

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092618\
 Data File : VU027201.D
 Acq On : 27 Sep 2018 01:11
 Operator : MD/SY
 Sample : J5048-04
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 MW-36-SEP18

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_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	2.286	333	346	367	rVB2	1293159	2131033	11.54%	4.079%
2	3.450	690	708	729	rVB	117680	258723	1.40%	0.495%
3	4.228	924	950	976	rBV	7758224	18465980	100.00%	35.348%
4	4.919	1138	1165	1179	rBV	1740761	4408293	23.87%	8.439%
5	4.987	1179	1186	1202	rVB	157121	324462	1.76%	0.621%
6	5.311	1271	1287	1308	rBV	139542	302933	1.64%	0.580%
7	5.887	1451	1466	1483	rBV	239198	468508	2.54%	0.897%
8	6.189	1542	1560	1576	rBV	6158523	11569536	62.65%	22.147%
9	7.565	1974	1988	2001	rBV	453404	790191	4.28%	1.513%
10	8.231	2180	2195	2231	rVB	3622447	6282332	34.02%	12.026%
11	8.977	2413	2427	2451	rBV	191989	579117	3.14%	1.109%
12	9.089	2452	2462	2486	rVB	368950	649520	3.52%	1.243%
13	9.372	2539	2550	2565	rBV	267012	436866	2.37%	0.836%
14	10.305	2825	2840	2884	rBV2	498891	1083178	5.87%	2.073%
15	11.485	3192	3207	3229	rBV	1002367	1928740	10.44%	3.692%
16	11.880	3319	3330	3345	rVB	153876	247862	1.34%	0.474%
17	12.565	3531	3543	3582	rBV	499935	1082737	5.86%	2.073%
18	13.575	3849	3857	3888	rBV	77929	210791	1.14%	0.404%
19	13.742	3899	3909	3926	rVB	118688	193762	1.05%	0.371%
20	15.234	4361	4373	4401	rBV4	305839	507514	2.75%	0.972%
21	16.102	4632	4643	4668	rBV2	191931	318132	1.72%	0.609%

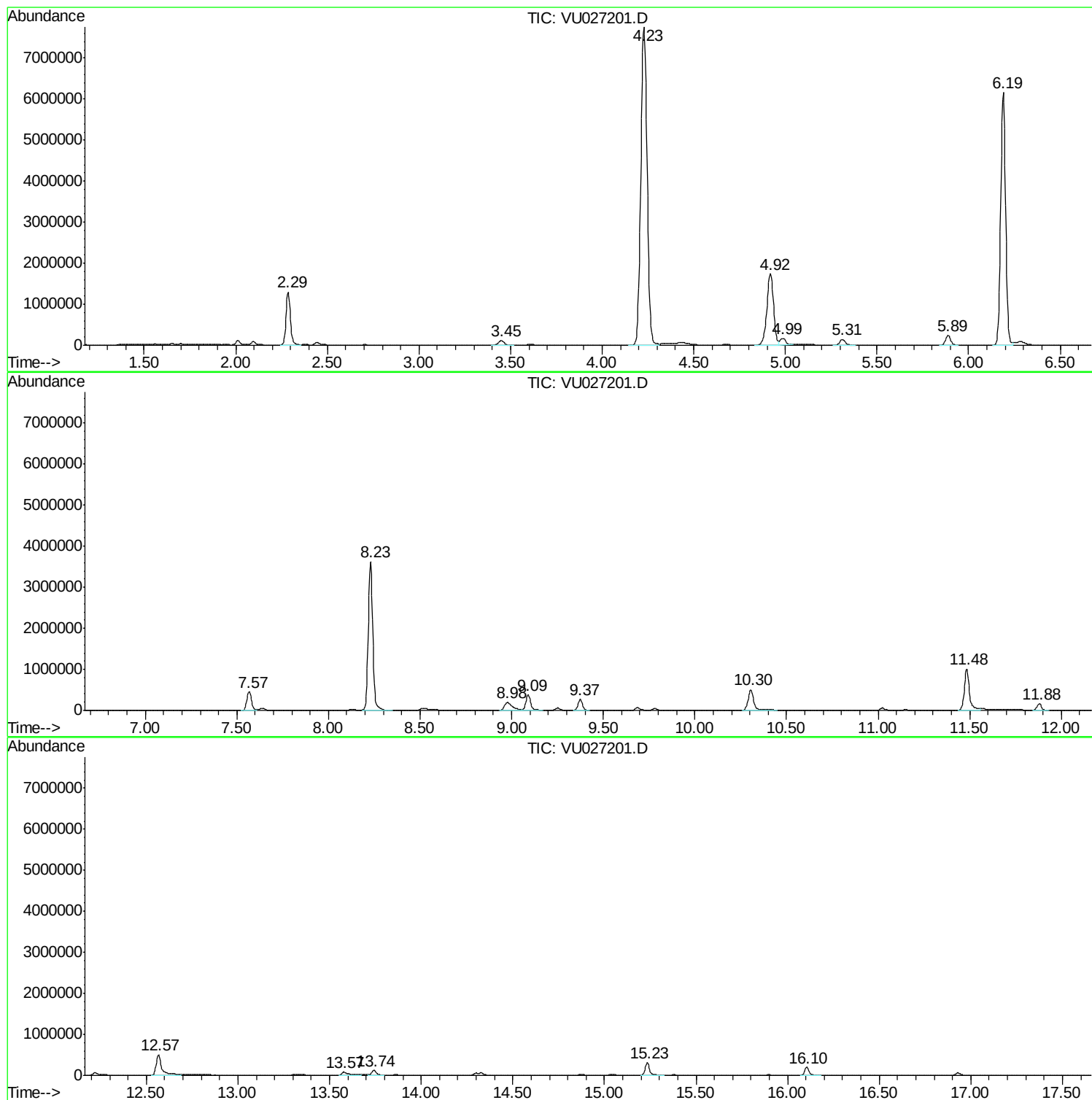
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ALS Vial : 42 Sample Multiplier: 1

