LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN012820\
Data File : VN059892.D
Acq On : 28 Jan 2020 13:09
Operator : JC/MD
Sample : L1238-01 5X
Misc : 3.33g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CLIFTON-POLES

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\82N011320W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.638	1812	1824	1851	rVB	253391	594209	1.09%	0.472%
2	8.564	2095	2112	2134	rBV	349374	723953	1.32%	0.576%
3	10.075	2566	2582	2596	rBV	546951	1005822	1.84%	0.800%
4	11.400	2980	2994	3008	rBV	504183	882408	1.61%	0.701%
5	12.397	3289	3304	3325	rBV	431323	714544	1.31%	0.568%
6	13.037	3487	3503	3513	rBV	428295	684843	1.25%	0.544%
7	13.339	3586	3597	3615	rBV2	553062	1149782	2.10%	0.914%
8	13.538	3639	3659	3668	rBV	1959713	3321258	6.07%	2.640%
9	14.471	3940	3949	3960	rBV	527643	834072	1.53%	0.663%
10	14.590	3973	3986	3997	rBV3	918627	1759576	3.22%	1.399%
11	14.654	3997	4006	4020	rVB	643441	1051735	1.92%	0.836%
12	14.738	4021	4032	4047	rVB	789951	1298346	2.37%	1.032%
13	14.850	4049	4067	4082	rBV6	236980	678253	1.24%	0.539%
14	15.059	4123	4132	4138	rBV2	331953	604352	1.11%	0.480%
15	15.133	4141	4155	4171	rVB	28267065	54686010	100.00%	43.474%
16	15.223	4172	4183	4197	rBV	1455383	2902796	5.31%	2.308%
17	16.094	4440	4454	4459	rBV3	330105	749902	1.37%	0.596%
18	16.159	4460	4474	4497	rVV	14409350	32215873	58.91%	25.611%
19	16.278	4499	4511	4518	rVV2	296933	669908	1.23%	0.533%
20	16.348	4519	4533	4552	rVB	8692764	19263263	35.23%	15.314%

Sum of corrected areas: 125790905

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Operator : JC/MD
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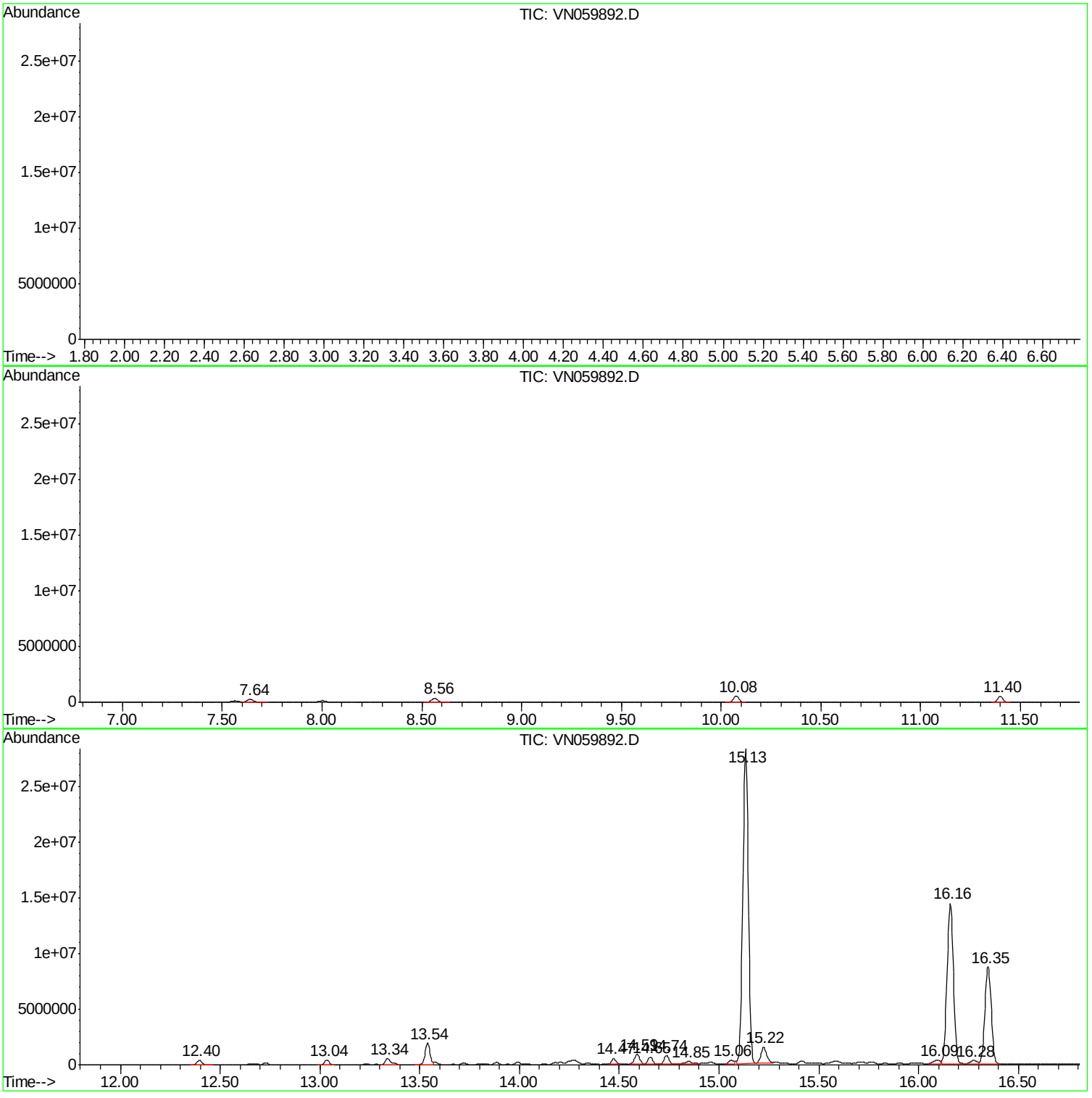
Misc : 3.33g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLIFTON-POLES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

