

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
 Data File : VN065839.D
 Acq On : 12 Feb 2021 15:29
 Operator : JC/MD
 Sample : M1341-04
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 26878

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\82N012521W.M

Title : SW846 8260

Signal : TIC: VN065839.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.798	8	18	32	rBV	100955	128443	2.63%	0.443%
2	2.142	116	125	141	rVB2	32770	57339	1.17%	0.198%
3	2.293	163	172	183	rVB	31920	50120	1.03%	0.173%
4	7.547	1788	1806	1817	rBV	96485	233770	4.78%	0.806%
5	7.621	1817	1829	1857	rVB	160634	386742	7.91%	1.334%
6	7.984	1924	1942	1973	rBV	103113	242665	4.96%	0.837%
7	8.547	2102	2117	2135	rBV	288997	590225	12.08%	2.035%
8	10.058	2569	2587	2605	rBV	475685	877186	17.95%	3.025%
9	11.376	2982	2997	3023	rBV	456773	822100	16.82%	2.835%
10	12.373	3294	3307	3327	rBV	342619	587437	12.02%	2.026%
11	13.312	3587	3599	3614	rBV	420255	715155	14.63%	2.466%
12	13.421	3622	3633	3657	rBV	799998	1282245	26.23%	4.422%
13	13.794	3739	3749	3763	rBV5	41174	80638	1.65%	0.278%
14	13.994	3800	3811	3823	rBV	67626	118907	2.43%	0.410%
15	14.093	3833	3842	3854	rVB2	58894	98656	2.02%	0.340%
16	14.177	3856	3868	3888	rBV	391403	664944	13.60%	2.293%
17	14.283	3890	3901	3903	rBV	529621	690345	14.12%	2.381%
18	14.312	3904	3910	3943	rVB	1498025	2535681	51.88%	8.745%
19	14.640	4000	4012	4042	rBV	3150588	4887915	100.00%	16.856%
20	14.836	4068	4073	4086	rVB3	49698	85007	1.74%	0.293%
21	14.942	4088	4106	4108	rBV	574651	821664	16.81%	2.834%
22	14.968	4109	4114	4127	rVB	1024948	1527181	31.24%	5.267%
23	15.090	4142	4152	4156	rBV	972937	1497122	30.63%	5.163%
24	15.122	4156	4162	4189	rVB	2095190	3694606	75.59%	12.741%
25	15.463	4255	4268	4298	rBV	2773964	4743706	97.05%	16.359%
26	15.756	4348	4359	4367	rBV2	224154	411696	8.42%	1.420%
27	15.807	4368	4375	4411	rVB2	198728	431149	8.82%	1.487%
28	15.958	4413	4422	4429	rBV2	129679	242118	4.95%	0.835%
29	16.003	4430	4436	4459	rVB2	175173	353045	7.22%	1.218%
30	16.408	4550	4562	4587	rBV3	50554	139444	2.85%	0.481%