Instrument :
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ClientSampled :
MW-36-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



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Instrument :
MSVOA_U
ClientSampleId :
MW-36-SEP18

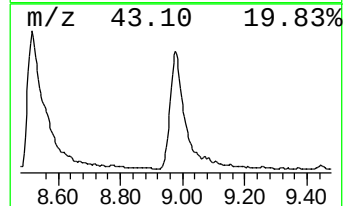
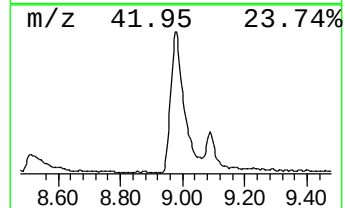
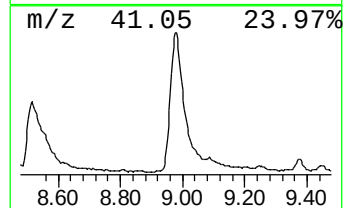
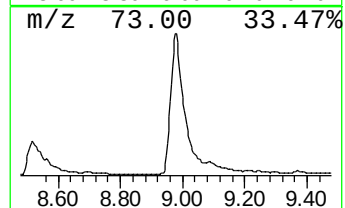
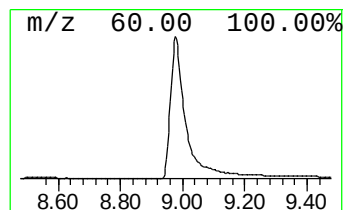
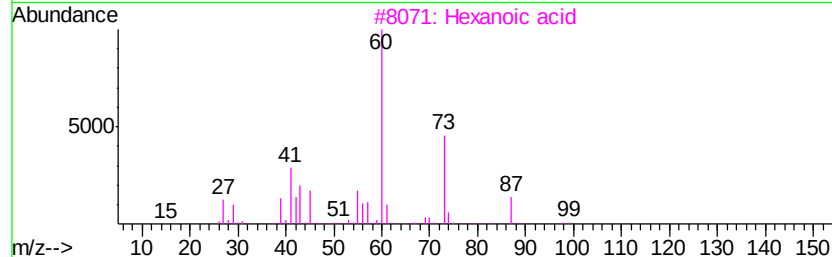
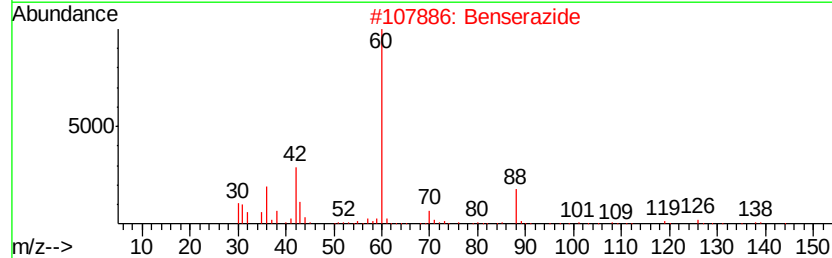
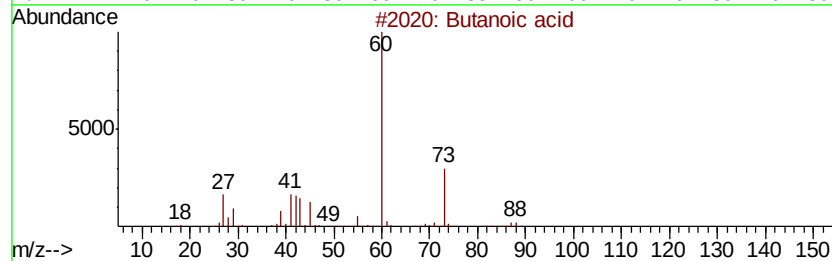
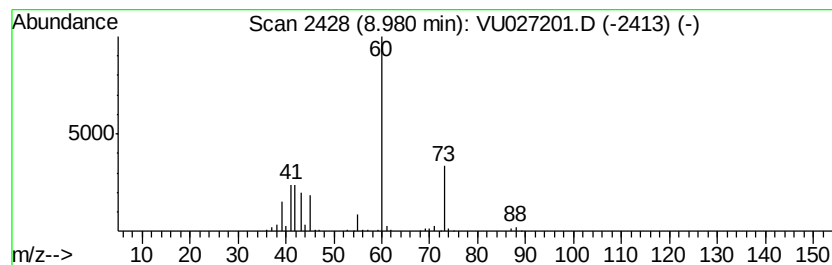
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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