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



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Acq On : 28 Jan 2020 13:09
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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CLIFTON-POLES

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Quant Title : SW846 8260

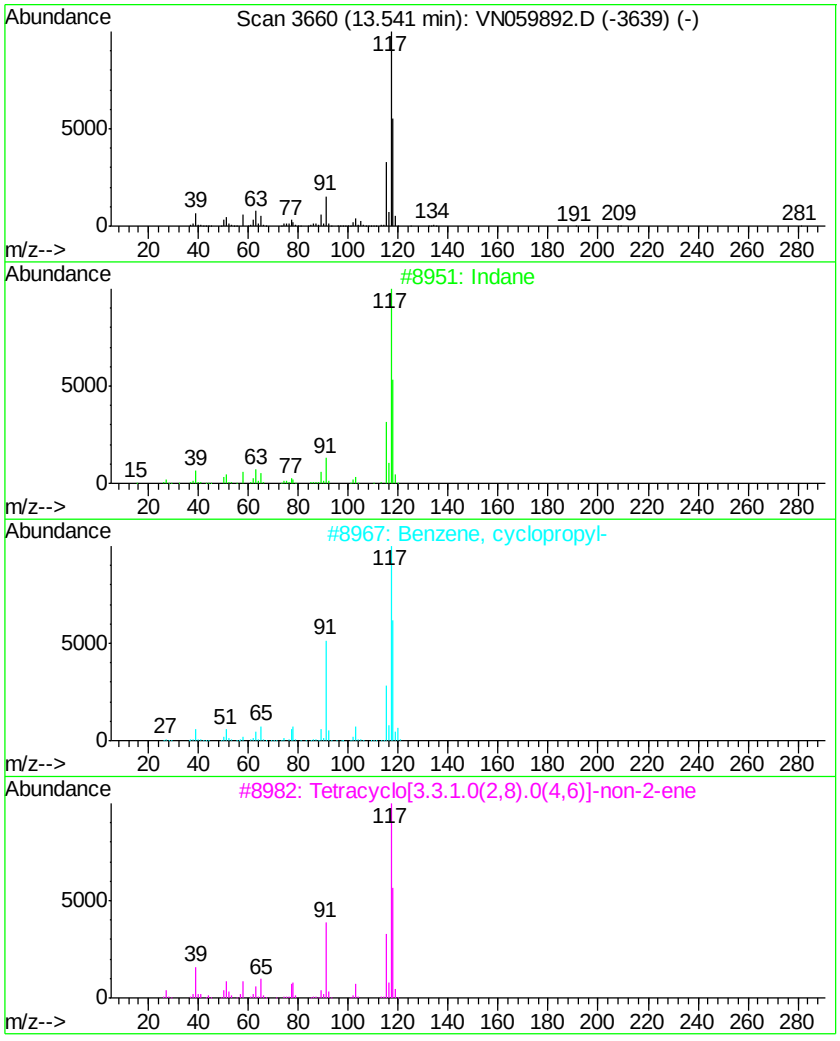
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

