

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
 Data File : VN065941.D
 Acq On : 18 Feb 2021 15:25
 Operator : JC/MD
 Sample : M1425-13
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41061

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\82N021721W.M

Title : SW846 8260

Signal : TIC: VN065941.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.255	450	471	493	rBV	120440	290062	7.79%	1.094%
2	3.788	619	637	656	rBV	243341	627127	16.85%	2.364%
3	4.049	697	718	750	rBV	189615	549370	14.76%	2.071%
4	6.801	1556	1574	1597	rBV2	23629	69960	1.88%	0.264%
5	7.550	1788	1807	1818	rBV3	116588	287399	7.72%	1.084%
6	7.627	1819	1831	1853	rVB	225377	531990	14.29%	2.006%
7	7.991	1925	1944	1968	rBV2	143067	337736	9.07%	1.273%
8	8.550	2103	2118	2142	rVB	333308	700002	18.81%	2.639%
9	8.759	2169	2183	2211	rBV	193262	423456	11.38%	1.597%
10	9.955	2543	2555	2571	rBV	50483	94531	2.54%	0.356%
11	10.058	2571	2587	2602	rBV	536182	991366	26.63%	3.738%
12	10.328	2658	2671	2691	rBV	27926	51299	1.38%	0.193%
13	10.576	2735	2748	2766	rBV2	35872	68936	1.85%	0.260%
14	11.376	2983	2997	3020	rBV	466567	828813	22.27%	3.125%
15	11.814	3119	3133	3148	rVB4	17987	40421	1.09%	0.152%
16	11.997	3176	3190	3208	rBV	156337	267767	7.19%	1.010%
17	12.087	3208	3218	3240	rVB	58197	111688	3.00%	0.421%
18	12.373	3294	3307	3331	rVB	355270	609130	16.36%	2.297%
19	12.656	3384	3395	3404	rBV2	26221	44940	1.21%	0.169%
20	13.061	3512	3521	3525	rBV2	33856	53679	1.44%	0.202%
21	13.097	3526	3532	3548	rVB5	49699	101918	2.74%	0.384%
22	13.312	3587	3599	3610	rBV	438004	743405	19.97%	2.803%
