

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
 Data File : VN081854.D
 Acq On : 25 Apr 2024 16:40
 Operator : JC\MD
 Sample : P2257-04
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41B

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: VN081854.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	rBV	155114	219155	4.36%	1.054%
2	2.665	117	121	132	rVB	41826	78810	1.57%	0.379%
3	4.712	459	469	480	rBV3	19092	64697	1.29%	0.311%
4	6.671	791	802	813	rBV3	52129	175838	3.50%	0.846%
5	7.224	886	896	913	rBV2	459829	1264495	25.13%	6.083%
6	8.165	1046	1056	1061	rBV	179558	430814	8.56%	2.073%
7	8.224	1061	1066	1076	rVB	327461	737701	14.66%	3.549%
8	8.577	1120	1126	1136	rVB2	206505	480910	9.56%	2.314%
9	9.100	1205	1215	1227	rBV	516140	1063081	21.13%	5.114%
10	9.265	1236	1243	1255	rBV2	65608	149798	2.98%	0.721%
11	9.653	1302	1309	1321	rVB3	63726	129232	2.57%	0.622%
12	10.565	1456	1464	1472	rBV	787885	1467727	29.17%	7.061%
13	11.865	1670	1685	1696	rBV	693688	1380333	27.44%	6.641%
14	12.376	1767	1772	1774	rBV2	50186	73966	1.47%	0.356%
15	12.418	1774	1779	1804	rVB	427819	749485	14.90%	3.606%
16	12.847	1843	1852	1859	rBV	549461	1041392	20.70%	5.010%
17	13.241	1913	1919	1922	rBV2	202589	360096	7.16%	1.732%
18	13.270	1922	1924	1929	rVV	182119	238269	4.74%	1.146%
19	13.335	1929	1935	1942	rVB	2283516	3484263	69.25%	16.763%
20	13.488	1956	1961	1965	rBV3	48024	74174	1.47%	0.357%
21	13.541	1965	1970	1978	rVB2	36209	71525	1.42%	0.344%
22	13.659	1981	1990	2005	rVB	81107	202320	4.02%	0.973%
23	13.794	2005	2013	2019	rBV	645524	1111375	22.09%	5.347%
24	13.870	2019	2026	2035	rVV	3168200	5031103	100.00%	24.204%
25	13.953	2035	2040	2046	rVB3	89180	138077	2.74%	0.664%
26	14.188	2068	2080	2086	rBV6	19171	53680	1.07%	0.258%
27	14.253	2086	2091	2095	rVB2	59281	92816	1.84%	0.447%
28	15.394	2279	2285	2291	rVB2	145869	240616	4.78%	1.158%
29	15.464	2291	2297	2304	rBV2	62718	104272	2.07%	0.502%
30	16.117	2401	2408	2413	rBV4	38000	75946	1.51%	0.365%

