

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN071918\
 Data File : VN049911.D
 Acq On : 19 Jul 2018 12:58
 Operator : MD\SY
 Sample : J4043-03
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SD-BASELINE-WATER

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_N\METHODS\82N071818W.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	1.658	5	21	44	rBV	983126	1520098	43.87%	6.590%
2	1.815	61	70	95	rVB2	103914	166071	4.79%	0.720%
3	2.018	120	133	142	rBV3	27267	52083	1.50%	0.226%
4	2.156	167	176	179	rBV	32744	44863	1.29%	0.195%
5	2.313	218	225	238	rVB	23849	39206	1.13%	0.170%
6	2.461	262	271	287	rBV2	53567	105002	3.03%	0.455%
7	3.133	471	480	492	rBV4	16538	34826	1.01%	0.151%
8	3.278	512	525	547	rVB	86959	215755	6.23%	0.935%
9	3.821	674	694	706	rBV	69683	189178	5.46%	0.820%
10	3.892	707	716	739	rVB2	49379	131812	3.80%	0.571%
11	4.053	748	766	793	rBV2	84676	251879	7.27%	1.092%
12	6.844	1610	1634	1652	rBV2	24562	82131	2.37%	0.356%
13	7.593	1846	1867	1878	rBV	467090	1177817	33.99%	5.106%
14	7.667	1878	1890	1915	rVB	699308	1660861	47.93%	7.201%
15	8.027	1984	2002	2025	rBV	462820	1094075	31.57%	4.743%
16	8.271	2042	2078	2080	rBV4	98355	409016	11.80%	1.773%
17	8.445	2122	2132	2152	rVB	304568	703553	20.30%	3.050%
18	8.586	2160	2176	2191	rBV	1038989	2154397	62.17%	9.341%
19	8.670	2192	2202	2226	rVB2	151281	330805	9.55%	1.434%
20	9.043	2308	2318	2332	rVB3	43929	86997	2.51%	0.377%
21	9.429	2428	2438	2455	rVB3	21617	44053	1.27%	0.191%
22	9.895	2572	2583	2601	rVB2	16803	37605	1.09%	0.163%
23	10.091	2629	2644	2667	rVV	1838042	3465080	100.00%	15.023%
24	10.194	2668	2676	2689	rVV	57924	113105	3.26%	0.490%
25	10.310	2692	2712	2723	rVV3	36225	121522	3.51%	0.527%
26	10.606	2795	2804	2827	rVB2	42901	87760	2.53%	0.380%
27	11.139	2958	2970	2986	rBV2	58470	106706	3.08%	0.463%
28	11.255	2994	3006	3018	rBV3	29488	55173	1.59%	0.239%
29	11.329	3019	3029	3040	rVV2	27938	51895	1.50%	0.225%
30	11.406	3040	3053	3071	rVV	1359204	2389238	68.95%	10.359%
31	11.496	3072	3081	3092	rVV	136668	249210	7.19%	1.080%
32	11.554	3093	3099	3112	rVB	29628	47873	1.38%	0.208%
33	12.152	3278	3285	3295	rVB2	35321	61343	1.77%	0.266%
34	12.265	3307	3320	3339	rBV9	25762	73131	2.11%	0.317%

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35	12.403	3351	3363	3382	rVB	1174736	2014581	58.14%	8.734%
36	12.609	3420	3427	3435	rVB2	27592	41608	1.20%	0.180%
37	12.728	3457	3464	3475	rVB4	33060	57602	1.66%	0.250%
38	13.014	3547	3553	3563	rVB3	33467	54423	1.57%	0.236%
39	13.159	3586	3598	3607	rBV4	31576	64886	1.87%	0.281%
40	13.236	3612	3622	3638	rVV2	179850	353982	10.22%	1.535%
41	13.345	3640	3656	3670	rVB	1208269	2058661	59.41%	8.925%
42	13.451	3679	3689	3702	rVB	382659	614275	17.73%	2.663%
43	13.618	3736	3741	3753	rVB4	36666	65515	1.89%	0.284%
44	13.763	3778	3786	3793	rBV4	23142	44368	1.28%	0.192%
45	13.821	3799	3804	3820	rVB5	33402	65234	1.88%	0.283%
46	14.062	3872	3879	3891	rBV4	37924	60400	1.74%	0.262%
47	14.380	3970	3978	3990	rVB8	27348	50182	1.45%	0.218%
48	14.467	3998	4005	4014	rVB4	29920	46333	1.34%	0.201%
49	14.525	4017	4023	4030	rVB6	24571	35659	1.03%	0.155%
50	14.657	4057	4064	4070	rBV5	23406	42471	1.23%	0.184%
51	14.850	4116	4124	4127	rBV3	28222	40798	1.18%	0.177%