23	13.376	3610	3619	3623	rVV2	112751	162432	4.36%	0.612%
24	13.418	3623	3632	3645	rVV	1953032	3009038	80.84%	11.345%
25	13.482	3647	3652	3660	rVB4	32627	53948	1.45%	0.203%
26	13.791	3737	3748	3776	rVB	192589	335603	9.02%	1.265%
27	13.990	3798	3810	3836	rBV2	2013325	3722194	100.00%	14.034%
28	14.177	3858	3868	3885	rBV2	83831	145346	3.90%	0.548%
29	14.312	3891	3910	3931	rBV	463788	983626	26.43%	3.709%
30	14.527	3970	3977	3992	rVB4	31820	57985	1.56%	0.219%
31	14.637	3993	4011	4029	rBV2	1721940	3063431	82.30%	11.550%
32	14.916	4089	4098	4100	rBV4	60847	88377	2.37%	0.333%
33	14.968	4109	4114	4118	rBV2	65868	80595	2.17%	0.304%
34	15.000	4118	4124	4135	rVB	211672	306678	8.24%	1.156%
35	15.125	4155	4163	4190	rVB2	538728	1060383	28.49%	3.998%
36	15.389	4237	4245	4255	rVB5	22871	38349	1.03%	0.145%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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37	15.463	4256	4268	4300	rBV	978549	1707352	45.87%	6.437%
38	15.685	4322	4337	4352	rBV	1954873	3449451	92.67%	13.005%
39	15.807	4370	4375	4388	rVB5	24156	41840	1.12%	0.158%
40	15.907	4398	4406	4415	rBV2	42929	73377	1.97%	0.277%
41	16.003	4428	4436	4449	rVB2	69993	137987	3.71%	0.520%
42	16.084	4453	4461	4484	rVB6	41392	105034	2.82%	0.396%
43	16.405	4549	4561	4577	rBV4	29448	75113	2.02%	0.283%

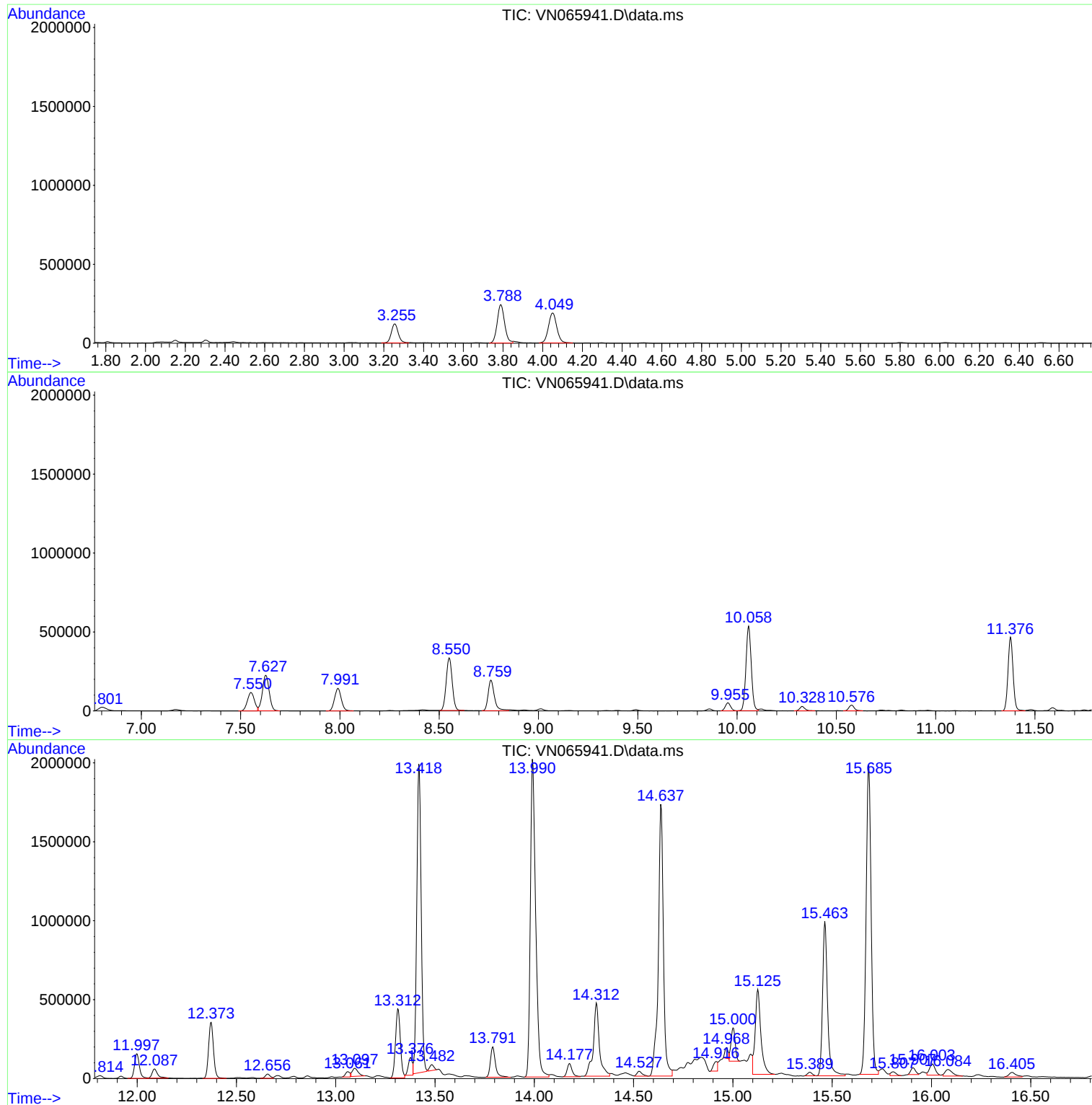
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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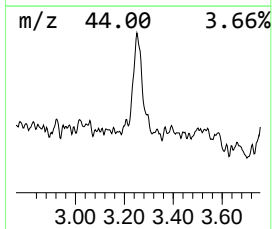
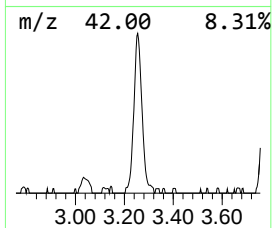
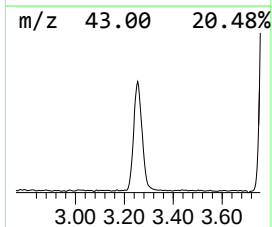
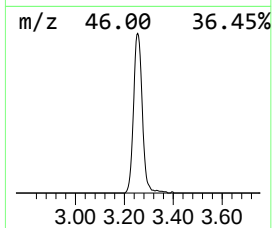
