

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN041620\
 Data File : VN061035.D
 Acq On : 17 Apr 2020 00:15
 Operator : JC/MD
 Sample : L2299-01
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 COMP-40860-861

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_N\METHODS\82N041620W.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	2.262	141	152	259	rBV	10714075	32509899	100.00%	61.913%
2	3.224	433	451	500	rBV	1407957	3314332	10.19%	6.312%
3	6.503	1448	1471	1498	rBV	498585	1485726	4.57%	2.829%
4	7.638	1812	1824	1846	rVB	210179	493772	1.52%	0.940%
5	7.998	1913	1936	1956	rBV2	138512	371998	1.14%	0.708%
6	8.564	2097	2112	2131	rVB	329311	683843	2.10%	1.302%
7	10.075	2564	2582	2596	rBV	534554	989074	3.04%	1.884%
8	11.397	2972	2993	3017	rBV2	582552	1028503	3.16%	1.959%
9	11.532	3017	3035	3056	rBV	3398675	5643469	17.36%	10.748%
10	12.394	3291	3303	3316	rVB	434052	729710	2.24%	1.390%
11	12.908	3451	3463	3479	rVB	386068	586025	1.80%	1.116%
12	13.098	3514	3522	3544	rVB	404669	640144	1.97%	1.219%
13	13.336	3583	3596	3614	rVB	495805	841100	2.59%	1.602%
14	13.442	3614	3629	3646	rBV2	1996107	3191573	9.82%	6.078%

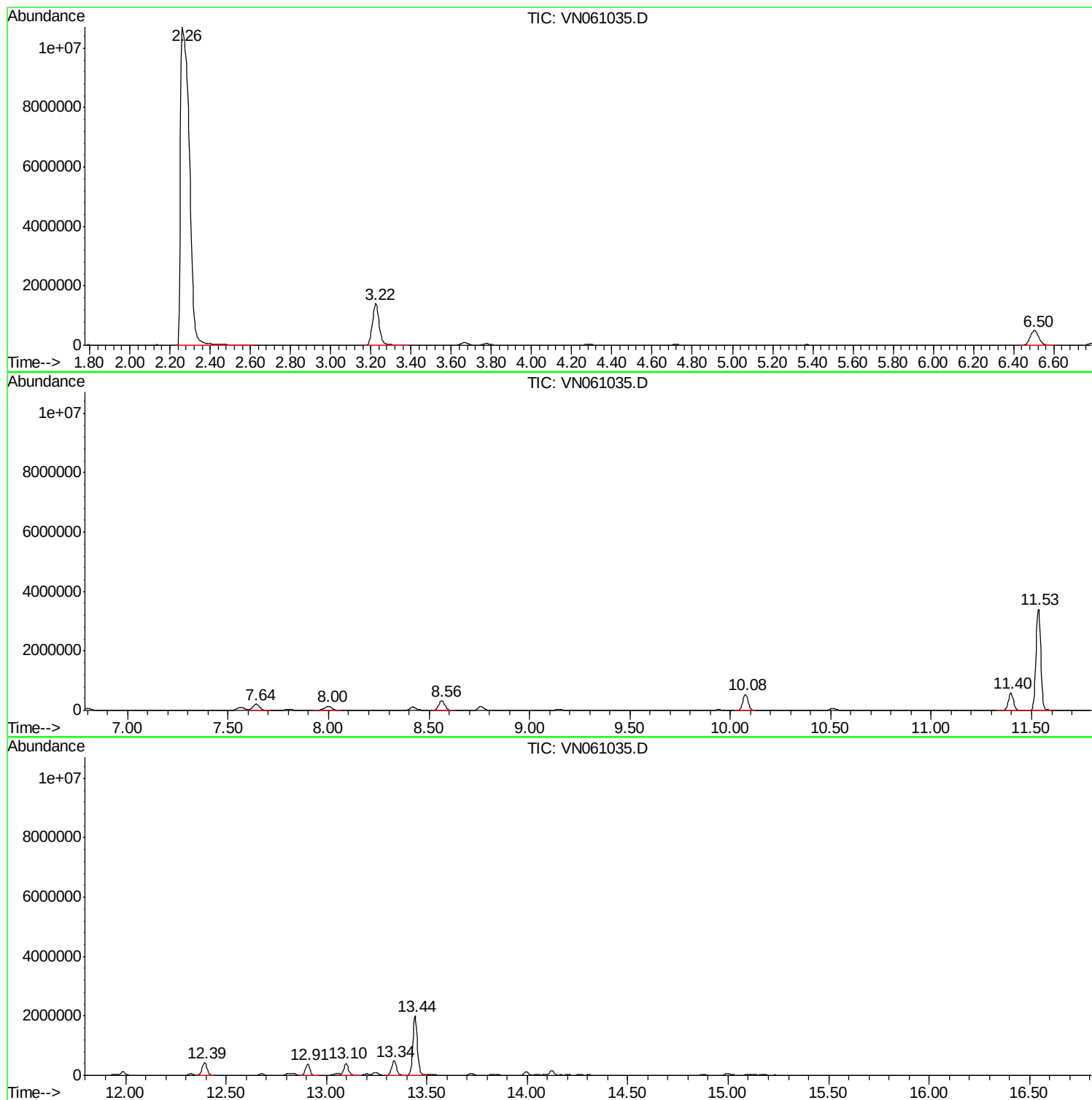
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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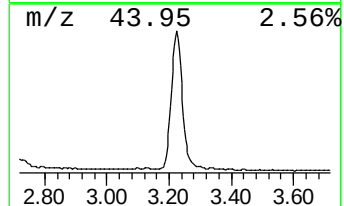
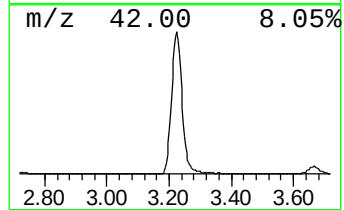
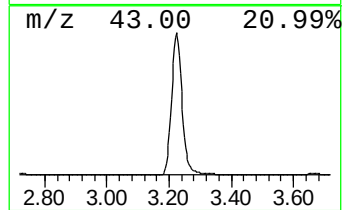
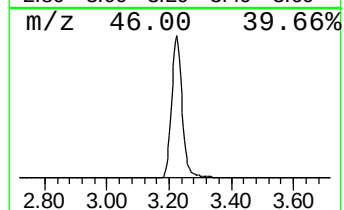
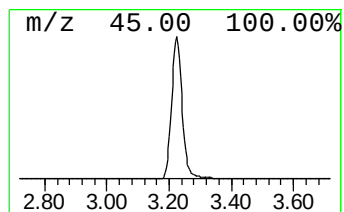
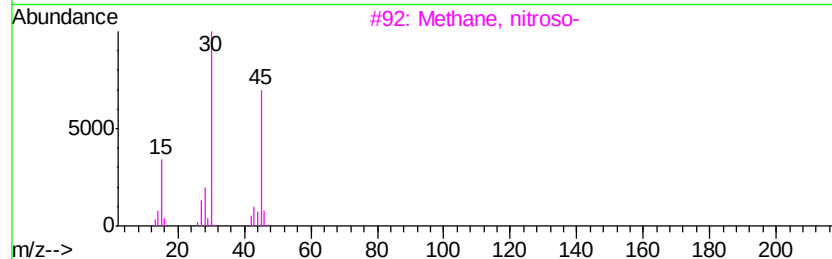
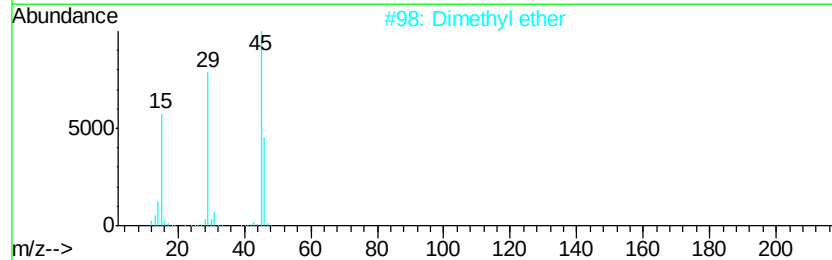
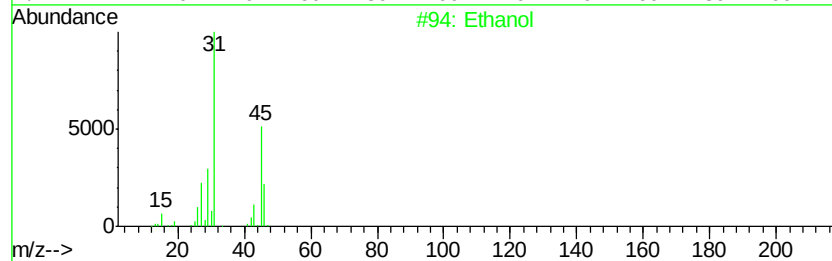
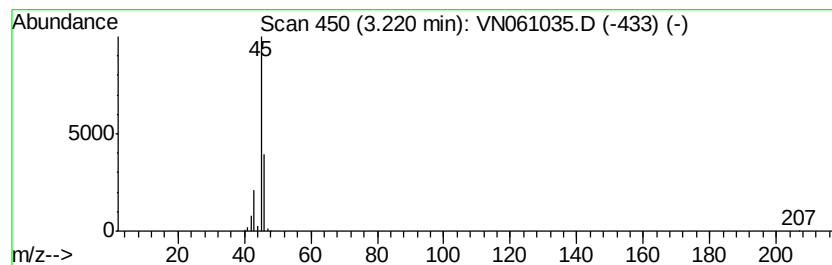
