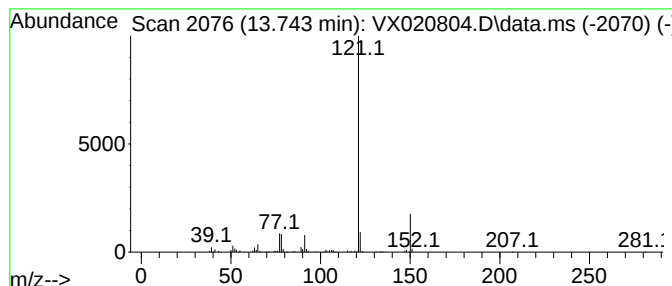
Instrument :
MSVOA_X
ClientSampleId :
1723-1724

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-methoxy-4-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.743	14.35 ug/l	412656	1,4-Dichlorobenzene-d4		12.061	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1-methoxy-4-propyl-		150	C10H14O	000104-45-0	91
2	Phenol, 4-(1-methylpropyl)-		150	C10H14O	000099-71-8	78
3	Phenol, 2-(1-methylpropyl)-		150	C10H14O	000089-72-5	72
4	4-Methoxybenzyl phenyl carbonate		258	C15H14O4	1000342-86-3	72
5	ortho-Hydroxypropiophenone		150	C9H10O2	000610-99-1	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013021\
Data File : VX020804.D
Acq On : 29 Jan 2021 15:06
Operator : JC/SP
Sample : M1217-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

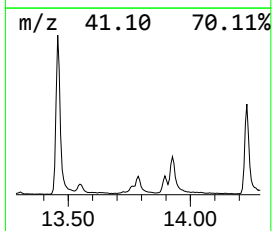
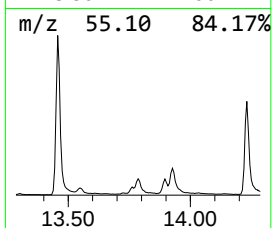
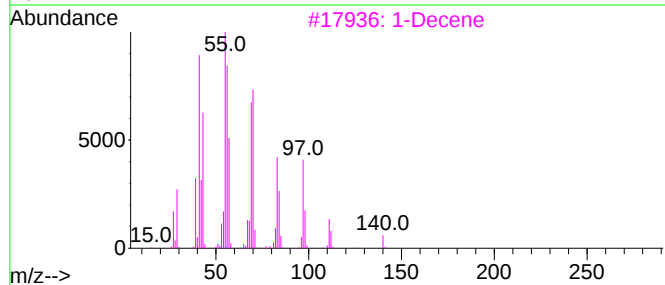
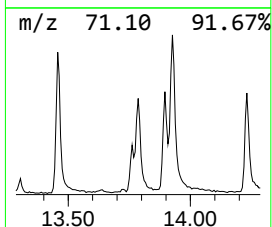
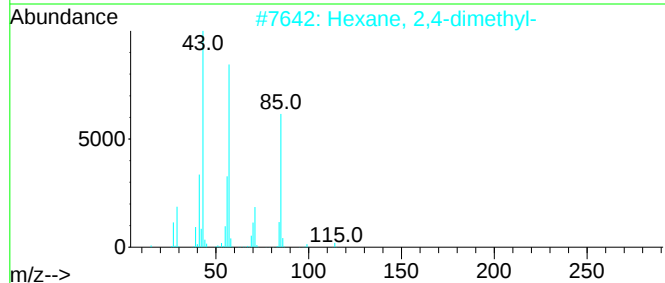
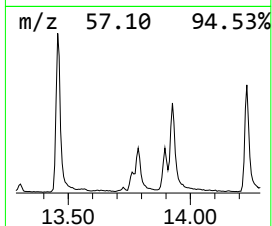
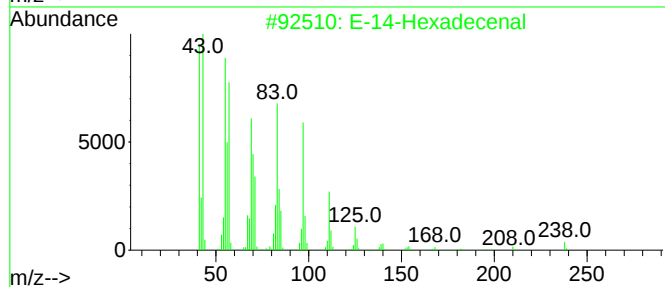
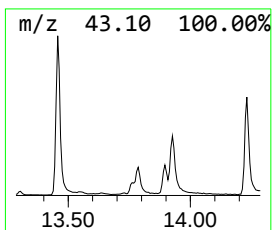
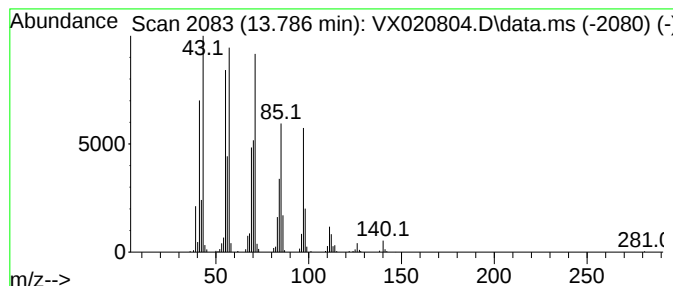
Instrument :
MSVOA_X
ClientSampleId :
1723-1724

