

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092618\
 Data File : VU027202.D
 Acq On : 27 Sep 2018 01:34
 Operator : MD/SY
 Sample : J5048-05
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DMW-35A-SEP18

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_U\METHOD\82U092218W.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	2.009	254	260	270	rVB	14523	20126	2.40%	0.308%
2	2.321	348	357	381	rVB	164494	263378	31.44%	4.026%
3	2.444	384	395	419	rVV	185367	315466	37.65%	4.822%
4	4.228	923	950	980	rBV3	40099	136189	16.26%	2.082%
5	4.884	1137	1154	1171	rBV	113420	257030	30.68%	3.929%
6	4.984	1172	1185	1210	rVB	159594	349466	41.71%	5.342%
7	5.312	1272	1287	1317	rBV	142389	339513	40.52%	5.190%
8	5.887	1450	1466	1488	rBV	243017	481498	57.47%	7.360%
9	6.189	1546	1560	1583	rBV	134785	267612	31.94%	4.091%
10	7.566	1973	1988	2004	rBV	451883	794228	94.80%	12.140%
11	8.228	2182	2194	2228	rVB	214068	384121	45.85%	5.872%
12	8.537	2280	2290	2312	rBV4	7205	28469	3.40%	0.435%
13	8.980	2416	2428	2450	rBV3	20979	79232	9.46%	1.211%
14	9.090	2451	2462	2487	rVB	351437	599650	71.57%	9.166%
15	9.688	2639	2648	2664	rBV2	10601	21518	2.57%	0.329%
16	10.308	2821	2841	2872	rBV	333893	584850	69.81%	8.940%
17	11.025	3056	3064	3083	rBV3	7901	14107	1.68%	0.216%
18	11.485	3190	3207	3239	rBV2	436415	837797	100.00%	12.806%
19	12.221	3429	3436	3450	rBV5	7619	13369	1.60%	0.204%
20	12.556	3531	3540	3581	rBV	120604	325591	38.86%	4.977%
21	13.575	3849	3857	3891	rBV	75181	207862	24.81%	3.177%
22	15.234	4363	4373	4390	rBV4	38884	65784	7.85%	1.006%
23	16.105	4634	4644	4669	rVB3	57542	100882	12.04%	1.542%
24	16.928	4891	4900	4918	rBV3	32441	54384	6.49%	0.831%

