

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX052020\
 Data File : VX016356.D
 Acq On : 20 May 2020 13:44
 Operator : JC/SP
 Sample : L2663-05 20X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1378

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\82X050420W.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	2.081	158	163	175	rBV	29829	47473	2.62%	0.367%
2	2.416	212	218	226	rVB	25109	41967	2.32%	0.324%
3	4.641	572	583	599	rBV2	9934	35972	1.99%	0.278%
4	5.464	706	718	731	rBV2	160320	459816	25.39%	3.550%
5	5.629	731	745	762	rVB	288559	807443	44.59%	6.235%
6	6.031	800	811	827	rBV	177356	472316	26.08%	3.647%
7	6.830	931	942	956	rBV	464044	1082341	59.77%	8.357%
8	8.695	1241	1248	1266	rBV	992106	1526871	84.32%	11.789%
9	10.098	1472	1478	1494	rVB	996553	1360563	75.14%	10.505%
10	11.122	1640	1646	1655	rVB	878668	1083846	59.85%	8.369%
11	11.518	1706	1711	1718	rVB	33770	42850	2.37%	0.331%
12	11.969	1781	1785	1789	rVB	34014	40962	2.26%	0.316%
13	12.061	1795	1800	1808	rBV	1104144	1366824	75.48%	10.554%
14	12.256	1828	1832	1844	rBV	39709	75609	4.18%	0.584%
15	12.896	1932	1937	1942	rBV	55669	66990	3.70%	0.517%
16	13.012	1951	1956	1966	rBV	62897	107228	5.92%	0.828%
17	13.109	1968	1972	1974	rBV	73896	98429	5.44%	0.760%
18	13.140	1974	1977	1993	rVB	203167	352630	19.47%	2.723%
19	13.304	2001	2004	2013	rVB4	17141	28564	1.58%	0.221%
20	13.463	2025	2030	2055	rBV	1194193	1810822	100.00%	13.982%
21	13.725	2069	2073	2077	rBV	46593	58796	3.25%	0.454%
22	13.792	2077	2084	2096	rVV3	94826	257356	14.21%	1.987%
23	13.902	2097	2102	2104	rVV	88316	127444	7.04%	0.984%
24	13.932	2104	2107	2129	rVB	184200	373954	20.65%	2.887%
25	14.237	2152	2157	2176	rBV	410007	769967	42.52%	5.945%
26	14.493	2194	2199	2202	rBV	58053	87540	4.83%	0.676%
27	14.530	2202	2205	2208	rVV2	31841	55058	3.04%	0.425%
28	14.560	2208	2210	2214	rVB	27542	30714	1.70%	0.237%