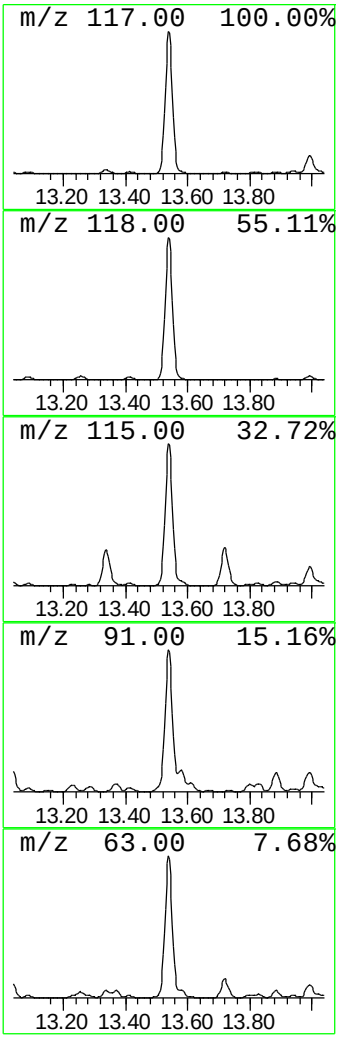
****

Peak Number 1 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	144.43 ug/l	3321260	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
4	Deltacyclene	118	C9H10	007785-10-6	72
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN012820\
Data File : VN059892.D
Acq On : 28 Jan 2020 13:09
Operator : JC/MD
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Misc : 3.33g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CLIFTON-POLES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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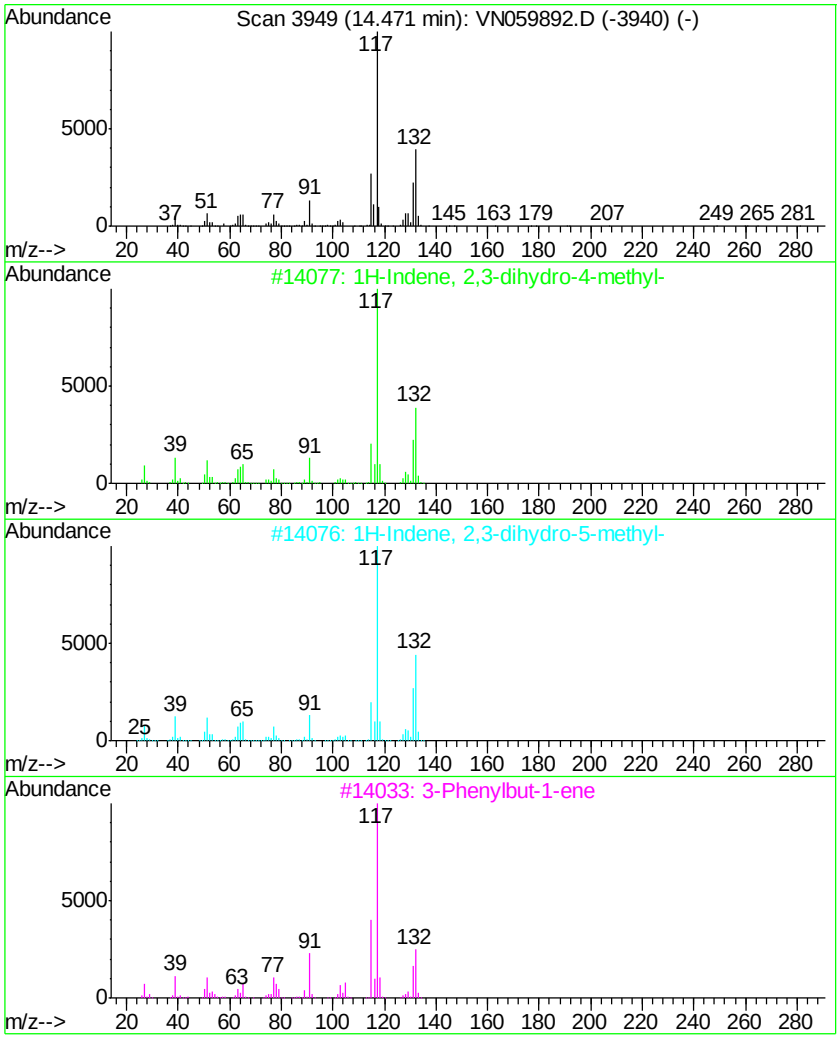
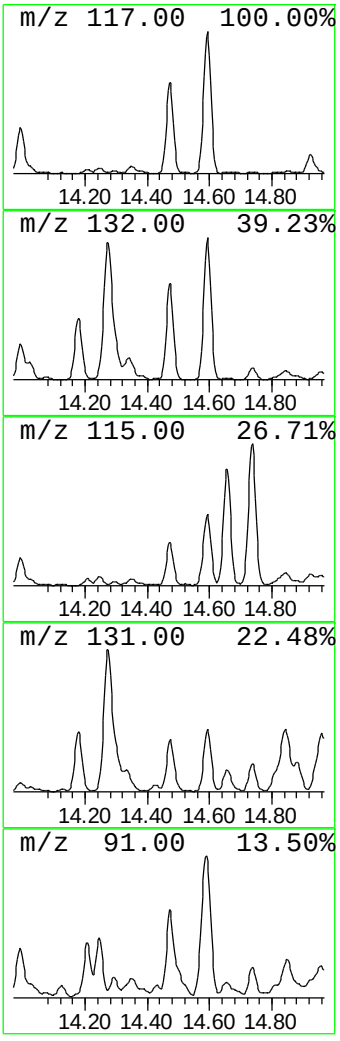
Peak Number 2 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	36.27 ug/l	834072	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
5	Indan, 1-methyl-	132	C10H12	000767-58-8	83





