

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030621\
 Data File : VX021016.D
 Acq On : 04 Mar 2021 15:59
 Operator : JC/MD
 Sample : M1553-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1729

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\82X022421W.M
 Title : SW846 8260

Signal : TIC: VX021016.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.417	219	226	237	rVB	97895	160557	1.41%	0.382%
2	2.999	315	325	339	rBV2	63905	156355	1.37%	0.372%
3	5.464	732	744	760	rBV2	149789	426637	3.75%	1.015%
4	5.629	760	772	793	rVB	227725	648417	5.69%	1.543%
5	6.029	829	840	854	rBV	162214	427132	3.75%	1.016%
6	6.829	962	976	1000	rVB	397409	946894	8.31%	2.253%
7	7.953	1161	1167	1178	rVB	85671	164582	1.45%	0.392%
8	8.694	1285	1293	1299	rBV	838029	1319160	11.58%	3.139%
9	8.765	1299	1305	1335	rVB	7241574	11387839	100.00%	27.099%
10	10.094	1520	1531	1547	rBV	818370	1141258	10.02%	2.716%
11	11.065	1690	1696	1701	rBV	1207317	1588829	13.95%	3.781%
12	11.118	1701	1705	1717	rVB	661679	886935	7.79%	2.111%
13	12.059	1859	1865	1873	rVB2	874544	1142206	10.03%	2.718%
14	12.142	1873	1879	1893	rVB	3685221	4673080	41.04%	11.120%
15	12.253	1893	1898	1921	rBV	2380762	3053479	26.81%	7.266%
16	12.895	2002	2007	2011	rBV	107100	129581	1.14%	0.308%
17	13.012	2021	2027	2039	rBV	299645	524232	4.60%	1.247%
18	13.106	2039	2043	2045	rVV	415919	518296	4.55%	1.233%
19	13.136	2045	2048	2073	rVV	1189473	1945786	17.09%	4.630%
20	13.459	2098	2103	2114	rBV	4022024	4777223	41.95%	11.368%
21	13.554	2114	2119	2129	rVB	703574	1032816	9.07%	2.458%
22	13.748	2145	2152	2156	rBV	535508	839210	7.37%	1.997%
23	13.789	2156	2159	2169	rVB	407960	638068	5.60%	1.518%
24	13.901	2174	2178	2180	rVV	344864	488544	4.29%	1.163%
25	13.930	2180	2183	2206	rVB	690616	1216150	10.68%	2.894%
26	14.236	2230	2235	2243	rBV	557011	894149	7.85%	2.128%
27	14.524	2281	2284	2293	rVB2	57173	115701	1.02%	0.275%
28	15.466	2440	2444	2449	rVB	126929	181169	1.59%	0.431%
29	15.795	2496	2500	2506	rVB2	147885	245607	2.16%	0.584%
30	16.148	2555	2560	2566	rBV	127911	220588	1.94%	0.525%
31	16.778	2662	2667	2669	rBV2	79064	132963	1.17%	0.316%

