

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021121\
 Data File : VN065828.D
 Acq On : 11 Feb 2021 21:01
 Operator : JC/MD
 Sample : M1384-01
 Misc : 1.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DRUM-1

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: VN065828.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.975	676	695	722	rVB	130626	336265	4.24%	1.034%
2	7.544	1787	1805	1816	rBV	114537	289328	3.65%	0.890%
3	7.618	1816	1828	1852	rVB	236075	567319	7.16%	1.744%
4	7.984	1925	1942	1969	rBV	136674	330092	4.17%	1.015%
5	8.544	2101	2116	2137	rBV	360217	750762	9.48%	2.308%
6	10.055	2571	2586	2601	rBV	576575	1070007	13.51%	3.290%
7	11.376	2982	2997	3018	rBV	507520	890396	11.24%	2.737%
8	11.601	3053	3067	3083	rBV4	56792	104120	1.31%	0.320%
9	12.306	3260	3286	3291	rBV5	27350	83257	1.05%	0.256%
10	12.373	3291	3307	3317	rVV	359134	623804	7.87%	1.918%
11	12.698	3394	3408	3437	rBV2	135274	250278	3.16%	0.769%
12	12.961	3484	3490	3499	rVB	72192	103375	1.30%	0.318%
13	13.074	3513	3525	3536	rBV	220614	386138	4.87%	1.187%
14	13.170	3542	3555	3564	rBV	158327	280016	3.53%	0.861%
15	13.228	3565	3573	3586	rVV3	108489	239300	3.02%	0.736%
16	13.315	3586	3600	3609	rVV	483348	911145	11.50%	2.801%
17	13.376	3609	3619	3638	rVB3	188181	494042	6.24%	1.519%
18	13.534	3660	3668	3682	rVB3	83079	150516	1.90%	0.463%
19	13.643	3694	3702	3710	rBV	181926	266151	3.36%	0.818%
20	14.029	3810	3822	3832	rVV5	65728	146314	1.85%	0.450%
21	14.129	3843	3853	3858	rBV5	224391	413091	5.21%	1.270%
22	14.199	3869	3875	3887	rVB3	244834	348757	4.40%	1.072%
23	14.267	3888	3896	3902	rBV2	329883	480670	6.07%	1.478%
24	14.495	3959	3967	3977	rBV	807793	1237300	15.62%	3.804%
25	14.563	3980	3988	3994	rBV4	478200	833237	10.52%	2.562%
26	14.611	3994	4003	4015	rVV	2298616	3726352	47.03%	11.456%
27	14.920	4091	4099	4107	rBV3	792228	1645777	20.77%	5.060%
28	15.010	4120	4127	4138	rVB2	2353546	3819803	48.21%	11.744%
29	15.080	4139	4149	4160	rBV2	4709478	7923036	100.00%	24.359%
30	15.296	4210	4216	4229	rVB	1013394	1573566	19.86%	4.838%
31	15.858	4384	4391	4402	rVB5	709934	1380226	17.42%	4.243%
32	15.990	4425	4432	4446	rVB3	514816	872099	11.01%	2.681%

