

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010522\
 Data File : VN070490.D
 Acq On : 5 Jan 2022 15:31
 Operator : JC/MD
 Sample : N1012-07
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31239

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\82N122721W.M

Title : SW846 8260

Signal : TIC: VN070490.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.236	77	92	147	rBV2	21563023	36740933	100.00%	36.547%
2	4.283	829	855	937	rBV	10371585	31031547	84.46%	30.867%
3	4.580	946	966	1020	rVB2	614904	2045686	5.57%	2.035%
4	6.584	1688	1713	1752	rBV5	175010	615646	1.68%	0.612%
5	7.061	1868	1891	1924	rBV3	174710	550463	1.50%	0.548%
6	8.021	2226	2249	2260	rBV2	623957	1503366	4.09%	1.495%
7	8.083	2261	2272	2300	rVB	1229348	2766066	7.53%	2.751%
8	8.437	2382	2404	2435	rBV	801642	1895795	5.16%	1.886%
9	8.968	2582	2602	2640	rBV	1840907	3886108	10.58%	3.866%
10	9.268	2700	2714	2735	rVB2	219319	427750	1.16%	0.425%
11	10.440	3133	3151	3167	rBV	2720744	5065080	13.79%	5.038%
12	11.186	3408	3429	3477	rBV	853446	1874295	5.10%	1.864%
13	11.744	3614	3637	3664	rBV	2496262	4568218	12.43%	4.544%
14	12.731	3992	4005	4031	rVB	1922720	3429033	9.33%	3.411%
15	13.675	4341	4357	4378	rBV	1770739	3146439	8.56%	3.130%
16	13.771	4380	4393	4415	rBV	566441	985292	2.68%	0.980%