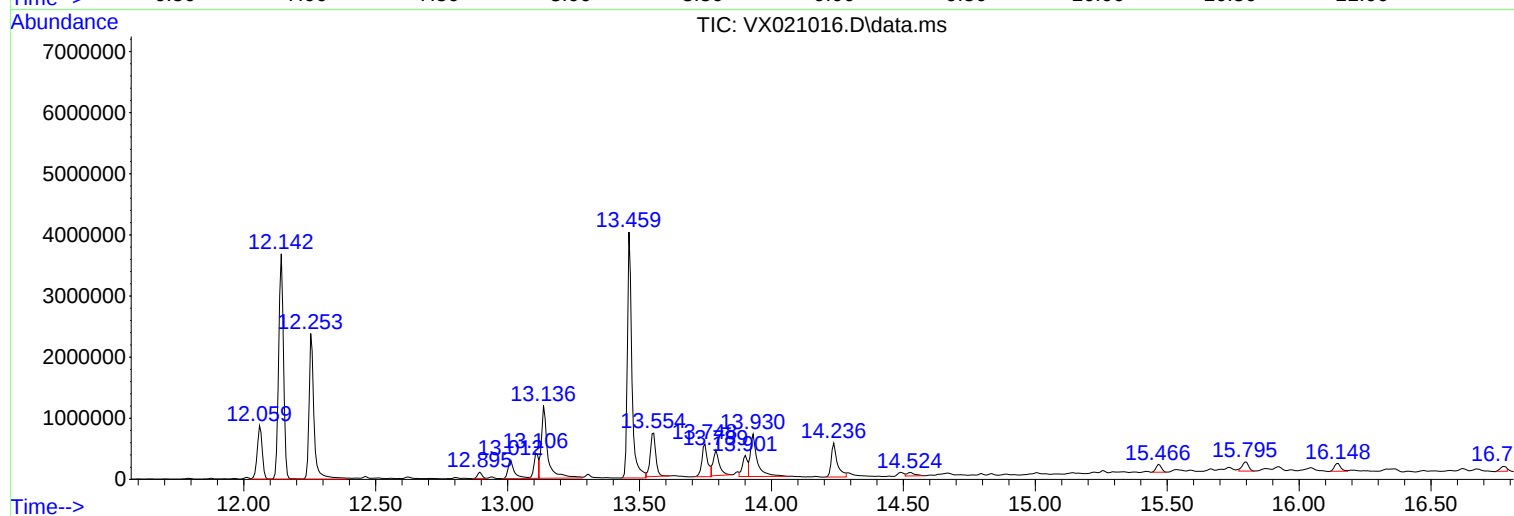
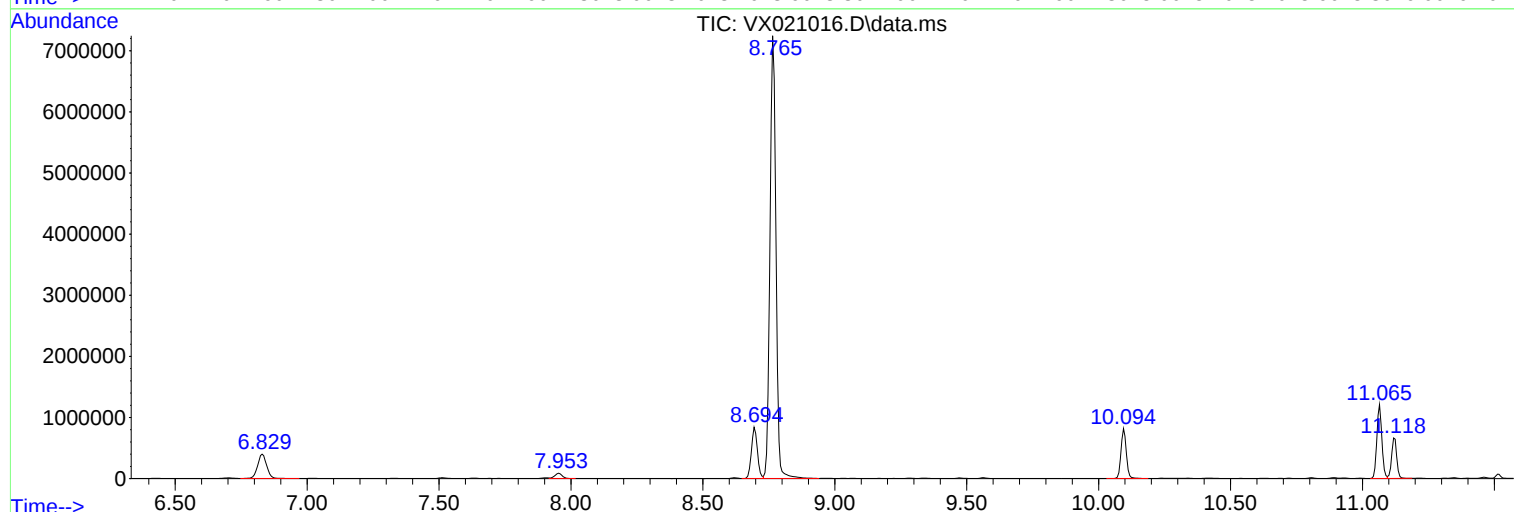
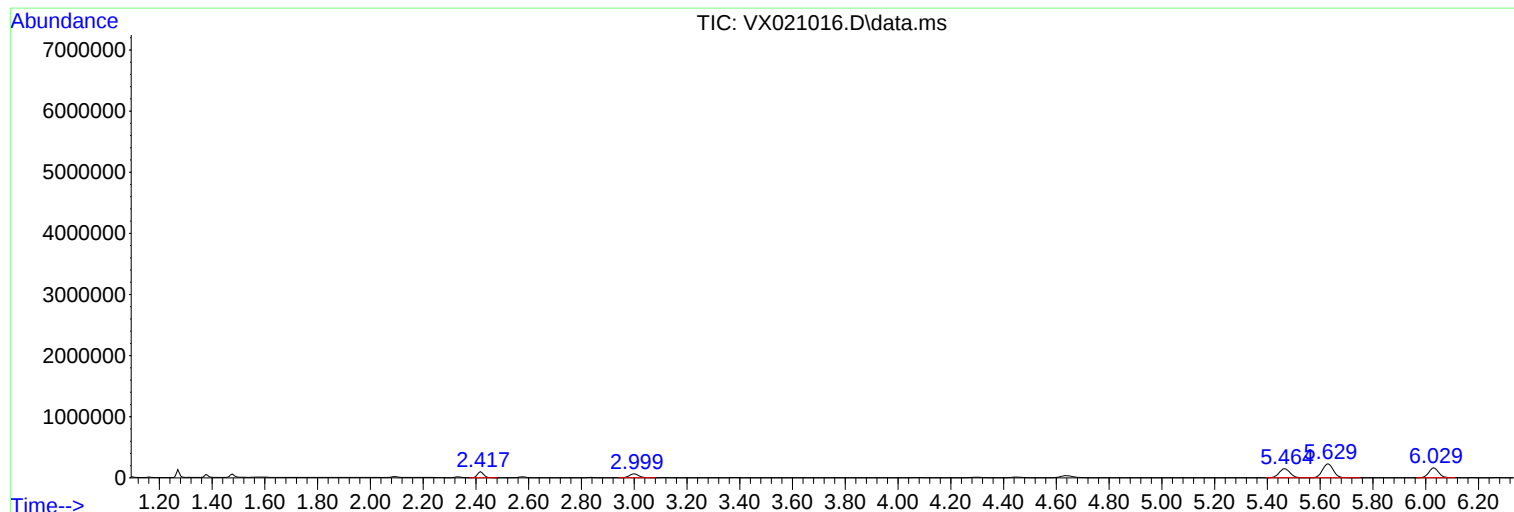
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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



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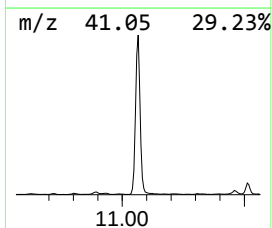
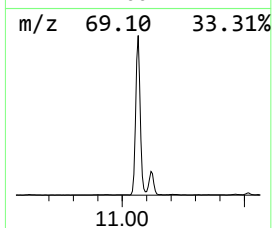
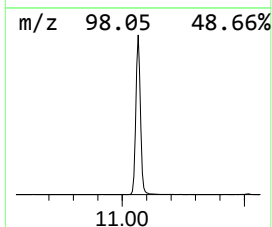
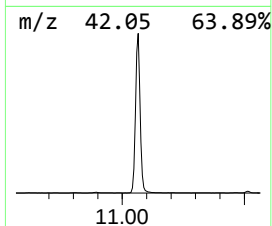
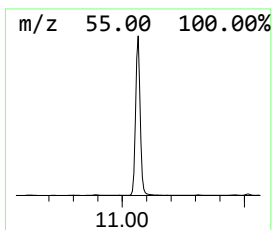
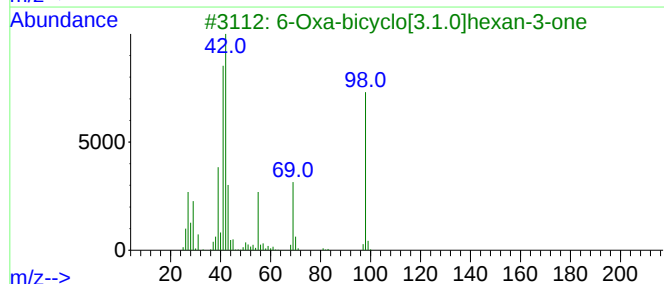
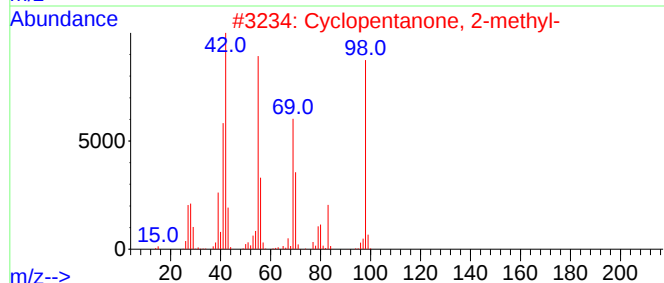
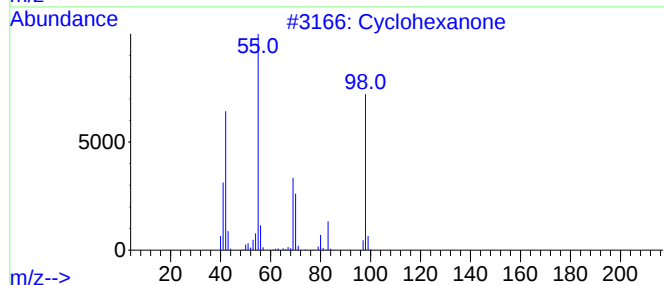
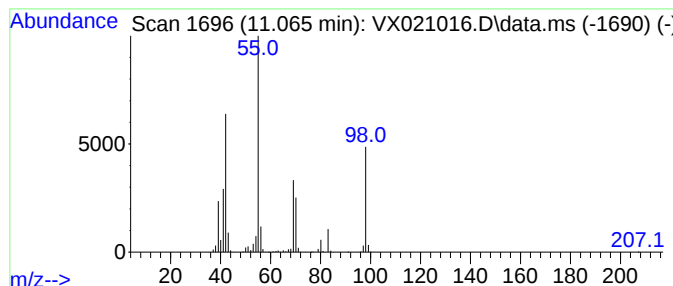
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.065	69.61 ug/l	1588830	Chlorobenzene-d5	10.094