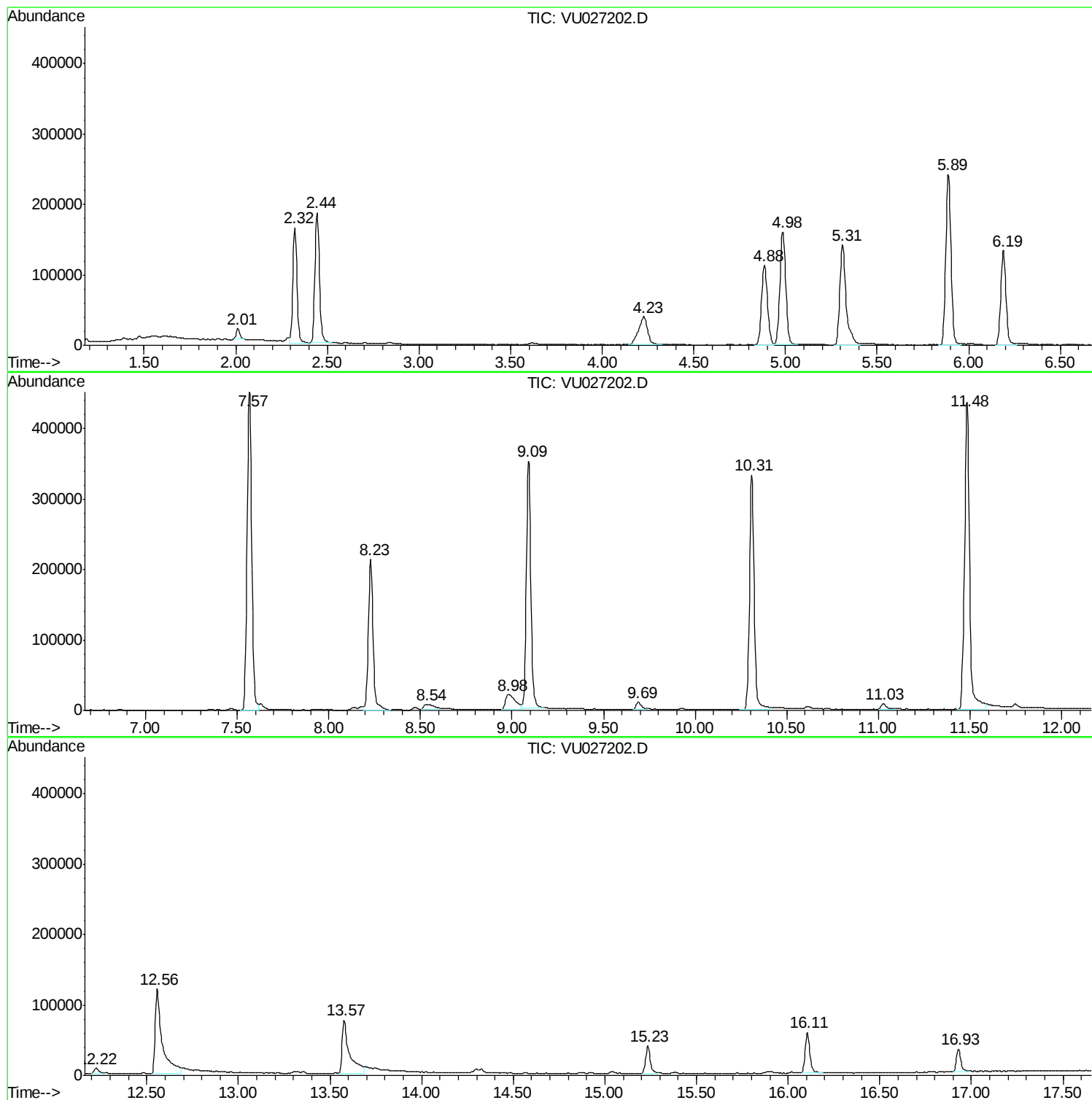
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU0922618\
Data File : VU027202.D
Acq On : 27 Sep 2018 01:34
Operator : MD/SY
Sample : J5048-05
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DMW-35A-SEP18

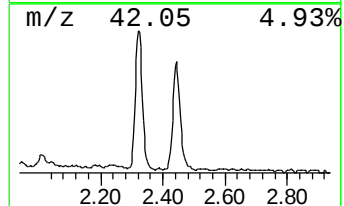
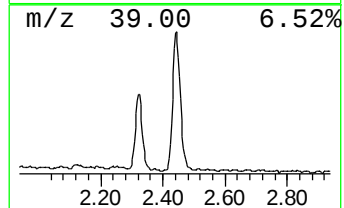
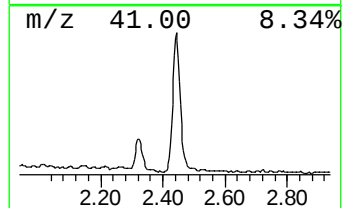
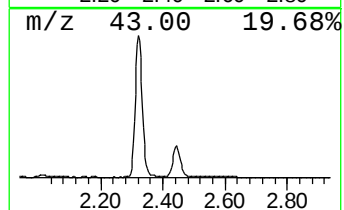
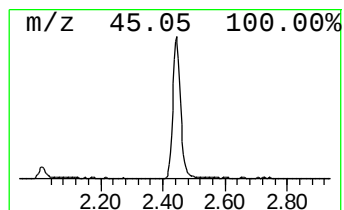
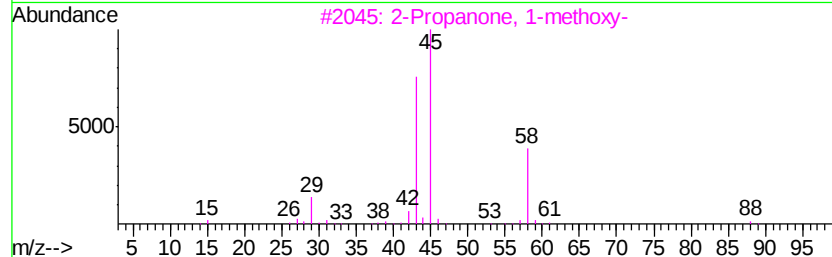
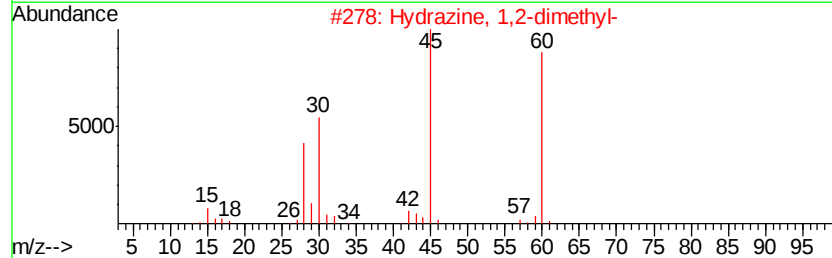
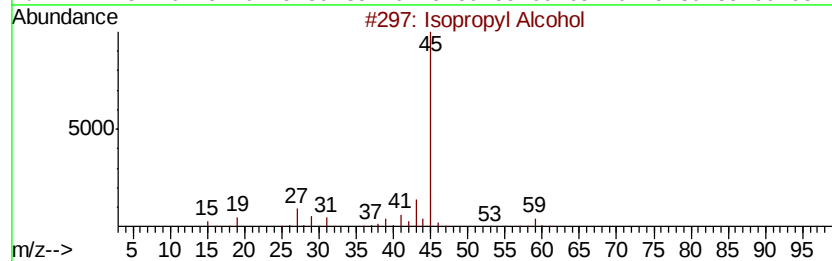
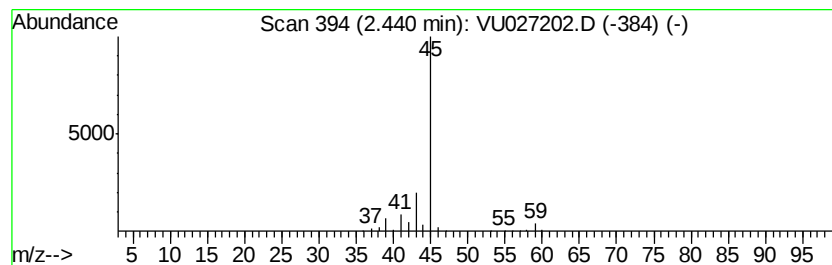
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	45.14 ug/l	315466	Pentafluorobenzene	4.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3		2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4