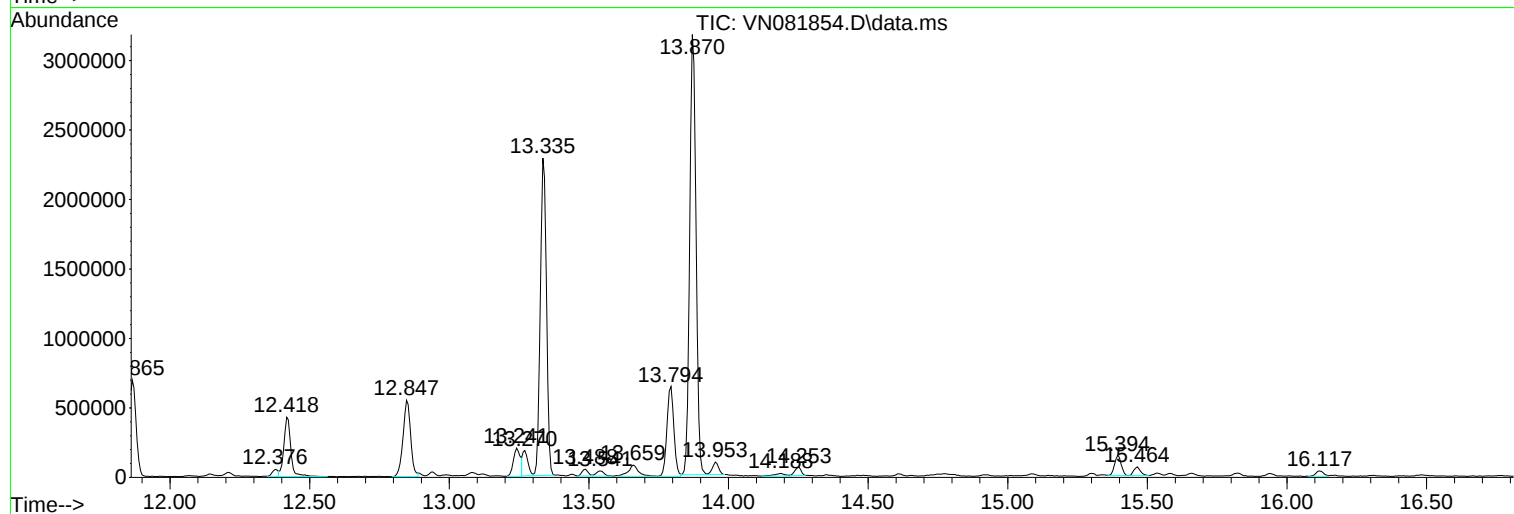
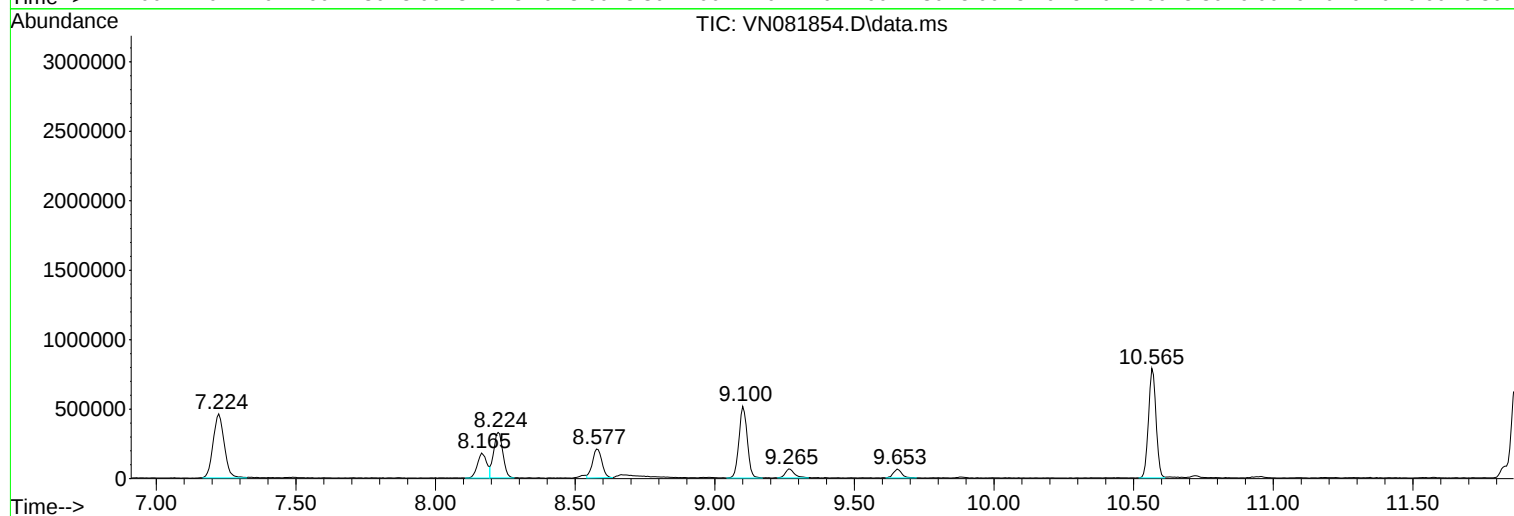
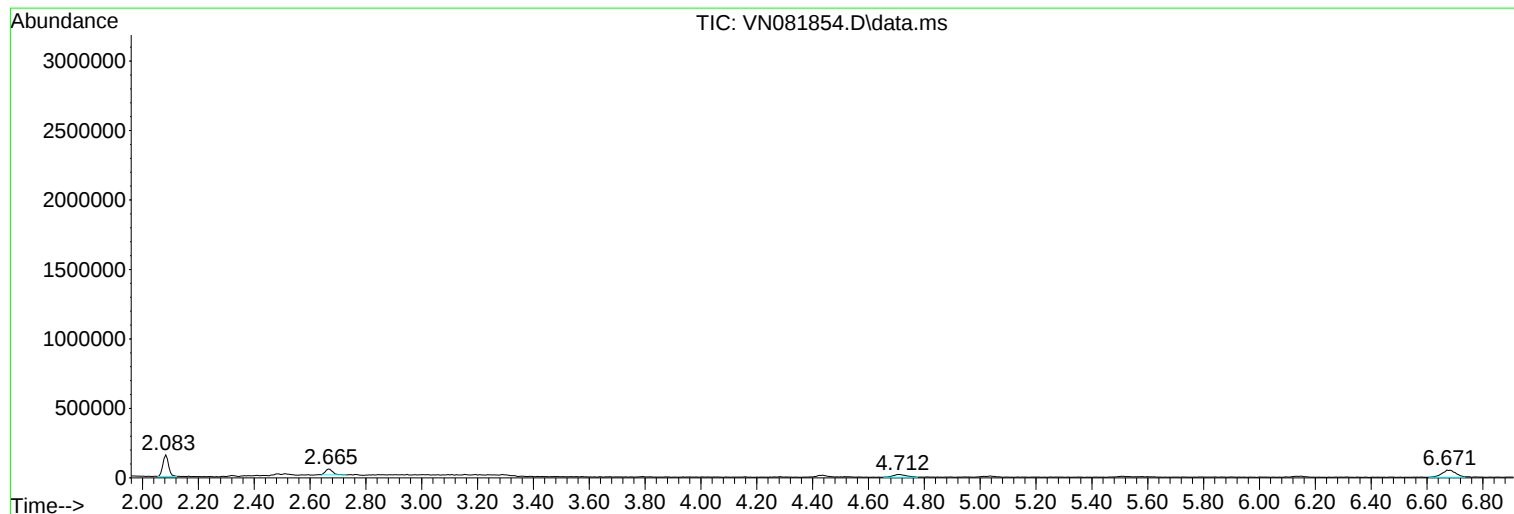
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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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



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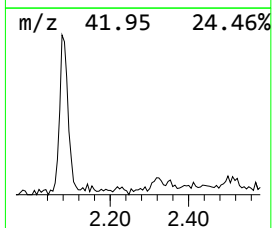
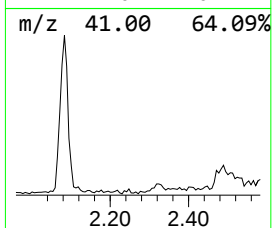
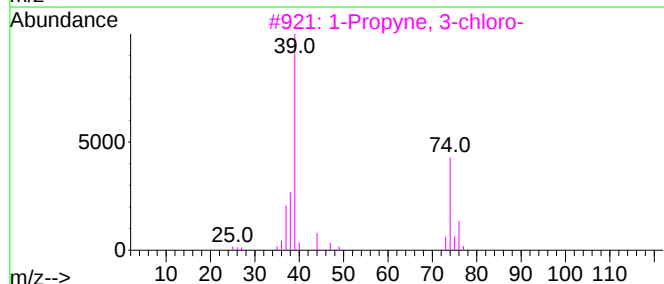
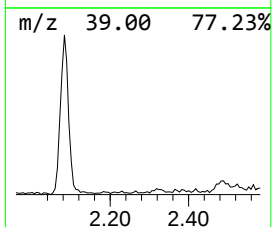
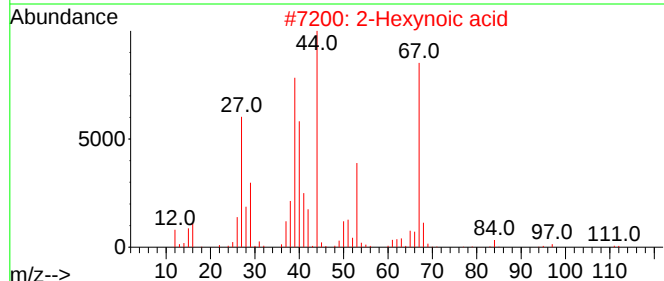
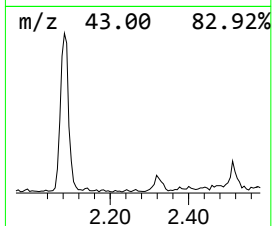
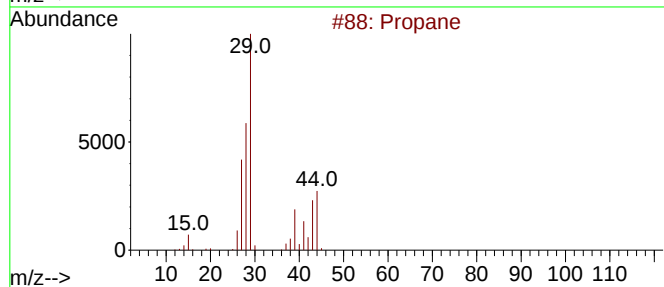
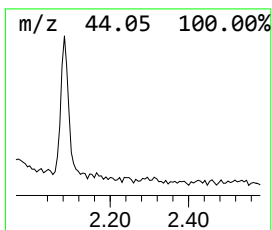
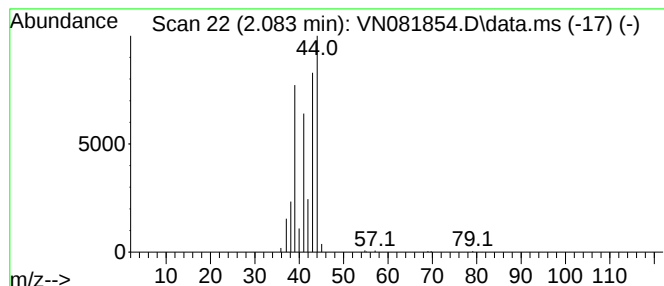
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	14.85 ug/l	219155	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	90
2			2-Hexynoic acid	112	C6H8O2	000764-33-0	43
3			1-Propyne, 3-chloro-	74	C3H3Cl	000624-65-7	9
4			Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	9
5			Propene	42	C3H6	000115-07-1	9



