

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
 Data File : VN070547.D
 Acq On : 10 Jan 2022 16:54
 Operator : JC/MD
 Sample : M5257-01ME
 Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 D3-12292021ME

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070547.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.016	2226	2247	2257	rBV	644476	1540452	3.55%	0.614%
2	8.078	2258	2270	2295	rVB	1539354	3625115	8.36%	1.444%
3	8.432	2384	2402	2434	rBV	846392	1943993	4.48%	0.775%
4	8.963	2582	2600	2630	rBV	2329325	5007146	11.55%	1.995%
5	10.438	3135	3150	3169	rBV	3053774	5791939	13.36%	2.308%
6	11.452	3519	3528	3537	rBV3	336510	578559	1.33%	0.231%
7	11.521	3544	3554	3580	rVB7	1291528	3456523	7.97%	1.377%
8	11.626	3581	3593	3616	rVB	1799607	3114212	7.18%	1.241%
9	11.744	3622	3637	3654	rBV	3072842	5805930	13.39%	2.313%
10	11.843	3662	3674	3694	rBV	4698661	8513976	19.63%	3.393%
11	11.948	3697	3713	3737	rBV2	20647083	43365870	100.00%	17.280%
12	12.173	3787	3797	3809	rVB3	2215584	4042938	9.32%	1.611%
13	12.251	3811	3826	3852	rBV5	5792933	19769127	45.59%	7.877%
14	12.366	3860	3869	3880	rVB	7835288	12171412	28.07%	4.850%
15	12.452	3881	3901	3903	rBV7	4143779	8274460	19.08%	3.297%
16	12.734	3996	4006	4011	rBV2	3611420	5445848	12.56%	2.170%
17	12.766	4013	4018	4027	rVB	4274931	5405275	12.46%	2.154%
18	12.895	4059	4066	4081	rVB5	4703238	8726983	20.12%	3.477%
19	12.978	4082	4097	4106	rVB8	3168828	7265890	16.75%	2.895%