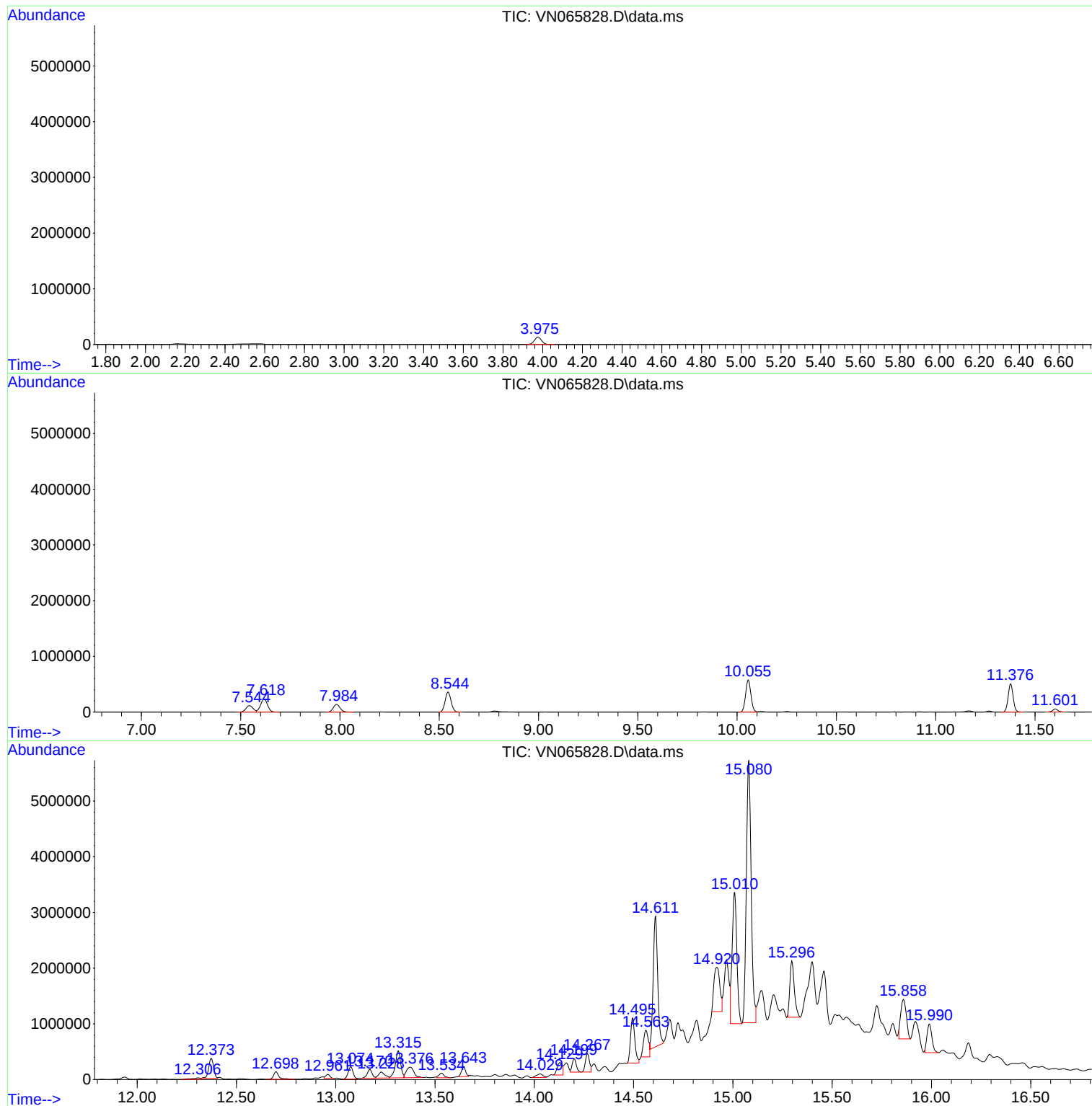
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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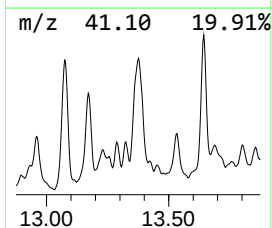
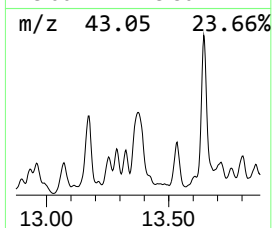
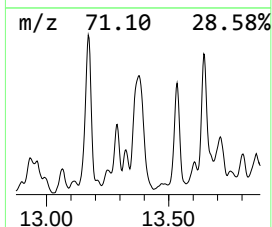
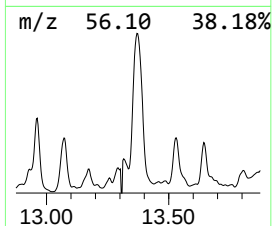
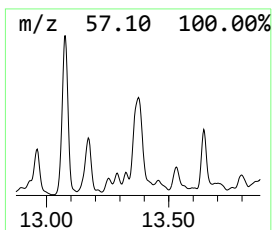
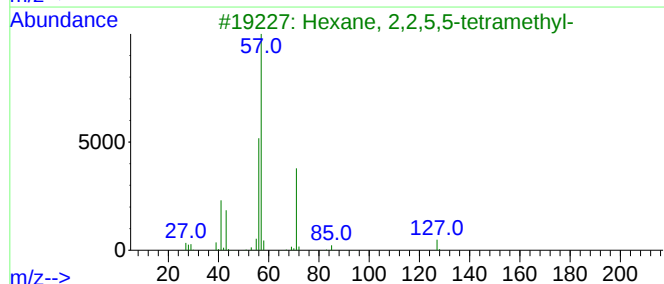
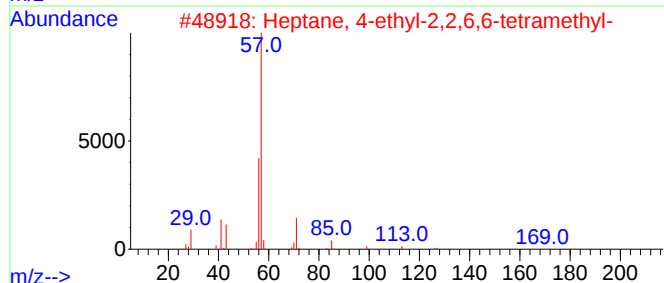
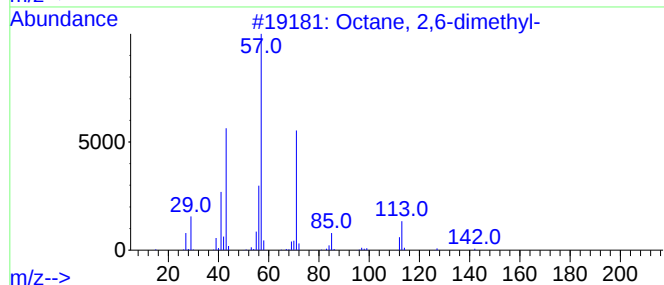
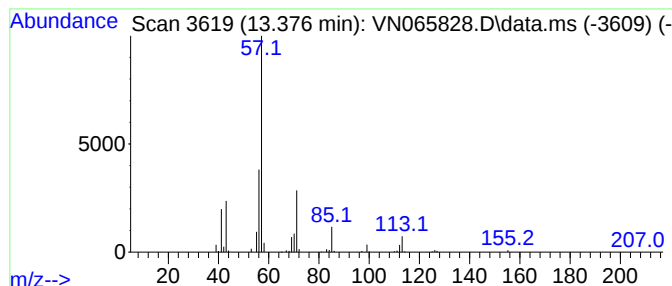
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 1 Octane, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.376	27.11 ug/l	494042	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
2			Heptane, 4-ethyl-2,2,6,6-tetrame...	184	C13H28	062108-31-0	72
3			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	59
4			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	53
5			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	53