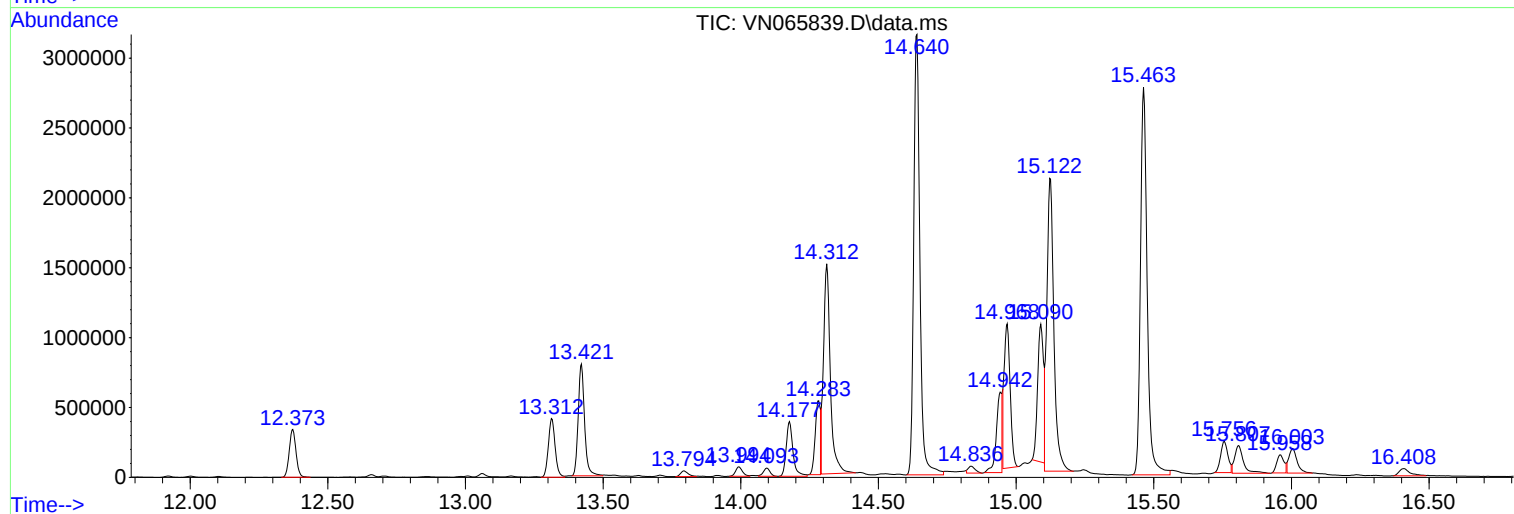
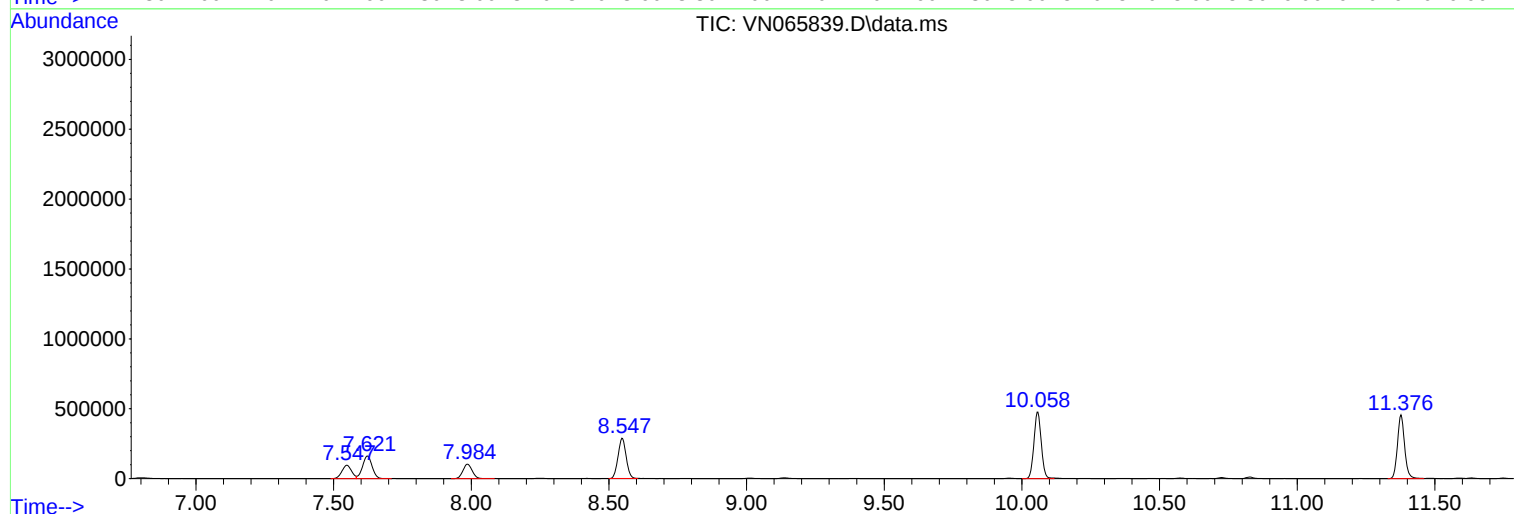
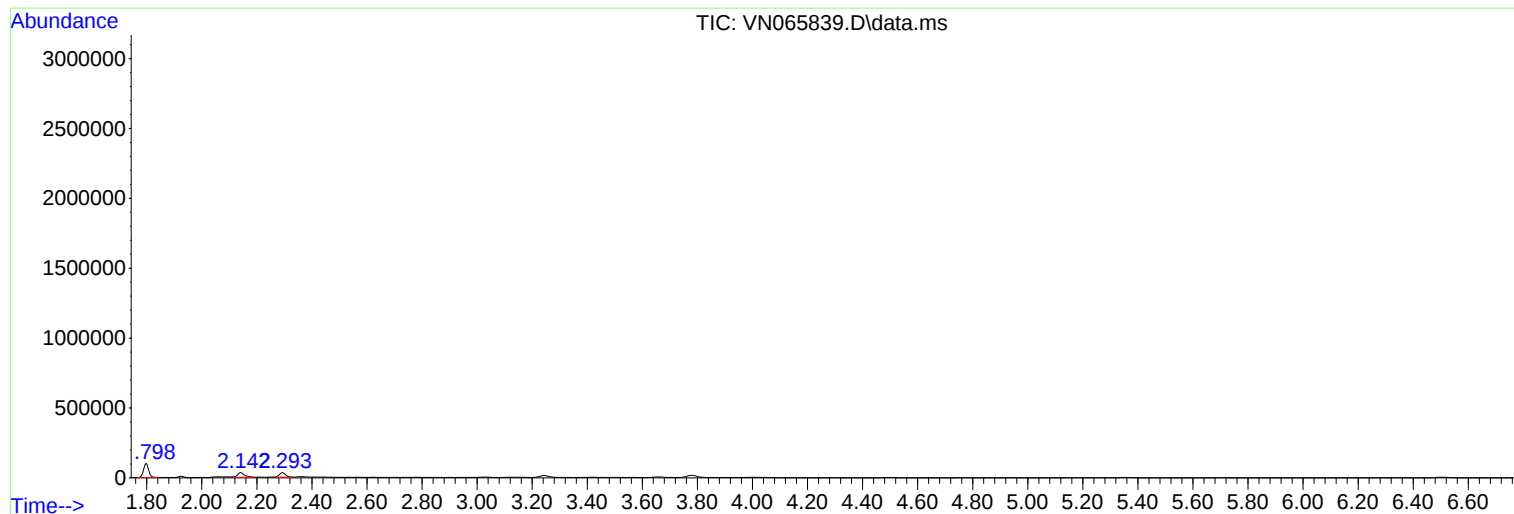
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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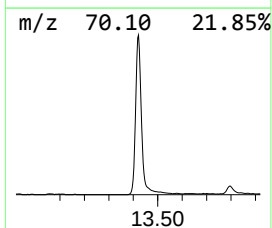
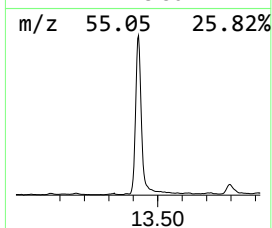
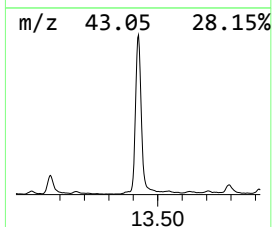
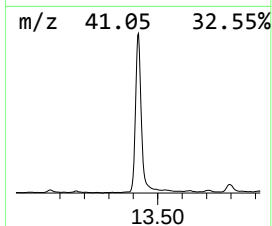
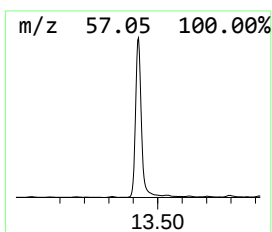
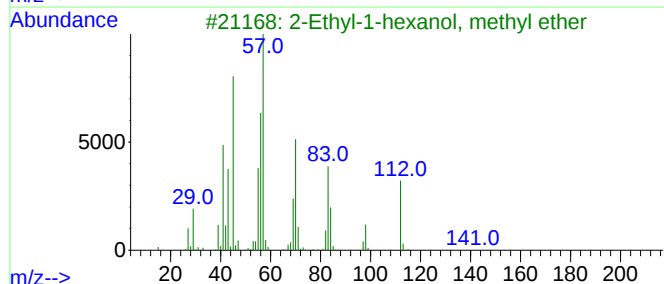
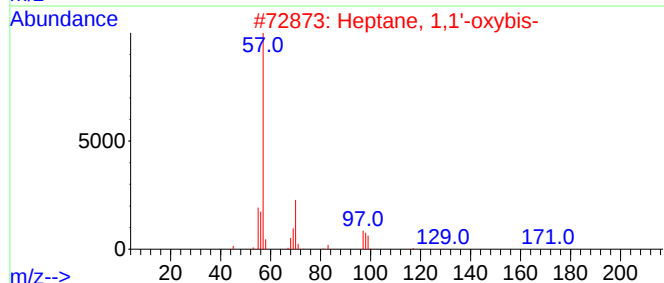
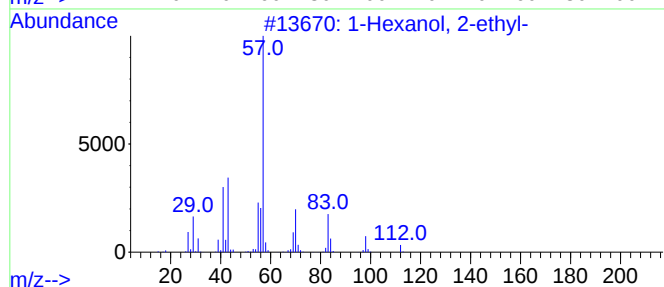
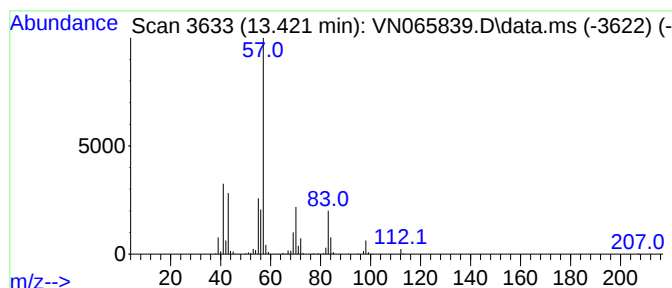
Instrument :
MSVOA_N
ClientSampleId :
26878

