

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112120\
 Data File : VX019522.D
 Acq On : 21 Nov 2020 03:10
 Operator : JC/MD
 Sample : L4779-03
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1623

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\82X112120W.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	1.337	34	41	44	rBV	29737	84856	1.12%	0.209%
2	1.563	76	78	95	rVB3	31307	77426	1.02%	0.190%
3	1.715	99	103	130	rVB3	20449	85696	1.13%	0.211%
4	2.428	213	220	236	rBV	572653	1356591	17.83%	3.336%
5	2.605	243	249	255	rBV	72487	167850	2.21%	0.413%
6	4.647	573	584	611	rVB	33190	129136	1.70%	0.318%
7	5.464	705	718	731	rBV	177773	504587	6.63%	1.241%
8	5.623	733	744	762	rVB	330870	934923	12.29%	2.299%
9	6.031	798	811	821	rBV	195842	530936	6.98%	1.306%
10	6.830	931	942	956	rBV	513905	1320071	17.35%	3.246%
11	8.695	1241	1248	1255	rBV	1018291	1579658	20.77%	3.884%
12	10.092	1469	1477	1487	rBV	923942	1322802	17.39%	3.253%
13	11.122	1640	1646	1653	rBV	752282	966221	12.70%	2.376%
14	11.878	1765	1770	1776	rBV	173691	219534	2.89%	0.540%
15	12.061	1794	1800	1807	rVB	999658	1220814	16.05%	3.002%
16	12.140	1808	1813	1825	rBV	1474067	1928364	25.35%	4.742%
17	12.256	1827	1832	1846	rBV	1165195	1540909	20.26%	3.789%
18	12.384	1849	1853	1858	rVB	88374	110031	1.45%	0.271%
19	12.493	1867	1871	1879	rVB3	58644	96870	1.27%	0.238%
20	12.725	1905	1909	1915	rBV	58836	78705	1.03%	0.194%
21	12.804	1917	1922	1925	rBV	146260	177773	2.34%	0.437%
22	12.896	1933	1937	1941	rBV	56137	77380	1.02%	0.190%
23	13.006	1951	1955	1964	rBV	221925	347964	4.57%	0.856%
24	13.134	1968	1976	1991	rBV	5628538	7607212	100.00%	18.706%
25	13.457	2024	2029	2039	rBV	269158	428059	5.63%	1.053%
26	13.548	2040	2044	2051	rVB	640983	828278	10.89%	2.037%
27	13.640	2052	2059	2066	rVB2	79615	154310	2.03%	0.379%
28	13.707	2066	2070	2076	rBV3	53637	103931	1.37%	0.256%
29	13.768	2076	2080	2081	rBV2	146069	192032	2.52%	0.472%
30	13.786	2081	2083	2087	rVB	208769	233653	3.07%	0.575%
31	13.926	2095	2106	2119	rBV	3626741	5543519	72.87%	13.631%
32	14.231	2152	2156	2170	rBV	305850	469648	6.17%	1.155%
33	14.481	2191	2197	2201	rBV3	126175	223585	2.94%	0.550%
34	14.524	2201	2204	2211	rVV	91956	183149	2.41%	0.450%

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Integration Parameters: RTEINT.P

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35	14.603	2213	2217	2224	rVV	737933	1373052	18.05%	3.376%
36	14.664	2224	2227	2234	rVV	1316017	1836646	24.14%	4.516%
37	14.731	2234	2238	2251	rVV	1078946	1865898	24.53%	4.588%
38	14.835	2251	2255	2269	rVV2	183645	487379	6.41%	1.198%
39	14.956	2270	2275	2302	rVB	678105	1143553	15.03%	2.812%
40	15.261	2320	2325	2327	rBV	272336	431686	5.67%	1.062%
41	15.298	2327	2331	2349	rVV	726597	1636212	21.51%	4.023%
42	15.456	2353	2357	2375	rVV	368225	877404	11.53%	2.158%
43	15.743	2400	2404	2423	rVB2	70483	188945	2.48%	0.465%

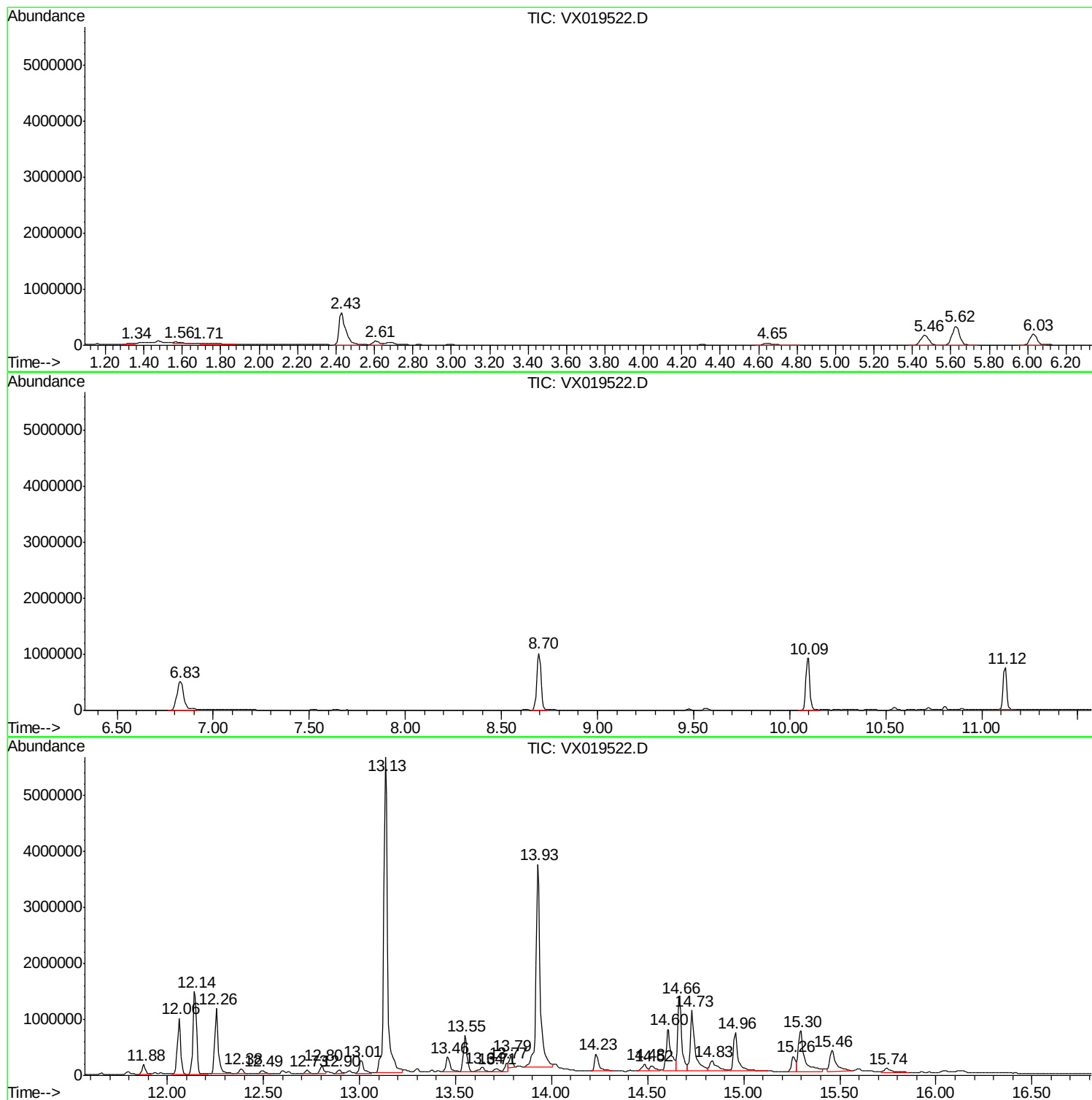
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Quant Title : SW846 8260