29	14.676	2220	2229	2233	rBV5	52388	112319	6.20%	0.867%
30	14.798	2245	2249	2251	rBV	35470	41280	2.28%	0.319%
31	14.822	2251	2253	2260	rVB2	17935	27568	1.52%	0.213%
32	14.963	2272	2276	2292	rVB9	13498	41749	2.31%	0.322%
33	15.292	2327	2330	2339	rVB8	13567	29895	1.65%	0.231%
34	15.536	2365	2370	2375	rVB3	18047	27995	1.55%	0.216%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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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

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Title : SW846 8260

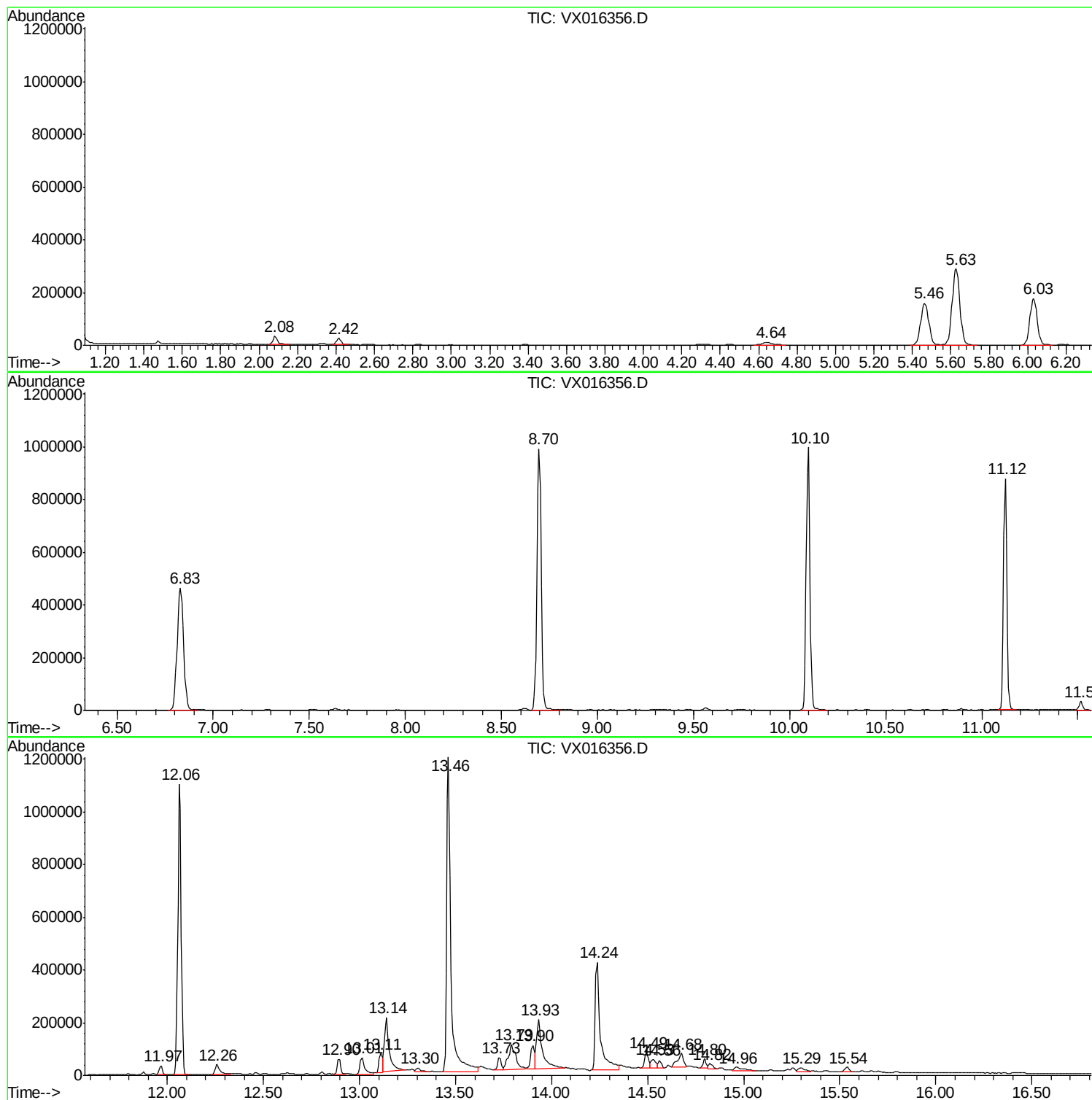
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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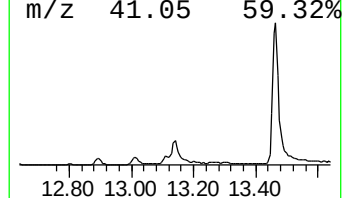
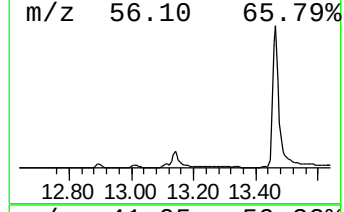
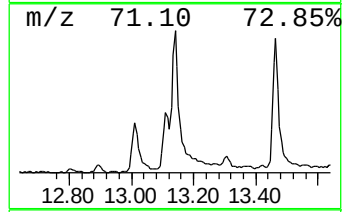
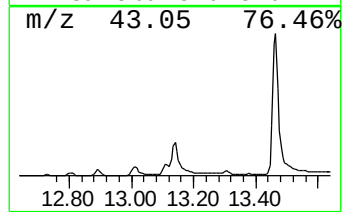
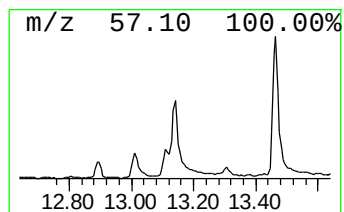