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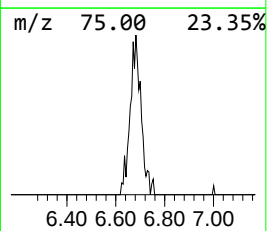
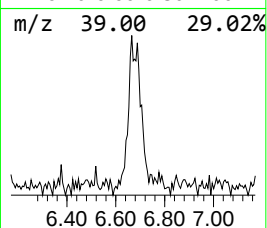
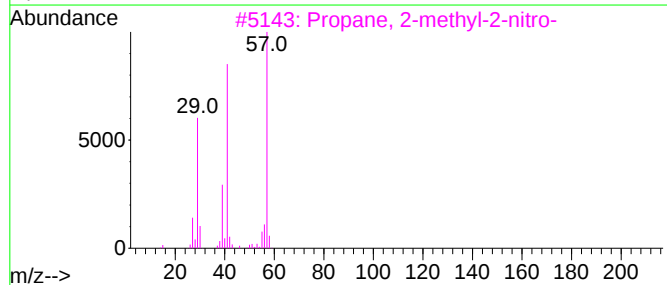
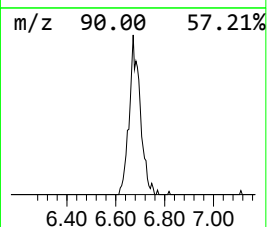
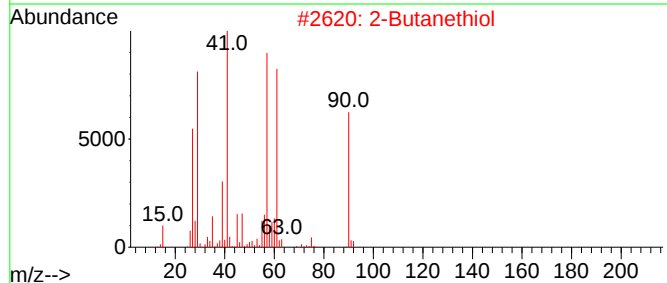
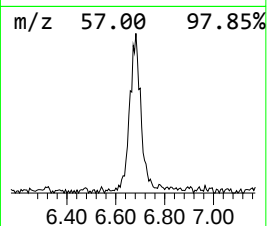
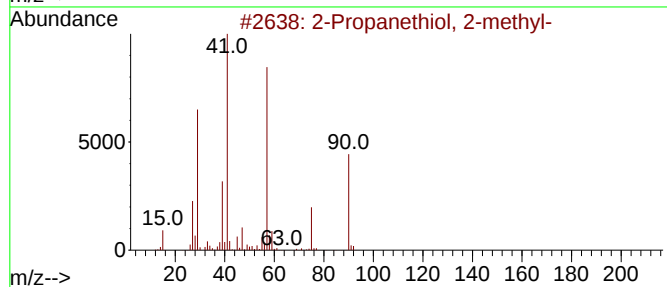
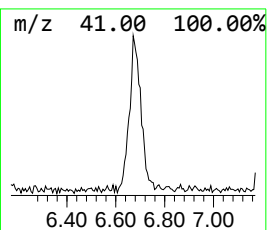
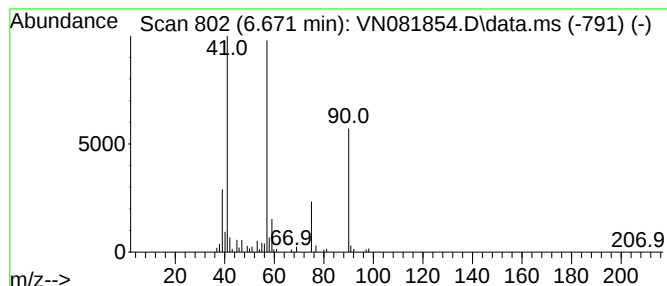
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Quant Title : SW846 8260

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

Peak Number 2 2-Propanethiol, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.671	11.92 ug/l	175838	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	86
2			2-Butanethiol	90	C4H10S	000513-53-1	36
3			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	14
4			Pivalyl chloride	120	C5H9ClO	003282-30-2	10
5			Butane, 2-nitro-	103	C4H9NO2	000600-24-8	10



