

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050222\
 Data File : VN072300.D
 Acq On : 02 May 2022 17:46
 Operator : JC\MD
 Sample : N2653-08RE
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 30992RE

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\82N042622W.M
 Title : SW846 8260

Signal : TIC: VN072300.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.034	3	8	18	rVB	28099	56480	3.95%	0.483%
2	2.234	37	42	44	rBV2	24605	38122	2.67%	0.326%
3	2.587	97	102	110	rVB	48463	80991	5.67%	0.692%
4	3.681	278	288	312	rBV	504263	1374703	96.19%	11.750%
5	4.298	383	393	400	rBV2	15173	43972	3.08%	0.376%
6	4.575	431	440	453	rVB2	9688	29999	2.10%	0.256%
7	7.057	848	862	879	rBV	491589	1429208	100.00%	12.216%
8	7.333	900	909	921	rBV	65113	175761	12.30%	1.502%
9	7.657	953	964	971	rBV4	5534	15422	1.08%	0.132%
10	8.016	1016	1025	1031	rBV	182838	453748	31.75%	3.878%
11	8.081	1031	1036	1047	rVB	288333	654975	45.83%	5.598%
12	8.433	1085	1096	1108	rBV	224615	538066	37.65%	4.599%
13	8.963	1177	1186	1196	rBV	406196	827566	57.90%	7.073%
14	9.151	1211	1218	1236	rBV	51390	135776	9.50%	1.161%