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	94
2			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	72
3			6-Oxa-bicyclo[3.1.0]hexan-3-one	98	C5H6O2	074017-10-0	47
4			Bis(1-hydroxycyclohexyl) peroxide	230	C12H22O4	002407-94-5	45
5			Cyclohexane, methyl-	98	C7H14	000108-87-2	42



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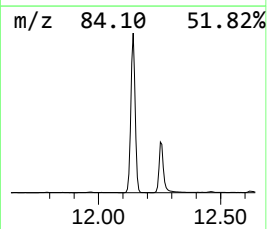
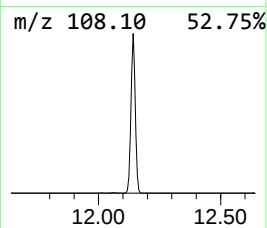
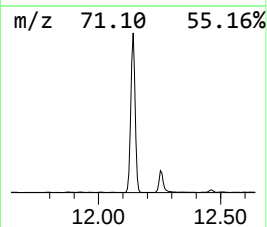
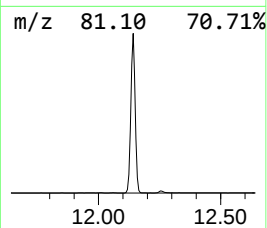
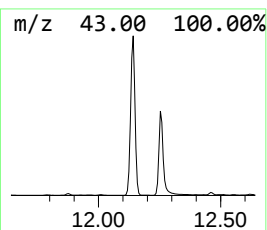
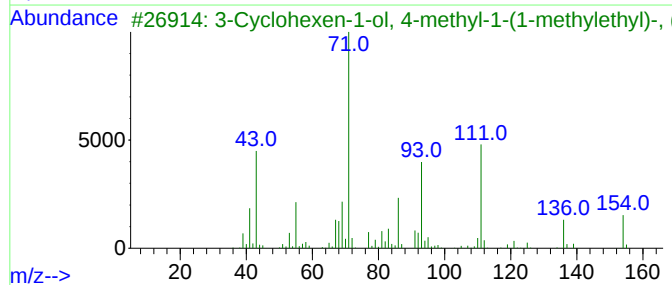
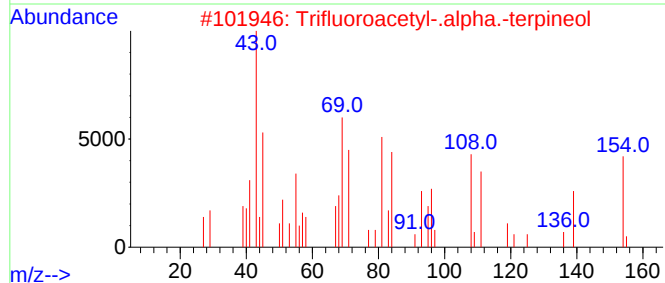
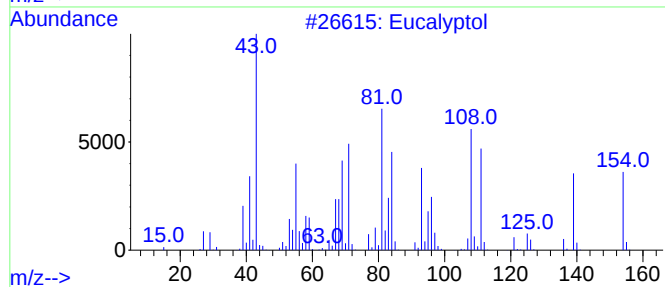
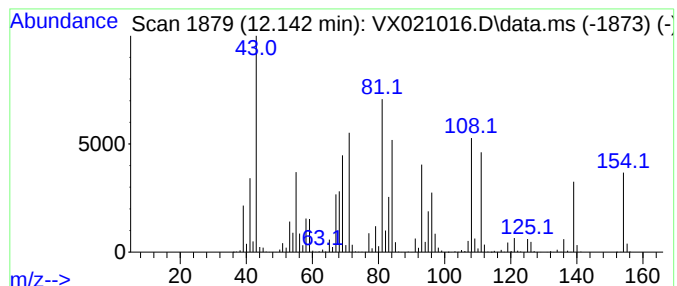
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Quant Title : SW846 8260

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

Peak Number 2 Eucalyptol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.142	204.56 ug/l	4673080	1,4-Dichlorobenzene-d4	12.059

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	64
3			3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-	154	C10H18O	020126-76-5	35
4			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	32
5			2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	27