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Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	335.61 ug/l	3314330	Pentafluorobenzene	7.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol	46	C2H6O	000064-17-5	74
2		Dimethyl ether	46	C2H6O	000115-10-6	9
3		Methane, nitroso-	45	CH3NO	000865-40-7	4
4		Formic acid	46	CH2O2	000064-18-6	4
5		Oxalic acid	90	C2H2O4	000144-62-7	4



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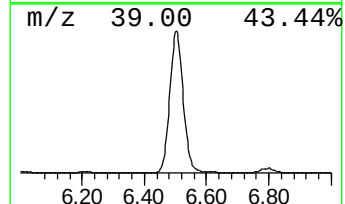
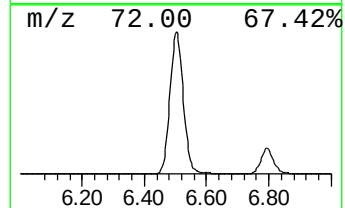
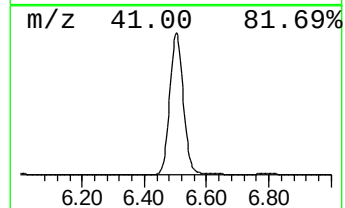
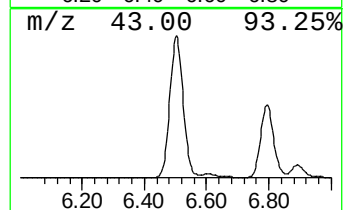
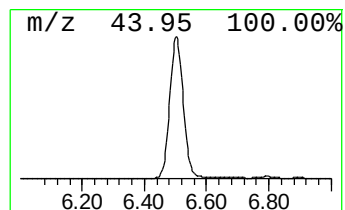
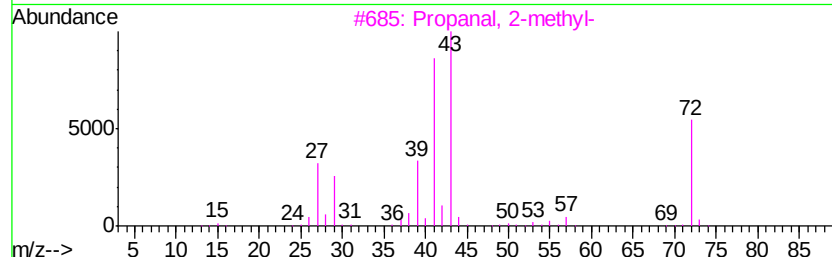
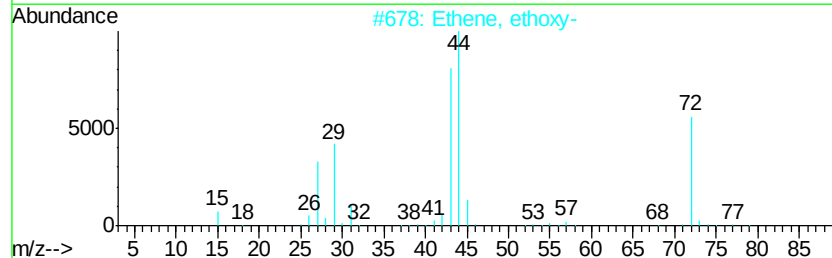
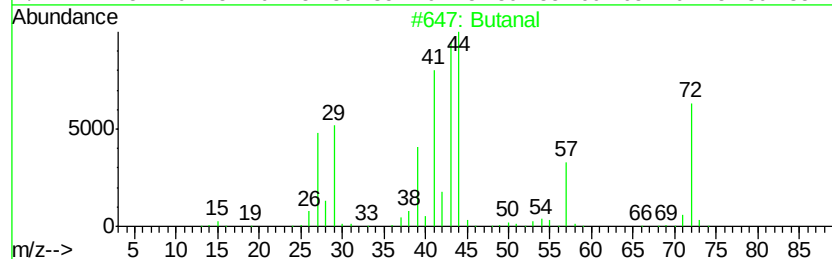
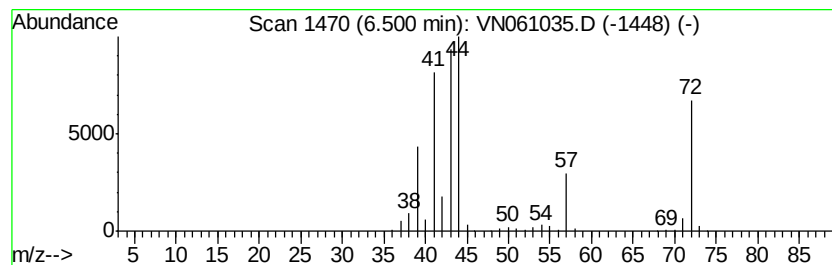
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Quant Title : SW846 8260