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



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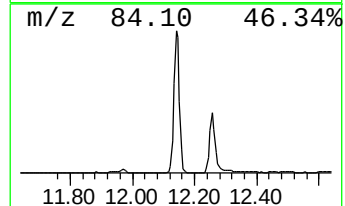
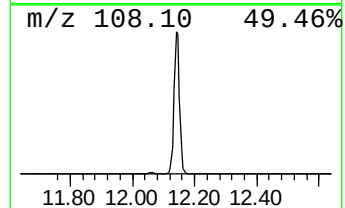
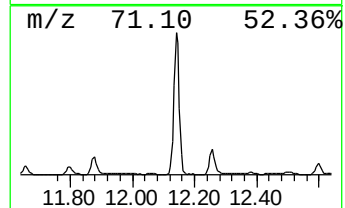
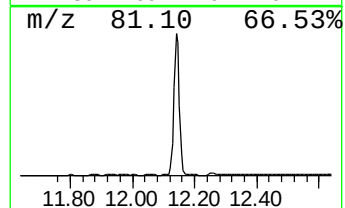
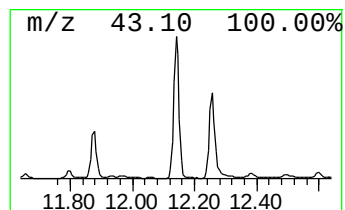
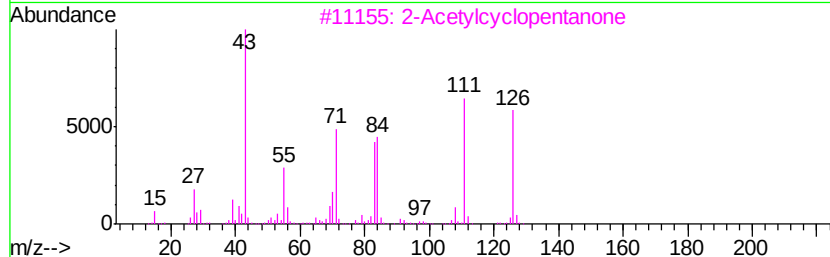
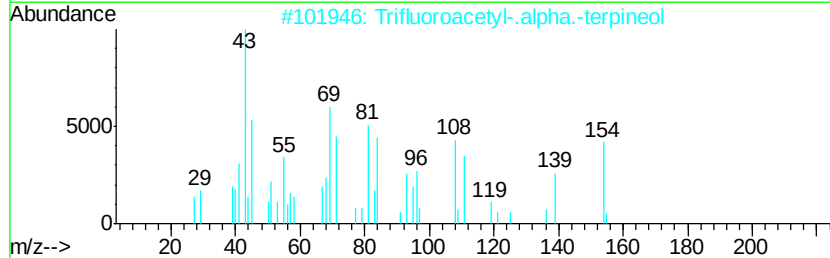
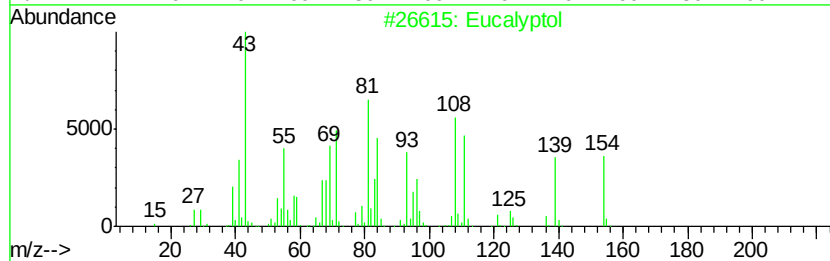
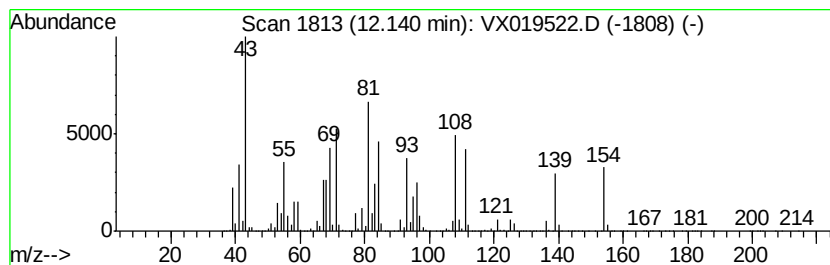
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

Peak Number 1 Eucalyptol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.14	78.98 ug/l	1928360	1,4-Dichlorobenzene-d4			12.06
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	43
3	2-Acetylcyclopentanone		126	C7H10O2	001670-46-8	35
4	5-Hepten-2-one, 6-methyl-		126	C8H14O	000110-93-0	32
5	2-Acetonilycyclohexanone		154	C9H14O2	006126-53-0	22