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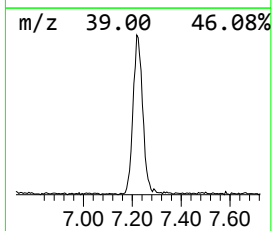
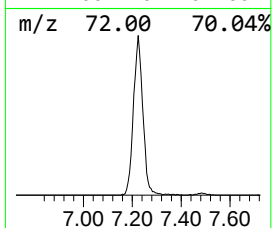
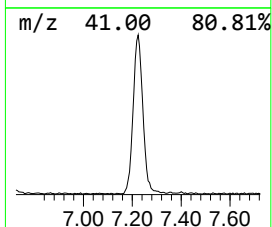
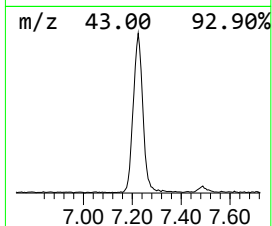
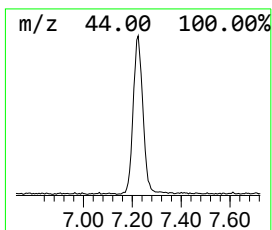
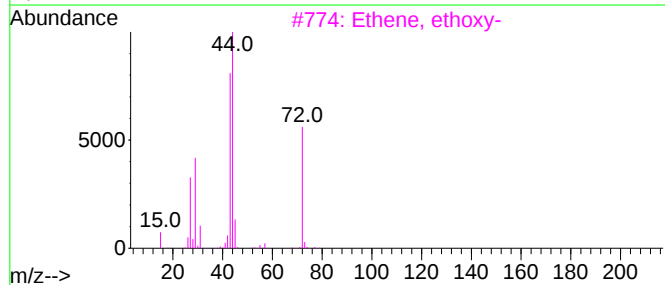
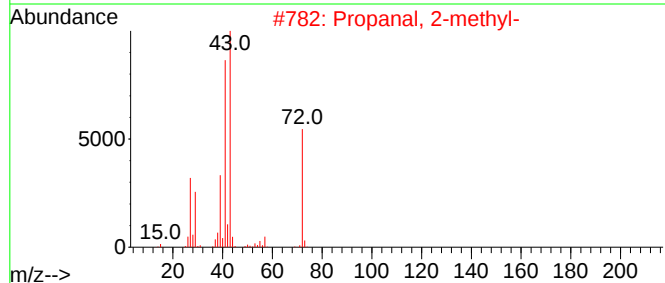
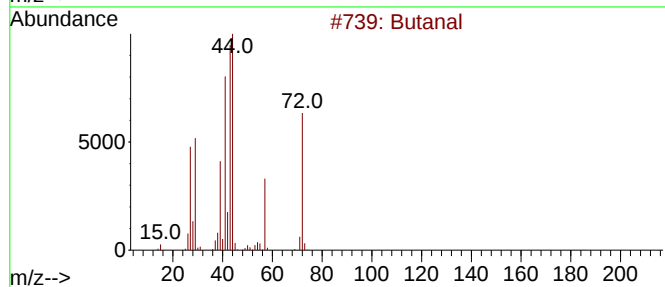
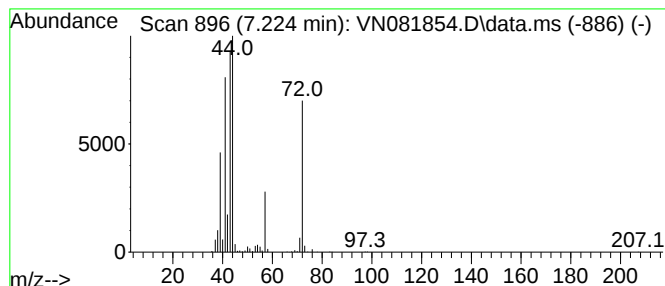
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	85.71 ug/l	1264500	Pentafluorobenzene	8.230

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	38
4			O-Methylisourea	74	C2H6N2O	002440-60-0	36
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32



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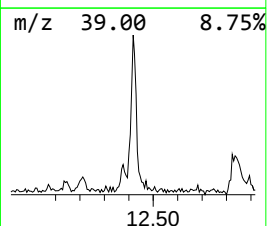
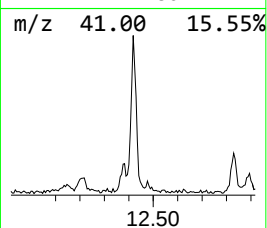
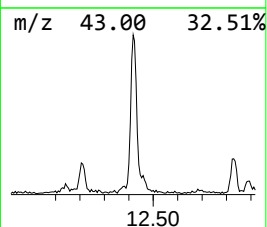
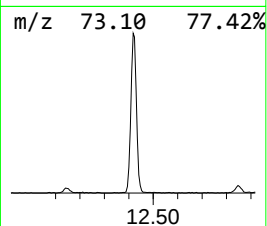
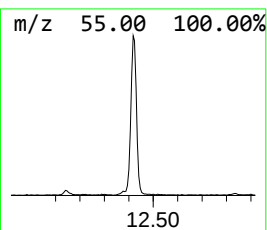
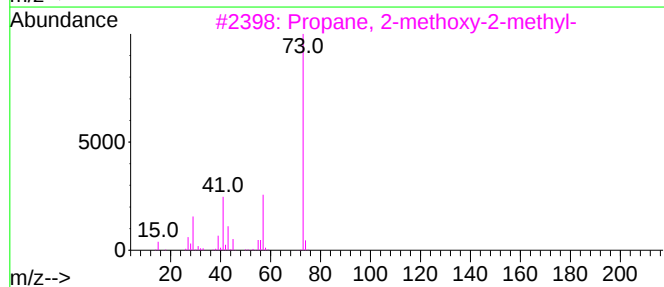
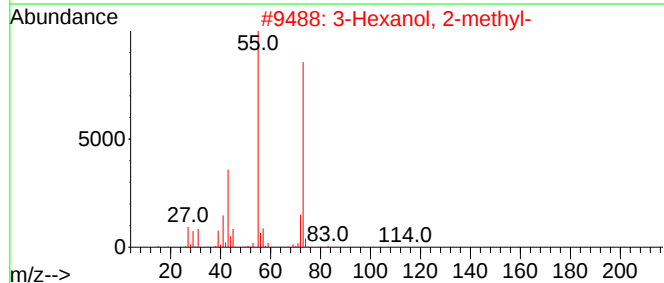
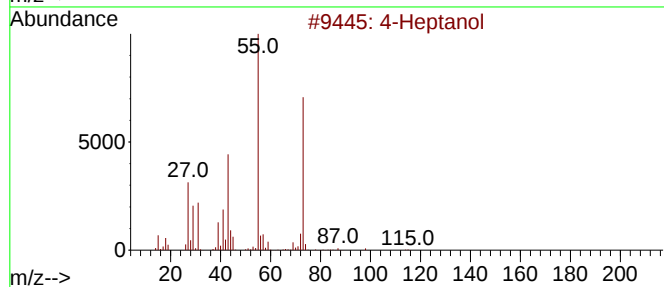
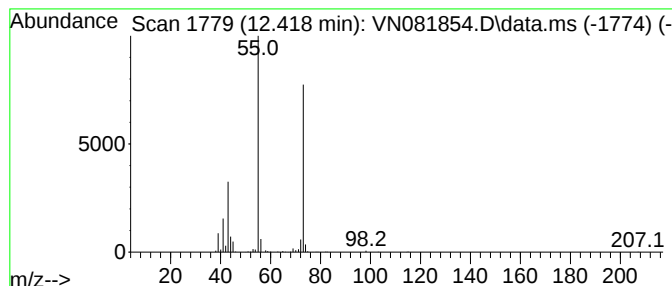
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Peak Number 4 4-Heptanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.418	27.15 ug/l	749485	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	78
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	72
3			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	32
4			1,3-Dioxolane	74	C3H6O2	000646-06-0	9
5			Pentanoic acid, 2-hydroxy-, meth...	132	C6H12O3	007445-76-3	9