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN012820\
Data File : VN059892.D
Acq On : 28 Jan 2020 13:09
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Sample : L1238-01 5X
Misc : 3.33g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CLIFTON-POLES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

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

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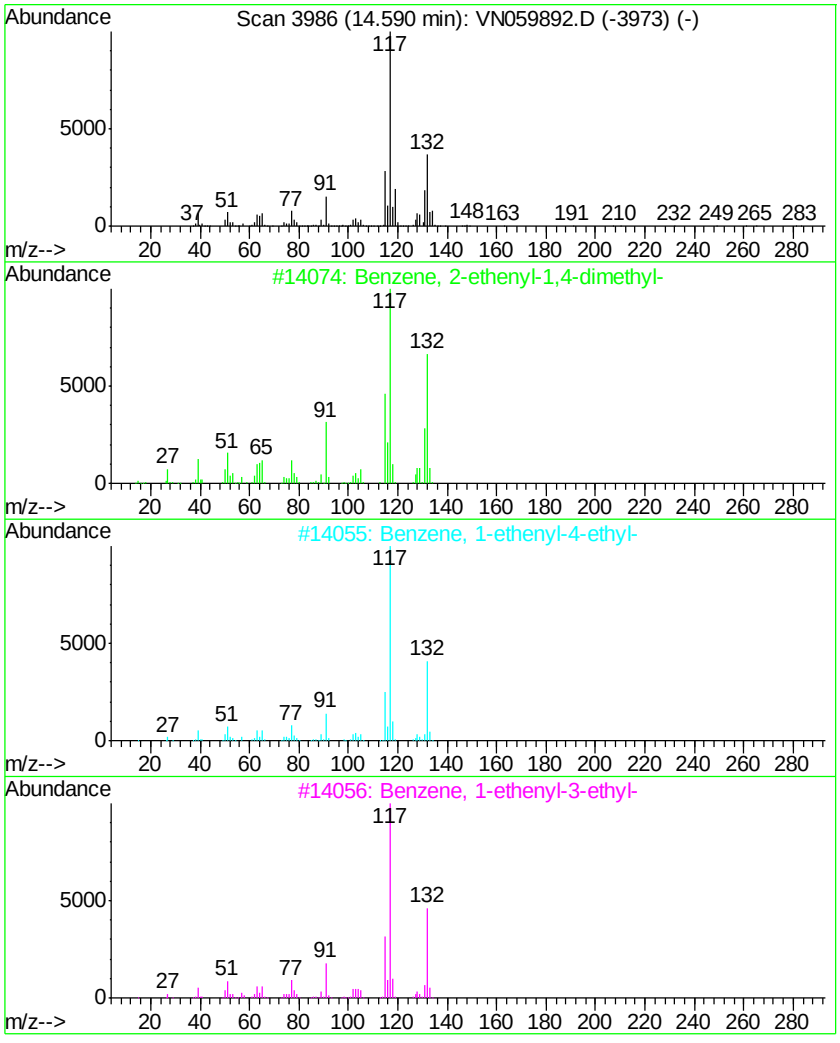
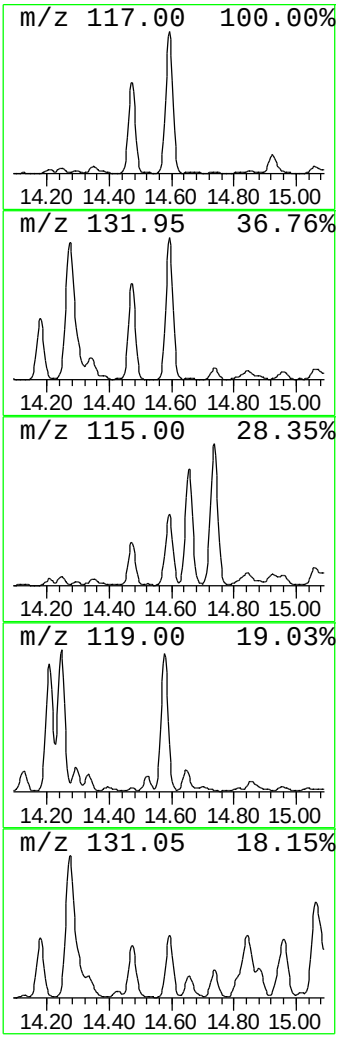
Peak Number 3 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	76.52 ug/l	1759580	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	83