15	9.527	1274	1282	1292	rBV2	69394	140576	9.84%	1.202%
16	10.439	1427	1437	1445	rBV	742716	1367429	95.68%	11.688%
17	10.598	1456	1464	1471	rBV7	7935	17823	1.25%	0.152%
18	10.857	1500	1508	1522	rBV2	47476	118337	8.28%	1.011%
19	11.739	1646	1658	1671	rBV	544367	1027316	71.88%	8.781%
20	12.098	1714	1719	1725	rBV2	9553	17199	1.20%	0.147%
21	12.268	1741	1748	1751	rBV3	9803	16944	1.19%	0.145%
22	12.316	1751	1756	1764	rVB2	41127	73693	5.16%	0.630%
23	12.727	1818	1826	1837	rBV	501551	861908	60.31%	7.367%
24	13.133	1887	1895	1898	rBV3	28106	53373	3.73%	0.456%
25	13.163	1898	1900	1905	rVV2	27712	39188	2.74%	0.335%
26	13.227	1907	1911	1919	rVB	34934	56505	3.95%	0.483%
27	13.386	1929	1938	1939	rBV4	10088	16979	1.19%	0.145%
28	13.421	1939	1944	1956	rVB	112189	201555	14.10%	1.723%
29	13.527	1956	1962	1967	rBV4	16559	27785	1.94%	0.237%
30	13.668	1977	1986	1995	rBV	440463	776424	54.33%	6.636%
31	13.768	1996	2003	2014	rBV	557838	980649	68.61%	8.382%
32	15.457	2282	2290	2295	rBV4	12262	24207	1.69%	0.207%
33	15.533	2295	2303	2309	rVB7	11306	26903	1.88%	0.230%

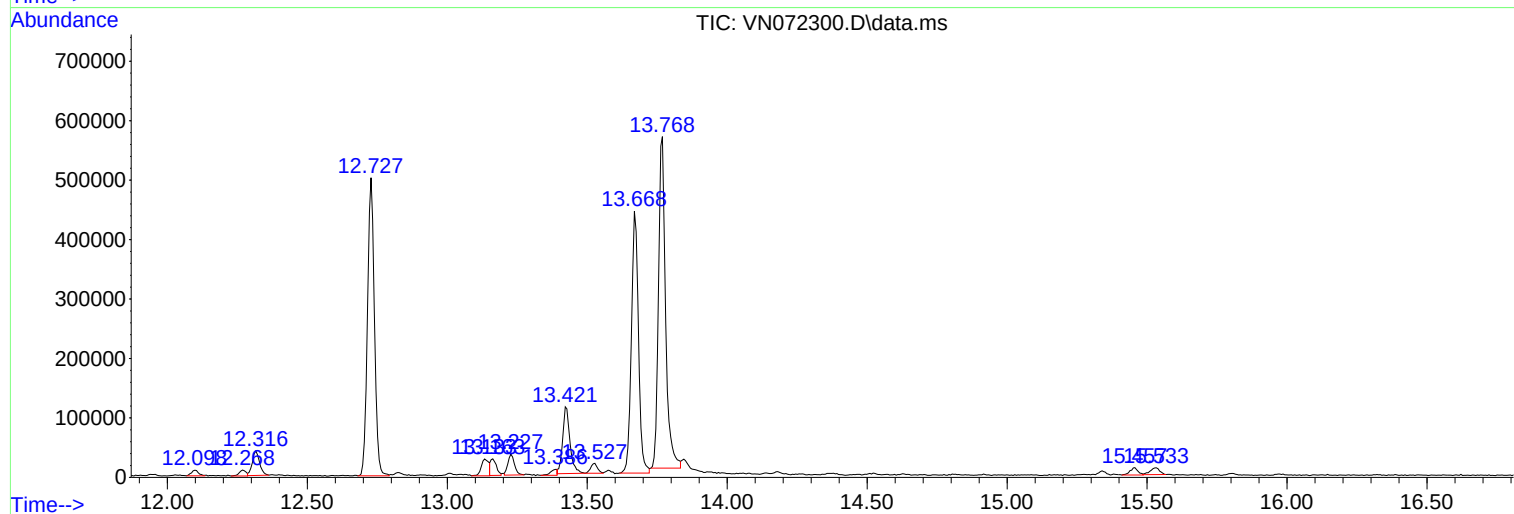