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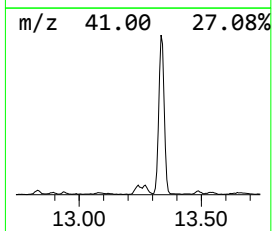
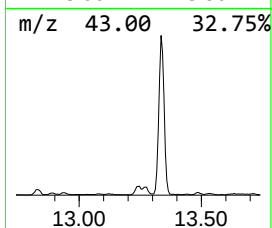
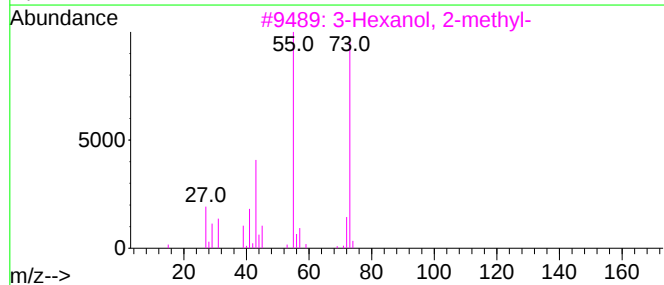
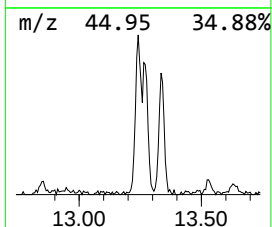
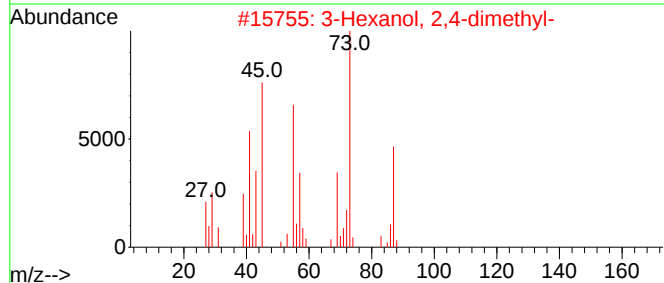
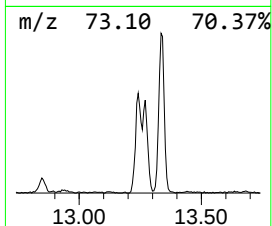
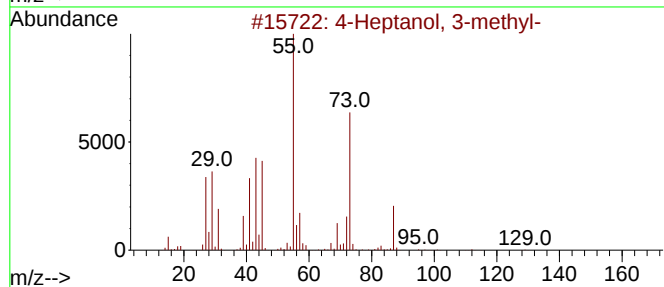
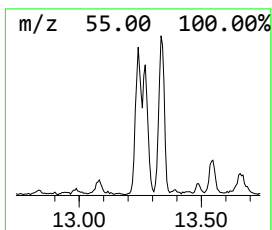
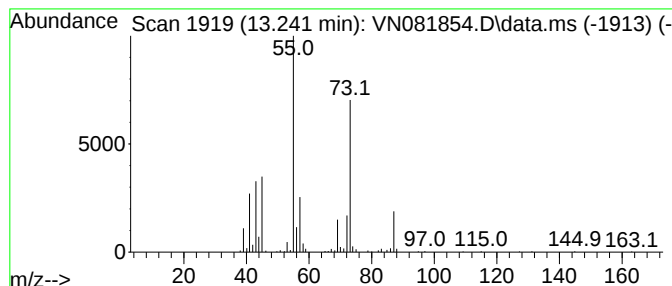
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 4-Heptanol, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.241	16.20 ug/l	360096	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	83
2			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	59
3			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	37
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
5			1-Butene, 3-propoxy-	114	C7H14O	037027-59-1	33



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ClientSampleId :
41B

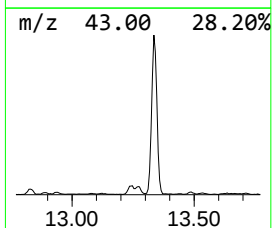
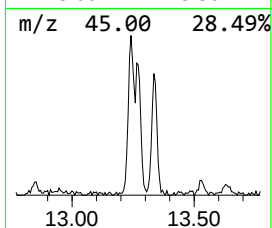
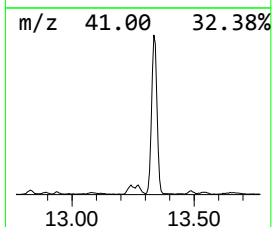
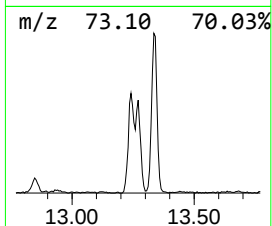
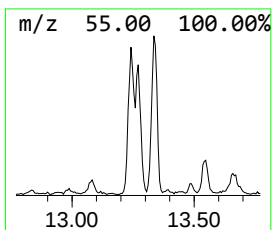
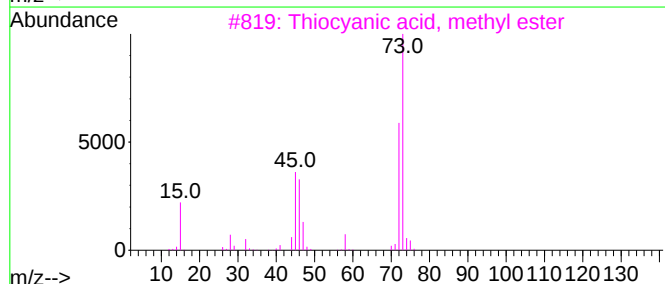
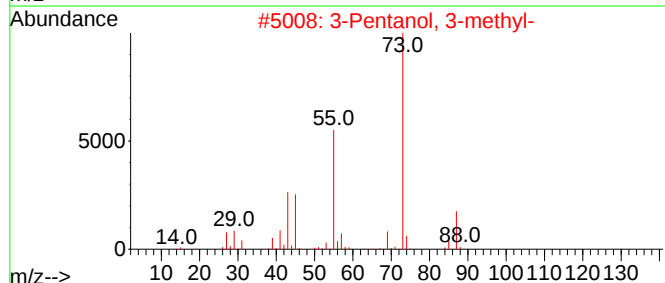
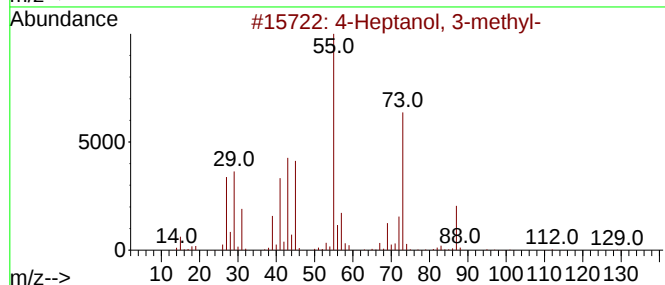
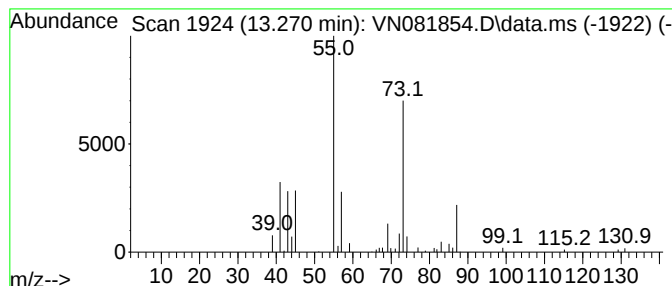
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Quant Title : SW846 8260