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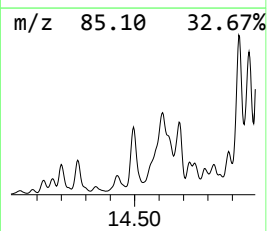
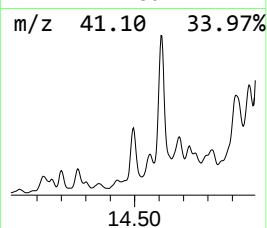
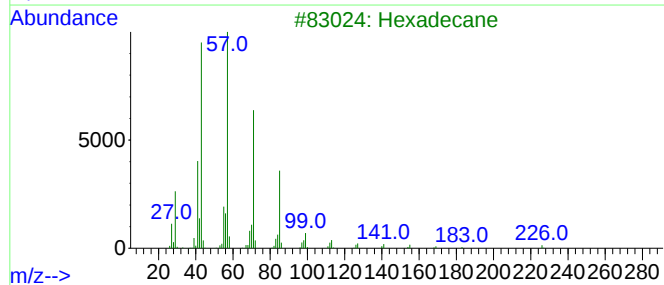
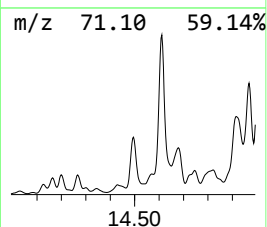
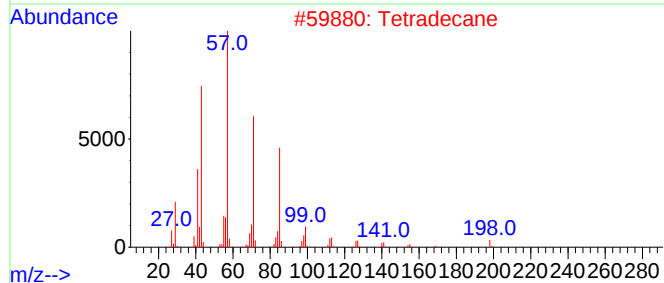
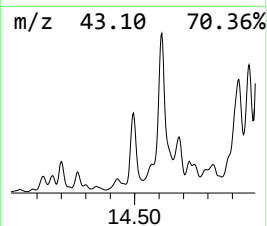
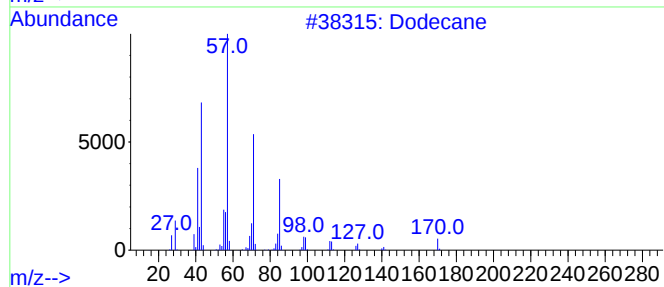
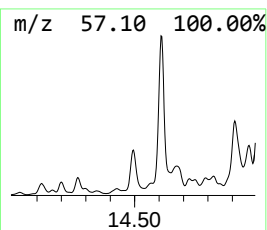
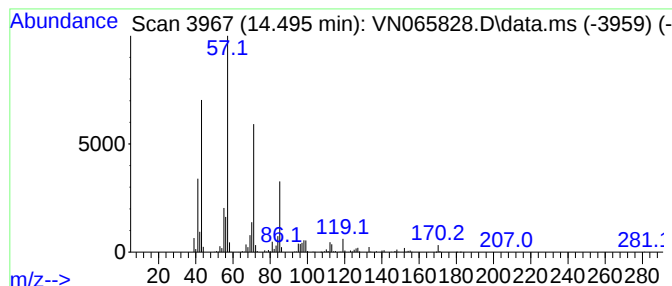
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.495	67.90 ug/l	1237300	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	93
2			Tetradecane	198	C14H30	000629-59-4	80
3			Hexadecane	226	C16H34	000544-76-3	80
4			Tridecane	184	C13H28	000629-50-5	72
5			Nonadecane	268	C19H40	000629-92-5	72



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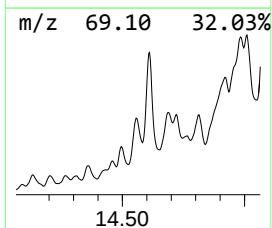
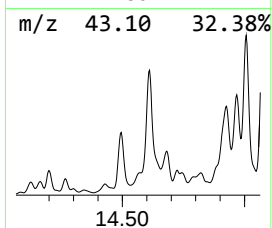
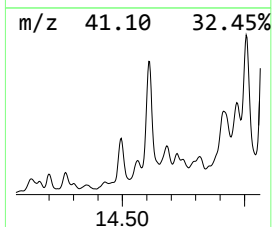
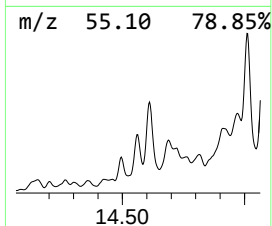
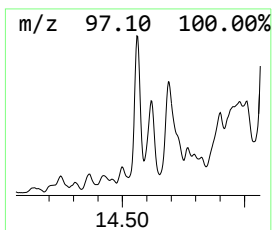
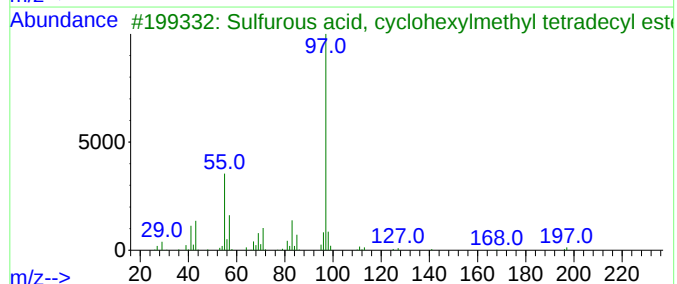
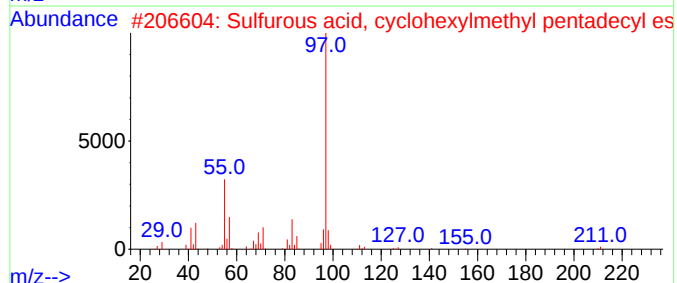
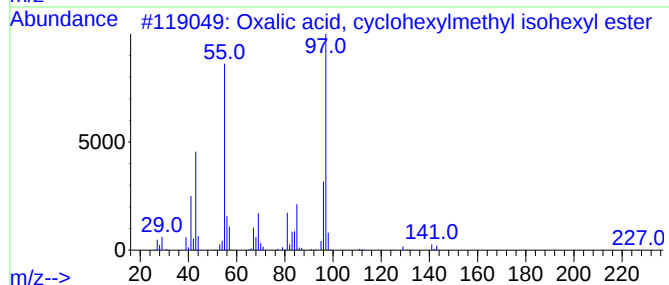
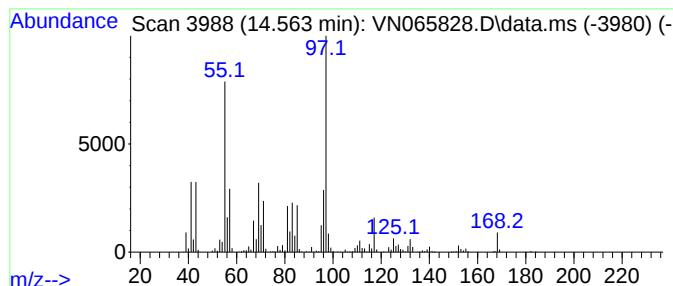
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Oxalic acid, cyclohexylmeth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.563	45.72 ug/l	833237	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclohexylmethyl is...	270	C15H26O4	1000309-68-3	58
2			Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	53
3			Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	53
4			Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	49
5			Cyclohexane, 1-methyl-3-pentyl-	168	C12H24	054411-02-8	49