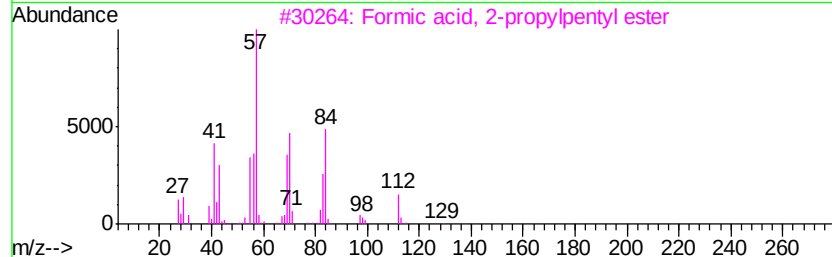
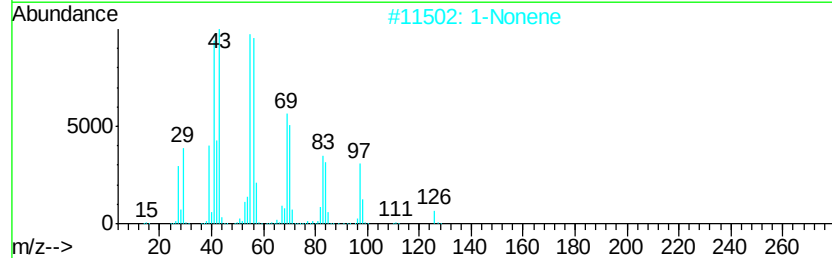
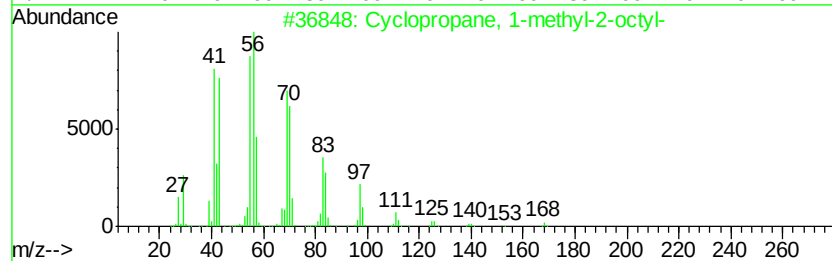
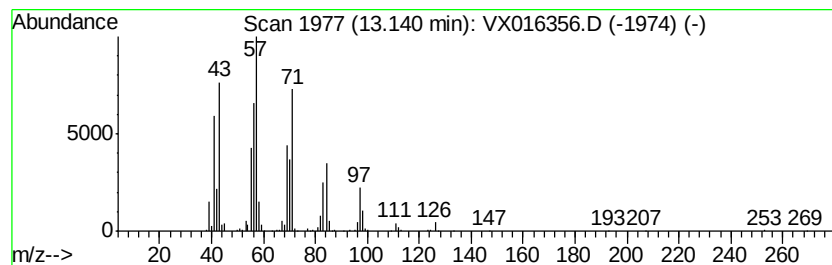
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
 Quant Title : SW846 8260

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

 Peak Number 1 unknown13.14 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.14	12.90 ug/l	352630	1,4-Dichlorobenzene-d4	12.06		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	47
2		1-Nonene	126	C9H18	000124-11-8	46
3		Formic acid, 2-propylpentyl ester	158	C9H18O2	1000368-74-8	43
4		Cyclobutane, 1,2-diethyl-, trans-	112	C8H16	019341-98-1	38
5		1-Undecene	154	C11H22	000821-95-4	38



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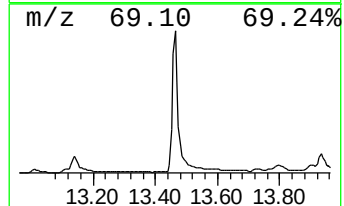
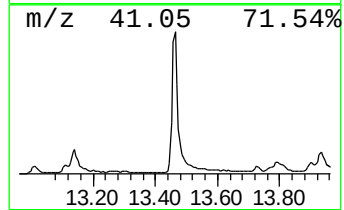
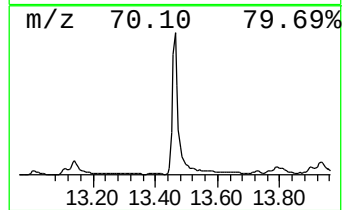
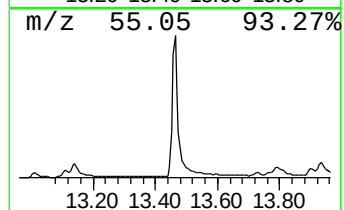