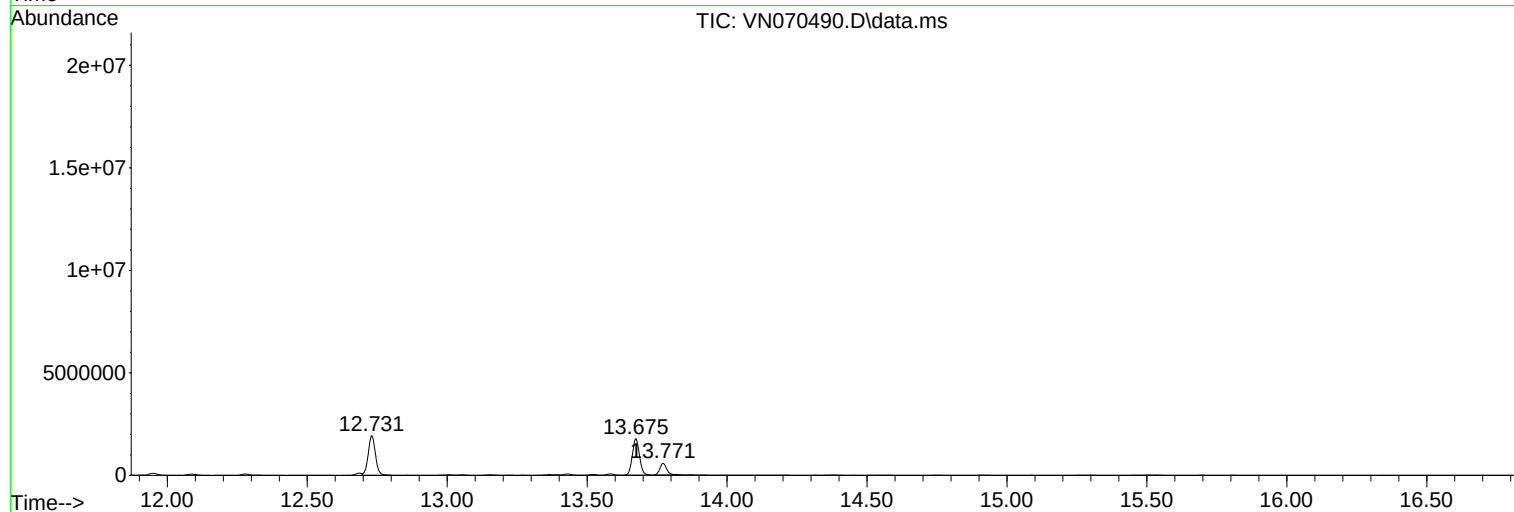
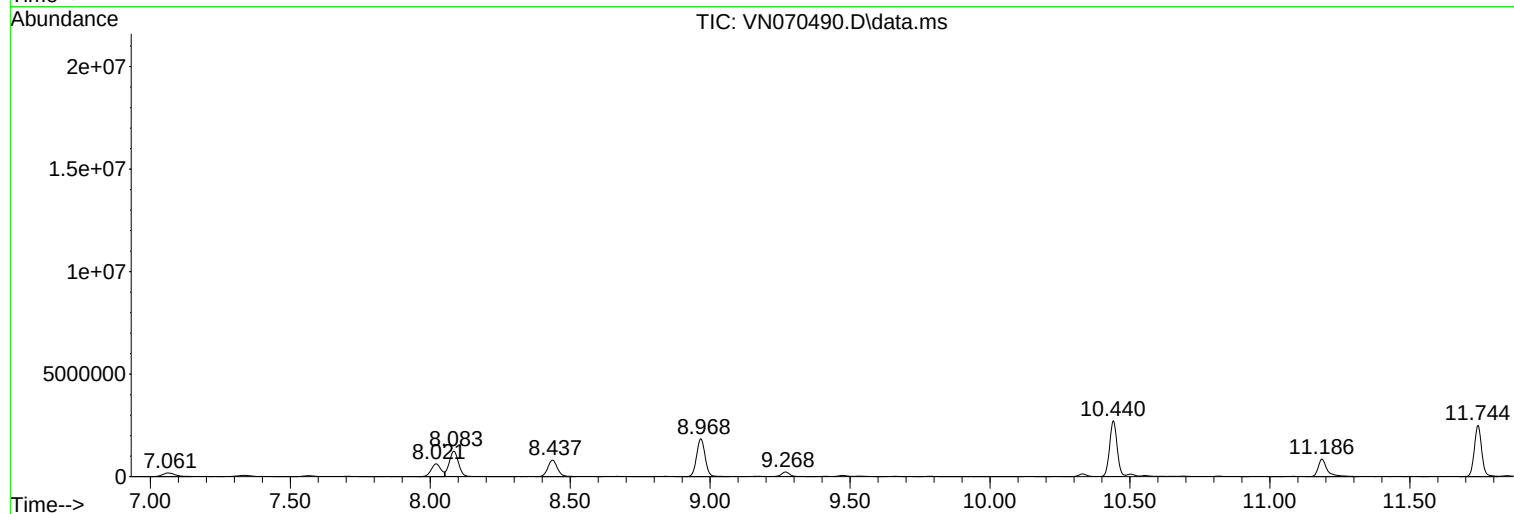
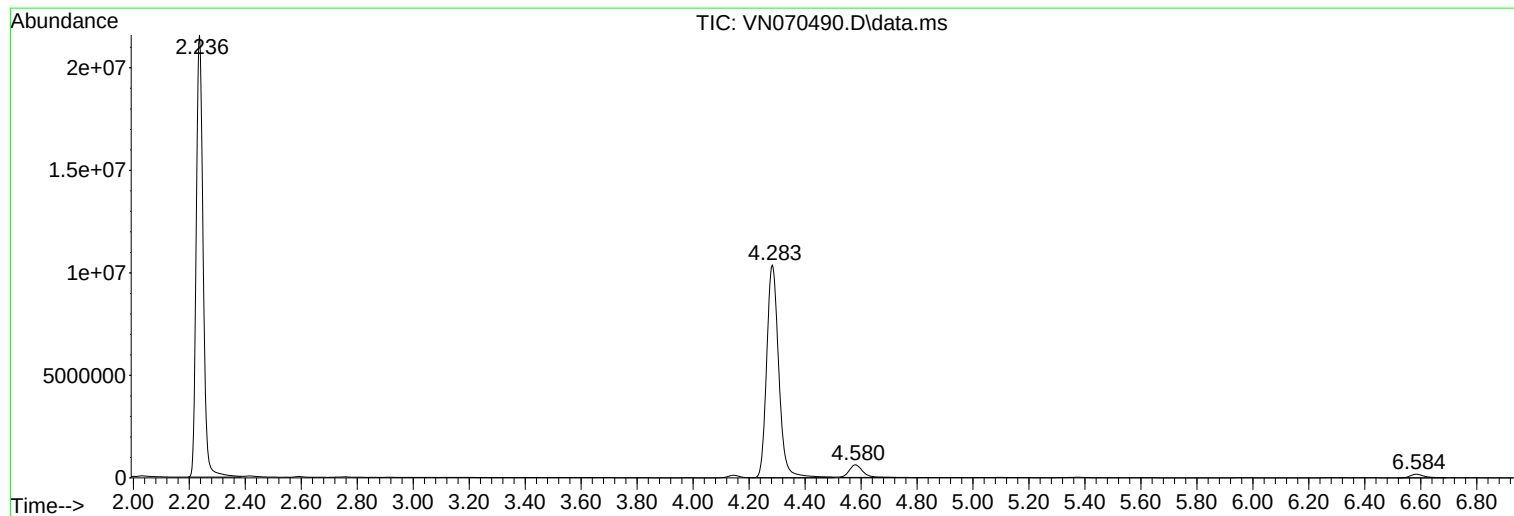
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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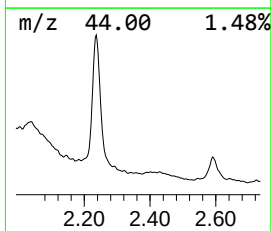
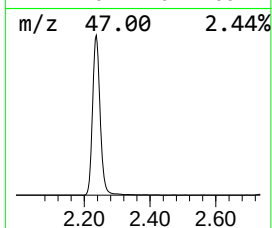
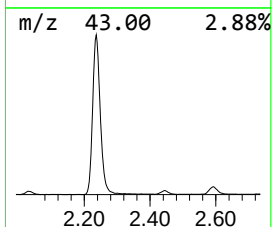
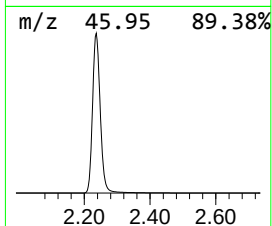
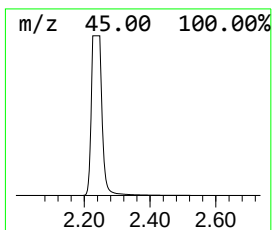
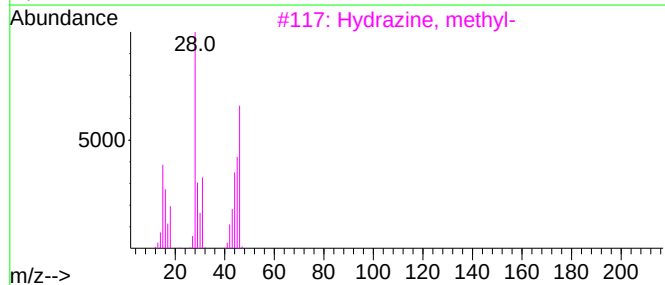
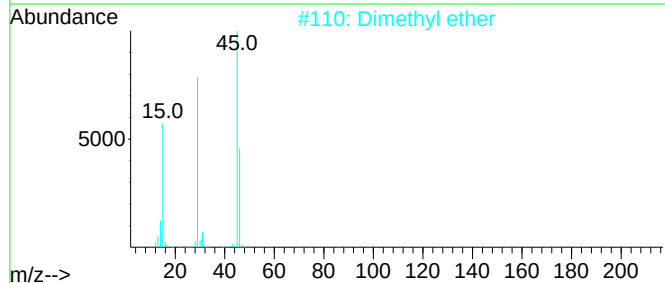
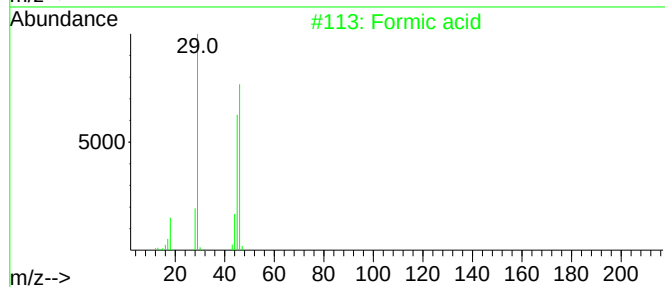
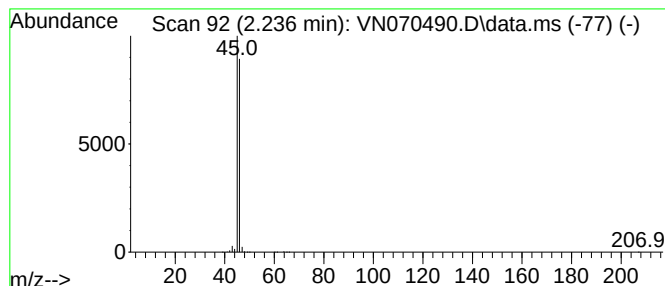
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 Formic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.236	664.14 ug/l	36740900	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formic acid	46	CH2O2	000064-18-6	74
