

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
 Data File : VN081793.D
 Acq On : 18 Apr 2024 17:30
 Operator : JC\MD
 Sample : P2121-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 4824

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\82N041524W.M
 Title : SW846 8260

Signal : TIC: VN081793.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	28	rBV	27811	40910	1.45%	0.292%
2	2.818	142	147	156	rVB4	14931	35082	1.24%	0.250%
3	4.436	411	422	431	rBV2	22976	67265	2.39%	0.480%
4	6.671	794	802	812	rBV4	9388	28213	1.00%	0.201%
5	7.224	887	896	906	rBV4	35277	97101	3.44%	0.693%
6	8.165	1046	1056	1061	rBV	181034	439306	15.58%	3.133%
7	8.224	1061	1066	1077	rVB	315088	696419	24.70%	4.967%
8	8.582	1118	1127	1137	rVB	196411	438473	15.55%	3.127%
9	9.100	1206	1215	1228	rBV	450398	933556	33.11%	6.658%
10	9.271	1237	1244	1259	rBV2	28592	80030	2.84%	0.571%
11	10.565	1454	1464	1473	rBV	679975	1286231	45.62%	9.174%
12	11.865	1673	1685	1698	rBV	628862	1154422	40.95%	8.234%
13	12.423	1774	1780	1798	rVB	82333	161424	5.73%	1.151%
14	12.853	1840	1853	1863	rBV	504341	918623	32.58%	6.552%
15	12.941	1863	1868	1874	rVV3	21357	34464	1.22%	0.246%
16	13.259	1914	1922	1929	rBV	942634	1544129	54.77%	11.013%
17	13.341	1929	1936	1951	rVB	1847878	2819161	100.00%	20.107%
18	13.506	1957	1964	1975	rBV	365184	611891	21.70%	4.364%
19	13.606	1976	1981	1989	rVB6	37443	69015	2.45%	0.492%
20	13.688	1989	1995	2002	rBV2	115723	205790	7.30%	1.468%
21	13.794	2006	2013	2019	rBV	670131	1133885	40.22%	8.087%
22	13.876	2019	2027	2035	rVV	372801	690863	24.51%	4.928%
23	13.953	2035	2040	2045	rVB6	23461	41075	1.46%	0.293%
24	14.241	2083	2089	2099	rBV9	28859	75255	2.67%	0.537%
25	15.347	2271	2277	2281	rBV6	42227	79382	2.82%	0.566%
26	15.394	2281	2285	2292	rVB2	76129	125065	4.44%	0.892%
27	15.517	2301	2306	2316	rBV8	20039	48720	1.73%	0.347%
28	15.823	2342	2358	2367	rVB6	39977	122161	4.33%	0.871%
29	15.941	2370	2378	2383	rBV6	18877	42636	1.51%	0.304%

