

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
 Data File : VN081857.D
 Acq On : 25 Apr 2024 17:52
 Operator : JC\MD
 Sample : P2257-08
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 413A

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\82N042524W.M
 Title : SW846 8260

Signal : TIC: VN081857.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	17	22	29	rVB	52090	75865	2.61%	0.524%
2	2.665	113	121	126	rBV	61464	118922	4.09%	0.821%
3	3.783	304	311	320	rBV	53861	137978	4.75%	0.952%
4	4.430	412	421	432	rBV	43877	134516	4.63%	0.928%
5	4.706	459	468	480	rBV	27719	88028	3.03%	0.607%
6	5.024	512	522	532	rBV2	25355	77405	2.66%	0.534%
7	7.224	884	896	908	rBV	96445	277264	9.55%	1.913%
8	7.488	932	941	952	rBV	49102	126192	4.34%	0.871%
9	8.165	1048	1056	1061	rBV2	170454	412008	14.18%	2.843%
10	8.224	1061	1066	1080	rVB	315700	701990	24.17%	4.845%
11	8.535	1109	1119	1120	rBV4	20343	40023	1.38%	0.276%
12	8.577	1120	1126	1132	rVV	189301	407115	14.02%	2.810%
13	8.647	1132	1138	1153	rVV2	66609	265799	9.15%	1.834%
14	9.100	1206	1215	1224	rBV	495506	1010227	34.78%	6.972%
15	9.265	1235	1243	1252	rBV3	21359	51924	1.79%	0.358%
16	9.659	1302	1310	1321	rVB4	27241	66901	2.30%	0.462%
17	10.565	1455	1464	1472	rBV	751572	1420245	48.89%	9.801%
18	11.865	1673	1685	1696	rBV	661860	1278065	44.00%	8.820%
19	12.206	1737	1743	1755	rVB	78419	136610	4.70%	0.943%
20	12.376	1765	1772	1776	rBV	116685	193360	6.66%	1.334%
21	12.418	1776	1779	1784	rVV	189155	301740	10.39%	2.082%
22	12.459	1784	1786	1795	rVB2	47148	65167	2.24%	0.450%
23	12.847	1845	1852	1862	rBV	512494	916294	31.55%	6.323%
24	12.988	1872	1876	1881	rVB2	23401	35386	1.22%	0.244%
25	13.241	1912	1919	1922	rBV3	61199	115168	3.96%	0.795%
26	13.270	1922	1924	1930	rVV3	58258	84918	2.92%	0.586%
27	13.335	1930	1935	1941	rVB	428786	647783	22.30%	4.470%
28	13.488	1956	1961	1966	rBV3	22029	39320	1.35%	0.271%
29	13.541	1966	1970	1976	rVB7	15533	29083	1.00%	0.201%
30	13.664	1979	1991	2006	rVB2	218788	605907	20.86%	4.181%
31	13.794	2006	2013	2019	rBV	617428	1047567	36.06%	7.229%
32	13.870	2019	2026	2035	rVV	1774269	2904714	100.00%	20.046%
33	13.953	2035	2040	2047	rVB3	57235	100361	3.46%	0.693%
34	14.188	2073	2080	2086	rBV6	20026	44004	1.51%	0.304%
35	14.253	2086	2091	2094	rVB4	17942	29472	1.01%	0.203%
36	14.464	2122	2127	2137	rVB6	16999	47872	1.65%	0.330%

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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

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37	14.629	2147	2155	2163	rBV5	25190	50117	1.73%	0.346%
38	14.747	2163	2175	2188	rBV5	73219	204038	7.02%	1.408%
39	15.300	2264	2269	2274	rBV2	39555	66440	2.29%	0.459%
40	15.394	2281	2285	2290	rVB3	25254	35280	1.21%	0.243%
41	15.464	2290	2297	2305	rBV2	51122	99285	3.42%	0.685%