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Hydrazine, methyl-	46	CH6N2	000060-34-4	4
4			Ethene, fluoro-	46	C2H3F	000075-02-5	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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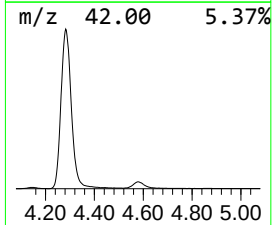
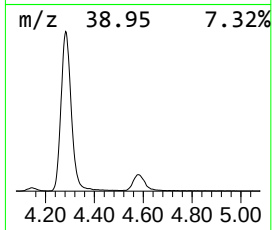
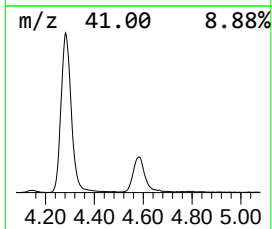
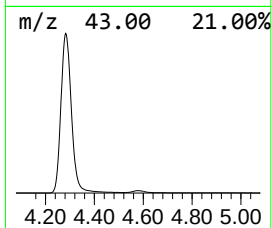
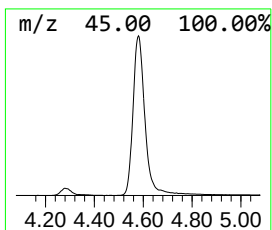
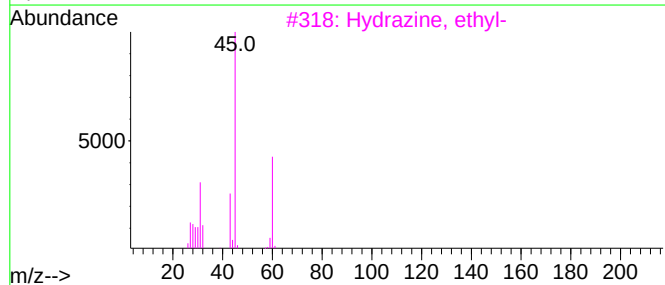
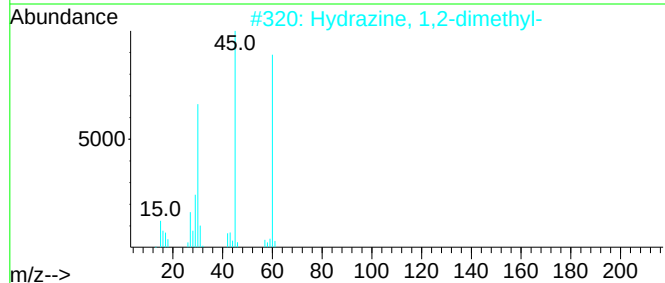
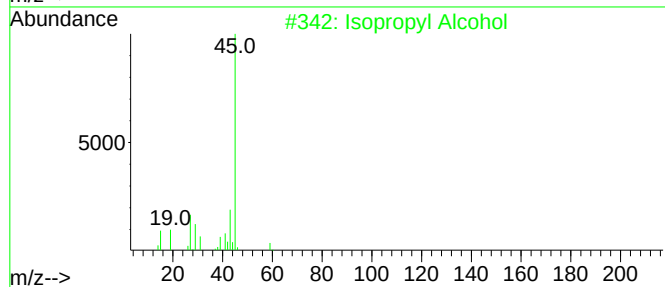
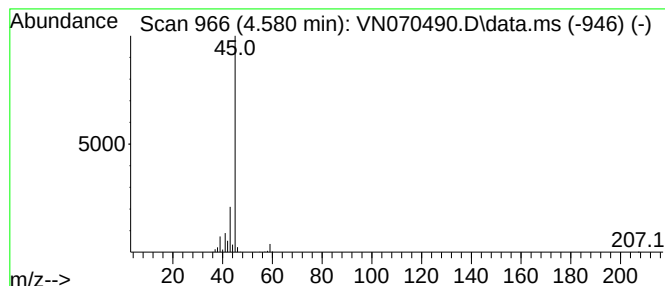
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.580	36.98 ug/l	2045690	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
4			Formamide	45	CH3NO	000075-12-7	4
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	4