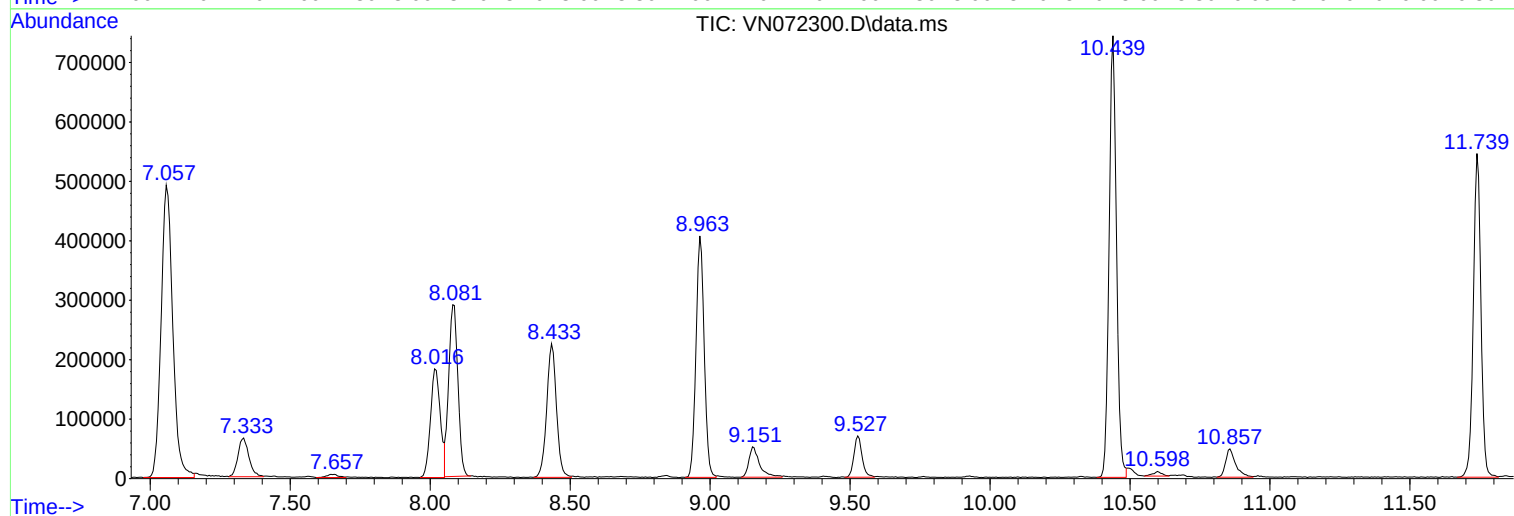
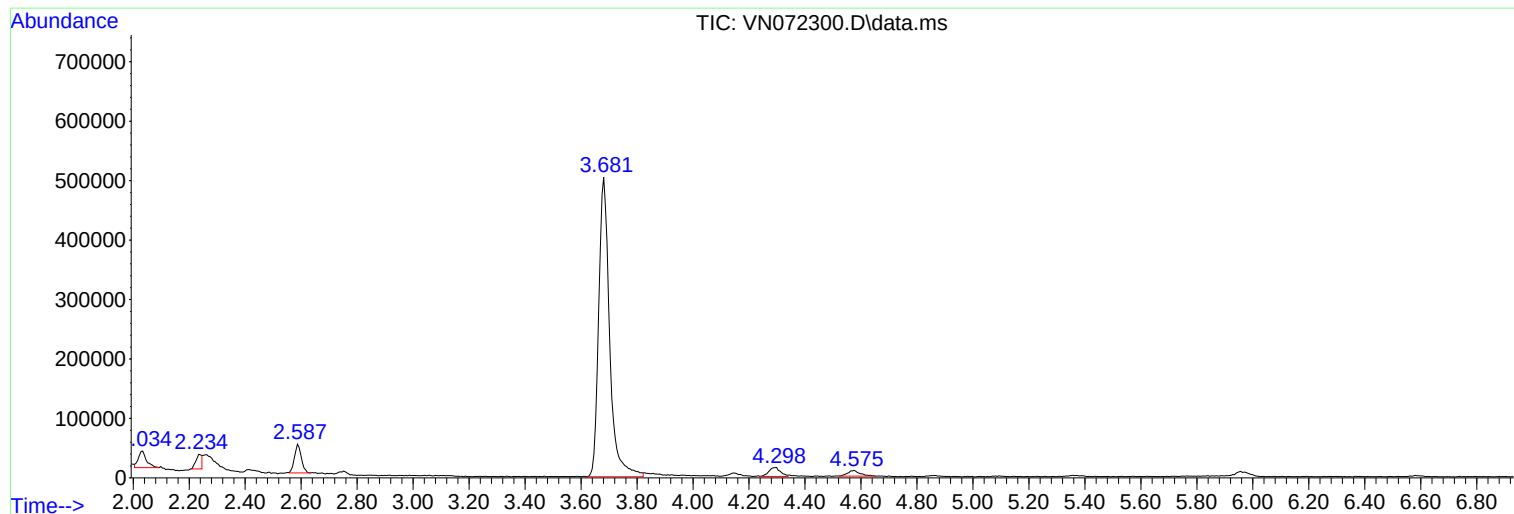
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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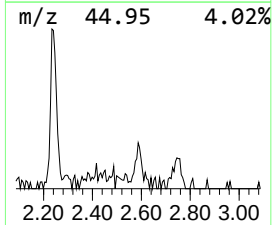
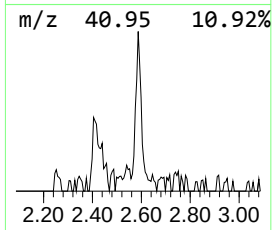
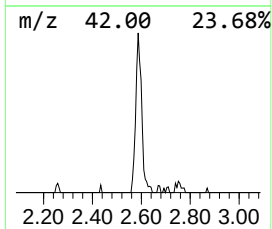
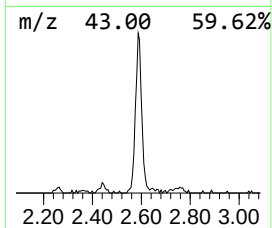
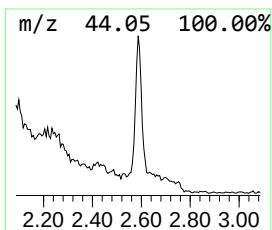
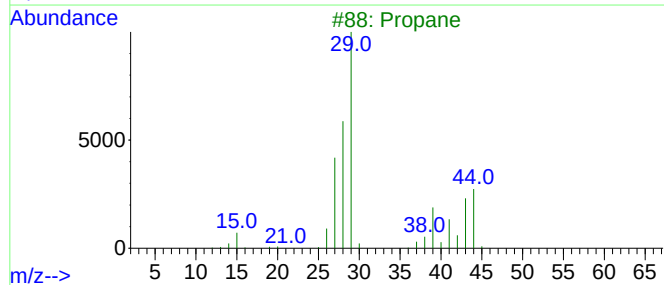
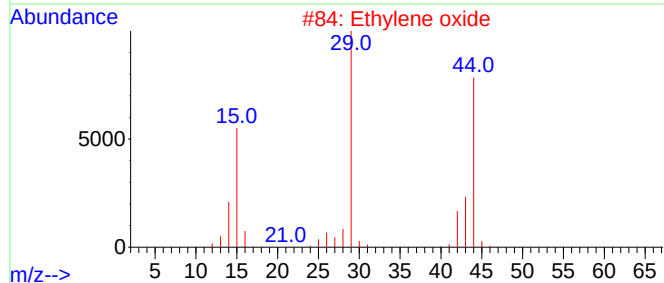
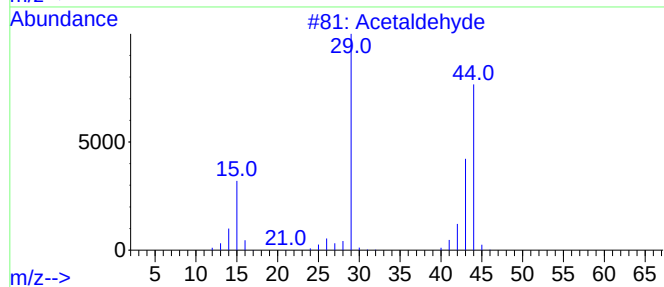
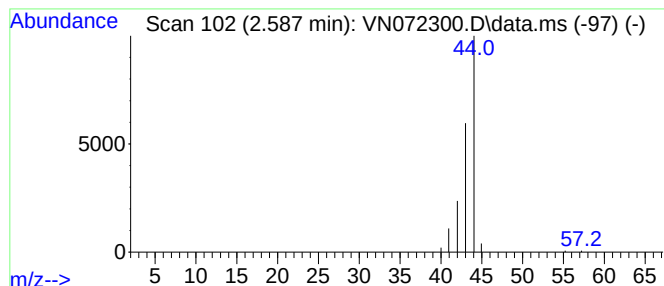
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.587	6.18 ug/l	80991	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Ethyne, fluoro-	44	C2HF	002713-09-9	3



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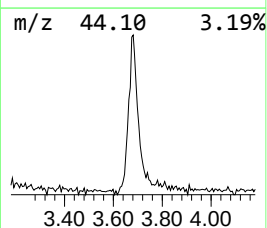
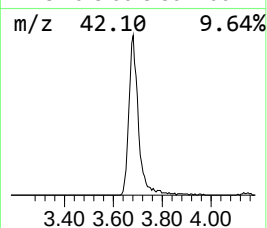
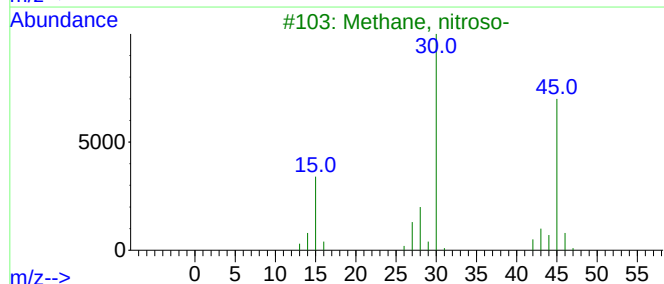
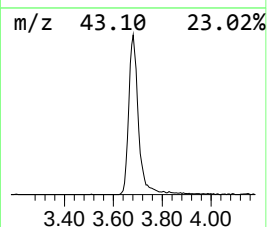
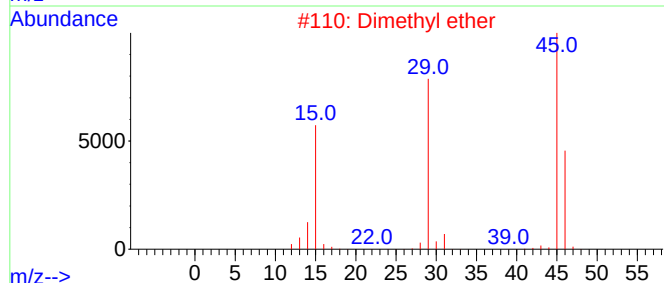
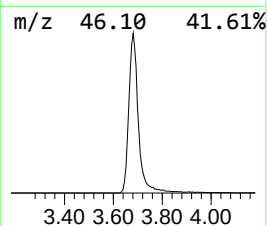
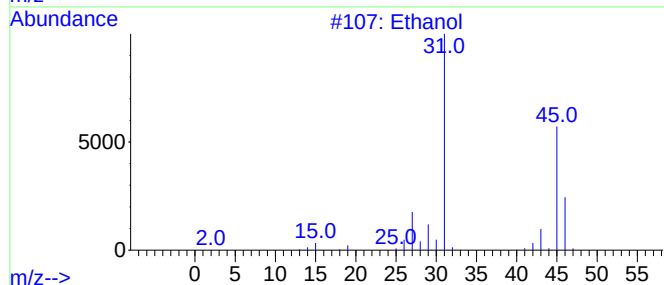
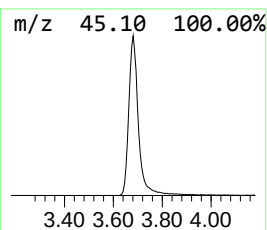
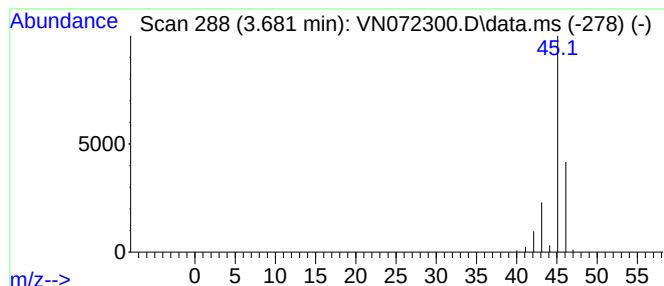
