

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061818\
 Data File : VU024706.D
 Acq On : 18 Jun 2018 21:04
 Operator : MD/SY
 Sample : J3477-11
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 S36-EB-2018-1

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\82U061318W.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	1.092	142	156	181	rBV	216642	271715	7.30%	2.240%
2	2.014	435	443	456	rVB	43033	65076	1.75%	0.537%
3	2.442	566	576	591	rBV	25727	43080	1.16%	0.355%
4	2.706	645	658	681	rBV	250893	455110	12.22%	3.752%
5	4.268	1132	1144	1164	rVB	16465	40345	1.08%	0.333%
6	4.638	1241	1259	1304	rBV	1564097	3723590	100.00%	30.698%
7	4.889	1322	1337	1354	rBV	179872	401642	10.79%	3.311%
8	4.989	1354	1368	1389	rVB	241426	534361	14.35%	4.405%
9	5.316	1454	1470	1492	rBV	182720	388549	10.43%	3.203%
10	5.799	1596	1620	1622	rBV	18039	53891	1.45%	0.444%
11	5.892	1636	1649	1669	rBV	366763	734006	19.71%	6.051%
12	7.570	2153	2171	2187	rBV	673091	1169750	31.41%	9.644%
13	7.863	2242	2262	2263	rBV3	38765	99275	2.67%	0.818%
14	9.094	2633	2645	2668	rVB	521478	862609	23.17%	7.112%
15	10.310	3011	3023	3041	rBV	523322	818887	21.99%	6.751%
16	11.487	3374	3389	3405	rBV	608960	944387	25.36%	7.786%
17	12.959	3837	3847	3869	rVB	81954	141202	3.79%	1.164%
18	13.323	3950	3960	3975	rBV2	40164	84748	2.28%	0.699%
19	15.130	4510	4522	4538	rBV7	16051	41266	1.11%	0.340%
20	15.689	4684	4696	4739	rBV	543171	1148303	30.84%	9.467%
21	16.020	4792	4799	4808	rVB2	44256	60714	1.63%	0.501%
22	16.888	5061	5069	5080	rVB2	32632	47109	1.27%	0.388%

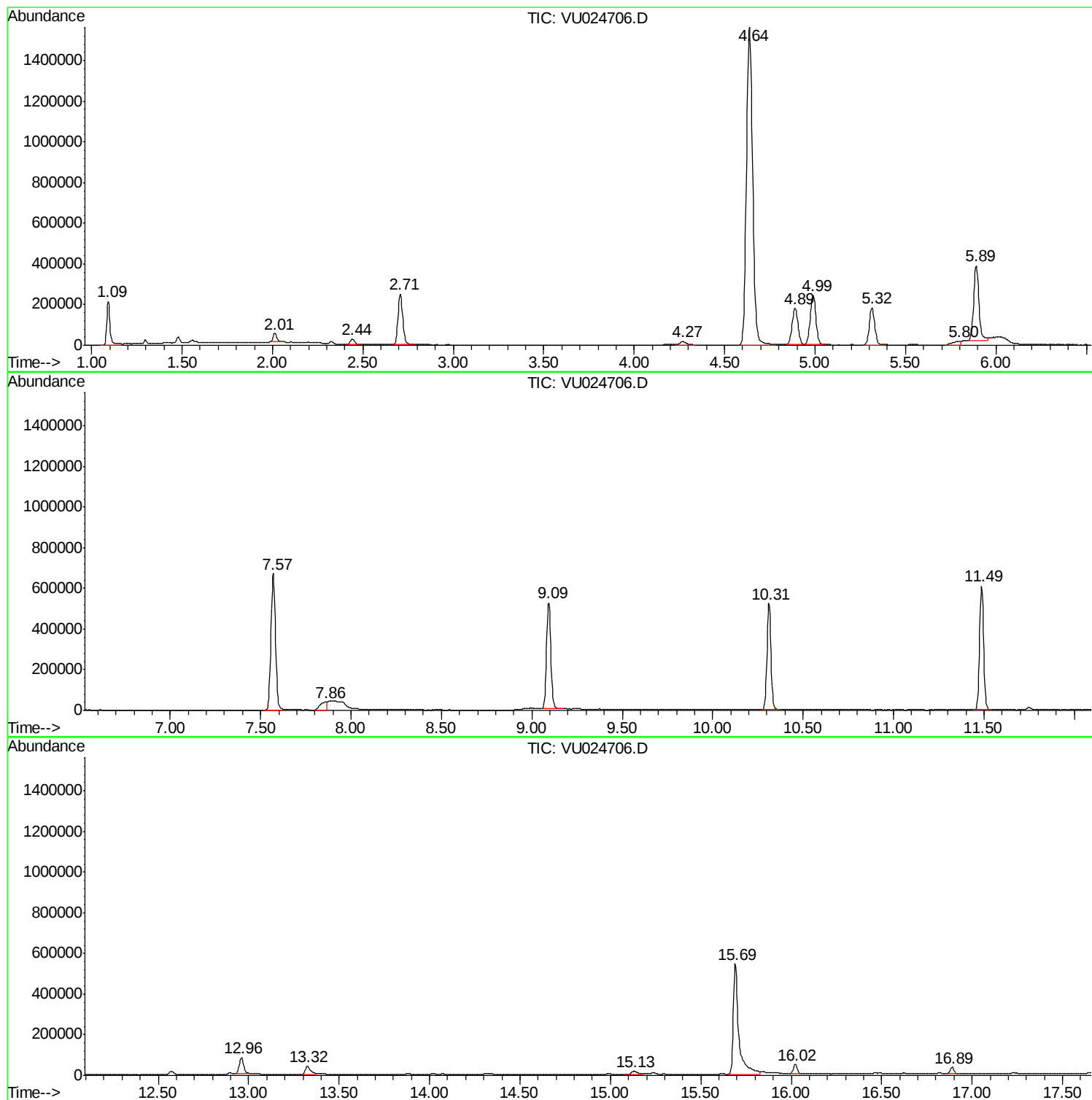
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