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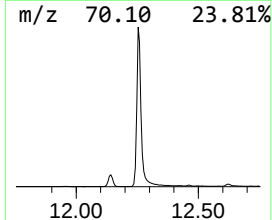
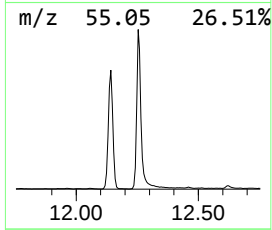
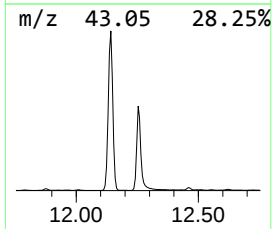
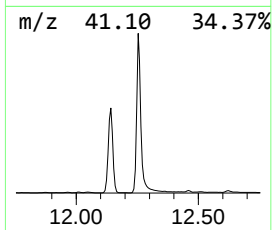
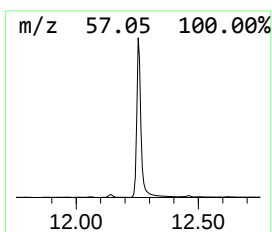
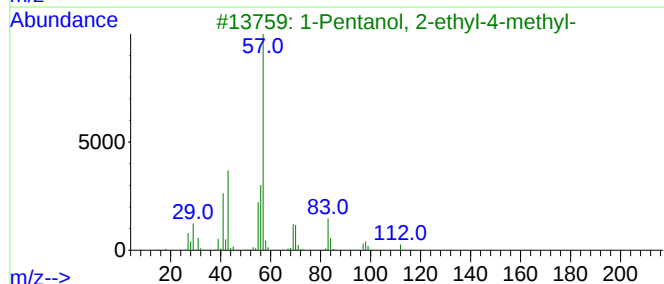
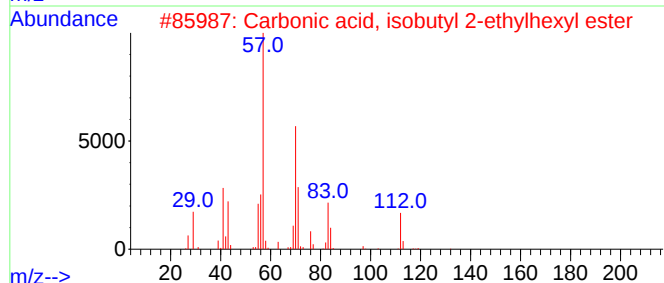
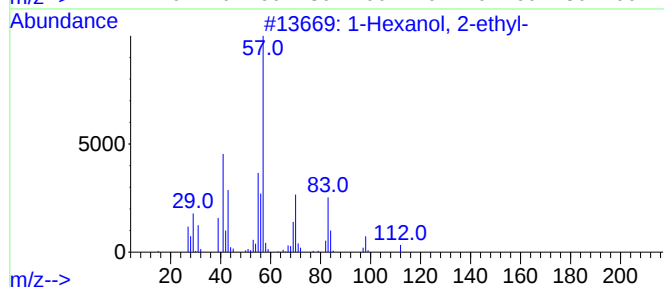
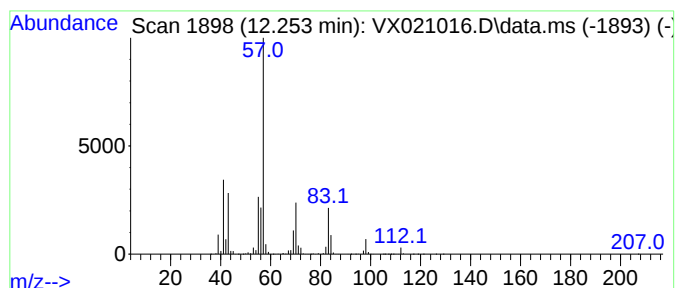
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.253	133.67 ug/l	3053480	1,4-Dichlorobenzene-d4	12.059	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



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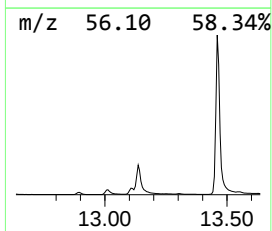
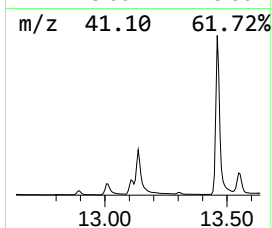
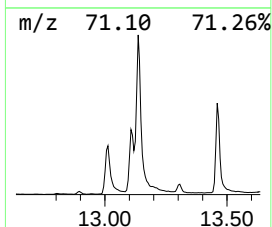
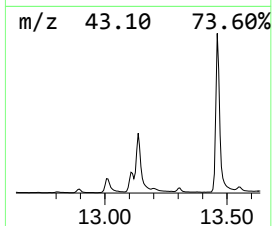
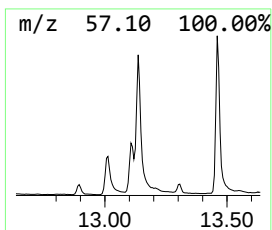
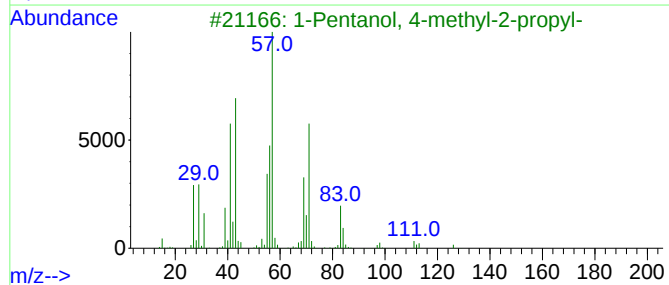
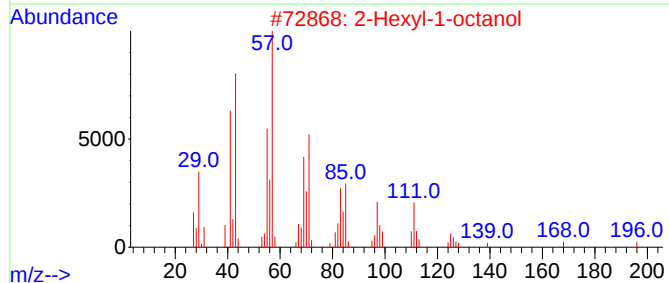
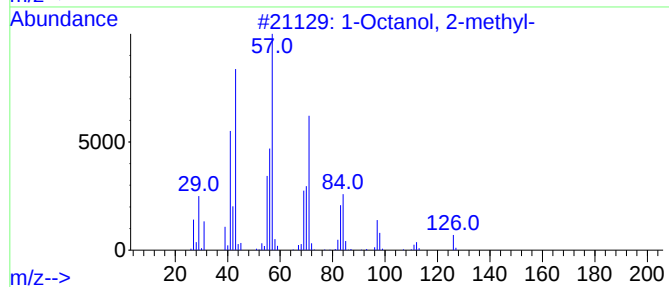
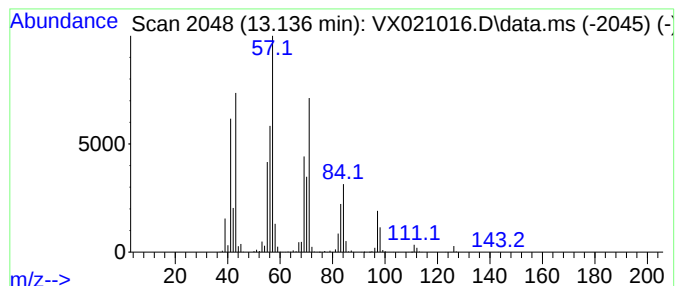
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Peak Number 4 1-Octanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.136	85.18 ug/l	1945790	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	78
2			2-Hexyl-1-octanol	214	C14H30O	019780-79-1	59
3			1-Pentanol, 4-methyl-2-propyl-	144	C9H20O	054004-41-0	59
4			Acetic acid, trichloro-, octyl e...	274	C10H17Cl3O2	016958-78-4	53
5			Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	49



