

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
 Data File : VN081856.D
 Acq On : 25 Apr 2024 17:28
 Operator : JC\MD
 Sample : P2257-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 45A

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: VN081856.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	15	22	32	rBV	99085	147973	3.57%	0.887%
2	2.665	116	121	129	rBV2	43242	80471	1.94%	0.482%
3	4.712	460	469	483	rVB2	28700	97011	2.34%	0.581%
4	6.677	791	803	817	rVB2	35987	122013	2.95%	0.731%
5	7.224	884	896	911	rBV	326735	935717	22.59%	5.607%
6	8.165	1046	1056	1061	rBV	179171	433307	10.46%	2.597%
7	8.224	1061	1066	1076	rVB	335984	727291	17.56%	4.358%
8	8.577	1106	1126	1133	rBV	213062	521120	12.58%	3.123%
9	8.653	1133	1139	1149	rBV3	41832	144983	3.50%	0.869%
10	9.100	1207	1215	1228	rVB	515962	1055181	25.47%	6.323%
11	9.265	1235	1243	1252	rBV2	63681	131453	3.17%	0.788%
12	9.653	1300	1309	1317	rBV	45145	99832	2.41%	0.598%
13	10.565	1453	1464	1473	rBV	761241	1437984	34.71%	8.617%
14	11.865	1672	1685	1694	rBV	678379	1341616	32.39%	8.039%
15	12.212	1738	1744	1753	rVB2	42390	83306	2.01%	0.499%
16	12.376	1766	1772	1775	rBV	76564	130372	3.15%	0.781%
17	12.418	1775	1779	1794	rVB	391513	666102	16.08%	3.992%
18	12.847	1843	1852	1863	rBV	537038	998278	24.10%	5.982%
19	13.241	1913	1919	1922	rBV2	179460	319548	7.71%	1.915%
20	13.271	1922	1924	1929	rVV2	162213	214951	5.19%	1.288%
21	13.335	1930	1935	1942	rVB	526289	786994	19.00%	4.716%
22	13.488	1956	1961	1965	rBV3	42562	69961	1.69%	0.419%
23	13.541	1965	1970	1976	rVB3	33479	65815	1.59%	0.394%
24	13.659	1976	1990	2002	rBV	83480	199540	4.82%	1.196%
25	13.794	2005	2013	2019	rBV	622969	1060220	25.59%	6.353%
26	13.871	2019	2026	2035	rVV	2631566	4142338	100.00%	24.822%
27	13.953	2035	2040	2046	rVB2	65620	108876	2.63%	0.652%
28	14.188	2071	2080	2085	rBV5	21583	55034	1.33%	0.330%
29	14.759	2166	2177	2192	rVB5	38292	153957	3.72%	0.923%
30	15.394	2278	2285	2292	rBV	124584	210763	5.09%	1.263%
31	15.465	2292	2297	2306	rBV3	45923	81689	1.97%	0.490%
32	16.117	2402	2408	2414	rBV3	33913	64290	1.55%	0.385%