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.421	89.65 ug/l	1282250	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	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47



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Instrument :
MSVOA_N
ClientSampled :
26878

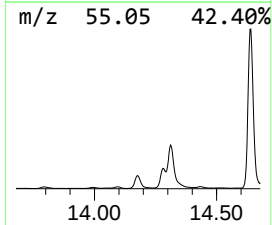
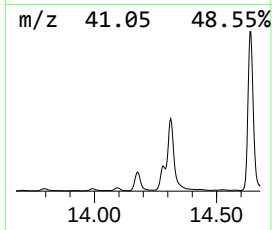
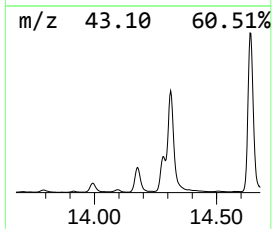
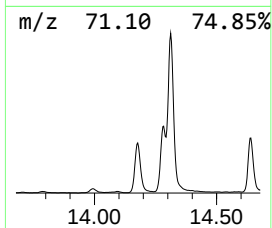
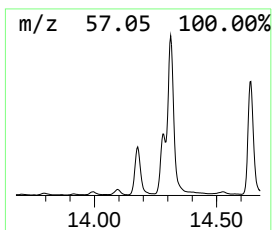
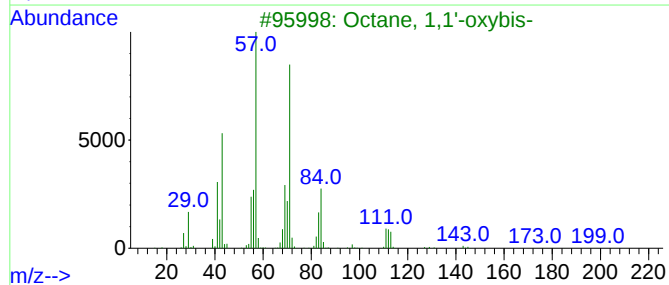
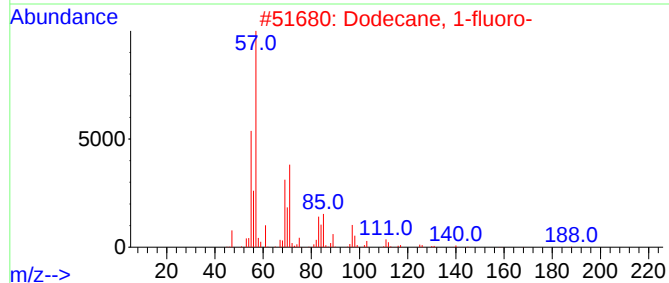
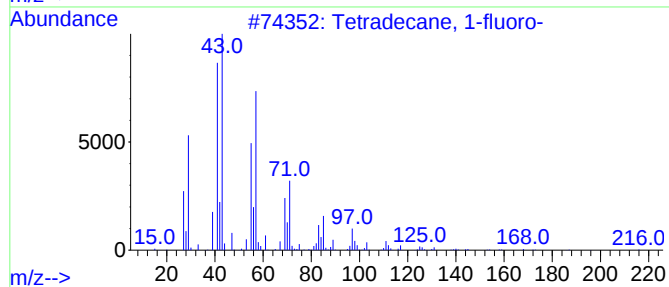
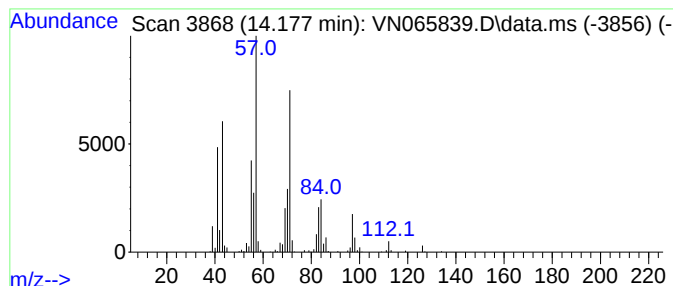
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 2 Tetradecane, 1-fluoro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.177	46.49 ug/l	664944	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-fluoro-	216	C14H29F	000593-33-9	78
2			Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	78
3			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
5			Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	47



