

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
 Data File : VN081136.D
 Acq On : 22 Feb 2024 15:35
 Operator : JC\MD
 Sample : P1546-08
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1331

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\82N021624W.M
 Title : SW846 8260

Signal : TIC: VN081136.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	16	22	31	rBV2	56123	88790	2.71%	0.449%
2	2.665	115	121	128	rVB2	49641	86633	2.64%	0.438%
3	2.818	141	147	153	rVB5	28768	54158	1.65%	0.274%
4	4.289	387	397	409	rBV2	36430	104809	3.19%	0.530%
5	4.424	411	420	433	rBV2	78461	236600	7.21%	1.197%
6	4.712	454	469	484	rBV	64064	215473	6.57%	1.090%
7	5.024	512	522	532	rBV2	18056	52407	1.60%	0.265%
8	7.230	885	897	908	rBV2	297657	849986	25.91%	4.299%
9	7.483	932	940	949	rVB2	18534	48935	1.49%	0.248%
10	8.171	1045	1057	1061	rBV	247708	594331	18.12%	3.006%
11	8.224	1061	1066	1077	rVB	481974	1084764	33.07%	5.487%
12	8.583	1110	1127	1133	rBV	265561	662862	20.21%	3.353%
13	8.659	1133	1140	1151	rVV3	44705	190076	5.79%	0.961%
14	9.106	1206	1216	1225	rVB	738870	1515642	46.20%	7.666%
15	9.271	1236	1244	1256	rBV	182129	403913	12.31%	2.043%
16	9.653	1298	1309	1316	rBV	46318	97704	2.98%	0.494%
17	10.571	1453	1465	1476	rBV	864686	1639995	49.99%	8.295%
18	10.959	1521	1531	1540	rBV3	47748	108018	3.29%	0.546%
19	11.300	1583	1589	1595	rBV2	22408	36727	1.12%	0.186%
20	11.871	1672	1686	1695	rBV	970466	1886487	57.51%	9.541%
21	12.212	1738	1744	1752	rVB2	44211	80676	2.46%	0.408%
22	12.376	1760	1772	1775	rBV	81472	139455	4.25%	0.705%
23	12.423	1775	1780	1785	rVB	267395	392217	11.96%	1.984%
24	12.853	1844	1853	1864	rBV	638681	1193275	36.38%	6.035%
25	13.123	1895	1899	1905	rVB2	31143	47278	1.44%	0.239%
26	13.247	1913	1920	1922	rBV2	121272	213561	6.51%	1.080%
27	13.270	1922	1924	1930	rVV	128400	200804	6.12%	1.016%
28	13.341	1930	1936	1950	rVB	1149416	1776128	54.14%	8.983%
29	13.488	1956	1961	1966	rBV3	19855	36207	1.10%	0.183%
30	13.541	1966	1970	1978	rVB7	17030	36577	1.12%	0.185%
31	13.665	1986	1991	2004	rVB	133446	302759	9.23%	1.531%
32	13.794	2005	2013	2020	rBV	953524	1587737	48.40%	8.030%
33	13.876	2020	2027	2036	rBV	2122334	3280436	100.00%	16.592%
34	13.959	2036	2041	2046	rVB5	53385	103662	3.16%	0.524%
35	14.253	2085	2091	2095	rBV5	29878	50270	1.53%	0.254%
36	14.559	2138	2143	2149	rVB4	30942	49386	1.51%	0.250%

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37	14.741	2164	2174	2179	rBV5	25513	60938	1.86%	0.308%
38	15.306	2263	2270	2273	rBV3	27349	48814	1.49%	0.247%
39	15.394	2281	2285	2291	rVB3	55905	96800	2.95%	0.490%
40	15.464	2291	2297	2302	rBV7	23251	38876	1.19%	0.197%
41	15.823	2354	2358	2369	rVV7	18501	43886	1.34%	0.222%
42	16.123	2403	2409	2413	rBV6	19593	33341	1.02%	0.169%

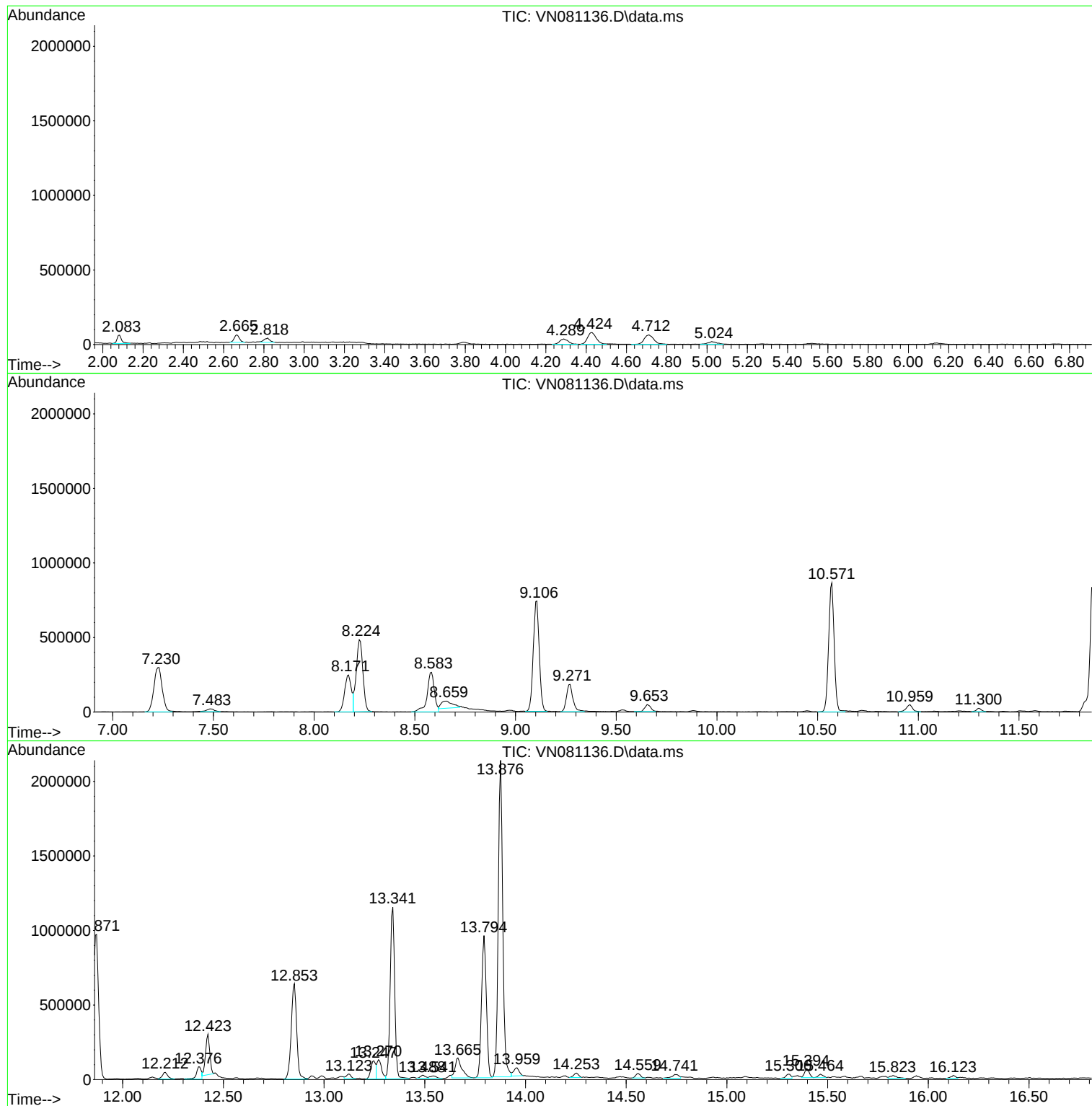
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