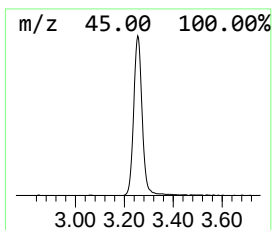
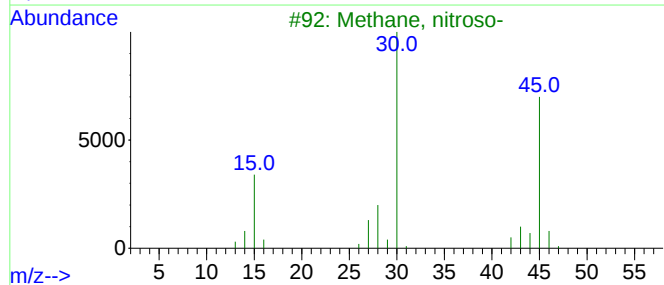
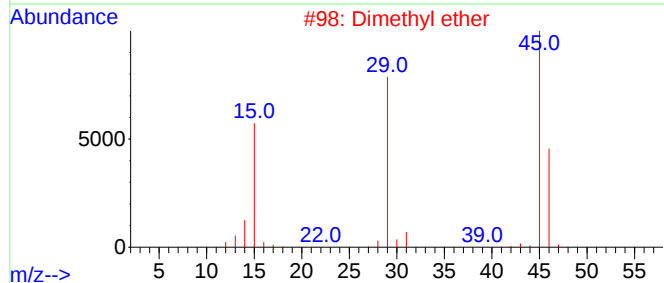
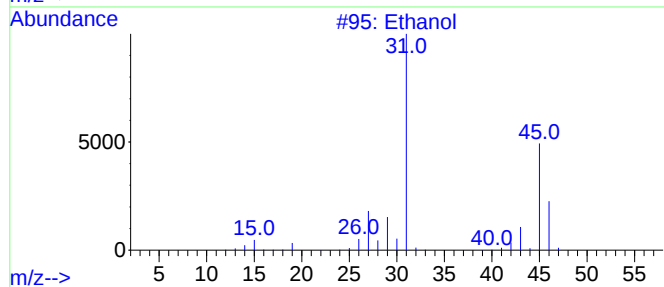
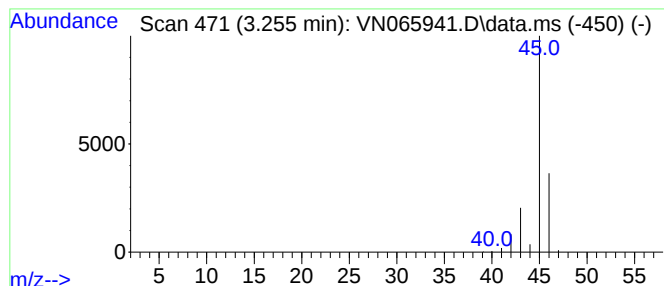
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.255	27.26 ug/l	290062	Pentafluorobenzene	7.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			L-Lactic acid	90	C3H6O3	000079-33-4	2



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Instrument :
MSVOA_N
ClientSampleId :
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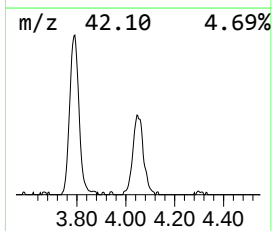
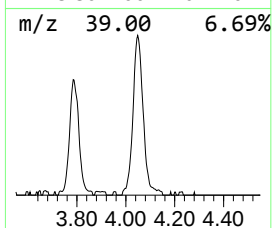
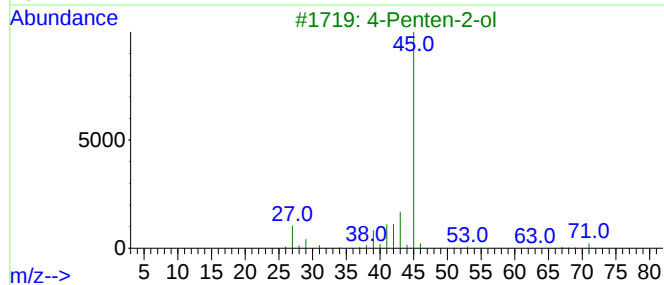
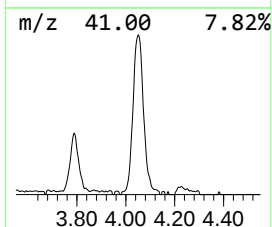
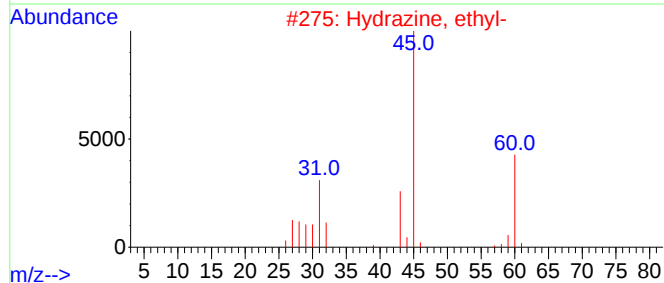
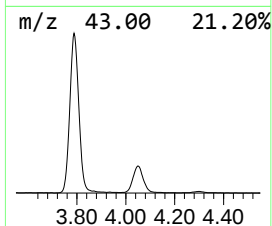
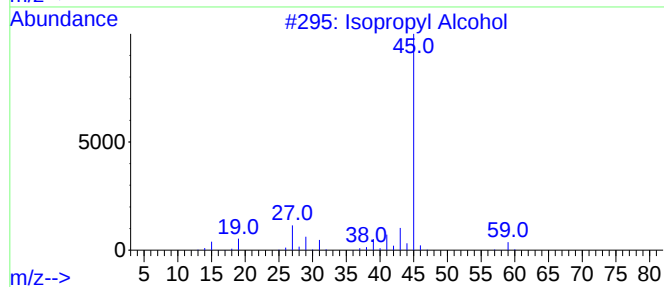
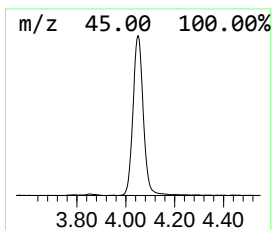
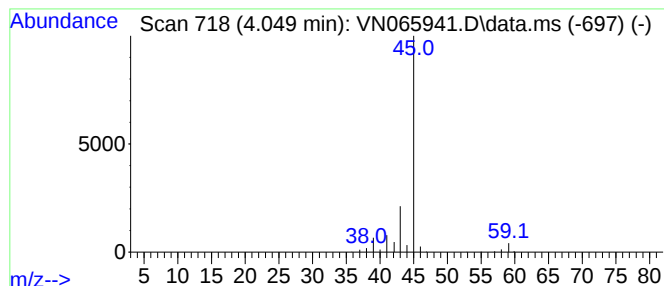
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.049	51.63 ug/l	549370	Pentafluorobenzene	7.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	90
2			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3			4-Penten-2-ol	86	C5H10O	000625-31-0	9
4			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5			Formamide	45	CH3NO	000075-12-7	5



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Sample : M1425-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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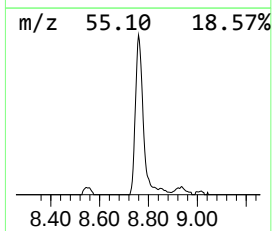
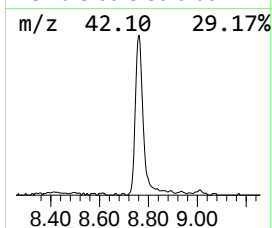
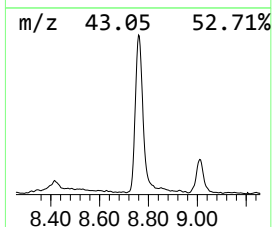