Peak Number 1 Butanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.98	44.58 ug/l	579117	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid	88	C4H8O2	000107-92-6	90
2		Benserazide	257	C10H15N3O5	000322-35-0	9
3		Hexanoic acid	116	C6H12O2	000142-62-1	9
4		Pentanoic acid	102	C5H10O2	000109-52-4	9
5		4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9



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ALS Vial : 42 Sample Multiplier: 1

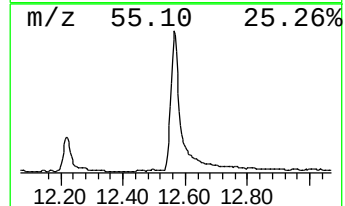
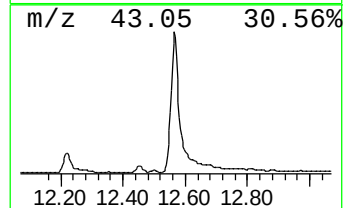
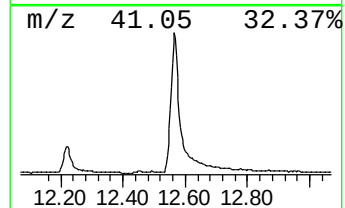
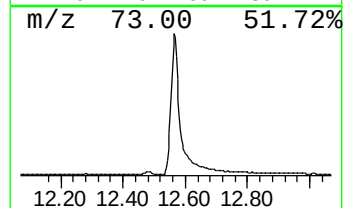
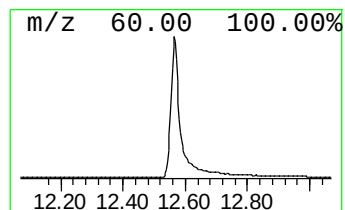
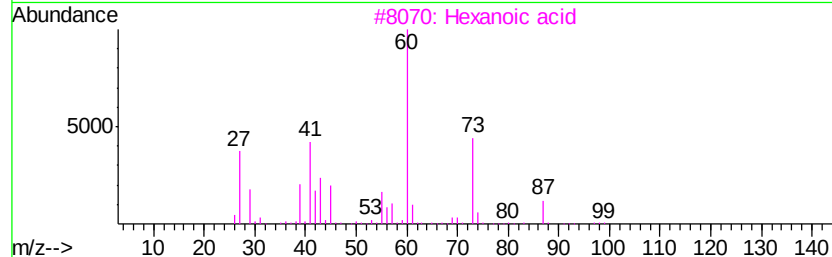
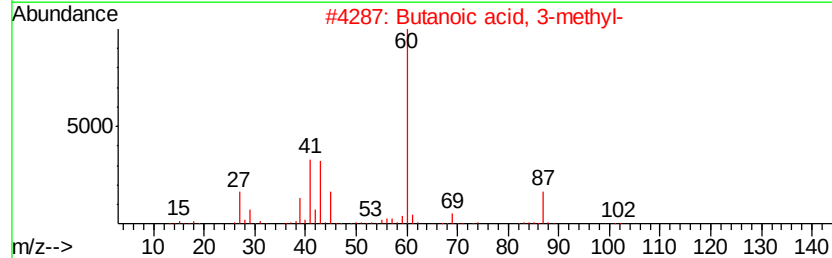
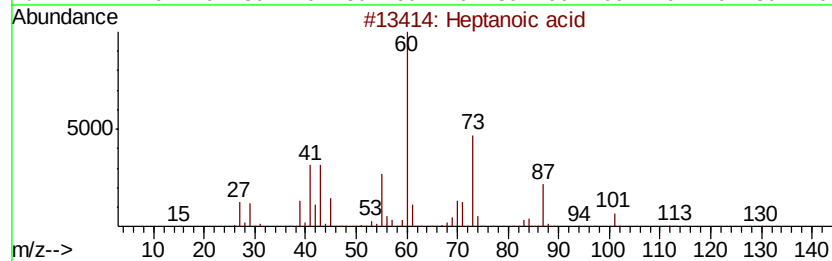
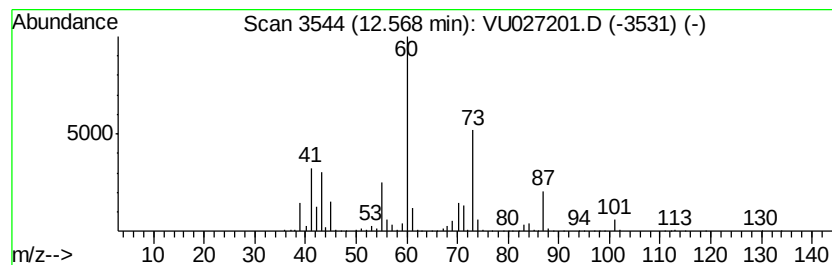
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	28.07 ug/l	1082740	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	Octanoic acid	144 C8H16O2	000124-07-2	45