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



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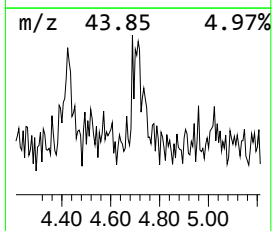
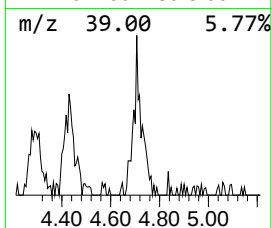
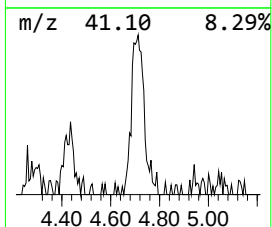
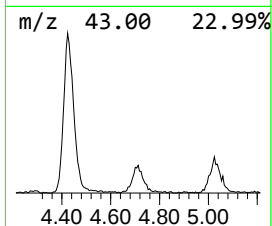
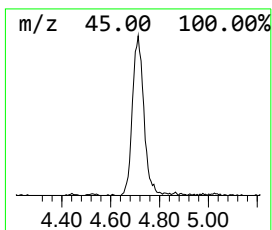
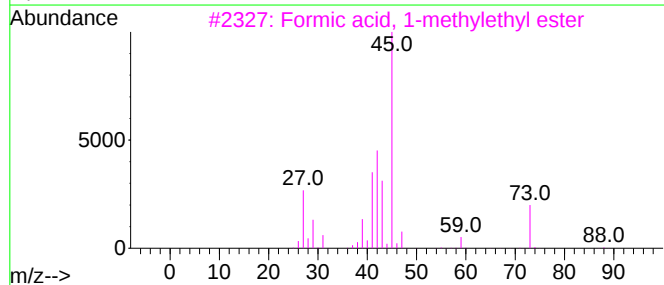
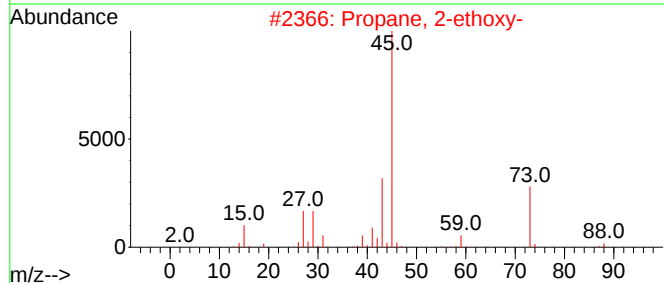
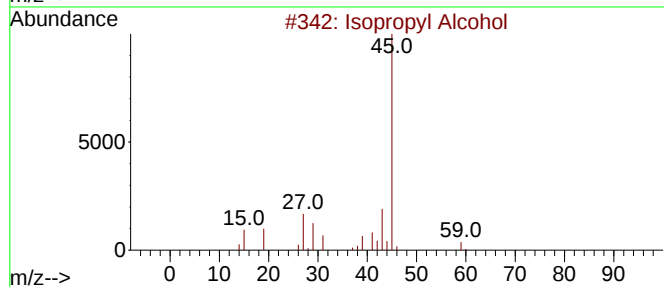
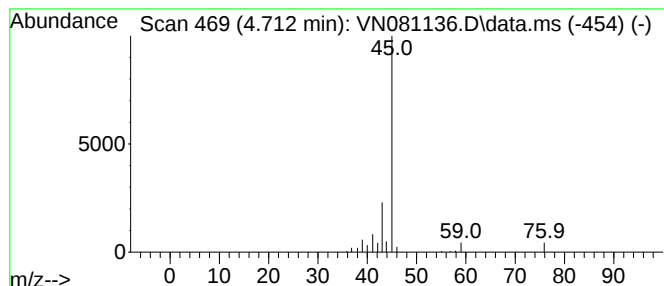
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.712	9.93 ug/l	215473	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
3			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	39
4			(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9
5			2-Pentanol	88	C5H12O	006032-29-7	9