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

Peak Number 6 unknown13.271 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.271	10.72 ug/l	238269	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	56
2		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
3		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
4		Aminocaproic acid	131	C6H13NO2	000060-32-2	9
5		3-Butyn-2-ol	70	C4H6O	002028-63-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081854.D
Acq On : 25 Apr 2024 16:40
Operator : JC\MD
Sample : P2257-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41B

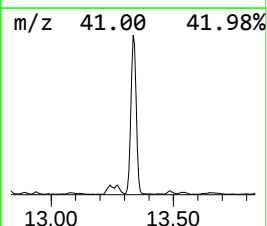
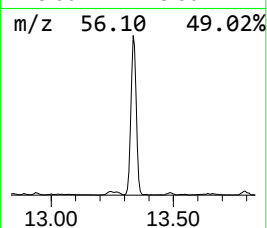
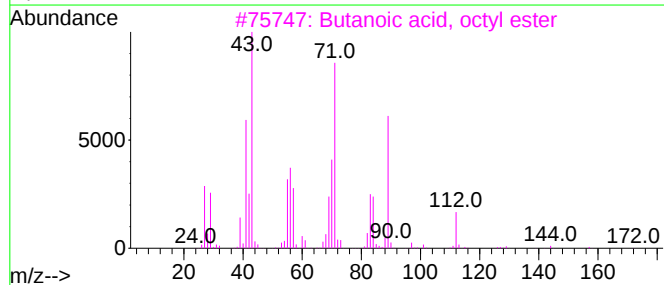
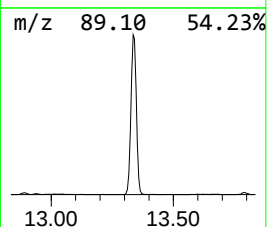
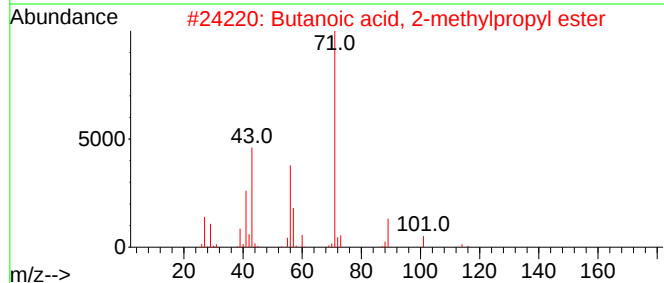
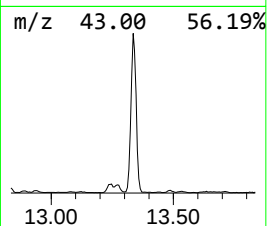
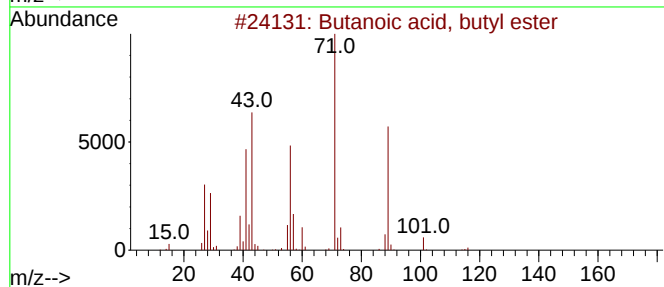
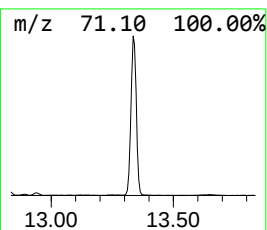
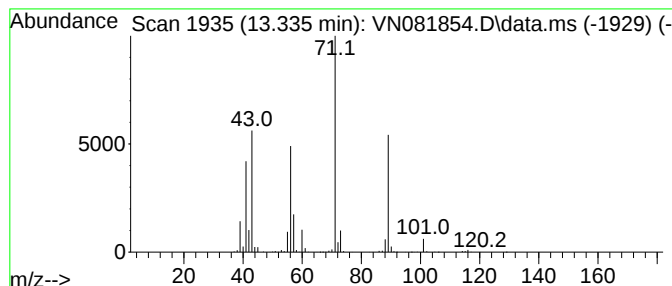
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Quant Title : SW846 8260