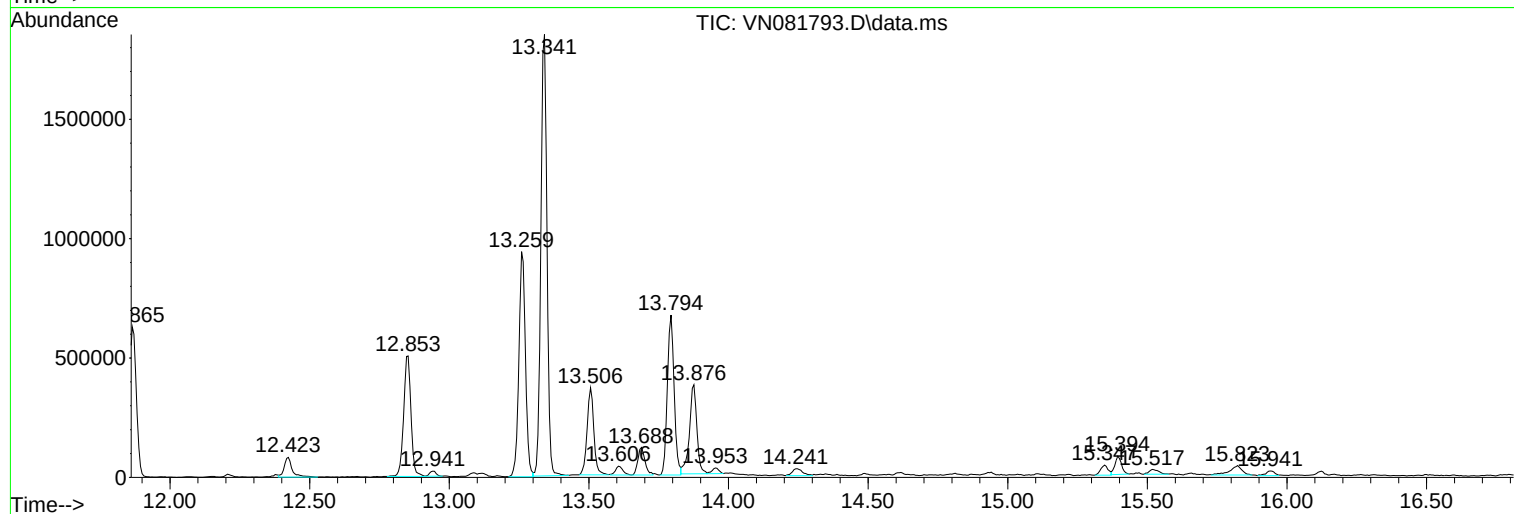
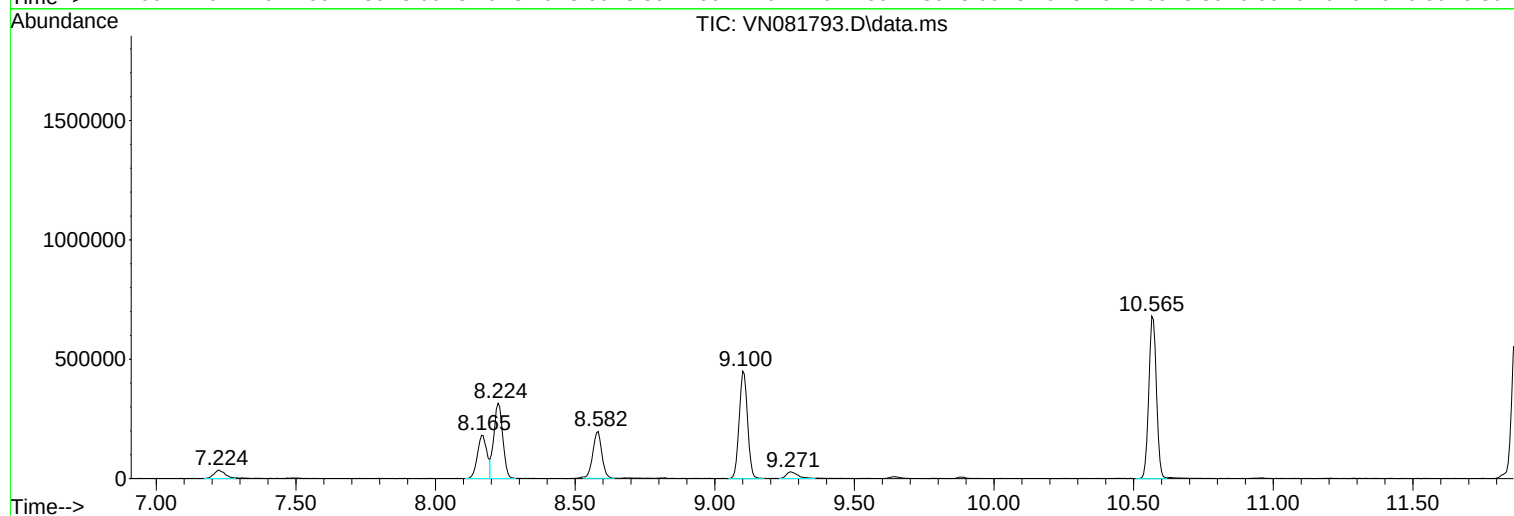
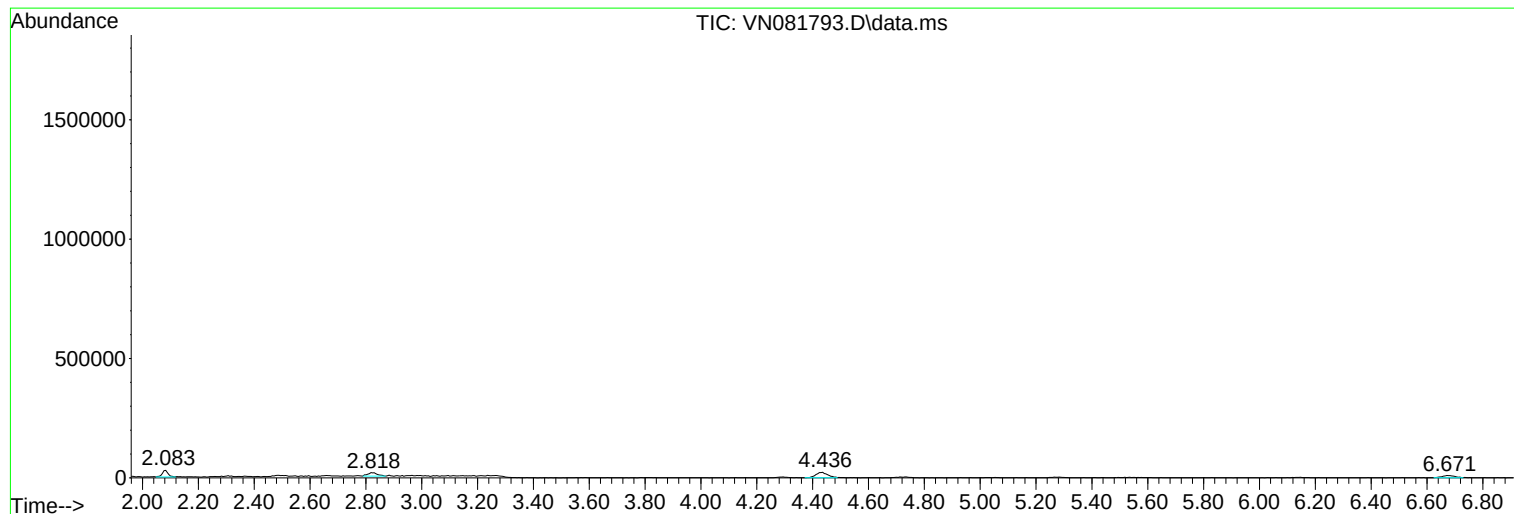
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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