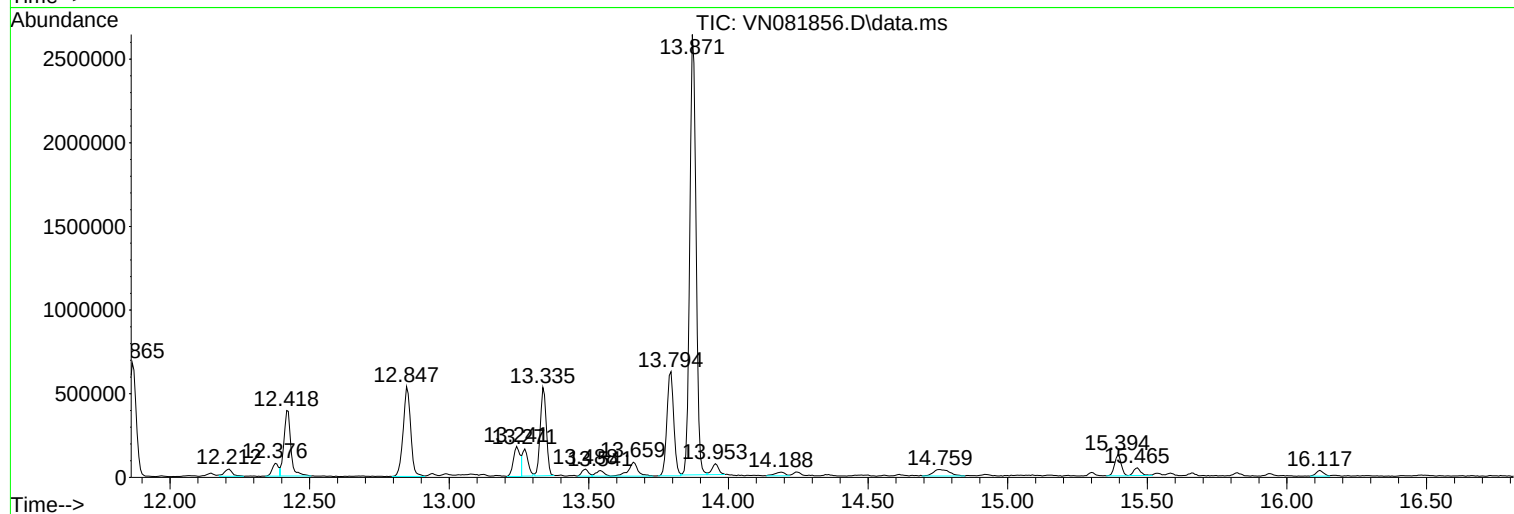
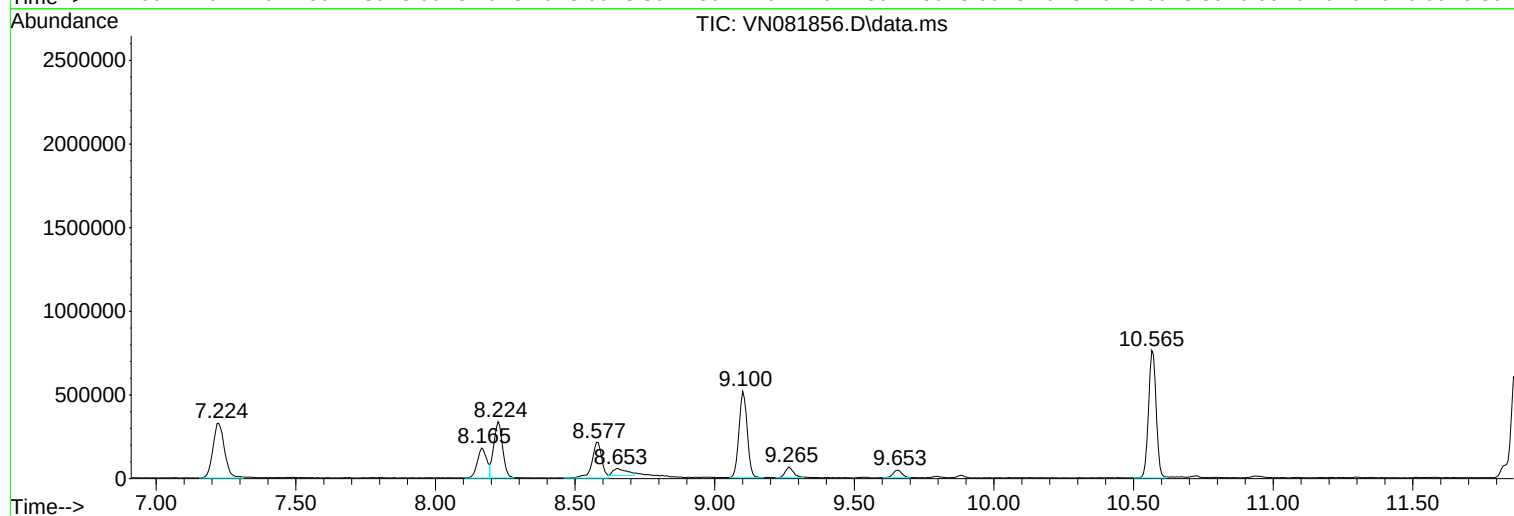
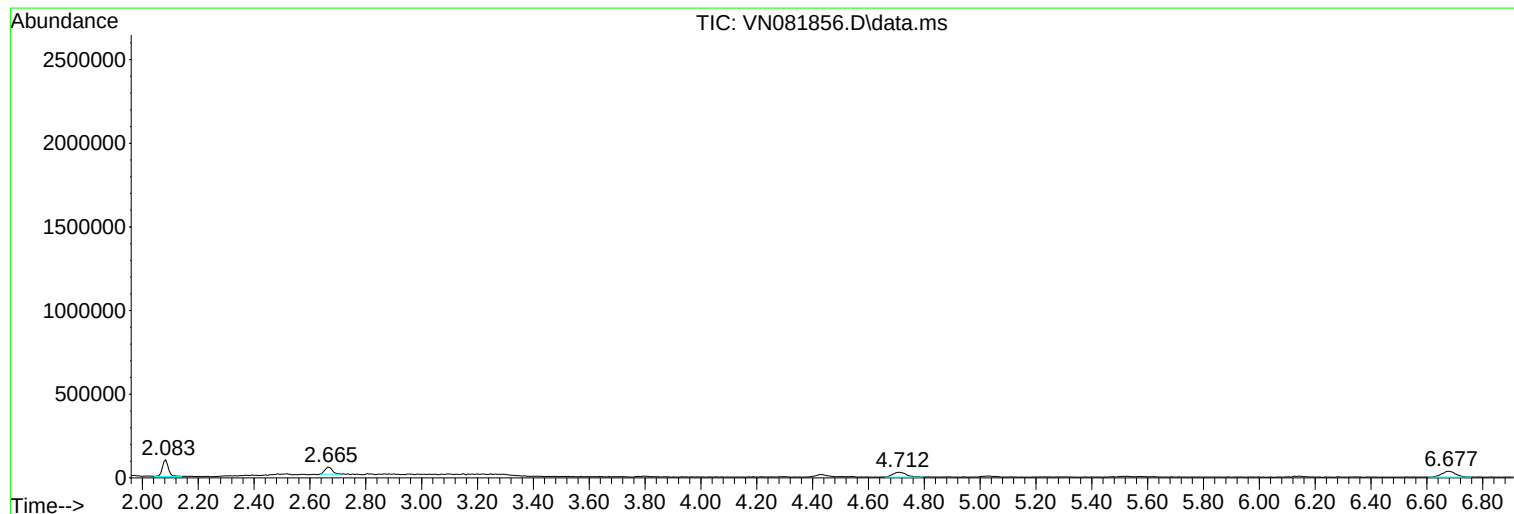
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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



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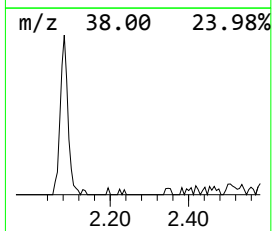
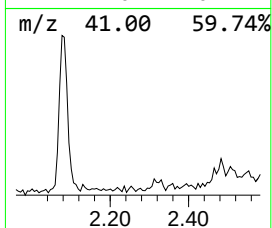
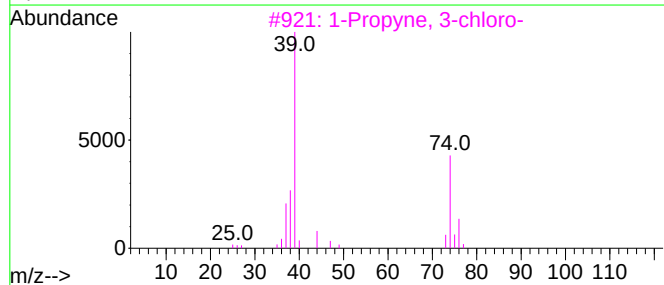
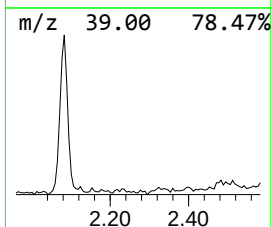
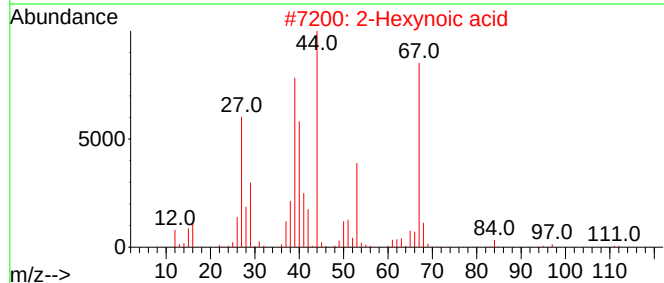
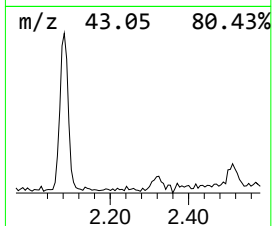
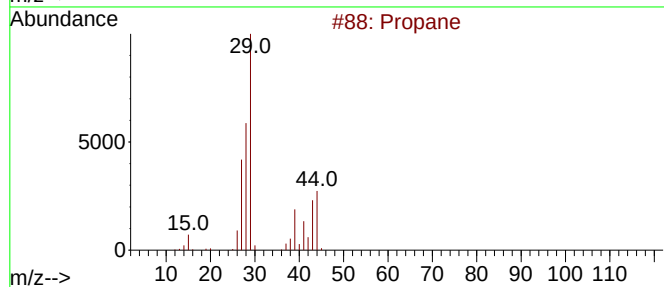
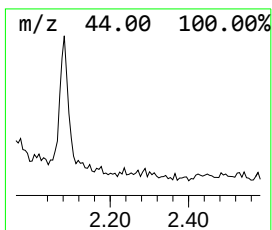
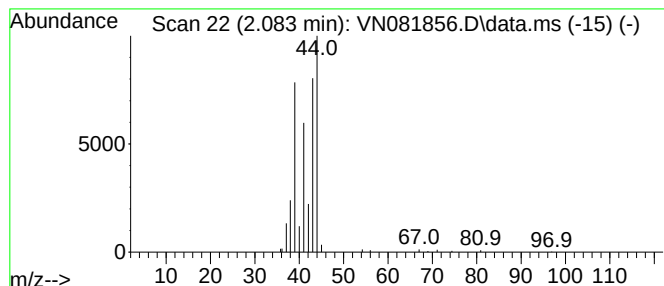
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Propane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	10.17 ug/l	147973	Pentafluorobenzene	8.224