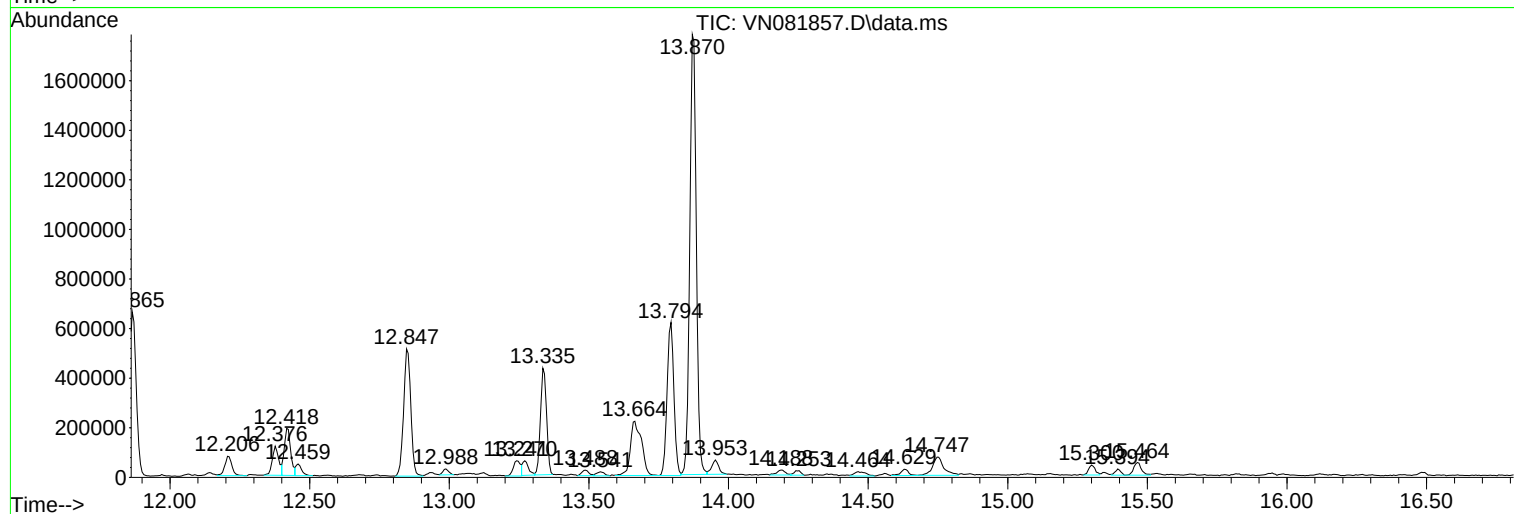
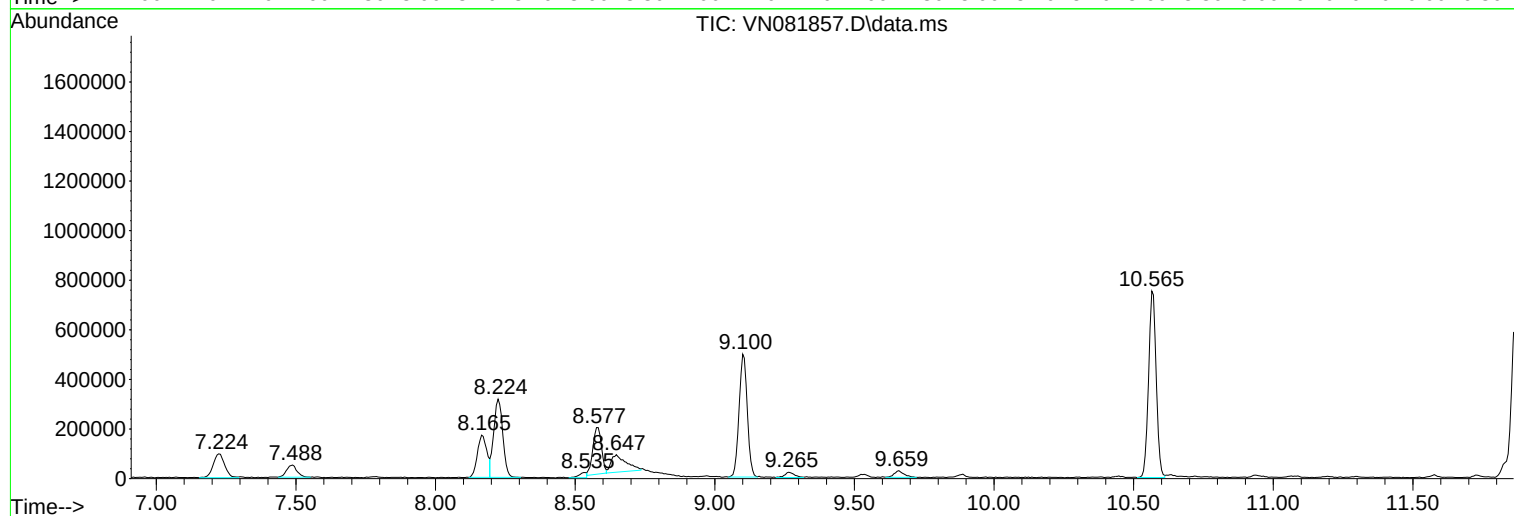
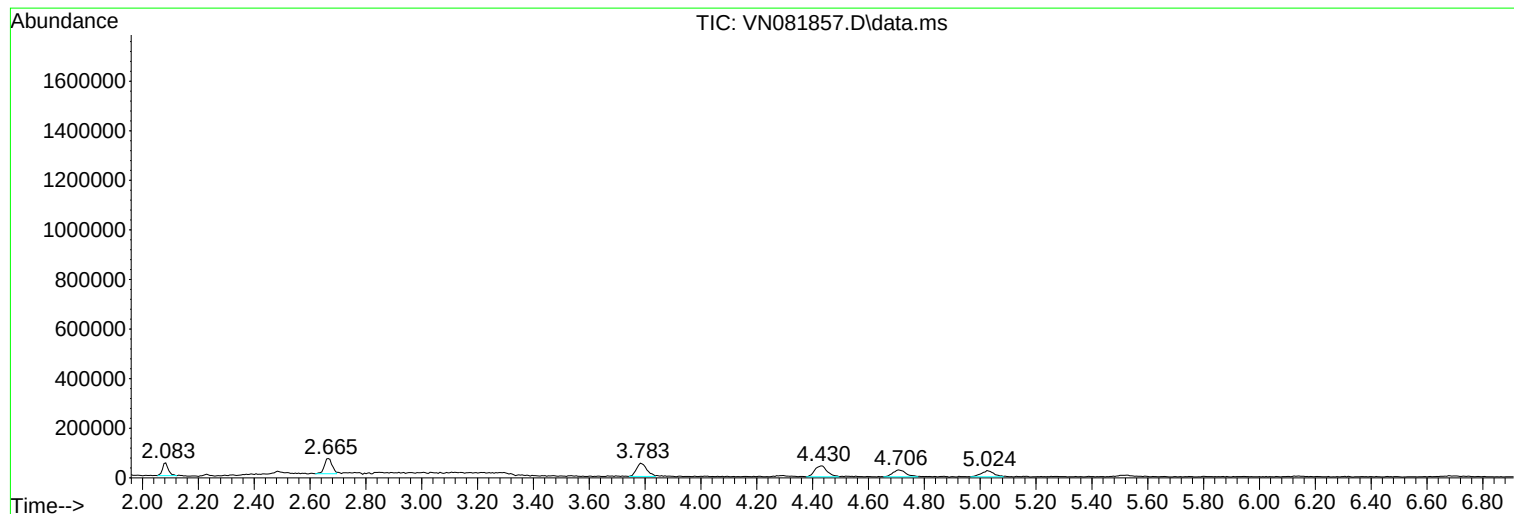
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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