4		Hydrazine, ethyl-	60	C2H8N2	000624-80-6	4
5		Formamide	45	CH3NO	000075-12-7	4



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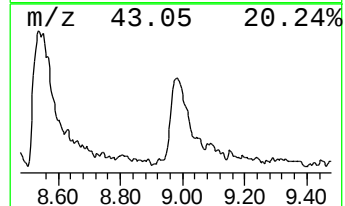
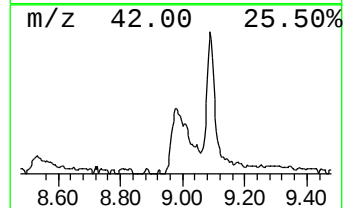
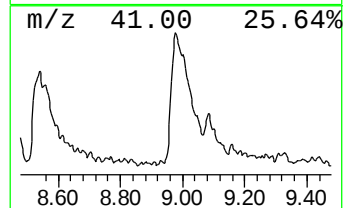
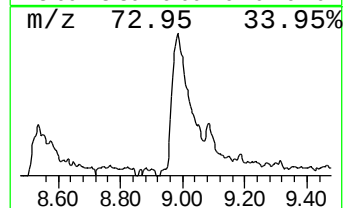
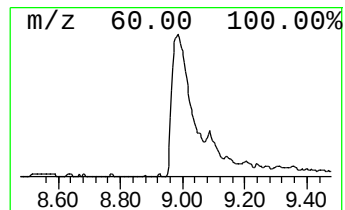
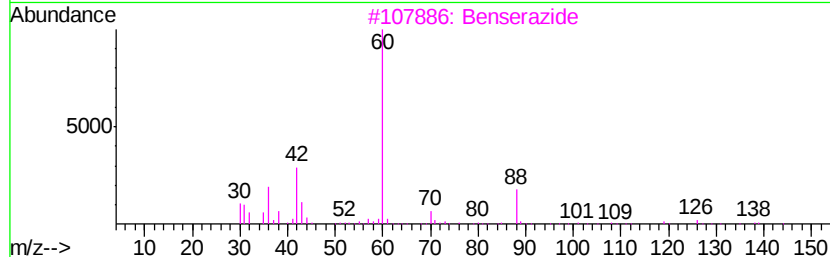
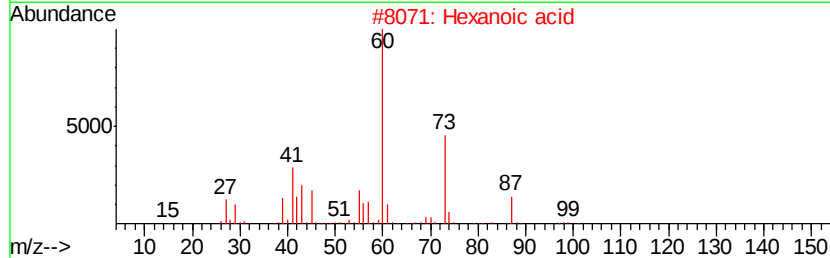
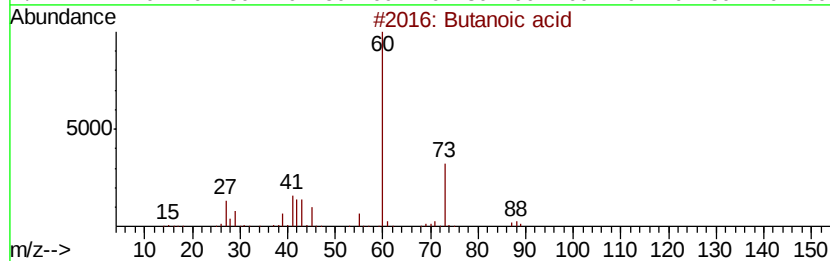
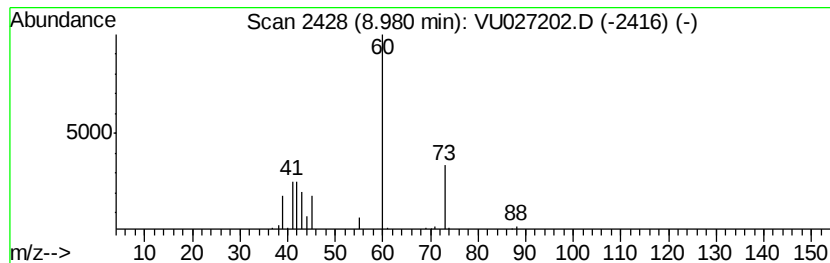
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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

Peak Number 2 Butanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.98	6.61 ug/l	79232	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid	88	C4H8O2	000107-92-6	80
