

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092718\
 Data File : VX004783.D
 Acq On : 27 Sep 2018 19:17
 Operator : JC/MD
 Sample : J5048-09
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 CMT-22-6-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_X\METHOD\82X092618W.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	1.318	17	27	35	rBV	46071	226413	15.26%	2.481%
2	2.111	154	157	165	rVB	12167	20537	1.38%	0.225%
3	2.617	234	240	248	rVB	79302	145031	9.77%	1.589%
4	3.019	299	306	316	rVB	28700	71063	4.79%	0.779%
5	4.598	556	565	576	rVB2	17633	48896	3.29%	0.536%
6	4.763	578	592	603	rBV2	18073	65789	4.43%	0.721%
7	5.506	700	714	728	rBV	181473	515958	34.77%	5.653%
8	5.665	728	740	757	rBV	223612	654136	44.08%	7.167%
9	6.067	794	806	823	rBV	194490	507910	34.22%	5.565%
10	6.860	924	936	964	rBV	365881	921515	62.09%	10.096%
11	7.213	986	994	1002	rBV	27728	58443	3.94%	0.640%
12	8.719	1233	1241	1267	rBV	862940	1484058	100.00%	16.259%
13	9.335	1333	1342	1350	rBV2	9557	16342	1.10%	0.179%
14	10.054	1455	1460	1464	rBV2	8279	18317	1.23%	0.201%
15	10.115	1464	1470	1489	rVB	800480	1153718	77.74%	12.640%
16	11.139	1630	1638	1652	rBV	826947	1089895	73.44%	11.941%
17	12.042	1780	1786	1788	rBV	70440	85731	5.78%	0.939%
18	12.078	1788	1792	1804	rVB	1059589	1302230	87.75%	14.267%
19	12.883	1919	1924	1935	rBV	155473	205775	13.87%	2.254%
20	13.663	2047	2052	2070	rBV	311065	421367	28.39%	4.616%
21	16.175	2458	2464	2472	rBV	37957	68725	4.63%	0.753%
22	16.614	2528	2536	2546	rBV3	22349	45743	3.08%	0.501%

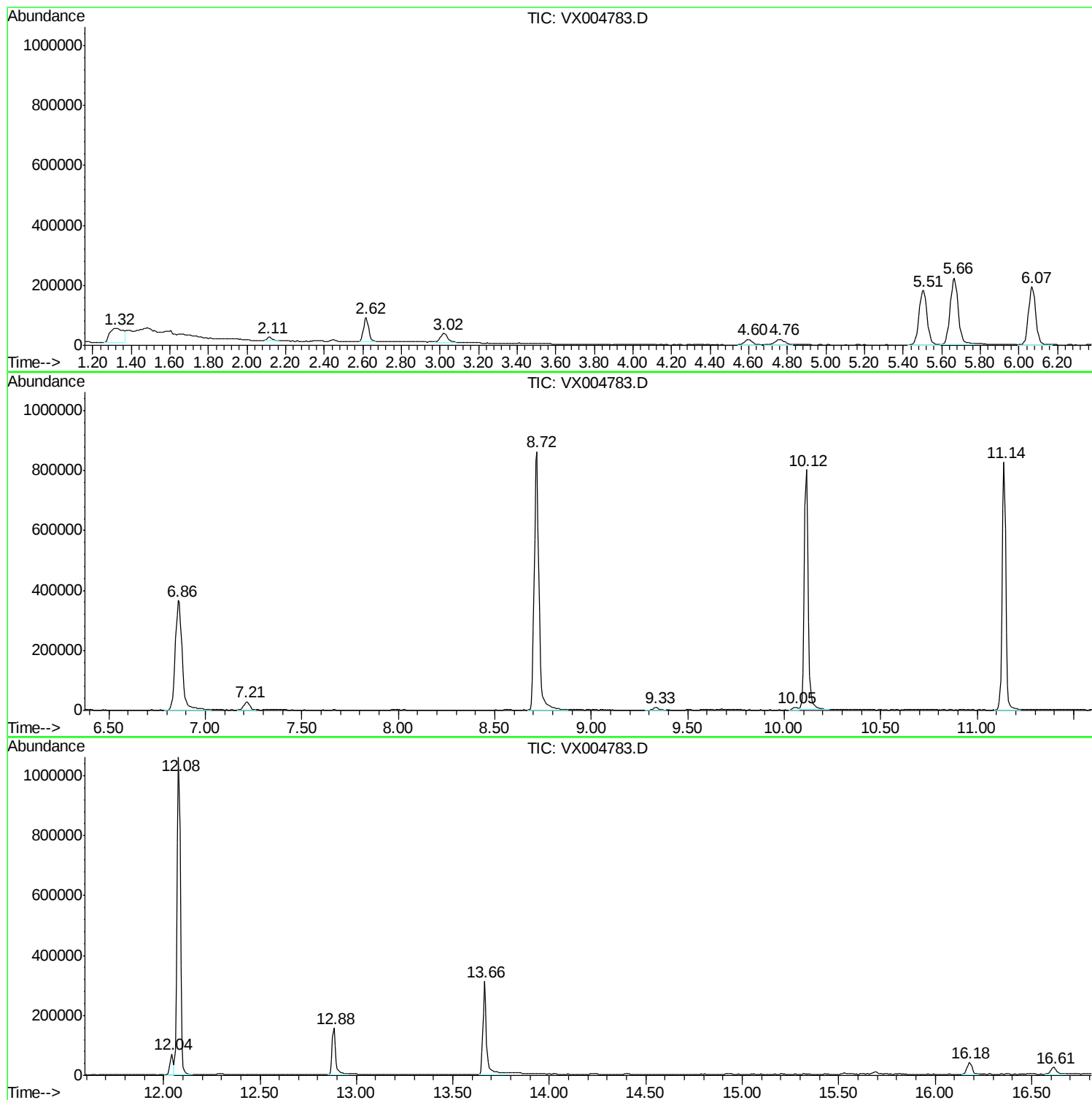
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Quant Title : SW846 8260

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



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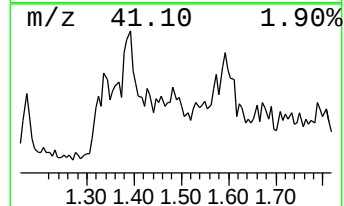
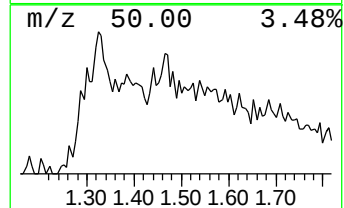