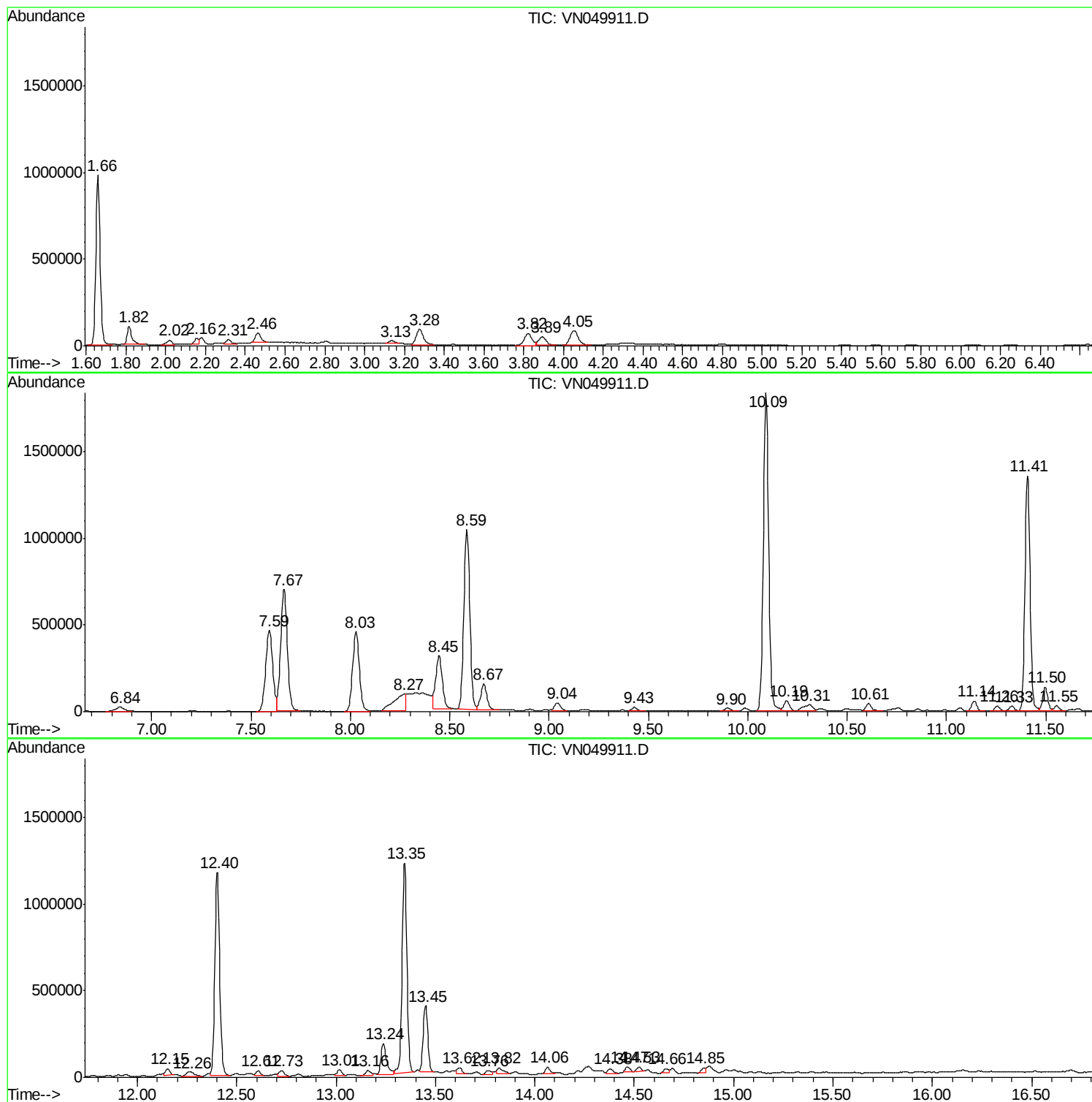
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N071818W.M
Quant Title : SW846 8260