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 6 E-14-Hexadecenal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.786	12.40 ug/l	356525	1,4-Dichlorobenzene-d4	12.061	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal	238	C16H30O	330207-53-9	52
2	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	30
3	1-Decene	140	C10H20	000872-05-9	30
4	Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	30
5	Heptane, 3-methyl-	114	C8H18	000589-81-1	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013021\
Data File : VX020804.D
Acq On : 29 Jan 2021 15:06
Operator : JC/SP
Sample : M1217-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1723-1724

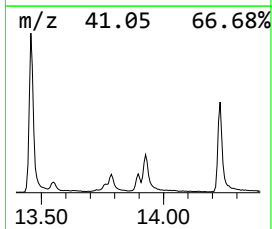
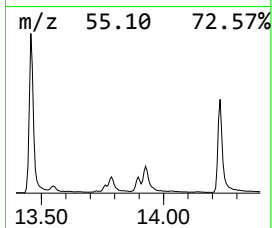
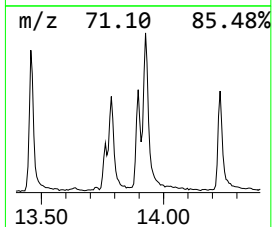
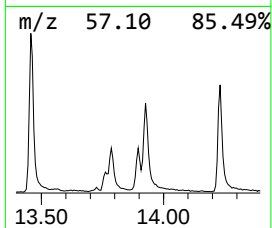
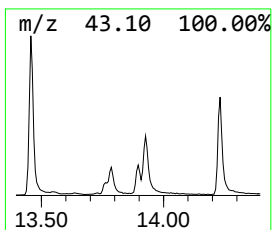
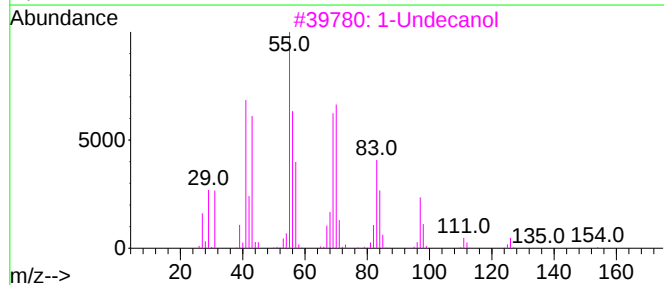
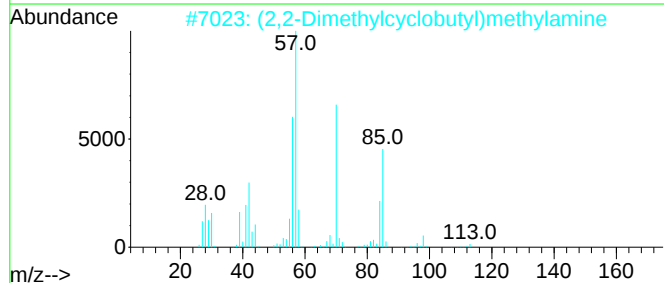
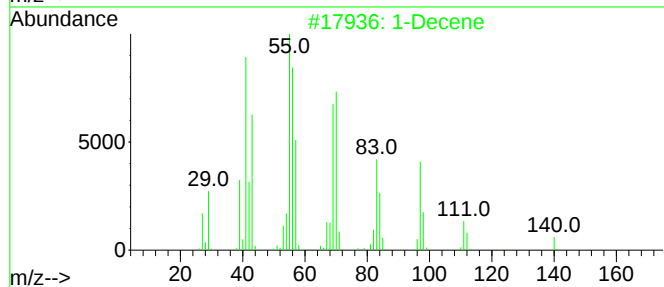
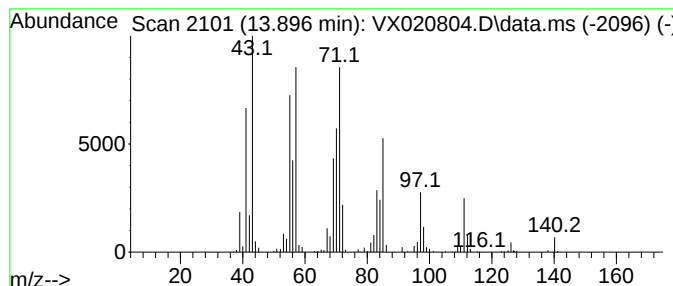
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Quant Title : SW846 8260