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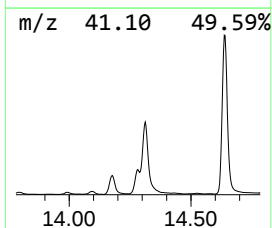
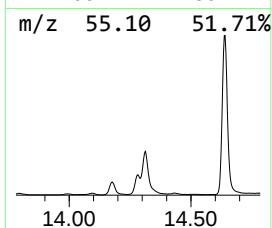
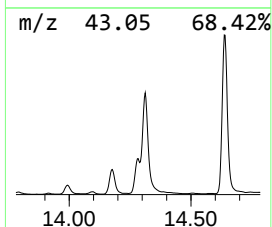
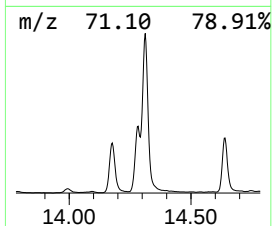
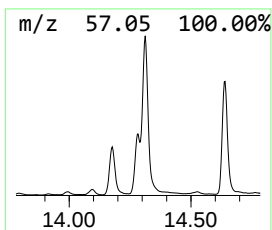
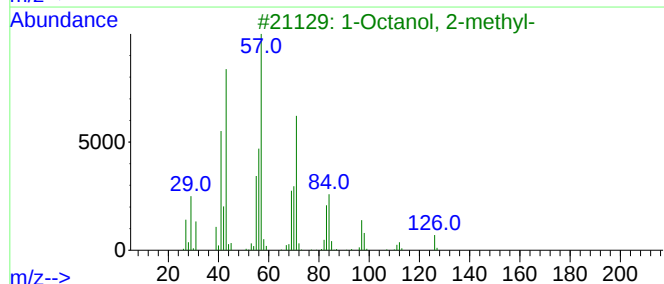
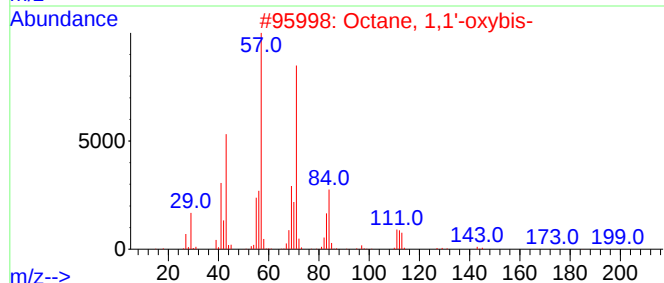
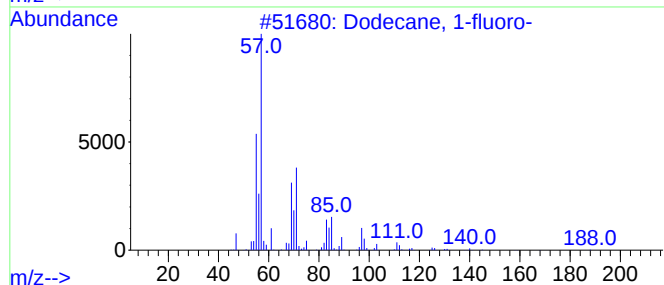
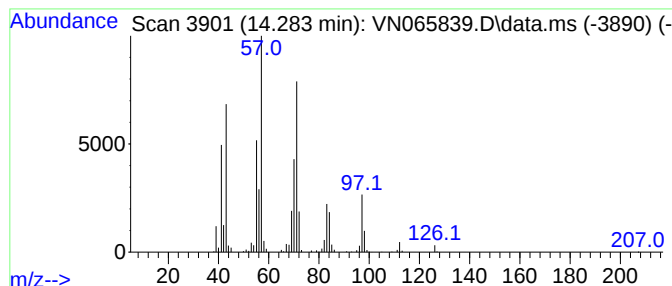
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Quant Title : SW846 8260

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

Peak Number 3 Dodecane, 1-fluoro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.283	48.27 ug/l	690345	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	64
2			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	50
3			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	47
4			Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	47
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	43



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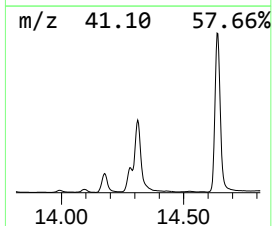
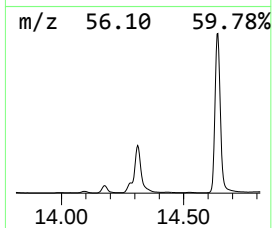
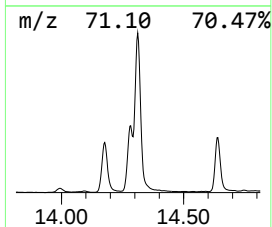
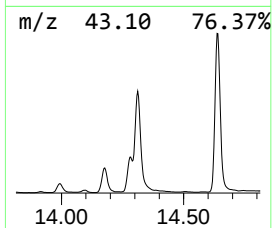
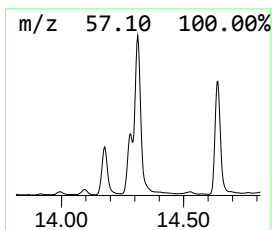
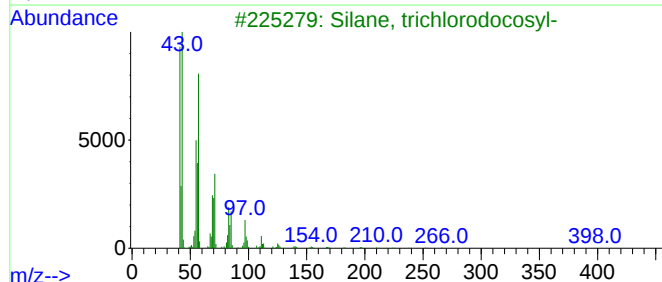
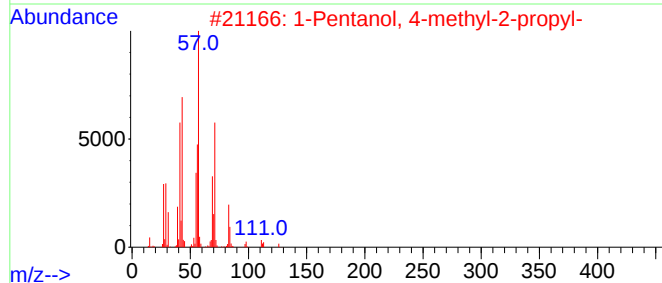
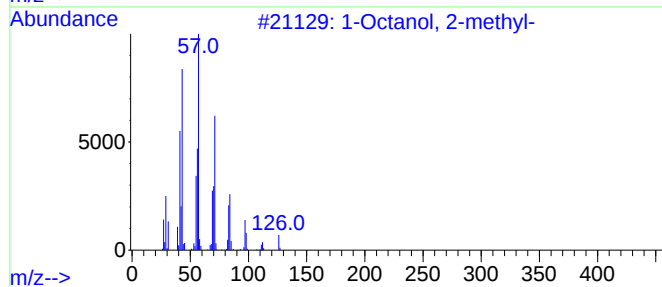
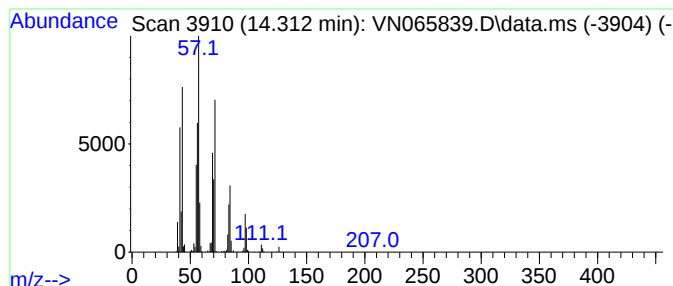
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 1-Octanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.312	177.28 ug/l	2535680	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	80
2			1-Pentanol, 4-methyl-2-propyl-	144	C9H20O	054004-41-0	53
3			Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	47
4			Nonyl chloroformate	206	C10H19ClO2	057045-82-6	47
5			Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	46