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



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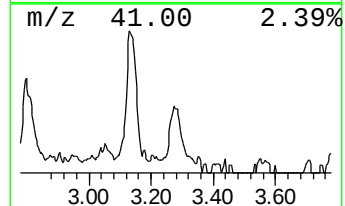
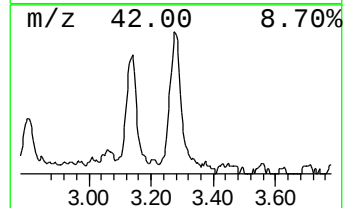
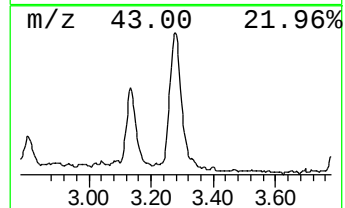
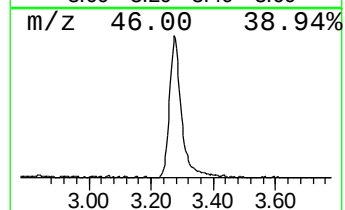
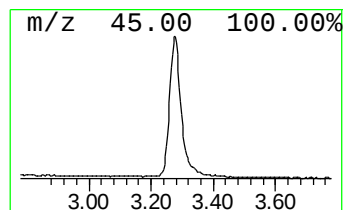
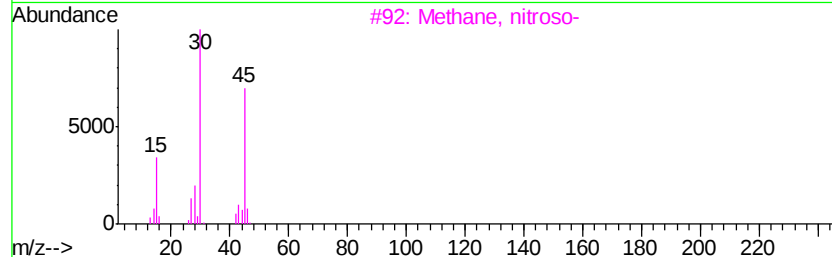
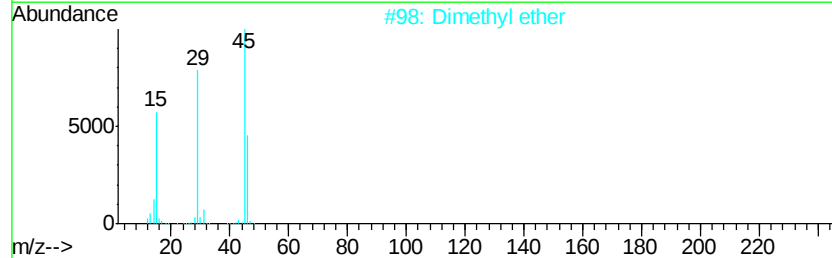
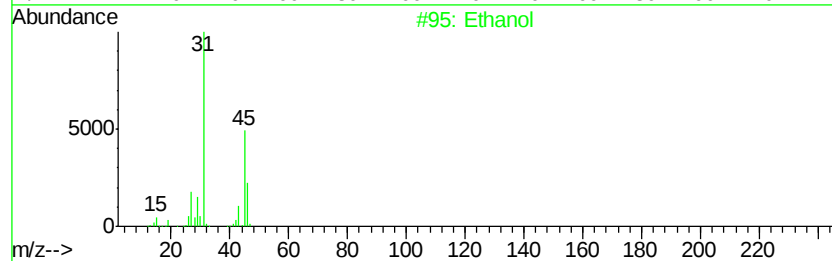
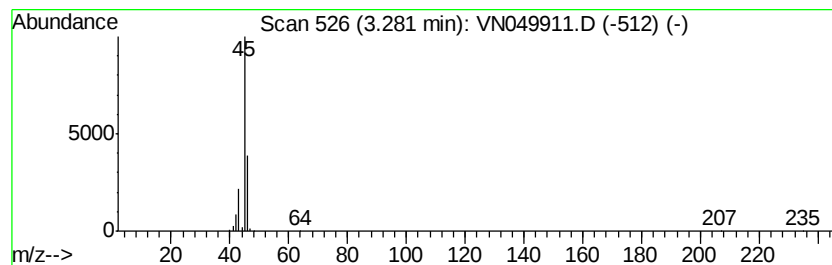
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N071818W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	6.50 ug/l	215755	Pentafluorobenzene	7.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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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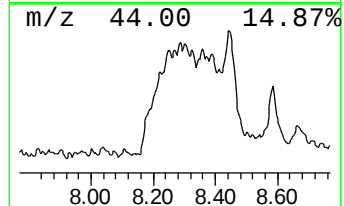
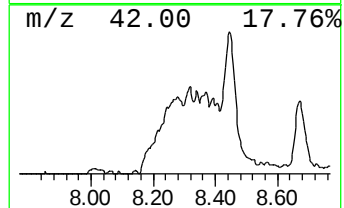
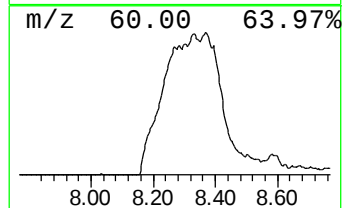
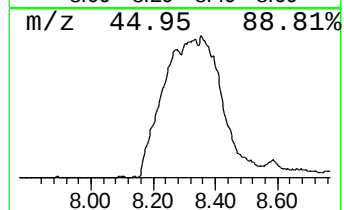
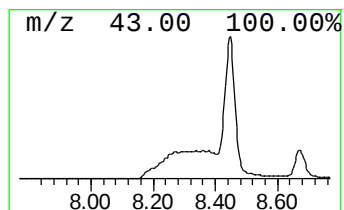
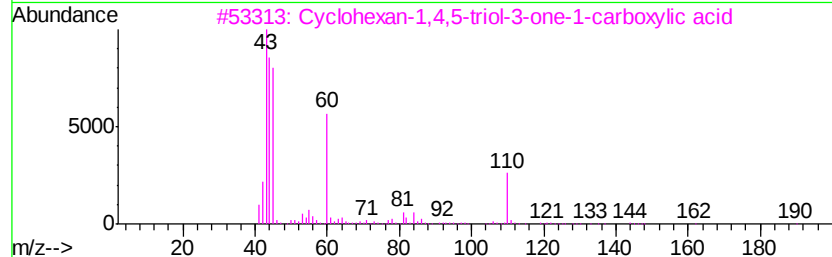
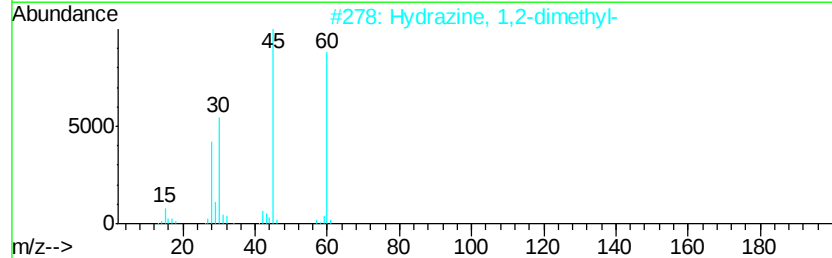
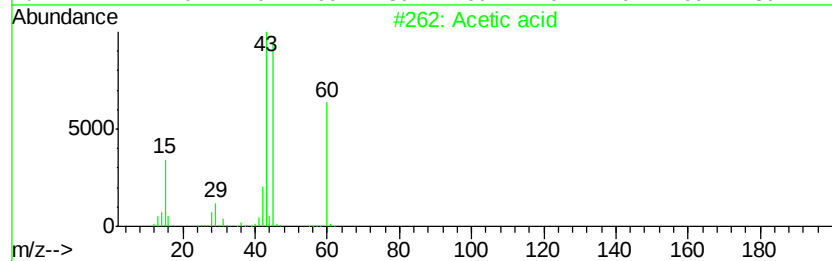
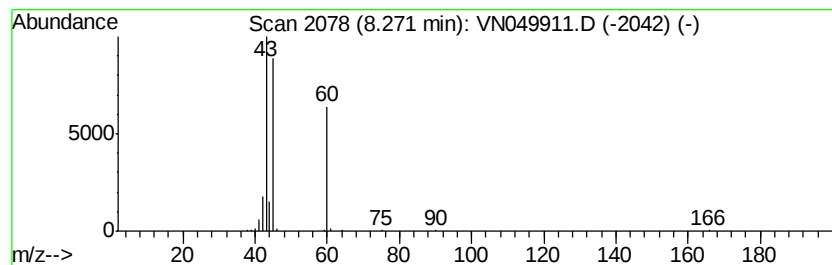
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Quant Title : SW846 8260

