LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-03-3.5-4.0

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\82N051421W.M
Title : SW846 8260

Signal : TIC: VN067147.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.652	1062	1086	1088	rBV4	17066	31344	1.26%	0.181%
2	7.514	2130	2153	2166	rBV2	313425	815925	32.90%	4.714%
3	7.589	2167	2181	2206	rVB	581227	1418155	57.18%	8.194%
4	7.798	2245	2259	2276	rBV2	12729	29350	1.18%	0.170%
5	7.956	2296	2318	2346	rBV2	302260	742285	29.93%	4.289%
6	8.139	2377	2386	2408	rVB4	11236	29712	1.20%	0.172%
7	8.519	2506	2528	2562	rBV	751682	1652446	66.63%	9.547%
8	9.016	2688	2713	2727	rBV5	41606	109506	4.42%	0.633%
9	9.305	2800	2821	2835	rVB5	11543	27912	1.13%	0.161%
10	9.455	2857	2877	2894	rBV5	24633	54348	2.19%	0.314%
11	9.600	2914	2931	2945	rBV6	18477	40065	1.62%	0.231%
12	9.812	2987	3010	3018	rBV5	23180	58198	2.35%	0.336%
13	10.035	3076	3093	3132	rBV	1281459	2479959	100.00%	14.328%
14	10.378	3212	3221	3232	rVB3	20808	35028	1.41%	0.202%
15	10.472	3241	3256	3270	rBV3	19952	50056	2.02%	0.289%
16	10.574	3284	3294	3307	rVB4	20584	33794	1.36%	0.195%
17	10.665	3317	3328	3341	rBV2	40152	66373	2.68%	0.383%
18	10.770	3354	3367	3383	rBV2	34096	69306	2.79%	0.400%
19	10.898	3410	3415	3423	rVB2	21514	26210	1.06%	0.151%
20	10.952	3423	3435	3448	rBV4	63122	112146	4.52%	0.648%
21	11.073	3467	3480	3489	rBV5	32632	59000	2.38%	0.341%
22	11.153	3489	3510	3531	rVB6	72186	212237	8.56%	1.226%
23	11.250	3534	3546	3569	rBV2	51327	109320	4.41%	0.632%
24	11.357	3571	3586	3608	rBV	855973	1667679	67.25%	9.635%
25	11.547	3647	3657	3667	rBV8	22062	40921	1.65%	0.236%
26	11.609	3671	3680	3689	rBV5	40015	70612	2.85%	0.408%
27	11.808	3746	3754	3763	rBV5	27194	40958	1.65%	0.237%
28	11.880	3765	3781	3795	rVV6	68644	175783	7.09%	1.016%
29	12.001	3817	3826	3838	rVB	109602	165068	6.66%	0.954%
30	12.073	3842	3853	3858	rBV5	69983	118392	4.77%	0.684%
31	12.360	3949	3960	3973	rBV	547127	977200	39.40%	5.646%
32	12.682	4066	4080	4093	rBV9	123349	326370	13.16%	1.886%
33	12.918	4160	4168	4183	rVB2	355967	583243	23.52%	3.370%
34	13.047	4210	4216	4227	rVB3	94399	143687	5.79%	0.830%
35	13.100	4229	4236	4252	rVB8	98990	204989	8.27%	1.184%
36	13.304	4302	4312	4332	rVB	686021	1275455	51.43%	7.369%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-03-3.5-4.0

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\82N051421W.M
Title : SW846 8260

37	13.615	4420	4428	4440	rBV	221036	370994	14.96%	2.143%
38	14.119	4605	4616	4634	rBV8	516786	1441013	58.11%	8.326%
39	14.597	4786	4794	4809	rVB2	655534	1061656	42.81%	6.134%
40	15.066	4963	4969	4978	rVB3	318243	381258	15.37%	2.203%