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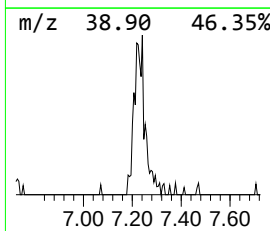
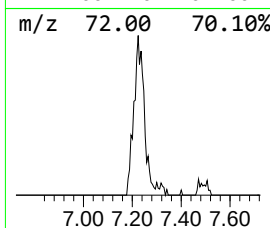
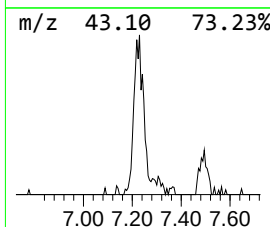
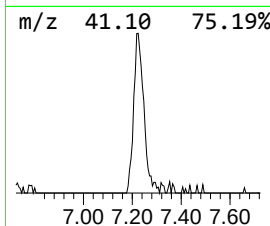
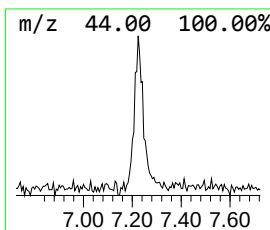
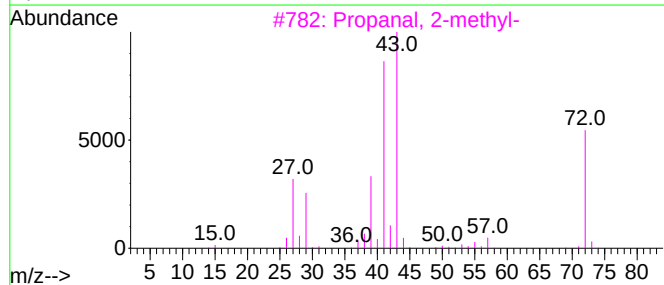
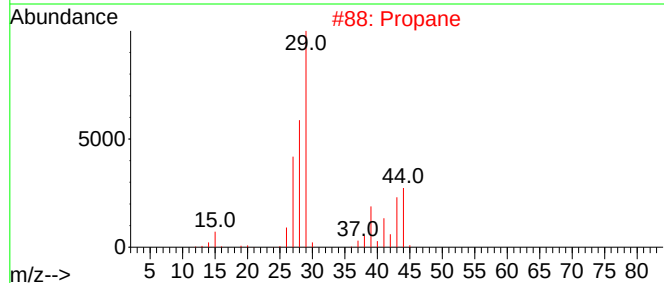
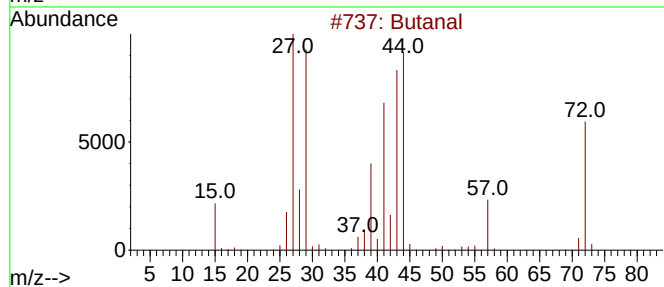
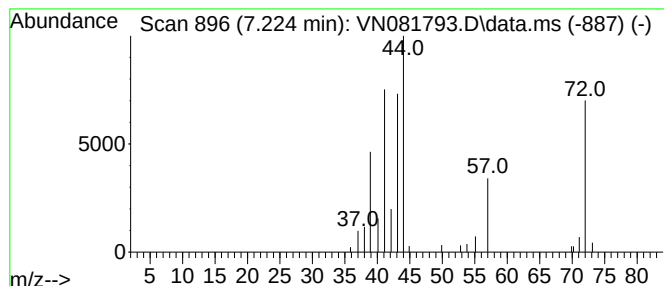
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Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	6.97 ug/l	97101	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propane	44	C3H8	000074-98-6	50
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			Ethene, ethoxy-	72	C4H8O	000109-92-2	32
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	27