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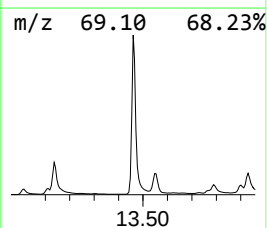
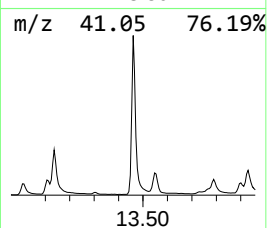
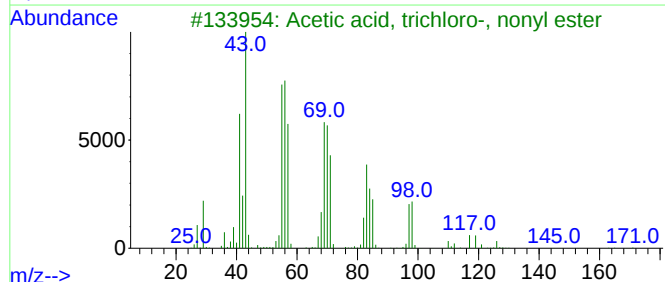
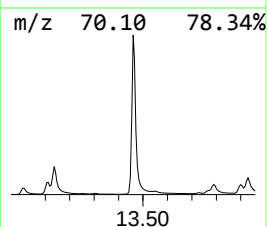
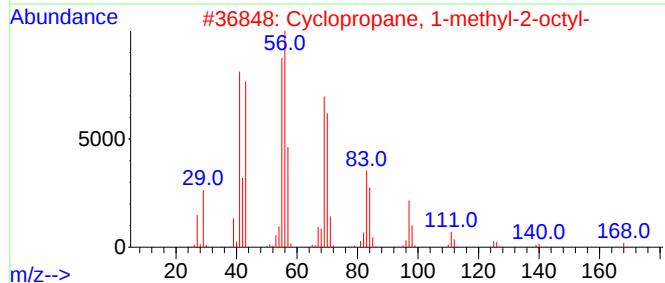
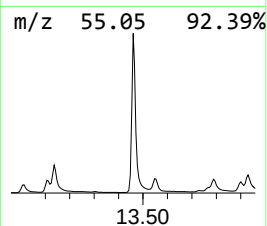
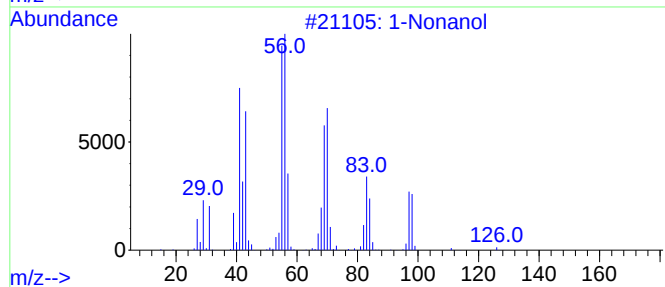
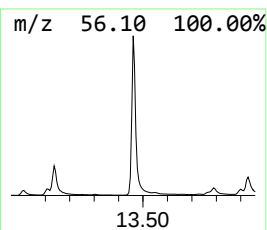
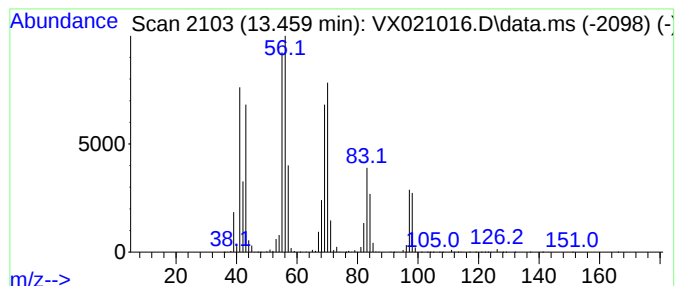
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.459	209.12 ug/l	4777220	1,4-Dichlorobenzene-d4	12.059

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	Acetic acid, trichloro-, nonyl e...			288	C11H19Cl3O2	065611-32-7	83
4	Cycloheptane			98	C7H14	000291-64-5	72
5	1-Octanol			130	C8H18O	000111-87-5	72



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ALS Vial : 14 Sample Multiplier: 1

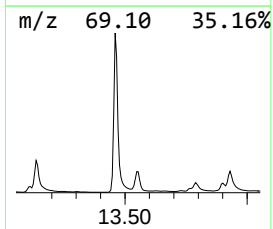
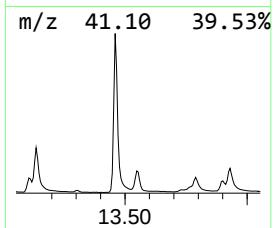
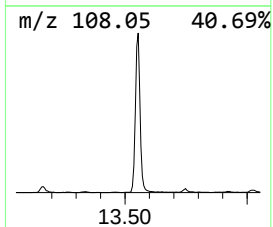
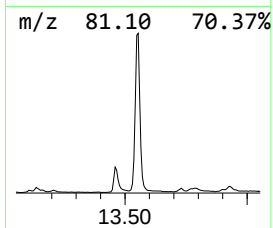
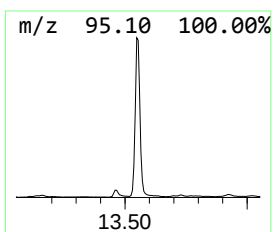
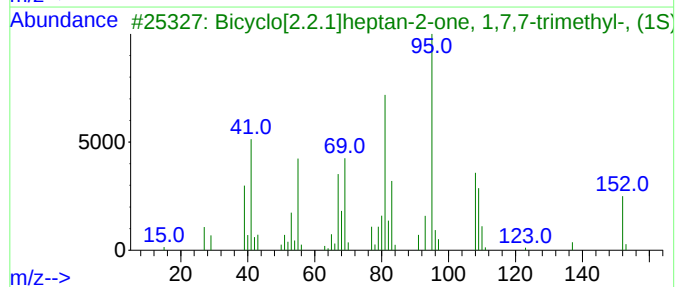
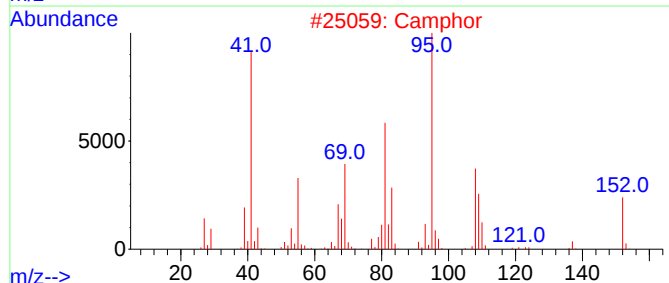
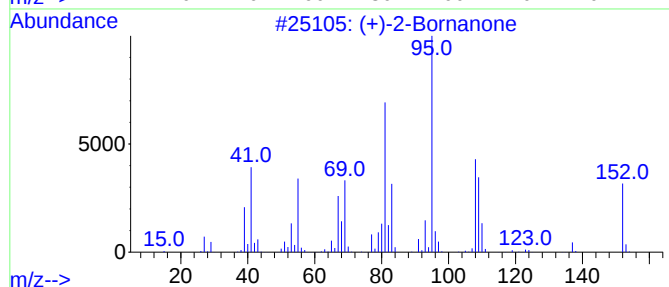
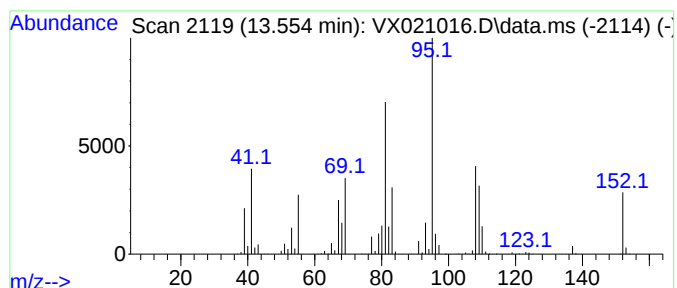
Instrument :
MSVOA_X
ClientSampleId :
1729