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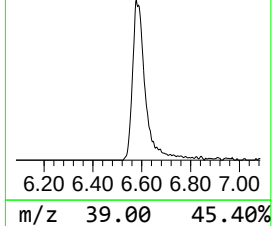
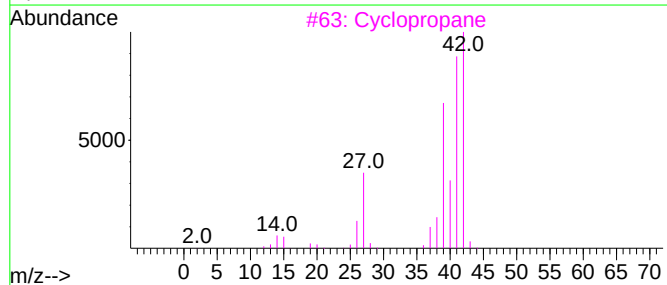
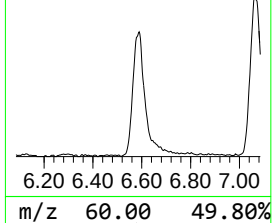
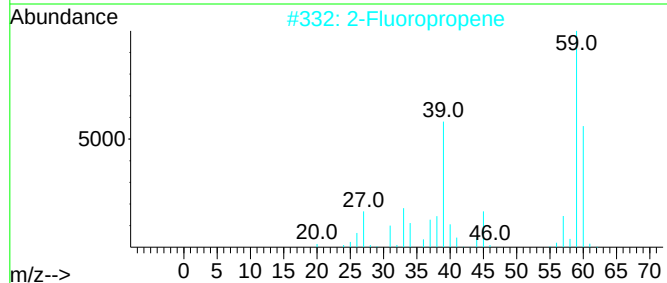
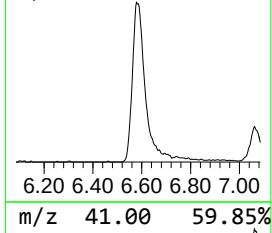
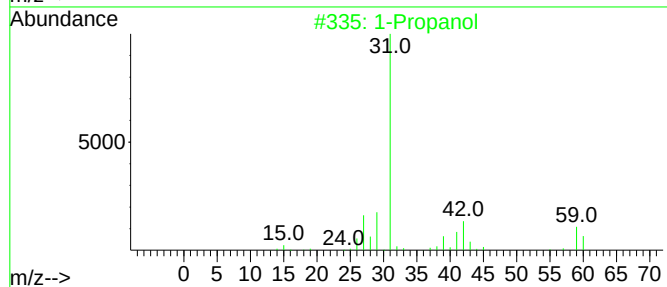
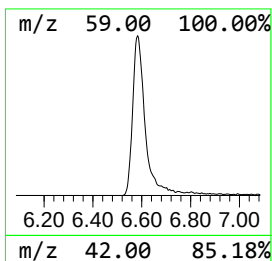
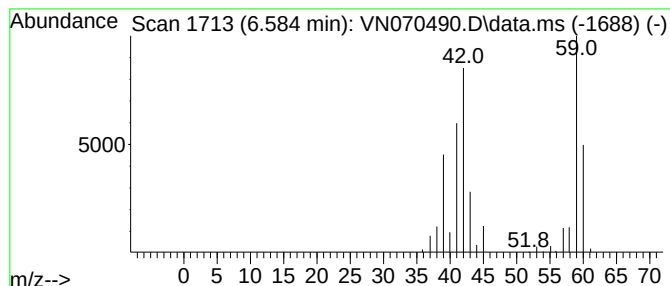
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Quant Title : SW846 8260