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	38
4			Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	38
5			Acetaldehyde	44	C2H4O	000075-07-0	9



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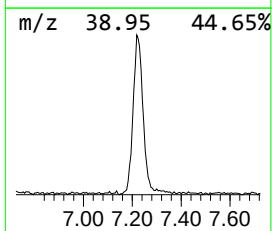
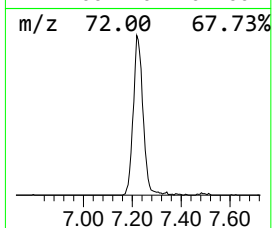
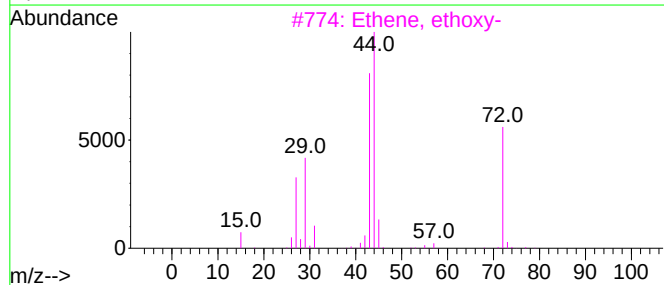
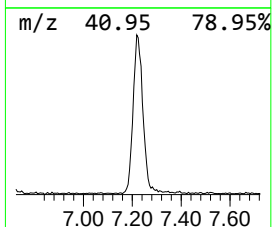
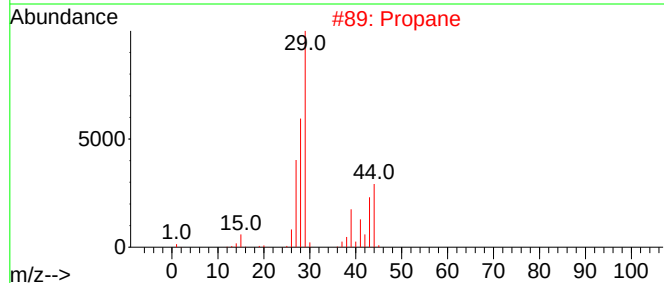
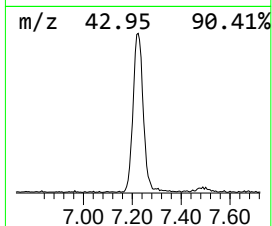
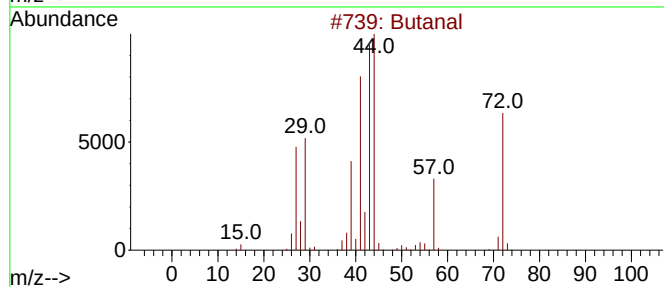
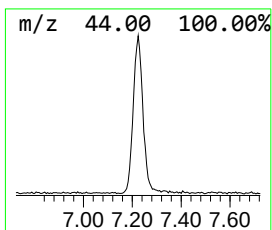
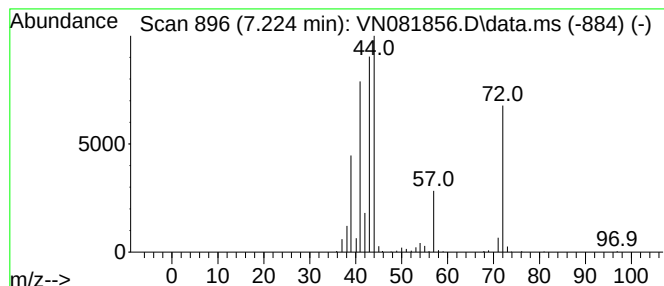
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Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	64.33 ug/l	935717	Pentafluorobenzene	8.224

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	94
2		Propane	44	C3H8	000074-98-6	53
3		Ethene, ethoxy-	72	C4H8O	000109-92-2	50
4		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
5		3-Butenamide	85	C4H7NO	028446-58-4	28