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

Peak Number 3 Acetic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.27	9.49 ug/l	409016	1,4-Difluorobenzene	8.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid	60	C2H4O2	000064-19-7	86
2		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	64
3		Cyclohexan-1,4,5-triol-3-one-1-c...	190	C7H10O6	1000128-45-5	40
4		Formic acid hydrazide	60	CH4N2O	000624-84-0	9
5		Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9



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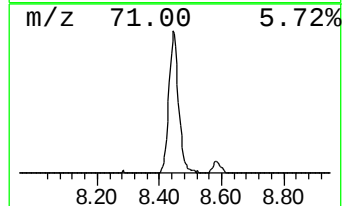
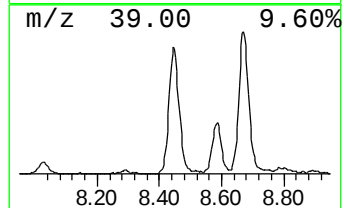
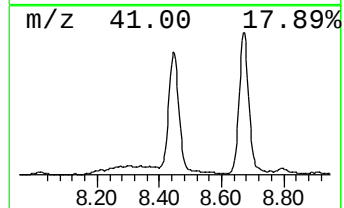
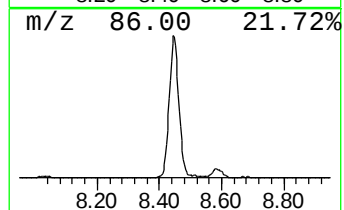
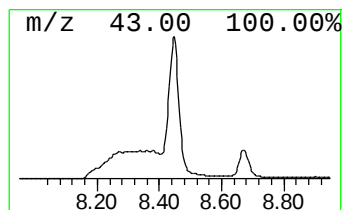
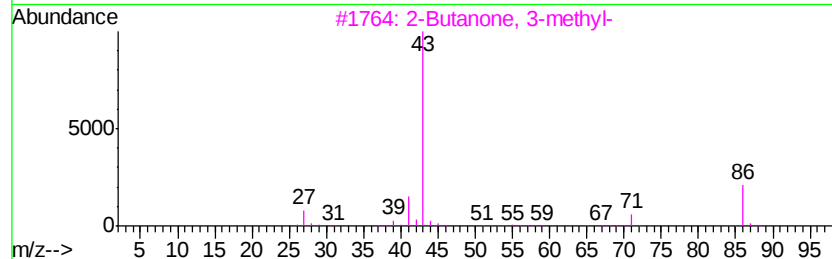
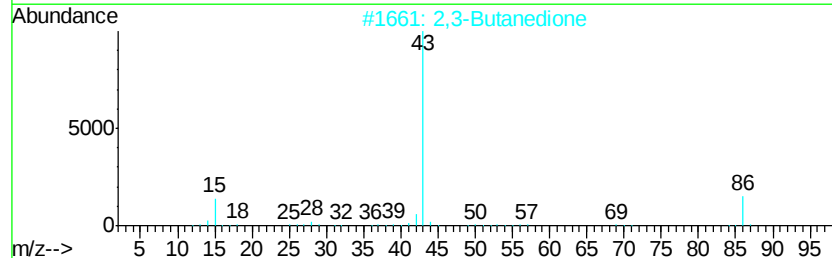
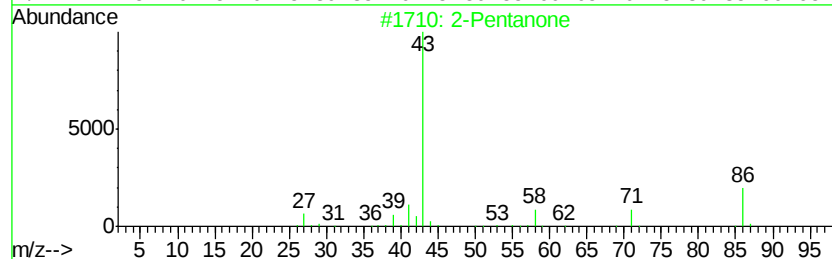
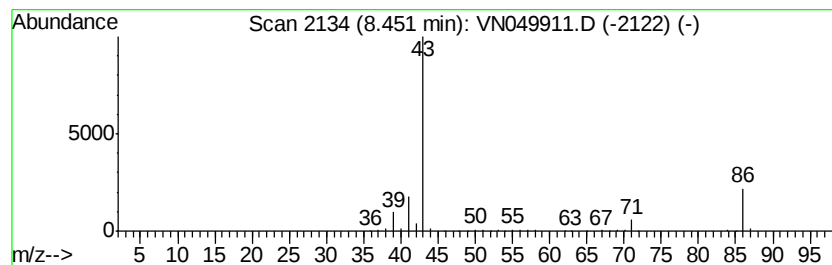
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	16.33 ug/l	703553	1,4-Difluorobenzene	8.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone	86	C5H10O	000107-87-9	64
2		2,3-Butanedione	86	C4H6O2	000431-03-8	50
3		2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	42
4		2-Imidazolidinone	86	C3H6N2O	000120-93-4	7
5		Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	5