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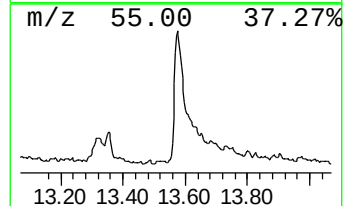
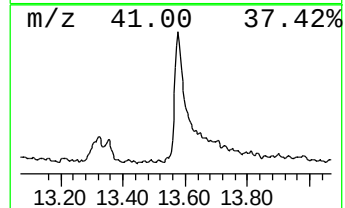
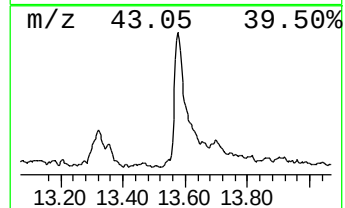
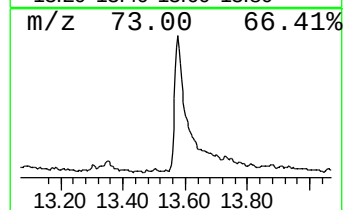
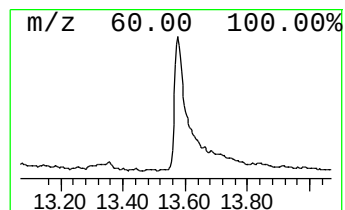
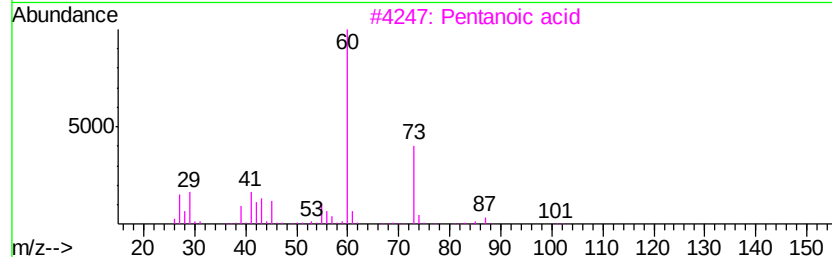
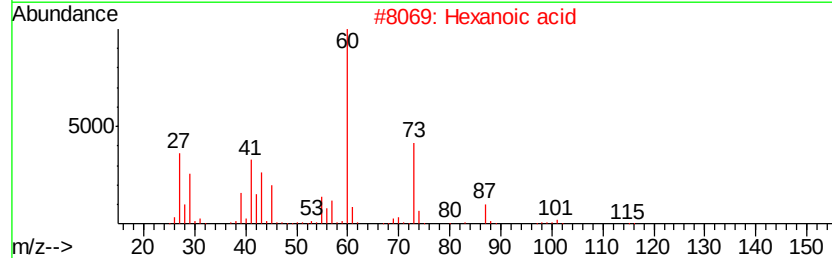
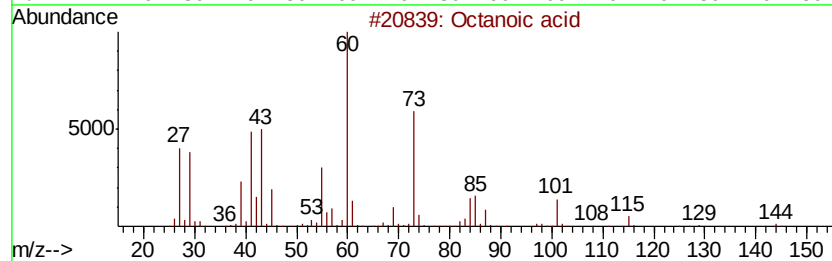
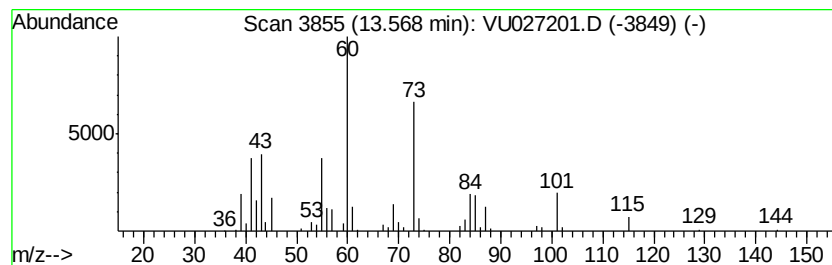
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	5.46 ug/l	210791	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octanoic acid	144 C8H16O2	000124-07-2	95
2	Hexanoic acid	116 C6H12O2	000142-62-1	53
3	Pentanoic acid	102 C5H10O2	000109-52-4	49
4	Heptanoic acid	130 C7H14O2	000111-14-8	47
5	Octanoic acid, silver(1+) salt	250 C8H15AgO2	024927-67-1	40



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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 42 Sample Multiplier: 1