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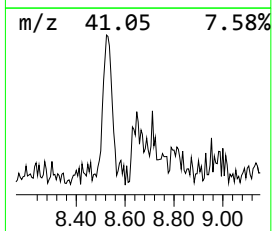
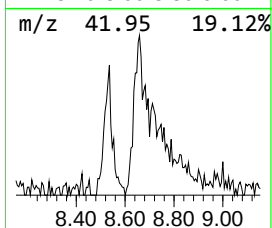
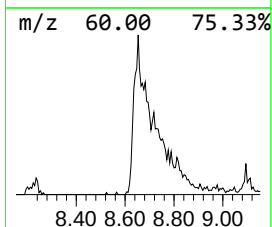
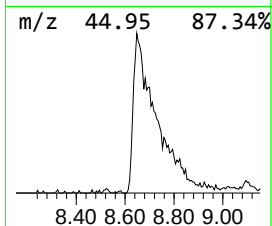
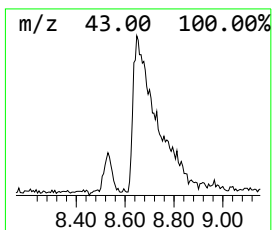
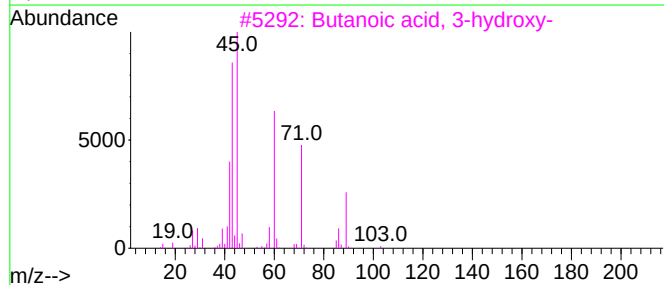
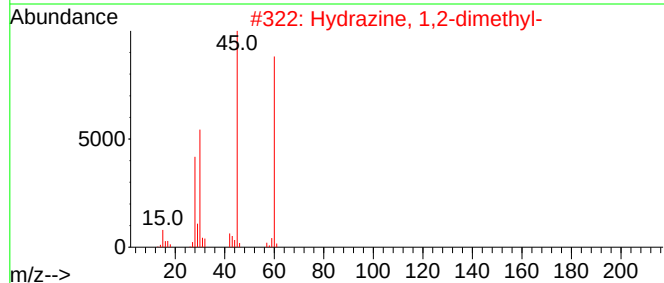
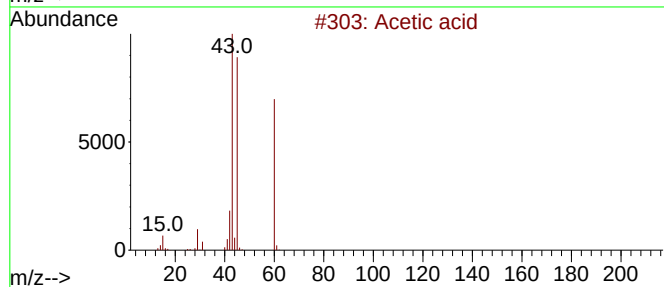
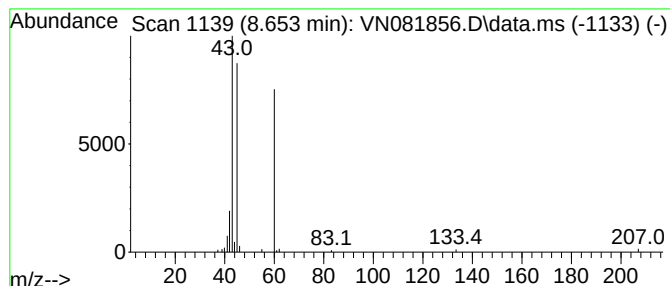
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Acetic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.653	9.97 ug/l	144983	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	90
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	50
3			Butanoic acid, 3-hydroxy-	104	C4H8O3	000300-85-6	40
4			N-Acetylisoaxazolidine	115	C5H9N2O2	115615-36-6	38
5			Thiirane	60	C2H4S	000420-12-2	9



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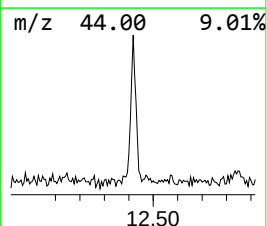
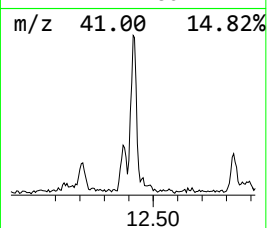
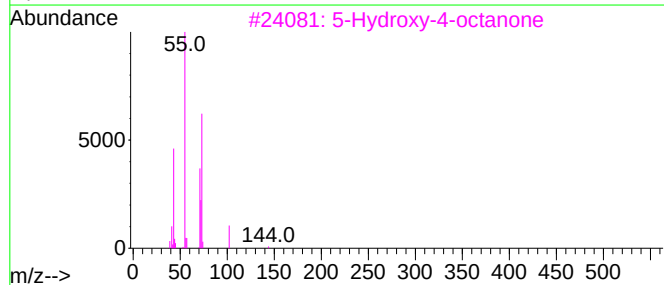
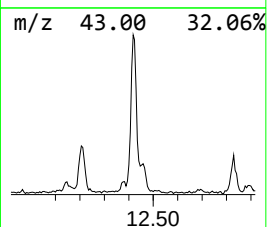
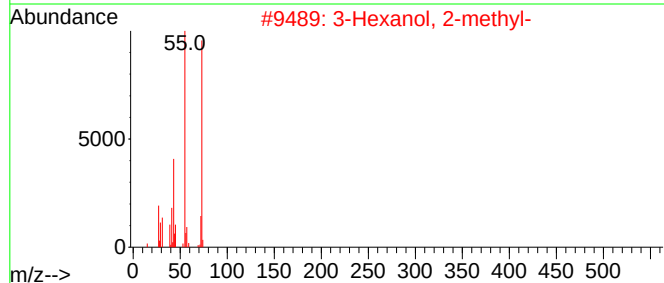
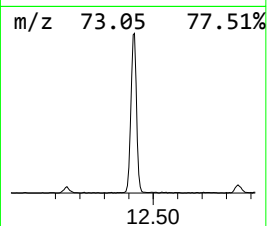
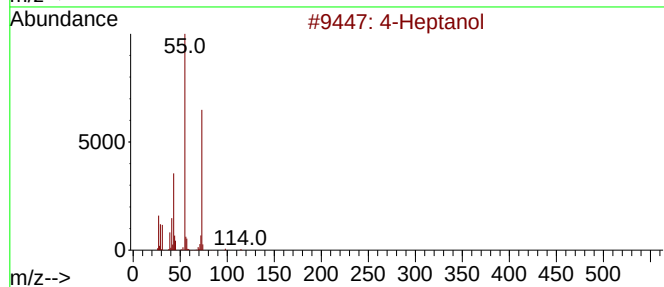
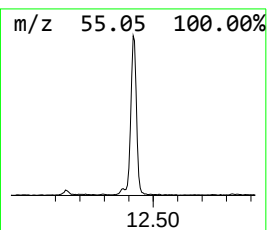
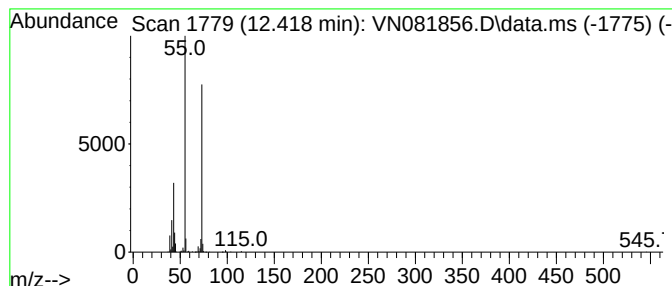
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4-Heptanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.418	24.82 ug/l	666102	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	72
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	50
3			5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	50
4			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
5			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9