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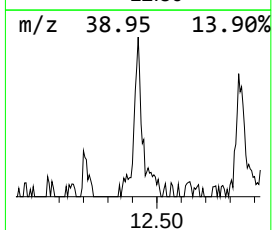
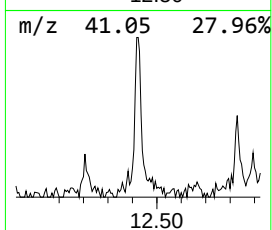
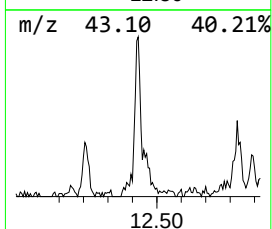
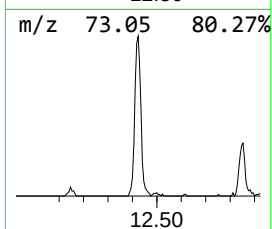
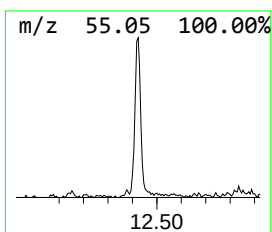
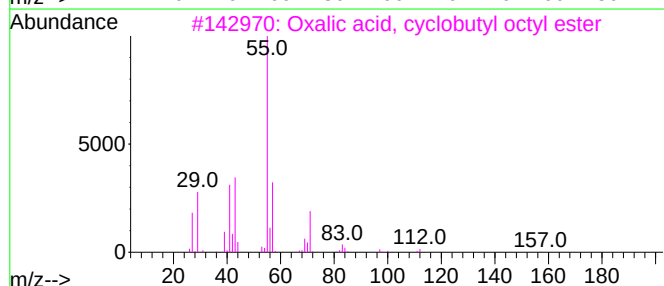
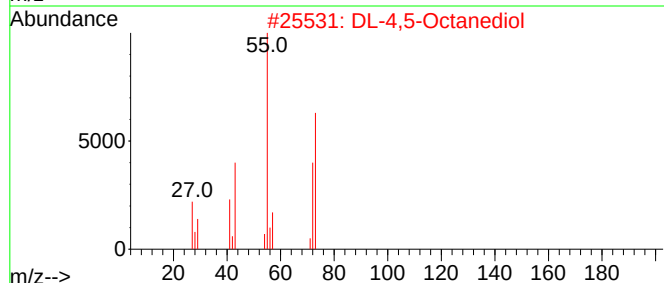
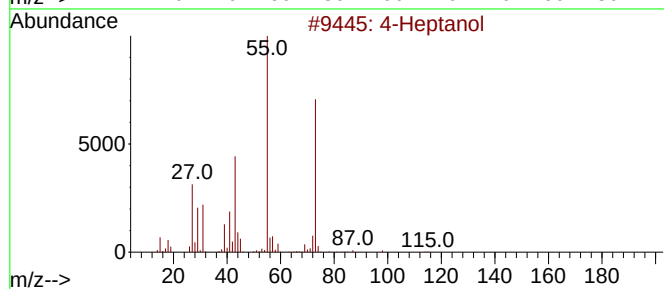
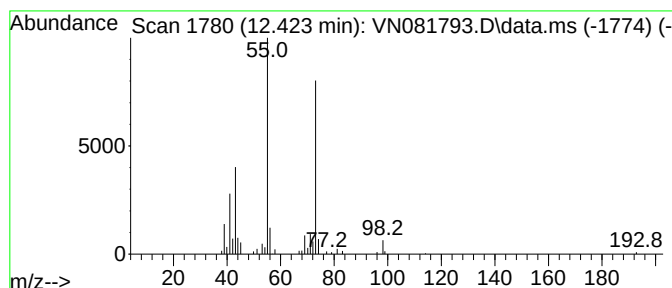
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Quant Title : SW846 8260

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

Peak Number 2 4-Heptanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.423	6.99 ug/l	161424	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	50
2			DL-4,5-Octanediol	146	C8H18O2	1000099-07-1	42
3			Oxalic acid, cyclobutyl octyl ester	256	C14H24O4	1000309-69-9	38
4			1-Heptyn-4-ol	112	C7H12O	022127-83-9	37
5			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	36