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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

Peak Number 6 (+)-2-Bornanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.554	45.21 ug/l	1032820	1,4-Dichlorobenzene-d4	12.059	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2	Camphor	152	C10H16O	000076-22-2	98
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
4	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46
5	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030621\
Data File : VX021016.D
Acq On : 04 Mar 2021 15:59
Operator : JC/MD
Sample : M1553-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
1729

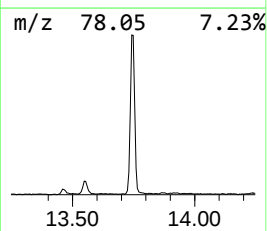
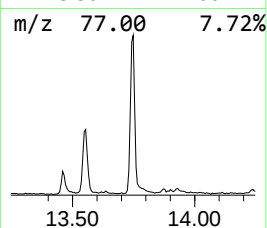
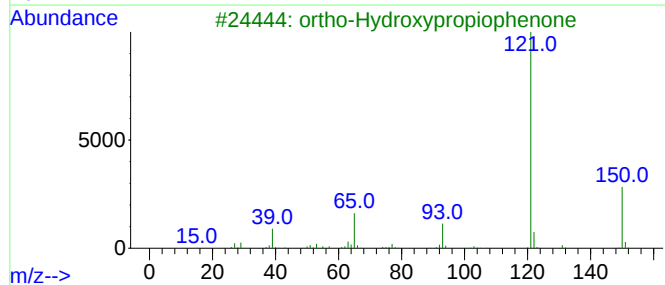
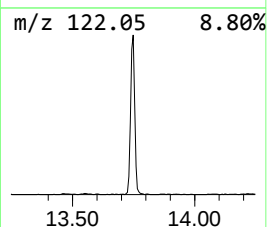
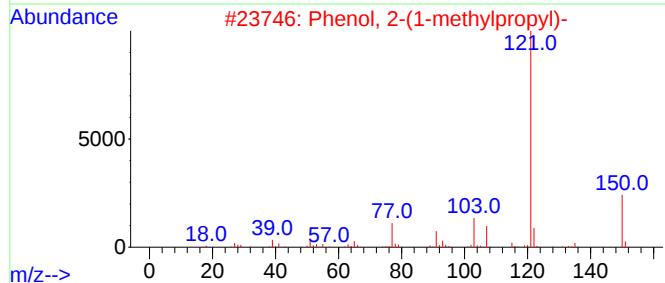
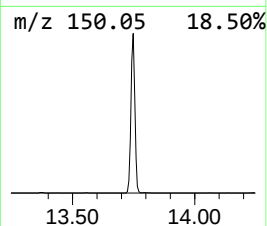
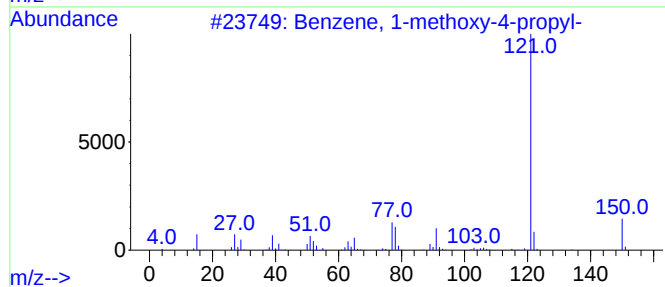
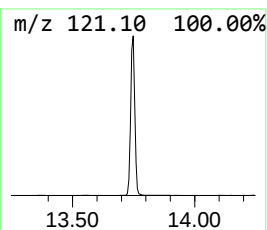
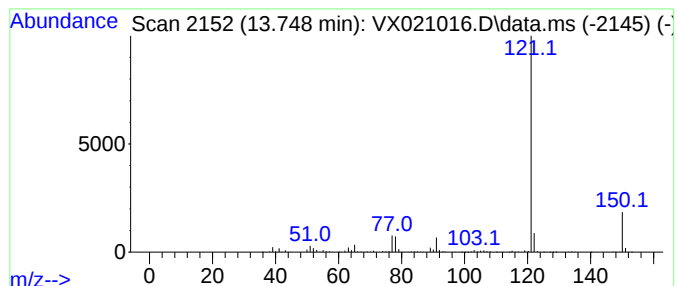
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-methoxy-4-propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.748	36.74 ug/l	839210	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	91
2			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	78
3			ortho-Hydroxypropiophenone	150	C9H10O2	000610-99-1	72
4			Benzene, 1-ethyl-4-methoxy-	136	C9H12O	001515-95-3	56
5			1-Methoxy-4-dimethyl(trimethylsi...	282	C14H26O2Si2	1000280-14-0	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030621\
Data File : VX021016.D
Acq On : 04 Mar 2021 15:59
Operator : JC/MD
Sample : M1553-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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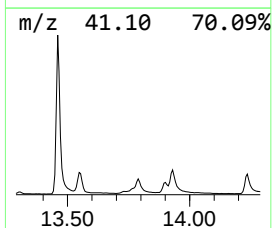
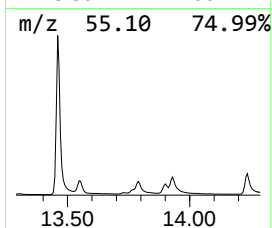
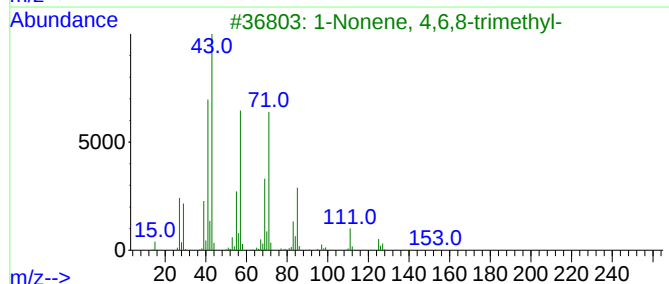
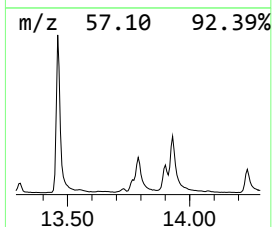
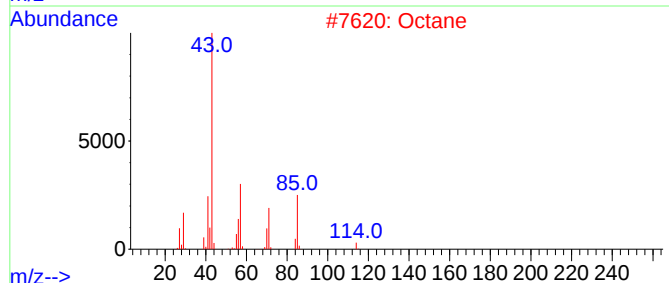
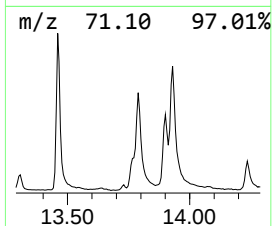
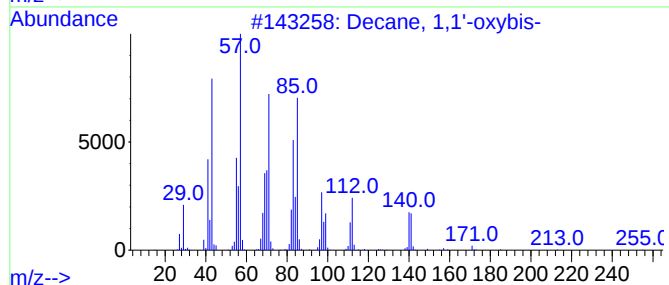
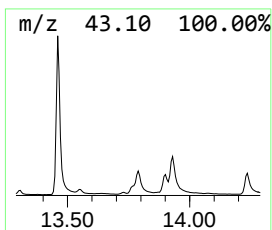
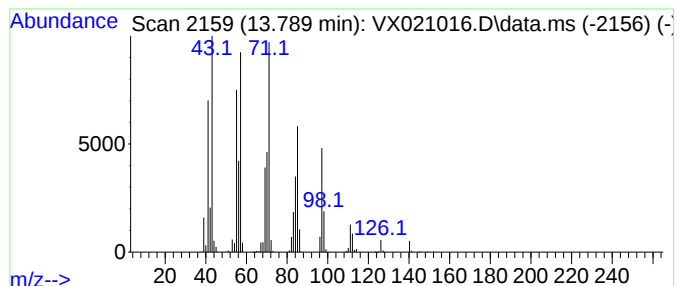
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Quant Title : SW846 8260