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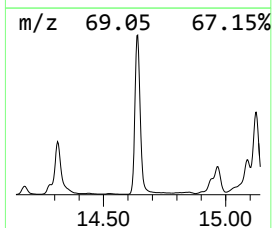
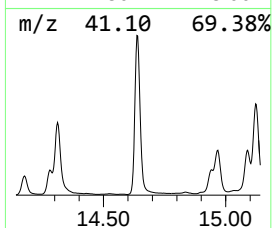
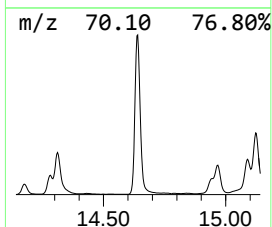
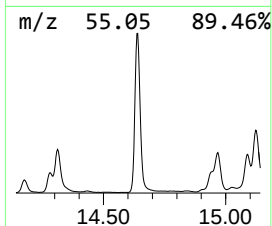
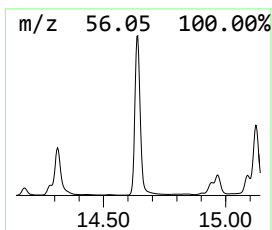
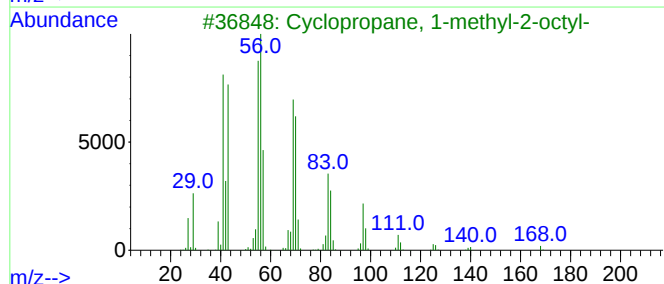
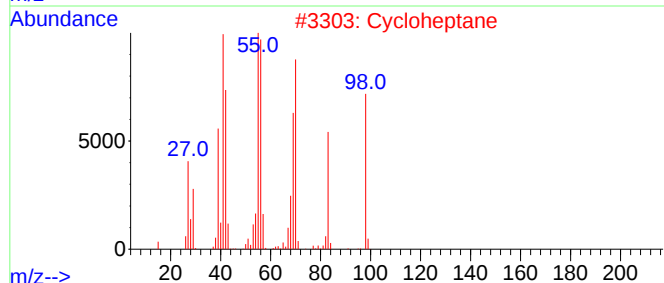
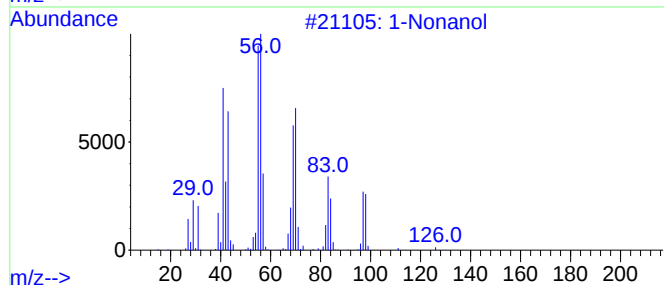
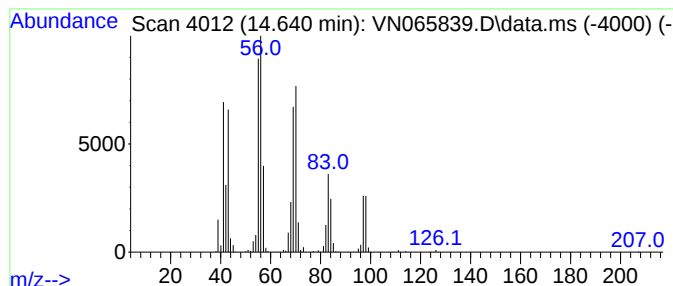
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Quant Title : SW846 8260

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

Peak Number 5 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	341.74 ug/l	4887920	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			Cycloheptane	98	C7H14	000291-64-5	87
3			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	80
4			1-Octanol	130	C8H18O	000111-87-5	80
5			Isopropylcyclobutane	98	C7H14	000872-56-0	68



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26878

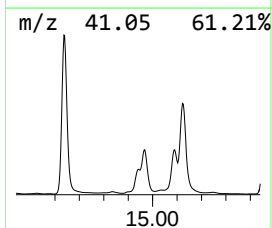
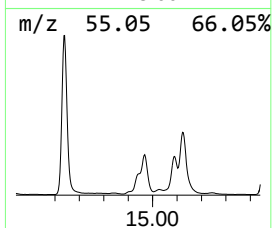
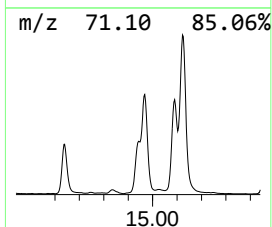
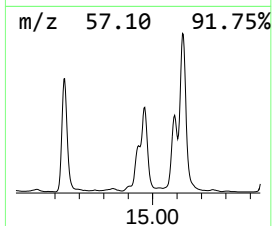
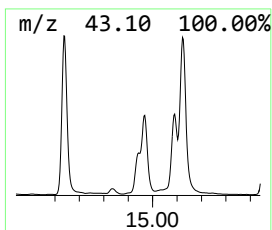
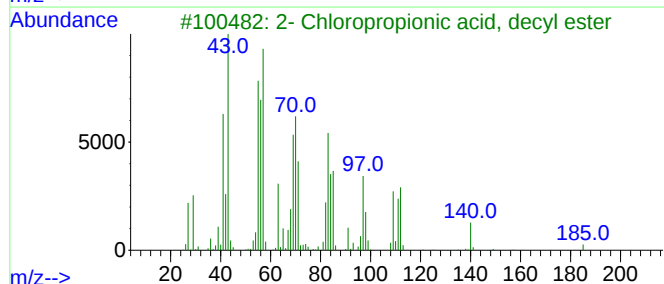
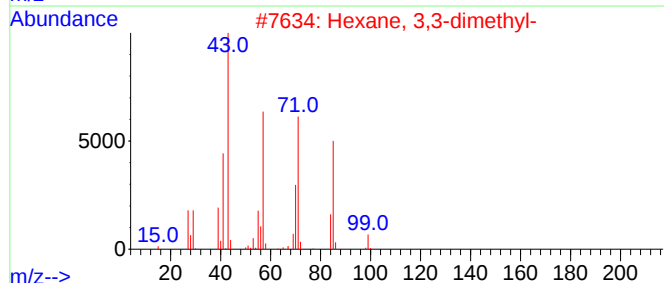
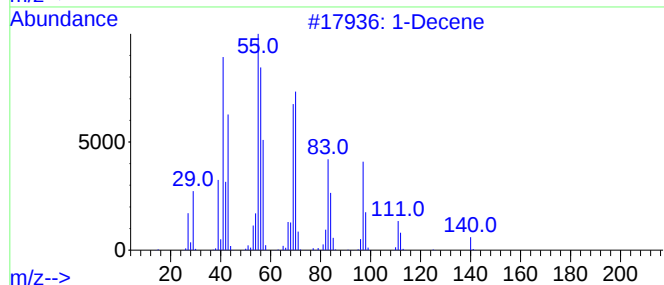
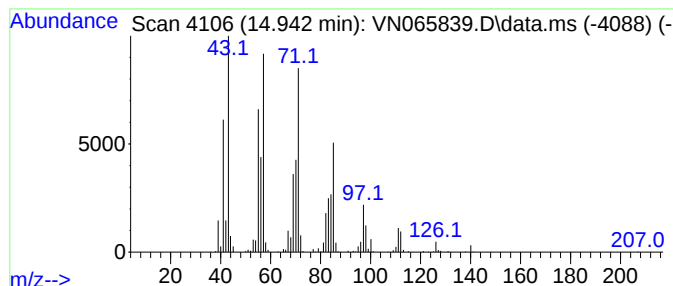
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Quant Title : SW846 8260