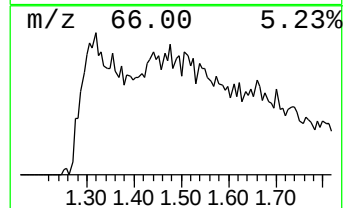
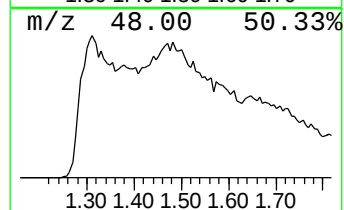
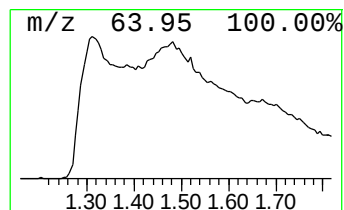
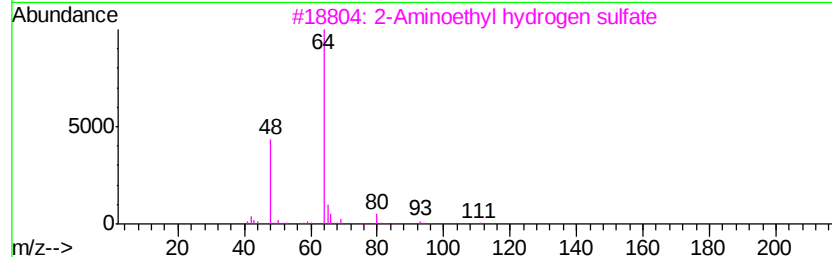
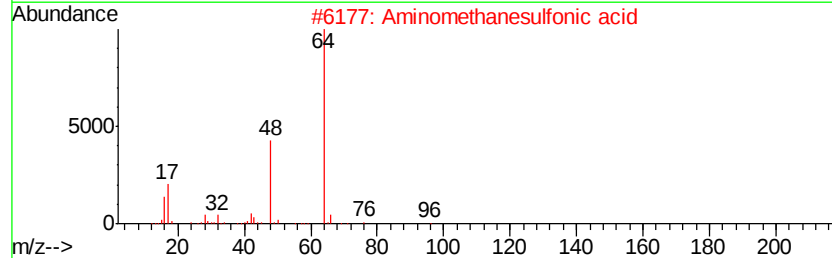
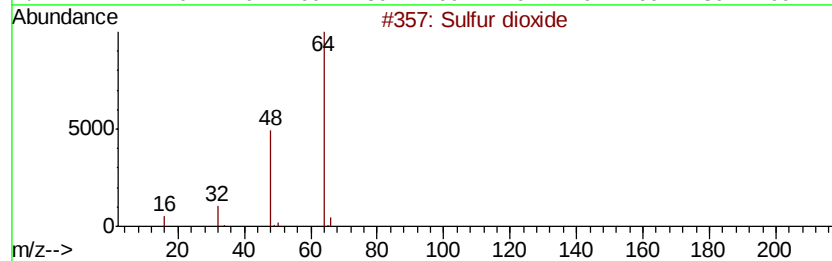
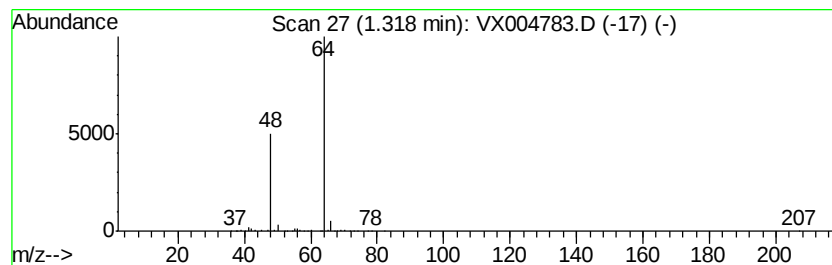
Instrument :
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ClientSampleId :
CMT-22-6-SEP18

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
1.32	17.31 ug/l	226413	Pentafluorobenzene	5.66		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfur dioxide	64	O2S	007446-09-5	83
2		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
3		2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4		S-2-[4-Glutarimidobutylamino]eth...	324	C11H20N2O5S2	031701-78-7	9
5		(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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CMT-22-6-SEP18