2		Hexanoic acid	116	C6H12O2	000142-62-1	9
3		Benserazide	257	C10H15N3O5	000322-35-0	9
4		CH3ON(CH3)2	75	C3H9NO	005669-39-6	9
5		4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9



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ALS Vial : 43 Sample Multiplier: 1

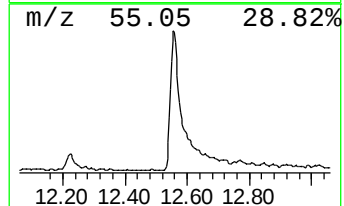
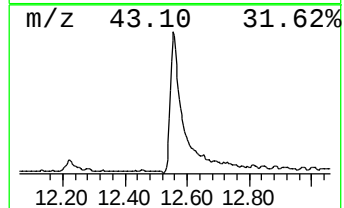
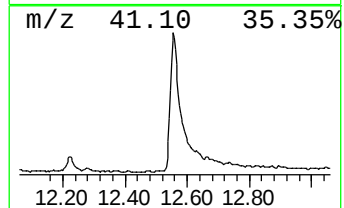
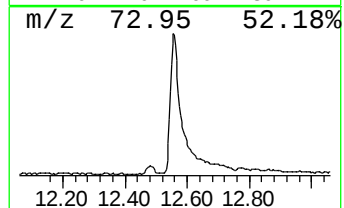
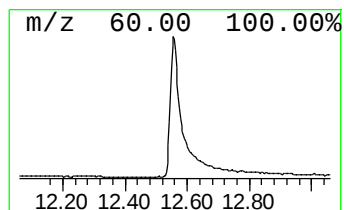
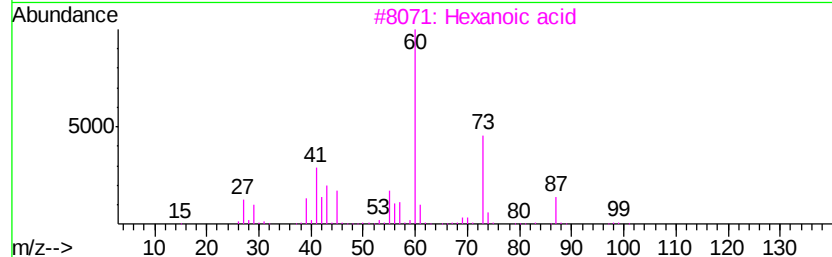
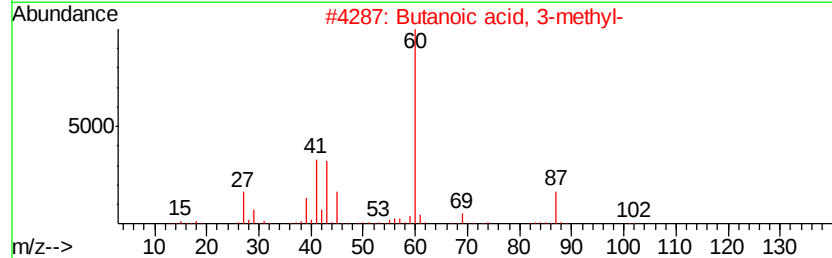
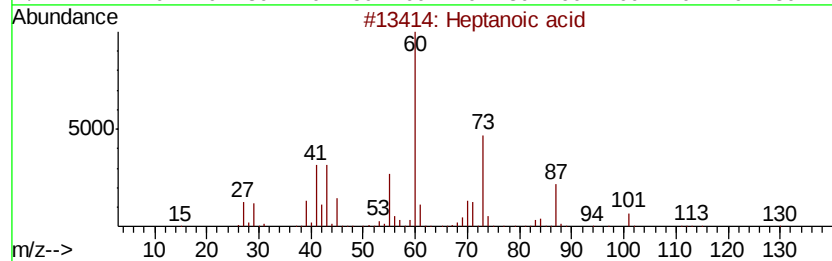
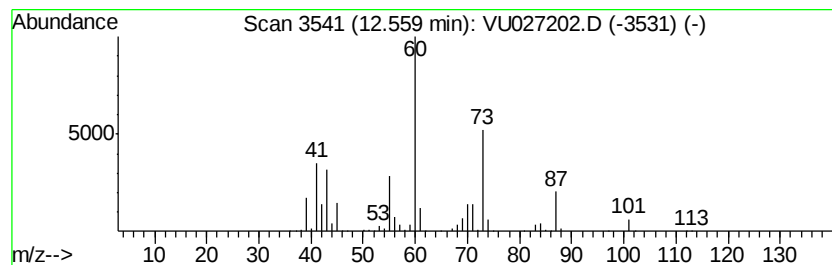
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	19.43 ug/l	325591	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptanoic acid	130 C7H14O2	000111-14-8	91
2	Butanoic acid, 3-methyl-	102 C5H10O2	000503-74-2	64