20	13.045	4110	4122	4137	rVV3	22121562	40834244	94.16%	16.271%
21	13.195	4170	4178	4186	rBV	3907249	5612125	12.94%	2.236%
22	13.246	4188	4197	4202	rVV4	4062918	6691784	15.43%	2.666%
23	13.281	4203	4210	4224	rVB	12001693	18242596	42.07%	7.269%
24	13.409	4252	4258	4267	rVB	2713776	3613603	8.33%	1.440%
25	13.603	4325	4330	4338	rVB	3068136	3431049	7.91%	1.367%
26	13.670	4349	4355	4365	rVB2	3689620	4870548	11.23%	1.941%
27	13.742	4377	4382	4397	rVB2	2131778	2983717	6.88%	1.189%
28	13.991	4465	4475	4487	rBV3	5909052	9474865	21.85%	3.775%
29	14.844	4786	4793	4807	rVB2	545846	825118	1.90%	0.329%
30	15.697	5103	5111	5133	rVB2	294882	537821	1.24%	0.214%

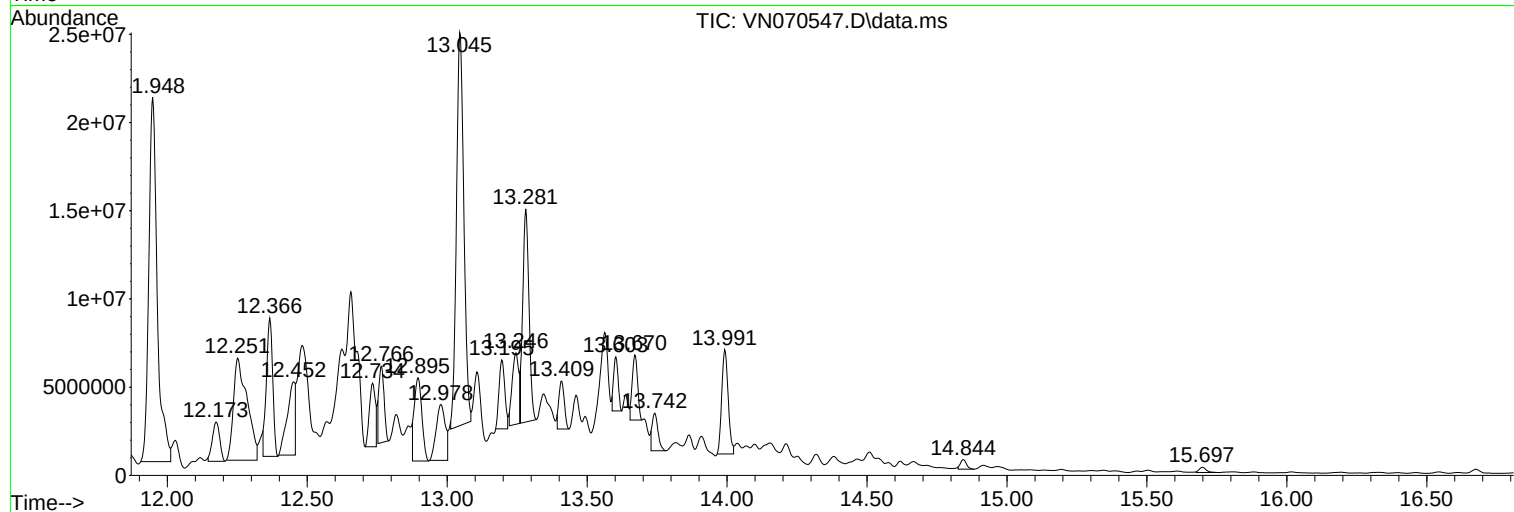
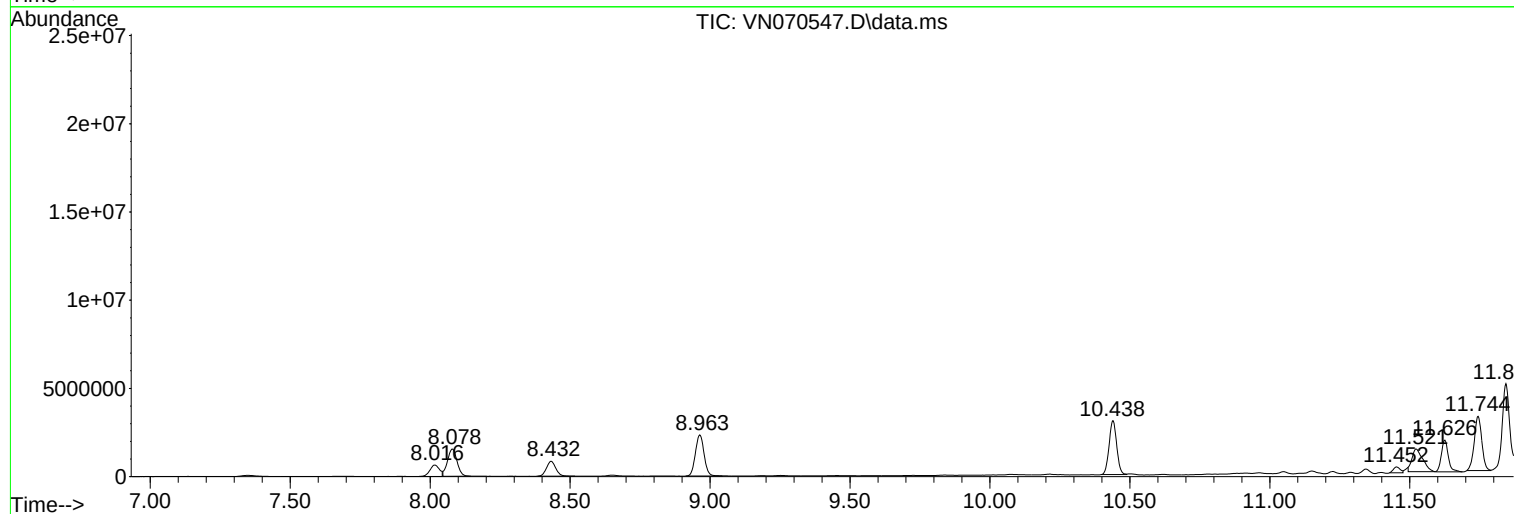
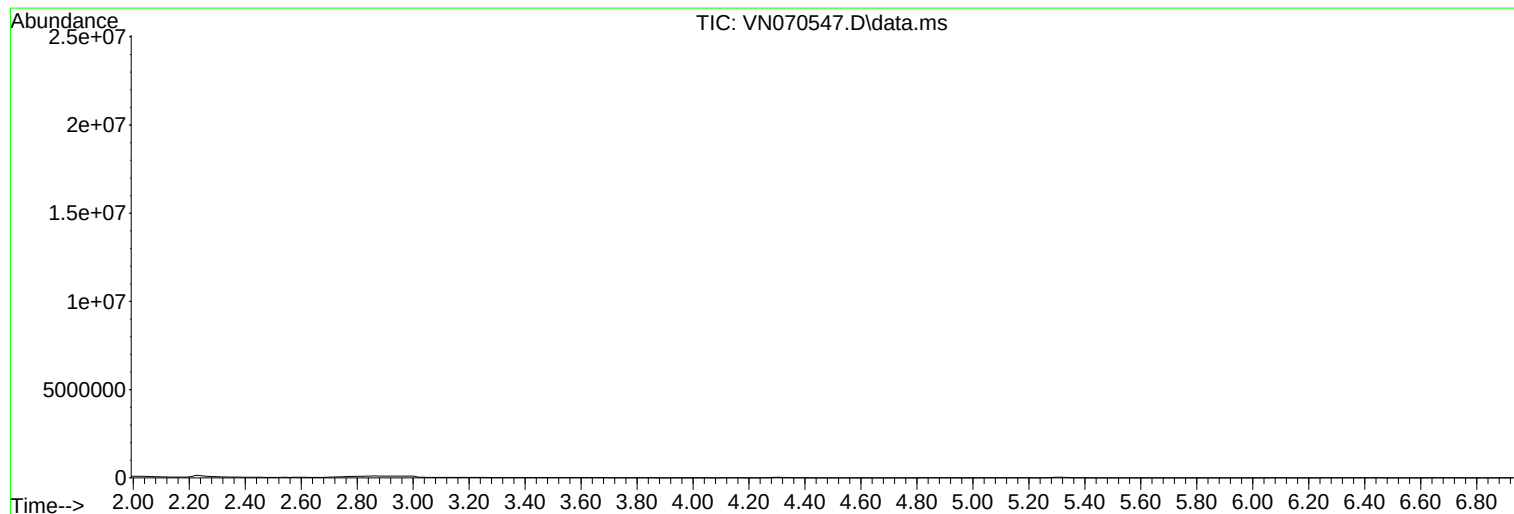
Sum of corrected areas: 250963118

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

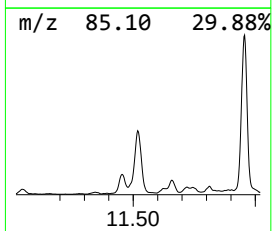
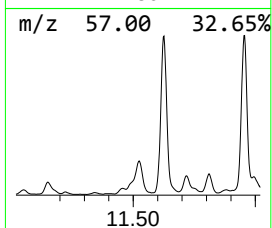
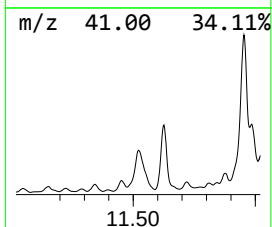
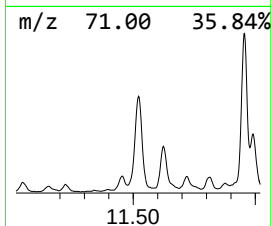
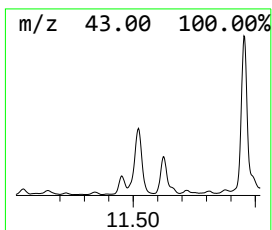
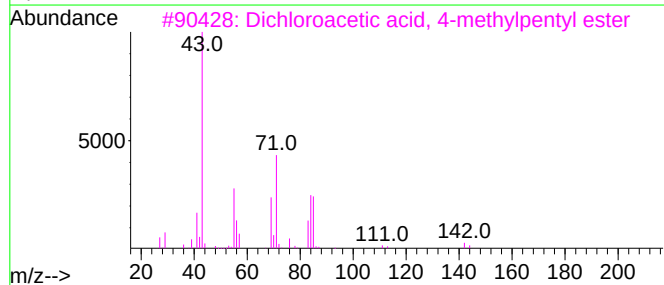
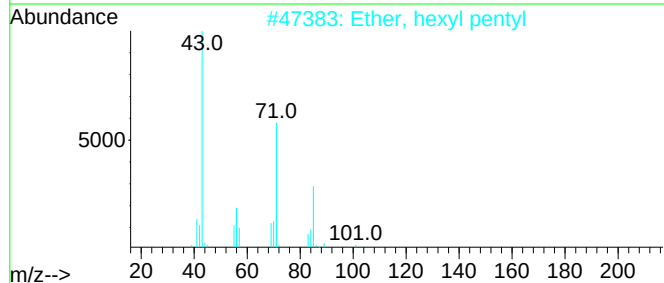
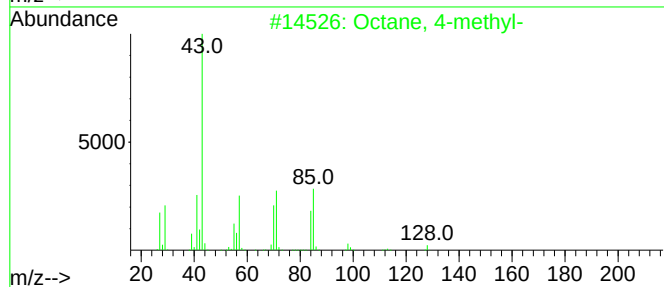
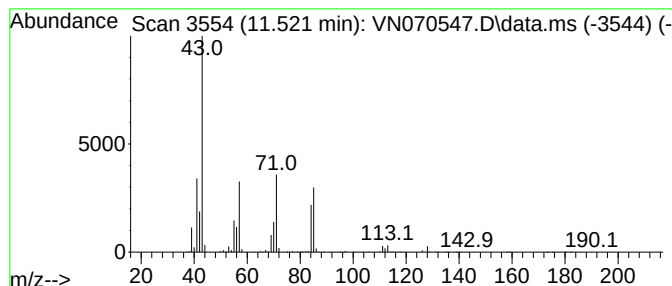
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 Octane, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.521	29.77 ug/l	3456520	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 4-methyl-	128	C9H20	002216-34-4	80