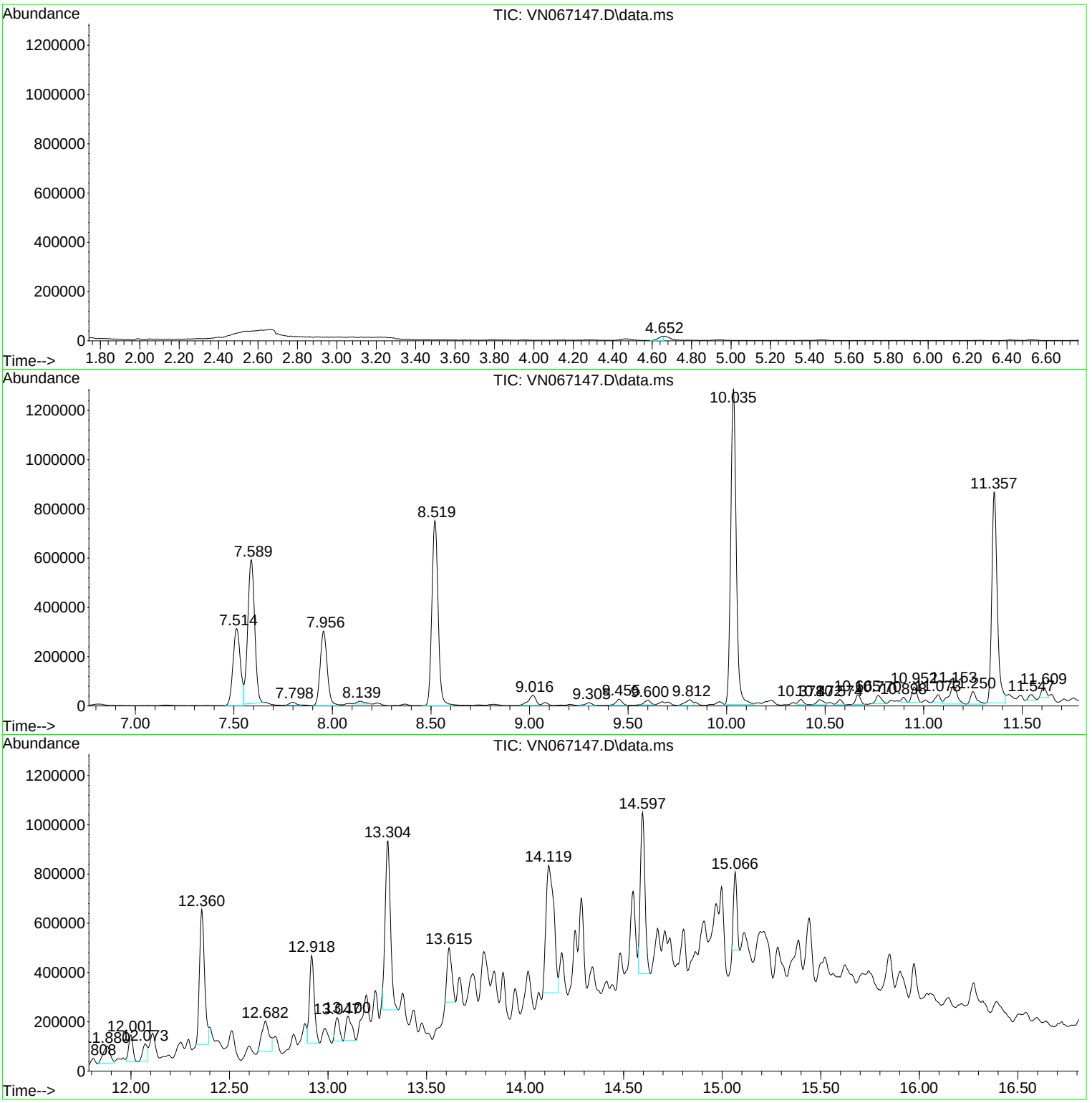
Sum of corrected areas: 17307953

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-03-3.5-4.0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-03-3.5-4.0

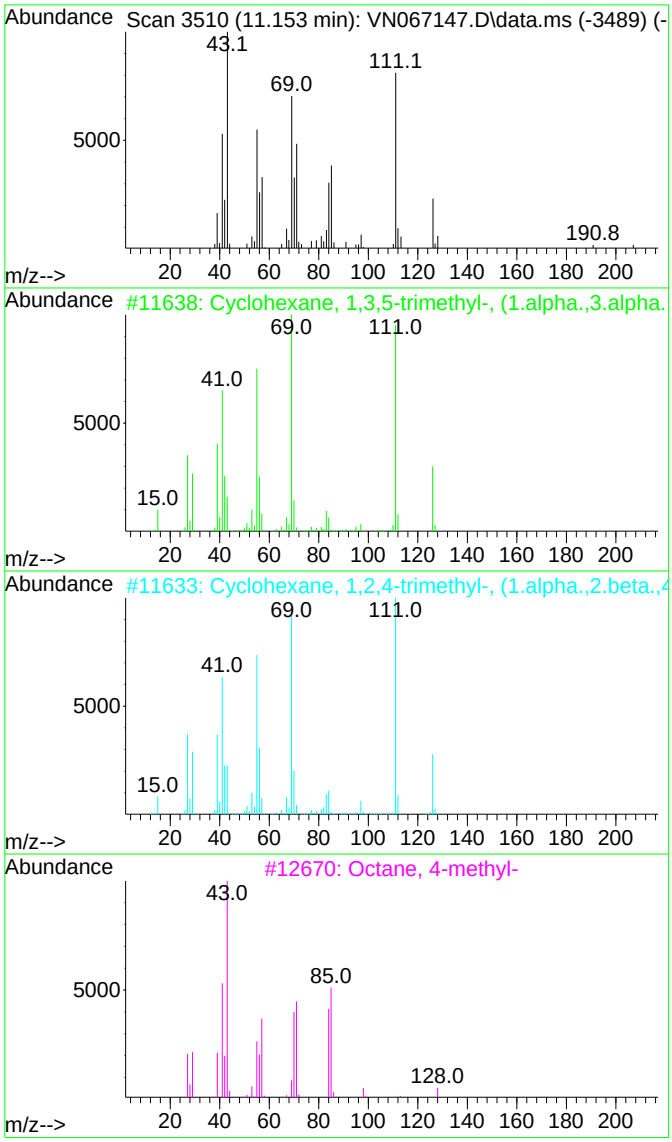
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

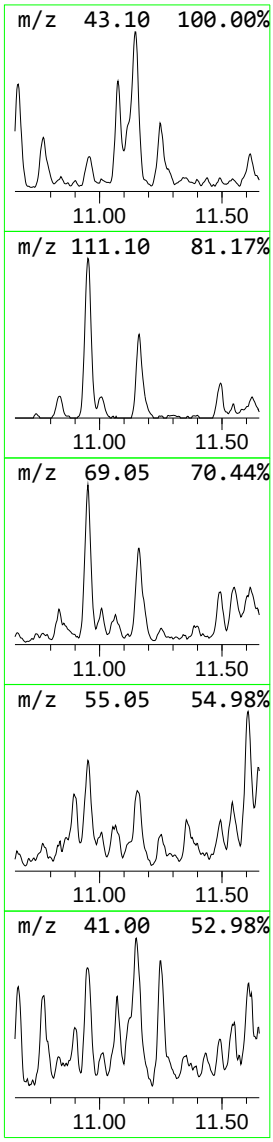
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclohexane, 1,3,5-trimethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.153	6.36 ug/l	212237	Chlorobenzene-d5	11.360

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	60
2	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	55
3	Octane, 4-methyl-	128	C9H20	002216-34-4	45
4	2-Propanamine, N,N'-methanetetra...	126	C7H14N2	000693-13-0	43
5	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-03-3.5-4.0