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Peak Number 3 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	150.45 ug/l	1485730	Pentafluorobenzene	7.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal		72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-		72	C4H8O	000109-92-2	52
3	Propanal, 2-methyl-		72	C4H8O	000078-84-2	49
4	Methacrolein		70	C4H6O	000078-85-3	22
5	Propane, 1-nitro-		89	C3H7NO2	000108-03-2	17



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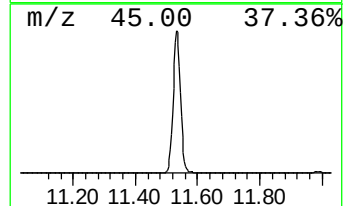
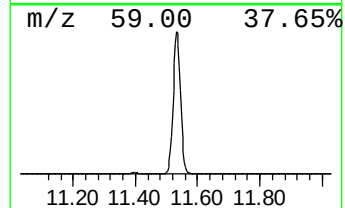
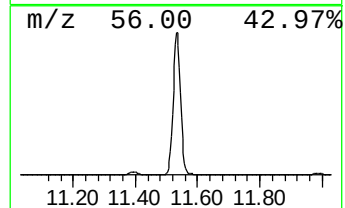
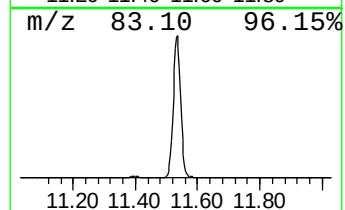
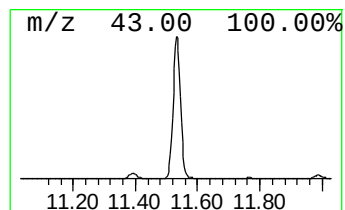
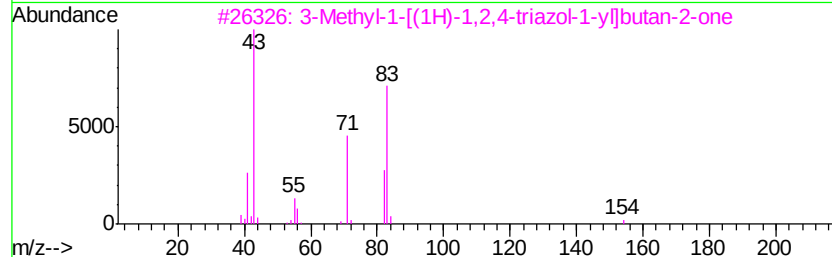
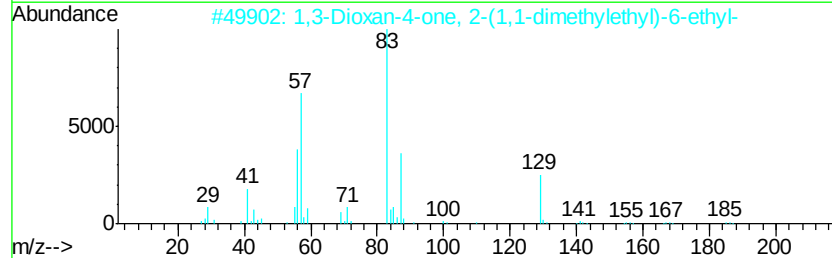
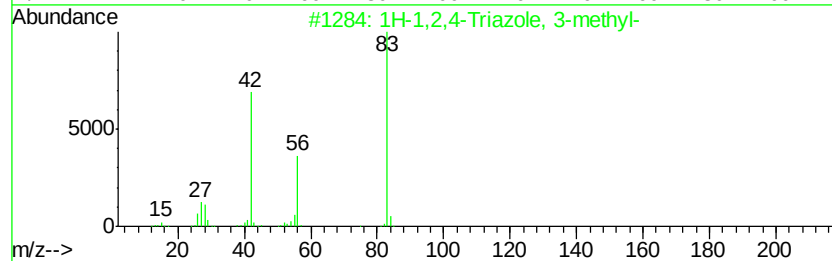
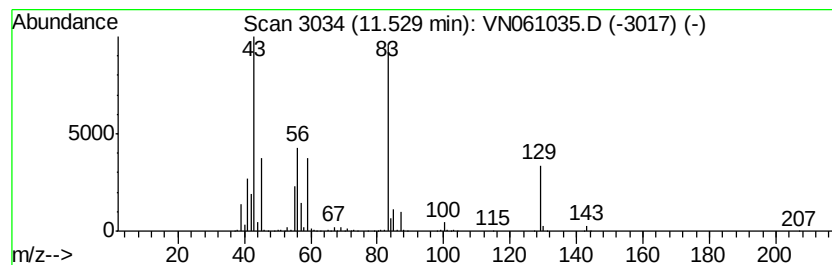