2			Ether, hexyl pentyl	172	C11H24O	032357-83-8	64
3			Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	59
4			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
5			Heptane, 4-ethyl-	128	C9H20	002216-32-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

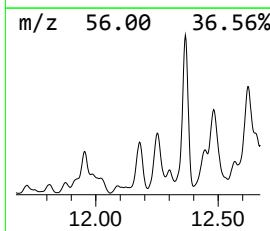
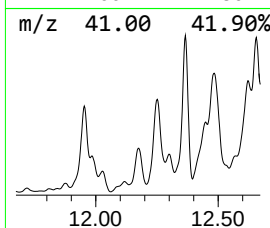
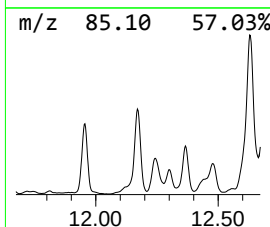
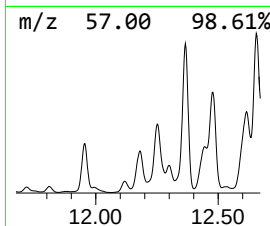
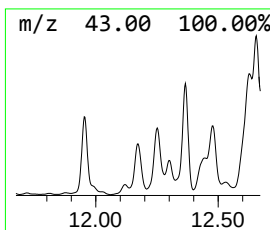
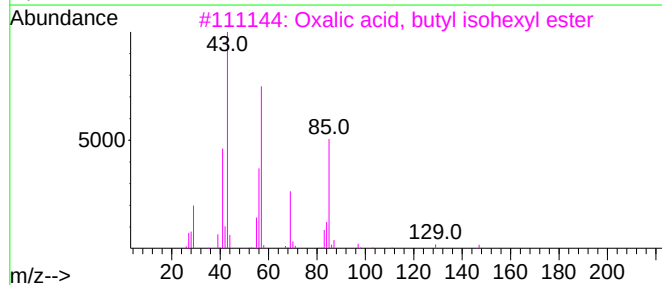
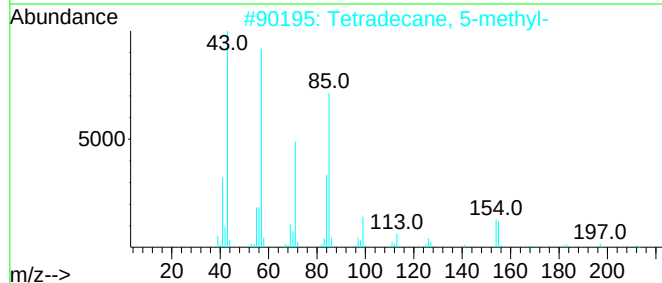
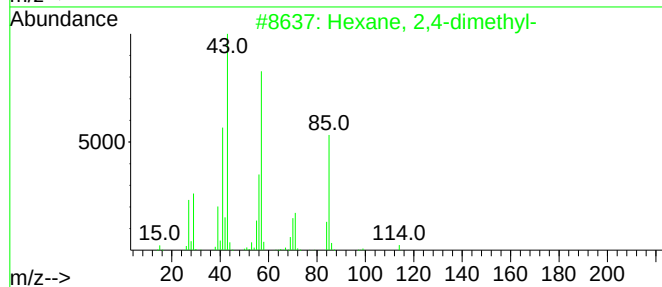
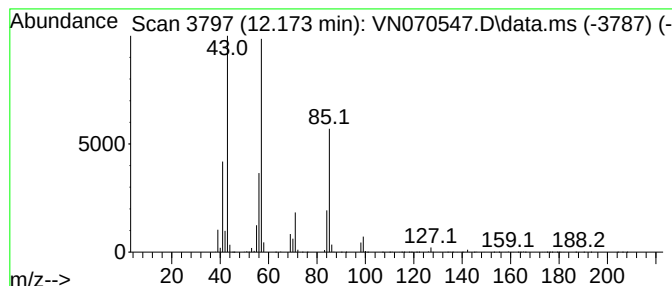
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 2 Hexane, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.173	34.82 ug/l	4042940	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
2			Tetradecane, 5-methyl-	212	C15H32	025117-32-2	64
3			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	64
4			Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	59
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

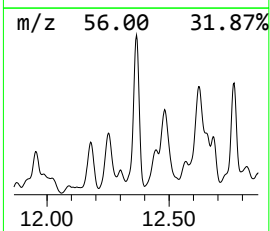
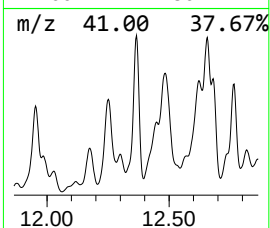
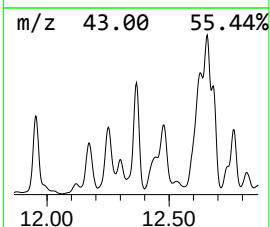
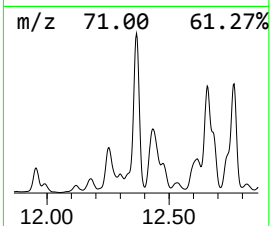
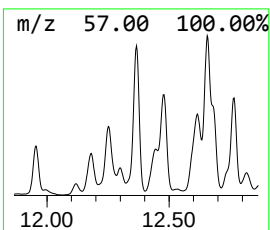
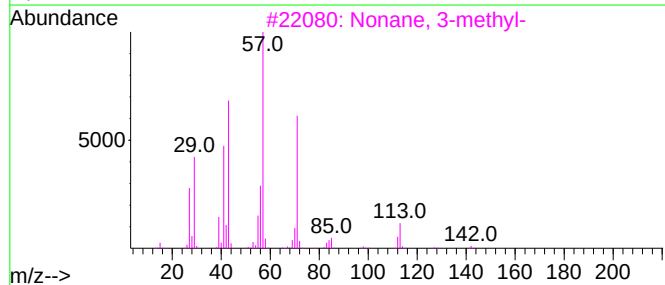
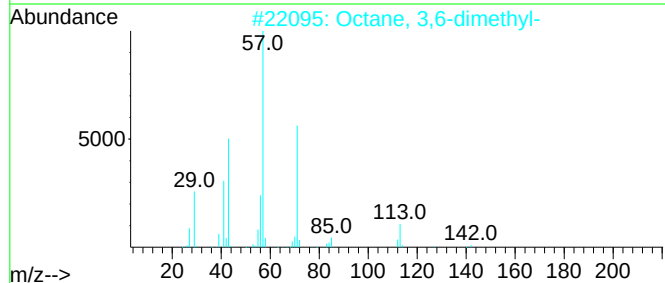
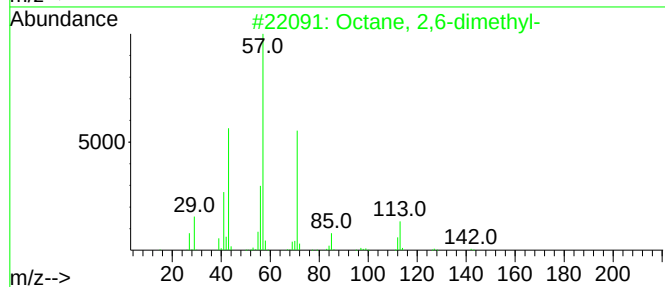
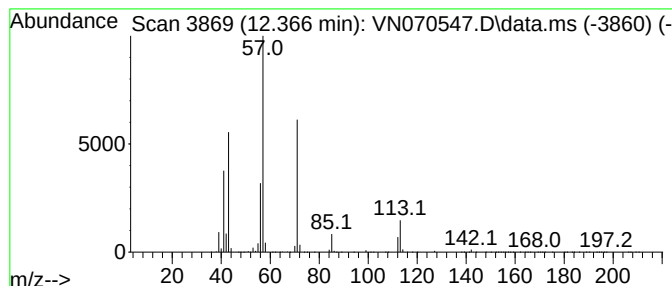