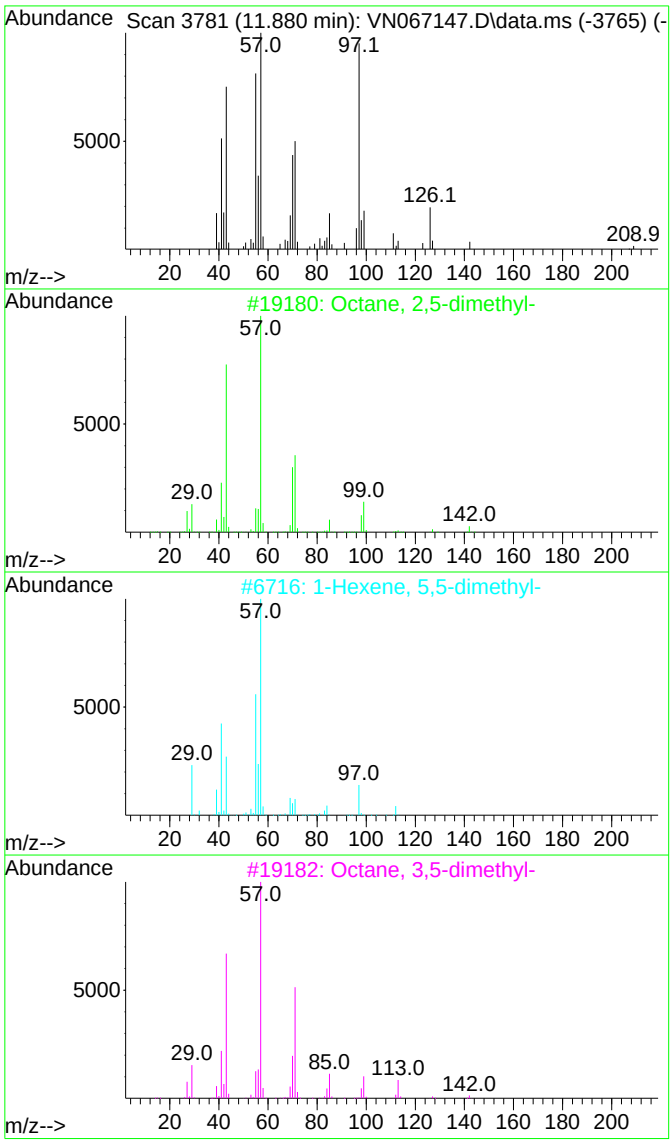
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

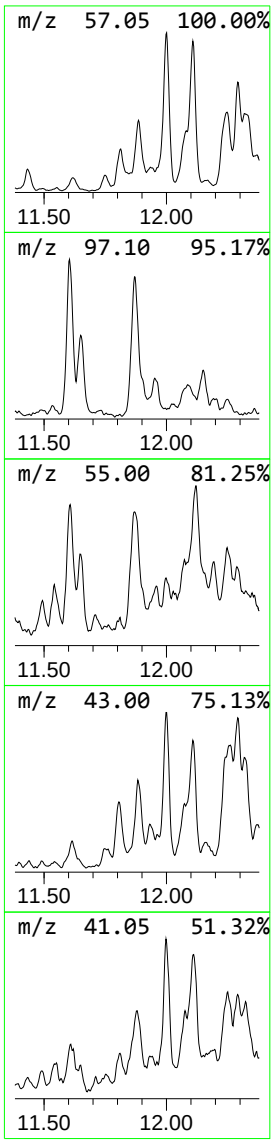
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown11.880 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	5.27 ug/l	175783	Chlorobenzene-d5	11.360

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	43
2	1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	38
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	38
4	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	38
5	4-Octen-3-one	126	C8H14O	014129-48-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-03-3.5-4.0

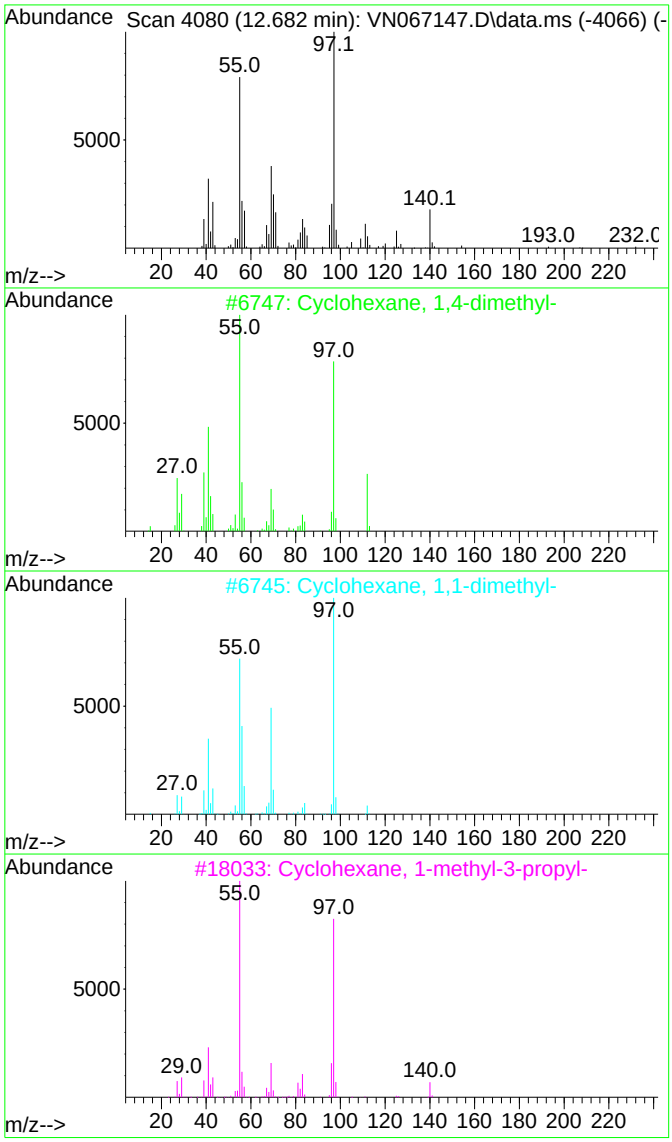
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