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Instrument :
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ClientSampled :
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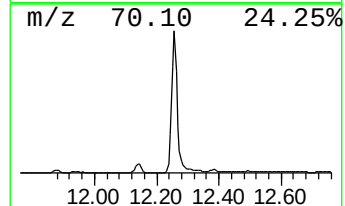
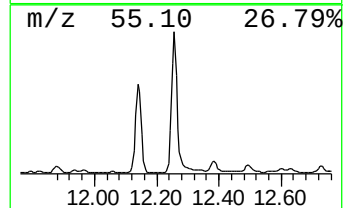
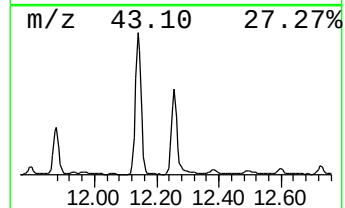
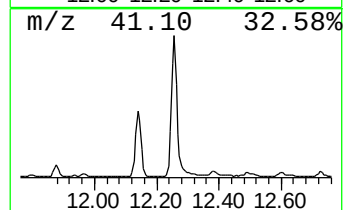
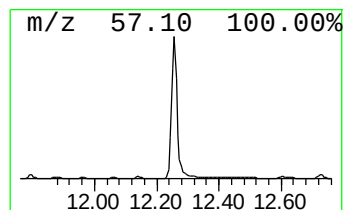
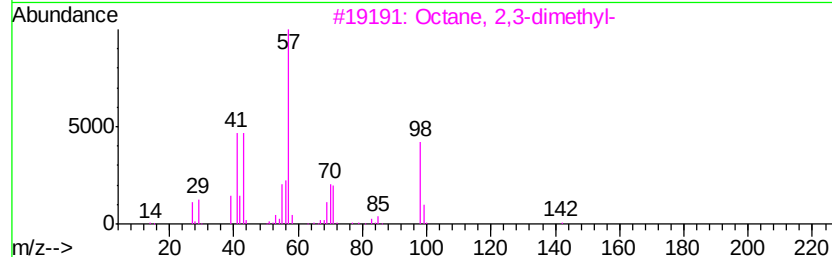
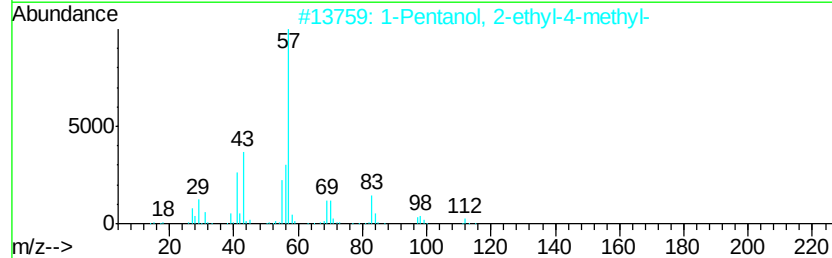
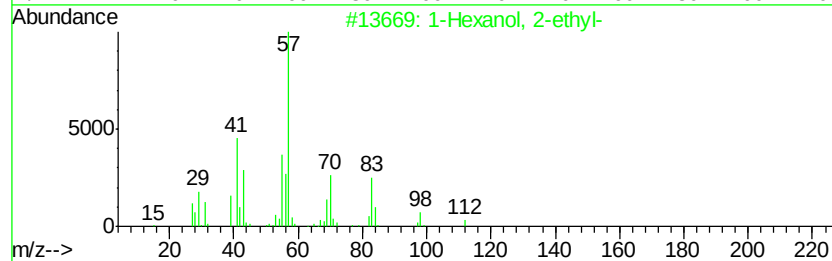
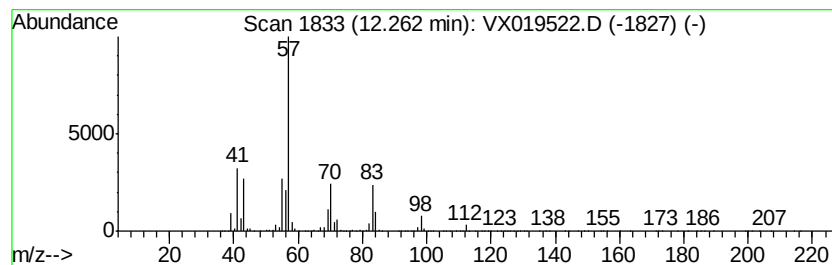
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Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	63.11 ug/l	1540910	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
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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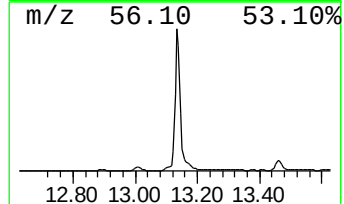
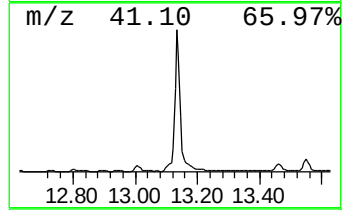
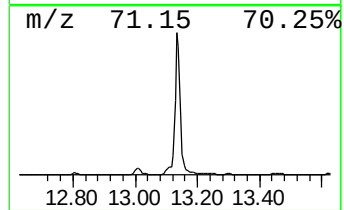
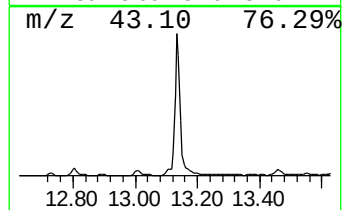
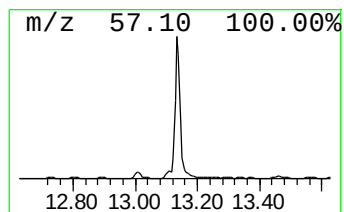
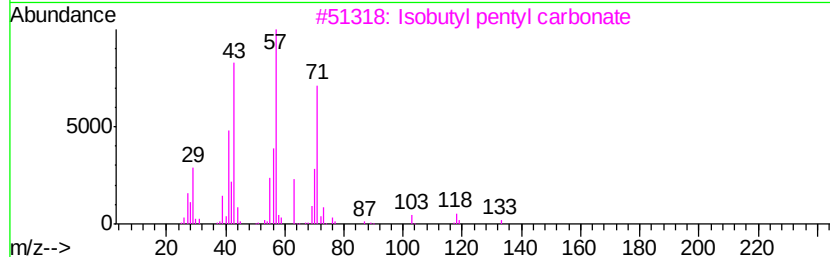
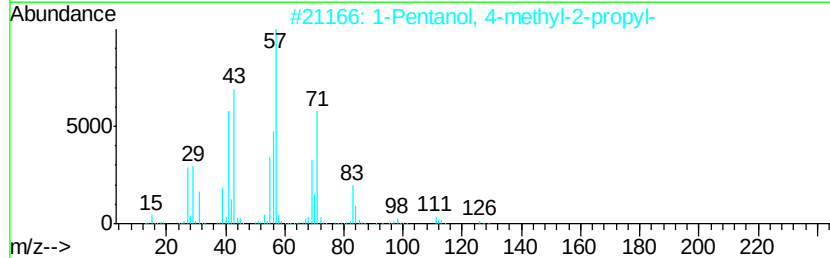
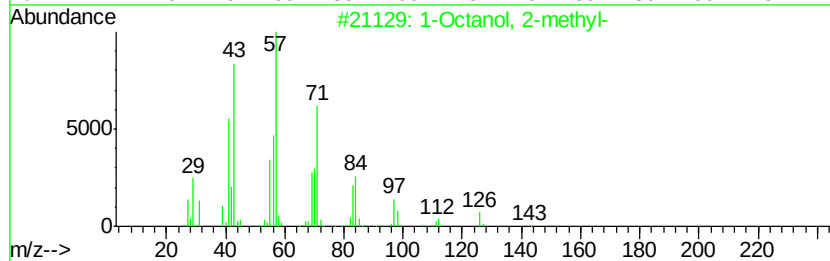
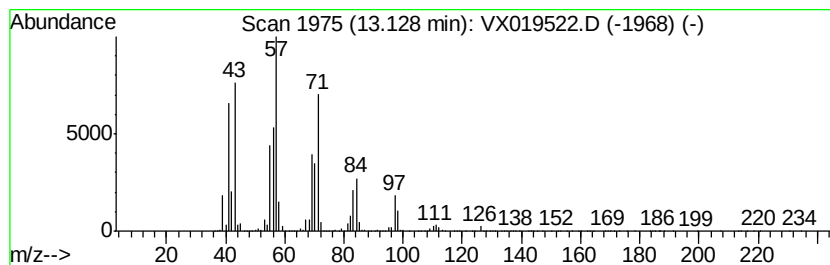
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Octanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.13	311.56 ug/l	7607210	1,4-Dichlorobenzene-d4	12.06		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-methyl-		144	C9H20O	000818-81-5	83
2	1-Pentanol, 4-methyl-2-propyl-		144	C9H20O	054004-41-0	59
3	Isobutyl pentyl carbonate		188	C10H20O3	178442-32-5	53
4	Isooctyl mercaptoacetate		204	C10H20O2S	025103-09-7	47
5	1-Dodecene		168	C12H24	000112-41-4	43