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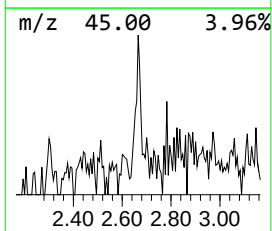
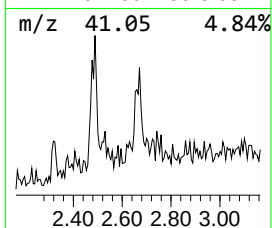
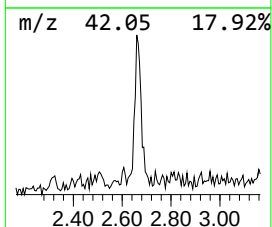
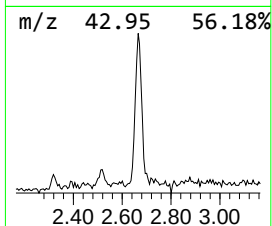
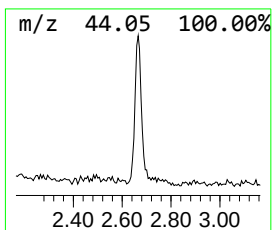
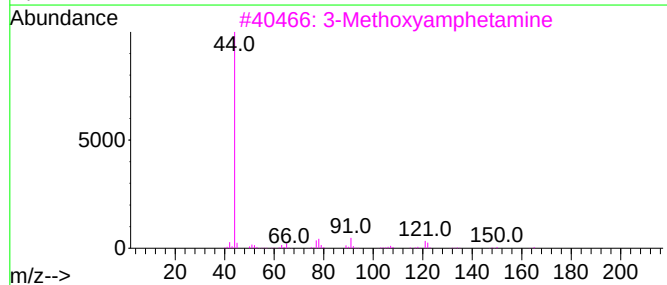
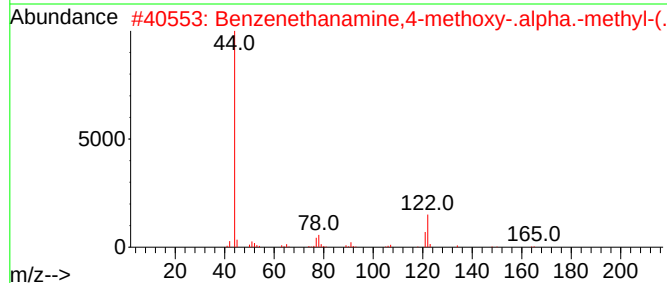
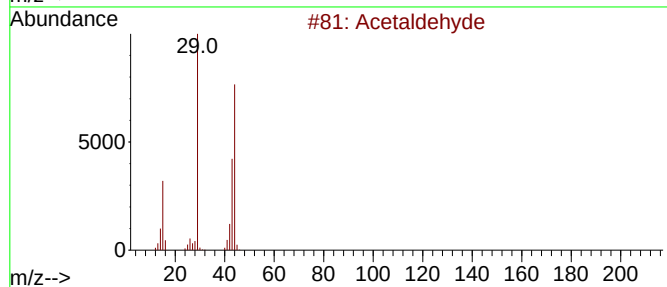
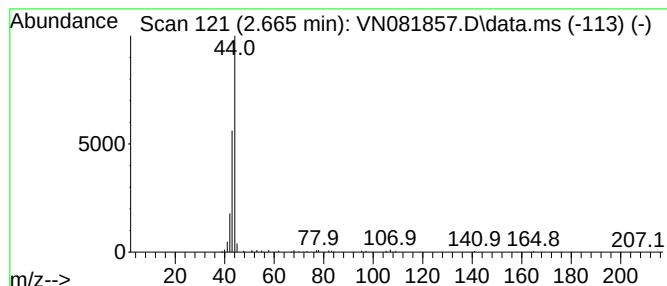
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.665	8.47 ug/l	118922	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	72
2			Benzenethanamine,4-methoxy-.alph...	165	C10H15NO	023239-32-9	7
3			3-Methoxyamphetamine	165	C10H15NO	017862-85-0	7
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Propane	44	C3H8	000074-98-6	4



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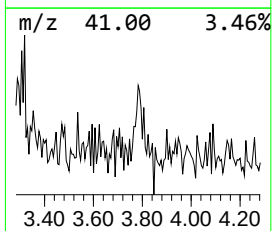
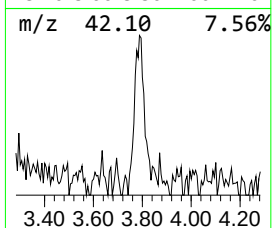
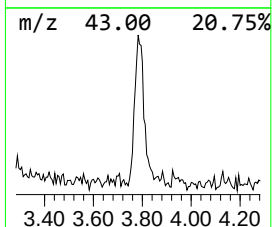
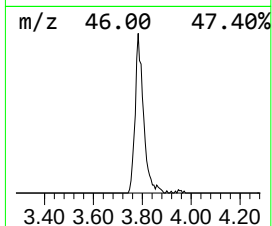
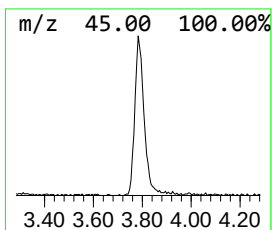
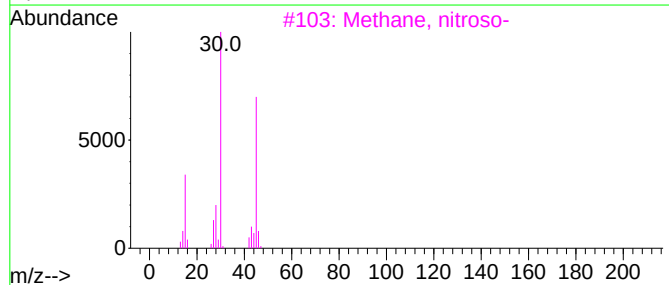
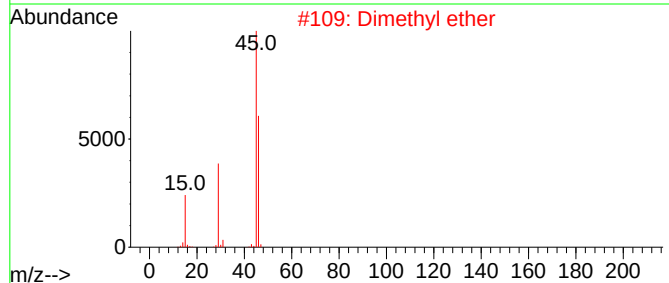
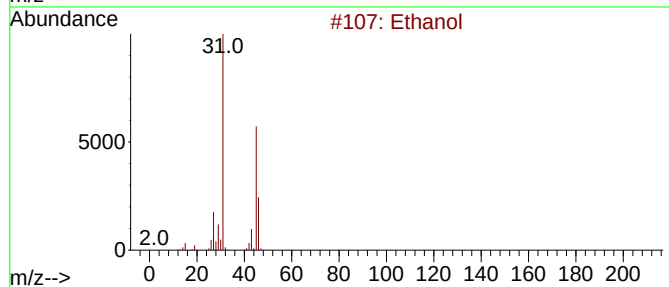
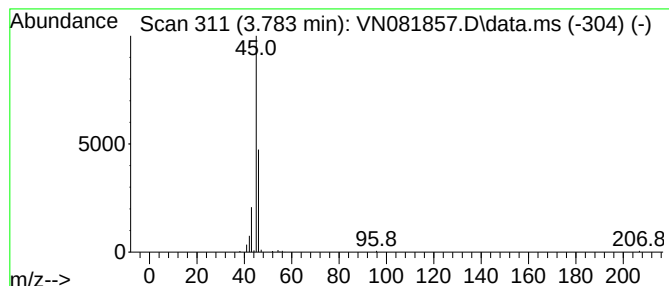
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.783	9.83 ug/l	137978	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	64
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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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