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Peak Number 3 1-Propanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.584	11.13 ug/l	615646	Pentafluorobenzene	8.086

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	64
2		2-Fluoropropene	60	C3H5F	001184-60-7	52
3		Cyclopropane	42	C3H6	000075-19-4	25
4		Propene	42	C3H6	000115-07-1	17
5		Allyl fluoride	60	C3H5F	000818-92-8	9



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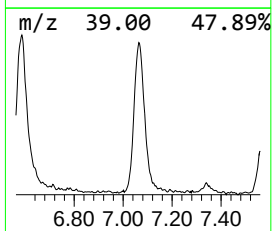
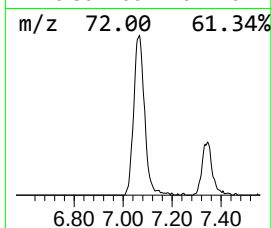
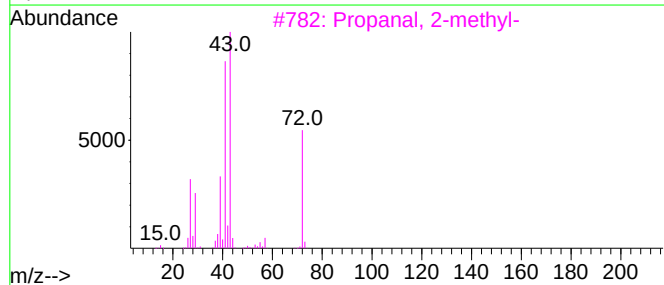
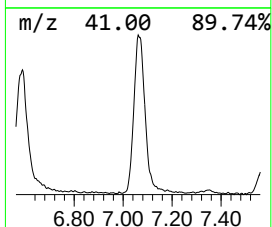
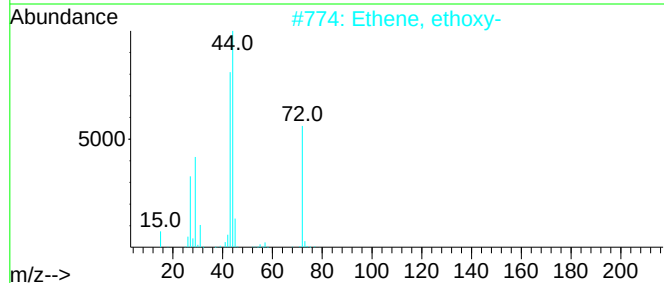
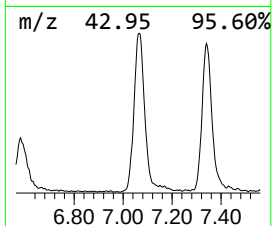
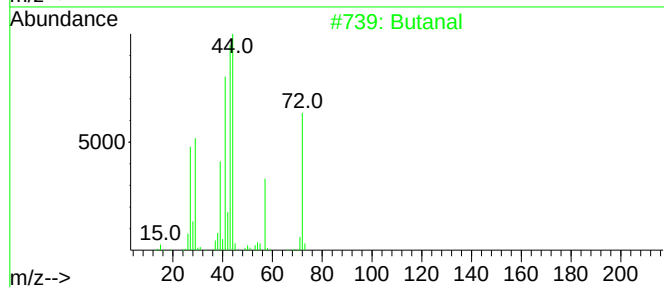
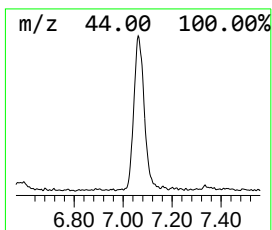
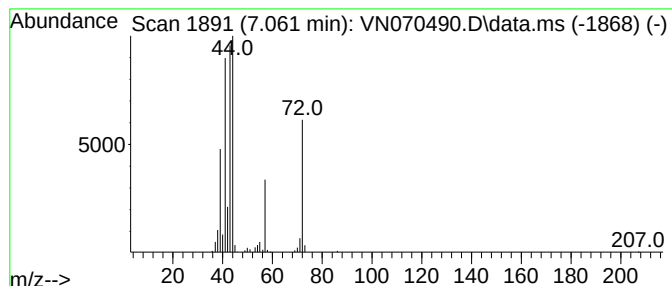
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.061	9.95 ug/l	550463	Pentafluorobenzene	8.086