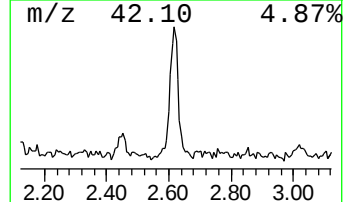
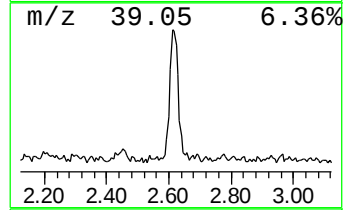
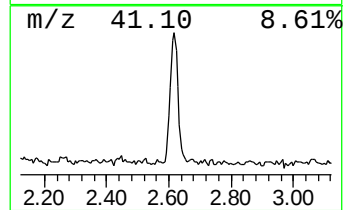
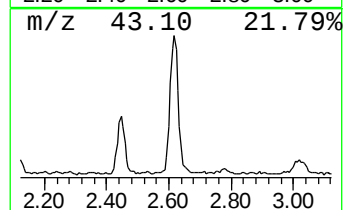
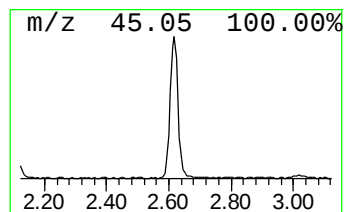
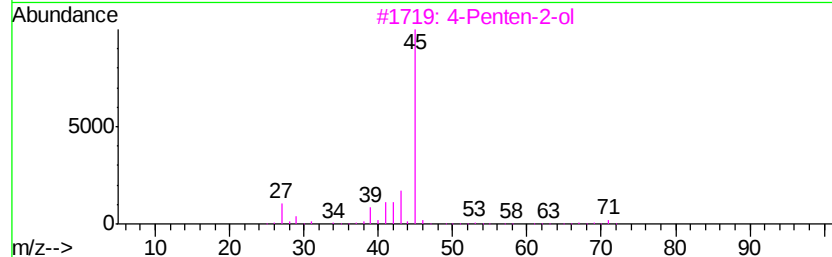
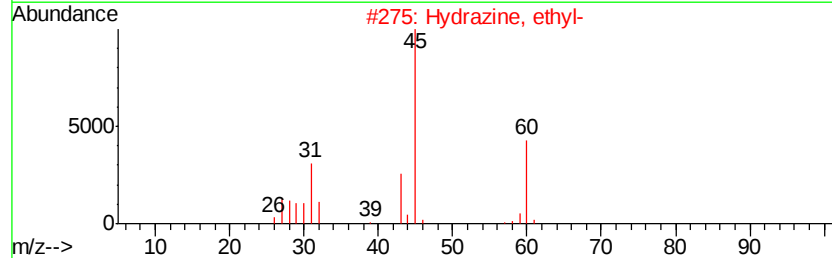
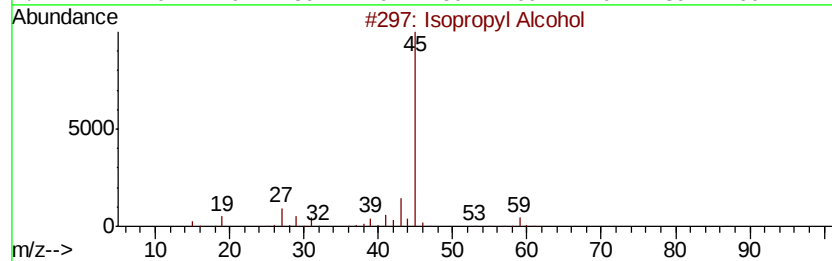
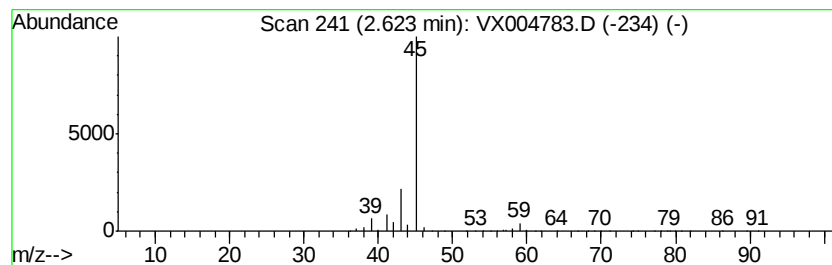
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Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.62	11.09 ug/l	145031	Pentafluorobenzene	5.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	90
2		Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3		4-Penten-2-ol	86	C5H10O	000625-31-0	9
4		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5		Formamide	45	CH3NO	000075-12-7	5



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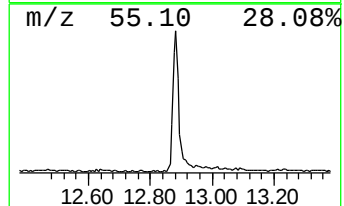
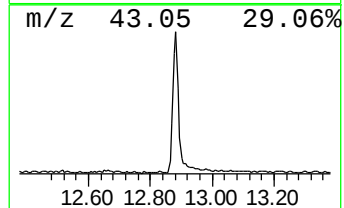
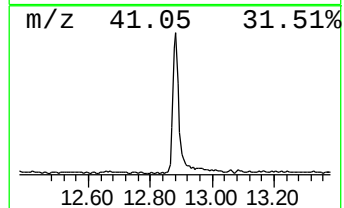