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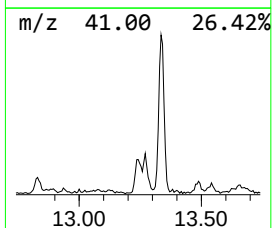
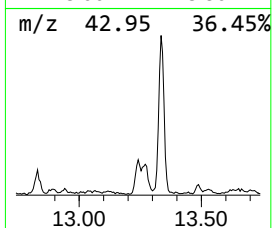
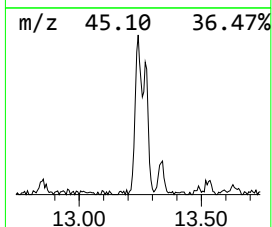
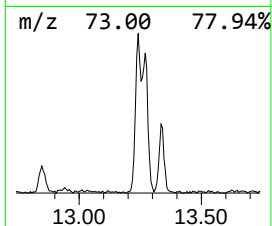
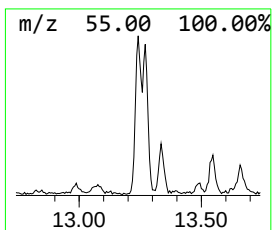
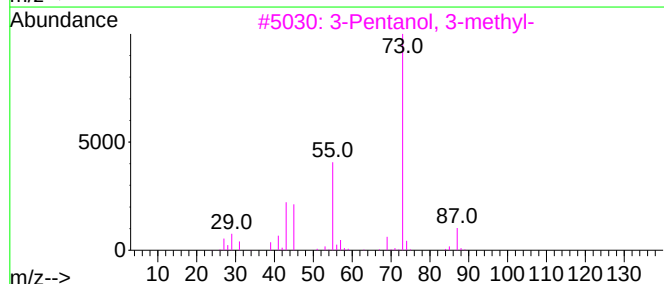
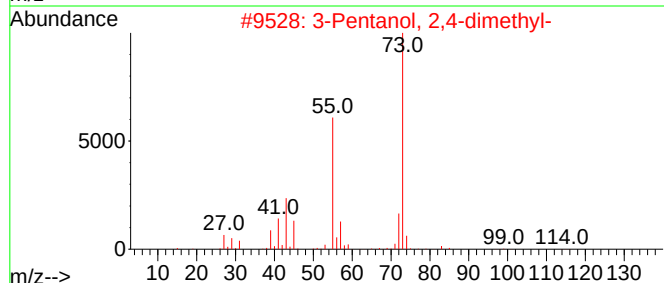
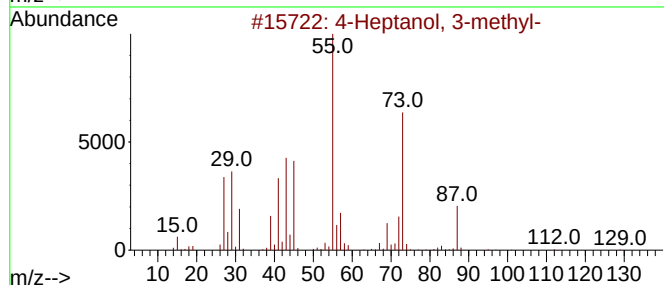
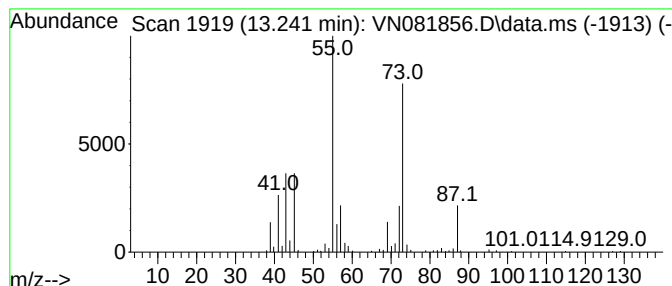
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Quant Title : SW846 8260

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

Peak Number 5 4-Heptanol, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.241	15.07 ug/l	319548	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	78
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	47
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	47
4			4-Heptanol	116	C7H16O	000589-55-9	43
5			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	43



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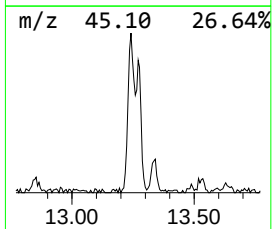
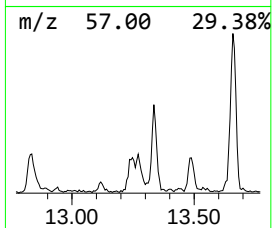
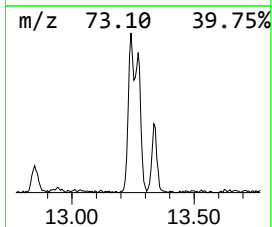
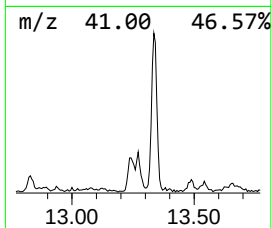
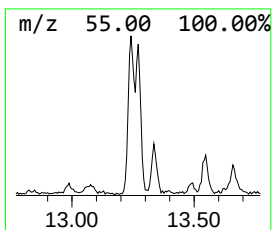
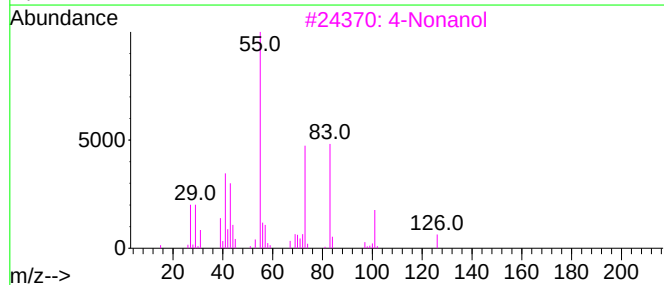
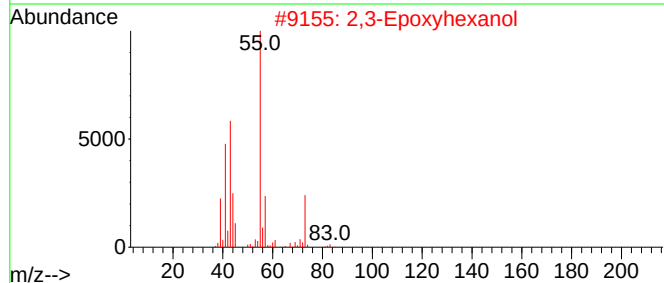
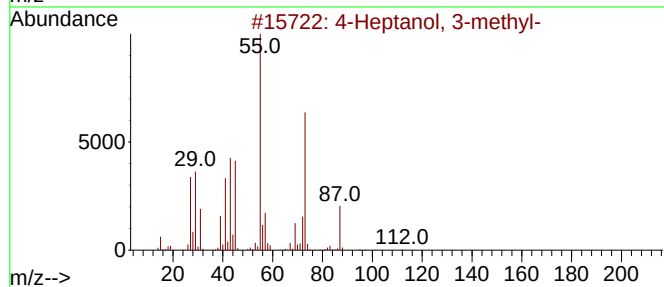
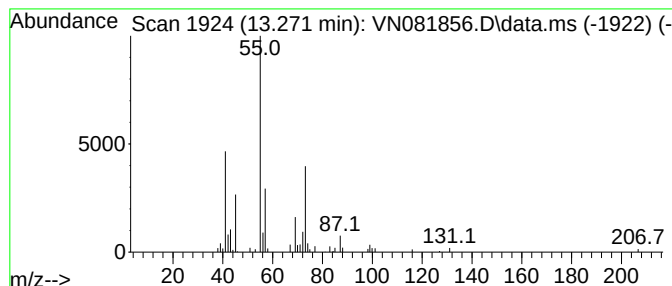
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Quant Title : SW846 8260