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

Peak Number 7 1-Decene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.896	9.98 ug/l	286985	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decene	140	C10H20	000872-05-9	50
2			(2,2-Dimethylcyclobutyl)methylamine	113	C7H15N	1000195-04-0	46
3			1-Undecanol	172	C11H24O	000112-42-5	43
4			Cyclooctane, methyl-	126	C9H18	001502-38-1	38
5			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013021\
Data File : VX020804.D
Acq On : 29 Jan 2021 15:06
Operator : JC/SP
Sample : M1217-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

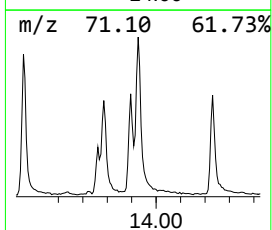
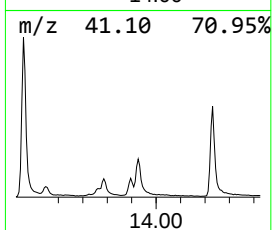
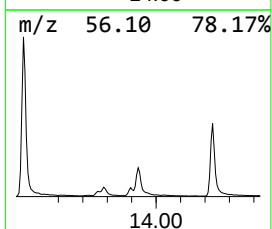
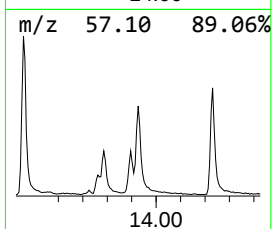
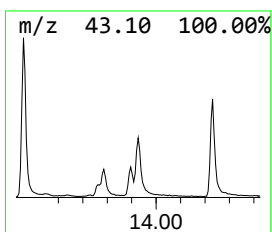
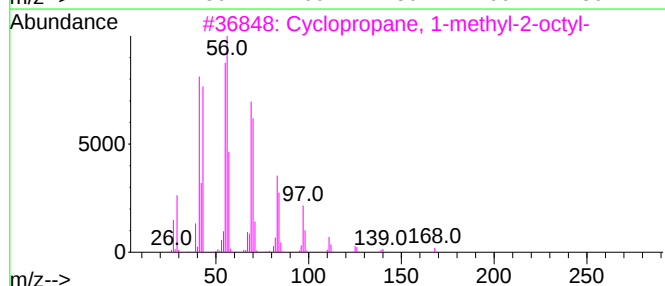
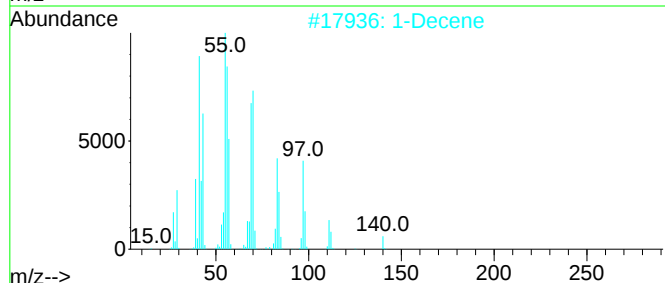
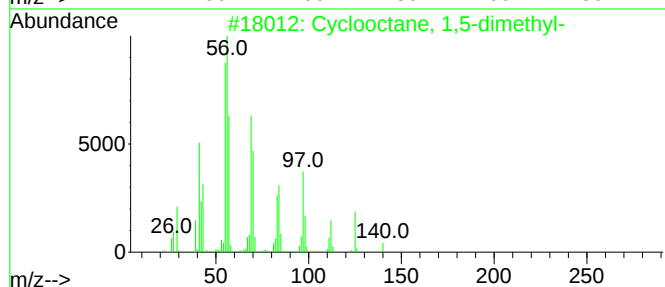
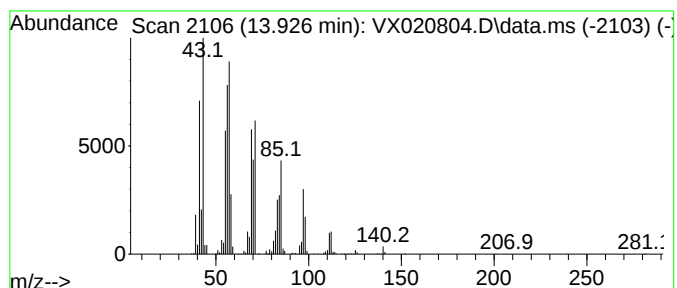
Instrument :
MSVOA_X
ClientSampleId :
1723-1724