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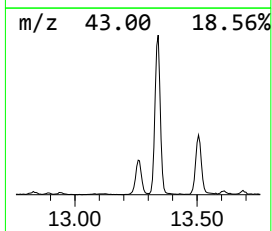
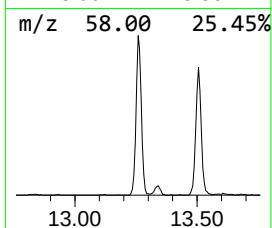
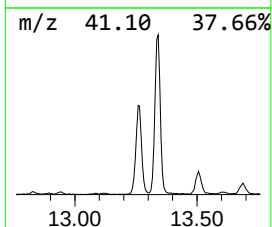
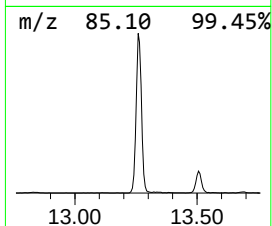
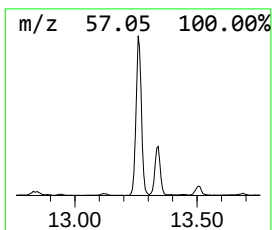
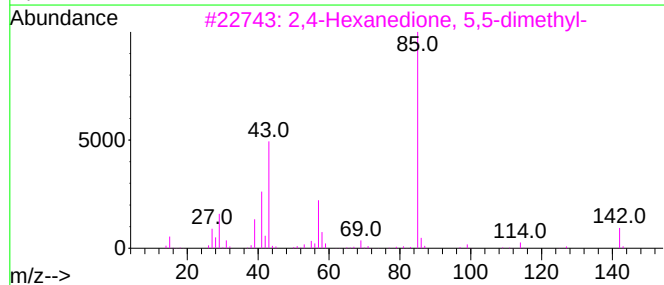
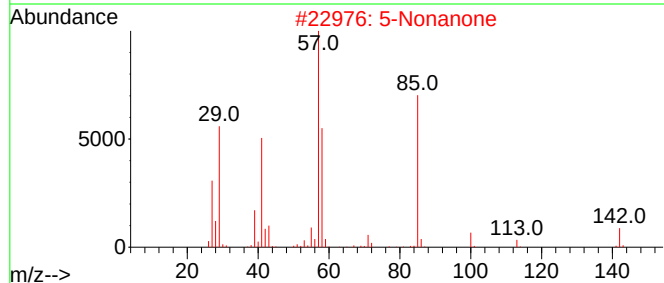
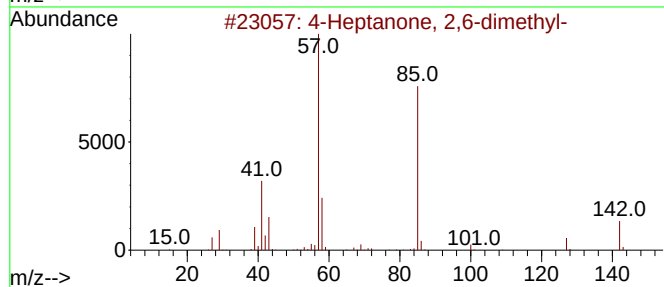
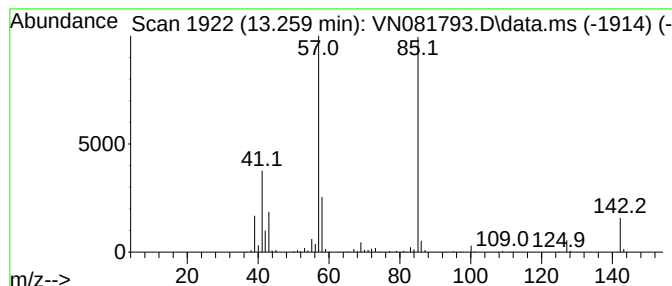
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 4-Heptanone, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	68.09 ug/l	1544130	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2			5-Nonanone	142	C9H18O	000502-56-7	64
3			2,4-Hexanedione, 5,5-dimethyl-	142	C8H14O2	007307-04-2	53
4			2,4-Heptanedione, 6-methyl-	142	C8H14O2	003002-23-1	53
5			t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	50