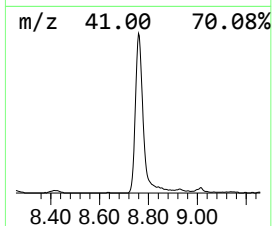
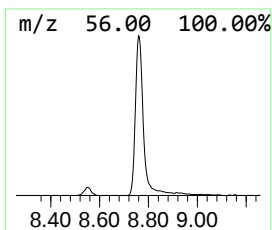
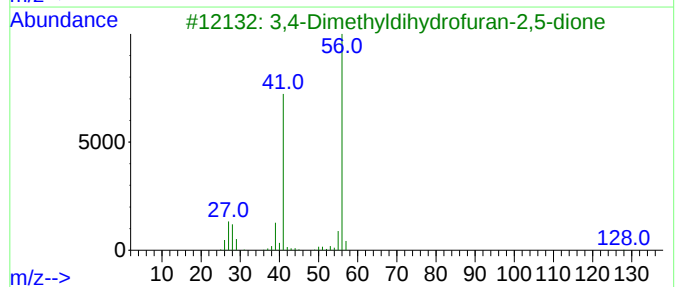
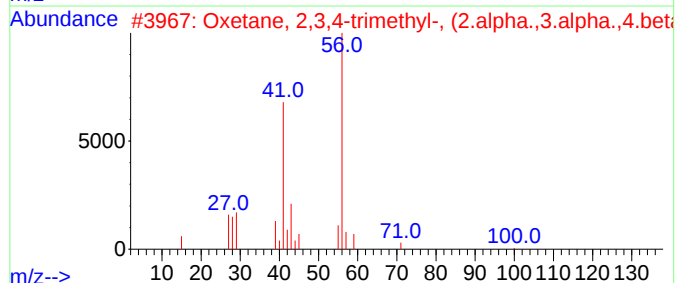
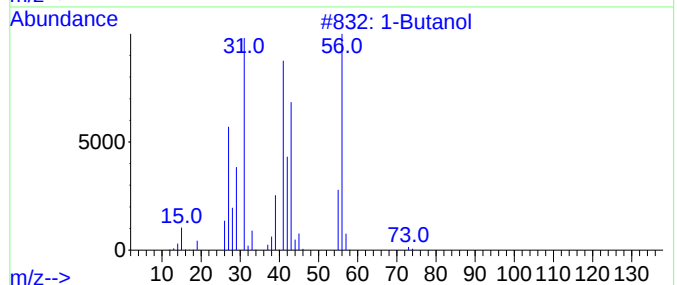
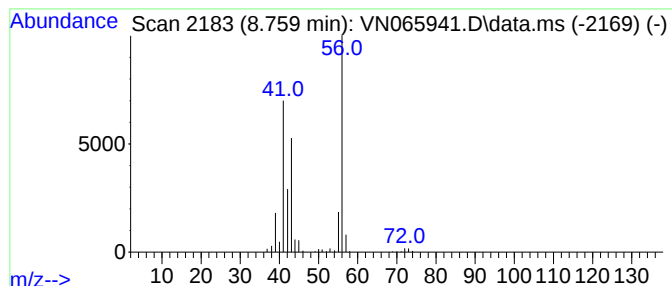
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Butanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.759	30.25 ug/l	423456	1,4-Difluorobenzene	8.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	90
2	Oxetane, 2,3,4-trimethyl-, (2.alpha...			100	C6H12O	032347-12-9	38
3	3,4-Dimethyldihydrofuran-2,5-dione			128	C6H8O3	007475-92-5	33
4	Formic acid, butyl ester			102	C5H10O2	000592-84-7	9
5	Butane, 1-chloro-			92	C4H9Cl	000109-69-3	9



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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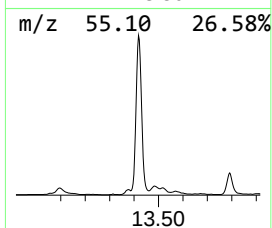
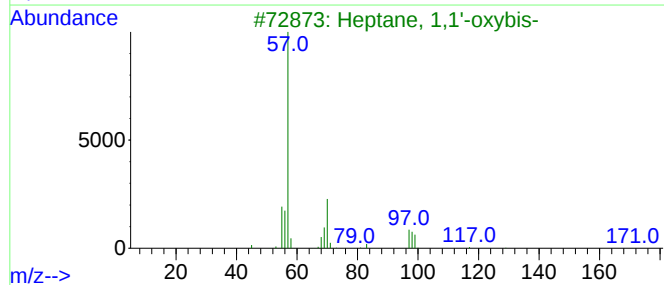
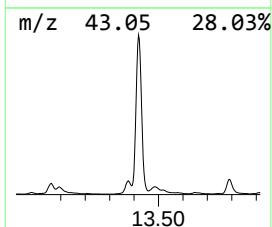
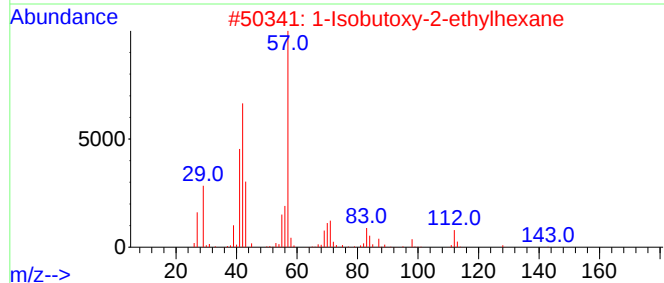
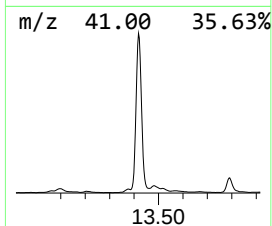
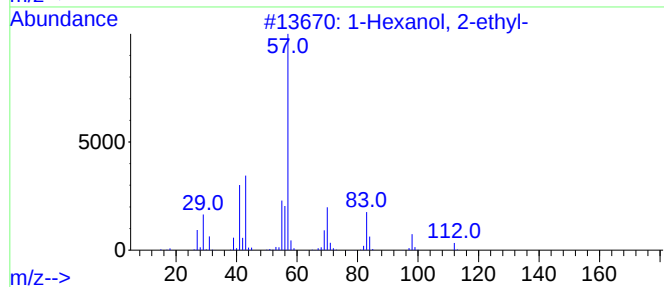
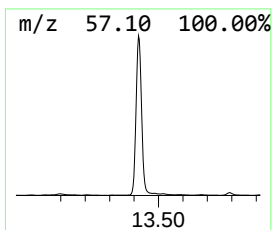
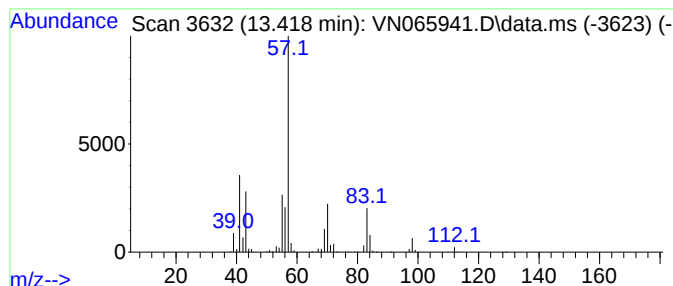
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.418	202.38 ug/l	3009040	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



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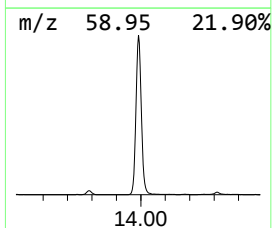
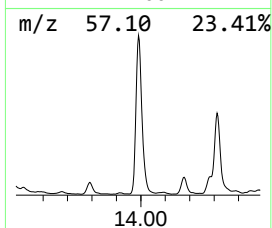
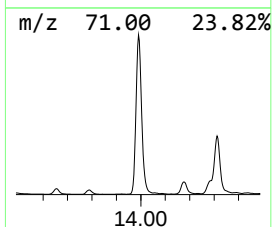
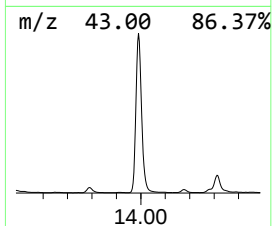
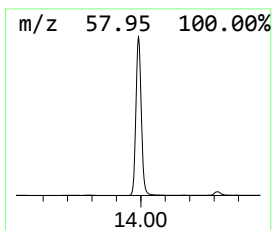
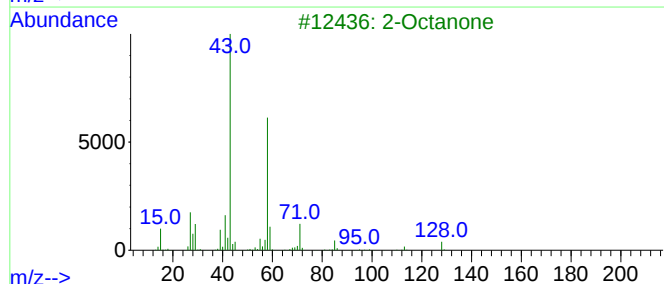
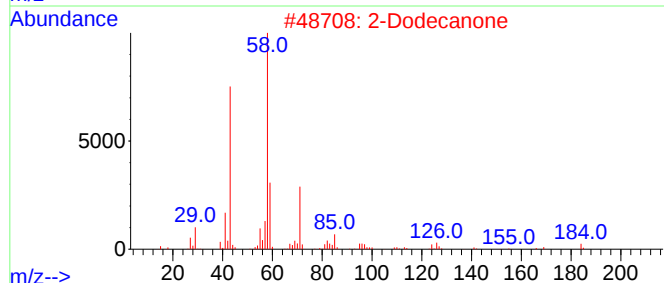