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 3 Octane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.366	104.82 ug/l	12171400	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
2			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	91
4			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	72
5			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

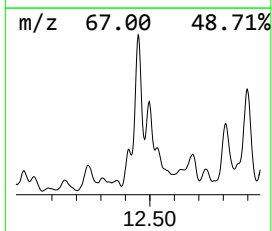
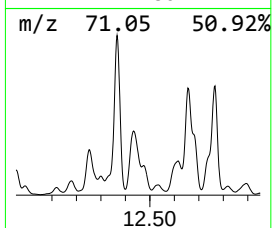
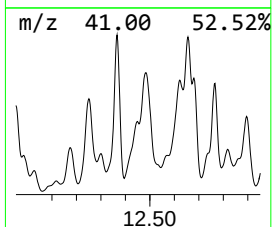
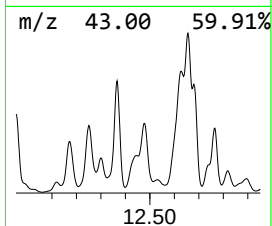
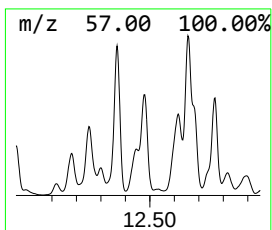
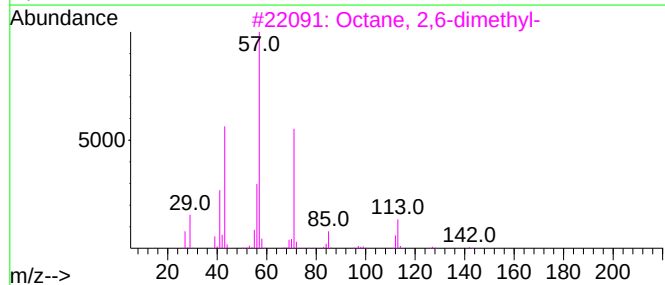
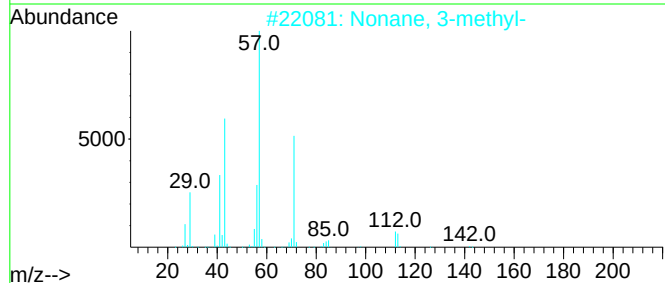
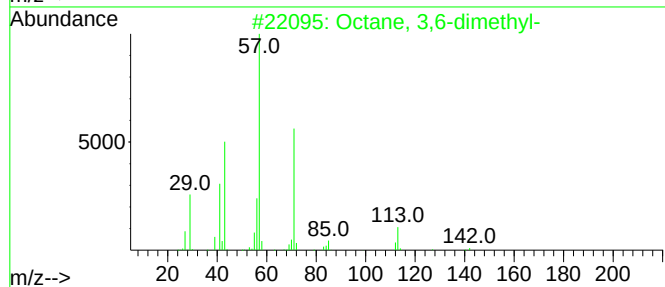
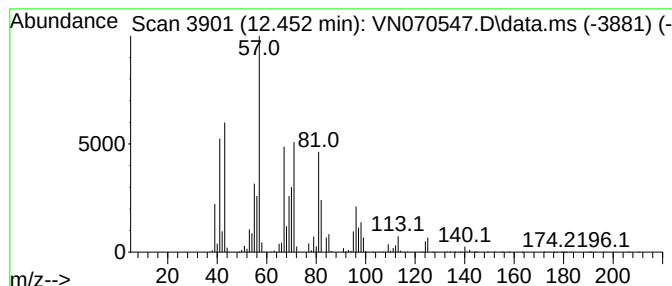
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown12.452 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.452	71.26 ug/l	8274460	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,6-dimethyl-		142	C10H22		015869-94-0	30
2	Nonane, 3-methyl-		142	C10H22		005911-04-6	30
3	Octane, 2,6-dimethyl-		142	C10H22		002051-30-1	27
4	2-Hexen-1-ol, acetate, (E)-		142	C8H14O2		002497-18-9	27
5	Pentane, 2,2,3,3-tetramethyl-		128	C9H20		007154-79-2	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

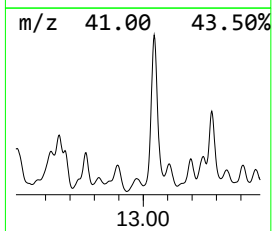
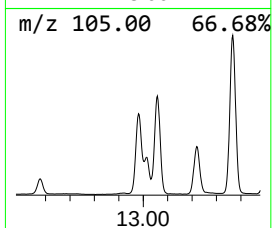
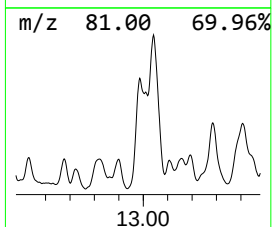
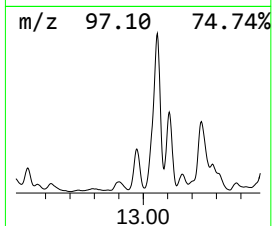
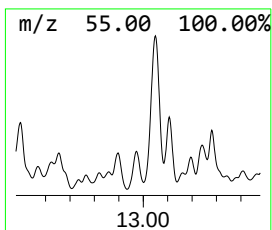
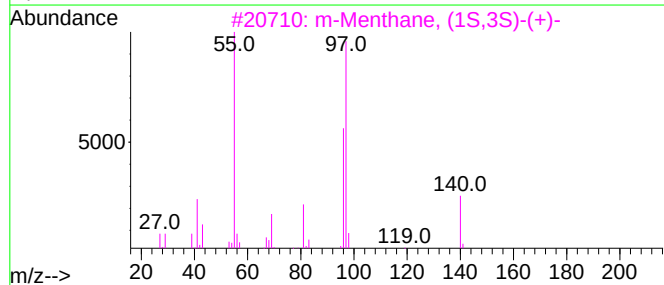