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	47
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			Adenine-9-propanoic acid, .alpha...	322	C13H18N6O4	055387-36-5	38
5			3-Iodopropionamide	199	C3H6INO	021437-81-0	32



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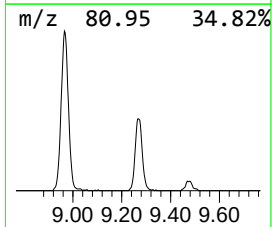
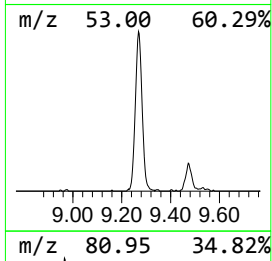
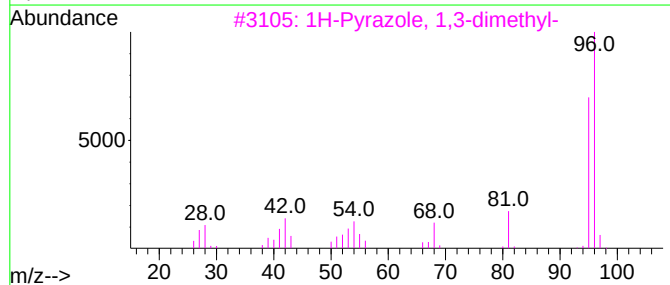
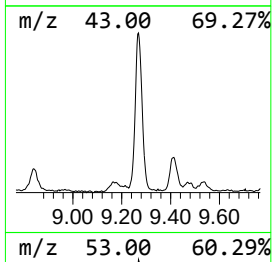
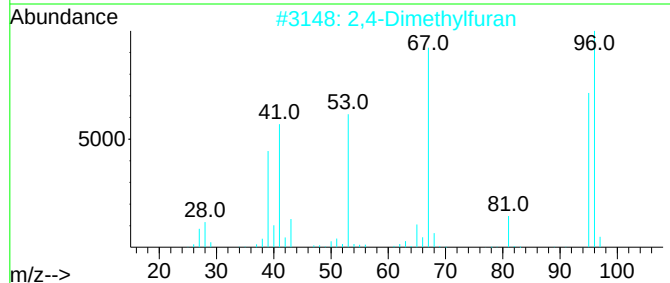
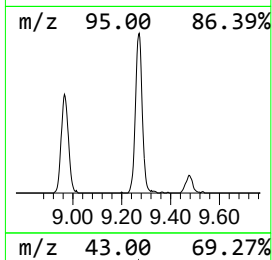
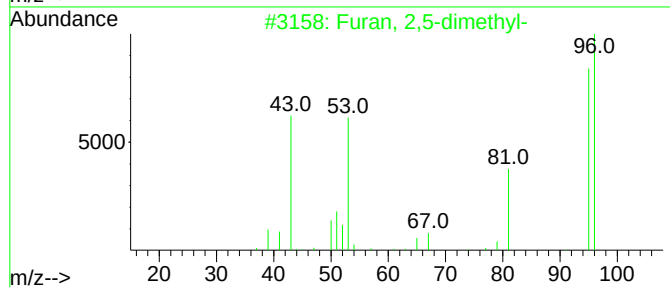
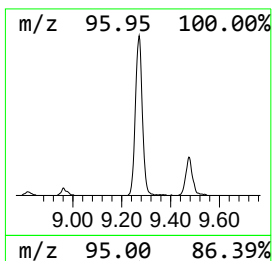
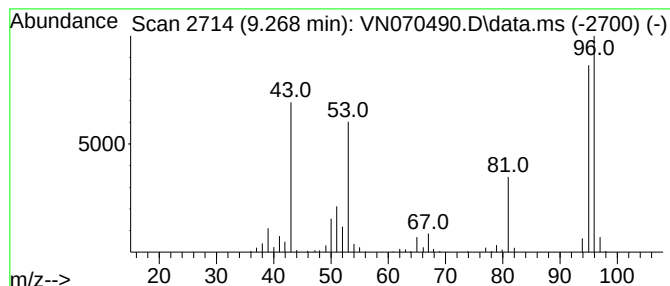
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Peak Number 5 Furan, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.268	5.50 ug/l	427750	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	97
2			2,4-Dimethylfuran	96	C6H8O	003710-43-8	80
3			1H-Pyrazole, 1,3-dimethyl-	96	C5H8N2	000694-48-4	43
4			1H-Imidazole, 4,5-dimethyl-	96	C5H8N2	002302-39-8	43
5			Furfural	96	C5H4O2	000098-01-1	38