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



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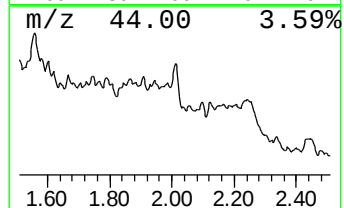
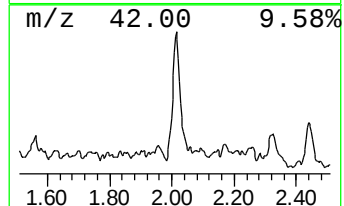
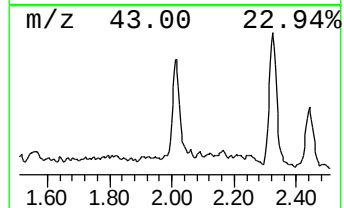
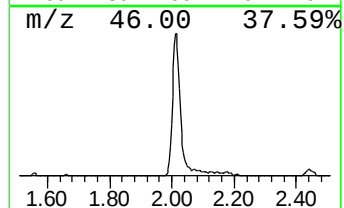
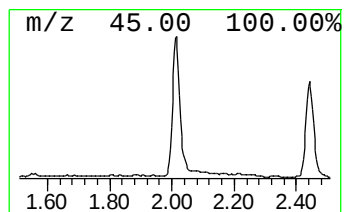
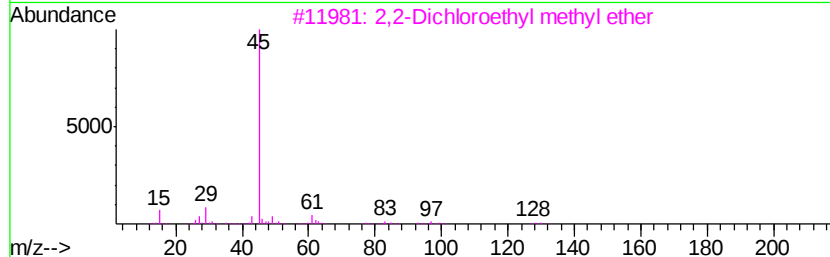
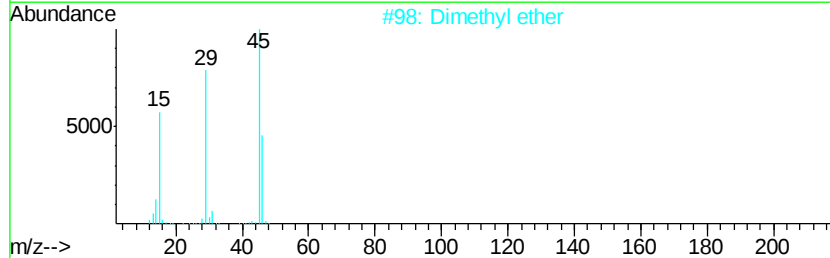
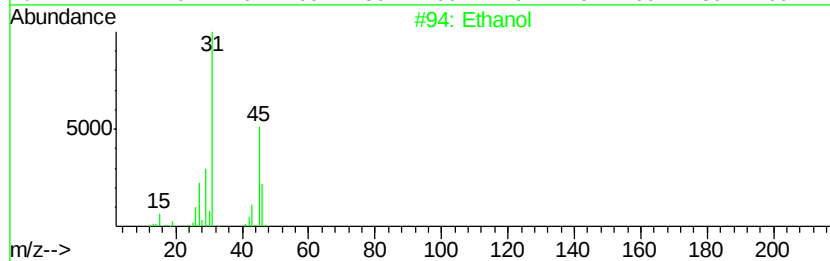
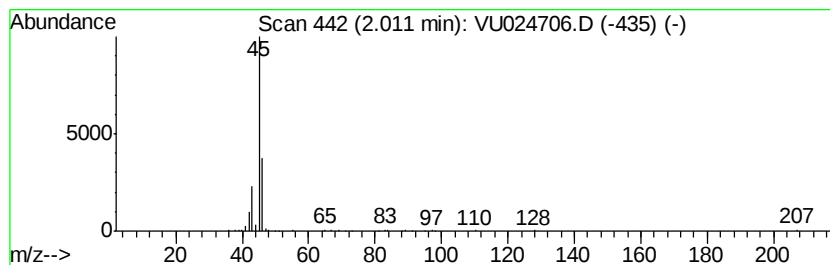
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	6.09 ug/l	65076	Pentafluorobenzene	4.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol	46	C2H6O	000064-17-5	56
2		Dimethyl ether	46	C2H6O	000115-10-6	9
3		2,2-Dichloroethyl methyl ether	128	C3H6Cl2O	034862-07-2	7
4		Methane, nitroso-	45	CH3NO	000865-40-7	4
5		Propanedioic acid, dihydroxy-	136	C3H4O6	000560-27-0	4