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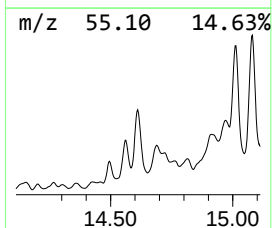
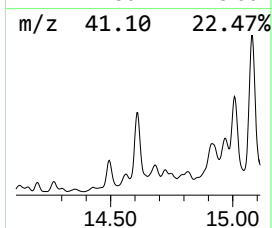
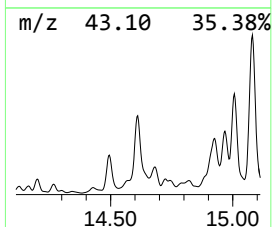
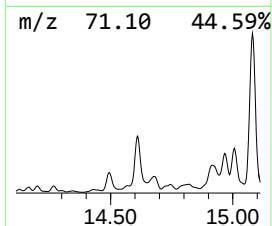
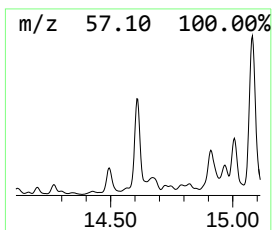
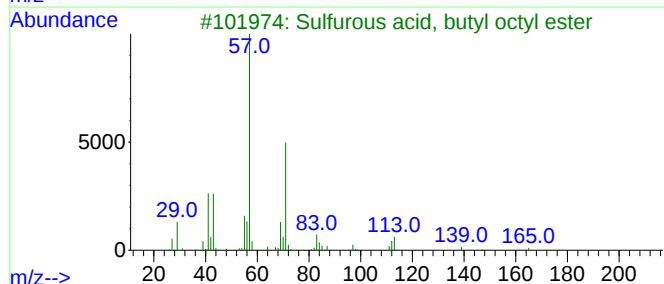
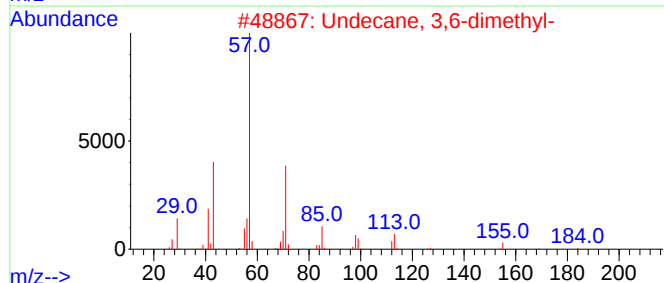
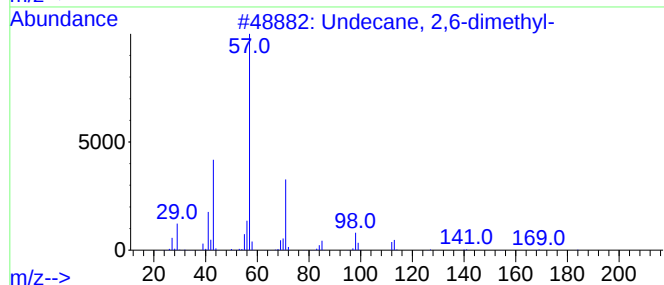
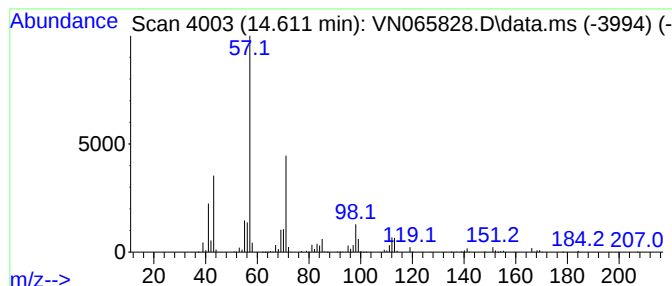
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Peak Number 4 Undecane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.611	204.49 ug/l	3726350	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	91
2			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	90
3			Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	80
4			Dodecane, 6-methyl-	184	C13H28	006044-71-9	76
5			Heptane, 3-(bromomethyl)-	192	C8H17Br	018908-66-2	64