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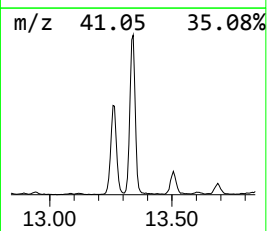
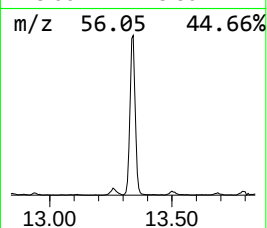
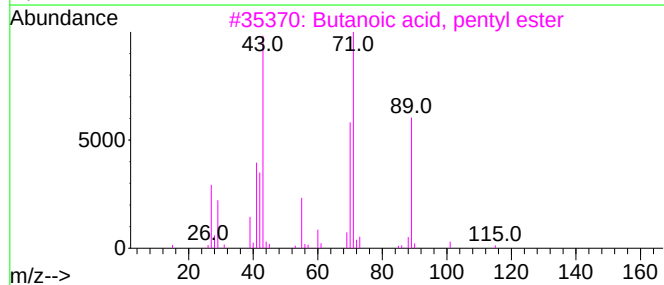
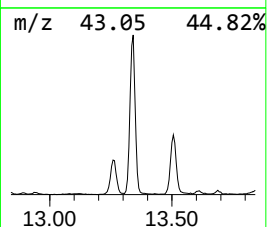
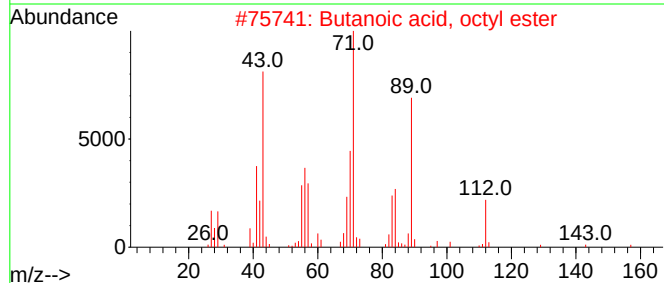
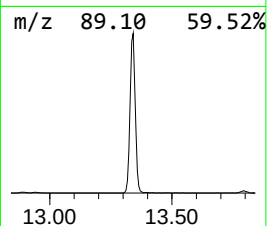
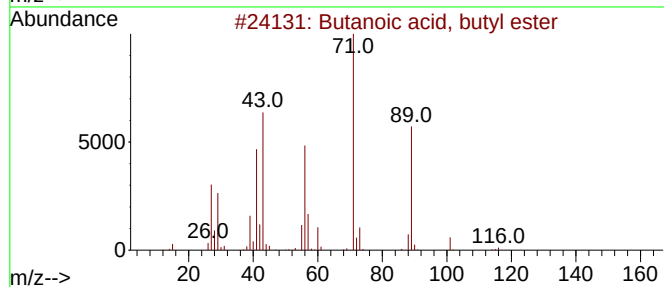
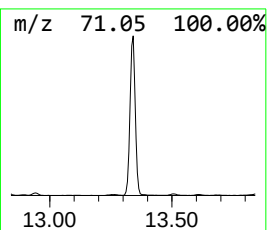
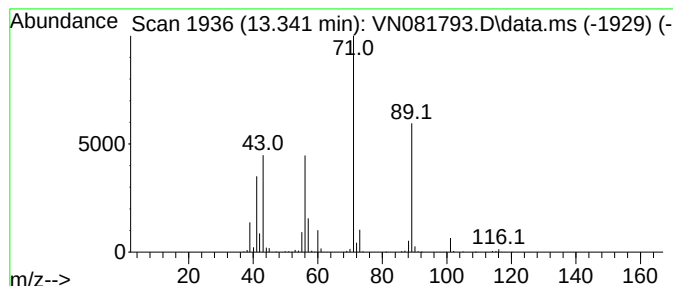
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	124.31 ug/l	2819160	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, octyl ester	200	C12H24O2	000110-39-4	59
3			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	53
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	50
5			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	50



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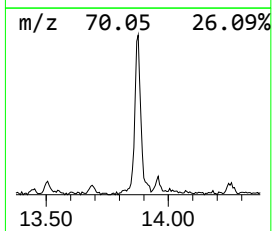
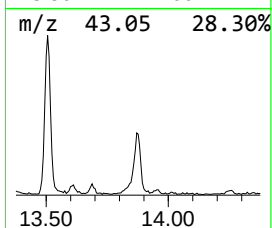
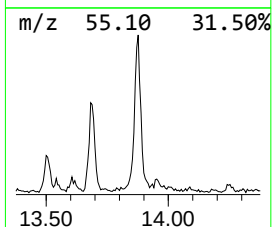
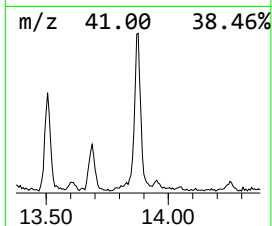
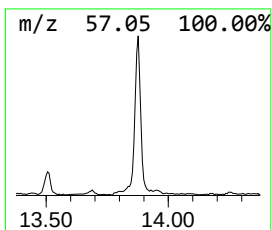
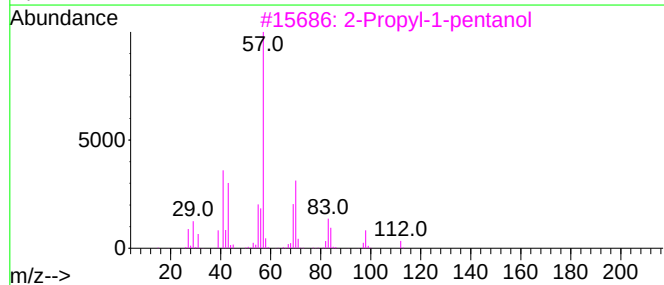
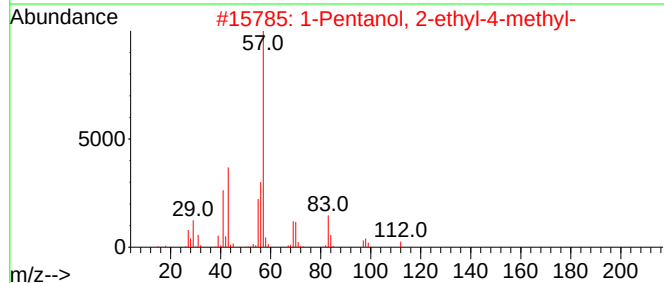
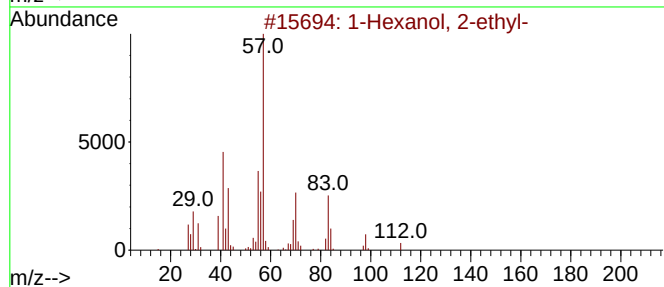
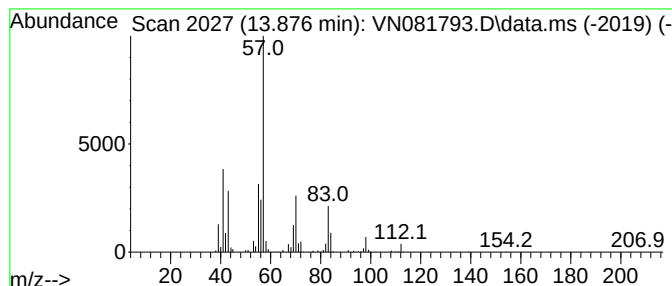
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	30.46 ug/l	690863	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	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			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47
5			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	47