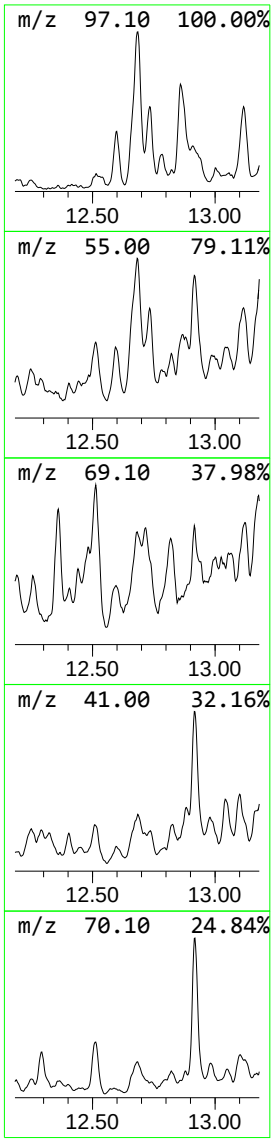
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, 1,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.682	12.79 ug/l	326370	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	59
2	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	49
3	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	49
4	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	47
5	2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	100463-01-2	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-03-3.5-4.0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

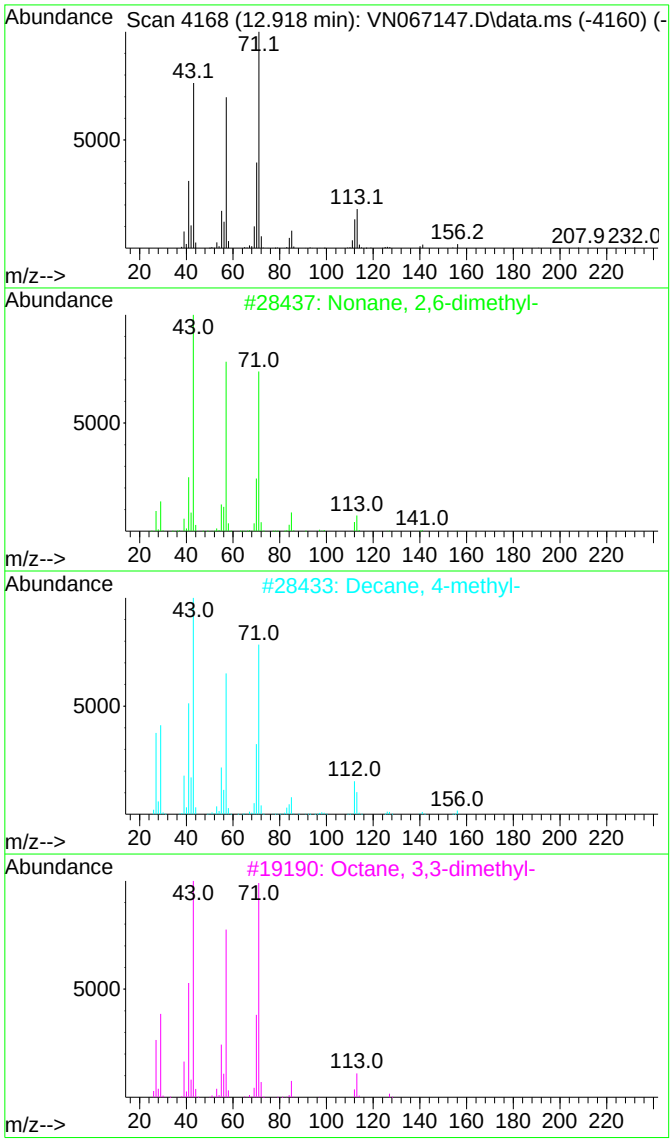
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

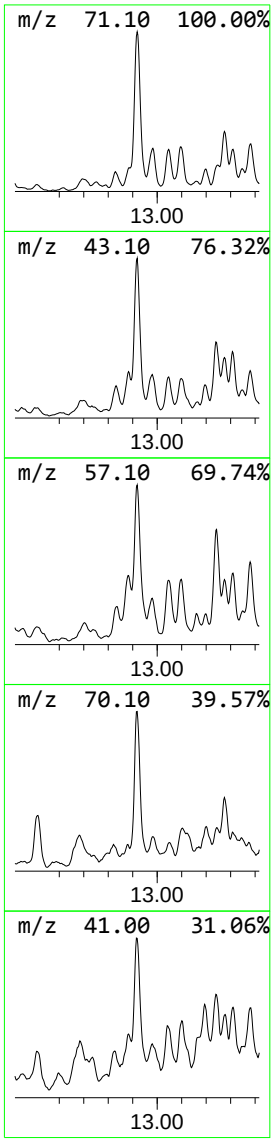
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.918	22.86 ug/l	583243	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	90
2	Decane, 4-methyl-	156	C11H24	002847-72-5	87
3	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	72
4	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	72
5	4-Methyl-3-heptanol, heptafluoro...	326	C12H17F7O2	1000365-51-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-03-3.5-4.0