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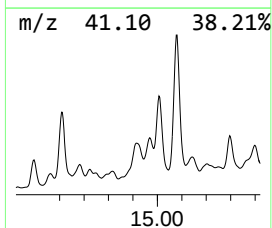
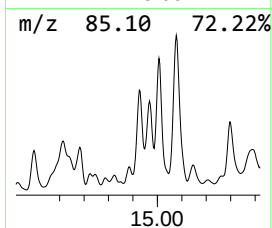
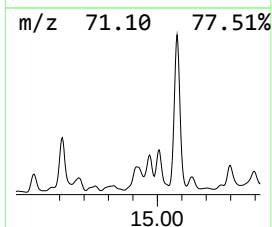
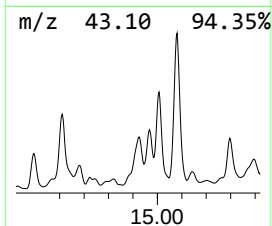
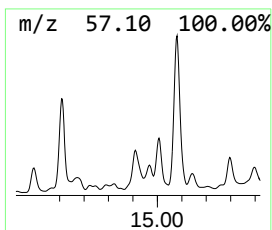
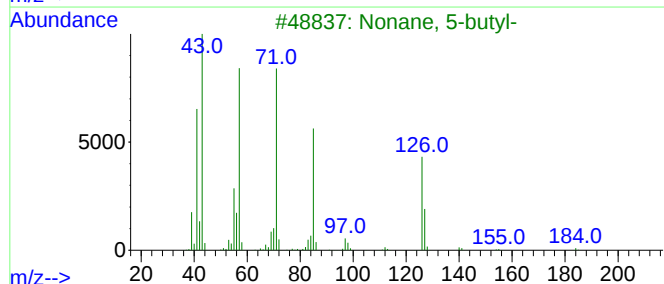
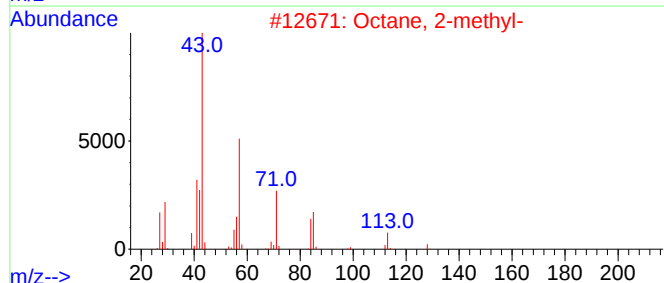
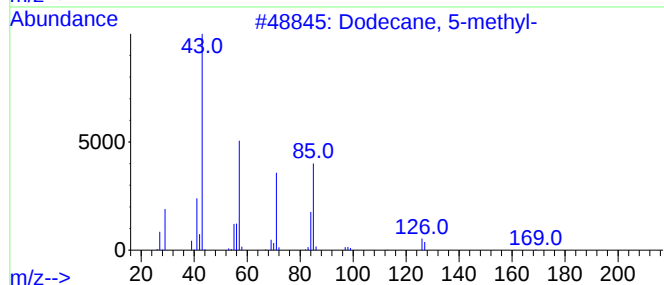
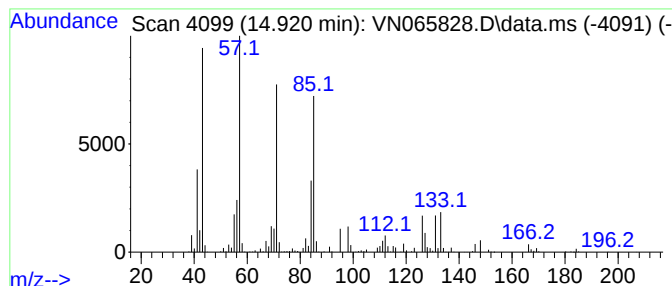
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane, 5-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.920	90.31 ug/l	1645780	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 5-methyl-	184	C13H28	017453-93-9	64
2			Octane, 2-methyl-	128	C9H20	003221-61-2	58
3			Nonane, 5-butyl-	184	C13H28	017312-63-9	58
4			Octane, 4-methyl-	128	C9H20	002216-34-4	52
5			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	52



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ClientSampleId :
DRUM-1

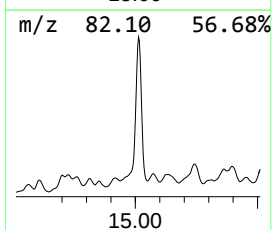
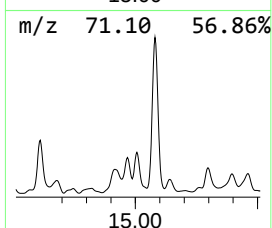
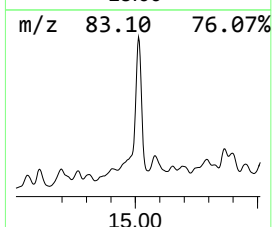
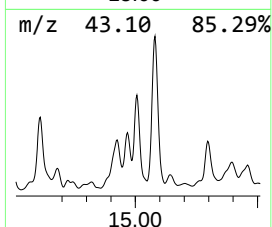
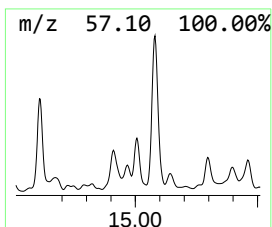
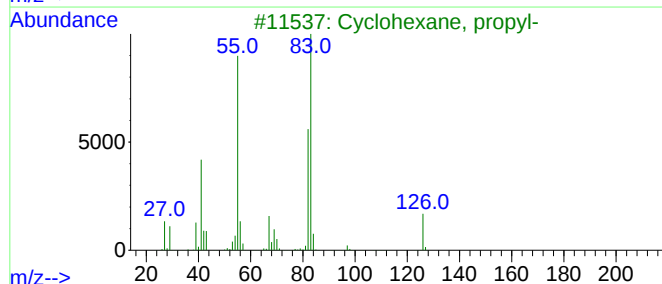
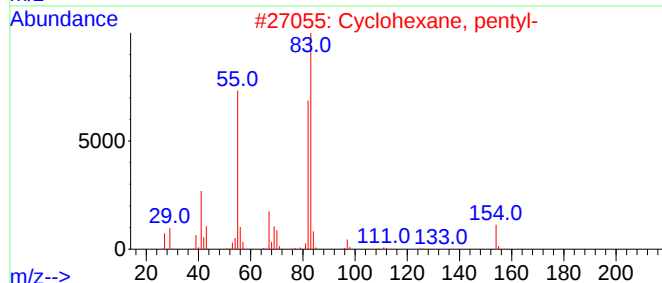
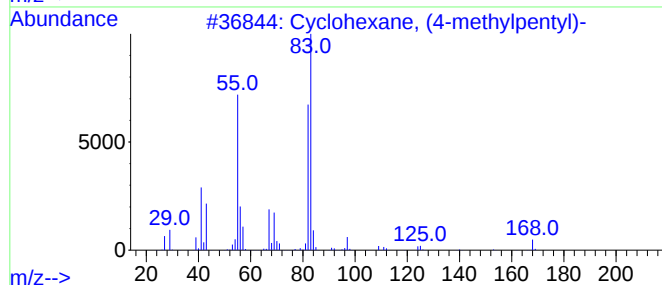
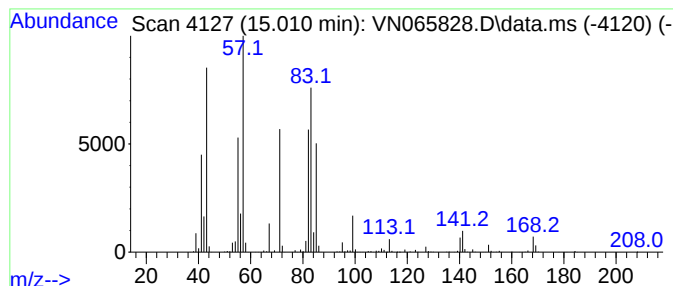
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Quant Title : SW846 8260