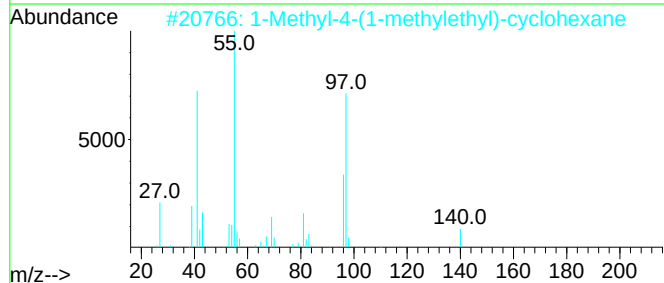
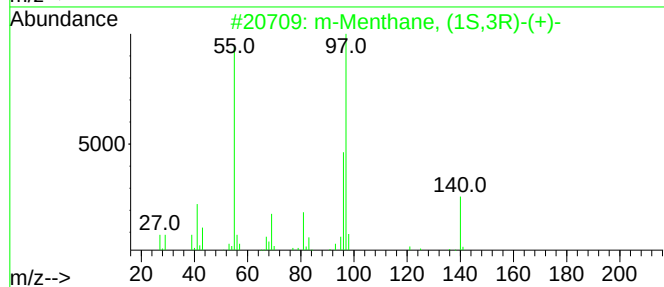
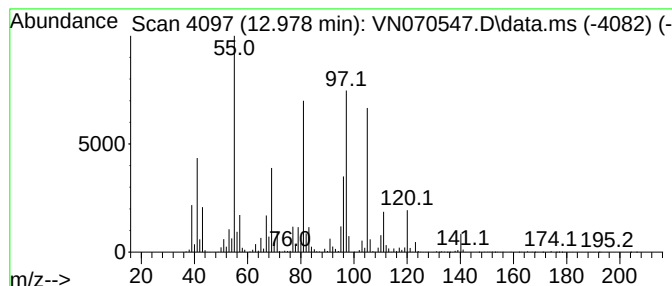
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 5 m-Menthane, (1S,3R)-(+)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.978	74.59 ug/l	7265890	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			m-Menthane, (1S,3R)-(+)-	140	C10H20	013837-66-6	64
2			1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	62
3			m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	58
4			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	58
5			Cyclopentane, 1-methyl-3-(2-meth...	140	C10H20	029053-04-1	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

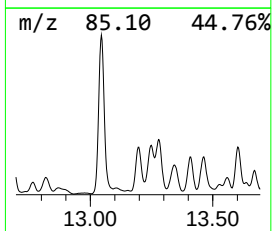
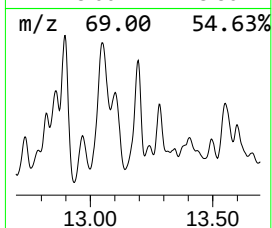
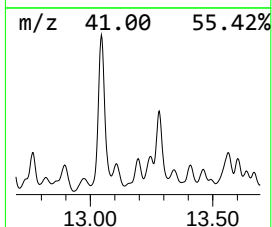
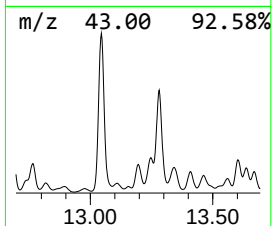
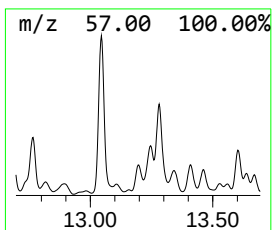
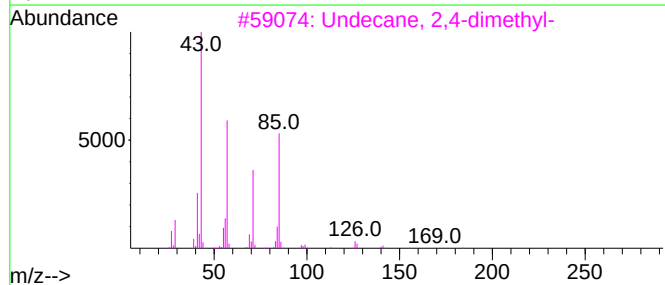
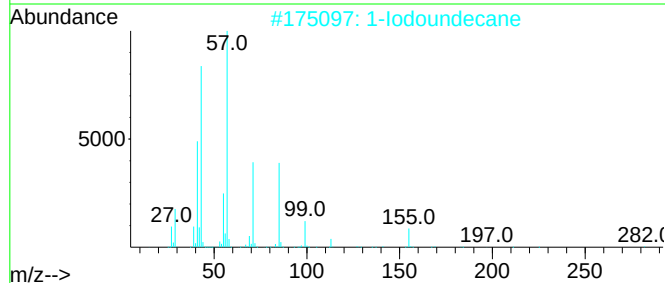
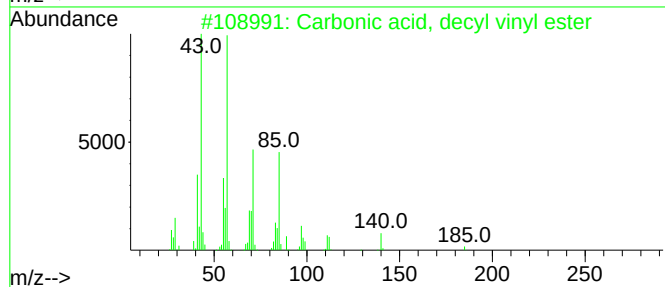
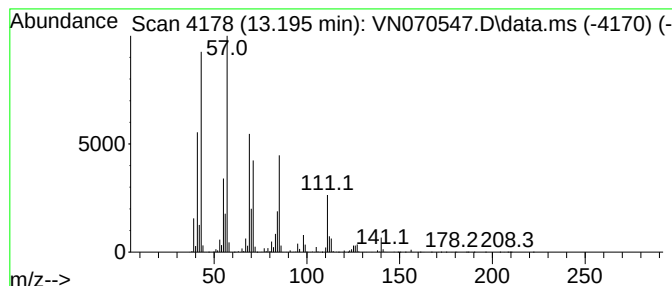
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 6 Carbonic acid, decyl vinyl ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.195	57.61 ug/l	5612130	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, decyl vinyl ester	228	C13H24O3	1000383-25-7	64
2			1-Iodoundecane	282	C11H23I	004282-44-4	50
3			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	47