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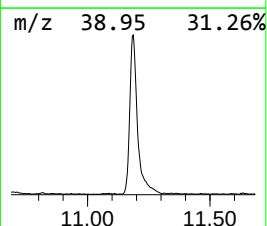
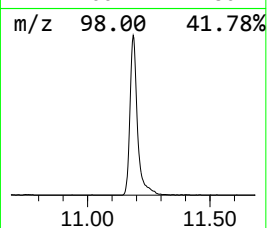
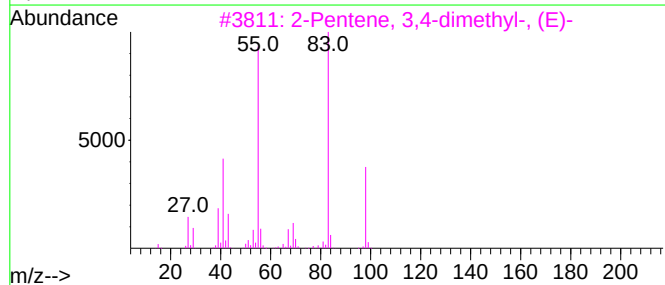
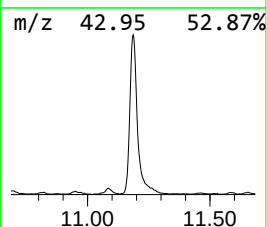
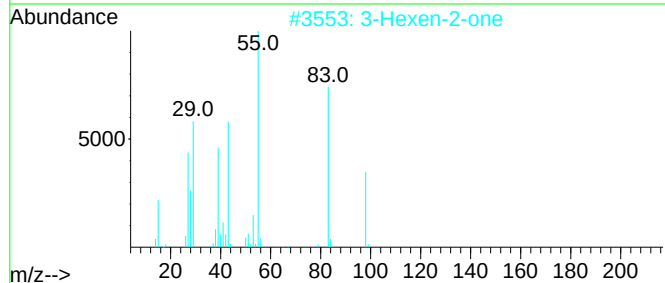
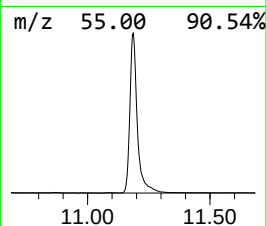
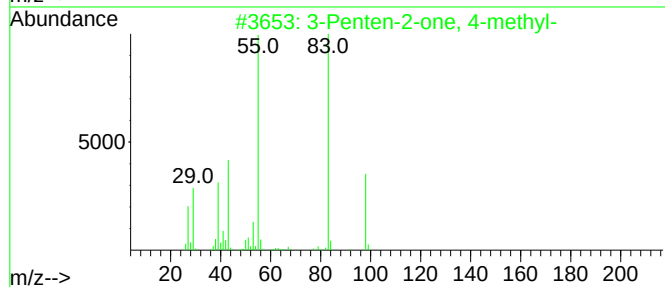
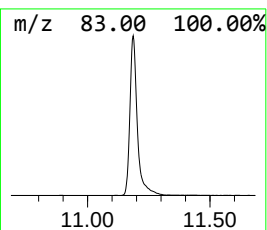
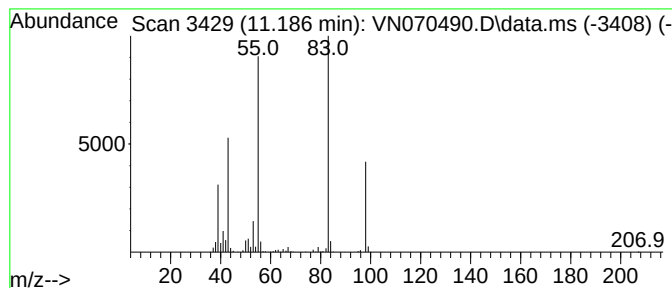
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Quant Title : SW846 8260