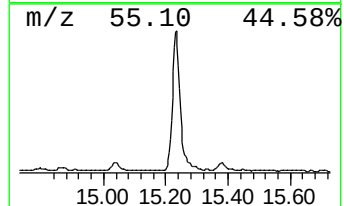
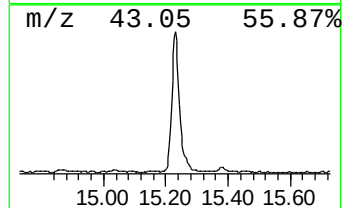
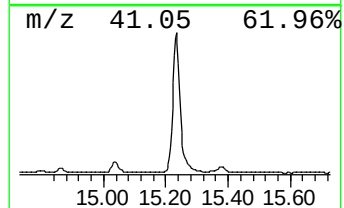
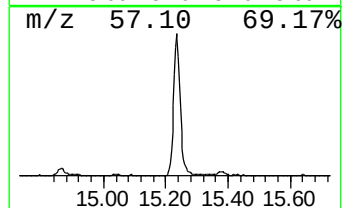
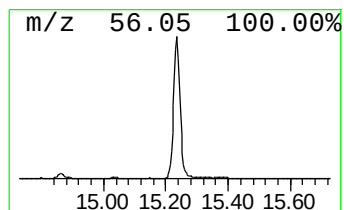
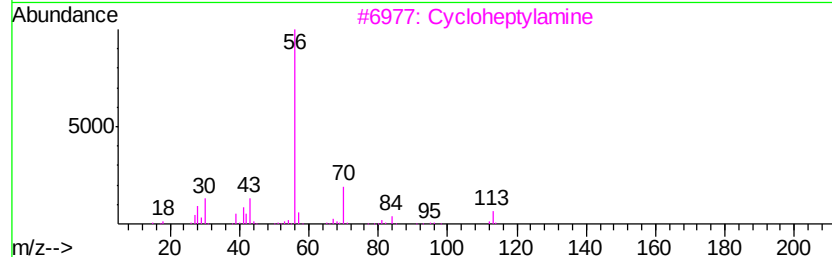
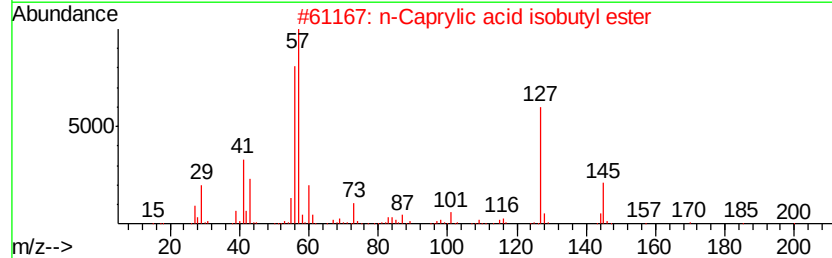
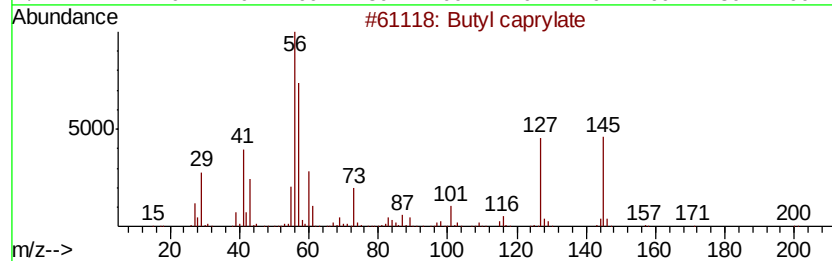
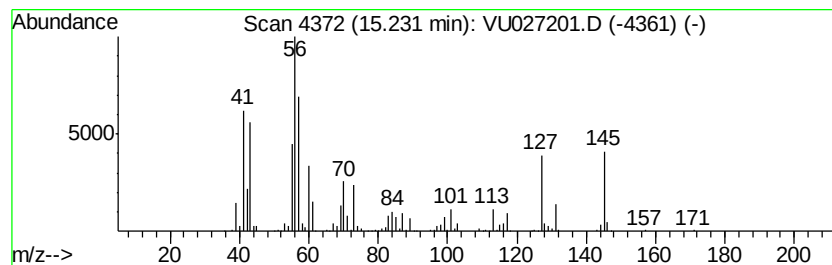
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butyl caprylate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	13.16 ug/l	507514	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Butyl caprylate	200 C12H24O2	000589-75-3 98
2		n-Caprylic acid isobutyl ester	200 C12H24O2	005461-06-3 38
3		Cycloheptylamine	113 C7H15N	005452-35-7 30
4		Cyclobutanone, 3,3-dimethyl-	98 C6H10O	001192-33-2 30
5		Heptyl caprylate	242 C15H30O2	004265-97-8 27