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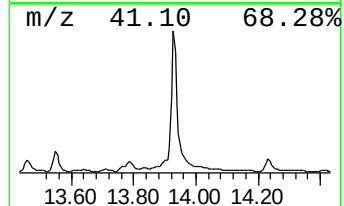
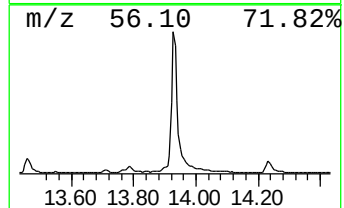
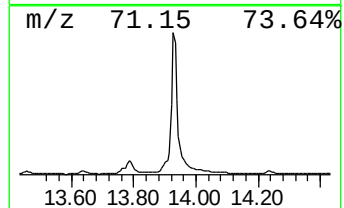
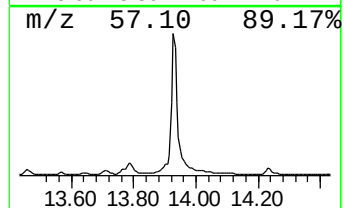
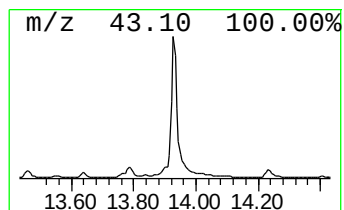
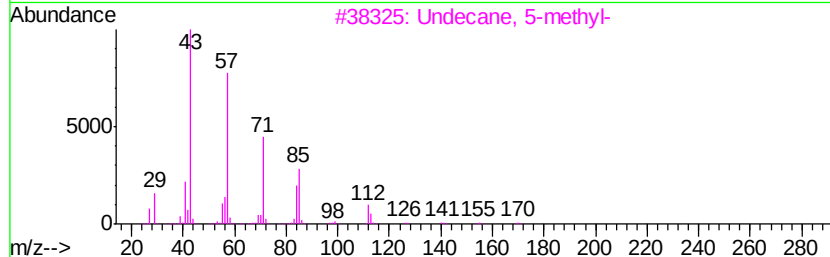
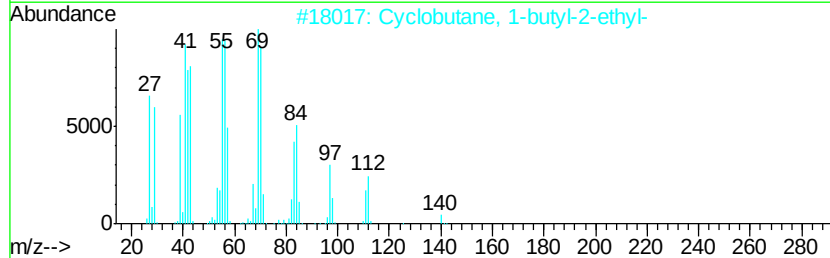
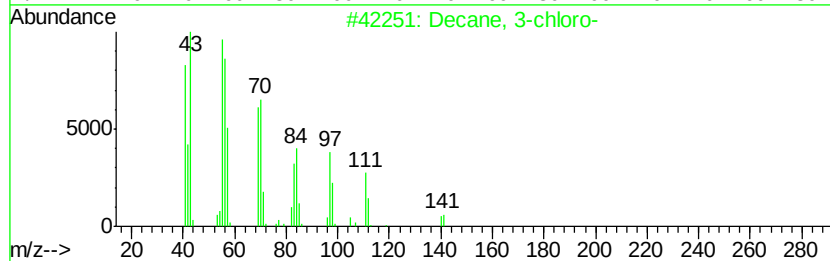
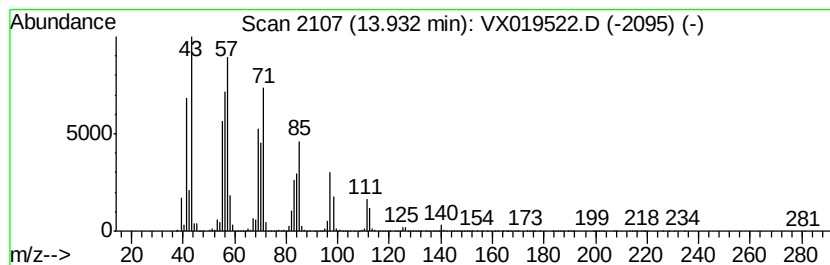
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Peak Number 4 Decane, 3-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	227.04 ug/l	5543520	1,4-Dichlorobenzene-d4	12.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3-chloro-	176	C10H21Cl	001002-11-5	58	
2	Cyclobutane, 1-butyl-2-ethyl-	140	C10H20	1000150-67-3	49	
3	Undecane, 5-methyl-	170	C12H26	001632-70-8	45	
4	Cyclooctane, 1,5-dimethyl-	140	C10H20	021328-57-4	43	
5	3-Octene, (E)-	112	C8H16	014919-01-8	38	