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.681	104.94 ug/l	1374700	Pentafluorobenzene	8.086

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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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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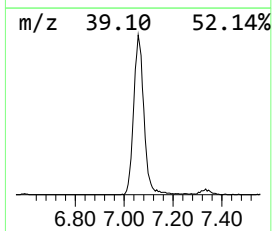
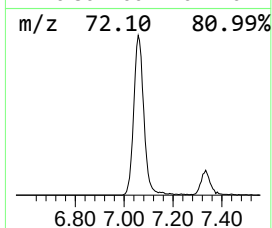
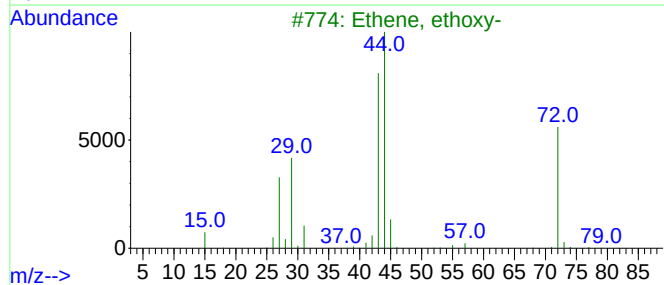
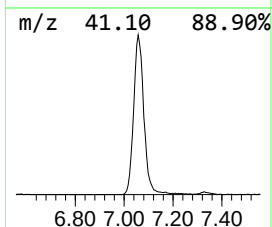
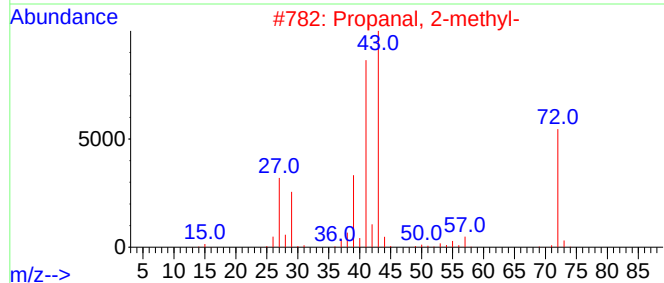
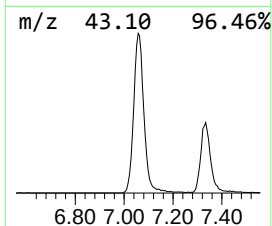
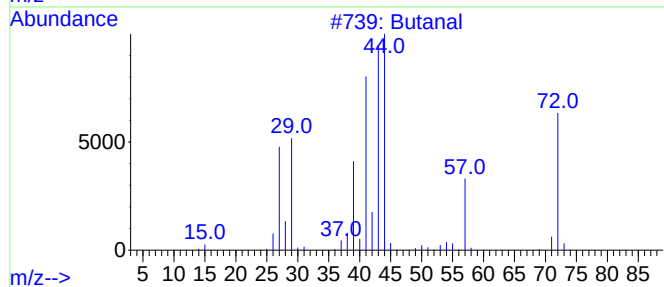
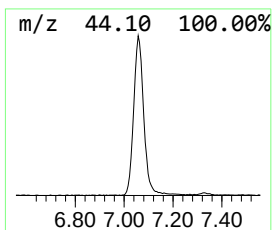
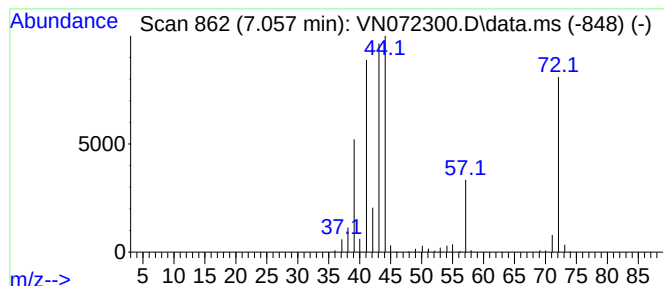
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.057	109.10 ug/l	1429210	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	40
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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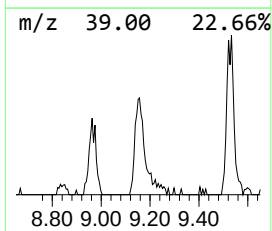
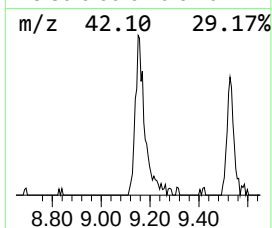
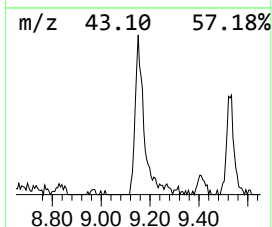
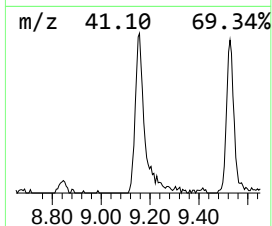