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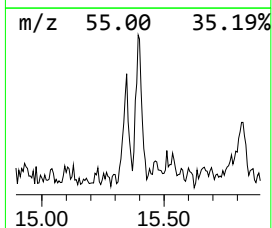
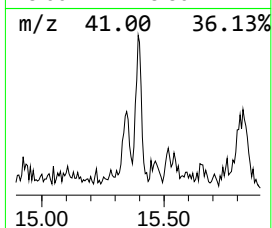
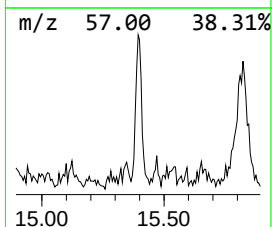
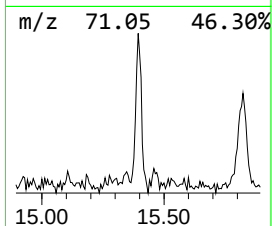
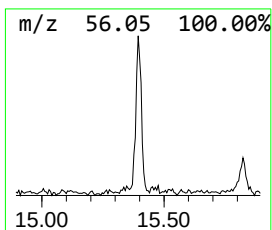
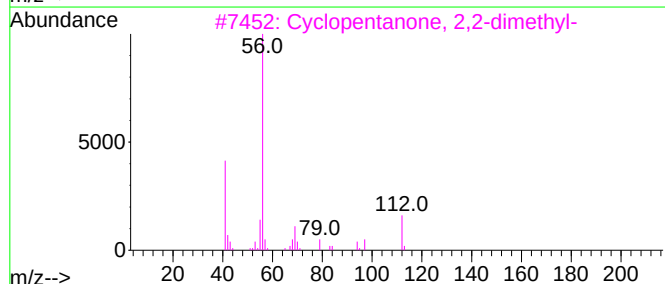
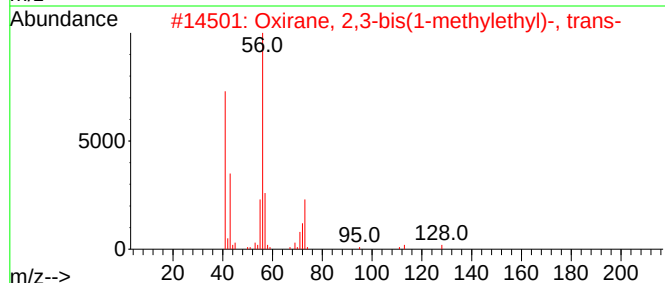
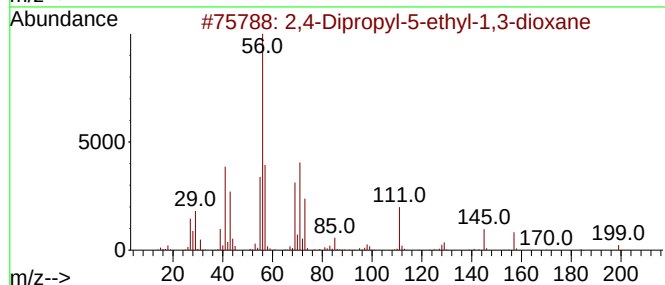
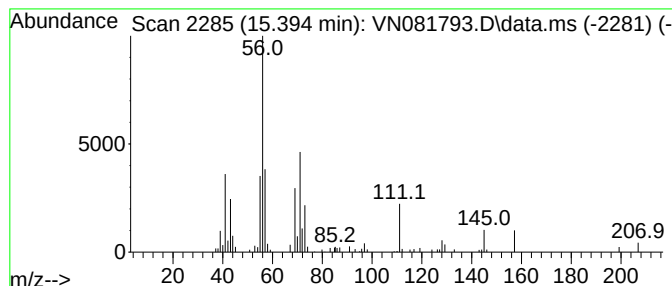
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Quant Title : SW846 8260

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

Peak Number 6 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.394	5.51 ug/l	125065	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	78
2		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37
3		Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	30
4		1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	27
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081793.D
Acq On : 18 Apr 2024 17:30
Operator : JC\MD
Sample : P2121-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
4824