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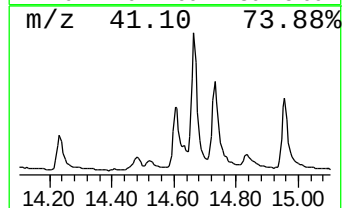
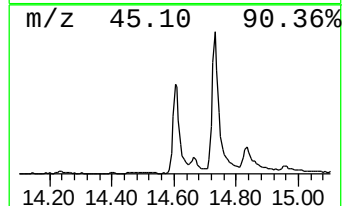
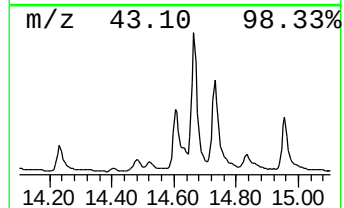
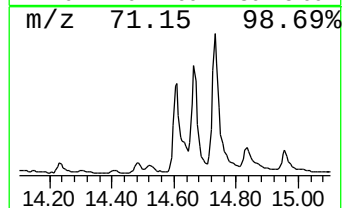
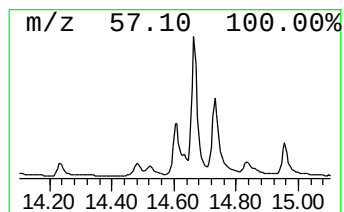
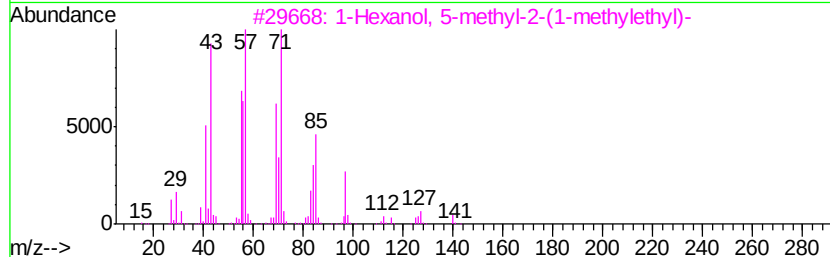
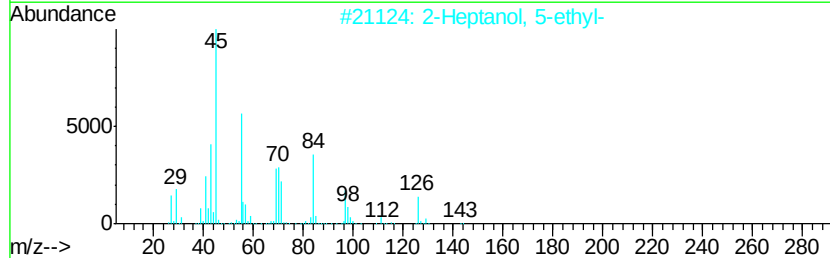
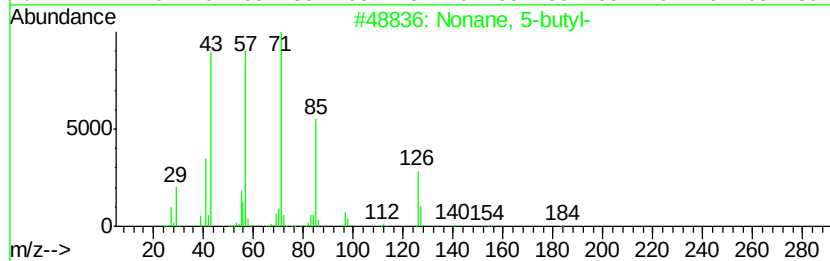
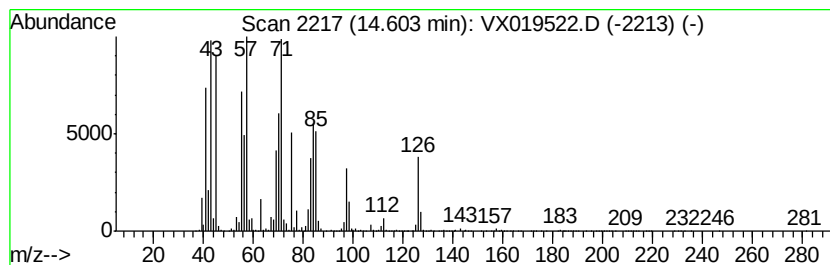
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TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown14.60 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	56.24 ug/l	1373050	1,4-Dichlorobenzene-d4	12.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonane, 5-butyl-	184	C13H28	017312-63-9	46
2		2-Heptanol, 5-ethyl-	144	C9H20O	019780-40-6	43
3		1-Hexanol, 5-methyl-2-(1-methyle...	158	C10H22O	002051-33-4	43
4		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	38
5		Propanal, 2-methyl-, 2-propenylh...	126	C7H14N2	066075-08-9	25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112120\
Data File : VX019522.D
Acq On : 21 Nov 2020 03:10
Operator : JC/MD
Sample : L4779-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
1623

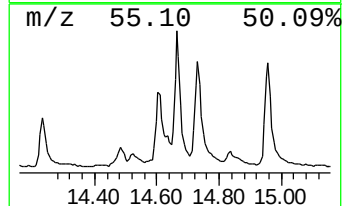
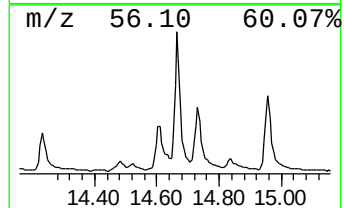
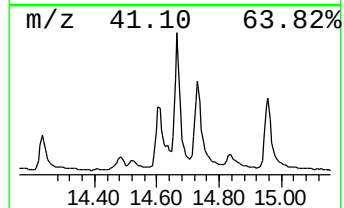
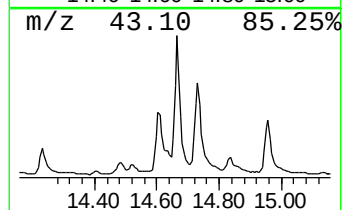
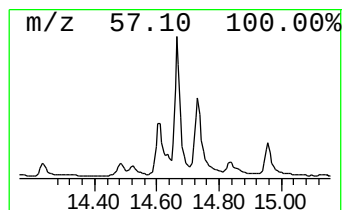
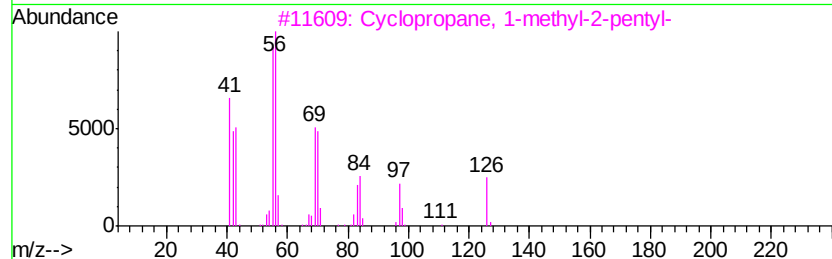
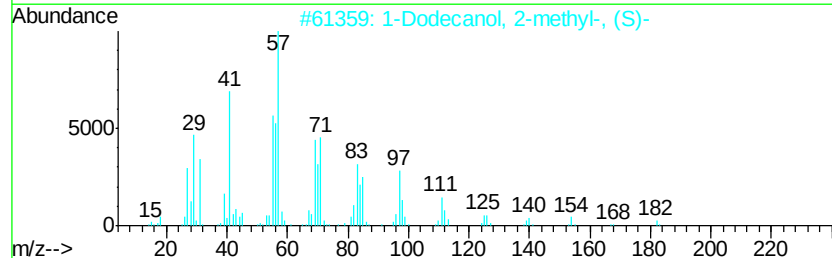
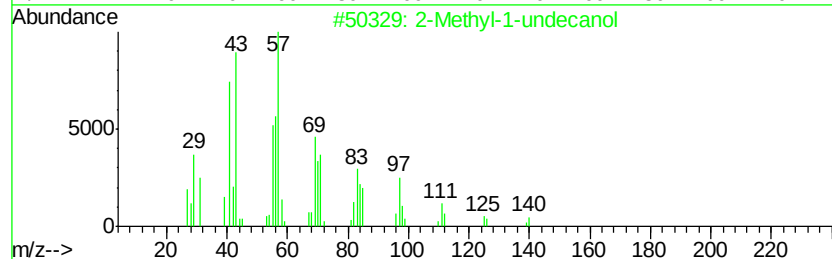
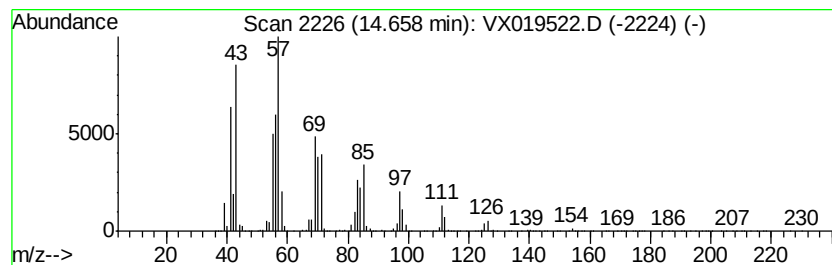
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Quant Title : SW846 8260