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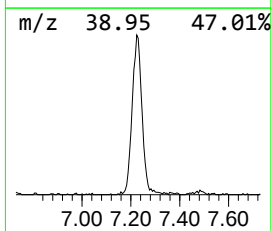
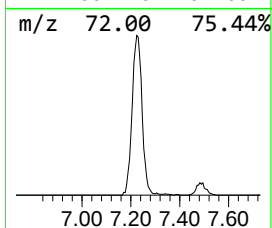
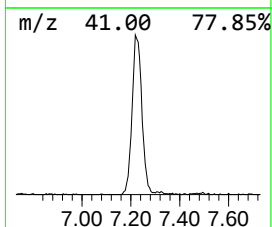
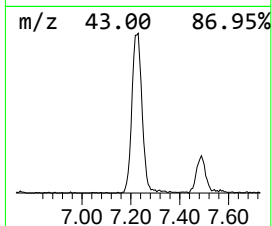
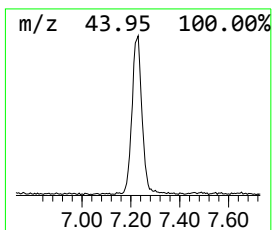
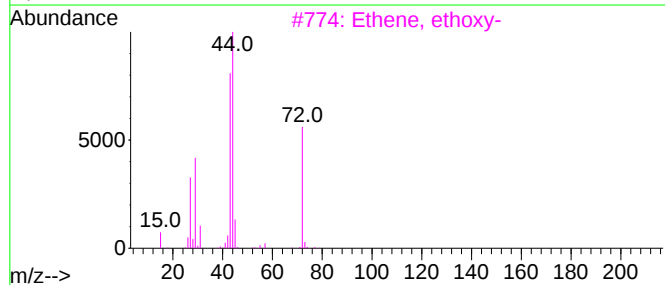
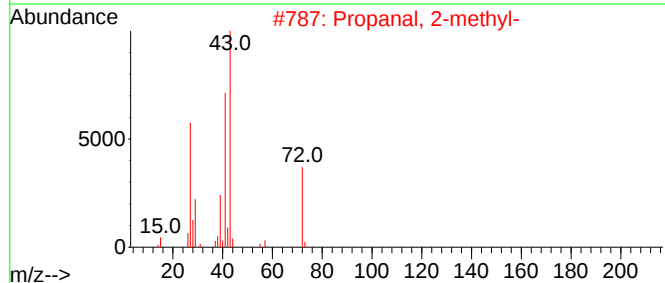
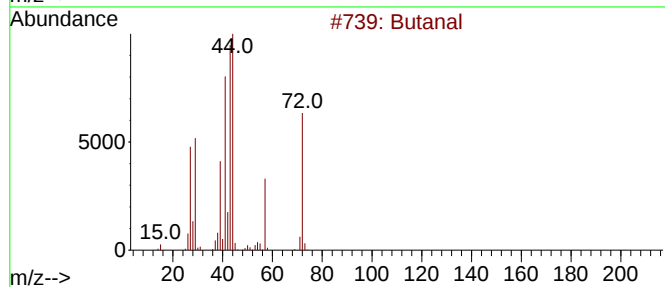
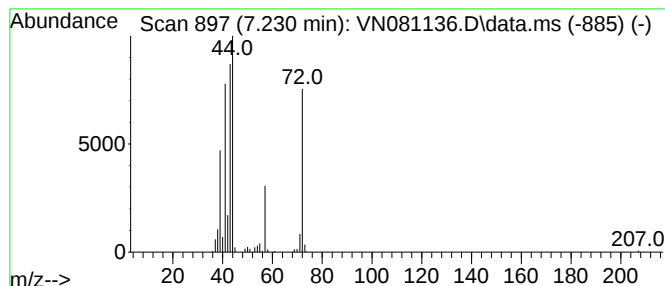
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
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Peak Number 2 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.230	39.18 ug/l	849986	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	42
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	40
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38



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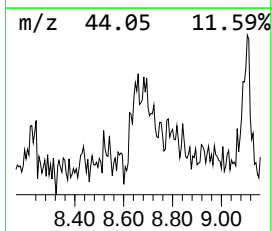
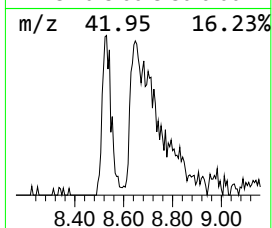
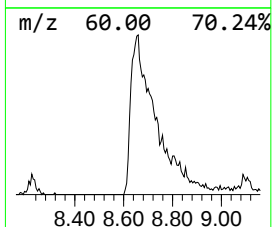
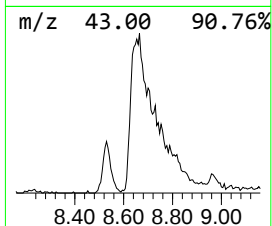
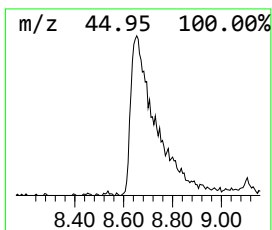
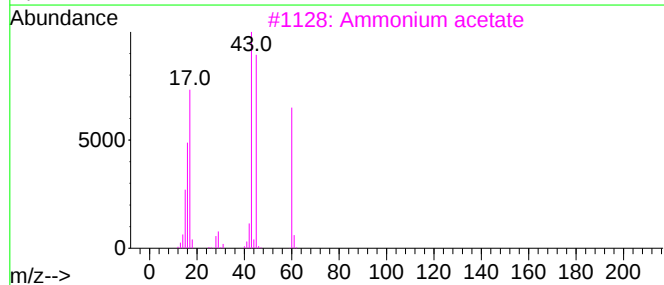
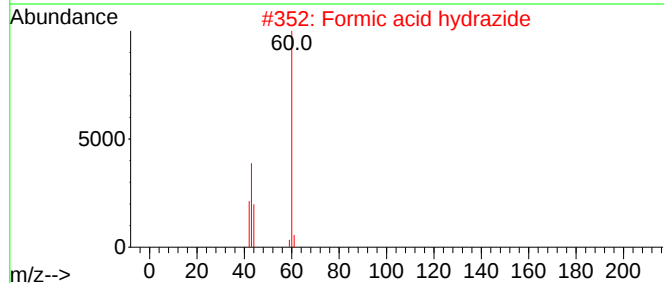
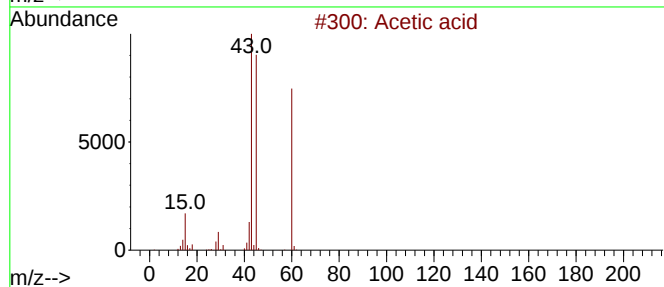
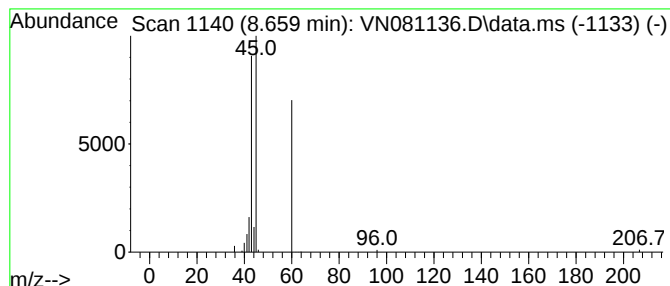
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Acetic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.659	8.76 ug/l	190076	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	86
2			Formic acid hydrazide	60	CH4N2O	000624-84-0	9
3			Ammonium acetate	77	C2H7NO2	000631-61-8	9
4			L-Cysteine, N-acetyl-	163	C5H9NO3S	000616-91-1	9
5			N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	9