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413A

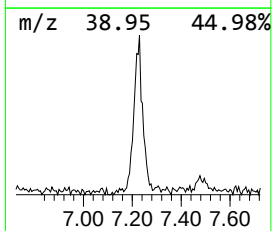
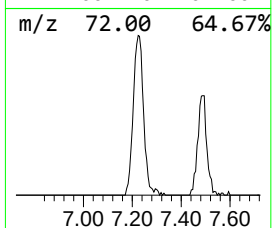
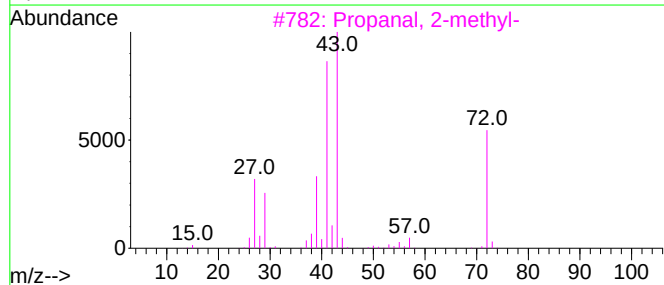
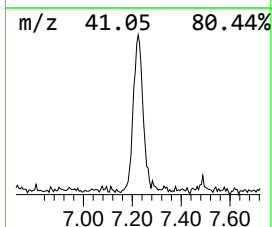
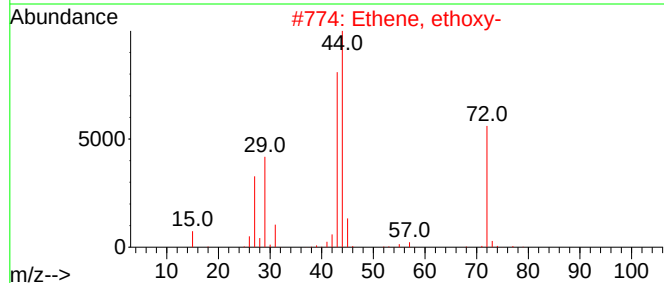
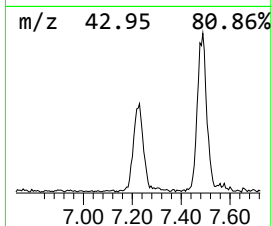
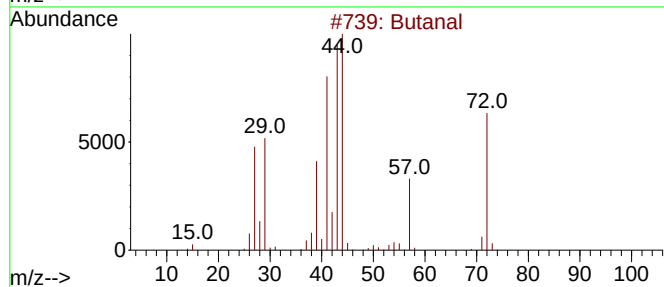
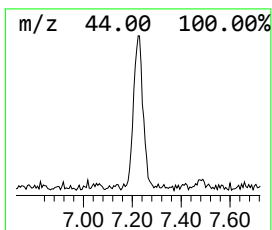
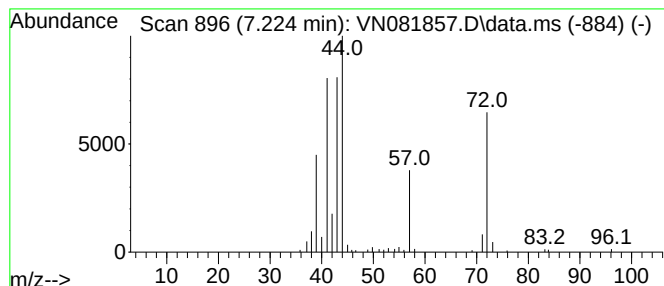
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	19.75 ug/l	277264	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	27



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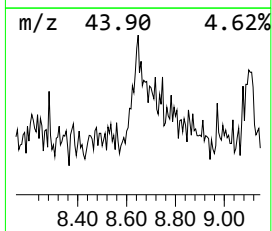
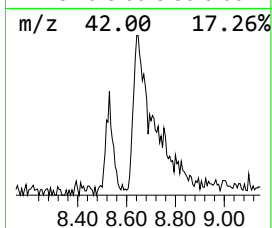
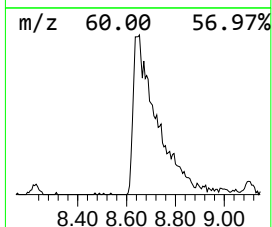
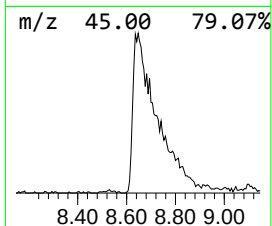
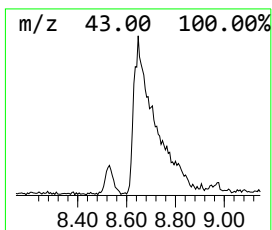
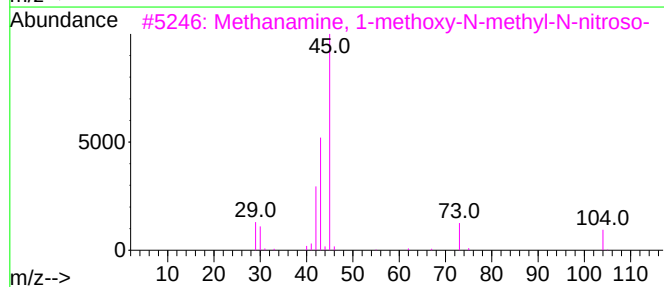
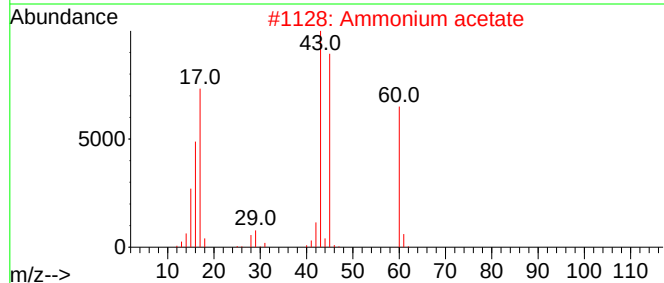
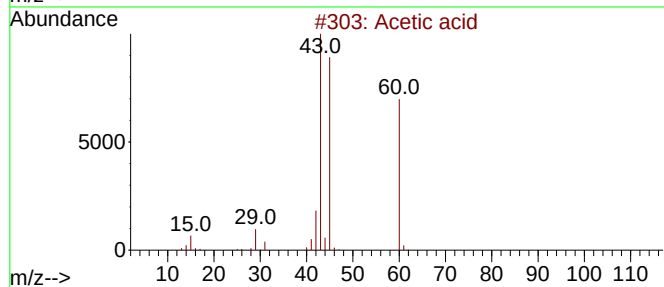
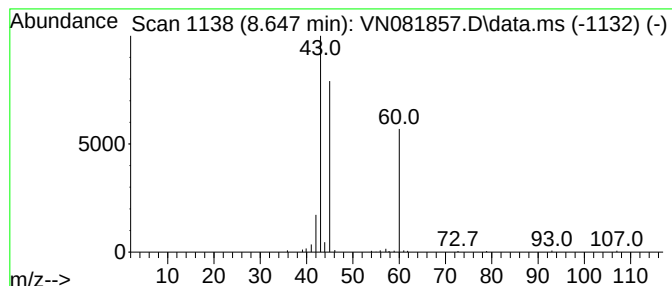
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Quant Title : SW846 8260