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

Peak Number 8 Decane, 1,1'-oxybis- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.789	27.93 ug/l	638068	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	64
2			Octane	114	C8H18	000111-65-9	43
3			1-Nonene, 4,6,8-trimethyl-	168	C12H24	054410-98-9	38
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	38
5			Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030621\
Data File : VX021016.D
Acq On : 04 Mar 2021 15:59
Operator : JC/MD
Sample : M1553-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
1729

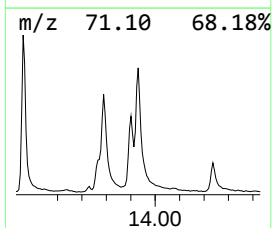
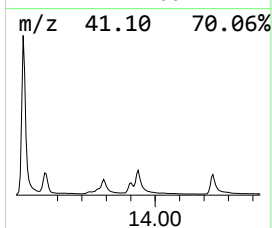
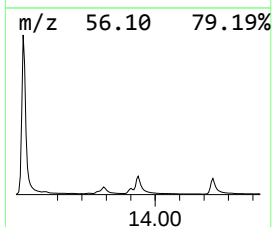
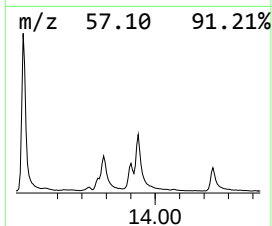
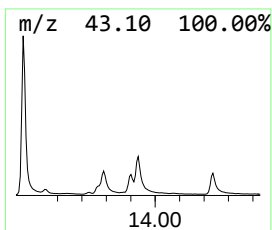
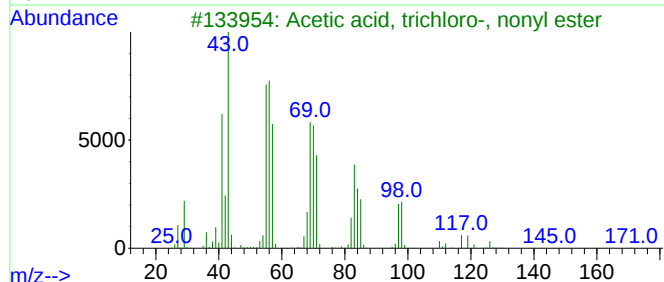
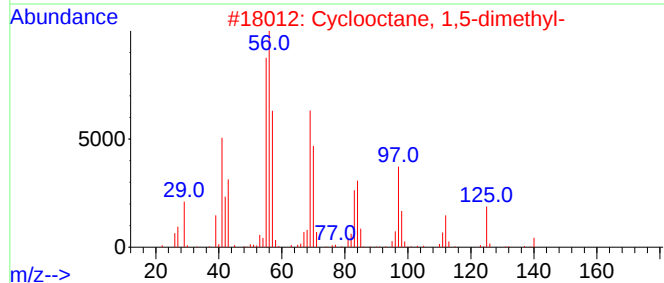
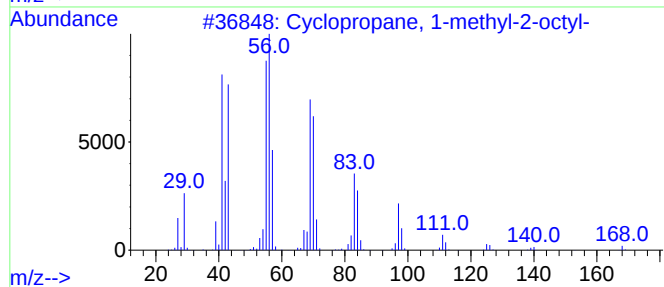
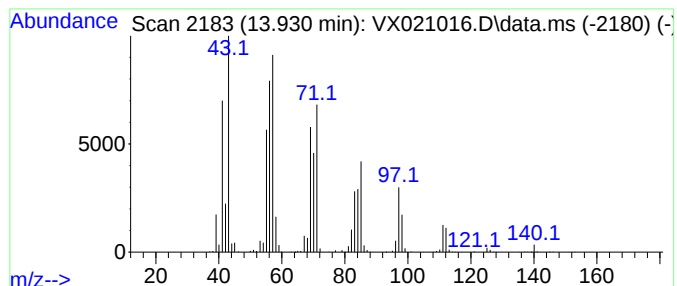
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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