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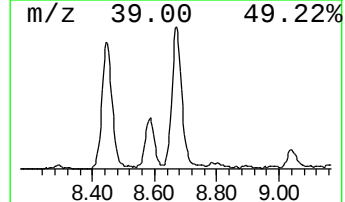
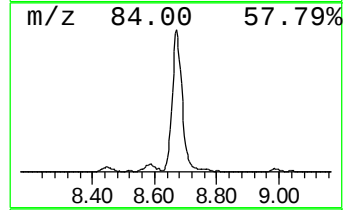
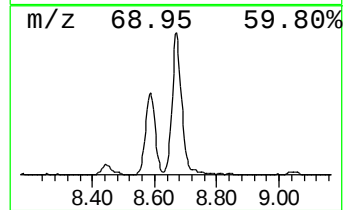
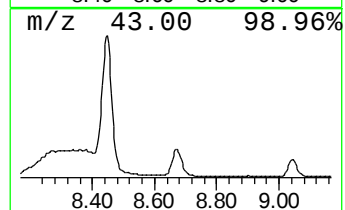
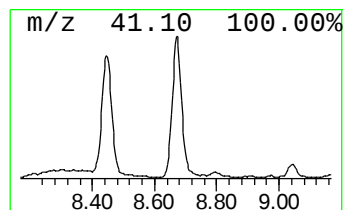
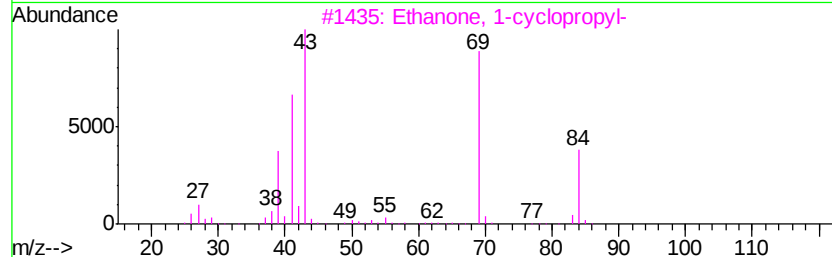
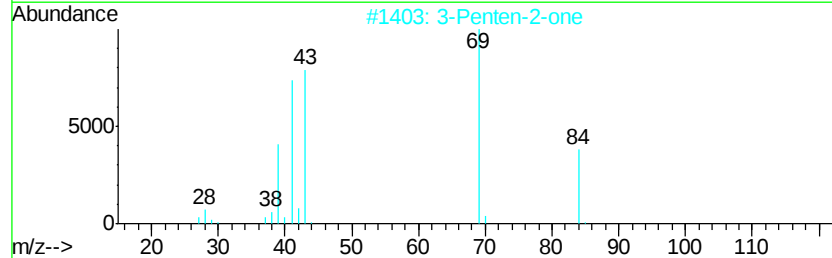
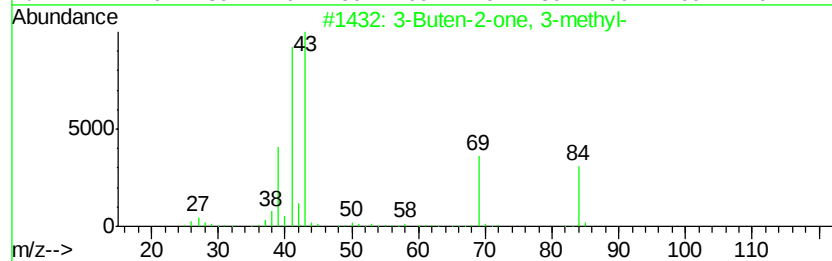
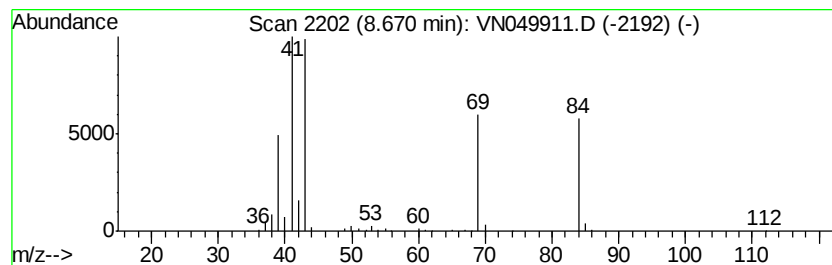
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Buten-2-one, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.67	7.68 ug/l	330805	1,4-Difluorobenzene	8.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	91
2		3-Penten-2-one	84	C5H8O	000625-33-2	90
3		Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	58
4		Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	50
5		2-Butanone, 4-hydroxy-3-(hydroxy...	132	C6H12O3	006868-97-9	42