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	156.76 ug/l	3484260	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	91
2			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
4			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
5			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081854.D
Acq On : 25 Apr 2024 16:40
Operator : JC\MD
Sample : P2257-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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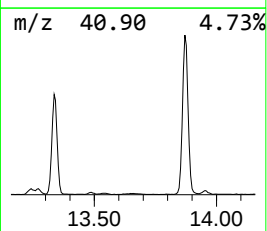
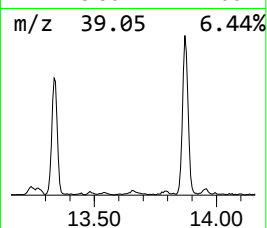
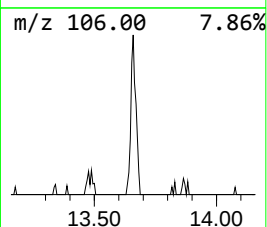
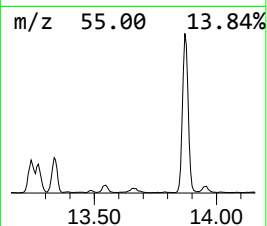
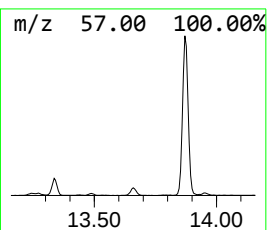
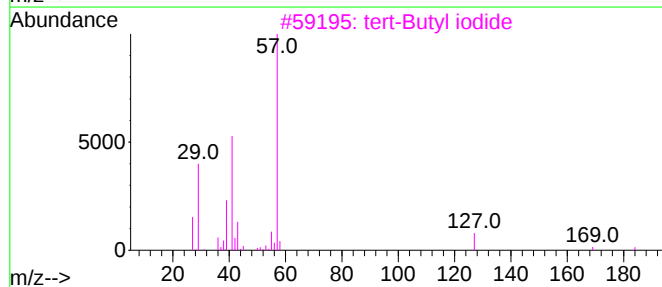
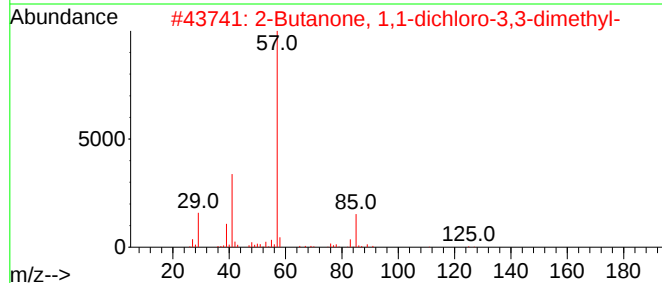
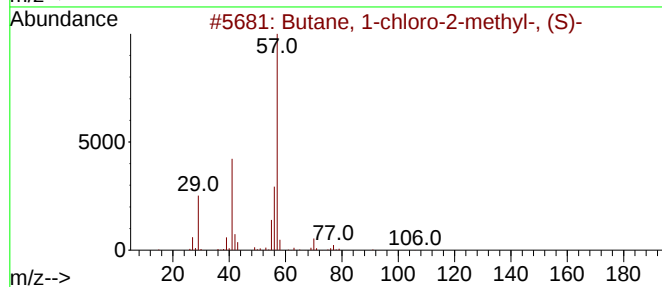
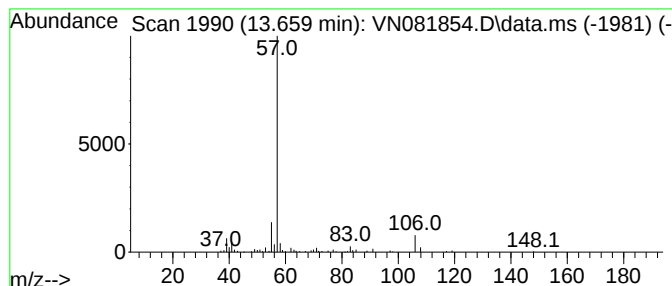
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.659 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.659	9.10 ug/l	202320	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-2-methyl-, (S)-	106	C5H11Cl	040560-29-0	25
2			2-Butanone, 1,1-dichloro-3,3-dimethyl-	168	C6H10Cl2O	022591-21-5	9
3			tert-Butyl iodide	184	C4H9I	000558-17-8	9
4			Propanoic acid, 2,2,2-trichloro-	218	C6H9Cl3O2	072037-39-9	9
5			2-Hexene, 3,5,5-trimethyl-	126	C9H18	026456-76-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081854.D
Acq On : 25 Apr 2024 16:40
Operator : JC\MD
Sample : P2257-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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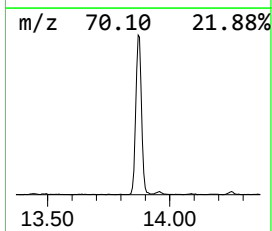
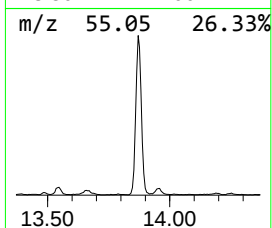
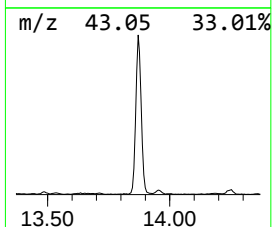
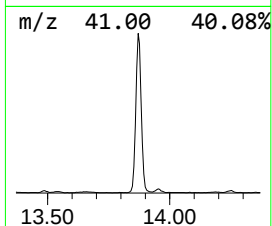
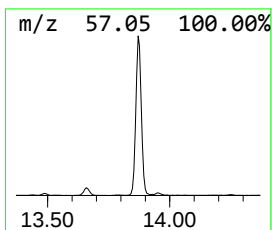
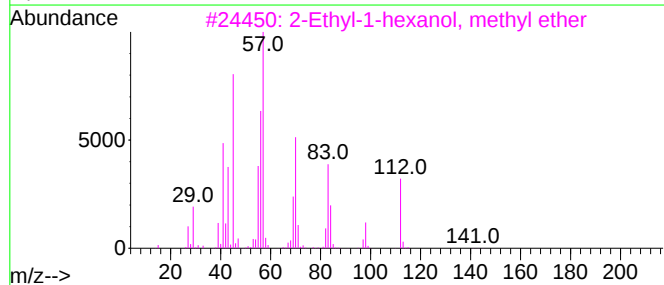
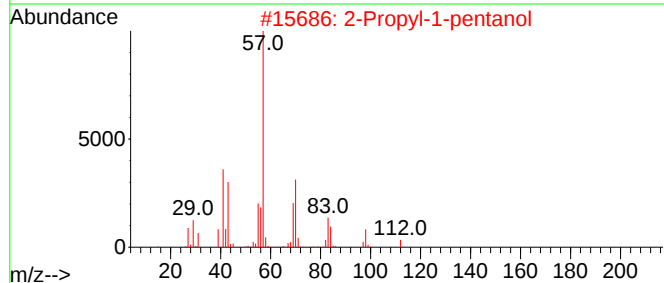
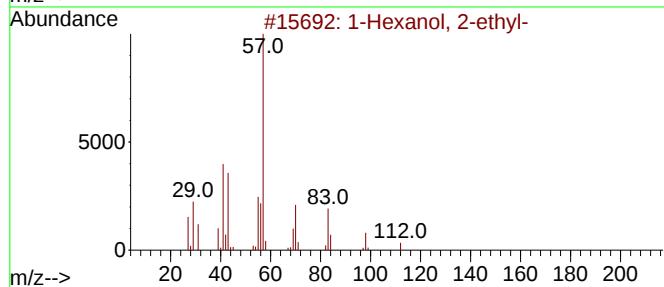
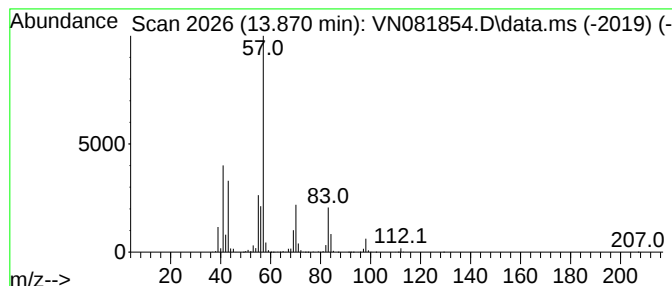
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Quant Title : SW846 8260