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Peak Number 4 unknown11.53 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	274.35 ug/l	5643470	Chlorobenzene-d5	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	37
2		1,3-Dioxan-4-one, 2-(1,1-dimethy...	186	C10H18O3	113505-80-9	36
3		3-Methyl-1-[(1H)-1,2,4-triazol-1...	153	C7H11N3O	064922-02-7	12
4		Oxalic acid, cyclohexyl butyl ester	228	C12H20O4	1000309-30-5	12
5		Oxalic acid, cyclohexyl isobutyl...	228	C12H20O4	1000309-30-4	12



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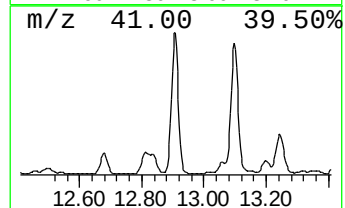
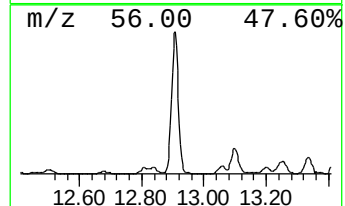
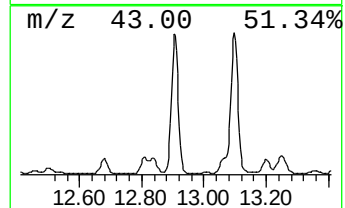
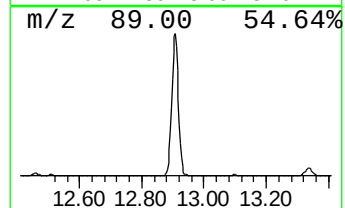
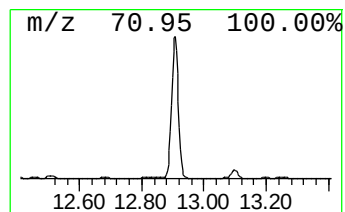
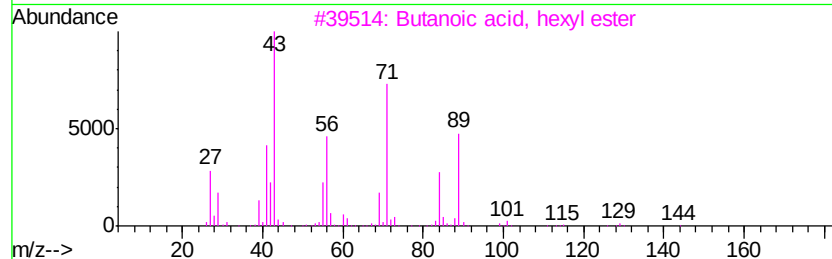
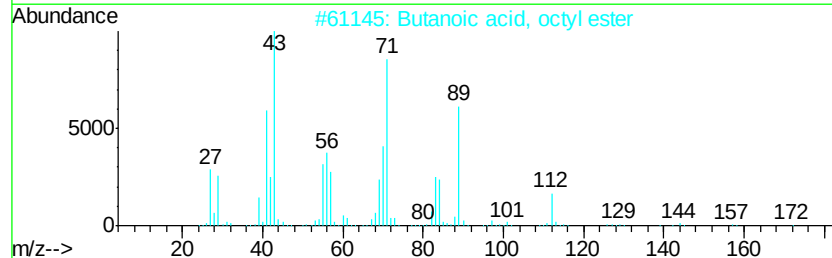
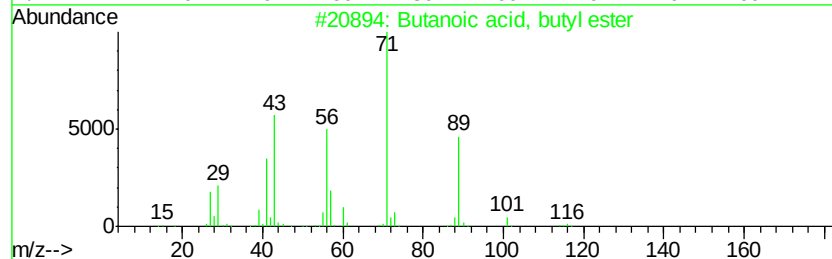
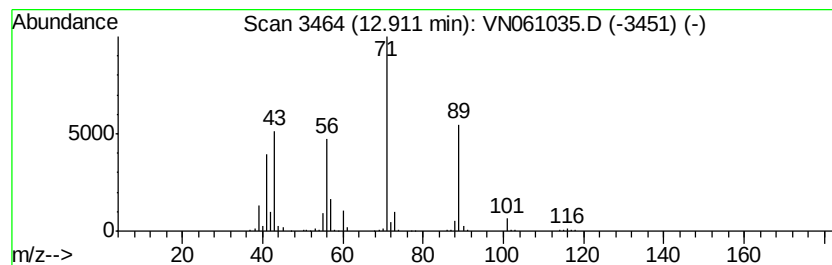