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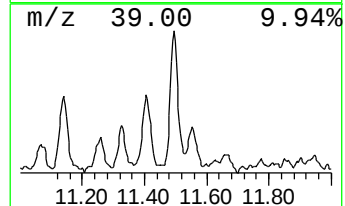
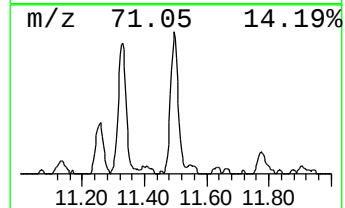
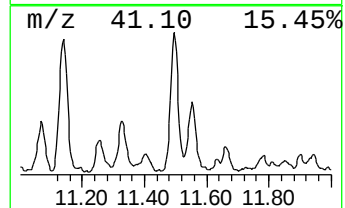
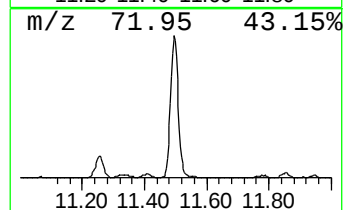
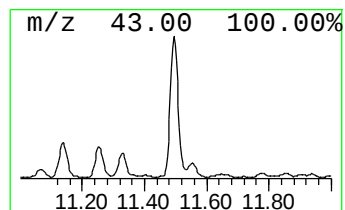
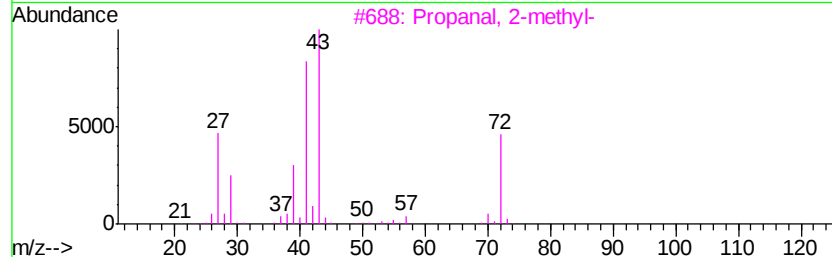
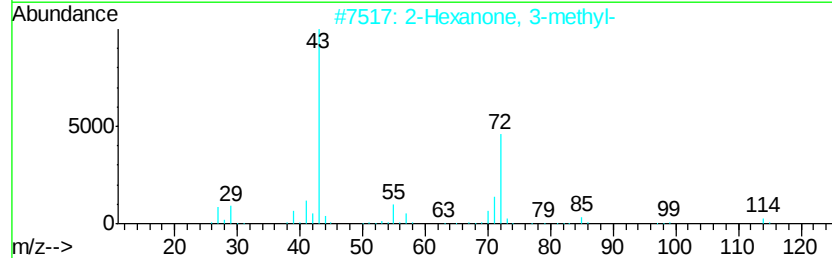
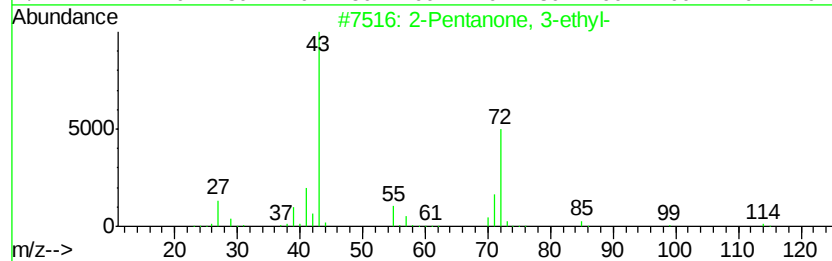
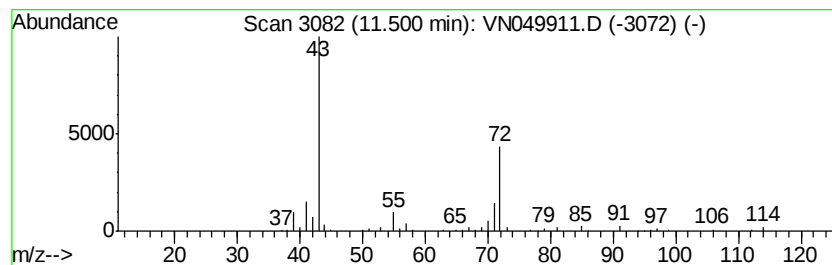
Instrument :
MSVOA_N
ClientSampleId :
SD-BASELINE-WATER

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N071818W.M
Quant Title : SW846 8260

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

Peak Number 6 2-Pentanone, 3-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.50	5.22 ug/l	249210	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Pentanone, 3-ethyl-	114 C7H14O	006137-03-7	91
2	2-Hexanone, 3-methyl-	114 C7H14O	002550-21-2	91
3	Propanal, 2-methyl-	72 C4H8O	000078-84-2	59
4	2-Hexanone, 3,4-dimethyl-	128 C8H16O	019550-10-8	42
5	1-Methylallyl acetate	114 C6H10O2	006737-11-7	38