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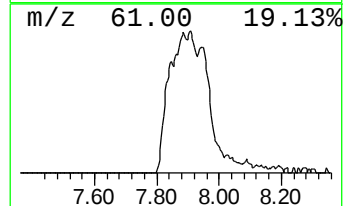
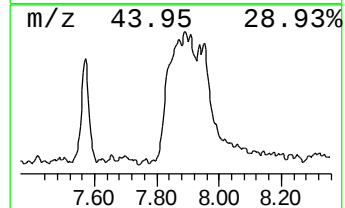
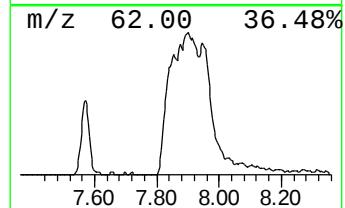
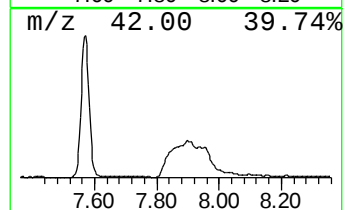
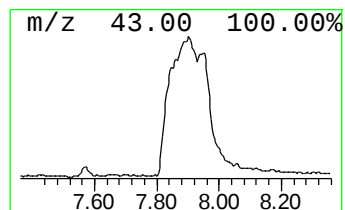
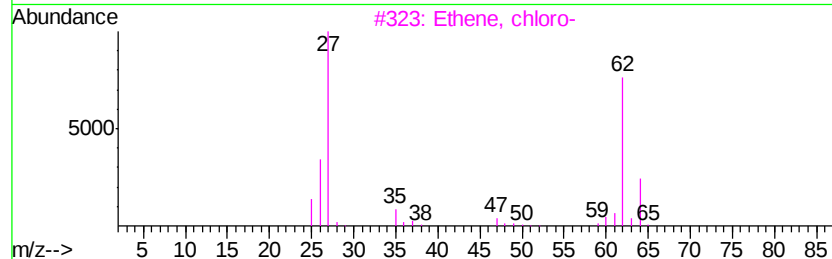
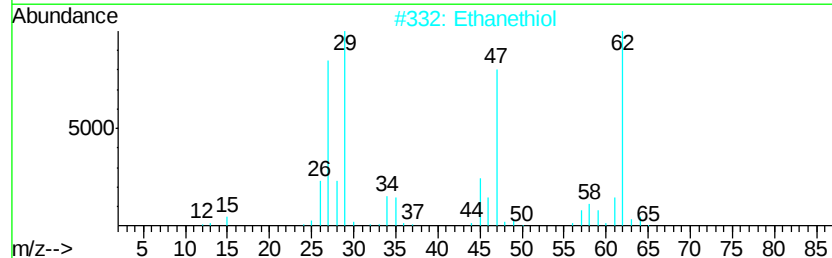
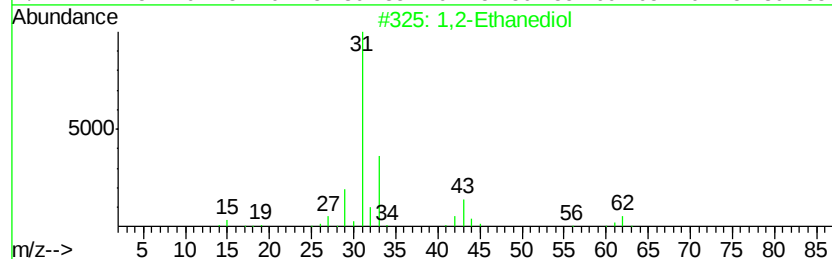
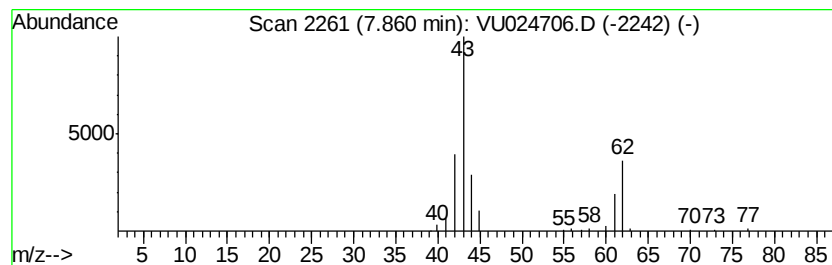
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Quant Title : SW846 8260