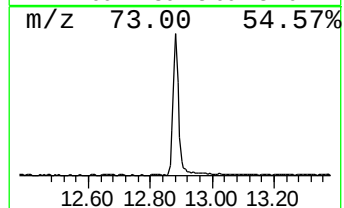
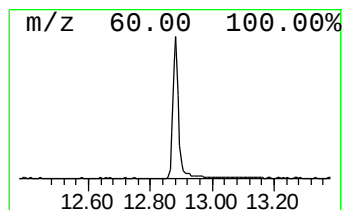
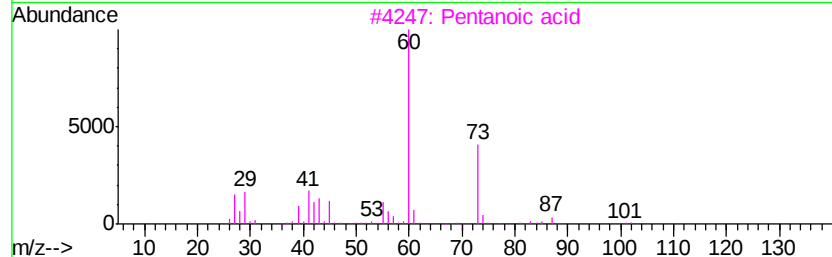
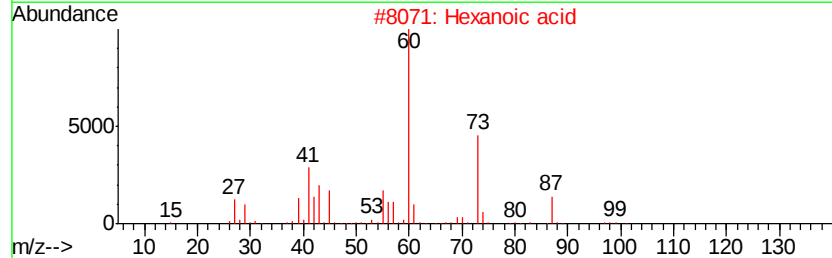
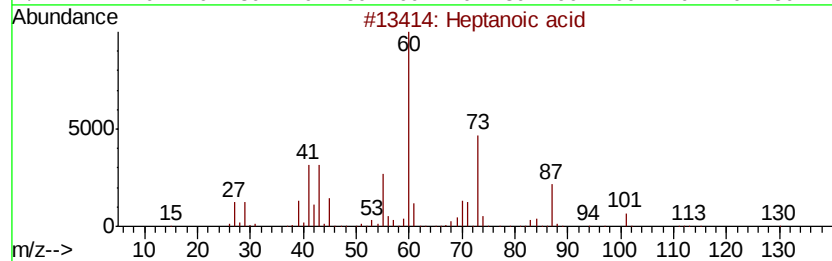
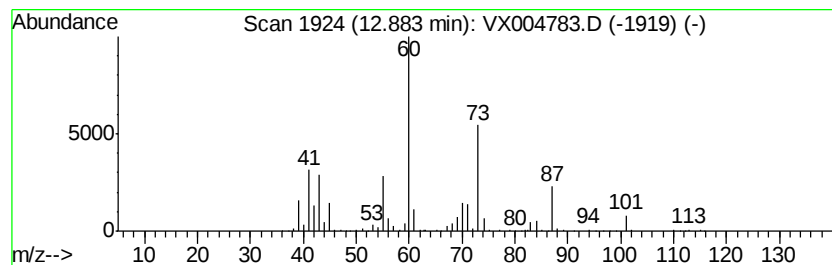
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Peak Number 5 Heptanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.88	7.90 ug/l	205775	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid		130	C7H14O2	000111-14-8	91
2	Hexanoic acid		116	C6H12O2	000142-62-1	59
3	Pentanoic acid		102	C5H10O2	000109-52-4	58
4	Octanoic acid		144	C8H16O2	000124-07-2	53
5	Butanoic acid, 3-methyl-		102	C5H10O2	000503-74-2	52



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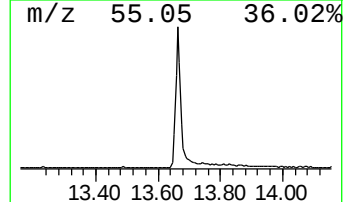
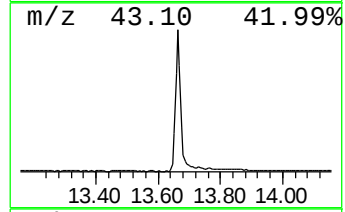
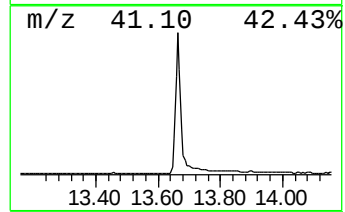
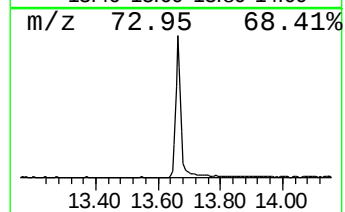