Peak Number 9 Cyclopropane, 1-methyl-2-oc... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.930	53.24 ug/l	1216150	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	64
2			Cyclooctane, 1,5-dimethyl-	140	C10H20	021328-57-4	60
3			Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	58
4			1-Decene	140	C10H20	000872-05-9	55
5			2-Chloropropionic acid, decyl e...	248	C13H25ClO2	086711-78-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030621\
Data File : VX021016.D
Acq On : 04 Mar 2021 15:59
Operator : JC/MD
Sample : M1553-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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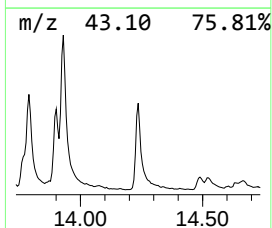
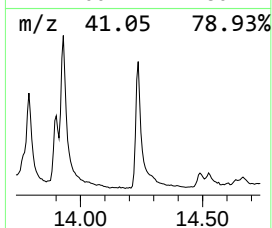
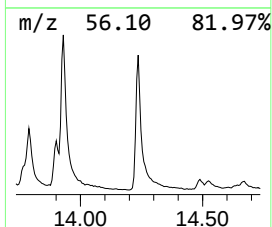
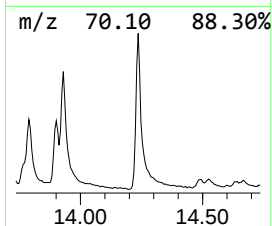
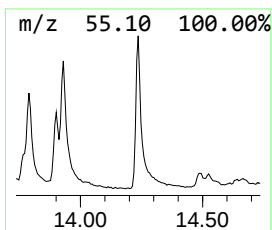
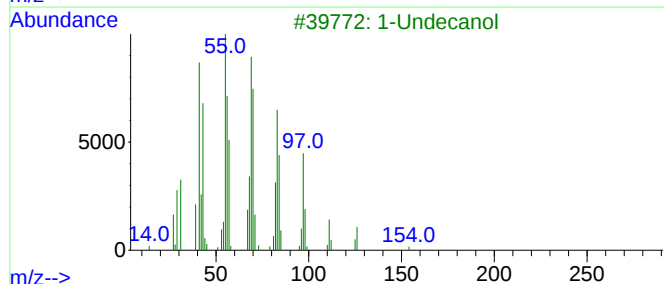
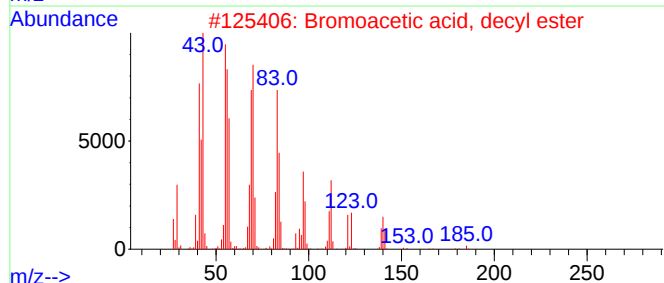
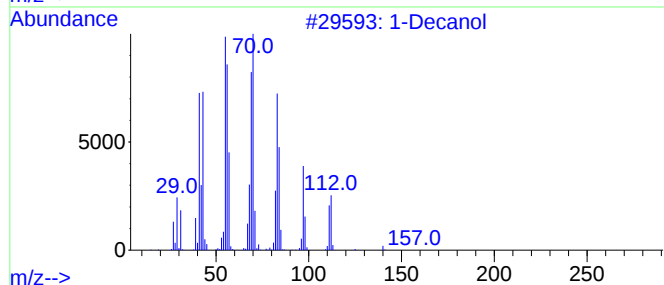
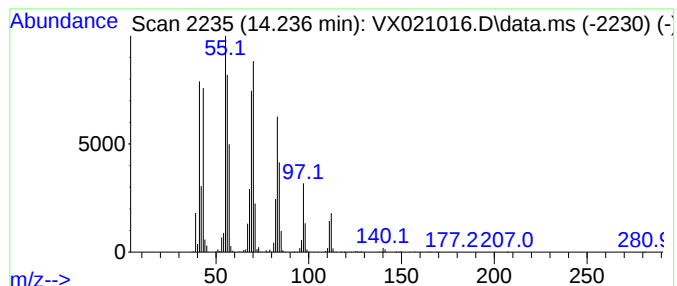
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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

Peak Number 10 1-Decanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.236	39.14 ug/l	894149	1,4-Dichlorobenzene-d4	12.059

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Decanol	158	C10H22O	000112-30-1	91
2		Bromoacetic acid, decyl ester	278	C12H23BrO2	005436-93-1	91
3		1-Undecanol	172	C11H24O	000112-42-5	91
4		1-Undecene	154	C11H22	000821-95-4	90
5		Cyclodecane	140	C10H20	000293-96-9	89



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030621\
Data File : VX021016.D
Acq On : 04 Mar 2021 15:59
Operator : JC/MD
Sample : M1553-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.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
Cyclohexanone	11.065	69.6	ug/l	1588830	3	10.094	1141260	50.0
Eucalyptol	12.142	204.6	ug/l	4673080	4	12.059	1142210	50.0
1-Hexanol, 2-et...	12.253	133.7	ug/l	3053480	4	12.059	1142210	50.0
1-Octanol, 2-me...	13.136	85.2	ug/l	1945790	4	12.059	1142210	50.0
1-Nonanol	13.459	209.1	ug/l	4777220	4	12.059	1142210	50.0
(+)-2-Bornanone	13.554	45.2	ug/l	1032820	4	12.059	1142210	50.0
Benzene, 1-meth...	13.748	36.7	ug/l	839210	4	12.059	1142210	50.0
Decane, 1,1'-ox...	13.789	27.9	ug/l	638068	4	12.059	1142210	50.0
Cyclopropane, 1...	13.930	53.2	ug/l	1216150	4	12.059	1142210	50.0
1-Decanol	14.236	39.1	ug/l	894149	4	12.059	1142210	50.0