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

Peak Number 3 unknown7.86 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.86	5.75 ug/l	99275	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Ethanediol	62	C2H6O2	000107-21-1	45
2	Ethanethiol	62	C2H6S	000075-08-1	5
3	Ethene, chloro-	62	C2H3Cl	000075-01-4	4
4	Monoethanolamine	61	C2H7NO	000141-43-5	4
5	Propylcarbamate	103	C4H9NO2	000627-12-3	4



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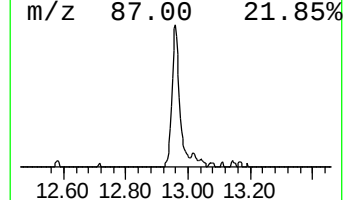
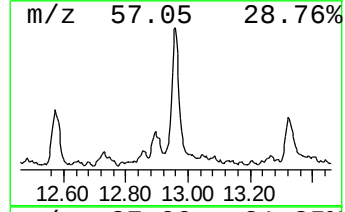
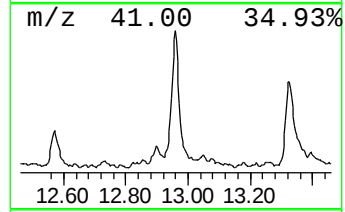
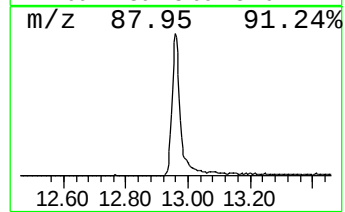
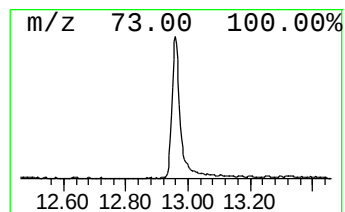
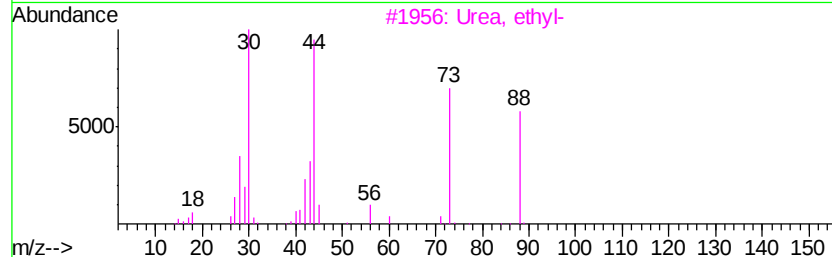
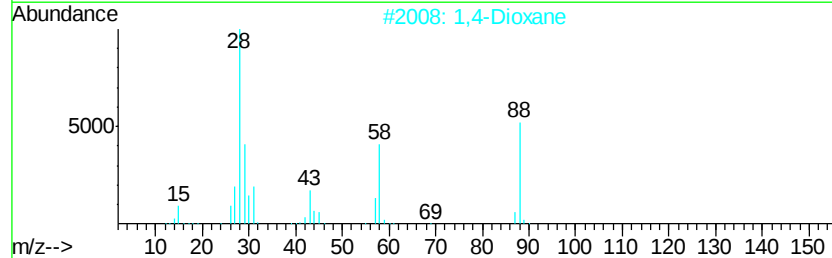
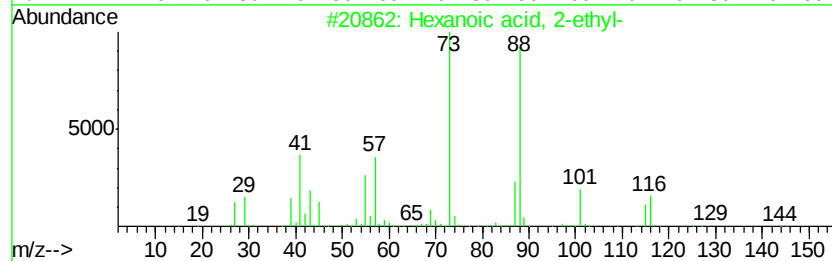
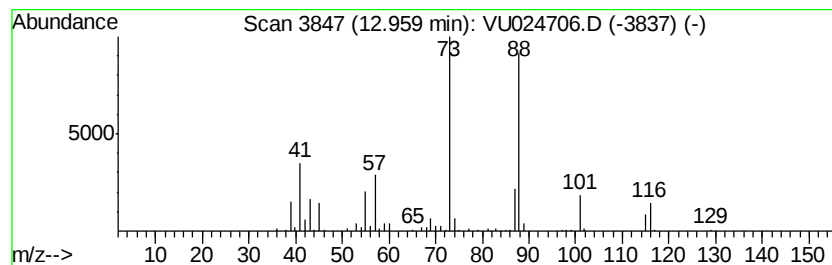
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Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	7.48 ug/l	141202	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		1,4-Dioxane	88	C4H8O2	000123-91-1	50
3		Urea, ethyl-	88	C3H8N2O	000625-52-5	36
4		Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	33
5		Heptanoic acid, 2,6-dimethyl-, m...	172	C10H20O2	033315-72-9	28