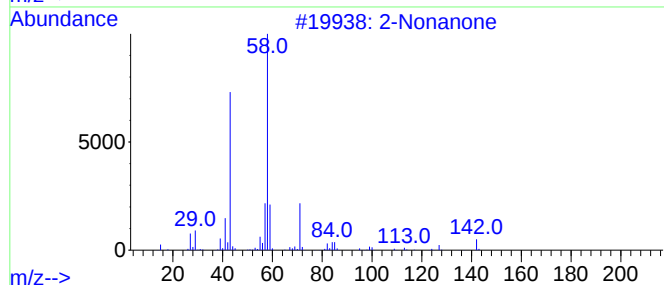
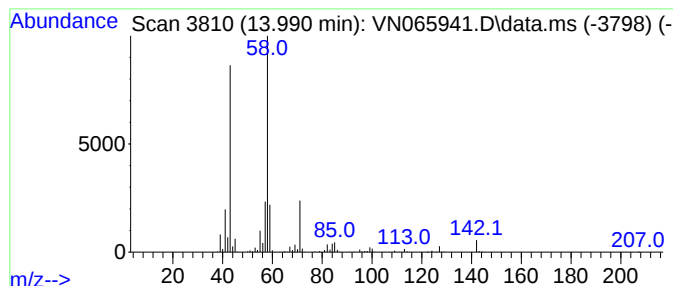
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Nonanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.990	250.35 ug/l	3722190	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone			142	C9H18O	000821-55-6	97
2	2-Dodecanone			184	C12H24O	006175-49-1	78
3	2-Octanone			128	C8H16O	000111-13-7	72
4	Pentanal, 2-methyl-			100	C6H12O	000123-15-9	58
5	Hexanal, 2-methyl-			114	C7H14O	000925-54-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
Data File : VN065941.D
Acq On : 18 Feb 2021 15:25
Operator : JC/MD
Sample : M1425-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41061

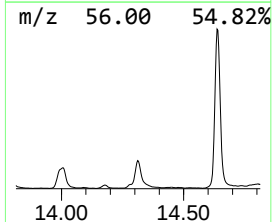
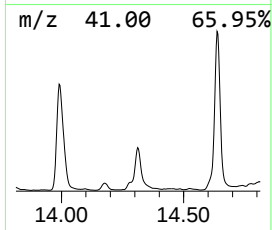
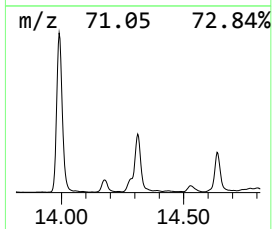
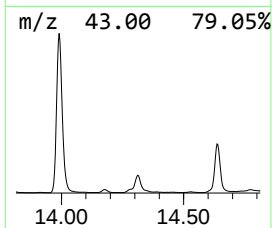
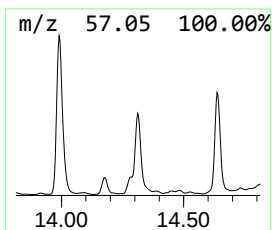
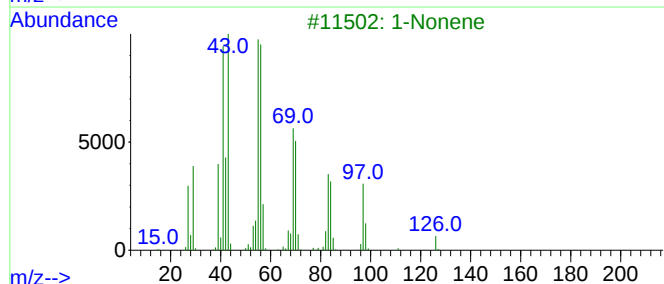
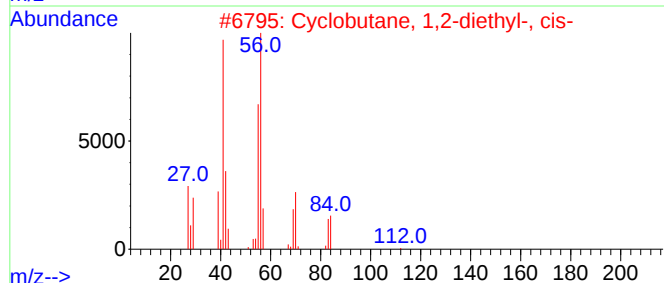
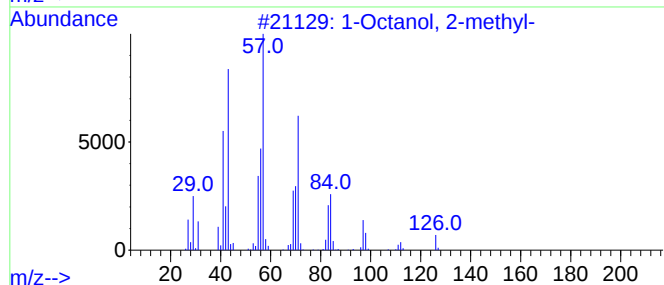
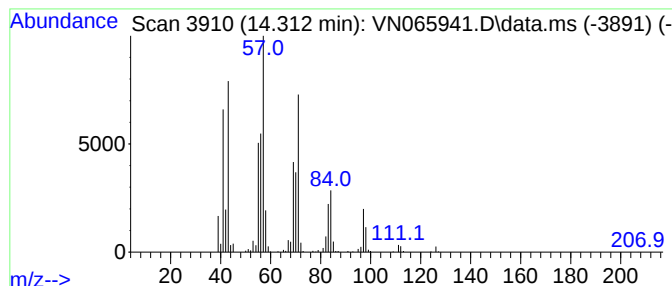
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Octanol, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.312	66.16 ug/l	983626	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	72
2			Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	43
3			1-Nonene	126	C9H18	000124-11-8	43
4			Isobutyl nonyl carbonate	244	C14H28O3	959311-27-4	43
5			Acetic acid, octyl ester	172	C10H20O2	000112-14-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
Data File : VN065941.D
Acq On : 18 Feb 2021 15:25
Operator : JC/MD