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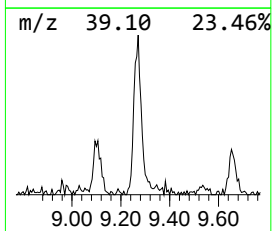
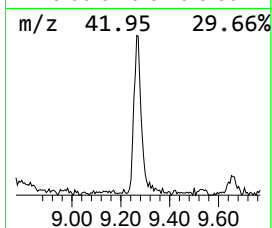
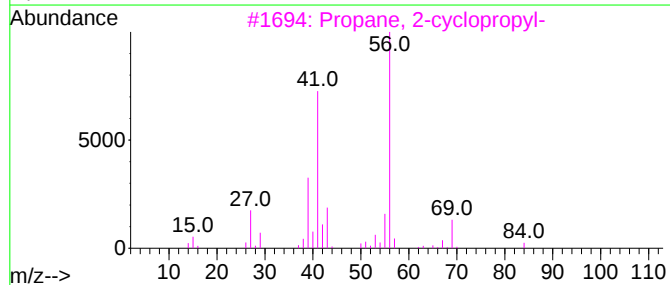
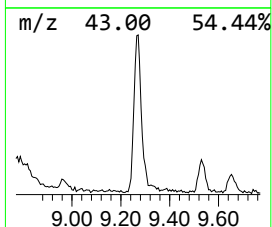
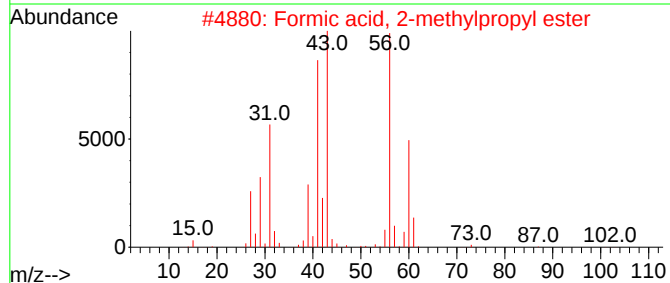
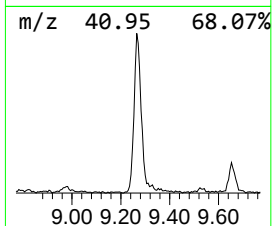
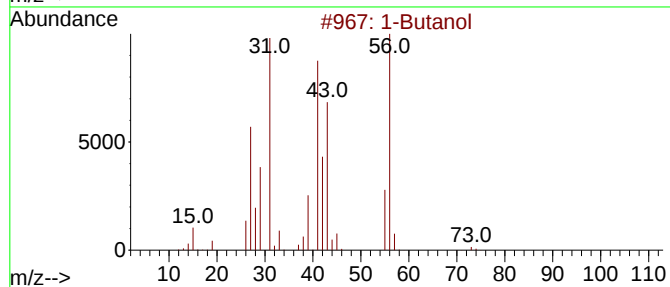
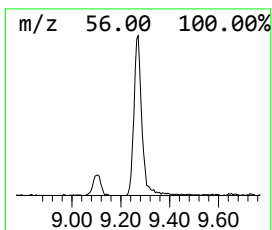
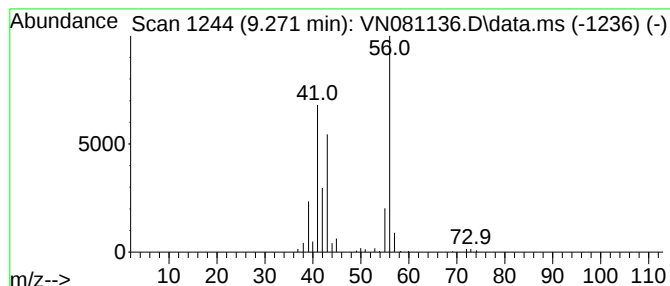
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Peak Number 4 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.271	13.32 ug/l	403913	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			Formic acid, 2-methylpropyl ester	102	C5H10O2	000542-55-2	40
3			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
5			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9