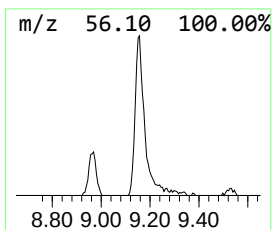
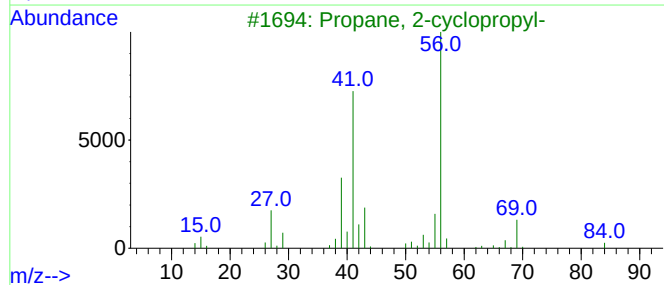
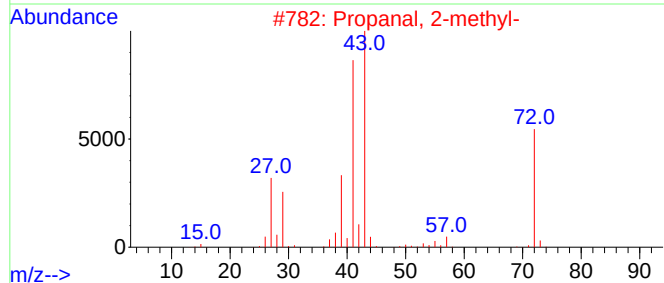
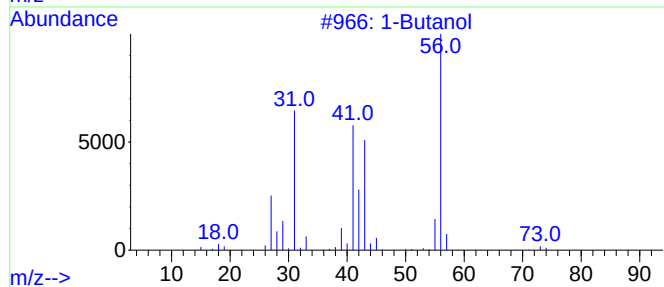
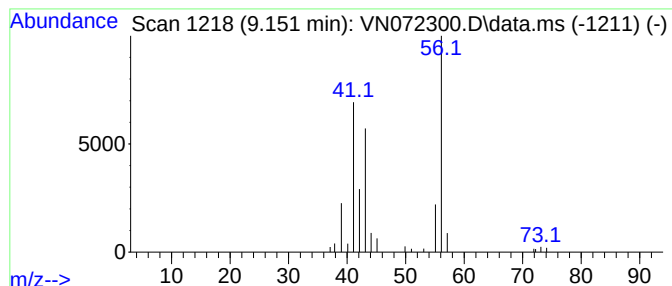
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.151	8.20 ug/l	135776	1,4-Difluorobenzene	8.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	10
3			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
5			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9



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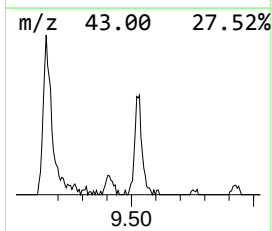
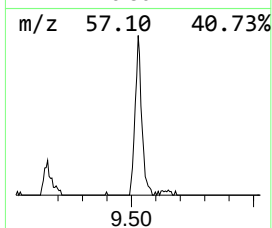
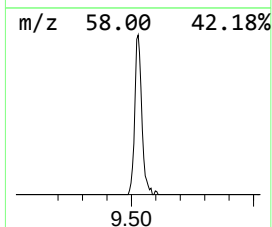
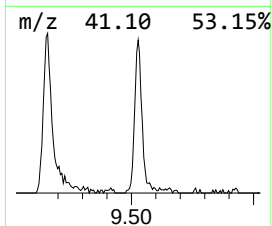
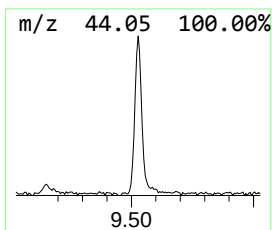
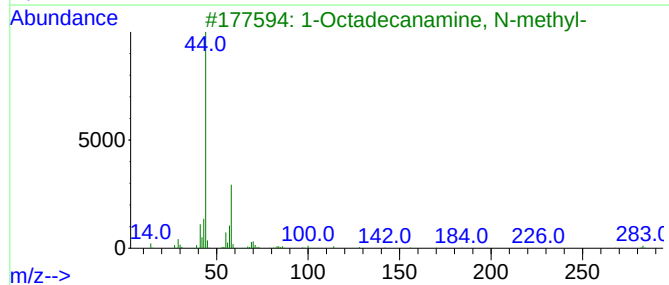
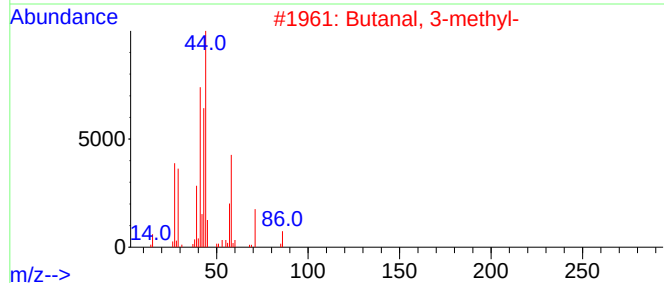
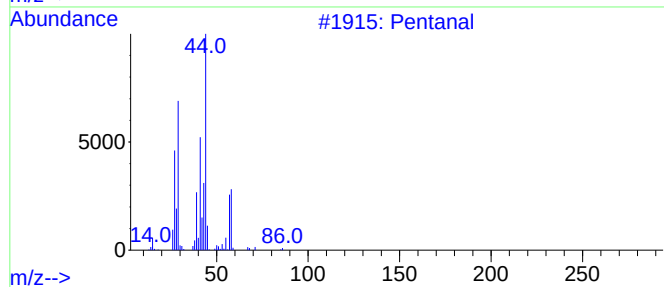
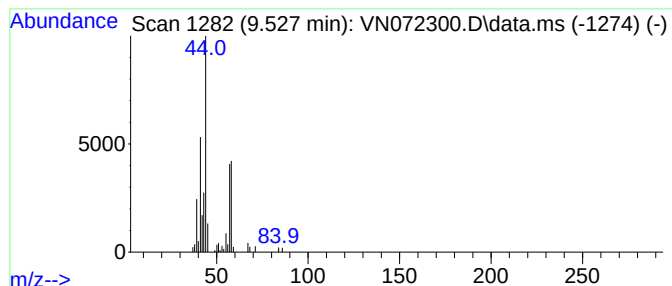
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.527	8.49 ug/l	140576	1,4-Difluorobenzene	8.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	86
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	78