4			Dodecane, 5-methyl-	184	C13H28	017453-93-9	47
5			Decane, 1-iodo-	268	C10H21I	002050-77-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

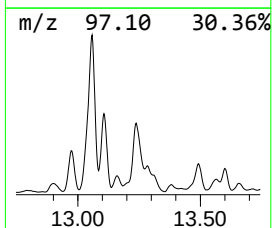
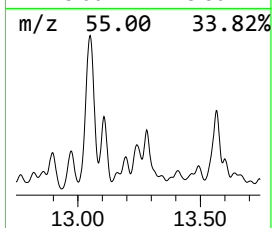
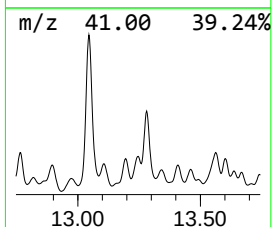
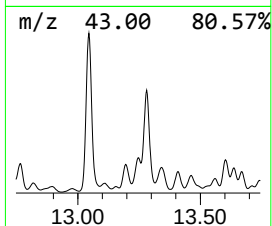
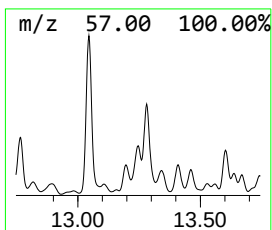
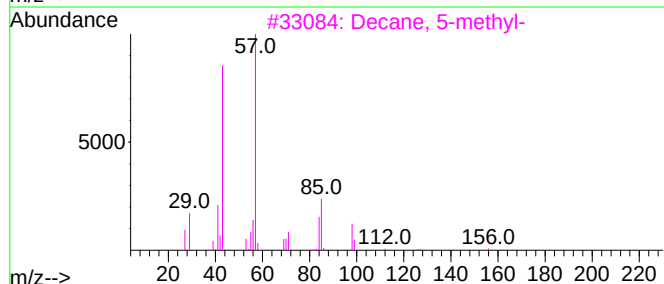
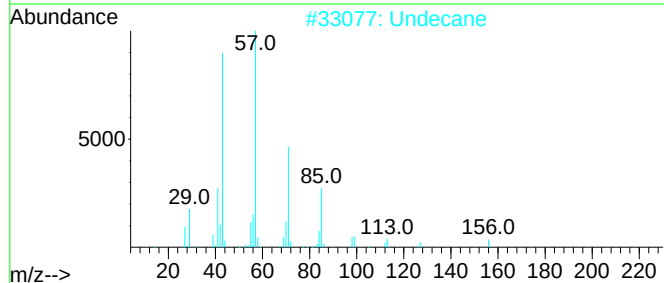
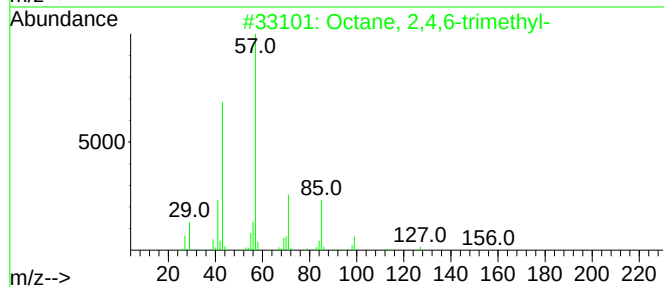
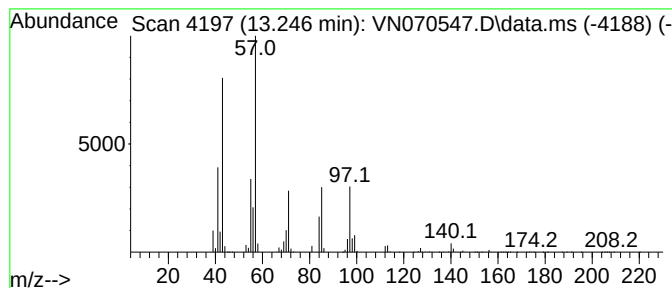
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 7 Octane, 2,4,6-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.246	68.70 ug/l	6691780	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	50
2			Undecane	156	C11H24	001120-21-4	49
3			Decane, 5-methyl-	156	C11H24	013151-35-4	49
4			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	47
5			Octane, 4-ethyl-	142	C10H22	015869-86-0	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

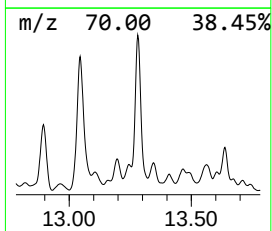
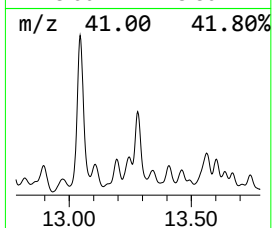
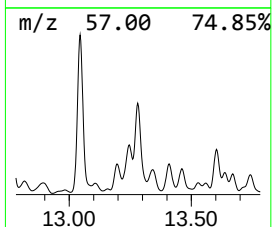
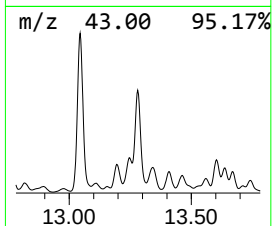
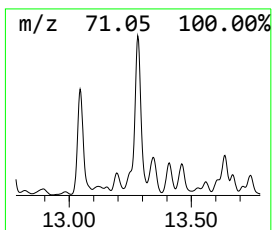
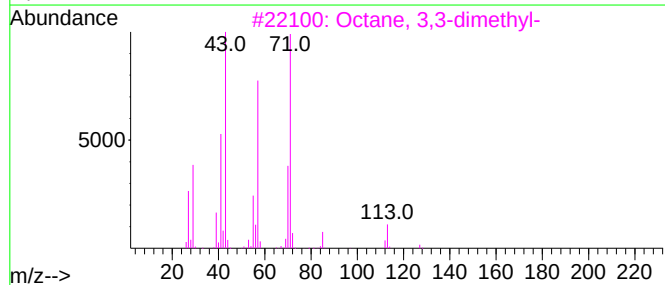
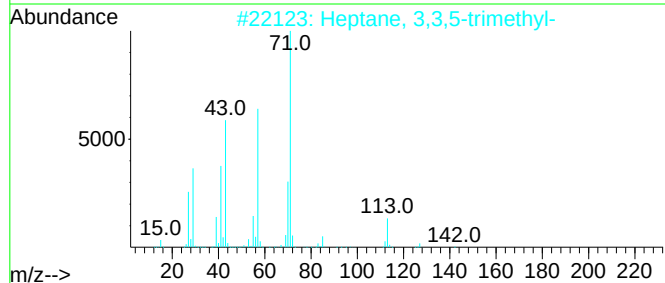
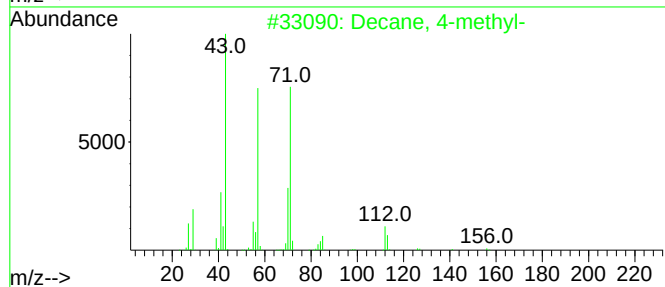
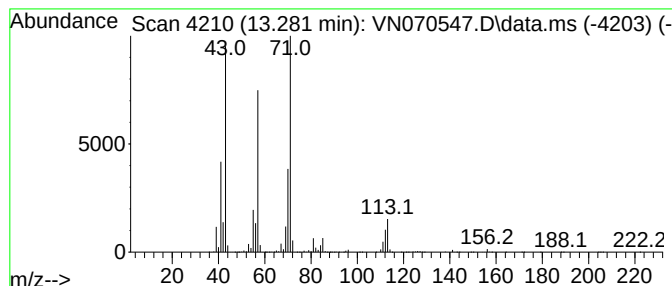
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 8 Decane, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.281	187.28 ug/l	18242600	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 4-methyl-	156	C11H24	002847-72-5	90