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

Peak Number 4 Acetic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.647	18.93 ug/l	265799	Pentafluorobenzene	8.224	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	Ammonium acetate	77	C2H7NO2	000631-61-8	64
3	Methanamine, 1-methoxy-N-methyl-...	104	C3H8N2O2	039885-14-8	9
4	Butanoic acid, 3-hydroxy-	104	C4H8O3	000300-85-6	9
5	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	7



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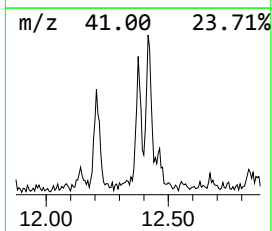
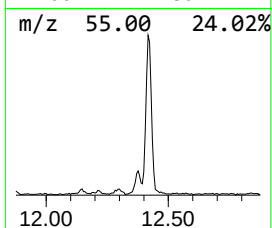
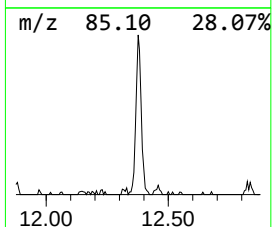
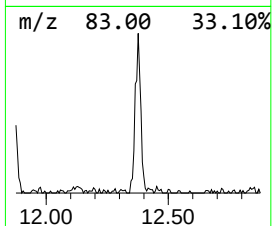
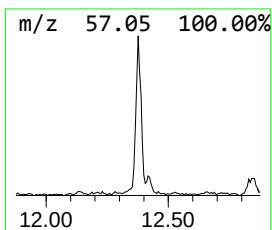
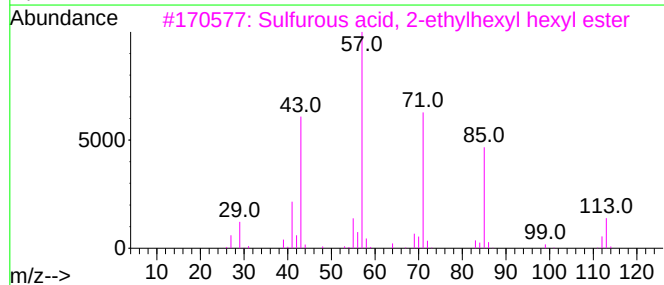
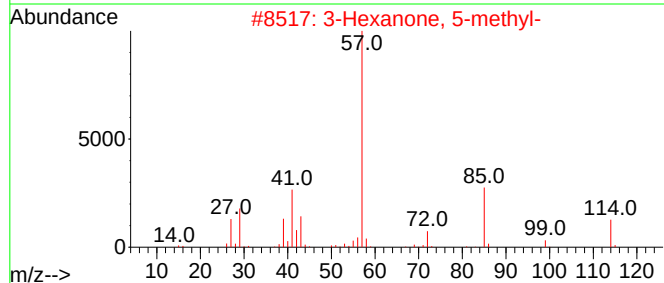
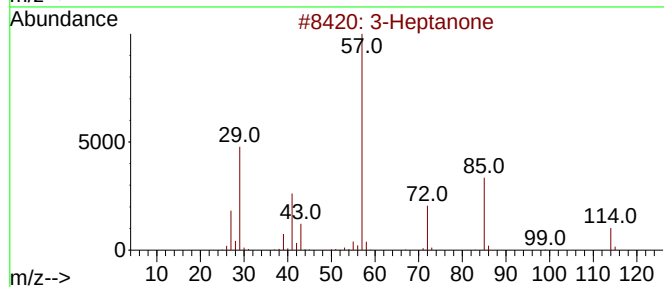
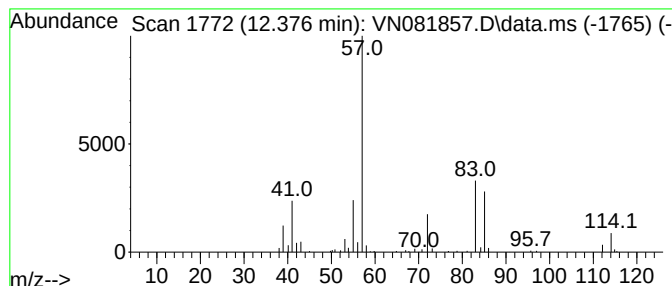
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 5 3-Heptanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.376	7.56 ug/l	193360	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanone	114	C7H14O	000106-35-4	52
2			3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	47
3			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	37
4			4-Methyl-5-nonanone	156	C10H20O	035900-26-6	32
5			3,5-Dimethyl-4-heptanone	142	C9H18O	019549-84-9	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081857.D
Acq On : 25 Apr 2024 17:52
Operator : JC\MD
Sample : P2257-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