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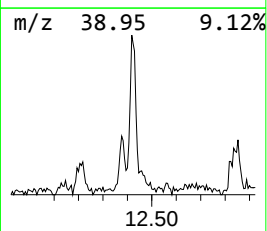
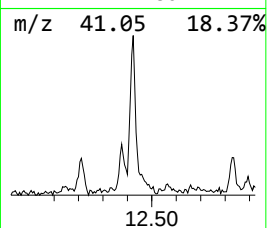
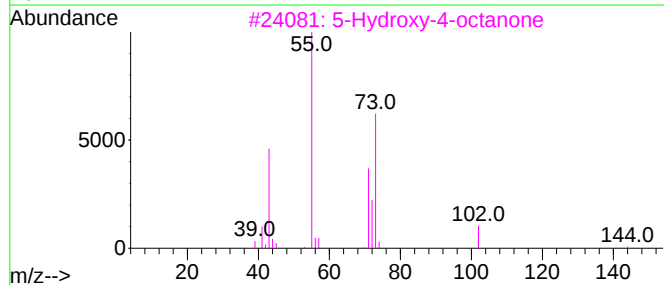
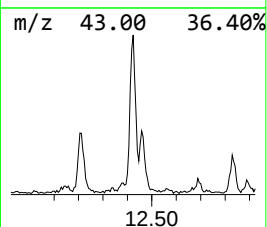
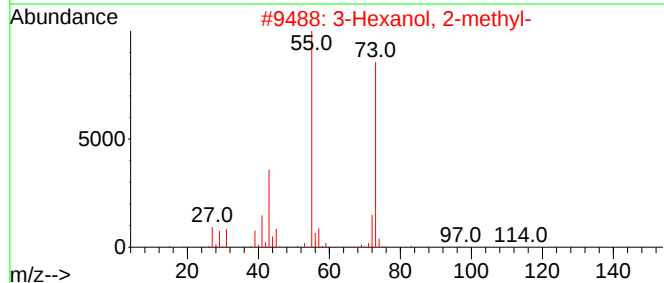
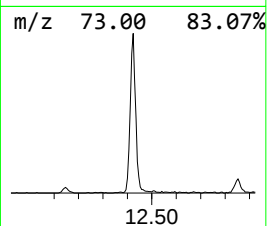
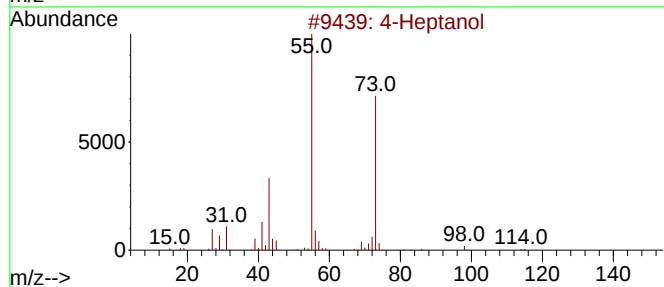
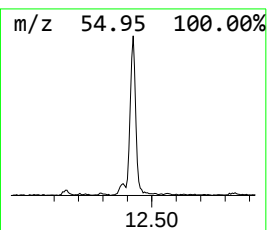
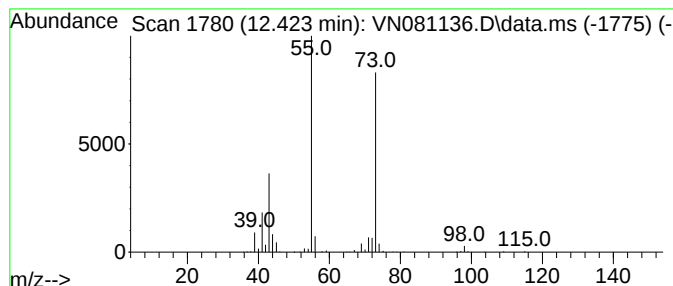
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4-Heptanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.424	10.40 ug/l	392217	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	83
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	45
3			5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	38
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	25
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081136.D
Acq On : 22 Feb 2024 15:35
Operator : JC\MD
Sample : P1546-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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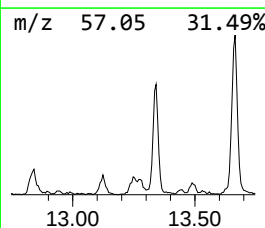
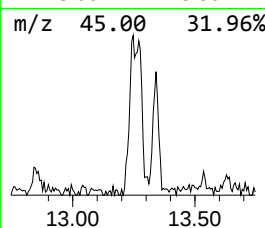
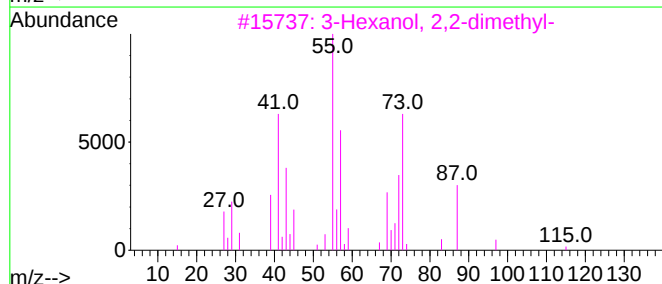
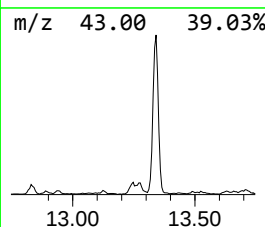
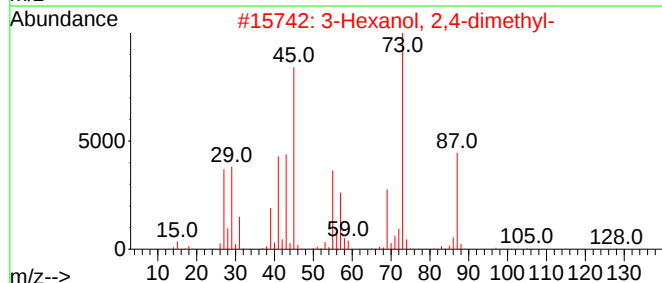
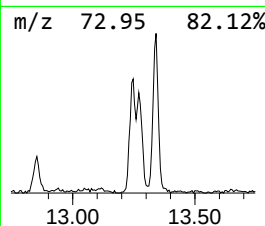
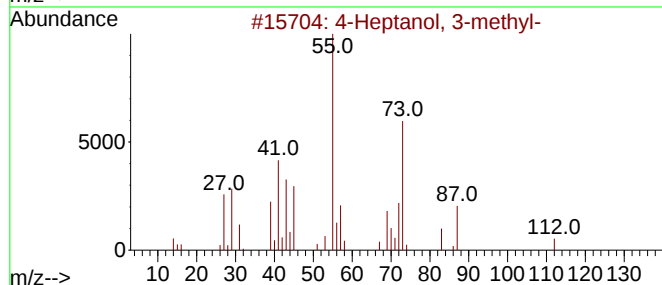
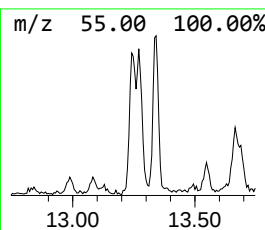
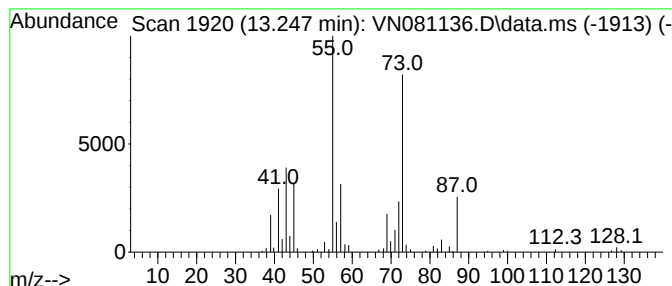
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Quant Title : SW846 8260