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN012820\
Data File : VN059892.D
Acq On : 28 Jan 2020 13:09
Operator : JC/MD
Sample : L1238-01 5X
Misc : 3.33g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CLIFTON-POLES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

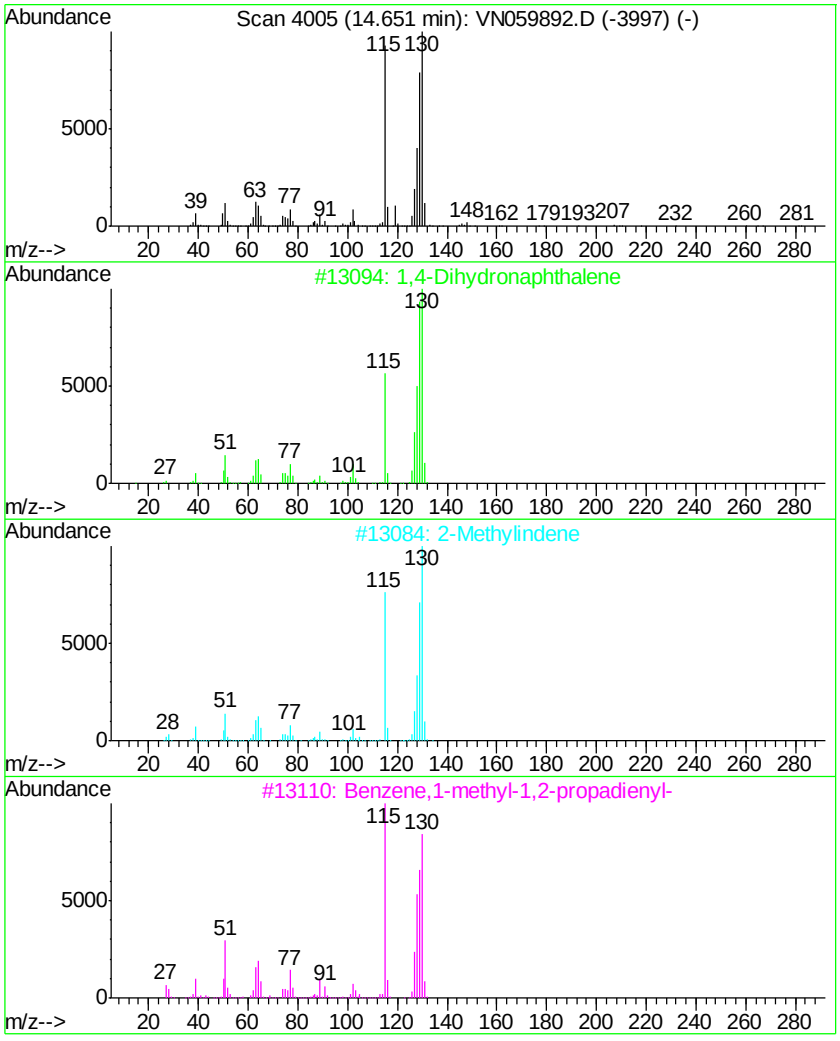
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

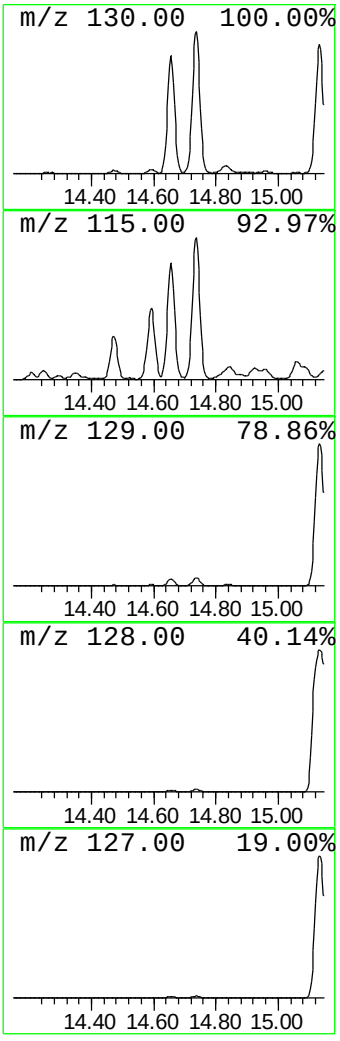
****

Peak Number 4 1,4-Dihydronaphthalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	45.74 ug/l	1051740	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	96
2	2-Methylindene	130	C10H10	002177-47-1	96
3	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
4	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
5	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN012820\
Data File : VN059892.D
Acq On : 28 Jan 2020 13:09
Operator : JC/MD
Sample : L1238-01 5X
Misc : 3.33g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CLIFTON-POLES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