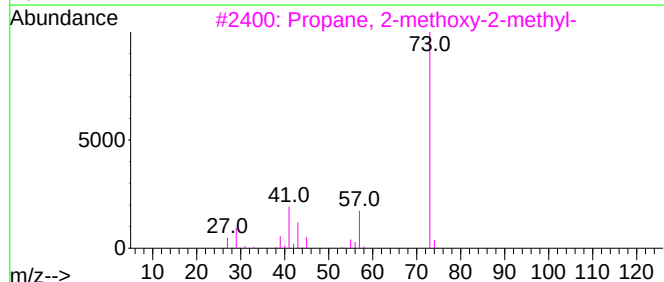
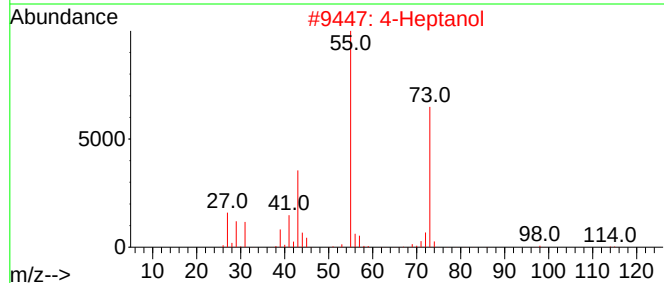
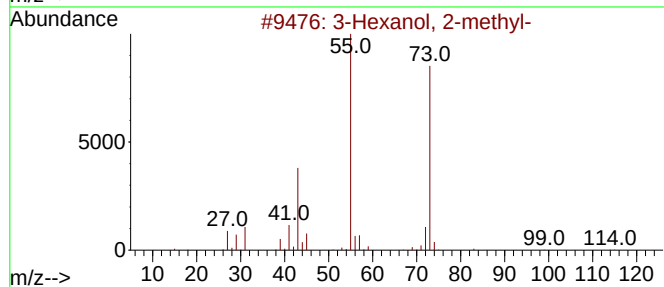
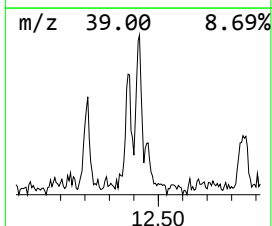
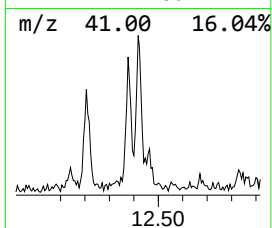
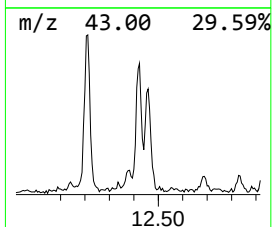
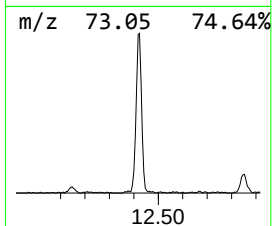
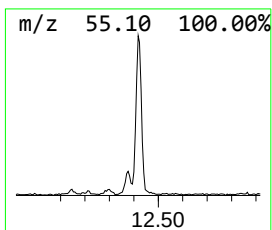
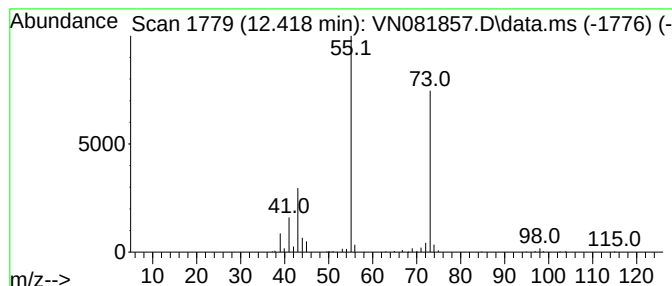
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 6 3-Hexanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.418	11.80 ug/l	301740	Chlorobenzene-d5		11.865	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Hexanol, 2-methyl-		116	C7H16O	000617-29-8	53
2	4-Heptanol		116	C7H16O	000589-55-9	38
3	Propane, 2-methoxy-2-methyl-		88	C5H12O	001634-04-4	25
4	2-Propenoic acid, ethenyl ester		98	C5H6O2	002177-18-6	9
5	1,3-Dioxolane, 2-ethyl-		102	C5H10O2	002568-96-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081857.D
Acq On : 25 Apr 2024 17:52
Operator : JC\MD
Sample : P2257-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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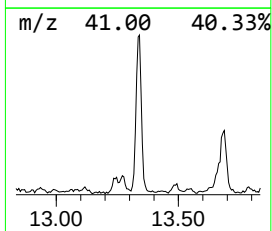
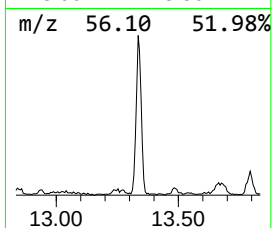
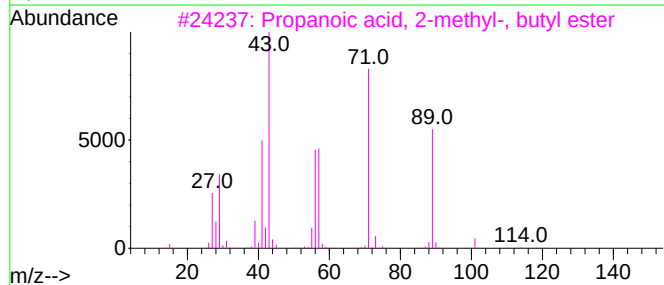
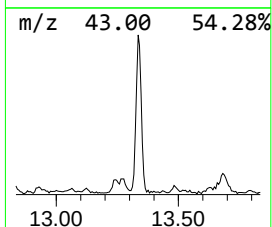
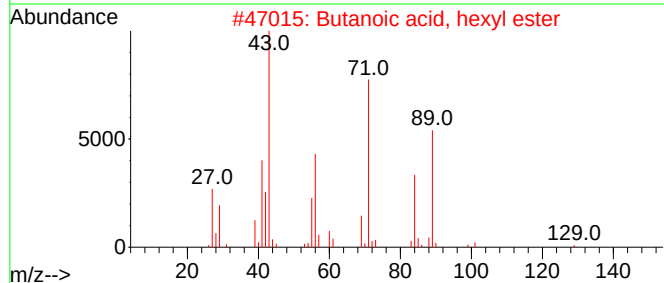
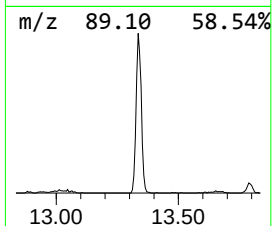
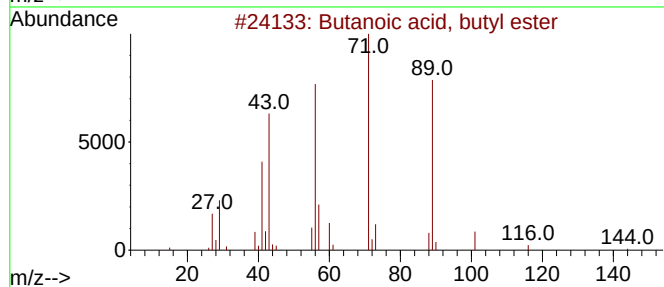
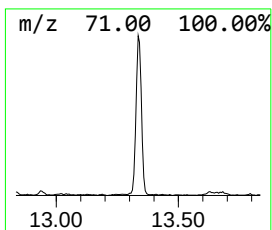
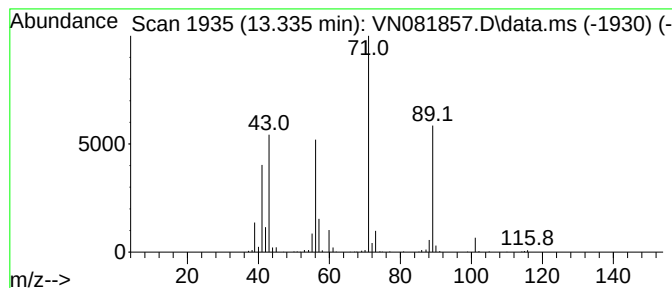
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Quant Title : SW846 8260