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

Peak Number 6 unknown15.010 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.010	209.62 ug/l	3819800	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	43
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	38
3			Cyclohexane, propyl-	126	C9H18	001678-92-8	38
4			Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	38
5			Cyclohexane, butyl-	140	C10H20	001678-93-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021121\
Data File : VN065828.D
Acq On : 11 Feb 2021 21:01
Operator : JC/MD
Sample : M1384-01
Misc : 1.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-1

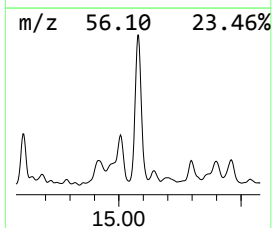
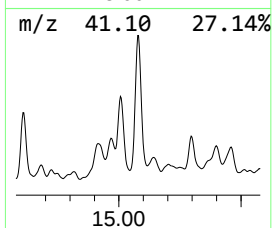
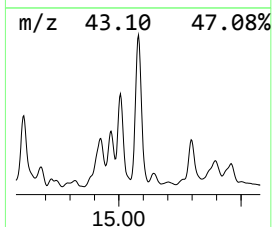
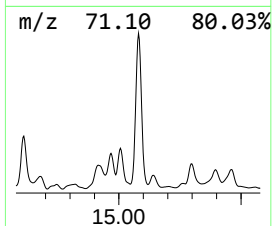
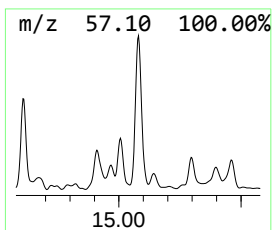
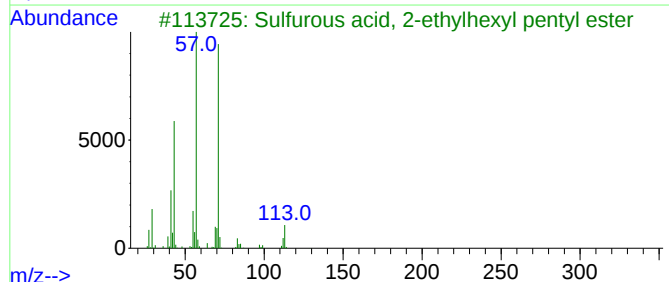
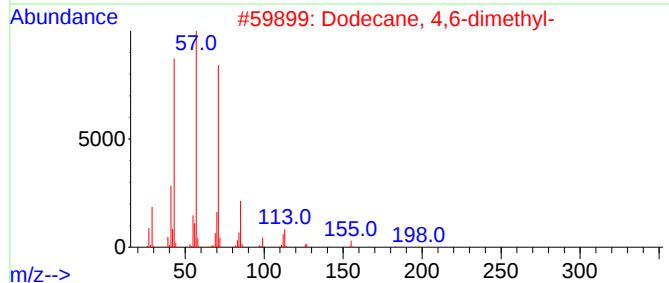
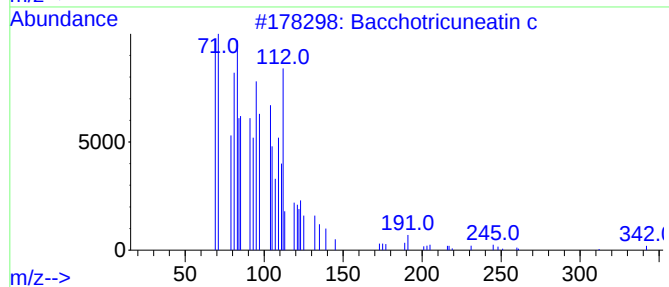
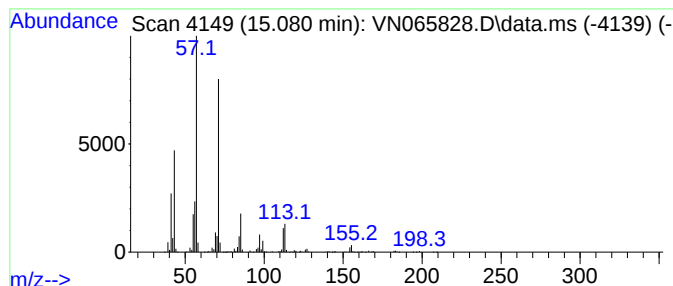
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Quant Title : SW846 8260

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

Peak Number 7 Bacchotricuneatin c Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	434.79 ug/l	7923040	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bacchotricuneatin c	342	C20H22O5	066563-30-2	80
2			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	72
3			Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	59
4			Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	59
5			Oxalic acid, butyl 2-ethylhexyl ...	258	C14H26O4	1000309-38-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021121\
Data File : VN065828.D
Acq On : 11 Feb 2021 21:01
Operator : JC/MD
Sample : M1384-01
Misc : 1.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-1