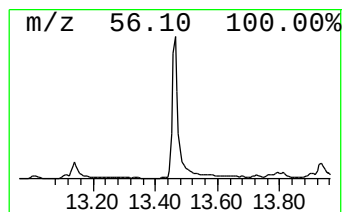
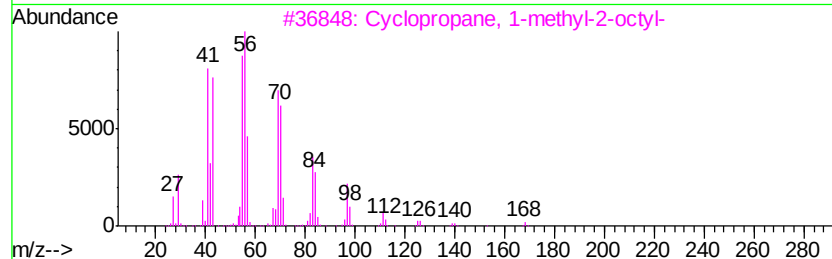
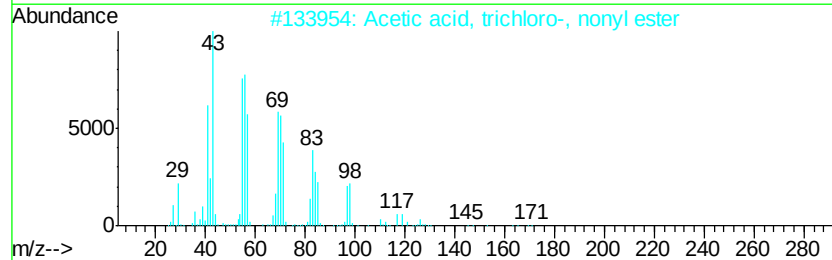
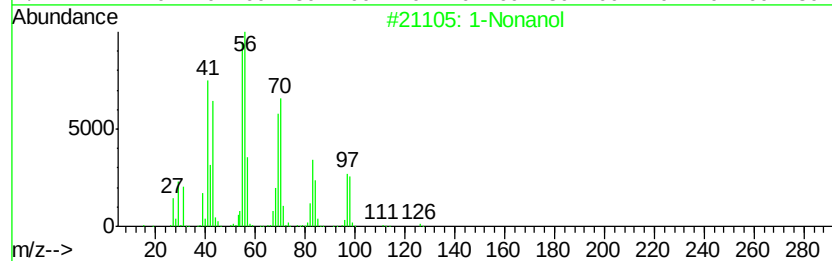
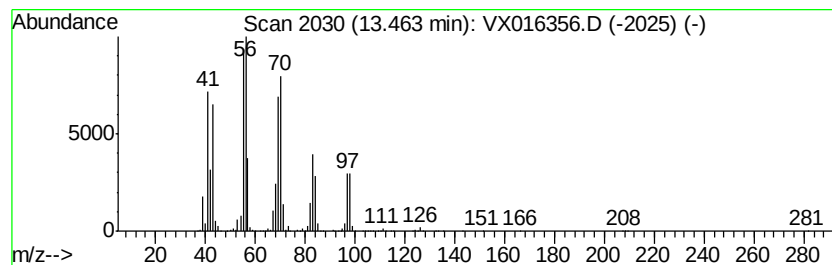
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.46	66.24 ug/l	1810820	1,4-Dichlorobenzene-d4	12.06		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol		144	C9H20O	000143-08-8	91
2	Acetic acid, trichloro-, nonyl e...		288	C11H19Cl3O2	065611-32-7	90
3	Cyclopropane, 1-methyl-2-octyl-		168	C12H24	037617-26-8	86
4	Cyclopropane, pentyl-		112	C8H16	002511-91-3	76
5	Cycloheptane		98	C7H14	000291-64-5	74



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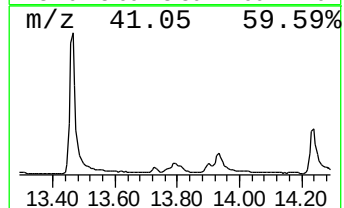
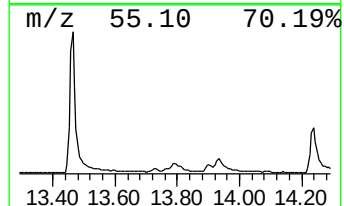
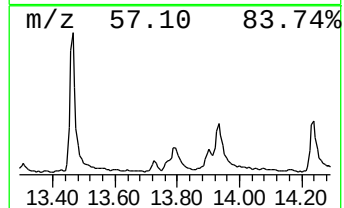
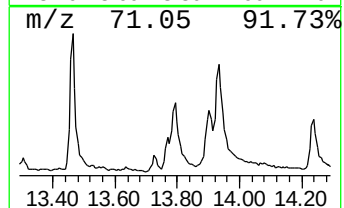
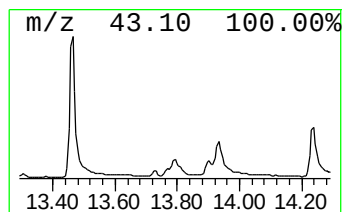
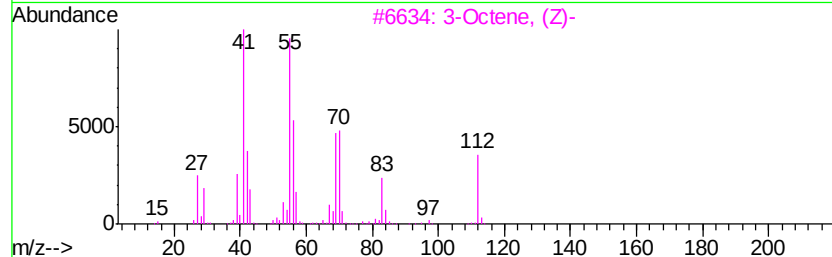