3			1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	40
4			Cyclopropyl carbinol	72	C4H8O	002516-33-8	28
5			2-Formylhistamine	139	C6H9N3O	1000132-95-8	9



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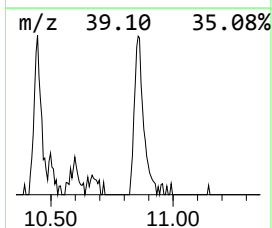
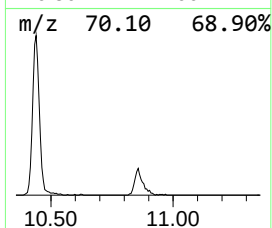
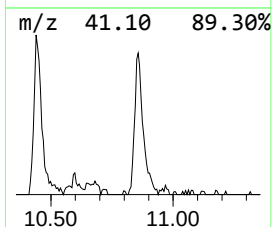
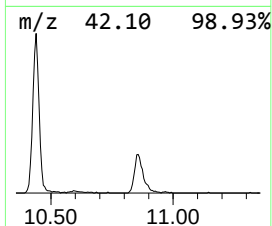
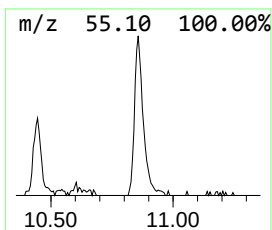
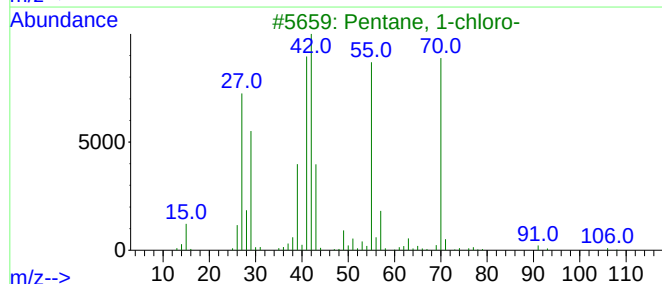
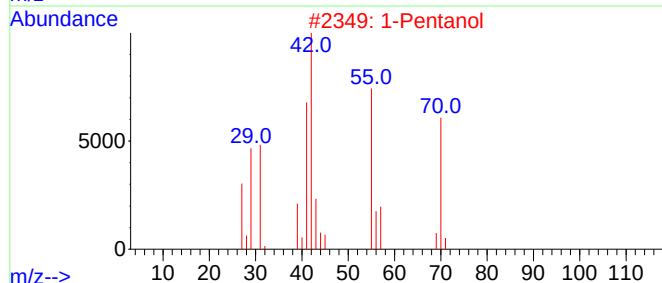
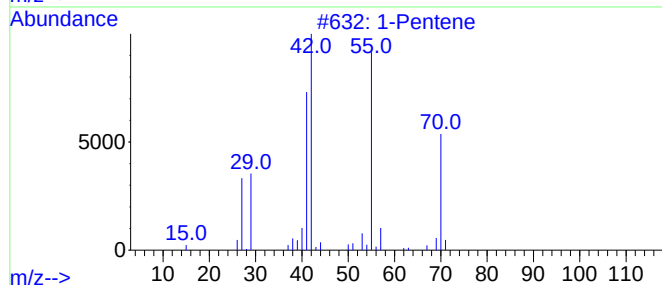
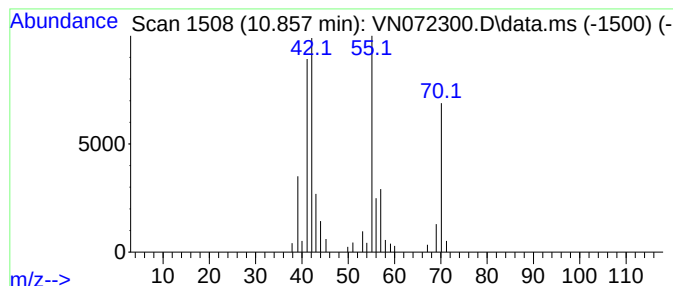
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Pentene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.857	5.76 ug/l	118337	Chlorobenzene-d5	11.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene	70	C5H10	000109-67-1	80
2			1-Pentanol	88	C5H12O	000071-41-0	78
3			Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	59
4			Cyclopentane	70	C5H10	000287-92-3	59
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050222\
Data File : VN072300.D
Acq On : 02 May 2022 17:46
Operator : JC\MD
Sample : N2653-08RE