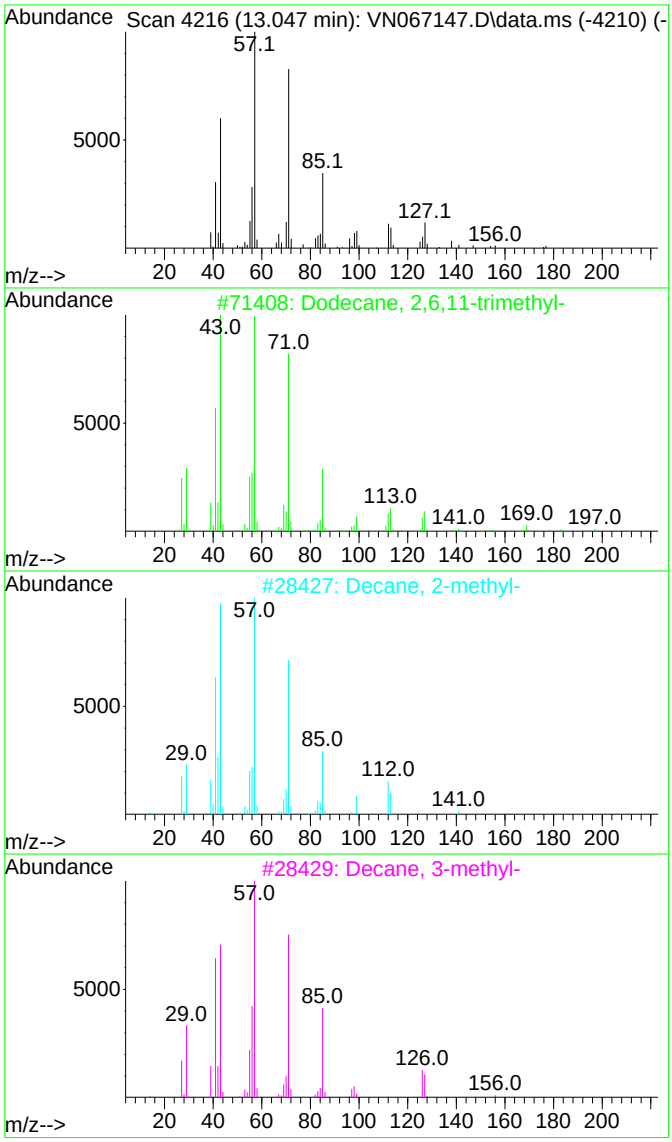
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

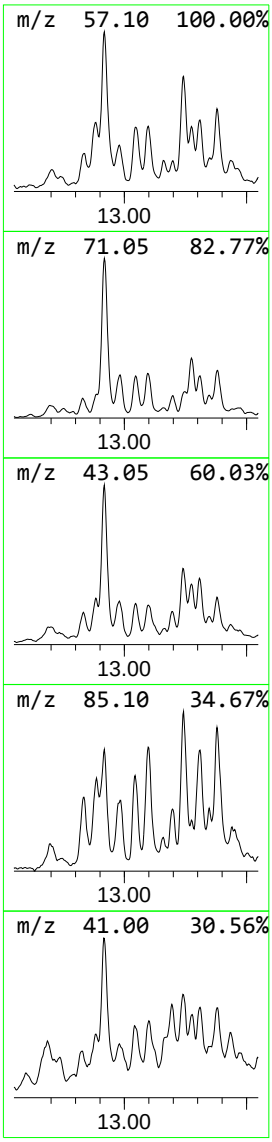
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Dodecane, 2,6,11-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.047	5.63 ug/l	143687	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	83
2	Decane, 2-methyl-	156	C11H24	006975-98-0	80
3	Decane, 3-methyl-	156	C11H24	013151-34-3	70
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
5	Decane, 4-methyl-	156	C11H24	002847-72-5	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-03-3.5-4.0

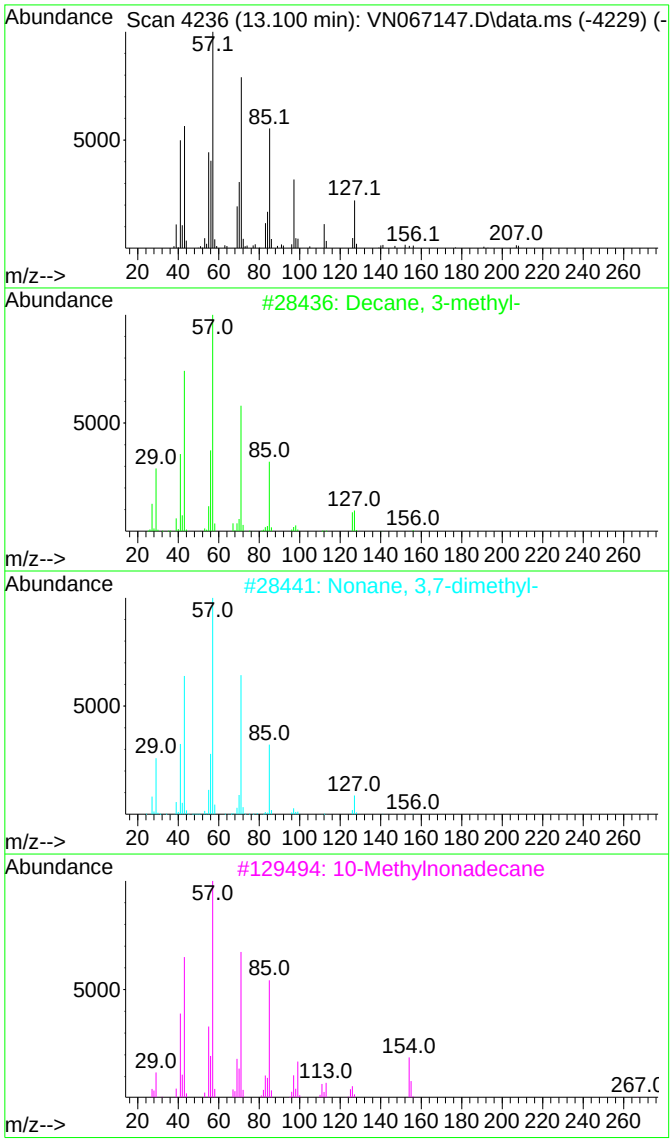
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