Sample : M1425-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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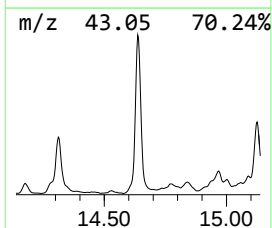
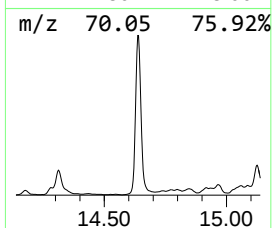
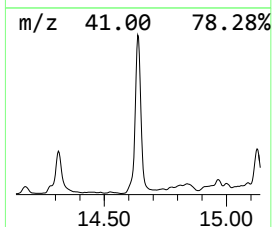
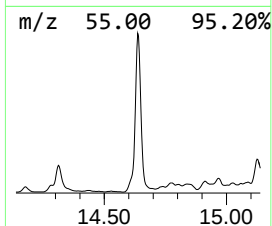
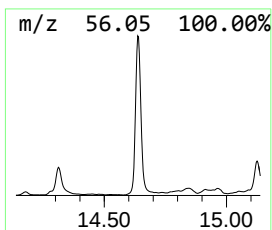
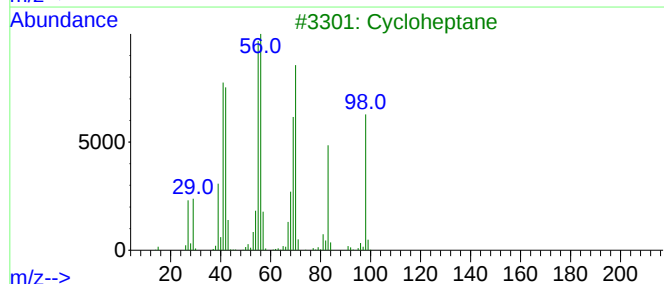
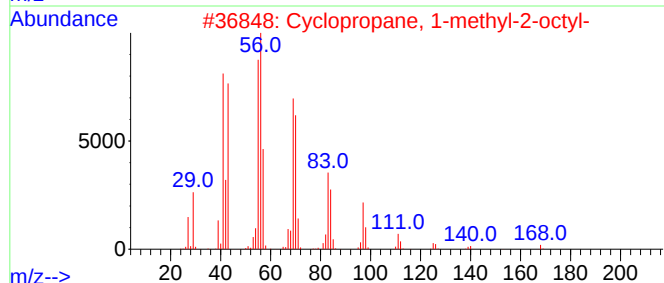
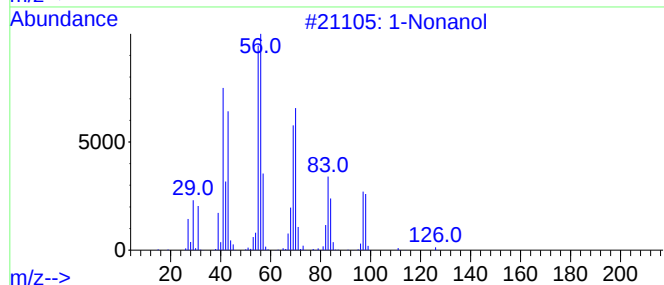
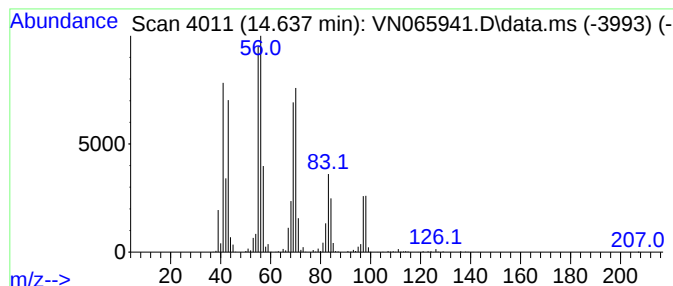
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Nonanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.637	206.04 ug/l	3063430	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol			144	C9H20O	000143-08-8	91
2	Cyclopropane, 1-methyl-2-octyl-			168	C12H24	037617-26-8	80
3	Cycloheptane			98	C7H14	000291-64-5	74
4	Isopropylcyclobutane			98	C7H14	000872-56-0	68
5	Cyclopentane, 1,2-dimethyl-, trans-			98	C7H14	000822-50-4	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
Data File : VN065941.D
Acq On : 18 Feb 2021 15:25
Operator : JC/MD
Sample : M1425-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41061

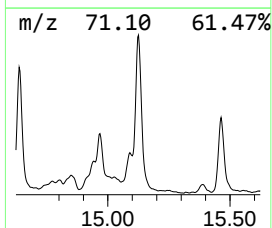
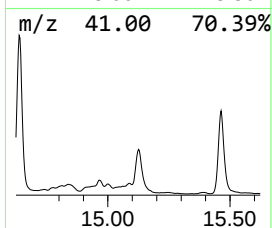
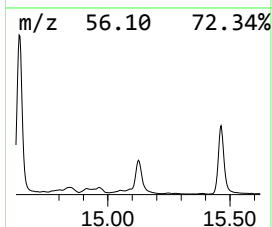
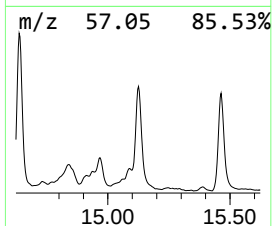
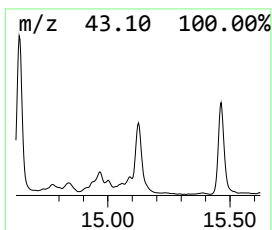
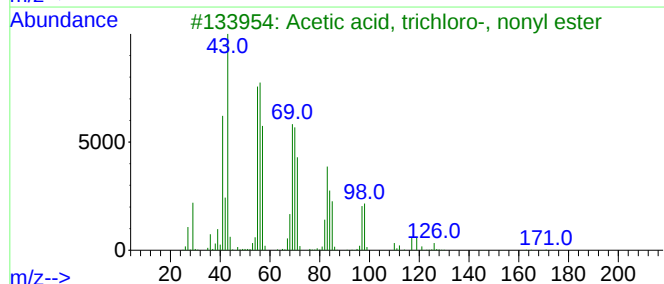
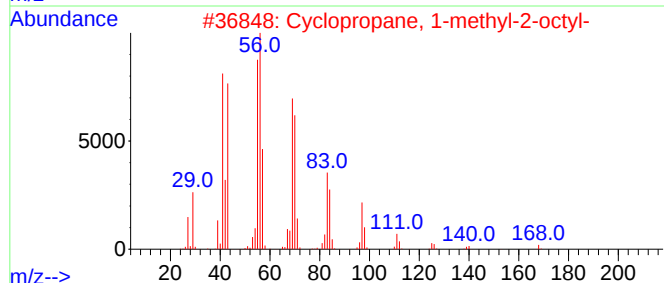
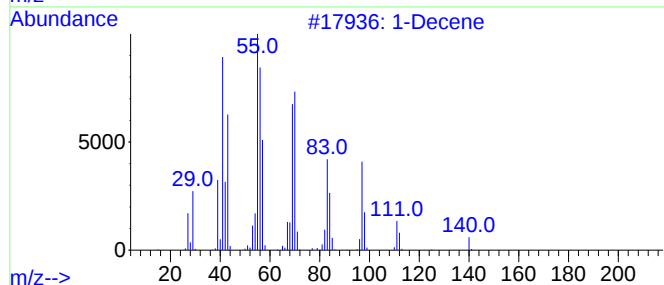
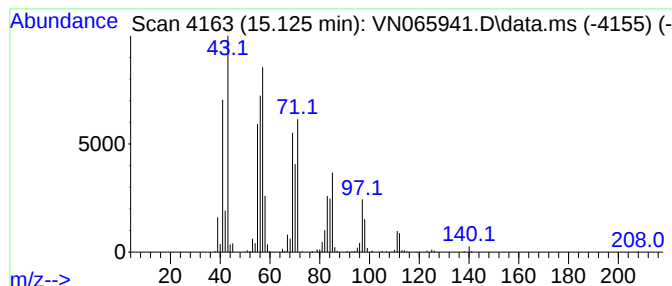