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

Peak Number 6 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.186	20.51 ug/l	1874300	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	86
5			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010522\
Data File : VN070490.D
Acq On : 5 Jan 2022 15:31
Operator : JC/MD
Sample : N1012-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31239

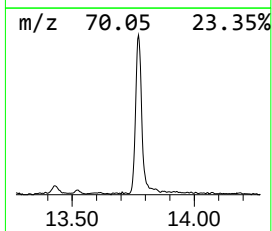
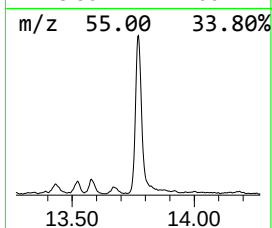
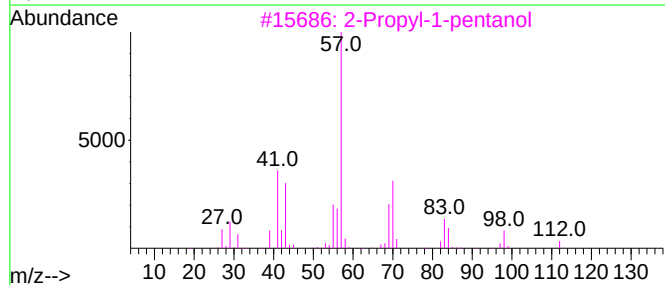
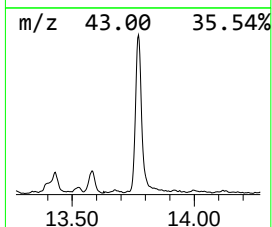
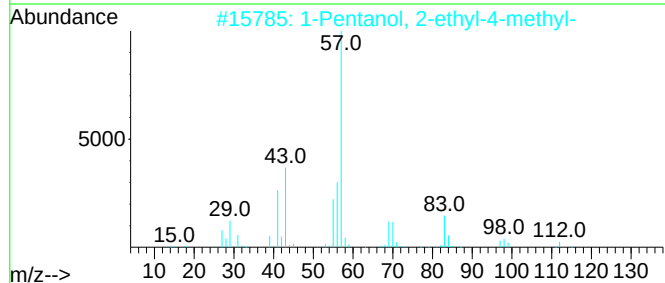
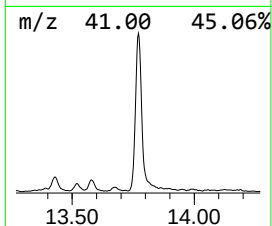
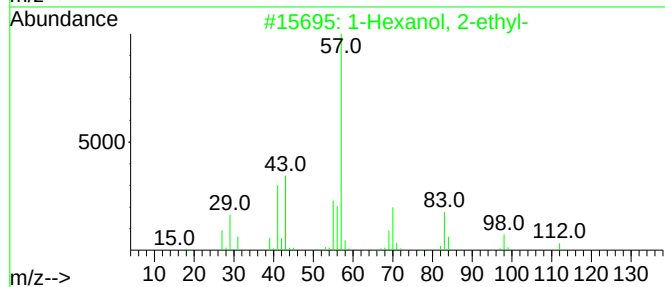
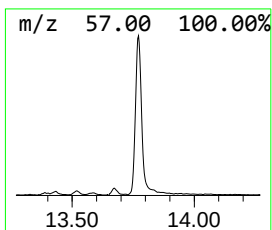
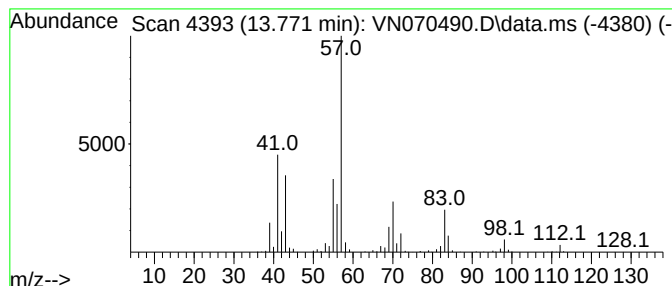
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.771	15.66 ug/l	985292	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	47
5			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010522\
Data File : VN070490.D
Acq On : 5 Jan 2022 15:31
Operator : JC/MD
Sample : N1012-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31239

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.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
Formic acid	2.236	664.1	ug/l	36740900	1	8.086	2766070	50.0
Isopropyl Alcohol	4.580	37.0	ug/l	2045690	1	8.086	2766070	50.0
1-Propanol	6.584	11.1	ug/l	615646	1	8.086	2766070	50.0
Butanal	7.061	9.9	ug/l	550463	1	8.086	2766070	50.0
Furan, 2,5-dime...	9.268	5.5	ug/l	427750	2	8.965	3886110	50.0
3-Penten-2-one,...	11.186	20.5	ug/l	1874300	3	11.744	4568220	50.0
1-Hexanol, 2-et...	13.771	15.7	ug/l	985292	4	13.675	3146440	50.0