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

Peak Number 7 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	30.92 ug/l	647783	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	72
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59
5			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081857.D
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Operator : JC\MD
Sample : P2257-08
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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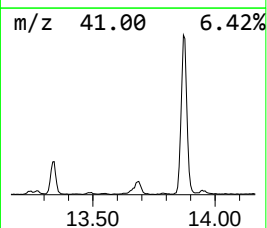
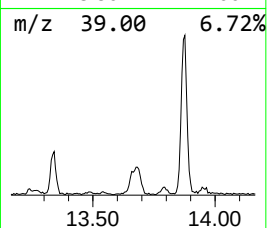
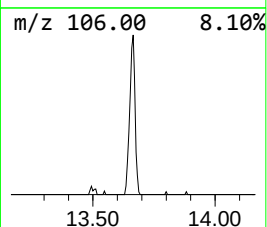
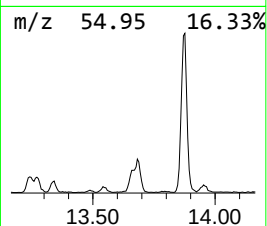
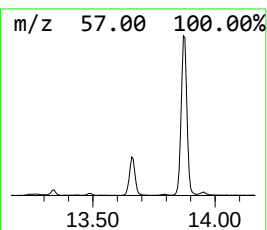
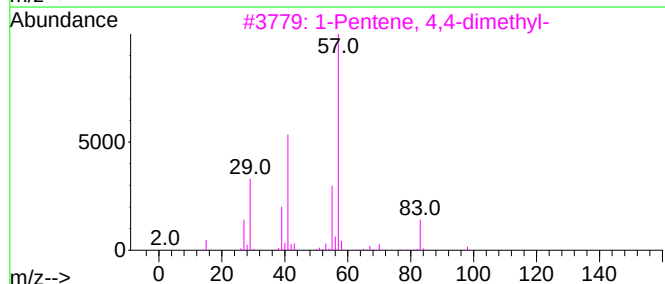
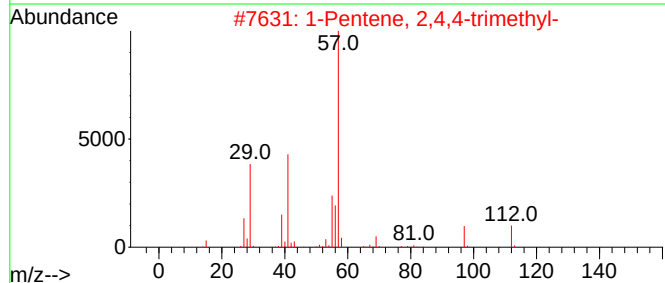
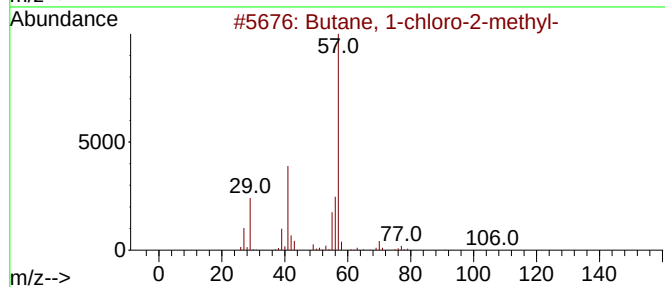
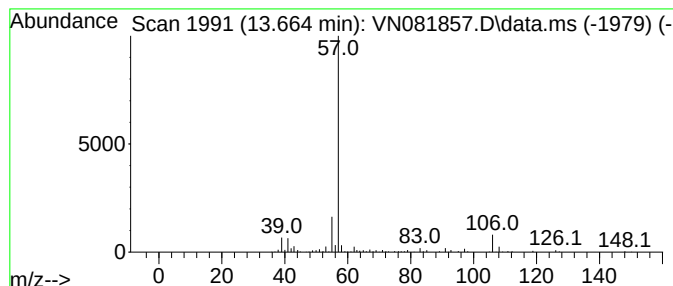
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.665 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.665	28.92 ug/l	605907	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	17
2			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	13
3			1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	9
4			Phosphinous chloride, (chloromet...	172	C5H11Cl2P	078055-63-7	9
5			3-Heptanone, 5-methylene-	126	C8H14O	020690-70-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081857.D
Acq On : 25 Apr 2024 17:52
Operator : JC\MD
Sample : P2257-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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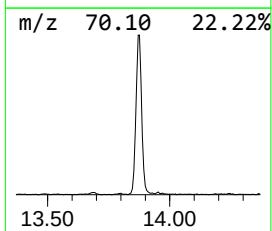
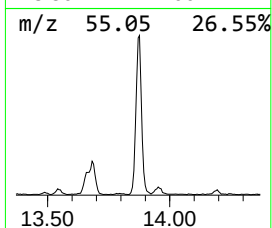
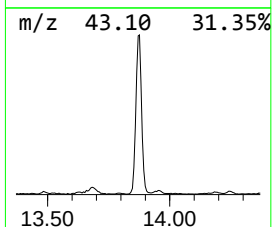
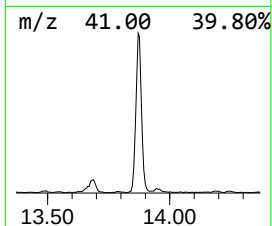
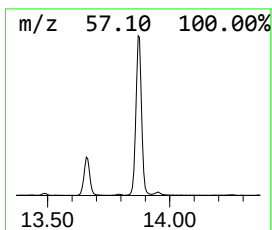
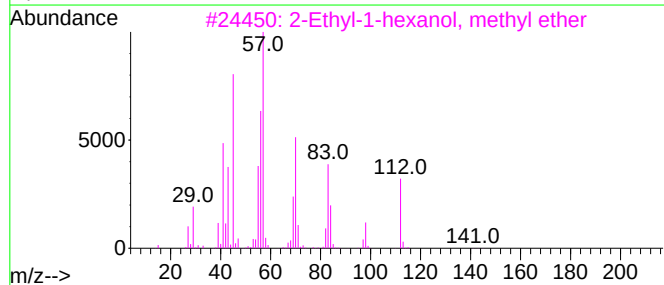
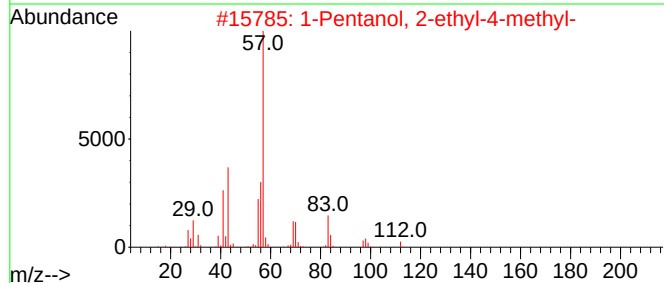
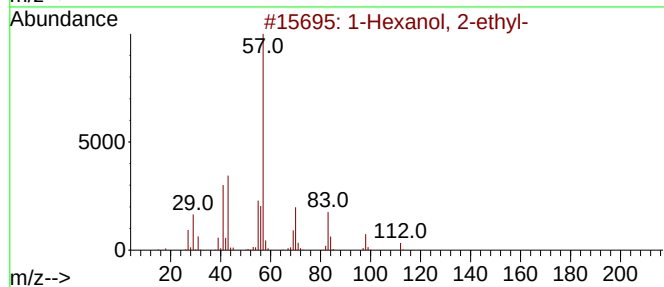
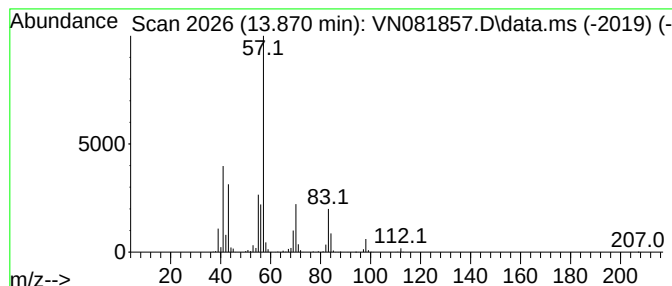
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Quant Title : SW846 8260