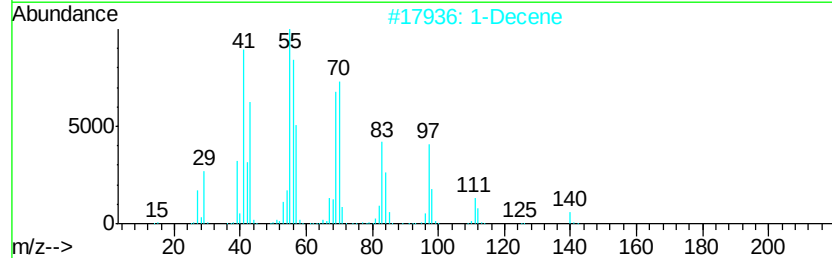
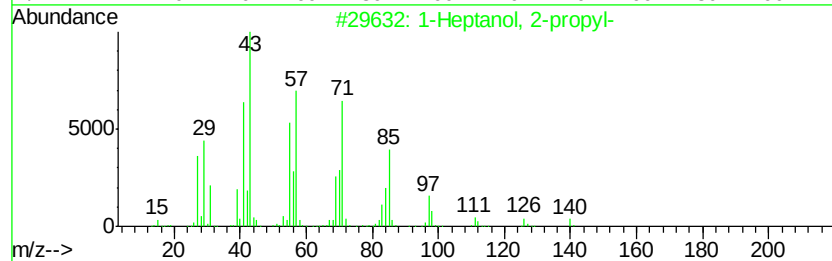
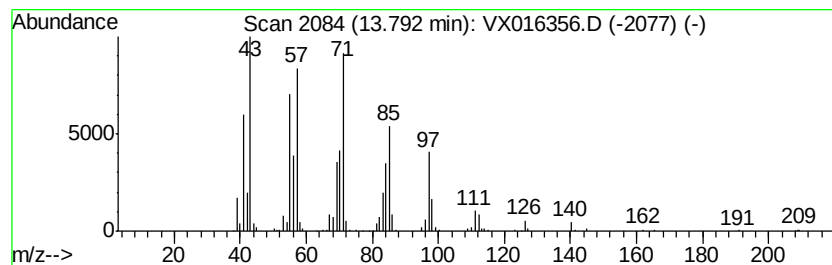
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Heptanol, 2-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.79	9.41 ug/l	257356	1,4-Dichlorobenzene-d4	12.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	72
2	1-Decene	140	C10H20	000872-05-9	41
3	3-Octene, (Z)-	112	C8H16	014850-22-7	38
4	Octane	114	C8H18	000111-65-9	38
5	Cycloheptane, methyl-	112	C8H16	004126-78-7	38



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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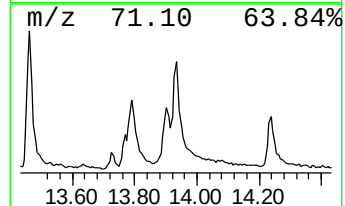
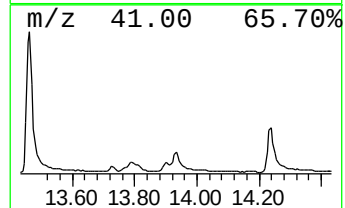
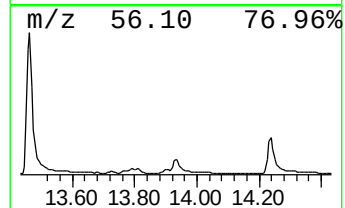
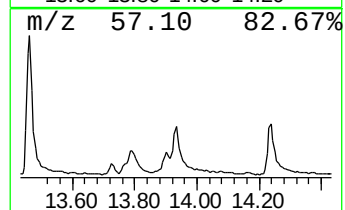
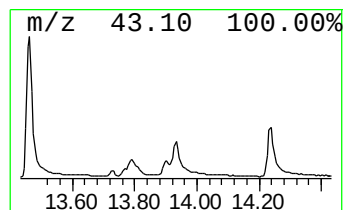
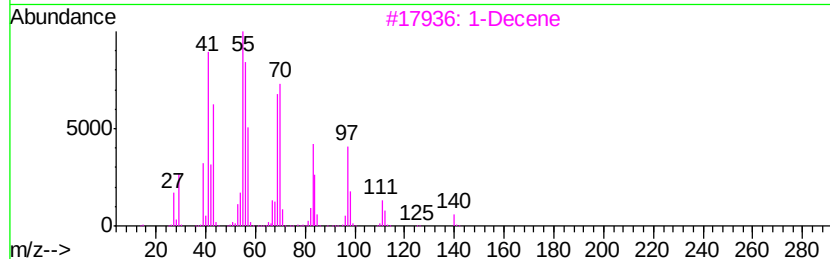
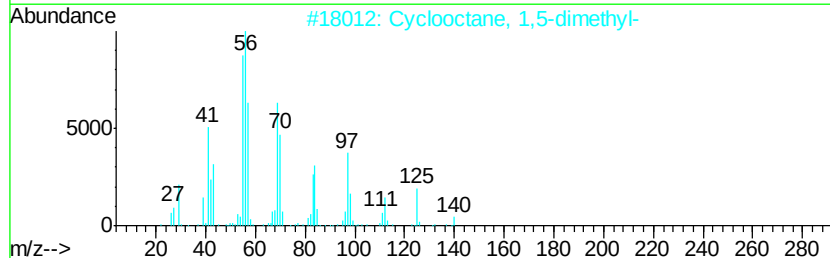
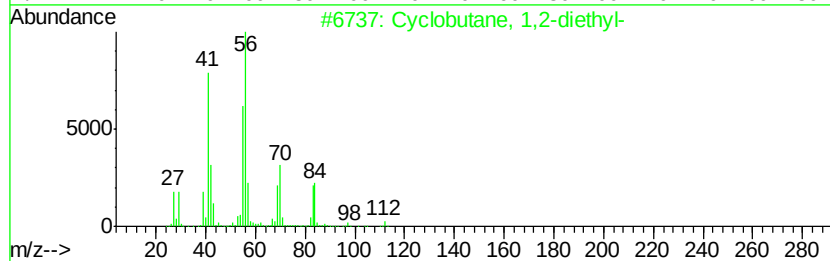