3	Hexanoic acid	116 C6H12O2	000142-62-1	59
4	Pentanoic acid	102 C5H10O2	000109-52-4	58
5	Pentanoic acid, 3-methyl-	116 C6H12O2	000105-43-1	45



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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DMW-35A-SEP18

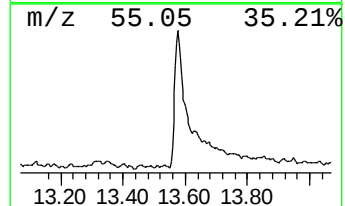
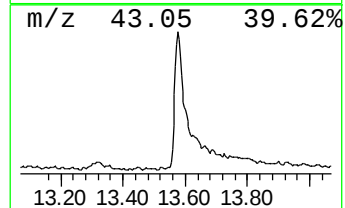
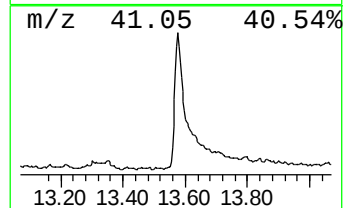
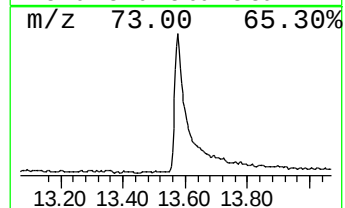
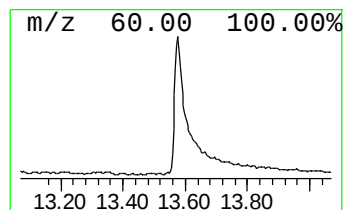
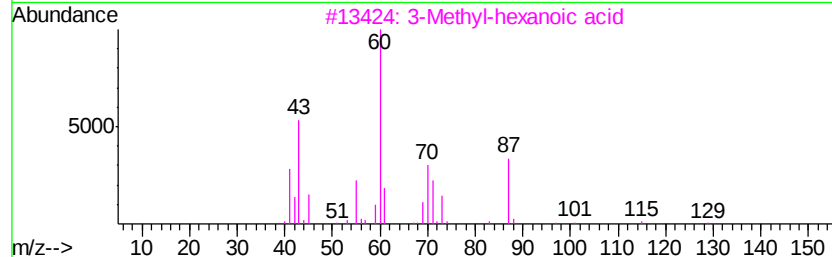
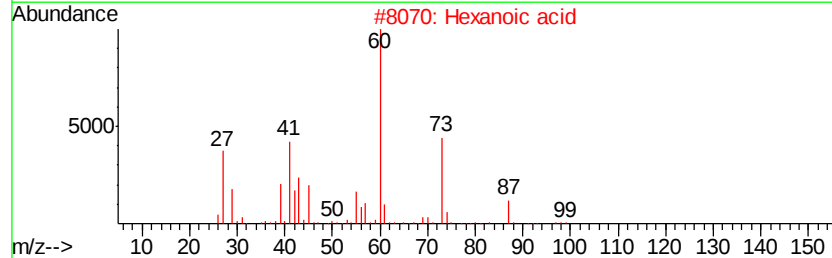
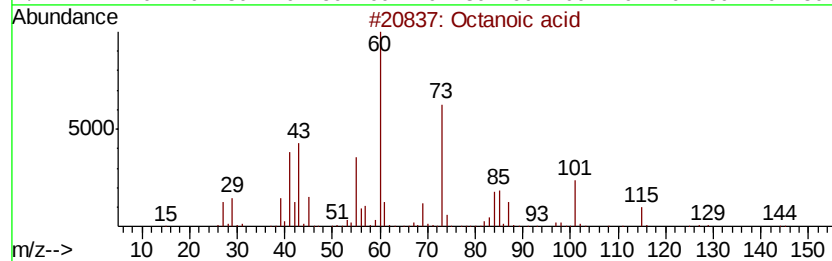
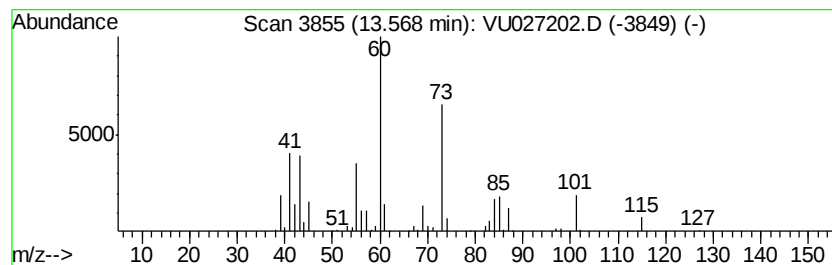
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Quant Title : SW846 8260

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