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

Peak Number 6 unknown13.271 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.271	10.14 ug/l	214951	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	78
2			2,3-Epoxyhexanol	116	C6H12O2	090528-63-5	33
3			4-Nonanol	144	C9H20O	005932-79-6	25
4			4-Heptanol	116	C7H16O	000589-55-9	25
5			(2S,3S)-(-)-3-Propyloxiranemethanol	116	C6H12O2	089321-71-1	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081856.D
Acq On : 25 Apr 2024 17:28
Operator : JC\MD
Sample : P2257-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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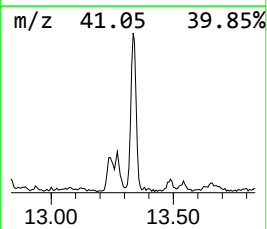
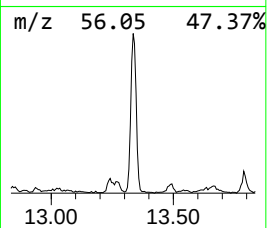
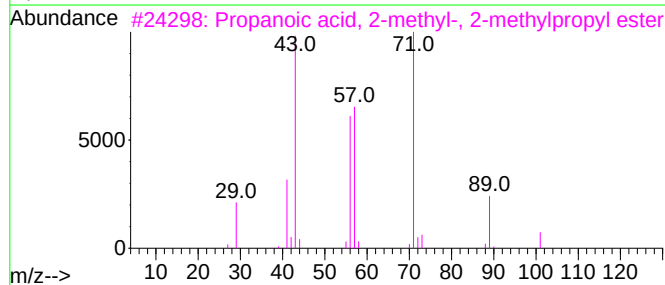
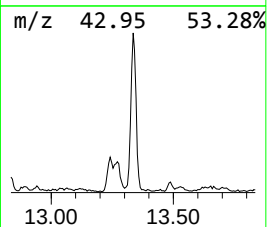
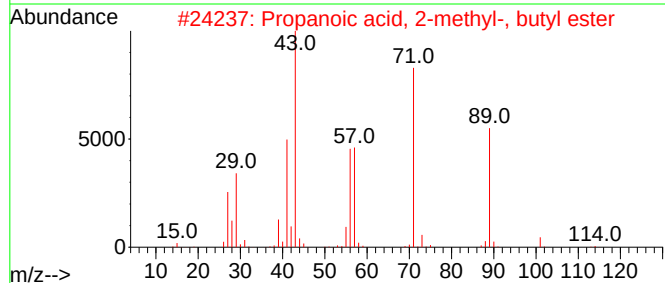
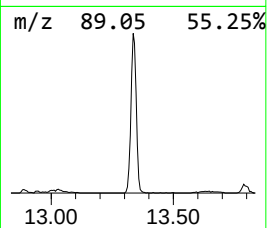
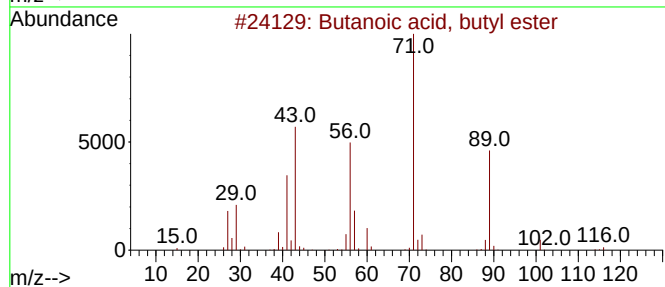
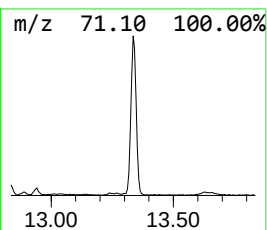
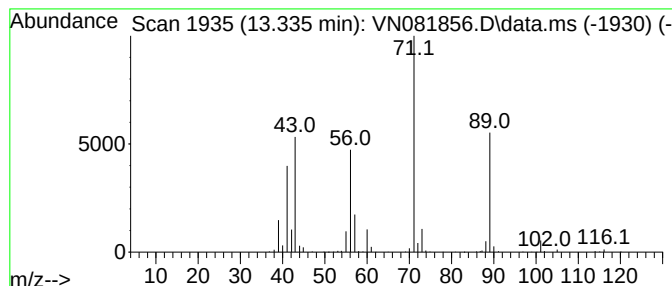
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Quant Title : SW846 8260