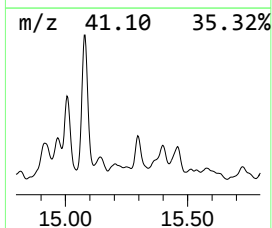
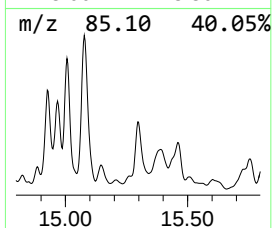
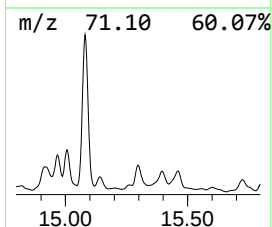
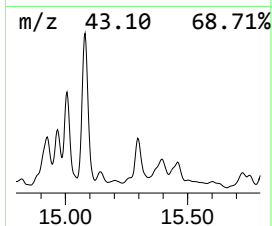
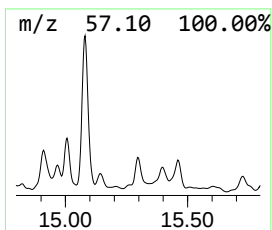
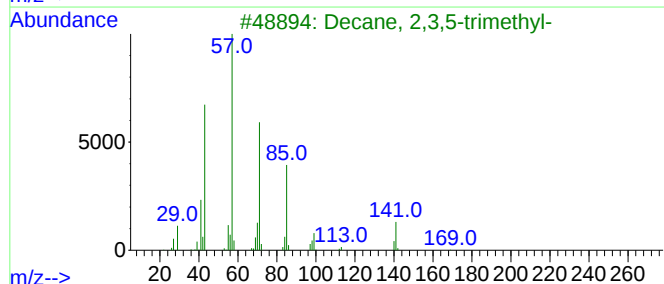
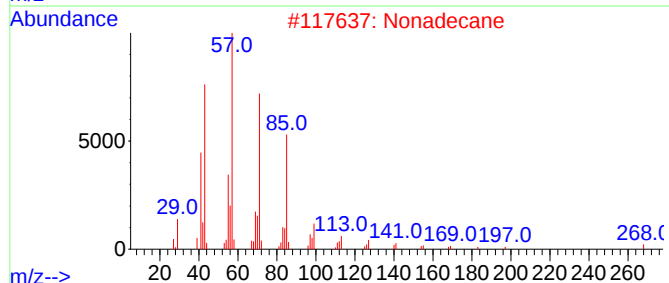
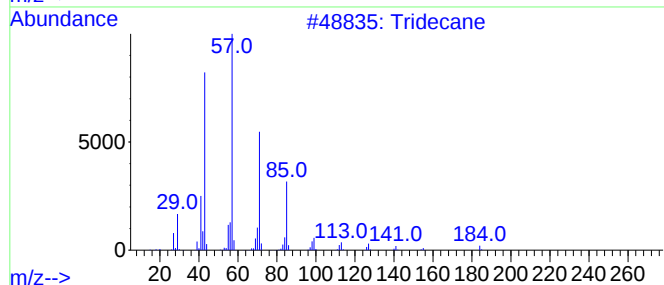
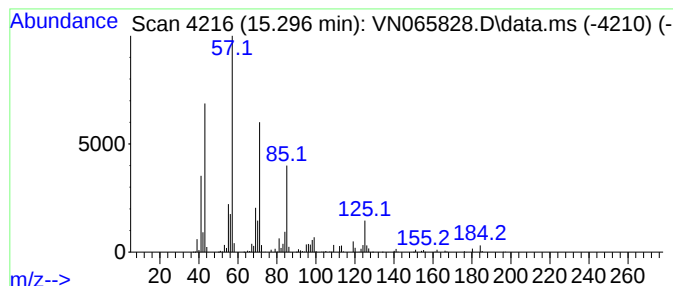
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.296	86.35 ug/l	1573570	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	83
2			Nonadecane	268	C19H40	000629-92-5	80
3			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72
4			Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	72
5			4-Methyl-5-nonanone	156	C10H20O	035900-26-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021121\
Data File : VN065828.D
Acq On : 11 Feb 2021 21:01
Operator : JC/MD
Sample : M1384-01
Misc : 1.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-1

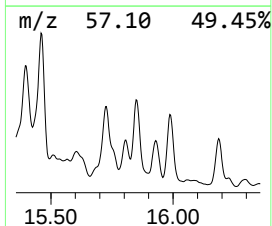
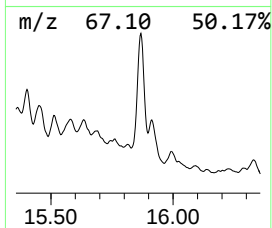
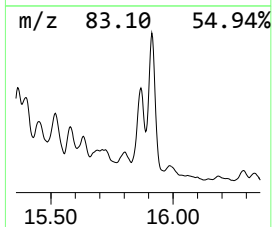
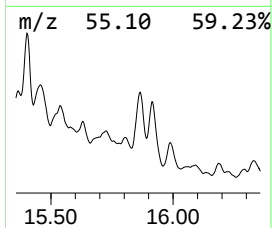
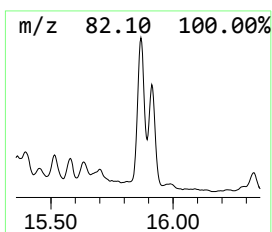
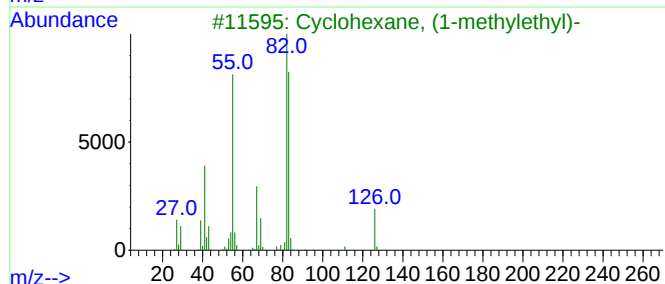
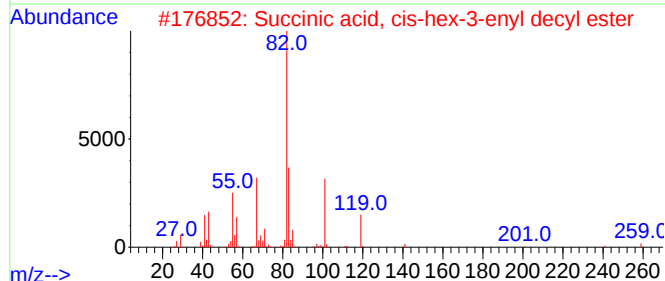
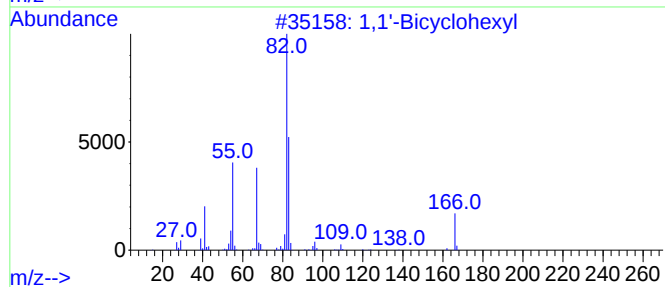
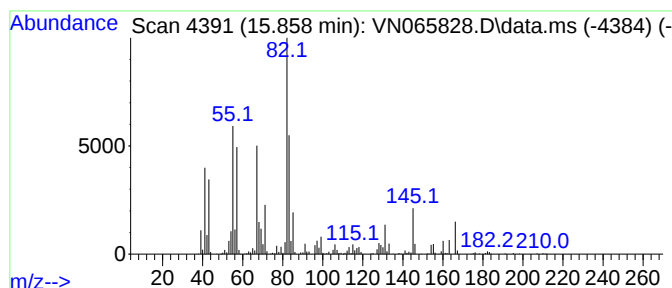
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 9 1,1'-Bicyclohexyl Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.858	75.74 ug/l	1380230	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1'-Bicyclohexyl	166	C12H22	000092-51-3	52
2			Succinic acid, cis-hex-3-enyl de...	340	C20H36O4	1000353-41-2	47
3			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	43
4			Fumaric acid, trans-hex-3-enyl t...	380	C23H40O4	1000348-89-3	38
5			Fumaric acid, trans-hex-3-enyl u...	352	C21H36O4	1000348-89-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021121\
Data File : VN065828.D
Acq On : 11 Feb 2021 21:01
Operator : JC/MD
Sample : M1384-01
Misc : 1.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-1