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.870	138.64 ug/l	2904710	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081857.D
Acq On : 25 Apr 2024 17:52
Operator : JC\MD
Sample : P2257-08
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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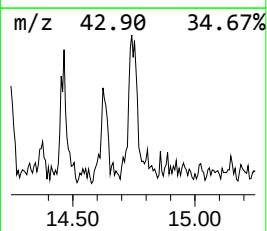
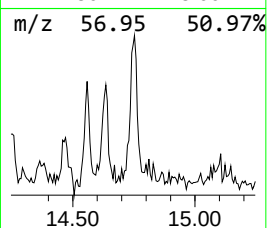
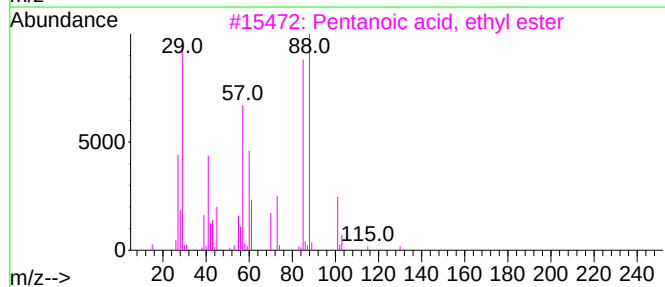
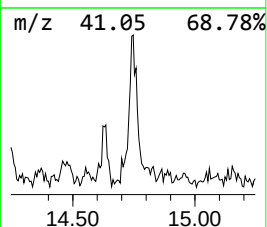
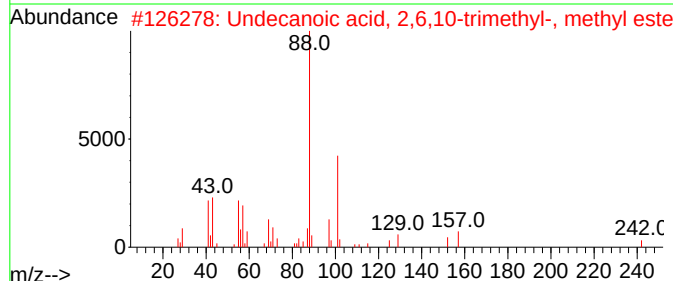
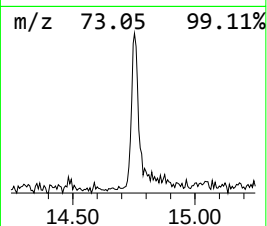
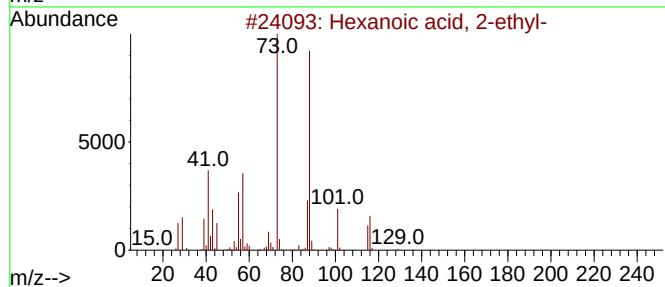
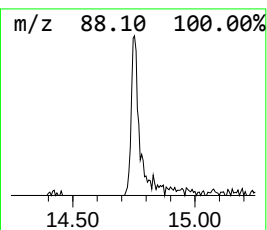
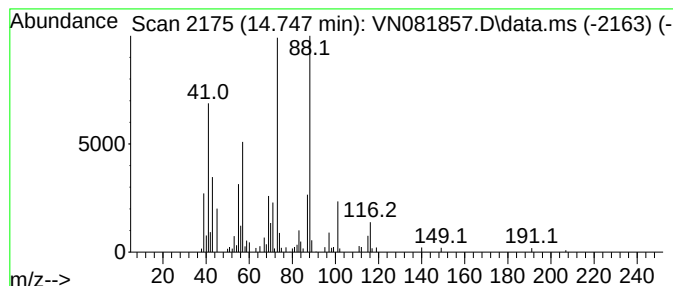
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Quant Title : SW846 8260

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

Peak Number 10 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.747	9.74 ug/l	204038	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	64
2			Undecanoic acid, 2,6,10-trimethyl-	242	C15H30O2	001001-79-2	53
3			Pentanoic acid, ethyl ester	130	C7H14O2	000539-82-2	53
4			Hexadecanoic acid, 2-methyl-, methyl ester	284	C18H36O2	002490-53-1	47
5			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081857.D
Acq On : 25 Apr 2024 17:52
Operator : JC\MD
Sample : P2257-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
413A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.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
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Ethanol	3.783	9.8	ug/l	137978	1	8.224	701990	50.0
Butanal	7.224	19.8	ug/l	277264	1	8.224	701990	50.0
Acetic acid	8.647	18.9	ug/l	265799	1	8.224	701990	50.0
3-Heptanone	12.376	7.6	ug/l	193360	3	11.865	1278070	50.0
3-Hexanol, 2-me...	12.418	11.8	ug/l	301740	3	11.865	1278070	50.0
Butanoic acid, ...	13.335	30.9	ug/l	647783	4	13.794	1047570	50.0
unknown13.665	13.665	28.9	ug/l	605907	4	13.794	1047570	50.0
1-Hexanol, 2-et...	13.870	138.6	ug/l	2904710	4	13.794	1047570	50.0
Hexanoic acid, ...	14.747	9.7	ug/l	204038	4	13.794	1047570	50.0