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

Peak Number 6 4-Heptanol, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.247	6.73 ug/l	213561	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	74
2			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	47
3			3-Hexanol, 2,2-dimethyl-	130	C8H18O	004209-90-9	45
4			4-Heptanol, 2-methyl-	130	C8H18O	021570-35-4	42
5			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081136.D
Acq On : 22 Feb 2024 15:35
Operator : JC\MD
Sample : P1546-08
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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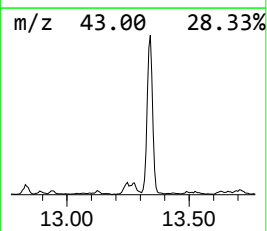
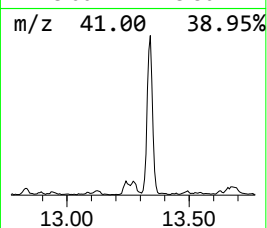
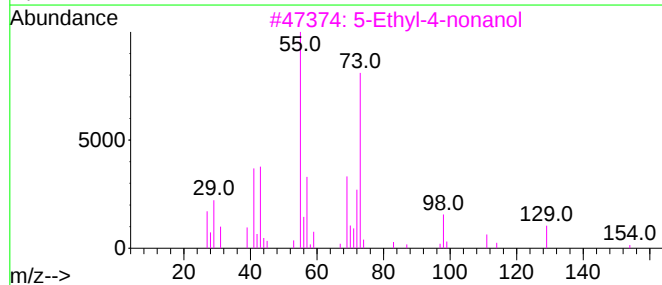
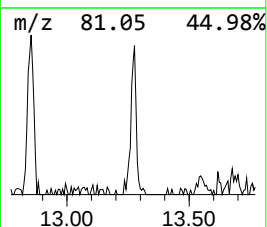
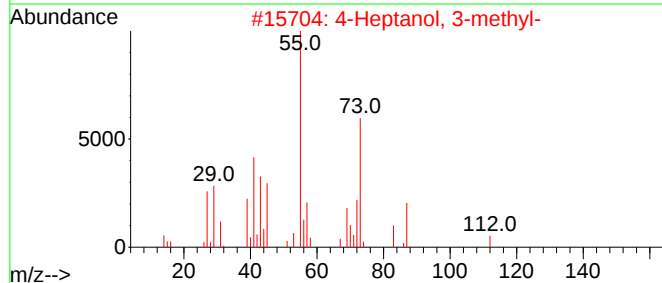
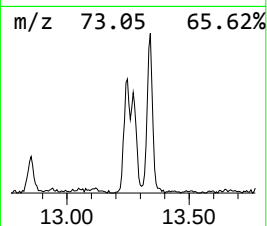
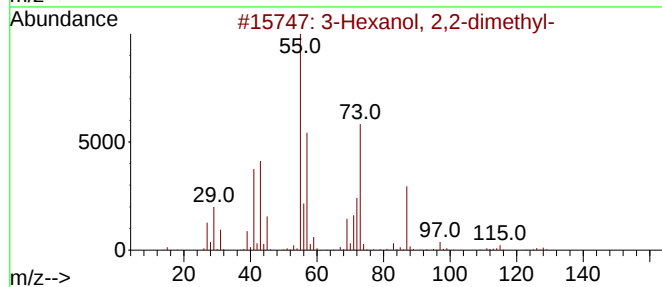
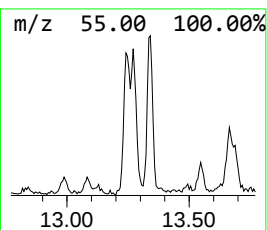
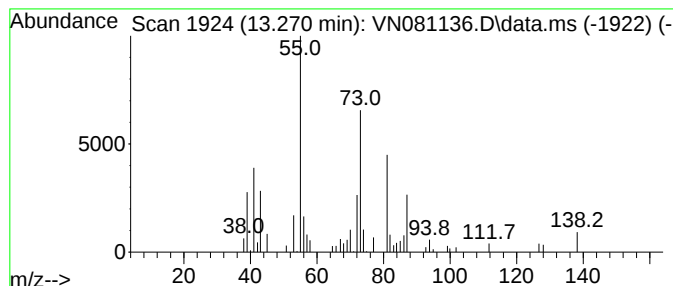
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Quant Title : SW846 8260