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

Peak Number 6 2-Methyl-1-undecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	75.22 ug/l	1836650	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Methyl-1-undecanol	186	C12H26O	010522-26-6	80
2		1-Dodecanol, 2-methyl-, (S)-	200	C13H28O	057289-26-6	72
3		Cyclopropane, 1-methyl-2-pentyl-	126	C9H18	041977-37-1	60
4		Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	58
5		1-Dodecene	168	C12H24	000112-41-4	52



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112120\
Data File : VX019522.D
Acq On : 21 Nov 2020 03:10
Operator : JC/MD
Sample : L4779-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
1623

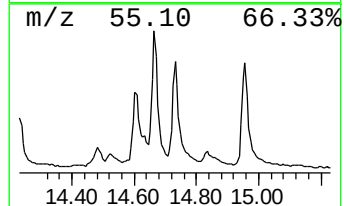
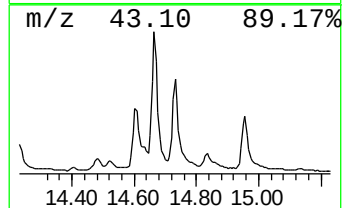
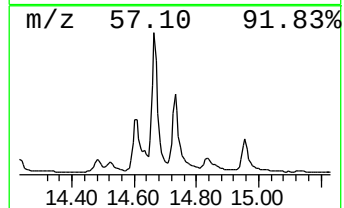
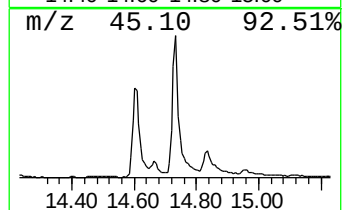
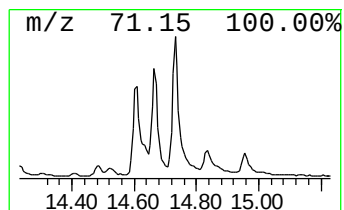
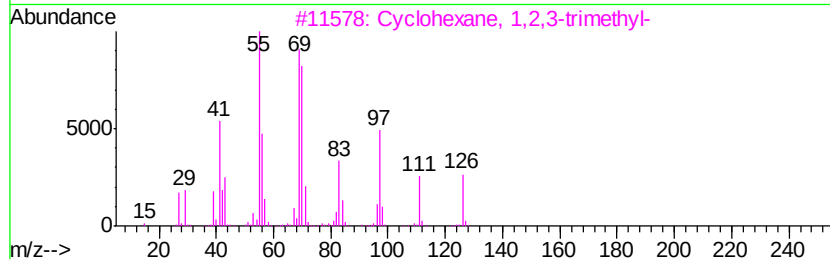
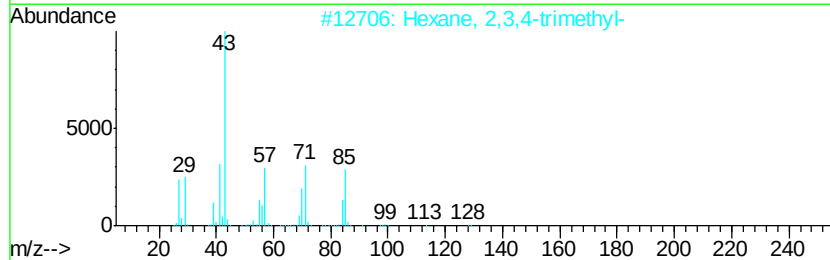
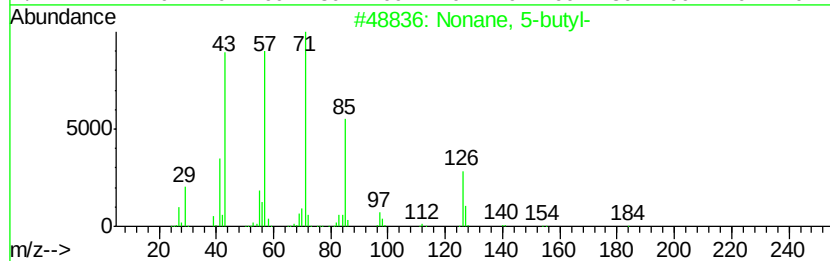
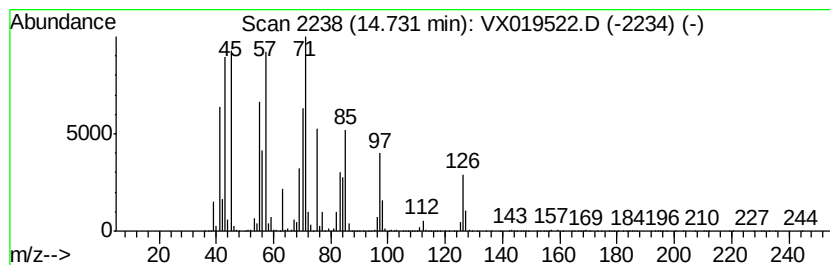
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.73 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	76.42 ug/l	1865900	1,4-Dichlorobenzene-d4	12.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonane, 5-butyl-	184	C13H28	017312-63-9	42
2		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	35
3		Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	30
4		Propanoic acid, nonyl ester	200	C12H24O2	053184-67-1	27
5		Hexadecane	226	C16H34	000544-76-3	27



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112120\
 Data File : VX019522.D
 Acq On : 21 Nov 2020 03:10
 Operator : JC/MD
 Sample : L4779-03
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 41 Sample Multiplier: 1