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN071918\
Data File : VN049911.D
Acq On : 19 Jul 2018 12:58
Operator : MD\SY
Sample : J4043-03
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SD-BASELINE-WATER

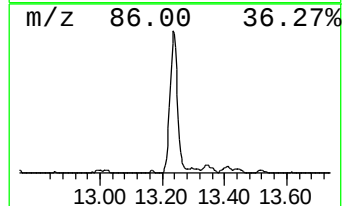
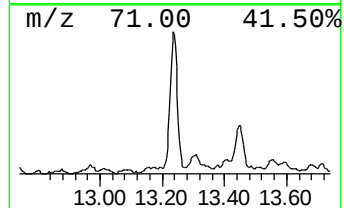
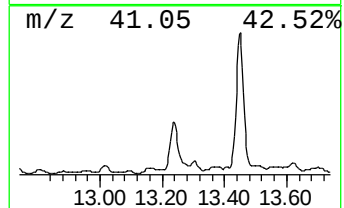
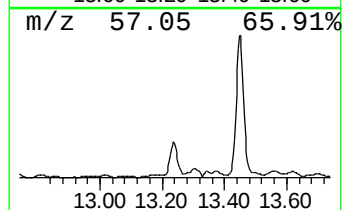
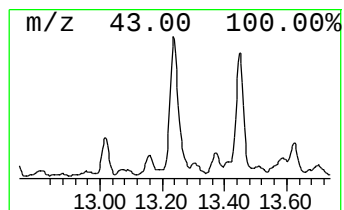
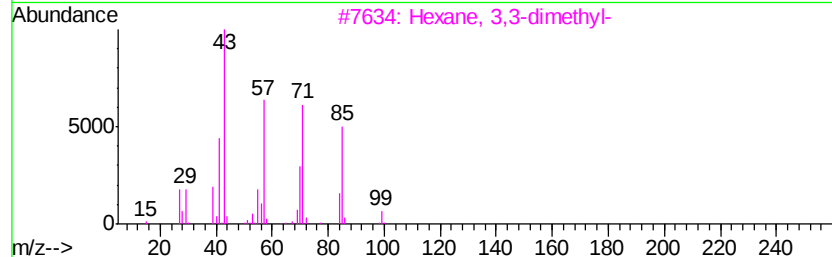
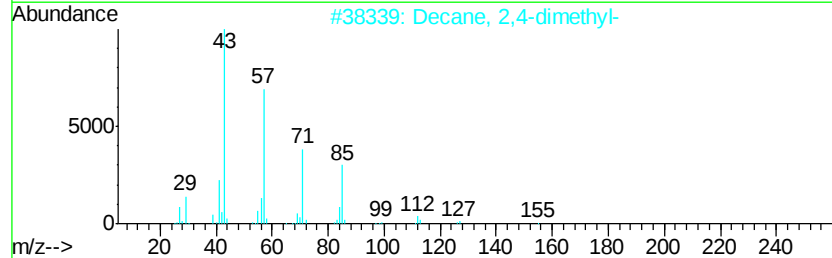
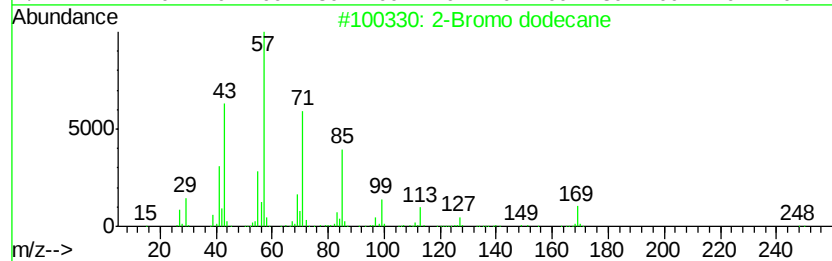
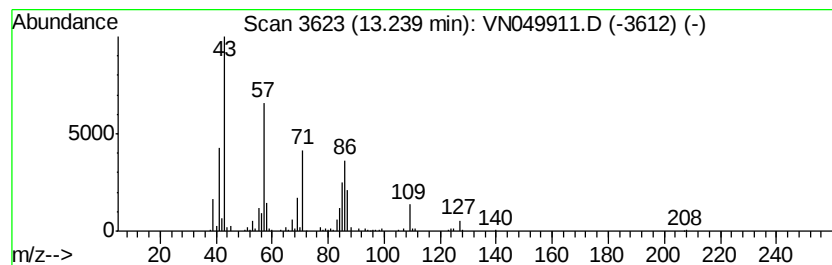
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.24 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	8.60 ug/l	353982	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Bromo dodecane	248	C12H25Br	013187-99-0	43
2		Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	43
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	43
4		Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	38
5		3-Heptanone, 4-methyl-	128	C8H16O	006137-11-7	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN071918\
Data File : VN049911.D
Acq On : 19 Jul 2018 12:58
Operator : MD\SY
Sample : J4043-03
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 8 Sample Multiplier: 1