2			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	78
3			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	78
4			4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	64
5			n-Amyl ether	158	C10H22O	000693-65-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

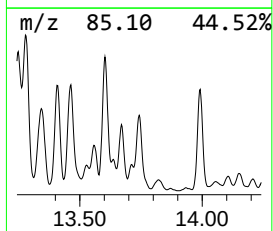
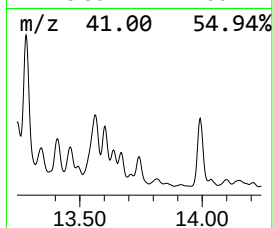
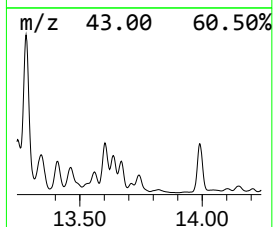
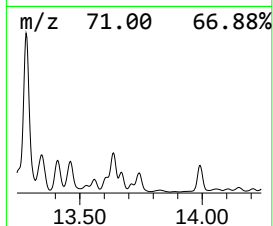
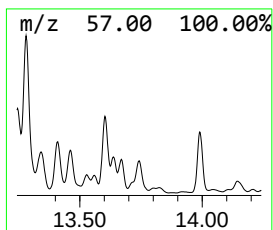
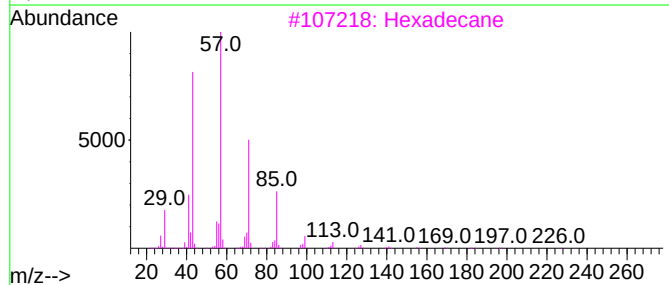
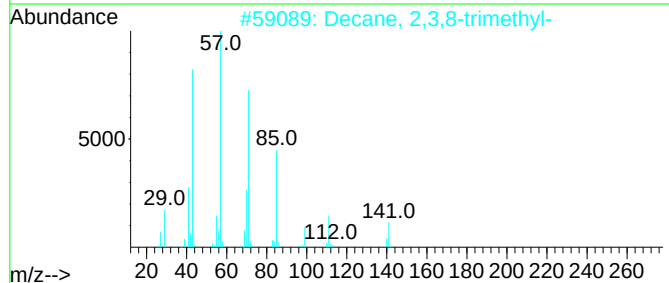
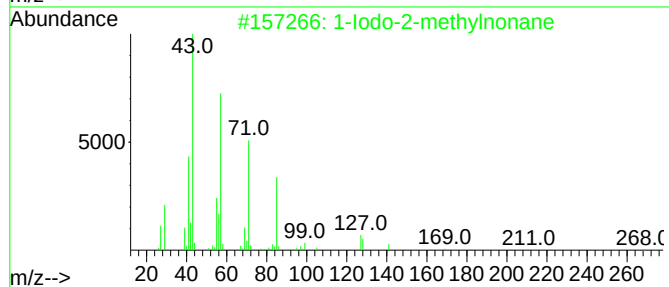
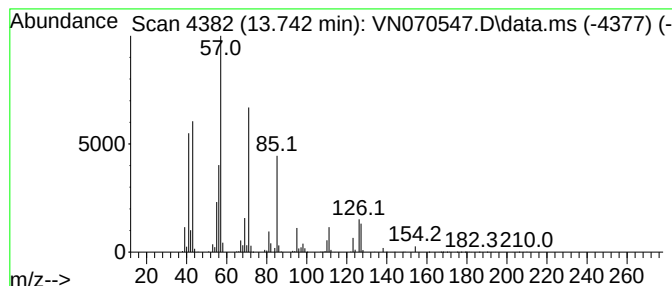
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 9 unknown13.742 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.742	30.63 ug/l	2983720	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	47
2			Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	47
3			Hexadecane	226	C16H34	000544-76-3	47
4			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	43
5			Oxalic acid, 6-ethyloct-3-yl pro...	272	C15H28O4	1000309-34-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

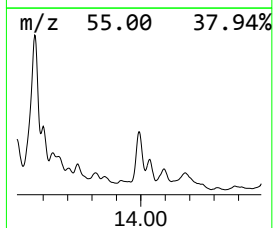
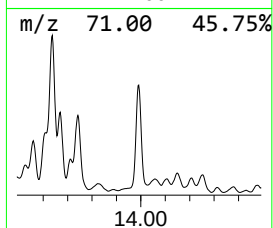
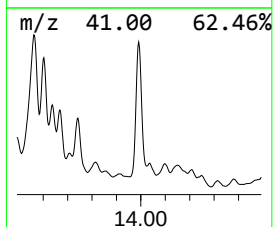
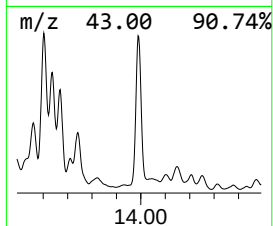
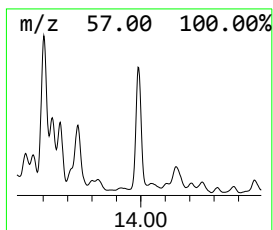