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30992RE

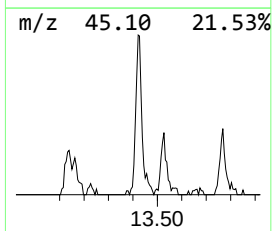
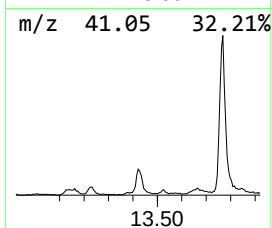
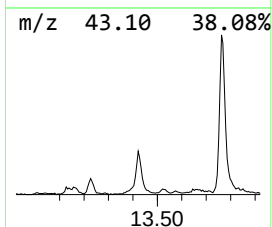
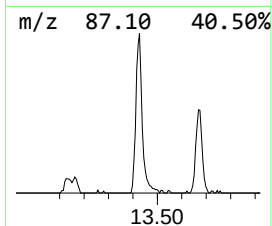
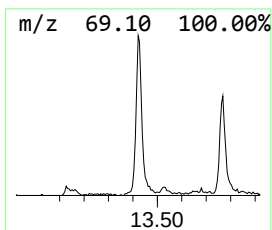
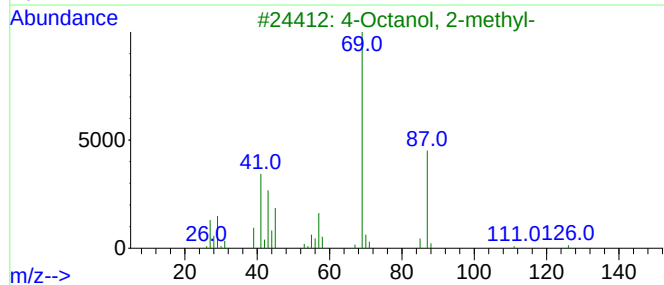
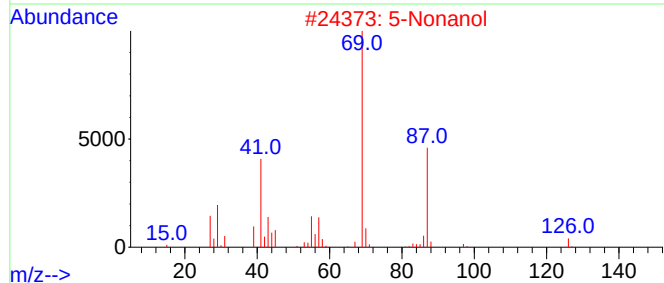
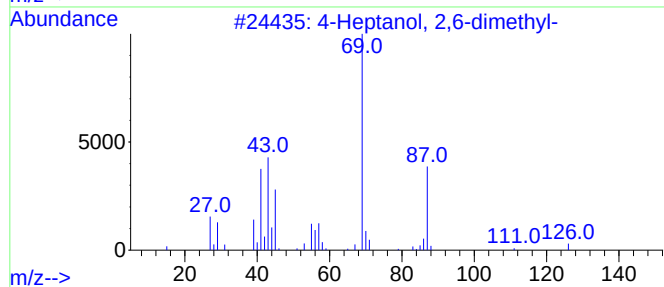
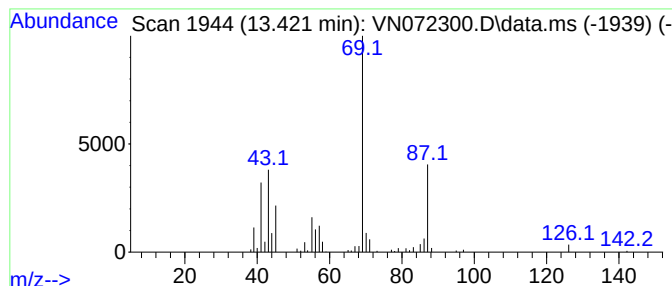
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 4-Heptanol, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.421	12.98 ug/l	201555	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	90
2			5-Nonanol	144	C9H20O	000623-93-8	72
3			4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	72
4			5-Decanol	158	C10H22O	005205-34-5	64
5			1,2-Hexanediol	118	C6H14O2	006920-22-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050222\
Data File : VN072300.D
Acq On : 02 May 2022 17:46
Operator : JC\MD
Sample : N2653-08RE
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30992RE

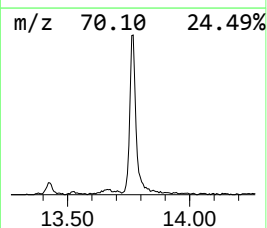
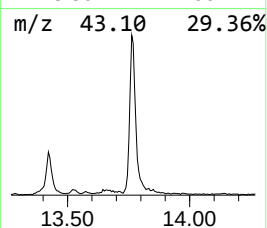