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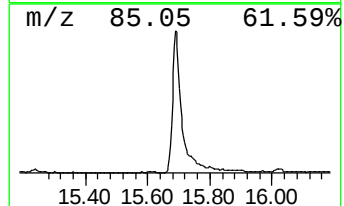
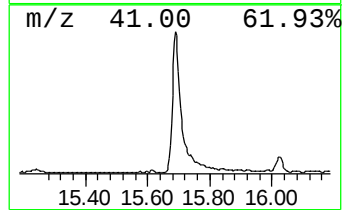
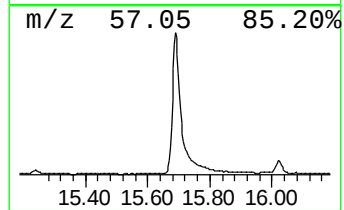
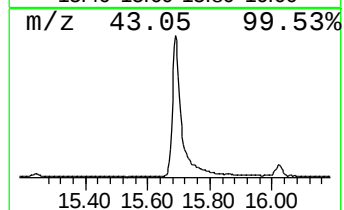
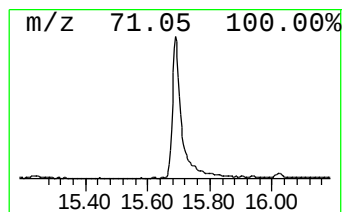
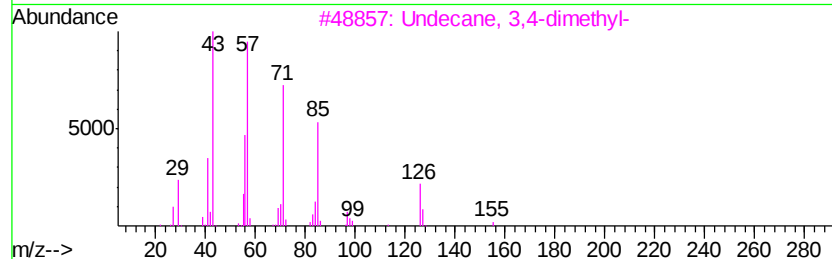
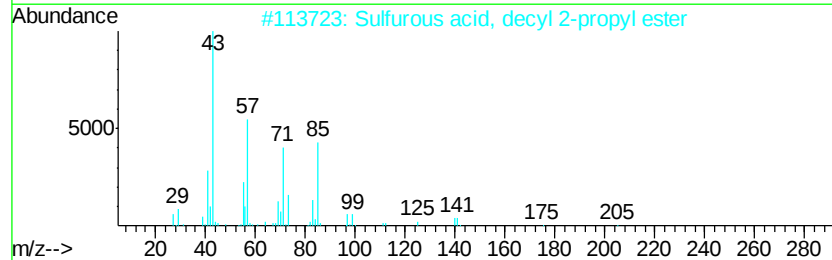
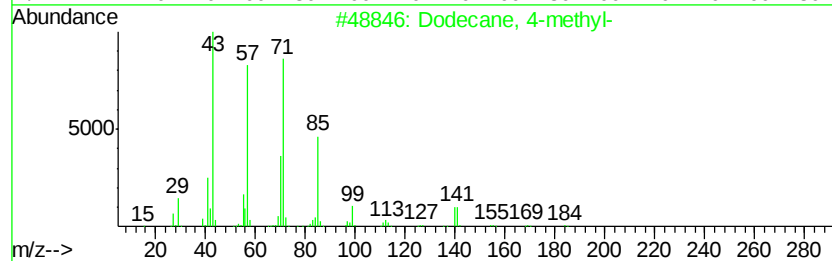
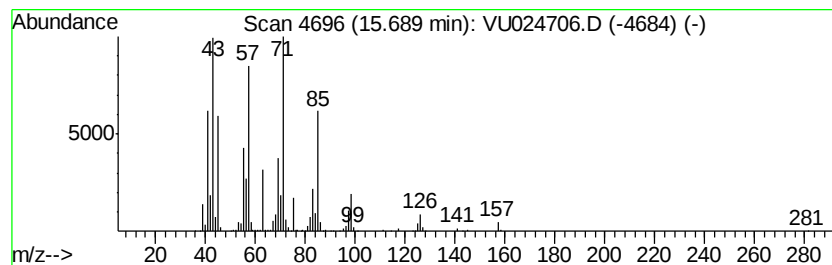
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Peak Number 5 Dodecane, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.69	60.80 ug/l	1148300	1,4-Dichlorobenzene-d4	11.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 4-methyl-	184	C13H28	006117-97-1	47
2	Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	43
3	Undecane, 3,4-dimethyl-	184	C13H28	017312-78-6	43
4	Ethanol, 2-(hexyloxy)-	146	C8H18O2	000112-25-4	43
5	Decane, 3-methyl-	156	C11H24	013151-34-3	38



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Ethanol	2.01	6.1	ug/l	65076	1	4.99	534361	50.0
unknown7.86	7.86	5.8	ug/l	99275	3	9.09	862609	50.0
Hexanoic acid, 2-...	12.96	7.5	ug/l	141202	4	11.49	944387	50.0
Dodecane, 4-methyl-	15.69	60.8	ug/l	1148300	4	11.49	944387	50.0