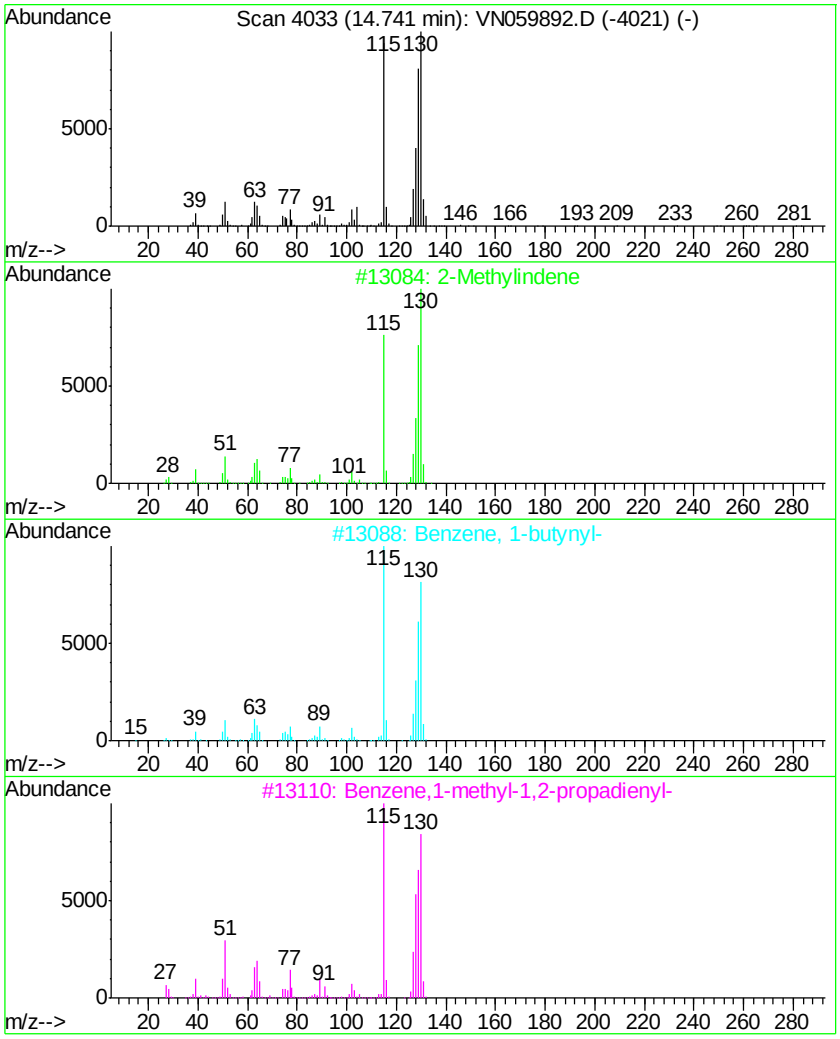
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

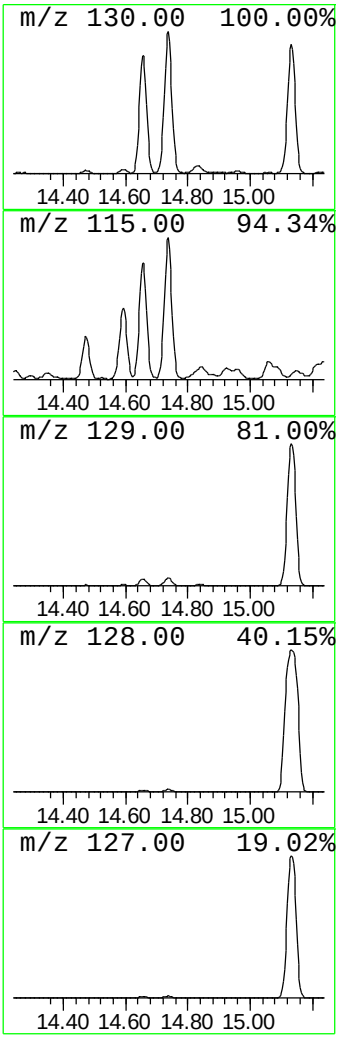
****

Peak Number 5 2-Methylindene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	56.46 ug/l	1298350	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	96
2	Benzene, 1-butynyl-	130	C10H10	000622-76-4	95
3	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
4	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
5	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	94