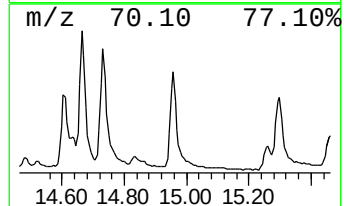
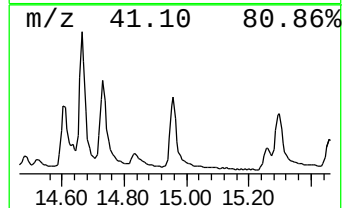
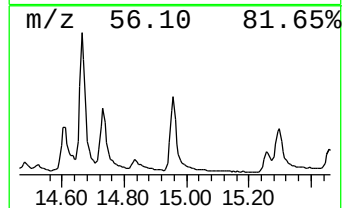
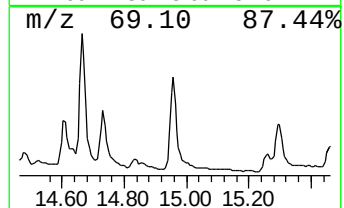
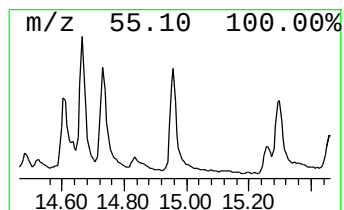
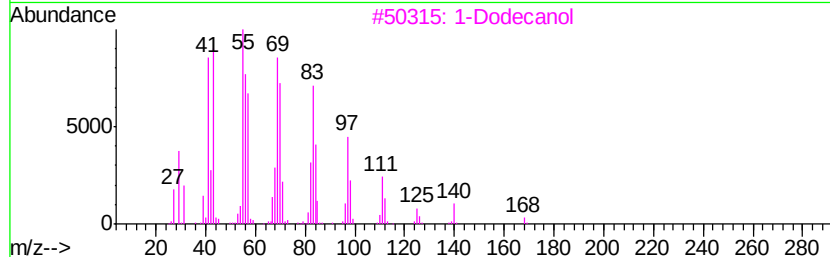
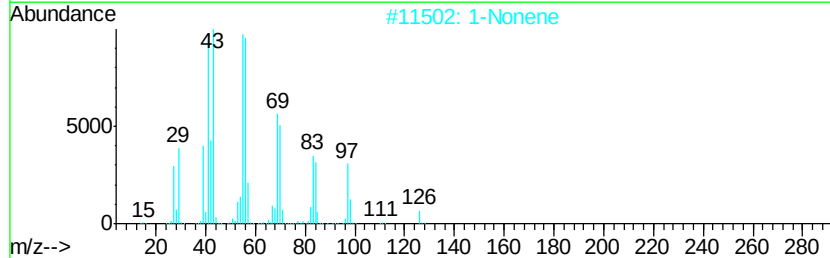
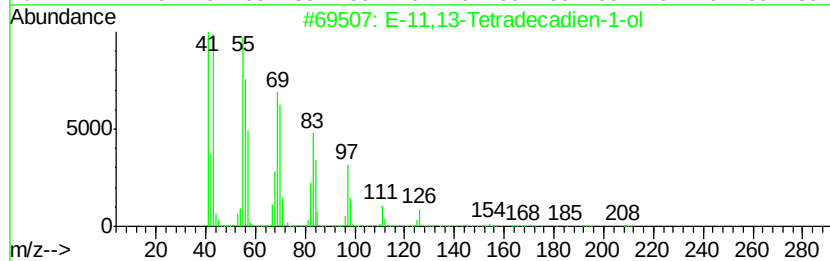
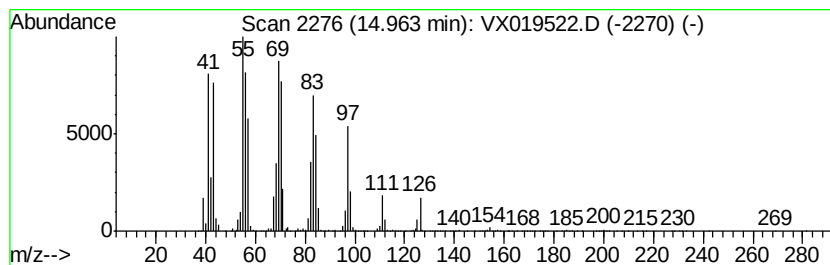
Instrument :
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 ClientSampleID :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
 Quant Title : SW846 8260

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

 Peak Number 8 E-11,13-Tetradecadien-1-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.96	46.84 ug/l	1143550	1,4-Dichlorobenzene-d4	12.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-11,13-Tetradecadien-1-ol	210	C14H26O	1000131-00-3	93
2	1-Nonene	126	C9H18	000124-11-8	91
3	1-Dodecanol	186	C12H26O	000112-53-8	91
4	1-Undecanol	172	C11H24O	000112-42-5	91
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112120\
Data File : VX019522.D
Acq On : 21 Nov 2020 03:10
Operator : JC/MD
Sample : L4779-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1623

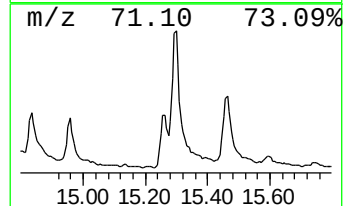
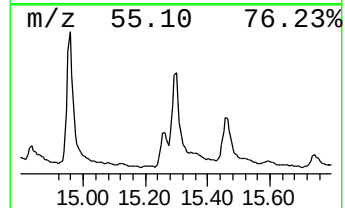
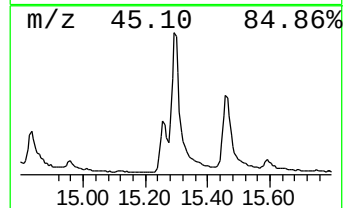
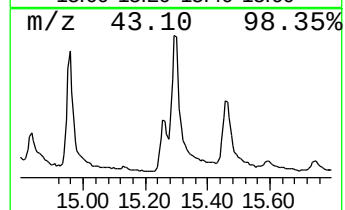
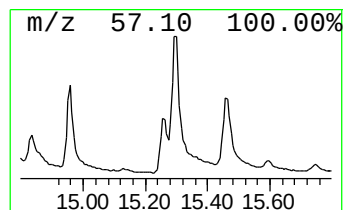
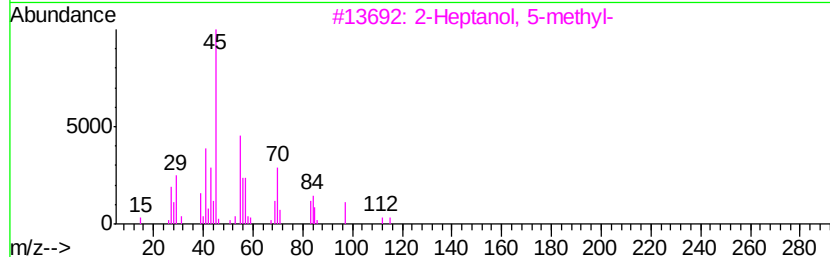
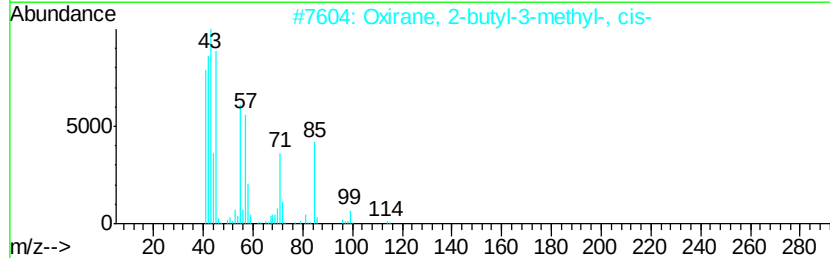
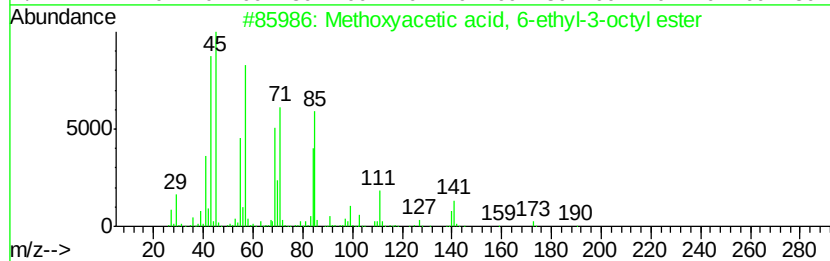
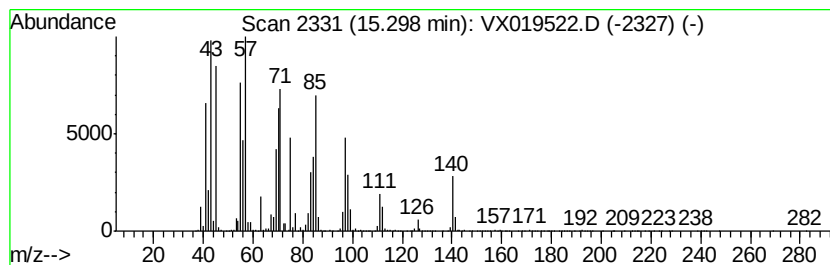
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Quant Title : SW846 8260