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 8 Cyclooctane, 1,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.926	25.43 ug/l	731039	1,4-Dichlorobenzene-d4			12.061
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclooctane, 1,5-dimethyl-		140	C10H20	021328-57-4	93
2	1-Decene		140	C10H20	000872-05-9	55
3	Cyclopropane, 1-methyl-2-octyl-		168	C12H24	037617-26-8	50
4	Cyclobutane, 1-butyl-2-ethyl-		140	C10H20	1000150-67-3	49
5	2- Chloropropionic acid, decyl e...		248	C13H25ClO2	086711-78-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013021\
Data File : VX020804.D
Acq On : 29 Jan 2021 15:06
Operator : JC/SP
Sample : M1217-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1723-1724

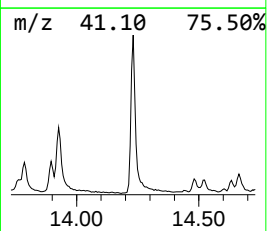
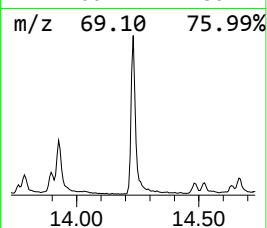
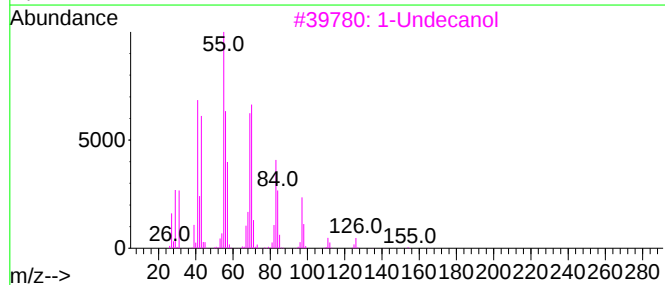
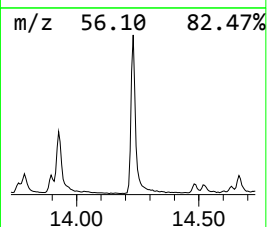
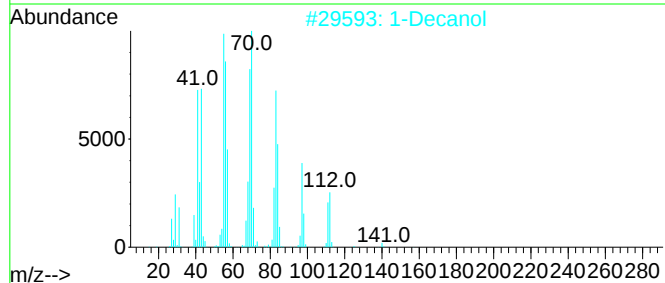
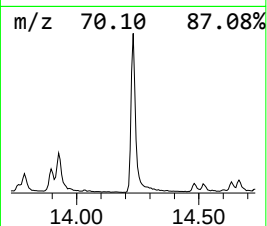
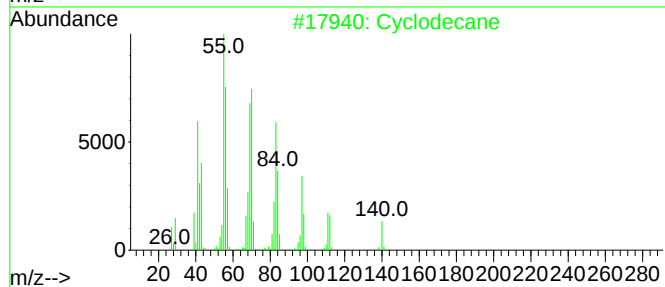
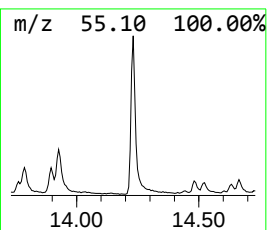
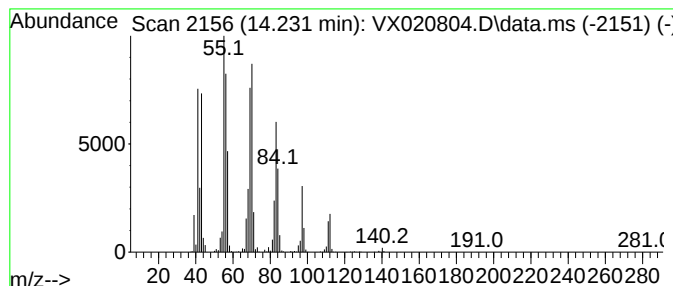
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Quant Title : SW846 8260

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

Peak Number 9 Cyclodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.231	55.06 ug/l	1582950	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodecane	140	C10H20	000293-96-9	93
2			1-Decanol	158	C10H22O	000112-30-1	91
3			1-Undecanol	172	C11H24O	000112-42-5	90
4			Cyclooctane	112	C8H16	000292-64-8	87
5			Cyclopropane, nonyl-	168	C12H24	074663-85-7	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013021\
Data File : VX020804.D
Acq On : 29 Jan 2021 15:06
Operator : JC/SP
Sample : M1217-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1723-1724