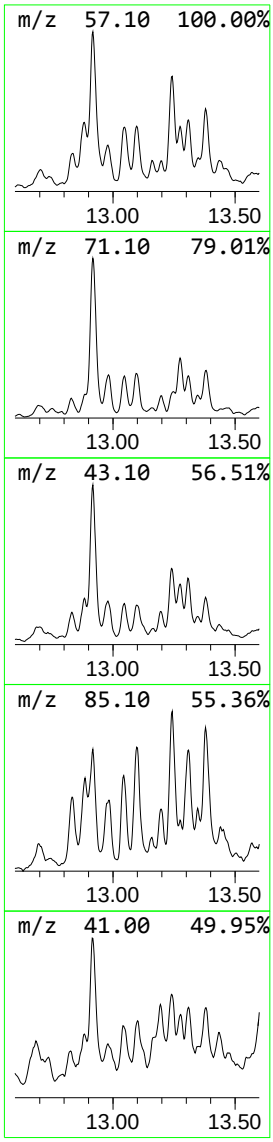
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Decane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	8.04 ug/l	204989	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3-methyl-	156	C11H24	013151-34-3	74
2	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	64
3	10-Methylnonadecane	282	C20H42	056862-62-5	53
4	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	47
5	Decane, 4-methyl-	156	C11H24	002847-72-5	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-03-3.5-4.0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

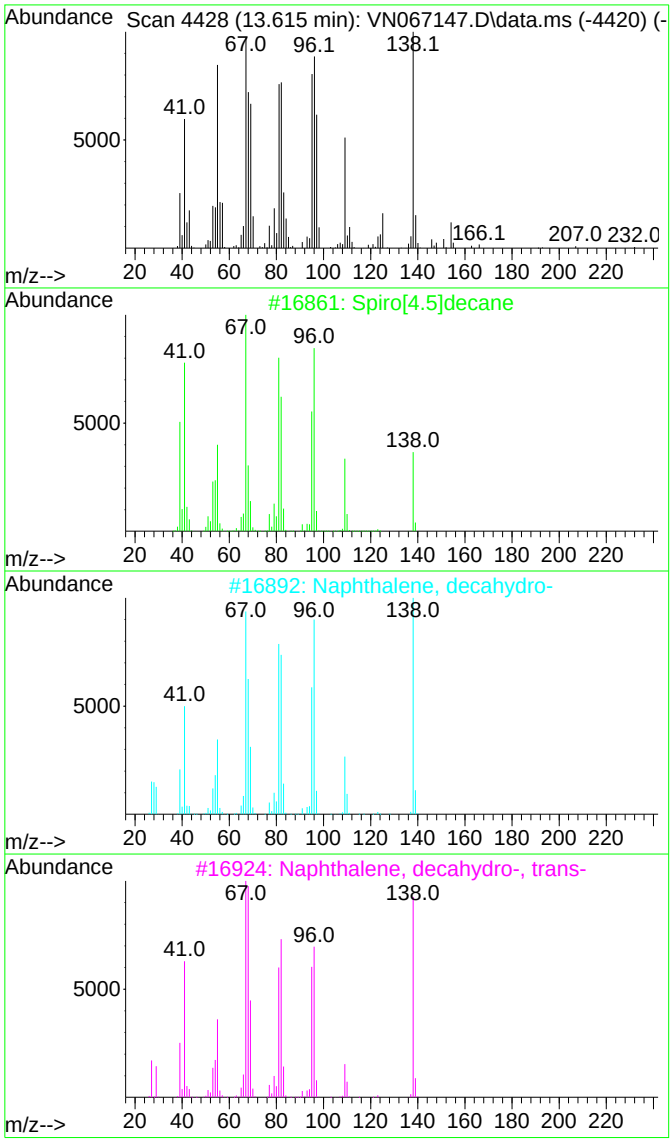
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

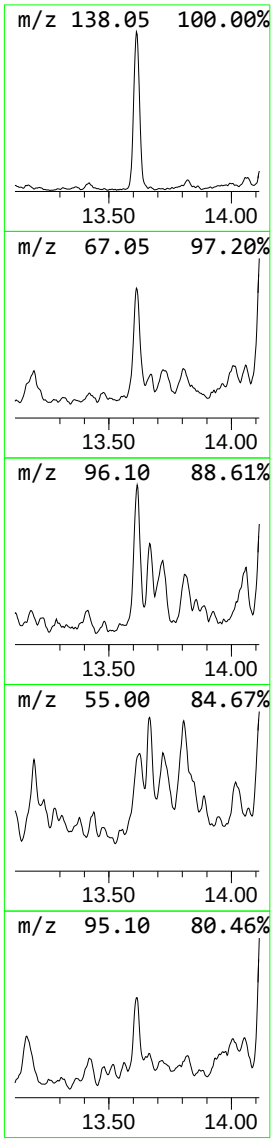
****

Peak Number 7 Spiro[4.5]decane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.615	14.54 ug/l	370994	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[4.5]decane	138	C10H18	000176-63-6	93
2	Naphthalene, decahydro-	138	C10H18	000091-17-8	93
3	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	90
4	2,6-Dimethylbicyclo[3.2.1]octane	138	C10H18	1000215-28-2	62
5	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	55