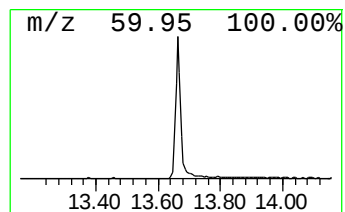
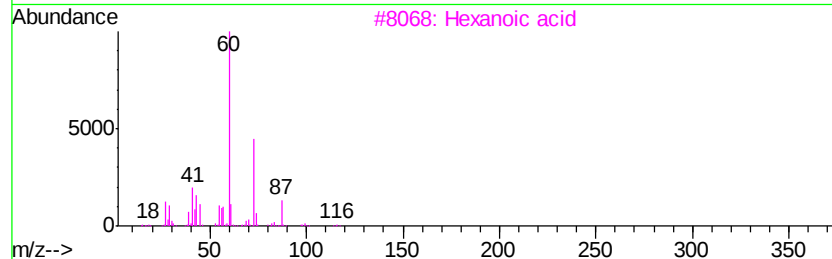
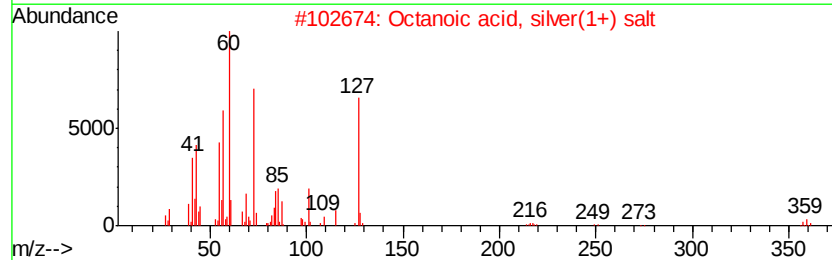
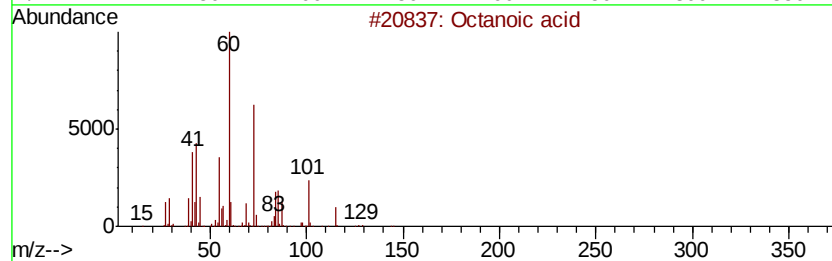
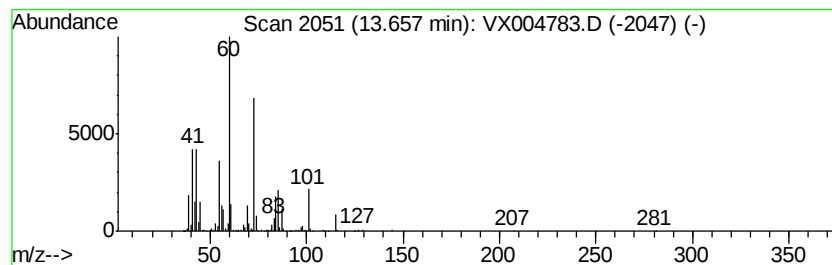
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Octanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	16.18 ug/l	421367	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid		144	C8H16O2	000124-07-2	98
2	Octanoic acid, silver(1+) salt		250	C8H15AgO2	024927-67-1	90
3	Hexanoic acid		116	C6H12O2	000142-62-1	55
4	Propanedioic acid, propyl-		146	C6H10O4	000616-62-6	47
5	3-Methyl-hexanoic acid		130	C7H14O2	1000365-65-4	43



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Sulfur dioxide	1.32	17.3	ug/l	226413	1	5.66	654136	50.0
Isopropyl Alcohol	2.62	11.1	ug/l	145031	1	5.66	654136	50.0
Heptanoic acid	12.88	7.9	ug/l	205775	4	12.08	1302230	50.0
Octanoic acid	13.66	16.2	ug/l	421367	4	12.08	1302230	50.0