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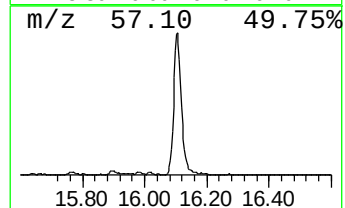
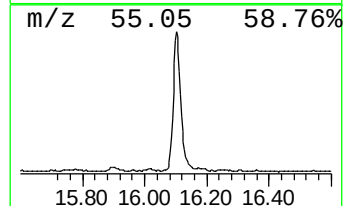
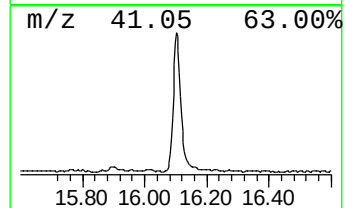
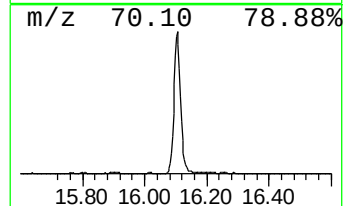
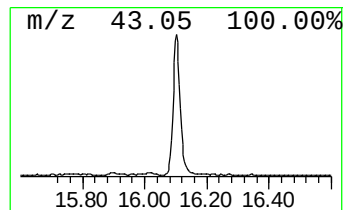
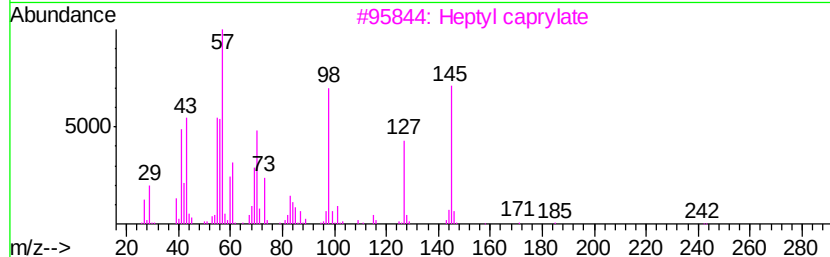
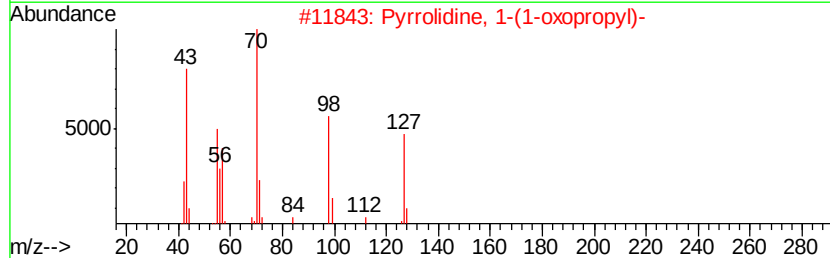
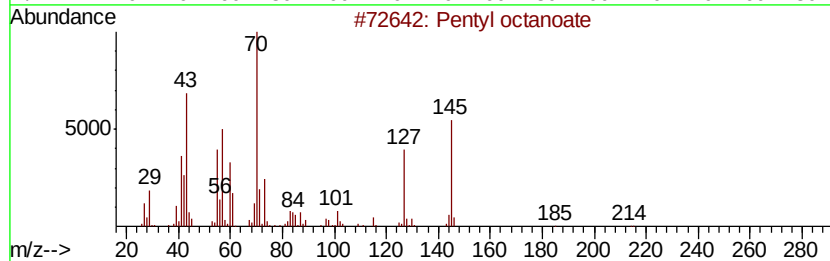
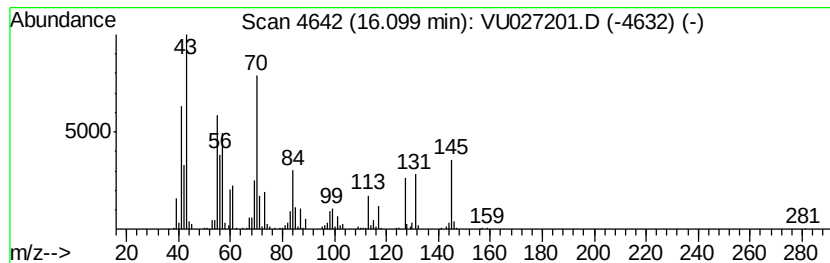
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentyl octanoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	8.25 ug/l	318132	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentyl octanoate	214 C13H26O2	000638-25-5	52
2	Pyrrolidine, 1-(1-oxopropyl)-	127 C7H13NO	004553-05-3	45
3	Heptyl caprylate	242 C15H30O2	004265-97-8	43
4	1-Butanol, 2-ethyl-	102 C6H14O	000097-95-0	35
5	Cyclohexylamine, N-methyl-4,4-di...	141 C9H19N	045815-91-6	25



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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
Butanoic acid	8.98	44.6	ug/l	579117	3	9.09	649520	50.0
Heptanoic acid	12.57	28.1	ug/l	1082740	4	11.48	1928740	50.0
Octanoic acid	13.57	5.5	ug/l	210791	4	11.48	1928740	50.0
Butyl caprylate	15.23	13.2	ug/l	507514	4	11.48	1928740	50.0
Pentyl octanoate	16.10	8.3	ug/l	318132	4	11.48	1928740	50.0