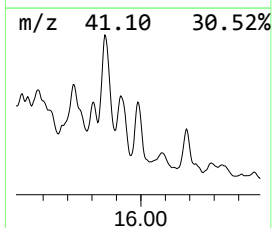
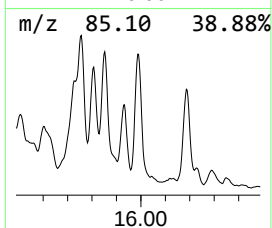
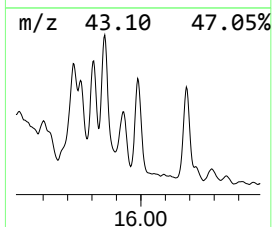
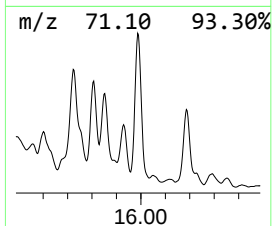
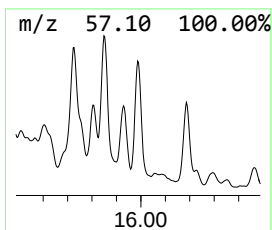
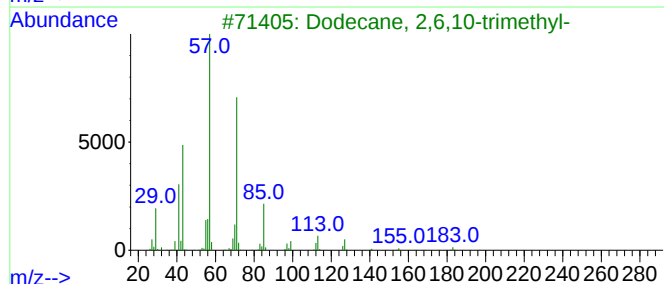
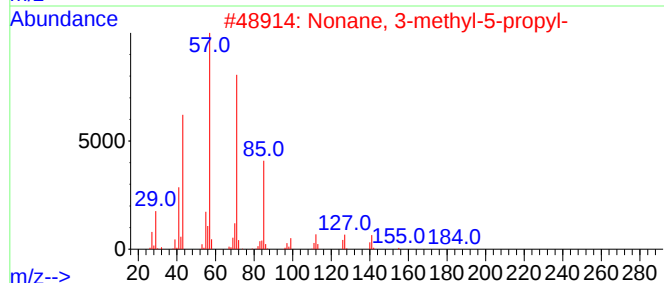
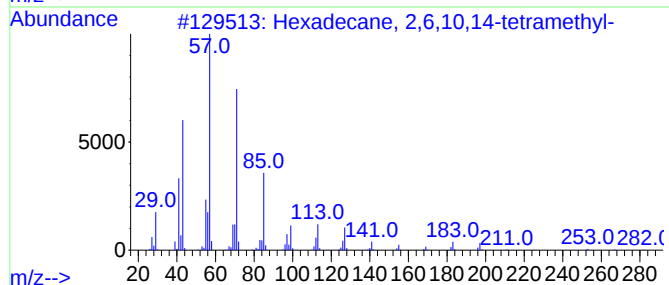
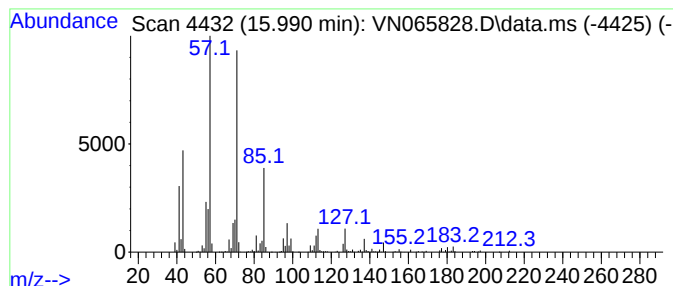
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 10 Hexadecane, 2,6,10,14-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.990	47.86 ug/l	872099	1,4-Dichlorobenzene-d4	13.315

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2		Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	72
3		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	72
4		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	72
5		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021121\
Data File : VN065828.D
Acq On : 11 Feb 2021 21:01
Operator : JC/MD
Sample : M1384-01
Misc : 1.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-1

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
Octane, 2,6-dim...	13.376	27.1	ug/l	494042	4	13.315	911145	50.0
Dodecane	14.495	67.9	ug/l	1237300	4	13.315	911145	50.0
Oxalic acid, cy...	14.563	45.7	ug/l	833237	4	13.315	911145	50.0
Undecane, 2,6-d...	14.611	204.5	ug/l	3726350	4	13.315	911145	50.0
Dodecane, 5-met...	14.920	90.3	ug/l	1645780	4	13.315	911145	50.0
unknown15.010	15.010	209.6	ug/l	3819800	4	13.315	911145	50.0
Bacchotricuneat...	15.080	434.8	ug/l	7923040	4	13.315	911145	50.0
Tridecane	15.296	86.3	ug/l	1573570	4	13.315	911145	50.0
1,1'-Bicyclohexyl	15.858	75.7	ug/l	1380230	4	13.315	911145	50.0
Hexadecane, 2,6...	15.990	47.9	ug/l	872099	4	13.315	911145	50.0