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

Peak Number 7 Butanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	37.11 ug/l	786994	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-, butyl...	144	C8H16O2	000097-87-0	72
3			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64
4			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	56
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081856.D
Acq On : 25 Apr 2024 17:28
Operator : JC\MD
Sample : P2257-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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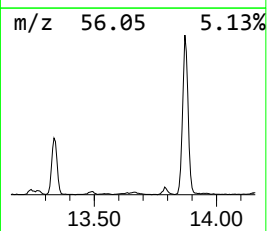
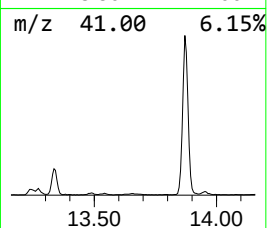
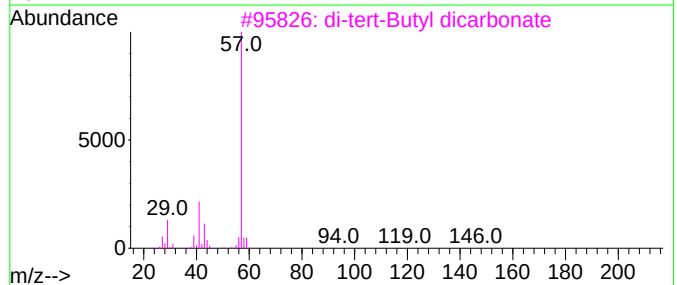
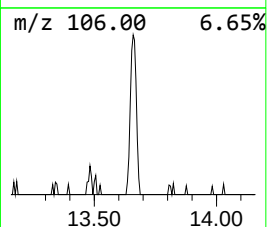
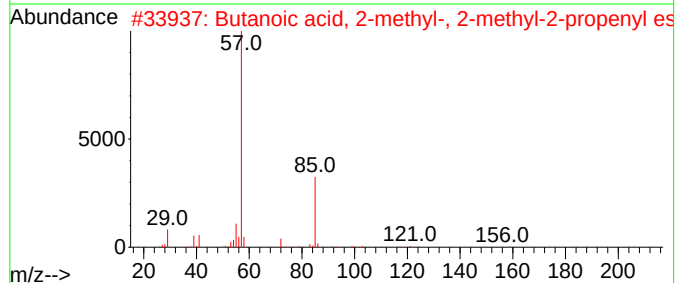
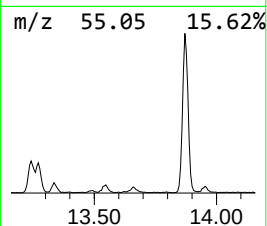
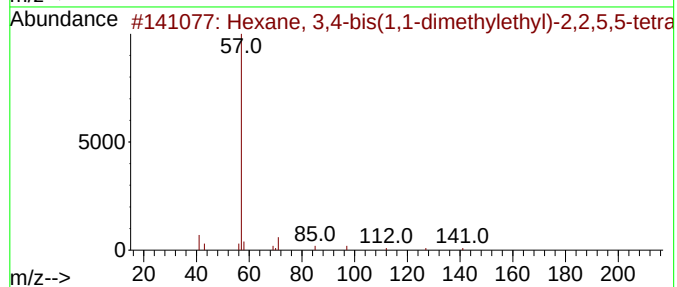
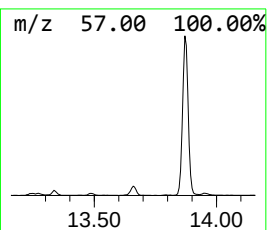
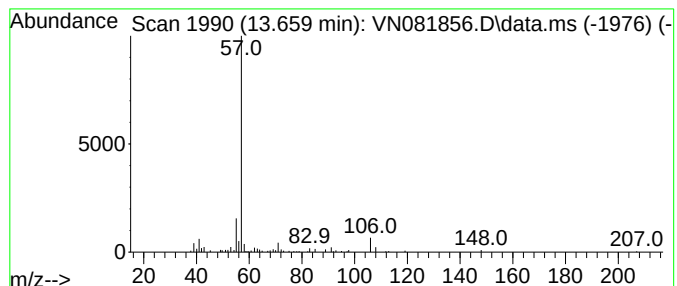
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Quant Title : SW846 8260

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	9.41 ug/l	199540	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3,4-bis(1,1-dimethylethy...	254	C18H38	062850-21-9	25
2			Butanoic acid, 2-methyl-, 2-meth...	156	C9H16O2	083783-90-8	12
3			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	12
4			1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	9
5			3-Oxobutan-2-yl 2-methylbutanoate	172	C9H16O3	1000372-70-6	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081856.D
Acq On : 25 Apr 2024 17:28
Operator : JC\MD
Sample : P2257-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
45A

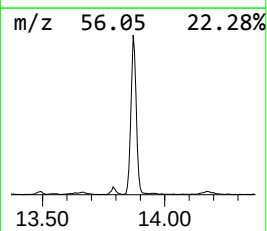
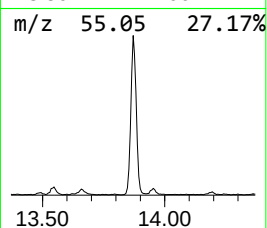
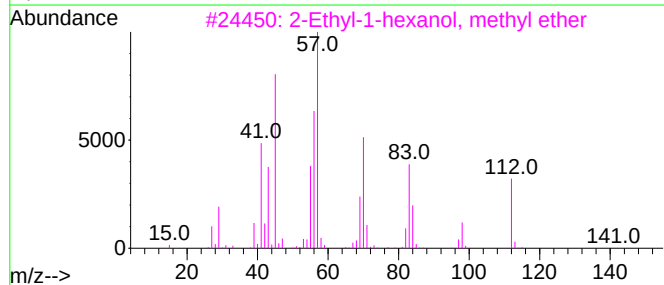
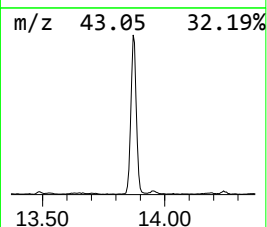
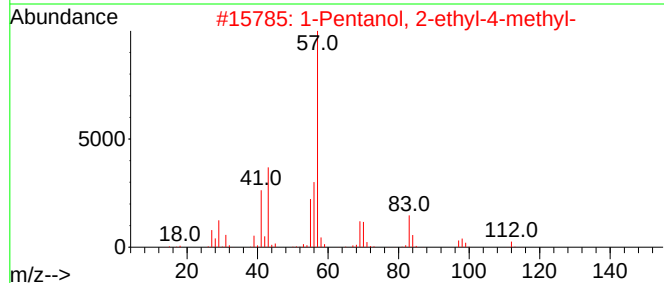
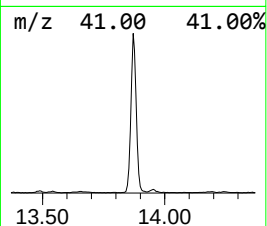
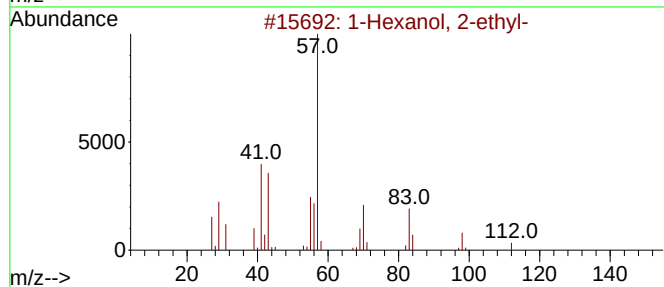
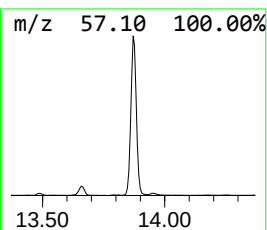
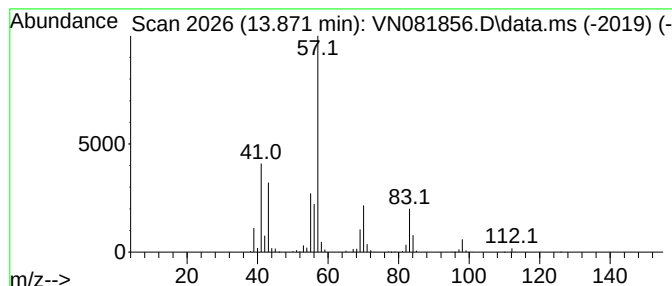
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Quant Title : SW846 8260