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Decene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.125	71.32 ug/l	1060380	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decene	140	C10H20	000872-05-9	60
2			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	58
3			Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	58
4			1-Dodecene	168	C12H24	000112-41-4	52
5			2-Chloropropionic acid, decyl e...	248	C13H25ClO2	086711-78-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
Data File : VN065941.D
Acq On : 18 Feb 2021 15:25
Operator : JC/MD
Sample : M1425-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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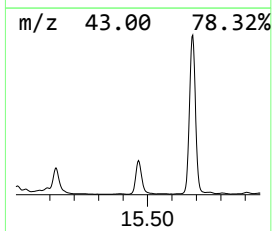
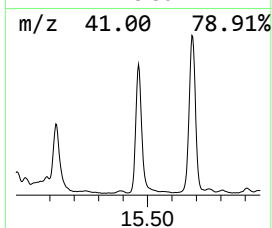
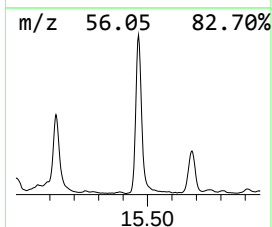
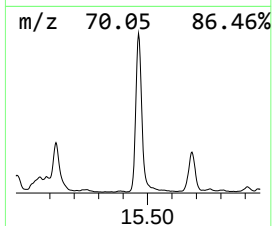
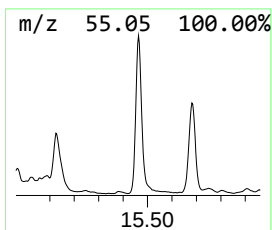
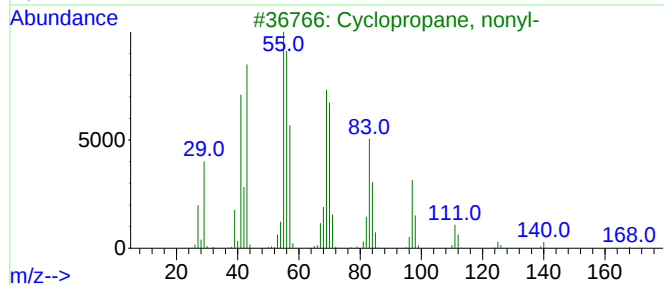
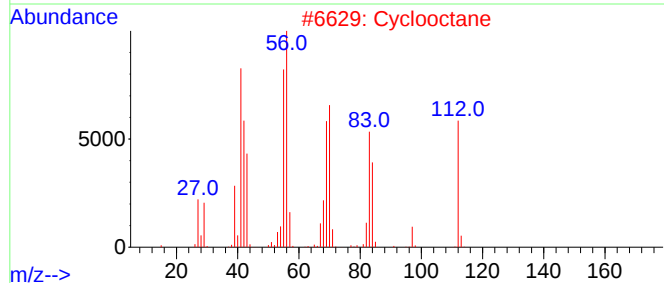
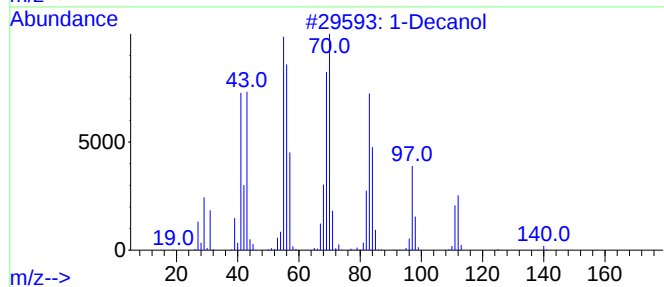
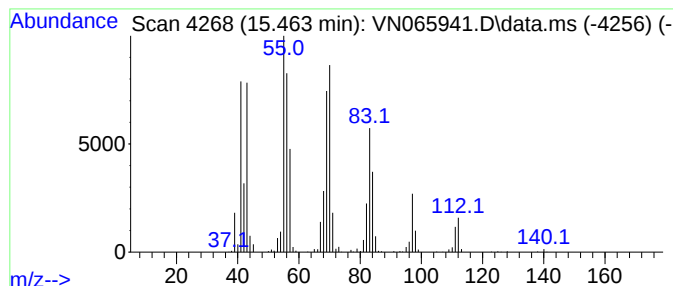
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Decanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.463	114.83 ug/l	1707350	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decanol	158	C10H22O	000112-30-1	91
2			Cyclooctane	112	C8H16	000292-64-8	87
3			Cyclopropane, nonyl-	168	C12H24	074663-85-7	86
4			Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	76
5			Cyclooctane, 1,4-dimethyl-, trans-	140	C10H20	013151-98-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
Data File : VN065941.D
Acq On : 18 Feb 2021 15:25
Operator : JC/MD