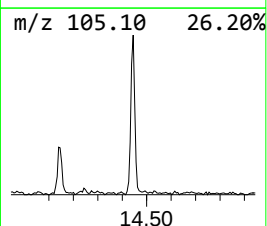
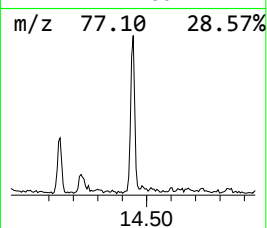
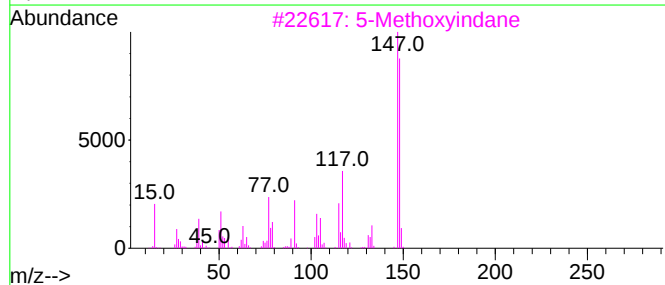
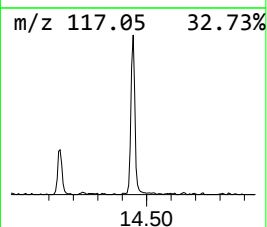
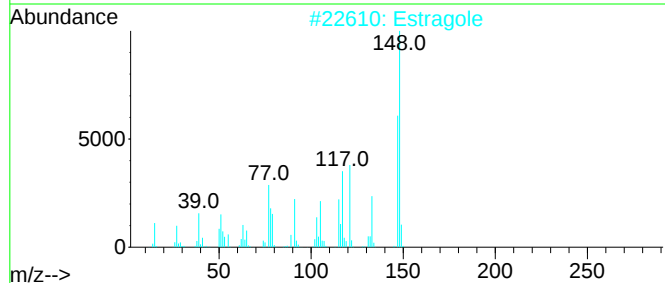
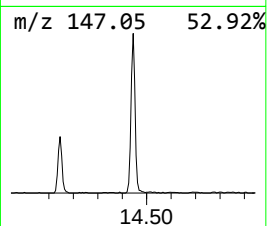
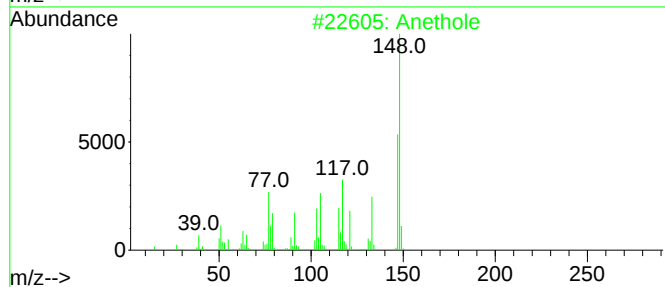
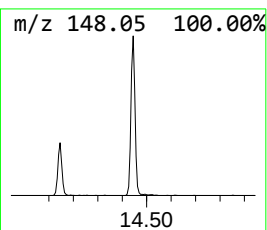
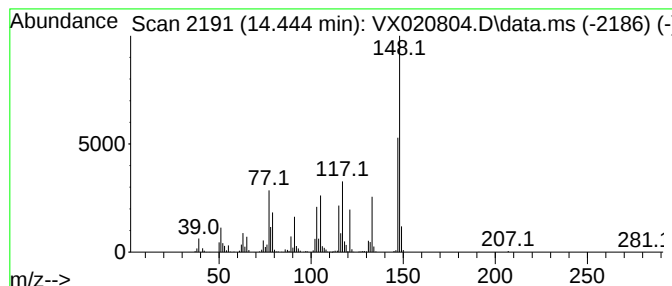
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Quant Title : SW846 8260

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

Peak Number 10 Anethole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	8.56 ug/l	246013	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anethole	148	C10H12O	000104-46-1	98
2			Estragole	148	C10H12O	000140-67-0	93
3			5-Methoxyindane	148	C10H12O	1000342-73-8	70
4			Benzene, (1-propynylthio)-	148	C9H8S	006212-77-7	53
5			Methanimidamide, N,N-dimethyl-N'...	148	C9H12N2	001783-25-1	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013021\
Data File : VX020804.D
Acq On : 29 Jan 2021 15:06
Operator : JC/SP
Sample : M1217-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1723-1724

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.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
Eucalyptol	12.140	19.1	ug/l	548833	4	12.061	1437550	50.0
1-Octanol, 2-me...	13.134	20.3	ug/l	584390	4	12.061	1437550	50.0
1-Nonanol	13.457	80.0	ug/l	2299510	4	12.061	1437550	50.0
(+)-2-Bornanone	13.548	8.0	ug/l	230750	4	12.061	1437550	50.0
Benzene, 1-meth...	13.743	14.4	ug/l	412656	4	12.061	1437550	50.0
E-14-Hexadecenal	13.786	12.4	ug/l	356525	4	12.061	1437550	50.0
1-Decene	13.896	10.0	ug/l	286985	4	12.061	1437550	50.0
Cyclooctane, 1,...	13.926	25.4	ug/l	731039	4	12.061	1437550	50.0
Cyclodecane	14.231	55.1	ug/l	1582950	4	12.061	1437550	50.0
Anethole	14.445	8.6	ug/l	246013	4	12.061	1437550	50.0