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN012820\
Data File : VN059892.D
Acq On : 28 Jan 2020 13:09
Operator : JC/MD
Sample : L1238-01 5X
Misc : 3.33g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CLIFTON-POLES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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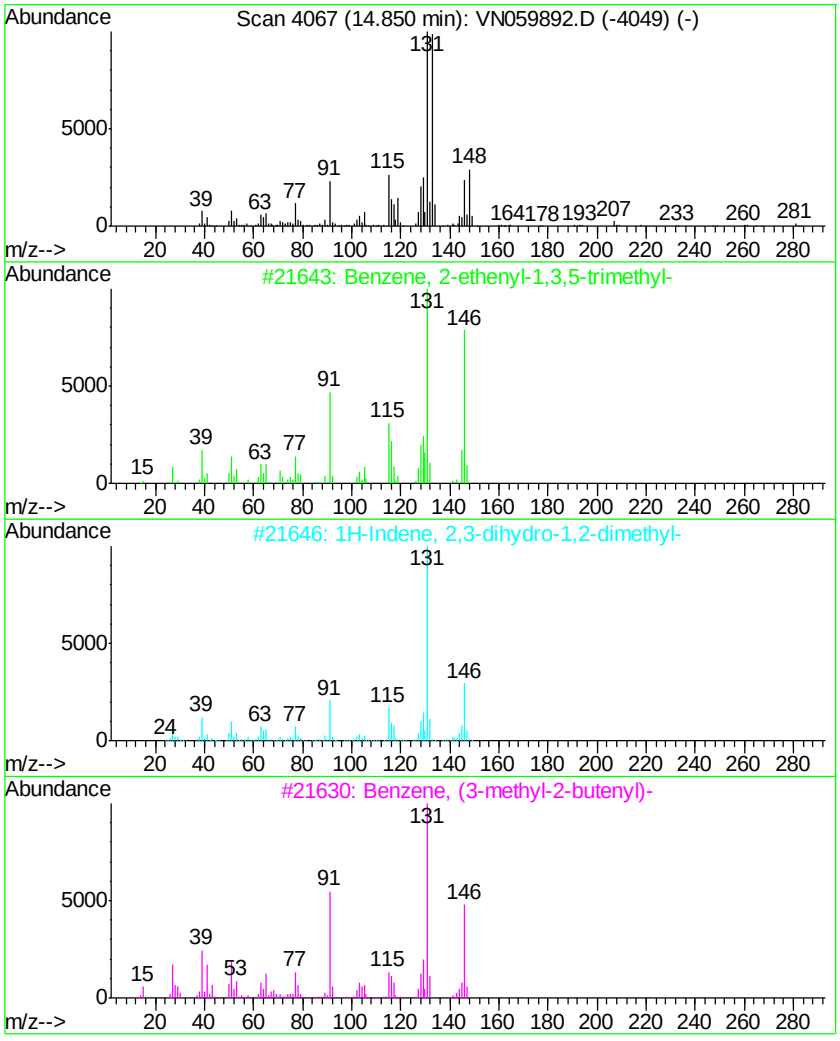
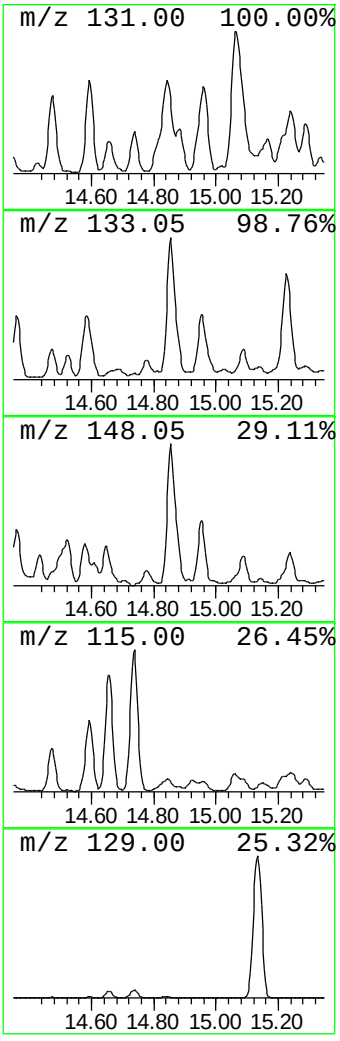
****