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-03-3.5-4.0

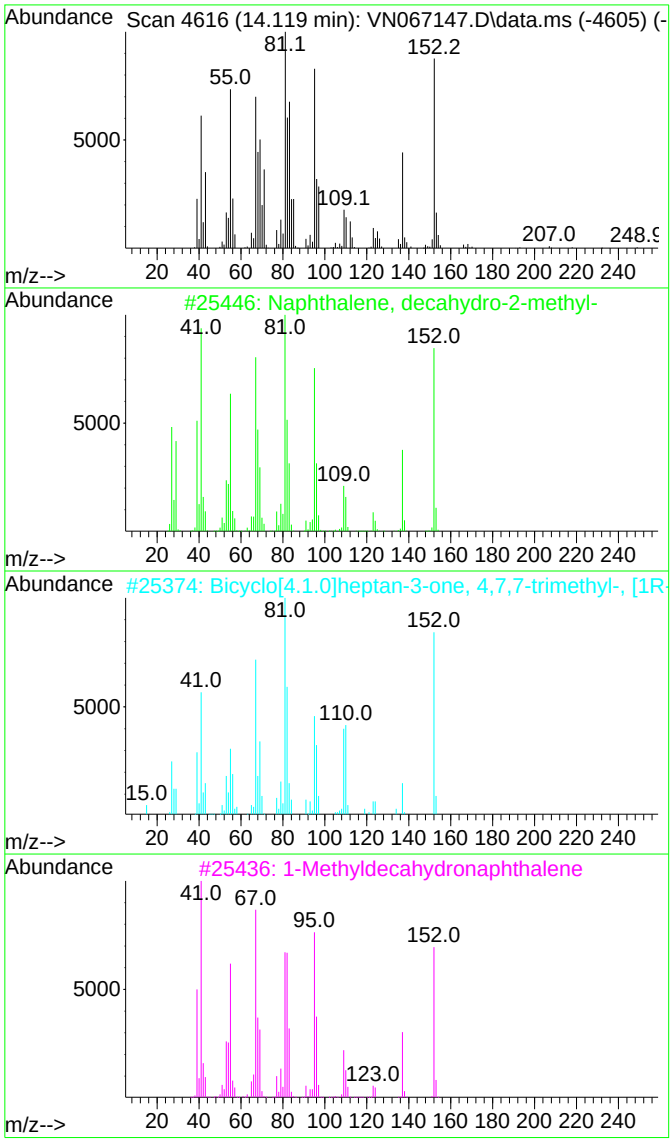
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

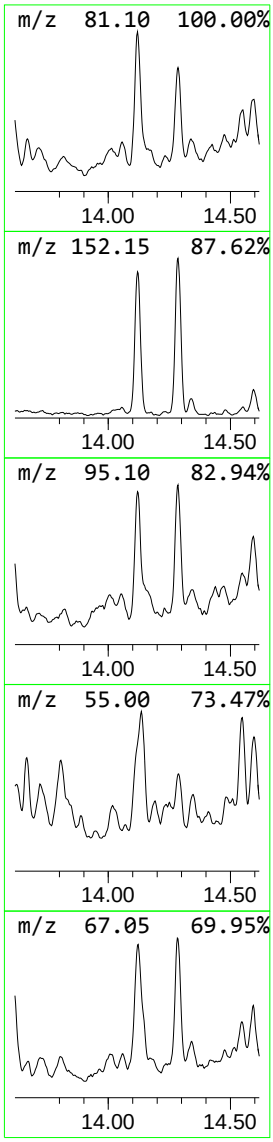
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, decahydro-2-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.119	56.49 ug/l	1441010	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	89
2	Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-04-9	60
3	1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	53
4	Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	52
5	Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-03-3.5-4.0

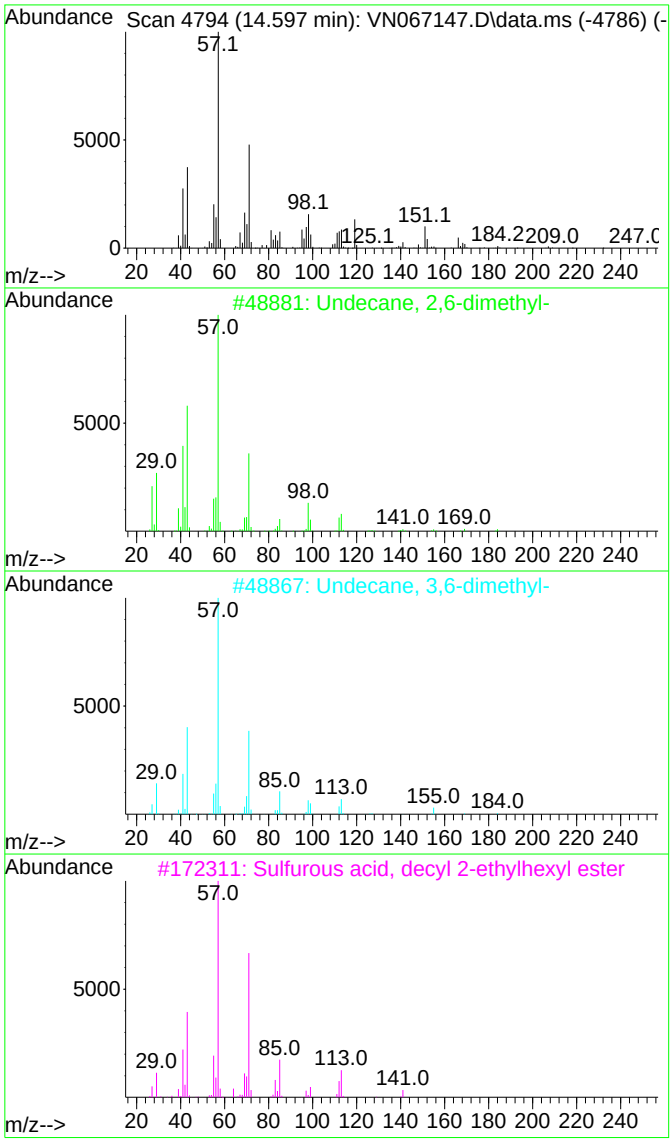
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