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

Peak Number 6 1-Decene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.942	57.45 ug/l	821664	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decene	140	C10H20	000872-05-9	55
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	49
3			2- Chloropropionic acid, decyl e...	248	C13H25ClO2	086711-78-6	47
4			Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	45
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065839.D
Acq On : 12 Feb 2021 15:29
Operator : JC/MD
Sample : M1341-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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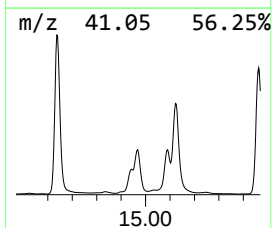
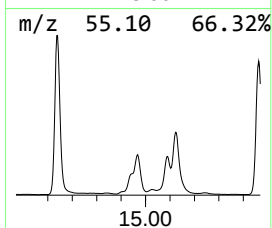
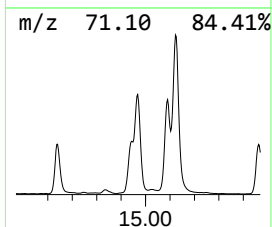
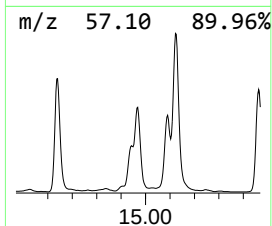
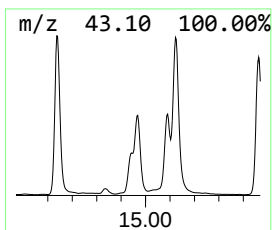
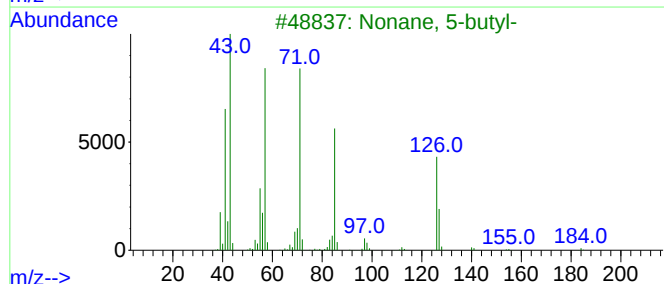
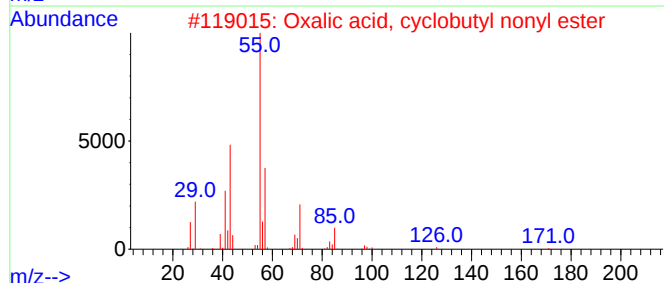
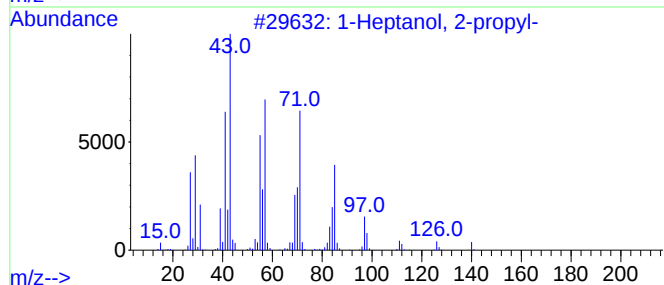
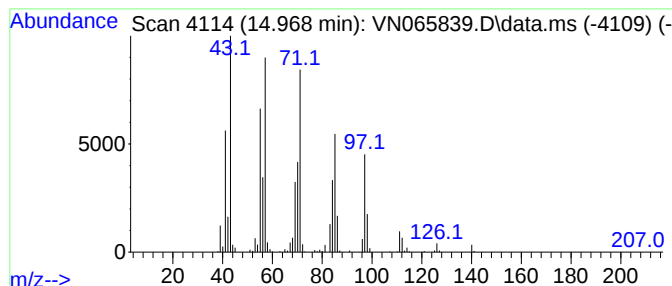
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Quant Title : SW846 8260