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	226.35 ug/l	5031100	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			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47
5			Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081854.D
Acq On : 25 Apr 2024 16:40
Operator : JC\MD
Sample : P2257-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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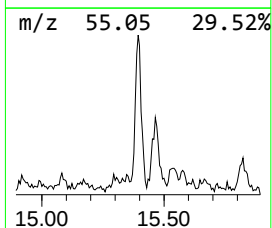
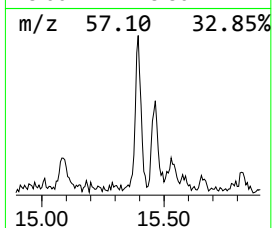
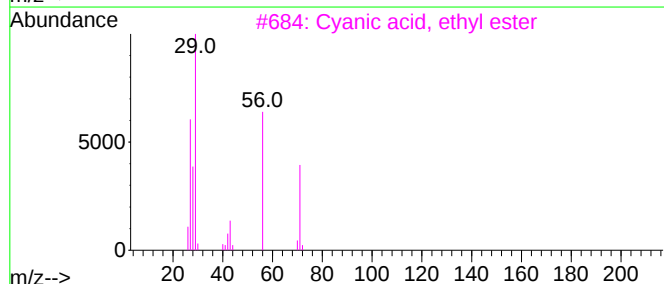
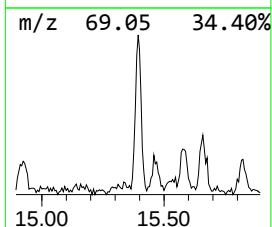
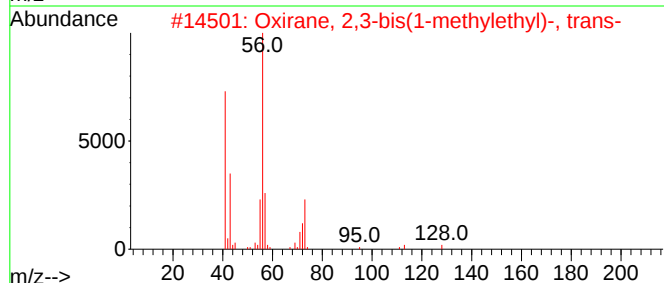
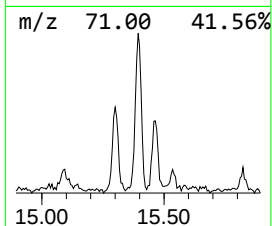
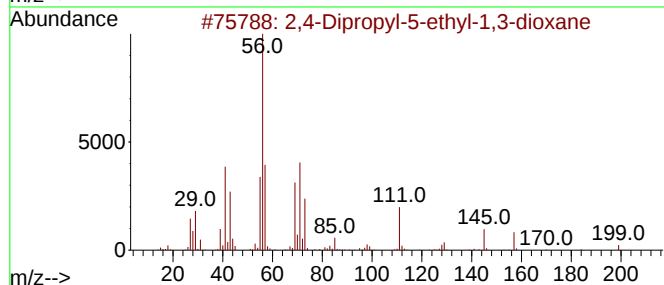
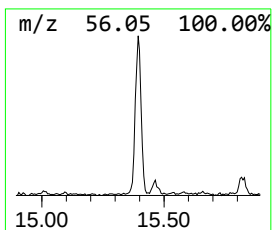
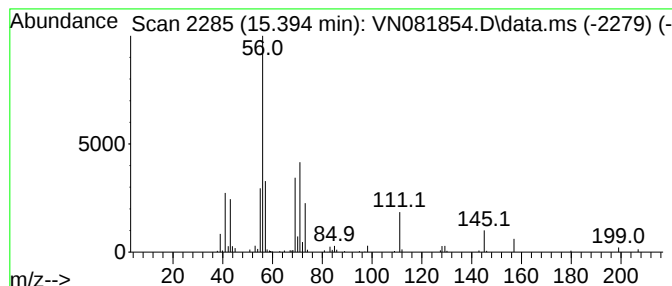
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Quant Title : SW846 8260

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

Peak Number 10 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.394	10.83 ug/l	240616	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	83
2		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	47
3		Cyanoic acid, ethyl ester	71	C3H5NO	000627-48-5	42
4		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	33
5		1-Octene, 2-methyl-	126	C9H18	004588-18-5	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081854.D
Acq On : 25 Apr 2024 16:40
Operator : JC\MD
Sample : P2257-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41B

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
Propane	2.083	14.9	ug/l	219155	1	8.230	737701	50.0
2-Propanethiol,...	6.671	11.9	ug/l	175838	1	8.230	737701	50.0
Butanal	7.224	85.7	ug/l	1264500	1	8.230	737701	50.0
4-Heptanol	12.418	27.1	ug/l	749485	3	11.865	1380330	50.0
4-Heptanol, 3-m...	13.241	16.2	ug/l	360096	4	13.794	1111380	50.0
unknown13.271	13.271	10.7	ug/l	238269	4	13.794	1111380	50.0
Butanoic acid, ...	13.335	156.8	ug/l	3484260	4	13.794	1111380	50.0
unknown13.659	13.659	9.1	ug/l	202320	4	13.794	1111380	50.0
1-Hexanol, 2-et...	13.870	226.3	ug/l	5031100	4	13.794	1111380	50.0
2,4-Dipropyl-5-...	15.394	10.8	ug/l	240616	4	13.794	1111380	50.0