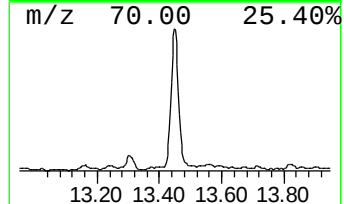
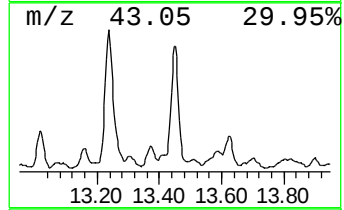
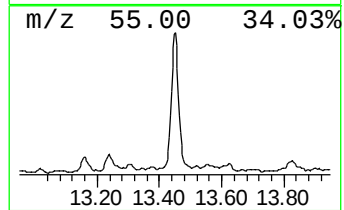
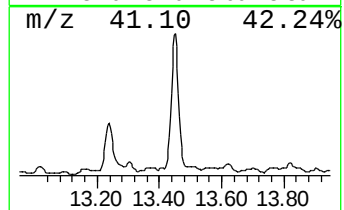
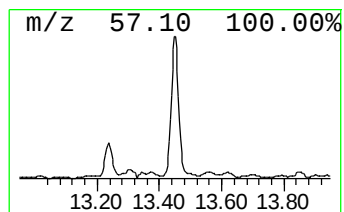
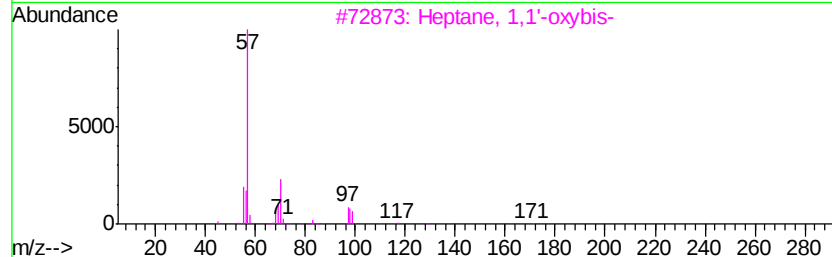
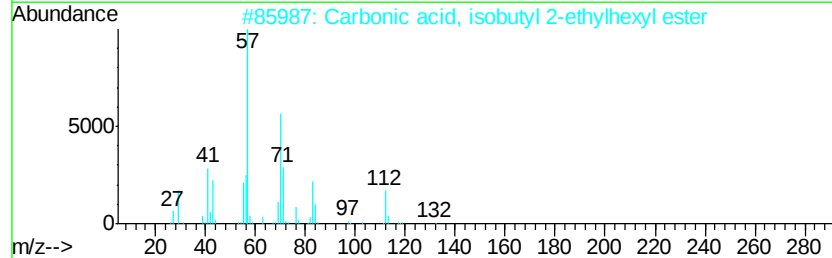
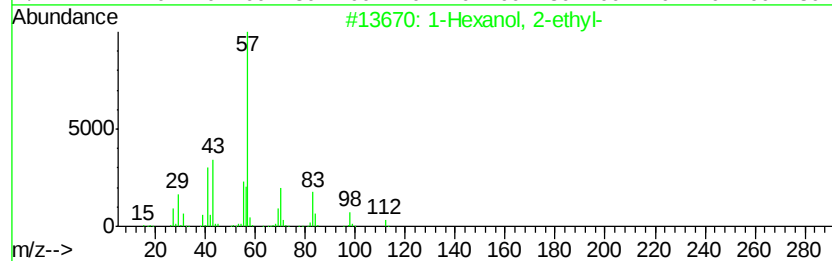
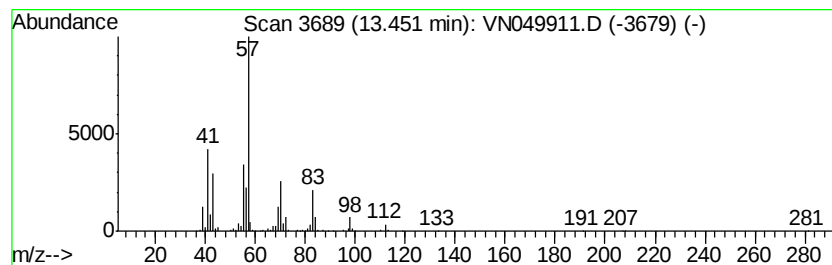
Instrument :
MSVOA_N
ClientSampleId :
SD-BASELINE-WATER

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N071818W.M
Quant Title : SW846 8260

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

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	14.92 ug/l	614275	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7 83
2		Carbonic acid, isobutyl 2-ethylh...	230 C13H26O3	1000357-82-9 50
3		Heptane, 1,1'-oxybis-	214 C14H30O	000629-64-1 50
4		2-Propyl-1-pentanol	130 C8H18O	058175-57-8 47
5		1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2 40



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN071918\
Data File : VN049911.D
Acq On : 19 Jul 2018 12:58
Operator : MD\SY
Sample : J4043-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SD-BASELINE-WATER

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N071818W.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	3.28	6.5	ug/l	215755	1	7.67	1660860	50.0
Acetic acid	8.27	9.5	ug/l	409016	2	8.59	2154400	50.0
2-Pentanone	8.45	16.3	ug/l	703553	2	8.59	2154400	50.0
3-Buten-2-one, 3-...	8.67	7.7	ug/l	330805	2	8.59	2154400	50.0
2-Pentanone, 3-et...	11.50	5.2	ug/l	249210	3	11.41	2389240	50.0
unknown13.24	13.24	8.6	ug/l	353982	4	13.35	2058660	50.0
1-Hexanol, 2-ethyl-	13.45	14.9	ug/l	614275	4	13.35	2058660	50.0