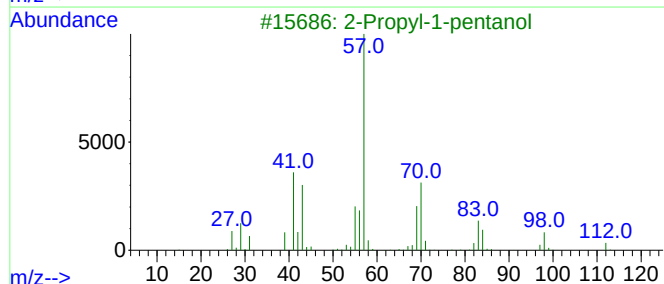
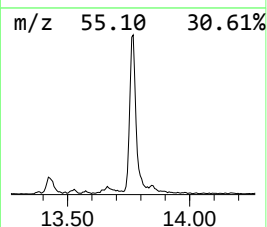
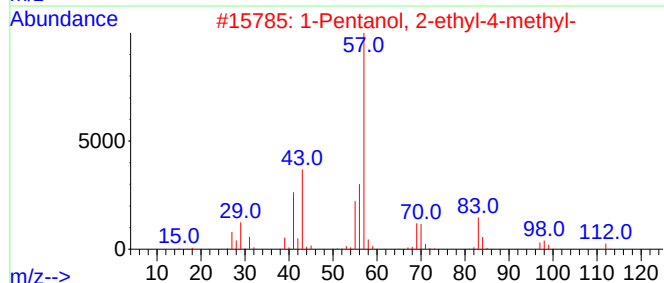
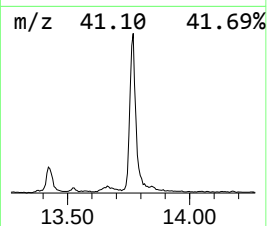
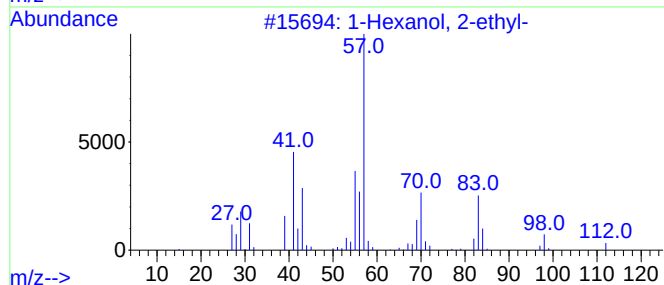
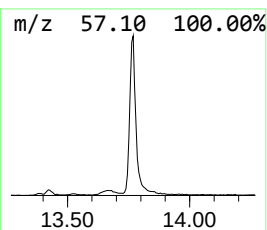
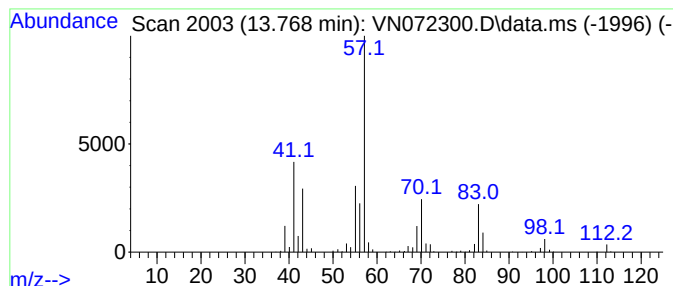
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.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.
13.768	63.15 ug/l	980649	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050222\
Data File : VN072300.D
Acq On : 02 May 2022 17:46
Operator : JC\MD
Sample : N2653-08RE
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30992RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.587	6.2	ug/l	80991	1	8.086	654975	50.0
Ethanol	3.681	104.9	ug/l	1374700	1	8.086	654975	50.0
Butanal	7.057	109.1	ug/l	1429210	1	8.086	654975	50.0
1-Butanol	9.151	8.2	ug/l	135776	2	8.963	827566	50.0
Pentanal	9.527	8.5	ug/l	140576	2	8.963	827566	50.0
1-Pentene	10.857	5.8	ug/l	118337	3	11.739	1027320	50.0
4-Heptanol, 2,6...	13.421	13.0	ug/l	201555	4	13.668	776424	50.0
1-Hexanol, 2-et...	13.768	63.1	ug/l	980649	4	13.668	776424	50.0