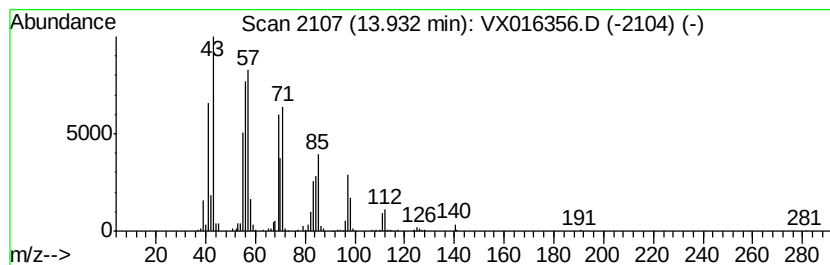
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Quant Title : SW846 8260

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

Peak Number 4 Cyclobutane, 1,2-diethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	13.68 ug/l	373954	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclobutane, 1,2-diethyl-	112	C8H16	061141-83-1	53
2		Cyclooctane, 1,5-dimethyl-	140	C10H20	021328-57-4	53
3		1-Decene	140	C10H20	000872-05-9	50
4		Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	49
5		Cyclobutane, 1-butyl-2-ethyl-	140	C10H20	1000150-67-3	43



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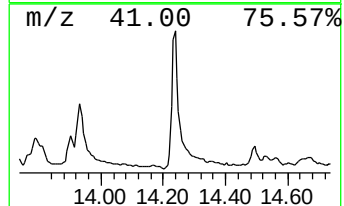
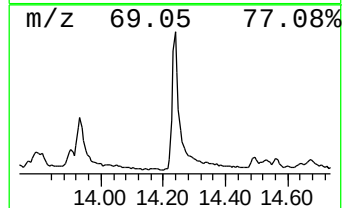
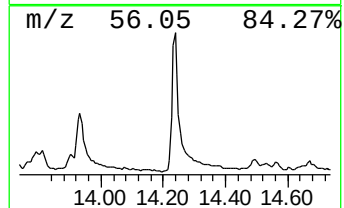
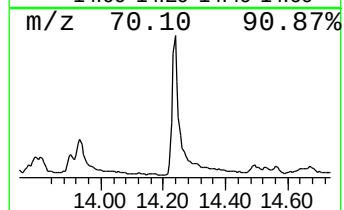
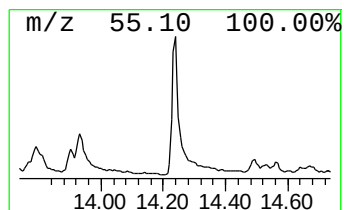
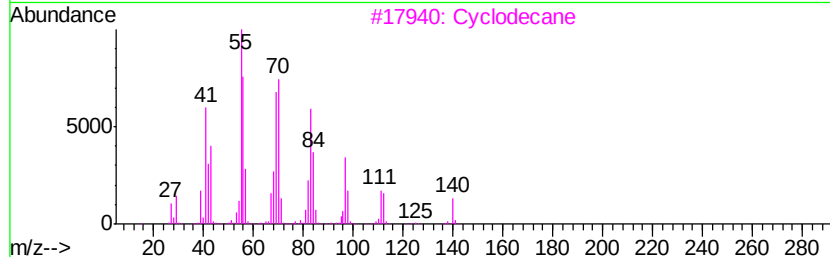