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.
13.871	195.35 ug/l	4142340	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	56
3			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	50
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081856.D
Acq On : 25 Apr 2024 17:28
Operator : JC\MD
Sample : P2257-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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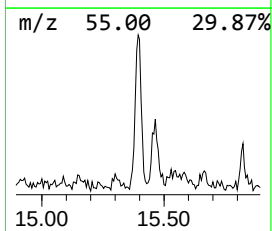
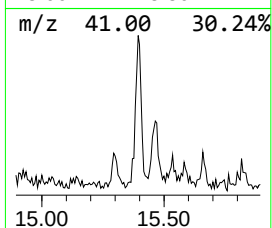
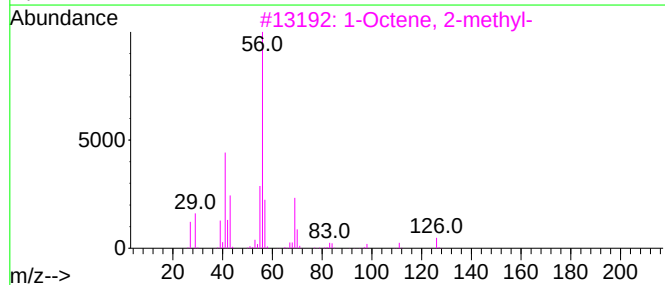
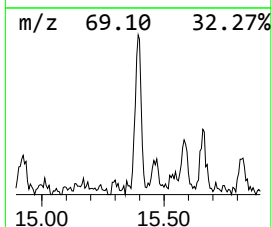
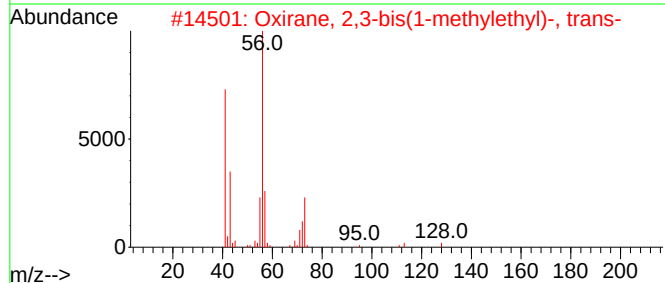
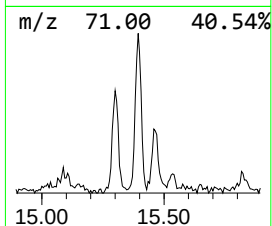
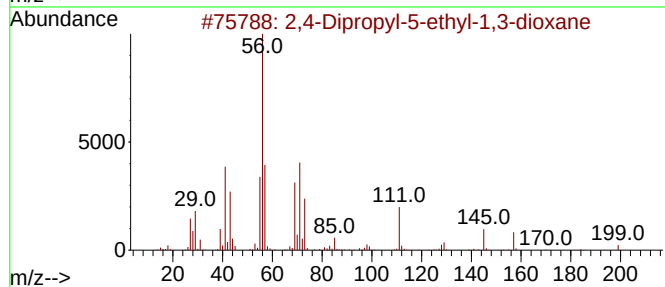
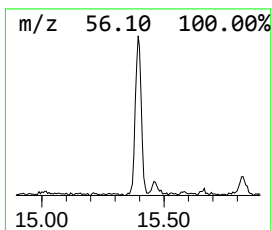
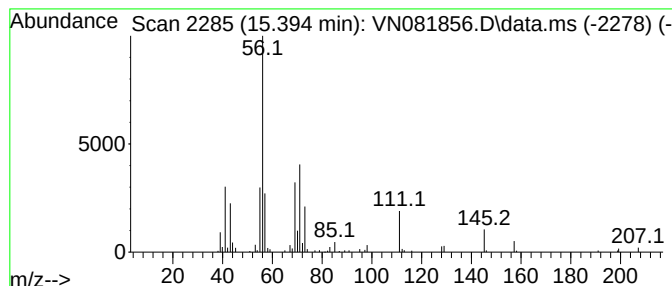
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Quant Title : SW846 8260

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

Peak Number 10 unknown15.394 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.394	9.94 ug/l	210763	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	47
2		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	43
3		1-Octene, 2-methyl-	126	C9H18	004588-18-5	38
4		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	35
5		3,4,5-Trimethyldihydrofuran-2-one	128	C7H12O2	1000194-05-2	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081856.D
Acq On : 25 Apr 2024 17:28
Operator : JC\MD
Sample : P2257-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
45A

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	10.2	ug/l	147973	1	8.224	727291	50.0
Butanal	7.224	64.3	ug/l	935717	1	8.224	727291	50.0
Acetic acid	8.653	10.0	ug/l	144983	1	8.224	727291	50.0
4-Heptanol	12.418	24.8	ug/l	666102	3	11.865	1341620	50.0
4-Heptanol, 3-m...	13.241	15.1	ug/l	319548	4	13.794	1060220	50.0
unknown13.271	13.271	10.1	ug/l	214951	4	13.794	1060220	50.0
Butanoic acid, ...	13.335	37.1	ug/l	786994	4	13.794	1060220	50.0
unknown13.659	13.659	9.4	ug/l	199540	4	13.794	1060220	50.0
1-Hexanol, 2-et...	13.871	195.3	ug/l	4142340	4	13.794	1060220	50.0
unknown15.394	15.394	9.9	ug/l	210763	4	13.794	1060220	50.0