Peak Number 4 Octanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	12.41 ug/l	207862	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanoic acid	144	C8H16O2	000124-07-2	91
2		Hexanoic acid	116	C6H12O2	000142-62-1	53
3		3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	50
4		Pentanoic acid	102	C5H10O2	000109-52-4	50
5		Heptanoic acid	130	C7H14O2	000111-14-8	45



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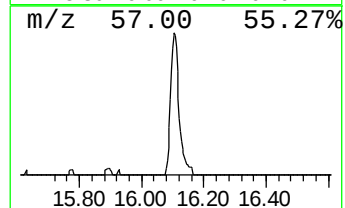
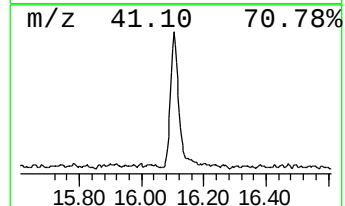
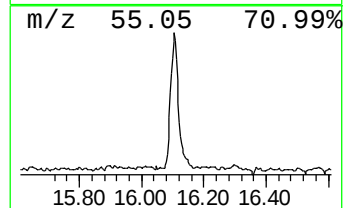
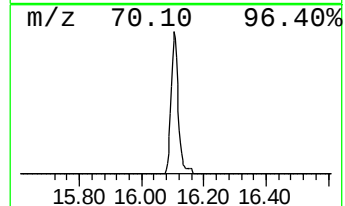
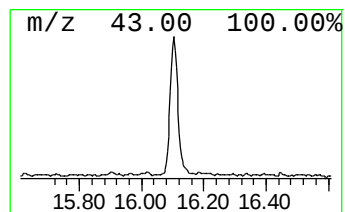
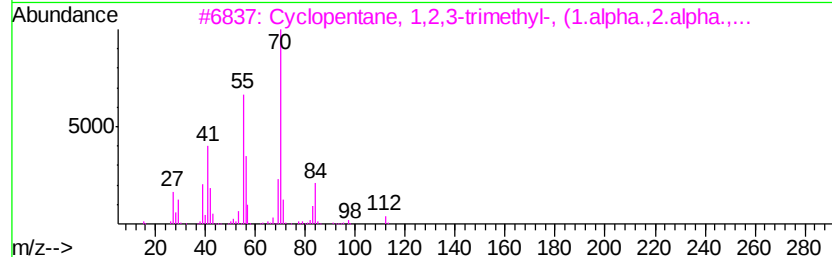
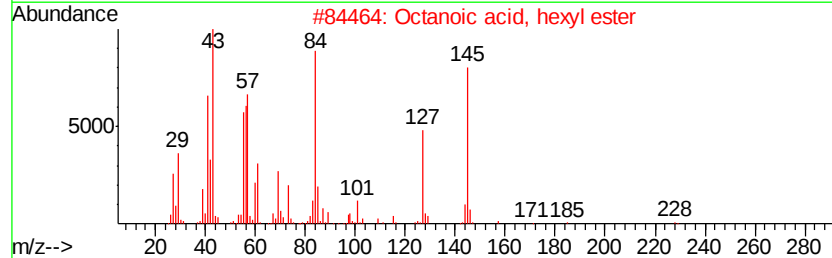
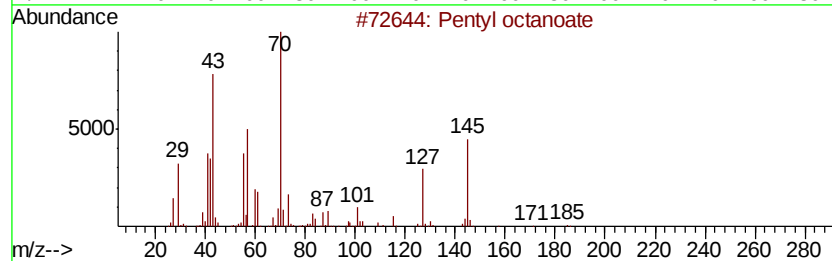
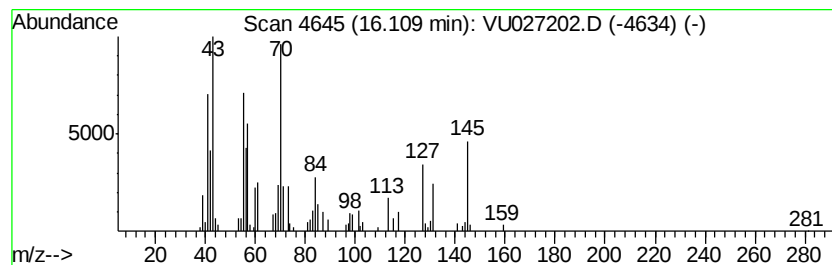
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentyl octanoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	6.02 ug/l	100882	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pentyl octanoate	214 C13H26O2	000638-25-5 76
2		Octanoic acid, hexyl ester	228 C14H28O2	001117-55-1 35
3		Cyclopentane, 1,2,3-trimethyl-, ...	112 C8H16	002613-69-6 35
4		1-Propanamine, N-nitroso-N-propyl-	130 C6H14N2O	000621-64-7 27
5		1-Butanol, 3-methyl-, acetate	130 C7H14O2	000123-92-2 27



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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
Isopropyl Alcohol	2.44	45.1	ug/l	315466	1	4.99	349466	50.0
Butanoic acid	8.98	6.6	ug/l	79232	3	9.09	599650	50.0
Heptanoic acid	12.56	19.4	ug/l	325591	4	11.48	837797	50.0
Octanoic acid	13.57	12.4	ug/l	207862	4	11.48	837797	50.0
Pentyl octanoate	16.11	6.0	ug/l	100882	4	11.48	837797	50.0