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Peak Number 5 Butanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	34.84 ug/l	586025	1,4-Dichlorobenzene-d4	13.34

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	72
4	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
5	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	56



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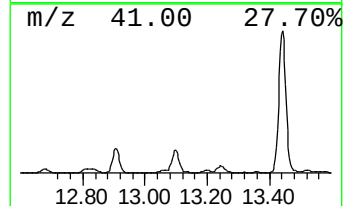
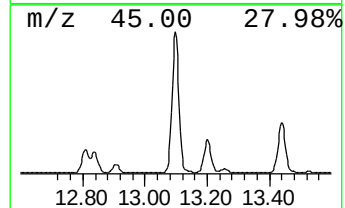
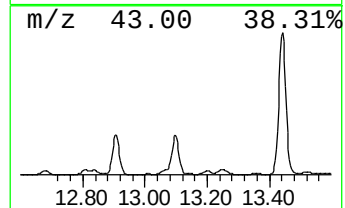
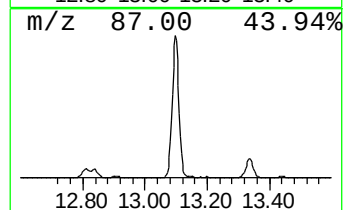
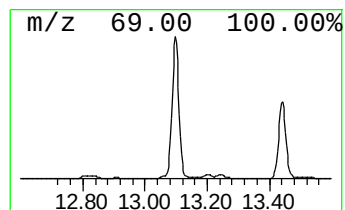
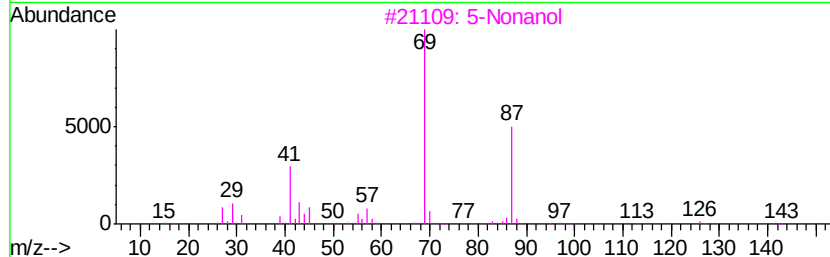
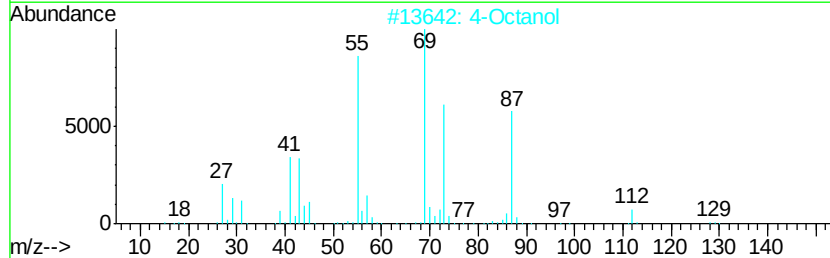
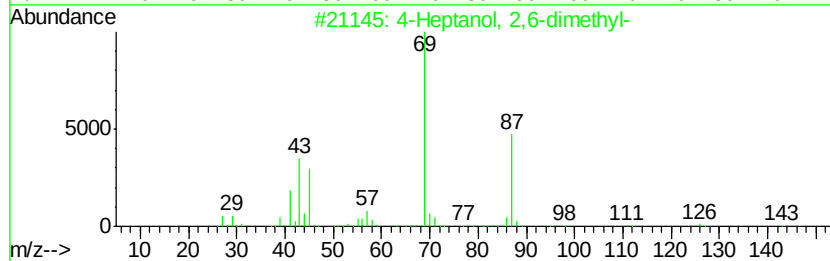
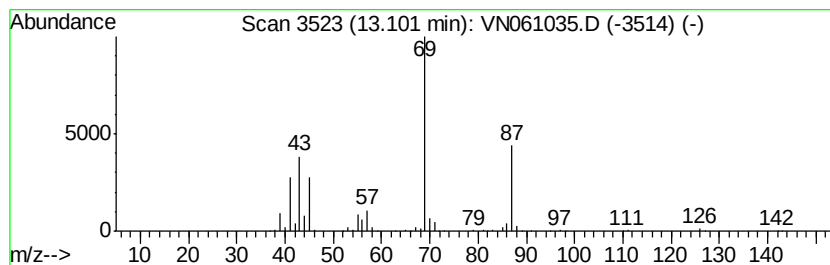