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

Peak Number 9 unknown15.30 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	67.01 ug/l	1636210	1,4-Dichlorobenzene-d4	12.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methoxyacetic acid, 6-ethyl-3-oc...	230	C13H26O3	1000282-69-8	49
2		Oxirane, 2-butyl-3-methyl-, cis-	114	C7H14O	056052-93-8	35
3		2-Heptanol, 5-methyl-	130	C8H18O	054630-50-1	22
4		Cyclodecane	140	C10H20	000293-96-9	22
5		Decane, 5-cyclohexyl-	224	C16H32	013151-76-3	22



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112120\
Data File : VX019522.D
Acq On : 21 Nov 2020 03:10
Operator : JC/MD
Sample : L4779-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 41 Sample Multiplier: 1

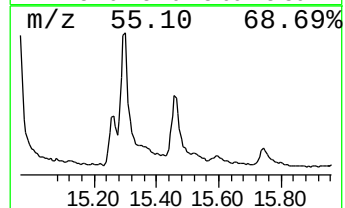
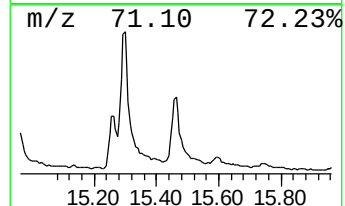
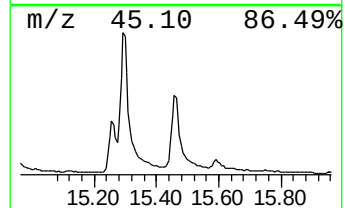
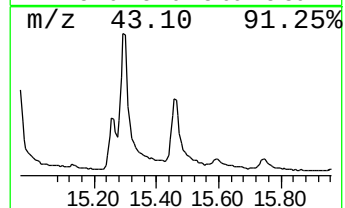
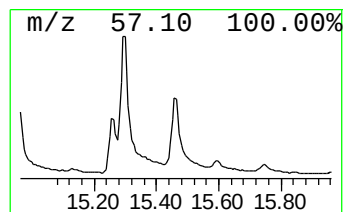
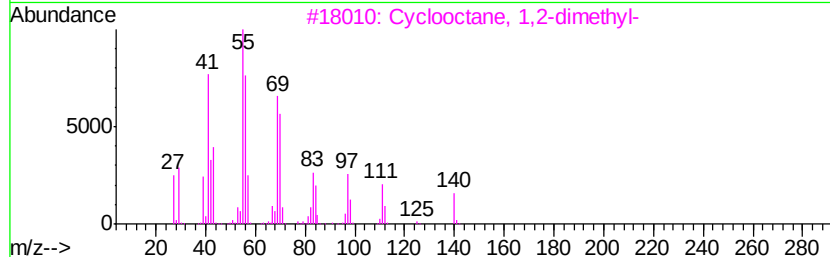
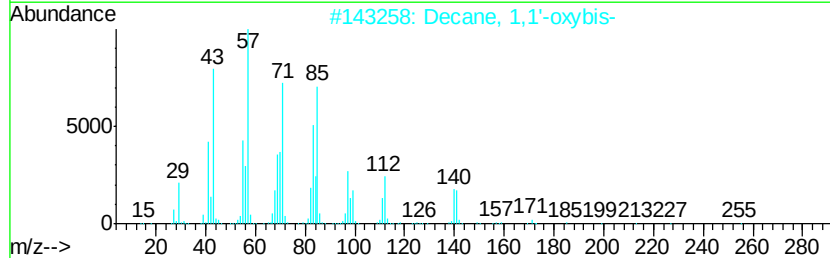
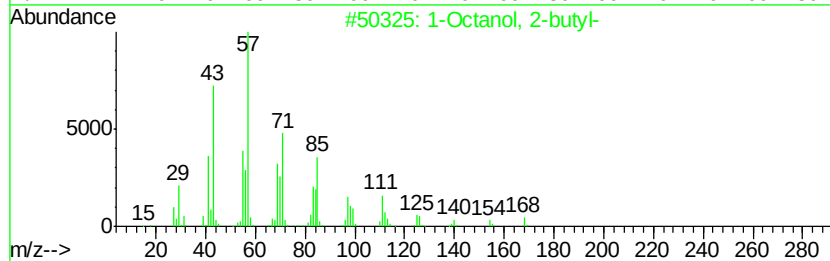
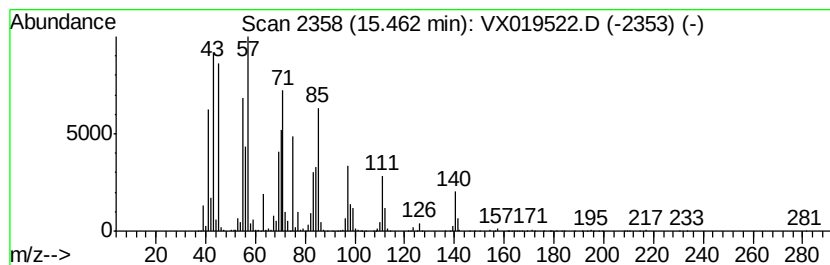
Instrument :
MSVOA_X
ClientSampled :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown15.46 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.46	35.94 ug/l	877404	1,4-Dichlorobenzene-d4	12.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	47
2	Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	43
3	Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	38
4	Cyclodecane	140	C10H20	000293-96-9	30
5	1-Tridecene	182	C13H26	002437-56-1	30



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
Data File : VX019522.D
Acq On : 21 Nov 2020 03:10
Operator : JC/MD
Sample : L4779-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.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
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1-Hexanol, 2-ethyl-	12.26	63.1	ug/l	1540910	4	12.06	1220810	50.0
1-Octanol, 2-methyl-	13.13	311.6	ug/l	7607210	4	12.06	1220810	50.0
Decane, 3-chloro-	13.93	227.0	ug/l	5543520	4	12.06	1220810	50.0
unknown14.60	14.60	56.2	ug/l	1373050	4	12.06	1220810	50.0
2-Methyl-1-undecanol	14.66	75.2	ug/l	1836650	4	12.06	1220810	50.0
unknown14.73	14.73	76.4	ug/l	1865900	4	12.06	1220810	50.0
E-11,13-Tetradeca...	14.96	46.8	ug/l	1143550	4	12.06	1220810	50.0
unknown15.30	15.30	67.0	ug/l	1636210	4	12.06	1220810	50.0
unknown15.46	15.46	35.9	ug/l	877404	4	12.06	1220810	50.0