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

Peak Number 7 3-Hexanol, 2,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.271	6.32 ug/l	200804	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexanol, 2,2-dimethyl-	130	C8H18O	004209-90-9	50
2			4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	42
3			5-Ethyl-4-nonanol	172	C11H24O	019780-73-5	25
4			Cyclobutylcarboxylic acid	100	C5H8O2	003721-95-7	23
5			2-Propenoic acid, ethyl ester	100	C5H8O2	000140-88-5	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081136.D
Acq On : 22 Feb 2024 15:35
Operator : JC\MD
Sample : P1546-08
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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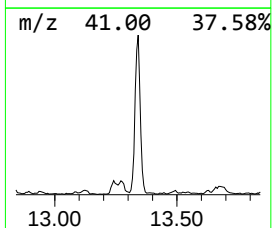
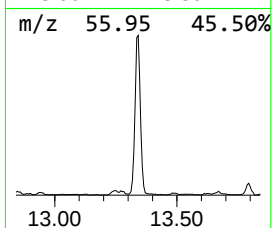
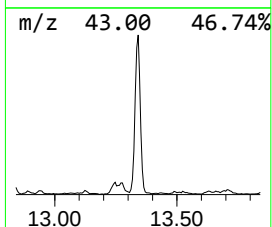
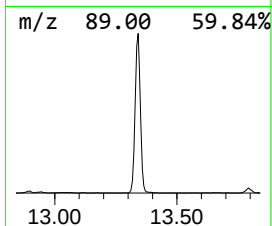
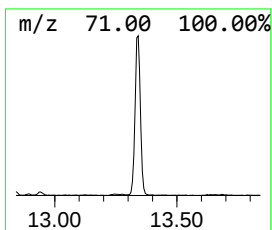
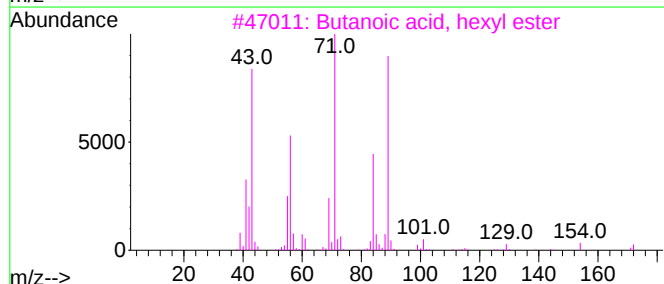
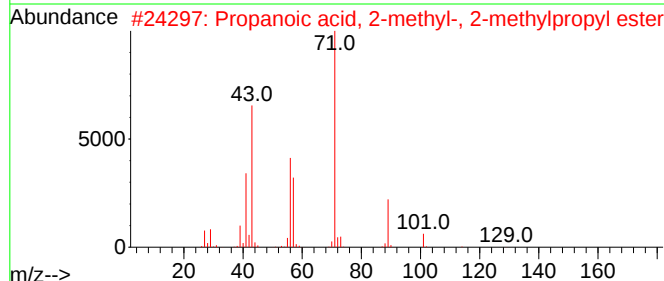
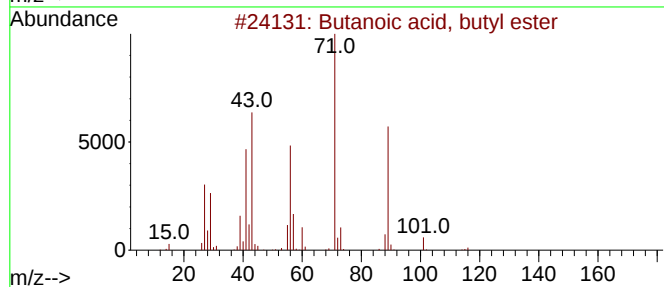
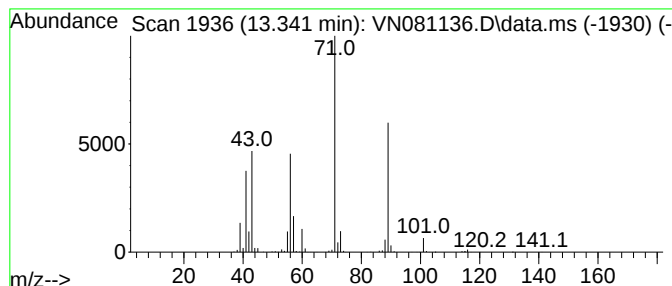
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Quant Title : SW846 8260

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

Peak Number 8 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	55.93 ug/l	1776130	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			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	53
5			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081136.D
Acq On : 22 Feb 2024 15:35
Operator : JC\MD
Sample : P1546-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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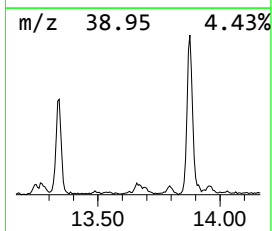
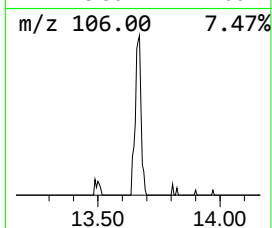
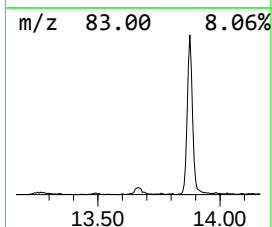
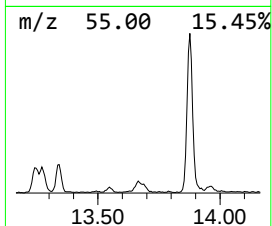
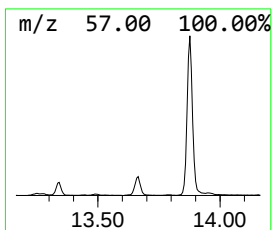
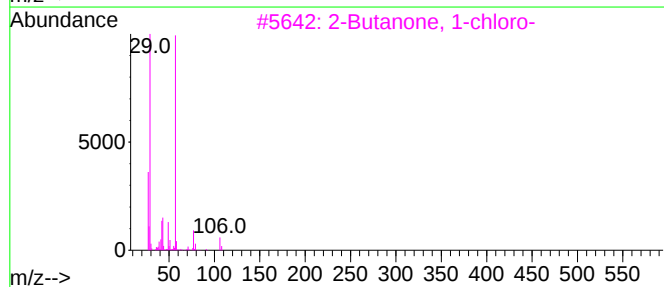
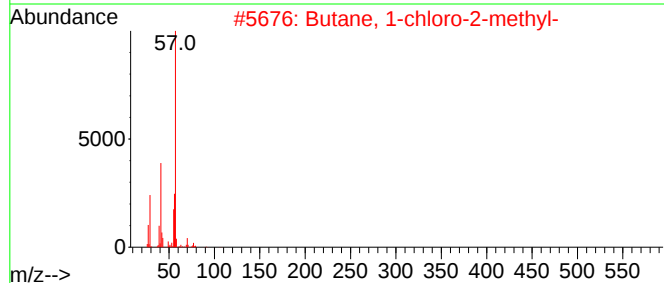
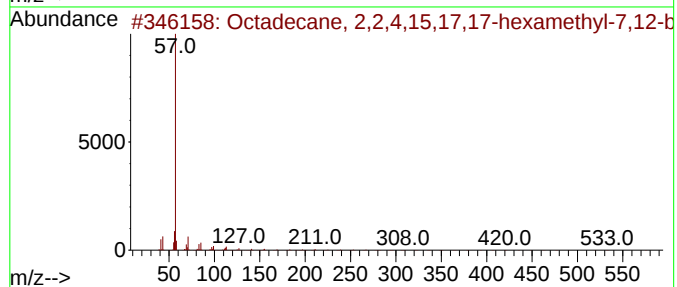
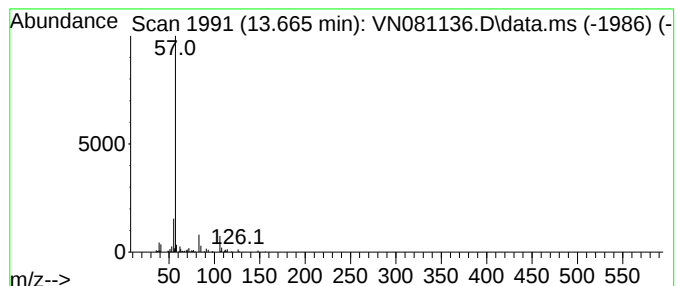
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Quant Title : SW846 8260