Sample : M1425-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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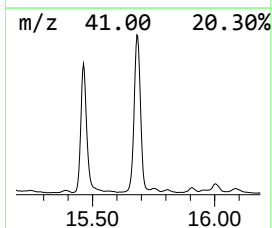
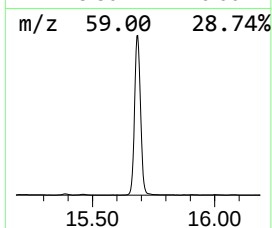
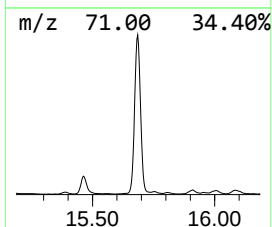
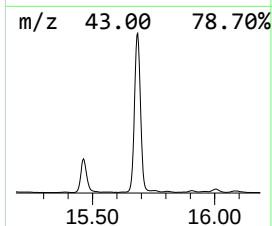
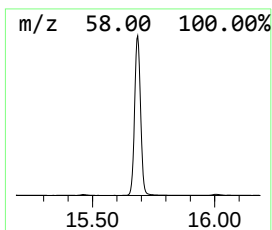
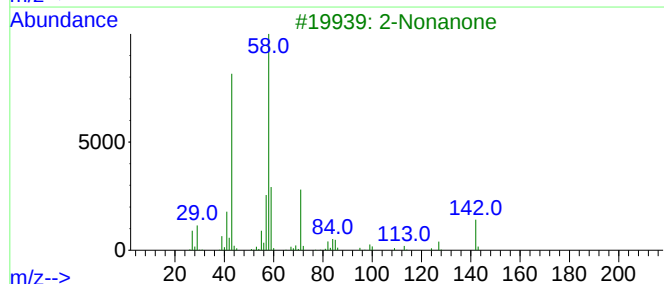
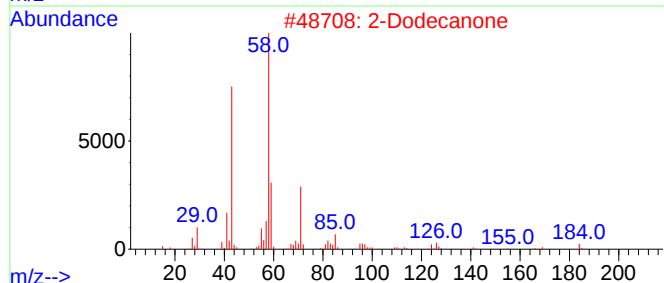
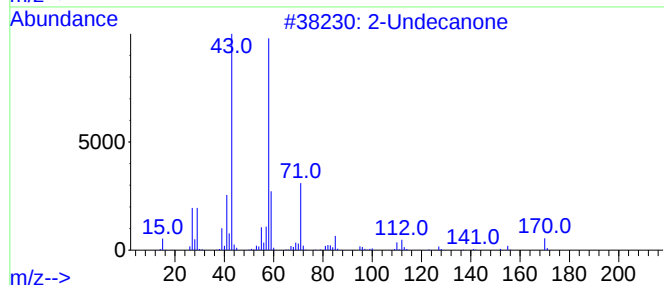
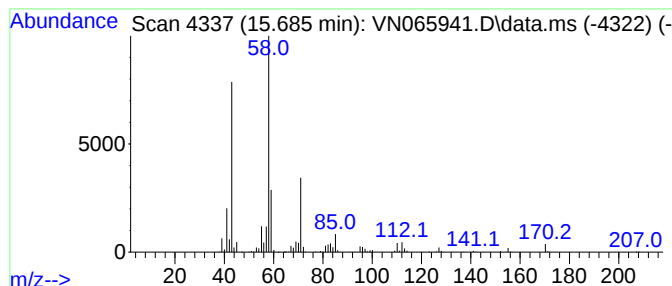
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 2-Undecanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.685	232.00 ug/l	3449450	1,4-Dichlorobenzene-d4	13.312

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Undecanone	170	C11H22O	000112-12-9	91
2		2-Dodecanone	184	C12H24O	006175-49-1	86
3		2-Nonanone	142	C9H18O	000821-55-6	72
4		1-Propene, 2-(1-methylethoxy)	100	C6H12O	004188-63-0	59
5		2-Octanone	128	C8H16O	000111-13-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
Data File : VN065941.D
Acq On : 18 Feb 2021 15:25
Operator : JC/MD
Sample : M1425-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Isopropyl Alcohol	4.049	51.6	ug/l	549370	1	7.627	531990	50.0
1-Butanol	8.759	30.3	ug/l	423456	2	8.550	700002	50.0
1-Hexanol, 2-et...	13.418	202.4	ug/l	3009040	4	13.312	743405	50.0
2-Nonanone	13.990	250.3	ug/l	3722190	4	13.312	743405	50.0
1-Octanol, 2-me...	14.312	66.2	ug/l	983626	4	13.312	743405	50.0
1-Nonanol	14.637	206.0	ug/l	3063430	4	13.312	743405	50.0
1-Decene	15.125	71.3	ug/l	1060380	4	13.312	743405	50.0
1-Decanol	15.463	114.8	ug/l	1707350	4	13.312	743405	50.0
2-Undecanone	15.685	232.0	ug/l	3449450	4	13.312	743405	50.0