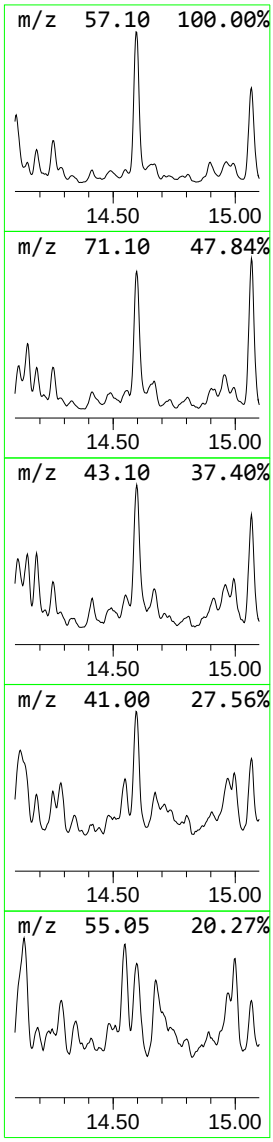
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Undecane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.597	41.62 ug/l	1061660	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	83
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
3	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	49
4	Tridecane, 6-methyl-	198	C14H30	013287-21-3	47
5	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-03-3.5-4.0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

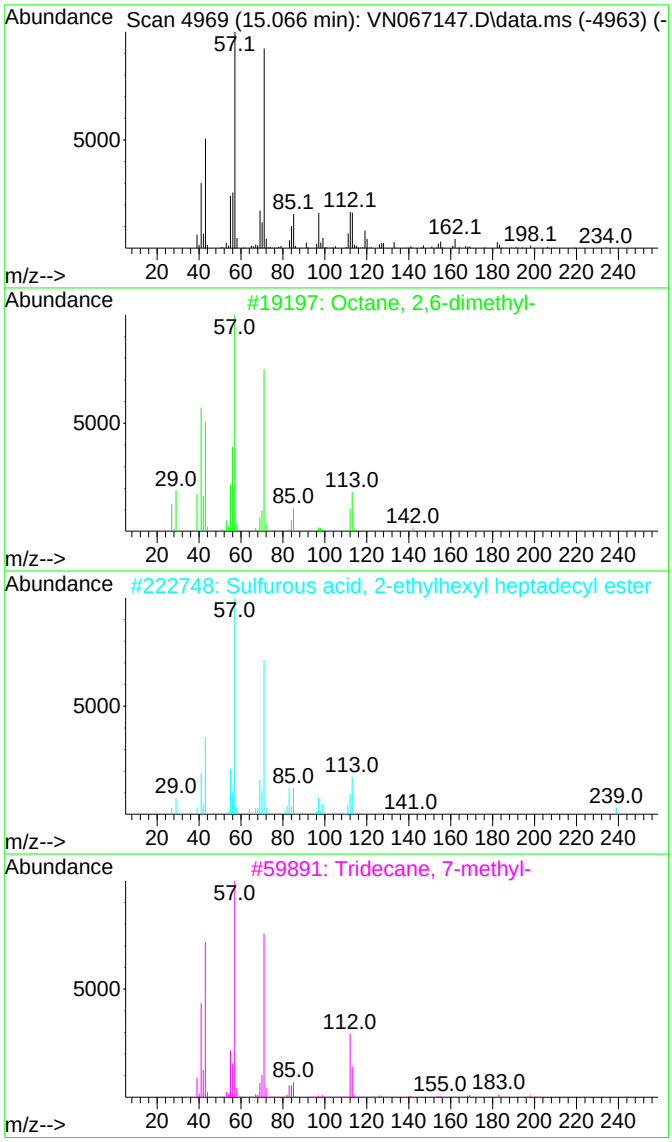
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

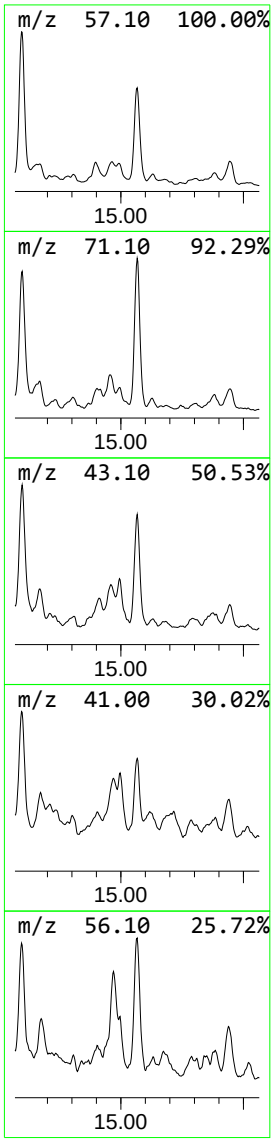
****

Peak Number 10 Octane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.066	14.95 ug/l	381258	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
2	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	83
3	Tridecane, 7-methyl-	198	C14H30	026730-14-3	64
4	Nonane, 3-methyl-	142	C10H22	005911-04-6	64
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051921\
Data File : VN067147.D
Acq On : 19 May 2021 13:32
Operator : JC/MD
Sample : M2392-07
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-03-3.5-4.0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclohexane, 1,...	11.153	6.4	ug/l	212237	3	11.360	1667680	50.0
unknown11.880	11.880	5.3	ug/l	175783	3	11.360	1667680	50.0
Cyclohexane, 1,...	12.682	12.8	ug/l	326370	4	13.301	1275460	50.0
Nonane, 2,6-dim...	12.918	22.9	ug/l	583243	4	13.301	1275460	50.0
Dodecane, 2,6,1...	13.047	5.6	ug/l	143687	4	13.301	1275460	50.0
Decane, 3-methyl-	13.100	8.0	ug/l	204989	4	13.301	1275460	50.0
Spiro[4.5]decane	13.615	14.5	ug/l	370994	4	13.301	1275460	50.0
Naphthalene, de...	14.119	56.5	ug/l	1441010	4	13.301	1275460	50.0
Undecane, 2,6-d...	14.597	41.6	ug/l	1061660	4	13.301	1275460	50.0
Octane, 2,6-dim...	15.066	14.9	ug/l	381258	4	13.301	1275460	50.0