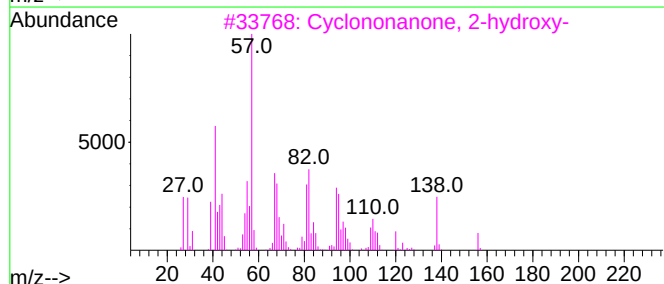
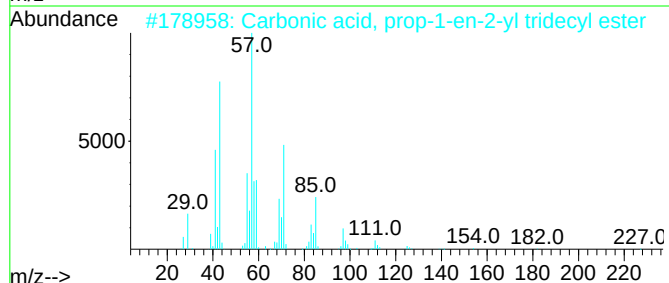
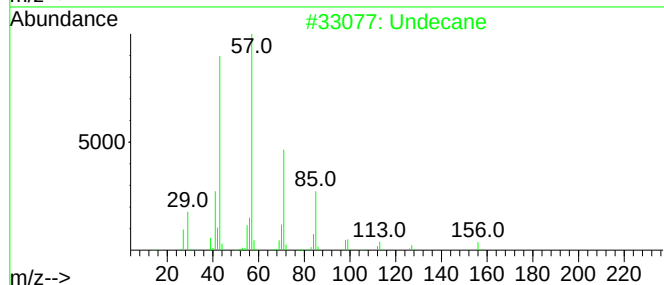
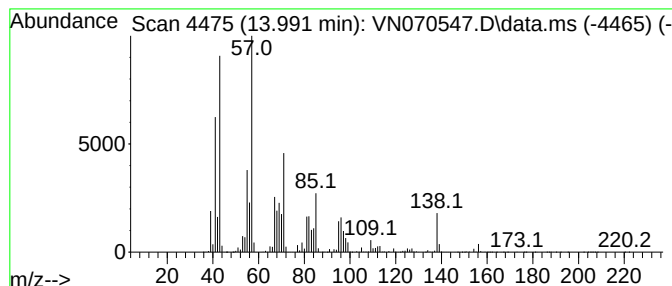
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown13.992 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	97.27 ug/l	9474870	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	46
2			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	45
3			Cyclononane, 2-hydroxy-	156	C9H16O2	000496-83-3	43
4			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	43
5			1-Decanol, 2-ethyl-	186	C12H26O	021078-65-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070547.D
Acq On : 10 Jan 2022 16:54
Operator : JC/MD
Sample : M5257-01ME
Misc : 4.99mL/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.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
Octane, 4-methyl-	11.521	29.8	ug/l	3456520	3	11.744	5805930	50.0
Hexane, 2,4-dim...	12.173	34.8	ug/l	4042940	3	11.744	5805930	50.0
Octane, 2,6-dim...	12.366	104.8	ug/l	12171400	3	11.744	5805930	50.0
unknown12.452	12.452	71.3	ug/l	8274460	3	11.744	5805930	50.0
m-Menthane, (1S...	12.978	74.6	ug/l	7265890	4	13.672	4870550	50.0
Carbonic acid, ...	13.195	57.6	ug/l	5612130	4	13.672	4870550	50.0
Octane, 2,4,6-t...	13.246	68.7	ug/l	6691780	4	13.672	4870550	50.0
Decane, 4-methyl-	13.281	187.3	ug/l	18242600	4	13.672	4870550	50.0
unknown13.742	13.742	30.6	ug/l	2983720	4	13.672	4870550	50.0
unknown13.992	13.992	97.3	ug/l	9474870	4	13.672	4870550	50.0