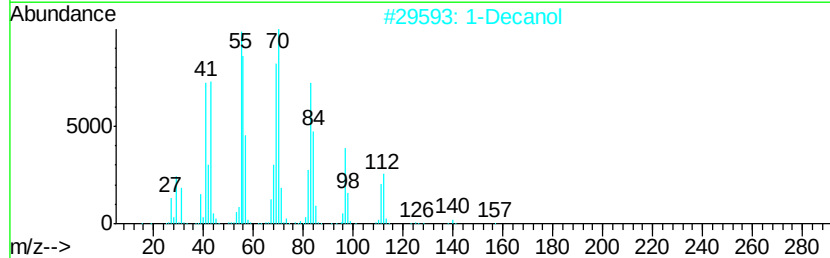
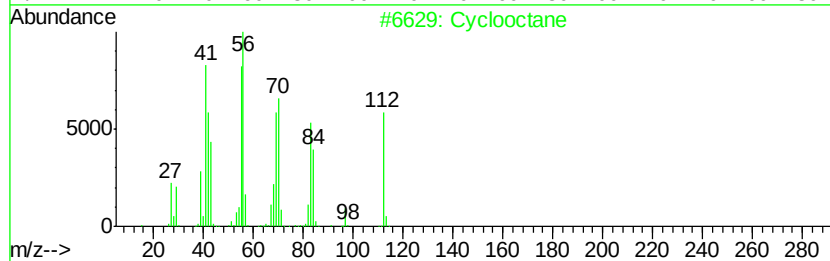
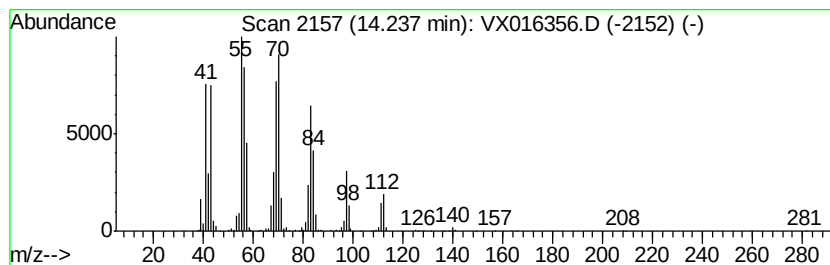
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclooctane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	28.17 ug/l	769967	1,4-Dichlorobenzene-d4	12.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclooctane	112	C8H16	000292-64-8	91
2		1-Decanol	158	C10H22O	000112-30-1	91
3		Cyclodecane	140	C10H20	000293-96-9	90
4		Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	86
5		Dichloroacetic acid, decyl ester	268	C12H22Cl2O2	083005-00-9	64



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown13.14	13.14	12.9	ug/l	352630	4	12.06	1366820	50.0
1-Nonanol	13.46	66.2	ug/l	1810820	4	12.06	1366820	50.0
1-Heptanol, 2-pro...	13.79	9.4	ug/l	257356	4	12.06	1366820	50.0
Cyclobutane, 1,2-...	13.93	13.7	ug/l	373954	4	12.06	1366820	50.0
Cyclooctane	14.24	28.2	ug/l	769967	4	12.06	1366820	50.0