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Peak Number 6 4-Heptanol, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	38.05 ug/l	640144	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	83
2		4-Octanol	130	C8H18O	000589-62-8	72
3		5-Nonanol	144	C9H20O	000623-93-8	72
4		1,2-Hexanediol	118	C6H14O2	006920-22-5	72
5		1,3-Dioxan-4-one, 2-(1,1-dimethyl-...	172	C9H16O3	113505-75-2	64



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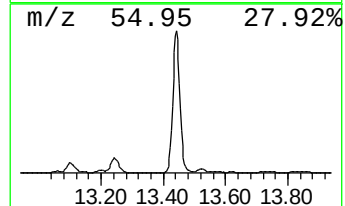
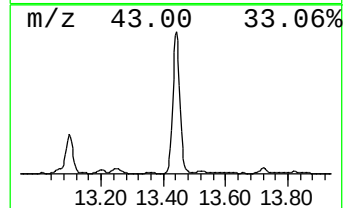
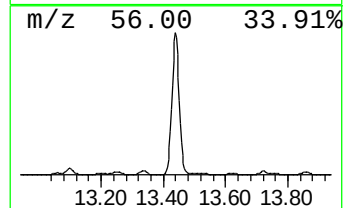
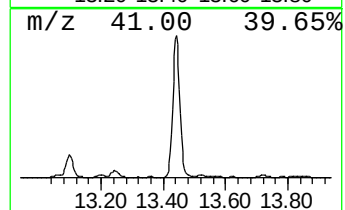
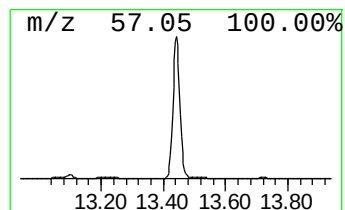
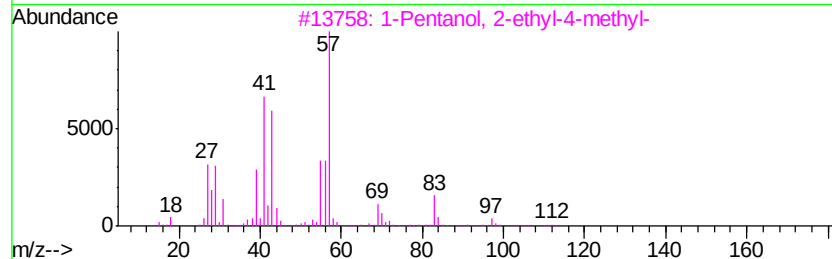
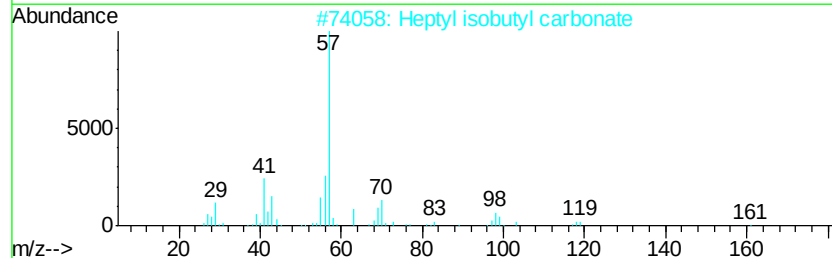
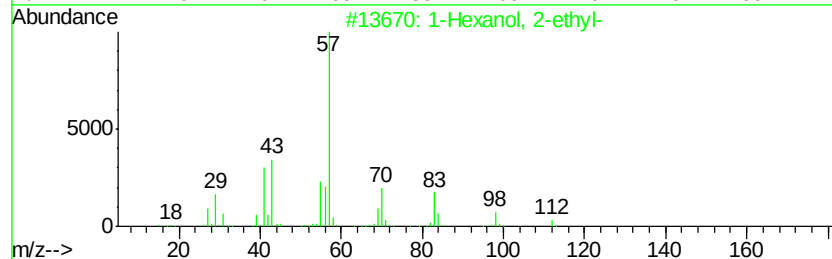
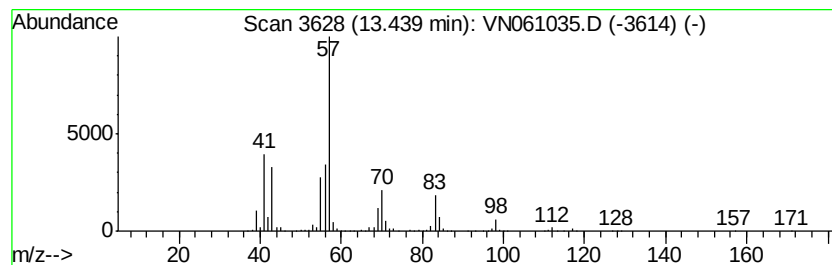
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TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	189.73 ug/l	3191570	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	74
2		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	64
3		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
4		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	45



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN041620\
Data File : VN061035.D
Acq On : 17 Apr 2020 00:15
Operator : JC/MD
Sample : L2299-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-40860-861

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	3.22	335.6	ug/l	3314330	1	7.64	493772	50.0
Butanal	6.50	150.4	ug/l	1485730	1	7.64	493772	50.0
unknown11.53	11.53	274.4	ug/l	5643470	3	11.40	1028500	50.0
Butanoic acid, bu...	12.91	34.8	ug/l	586025	4	13.34	841100	50.0
4-Heptanol, 2,6-d...	13.10	38.0	ug/l	640144	4	13.34	841100	50.0
1-Hexanol, 2-ethyl-	13.44	189.7	ug/l	3191570	4	13.34	841100	50.0