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

Peak Number 9 unknown13.665 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.665	9.53 ug/l	302759	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 2,2,4,15,17,17-hexam...	591	C42H86	055470-97-8	25
2			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	9
3			2-Butanone, 1-chloro-	106	C4H7ClO	000616-27-3	7
4			3-Decanone	156	C10H20O	000928-80-3	7
5			1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081136.D
Acq On : 22 Feb 2024 15:35
Operator : JC\MD
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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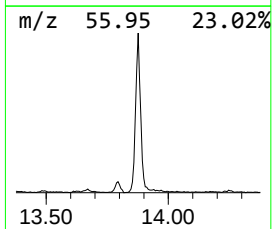
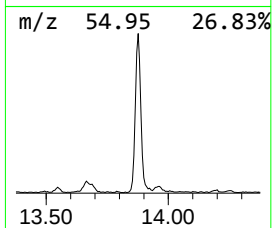
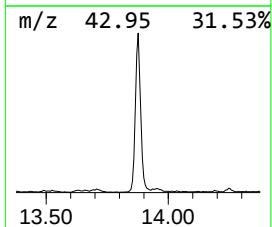
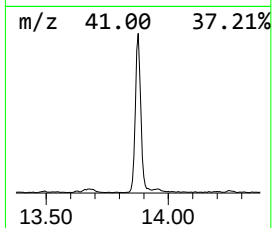
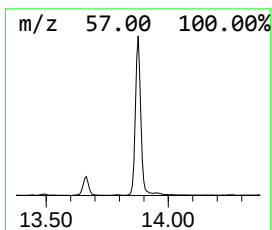
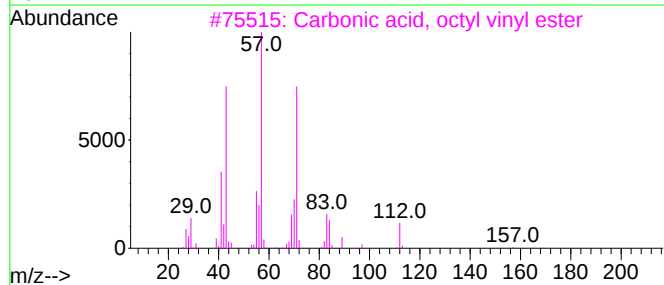
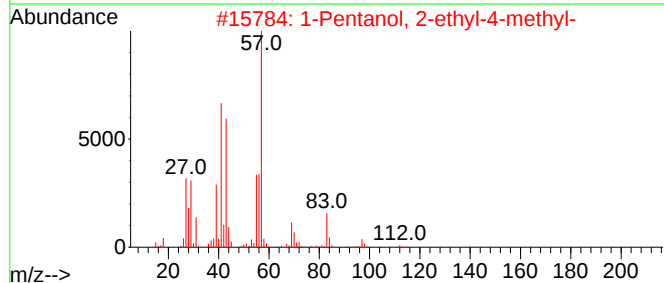
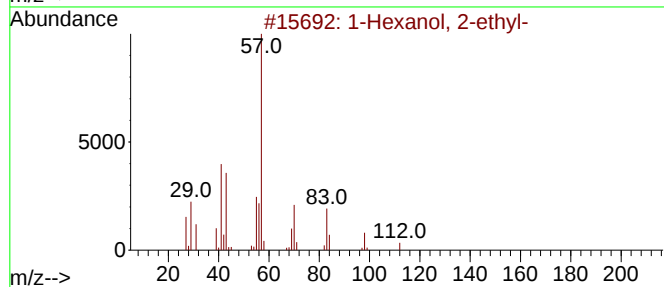
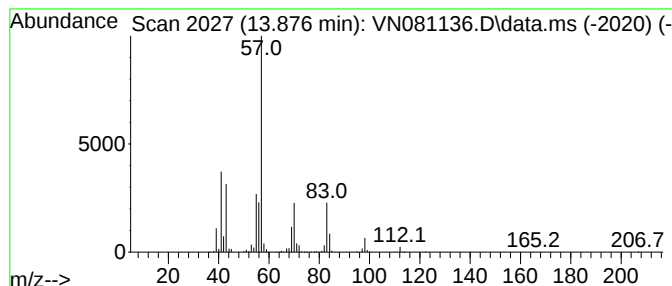
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Quant Title : SW846 8260

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	103.31 ug/l	3280440	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	64
3			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	59
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081136.D
Acq On : 22 Feb 2024 15:35
Operator : JC\MD
Sample : P1546-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.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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Butanal	7.230	39.2	ug/l	849986	1	8.224	1084760	50.0
Acetic acid	8.659	8.8	ug/l	190076	1	8.224	1084760	50.0
1-Butanol	9.271	13.3	ug/l	403913	2	9.106	1515640	50.0
4-Heptanol	12.424	10.4	ug/l	392217	3	11.865	1886490	50.0
4-Heptanol, 3-m...	13.247	6.7	ug/l	213561	4	13.794	1587740	50.0
3-Hexanol, 2,2-...	13.271	6.3	ug/l	200804	4	13.794	1587740	50.0
Butanoic acid, ...	13.341	55.9	ug/l	1776130	4	13.794	1587740	50.0
unknown13.665	13.665	9.5	ug/l	302759	4	13.794	1587740	50.0
1-Hexanol, 2-et...	13.876	103.3	ug/l	3280440	4	13.794	1587740	50.0