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

Peak Number 7 1-Heptanol, 2-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	106.77 ug/l	1527180	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	59
2			Oxalic acid, cyclobutyl nonyl ester	270	C15H26O4	1000309-70-0	47
3			Nonane, 5-butyl-	184	C13H28	017312-63-9	43
4			4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	38
5			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065839.D
Acq On : 12 Feb 2021 15:29
Operator : JC/MD
Sample : M1341-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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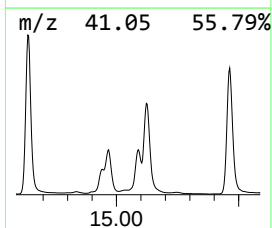
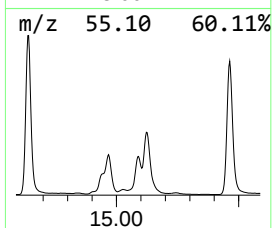
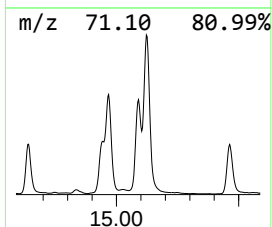
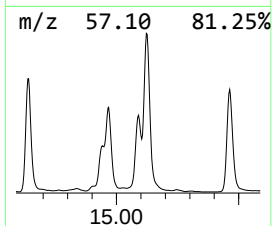
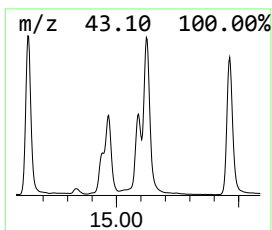
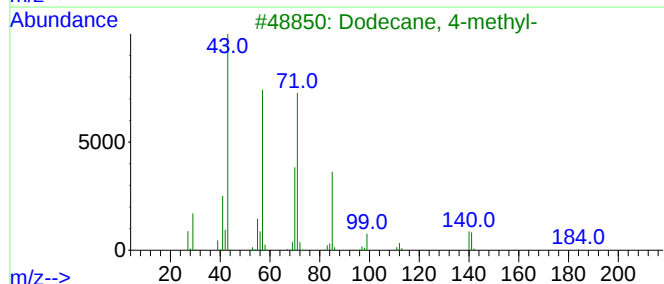
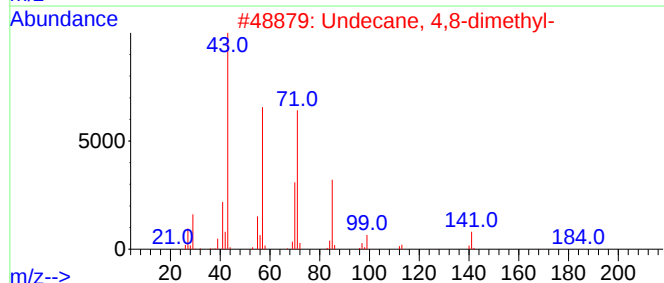
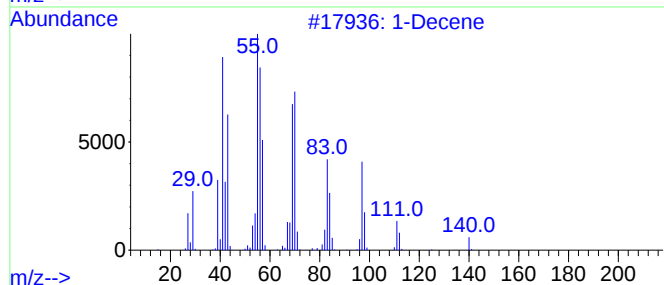
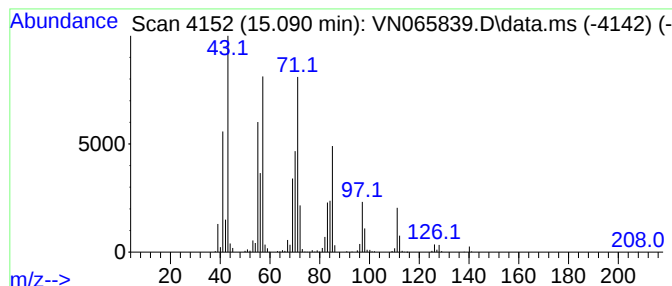
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Quant Title : SW846 8260

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

Peak Number 8 Undecane, 4,8-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.090	104.67 ug/l	1497120	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decene	140	C10H20	000872-05-9	70
2			Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	50
3			Dodecane, 4-methyl-	184	C13H28	006117-97-1	50
4			Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	43
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065839.D
Acq On : 12 Feb 2021 15:29
Operator : JC/MD
Sample : M1341-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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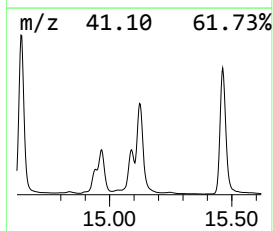
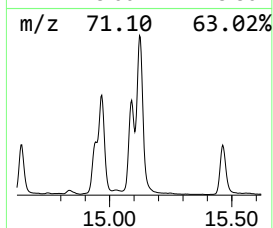
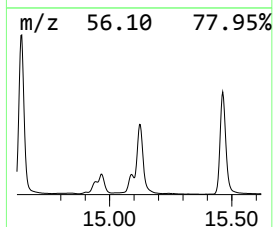
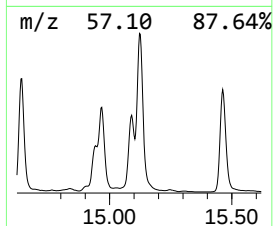
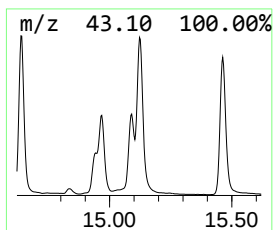
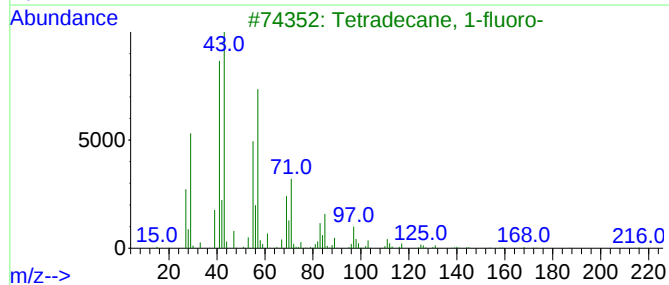
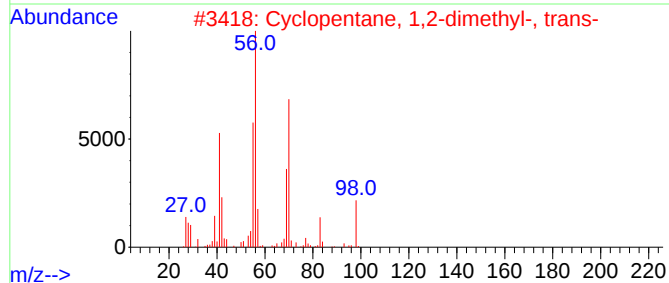
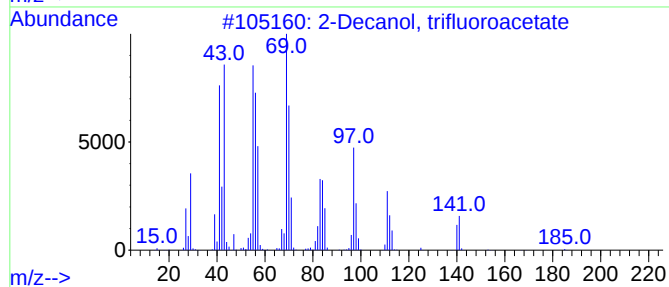
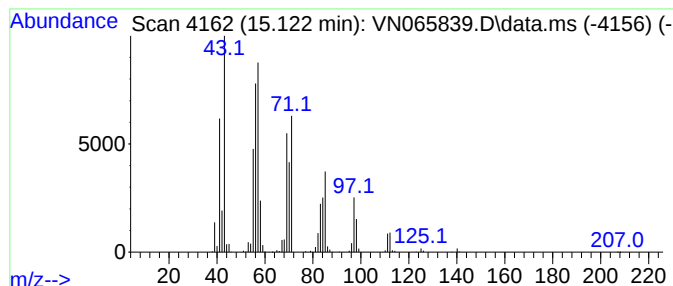
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Quant Title : SW846 8260