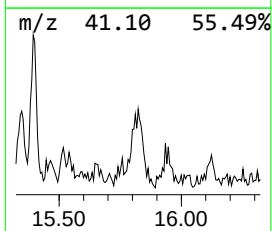
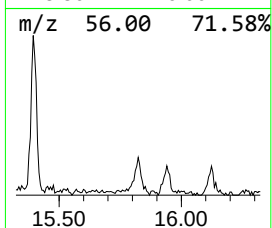
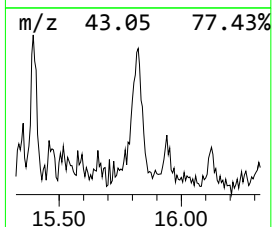
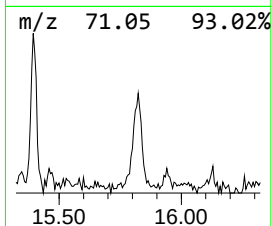
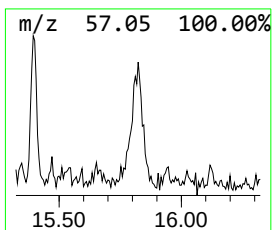
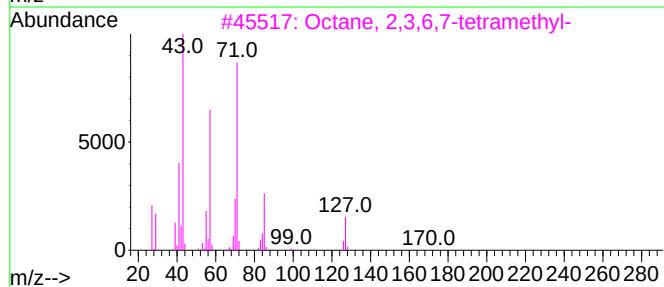
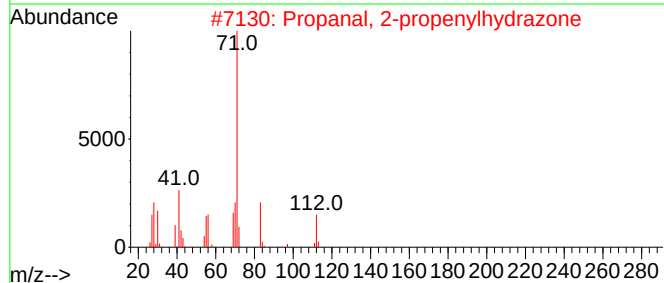
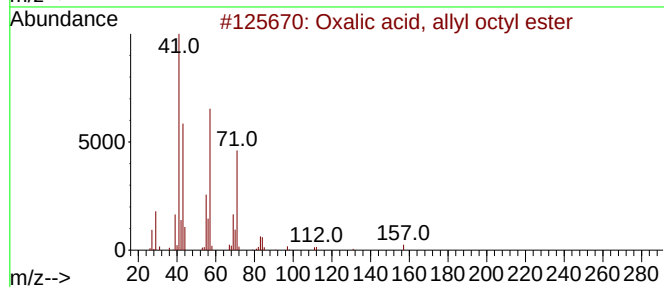
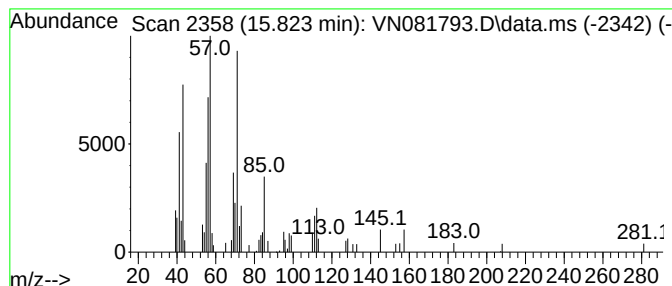
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.823 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.823	5.39 ug/l	122161	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	43
2			Propanal, 2-propenylhydrazone	112	C6H12N2	019031-78-8	38
3			Octane, 2,3,6,7-tetramethyl-	170	C12H26	052670-34-5	35
4			Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	35
5			Nonane, 2,3-dimethyl-	156	C11H24	002884-06-2	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081793.D
Acq On : 18 Apr 2024 17:30
Operator : JC\MD
Sample : P2121-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
4824

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	7.224	7.0	ug/l	97101	1	8.224	696419	50.0
4-Heptanol	12.423	7.0	ug/l	161424	3	11.865	1154420	50.0
4-Heptanone, 2,...	13.259	68.1	ug/l	1544130	4	13.794	1133890	50.0
Butanoic acid, ...	13.341	124.3	ug/l	2819160	4	13.794	1133890	50.0
1-Hexanol, 2-et...	13.876	30.5	ug/l	690863	4	13.794	1133890	50.0
2,4-Dipropyl-5-...	15.394	5.5	ug/l	125065	4	13.794	1133890	50.0
unknown15.823	15.823	5.4	ug/l	122161	4	13.794	1133890	50.0