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

Peak Number 9 2-Decanol, trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.122	258.31 ug/l	3694610	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Decanol, trifluoroacetate	254	C12H21F3O2	1000352-32-8	50
2			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	43
3			Tetradecane, 1-fluoro-	216	C14H29F	000593-33-9	43
4			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	43
5			Isopropylcyclobutane	98	C7H14	000872-56-0	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065839.D
Acq On : 12 Feb 2021 15:29
Operator : JC/MD
Sample : M1341-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
26878

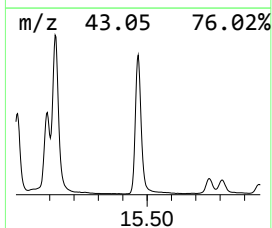
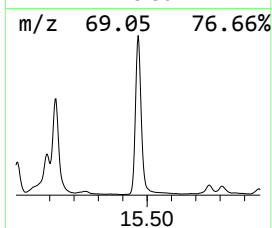
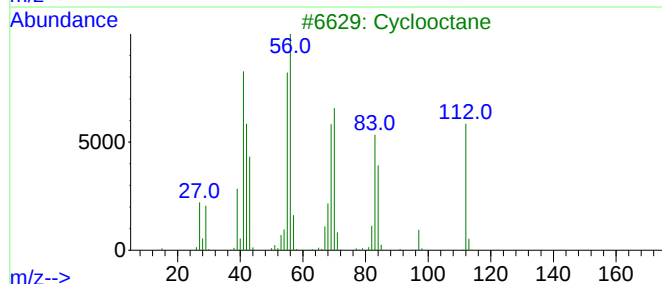
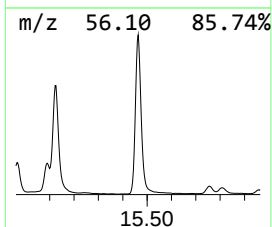
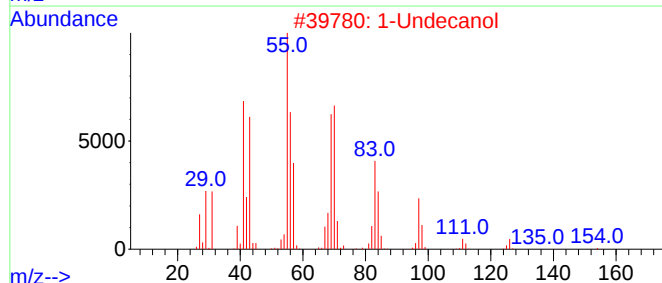
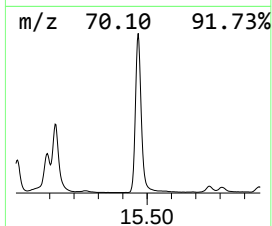
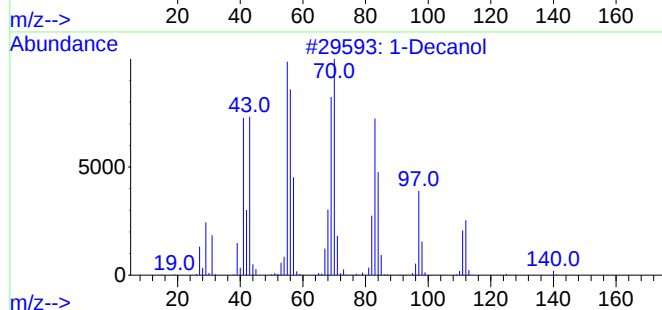
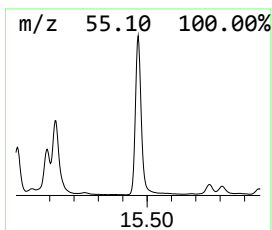
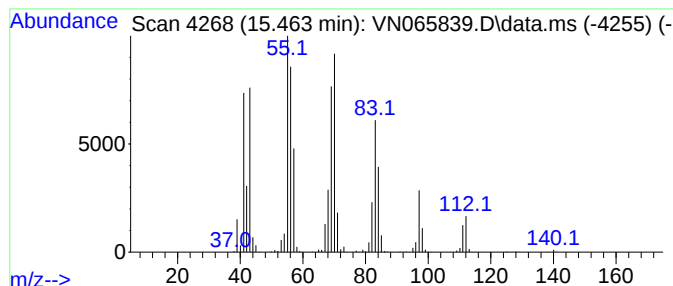
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 10 1-Decanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.463	331.66 ug/l	4743710	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		1-Undecanol	172	C11H24O	000112-42-5	90
3		Cyclooctane	112	C8H16	000292-64-8	87
4		Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	86
5		Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065839.D
Acq On : 12 Feb 2021 15:29
Operator : JC/MD
Sample : M1341-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
26878

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.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
1-Hexanol, 2-et...	13.421	89.7	ug/l	1282250	4	13.312	715155	50.0
Tetradecane, 1-...	14.177	46.5	ug/l	664944	4	13.312	715155	50.0
Dodecane, 1-flu...	14.283	48.3	ug/l	690345	4	13.312	715155	50.0
1-Octanol, 2-me...	14.312	177.3	ug/l	2535680	4	13.312	715155	50.0
1-Nonanol	14.640	341.7	ug/l	4887920	4	13.312	715155	50.0
1-Decene	14.942	57.5	ug/l	821664	4	13.312	715155	50.0
1-Heptanol, 2-p...	14.968	106.8	ug/l	1527180	4	13.312	715155	50.0
Undecane, 4,8-d...	15.090	104.7	ug/l	1497120	4	13.312	715155	50.0
2-Decanol, trif...	15.122	258.3	ug/l	3694610	4	13.312	715155	50.0
1-Decanol	15.463	331.7	ug/l	4743710	4	13.312	715155	50.0