Peak Number 6 Benzene, 2-ethenyl-1,3,5-tr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	29.49 ug/l	678253	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	55
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	50
3	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	50
4	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	46
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	46





Library Search Compound Report

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Quant Title : SW846 8260

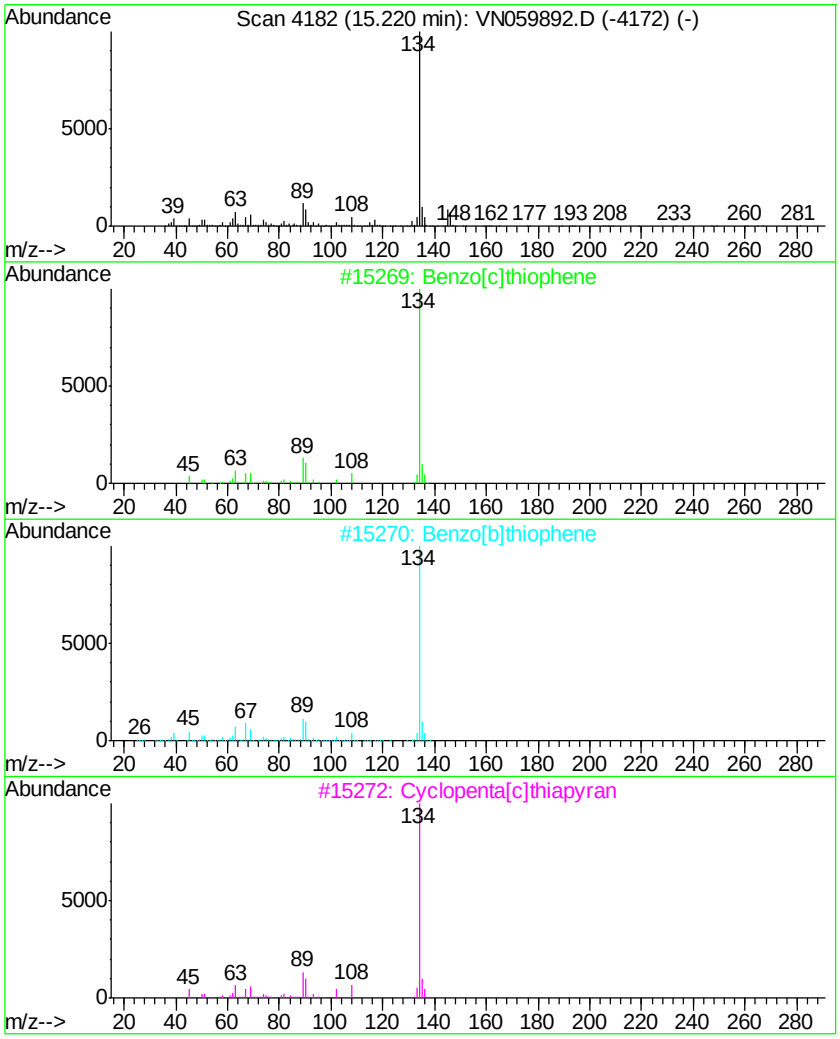
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

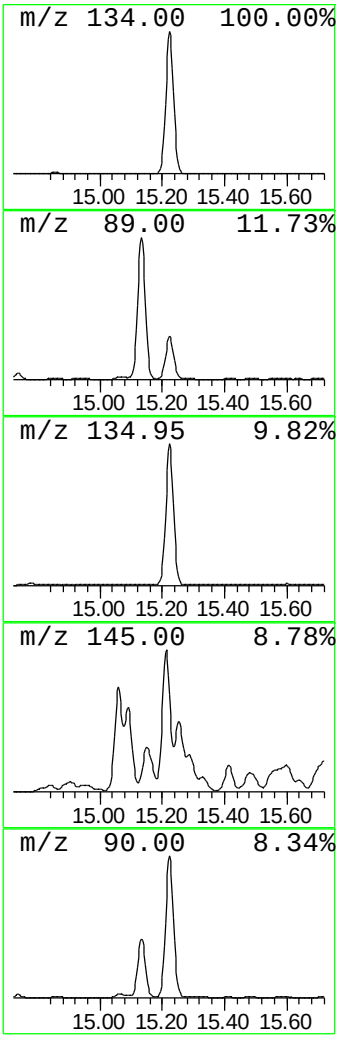
****

Peak Number 7 Benzo[c]thiophene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	126.23 ug/l	2902800	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]thiophene	134	C8H6S	000270-82-6	95
2	Benzo[b]thiophene	134	C8H6S	000095-15-8	91
3	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
4	5H-Pyrrolo(3,2-d)pyrimidin-4-amine	134	C6H6N4	002227-98-7	59
5	[1]Benzothieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	39





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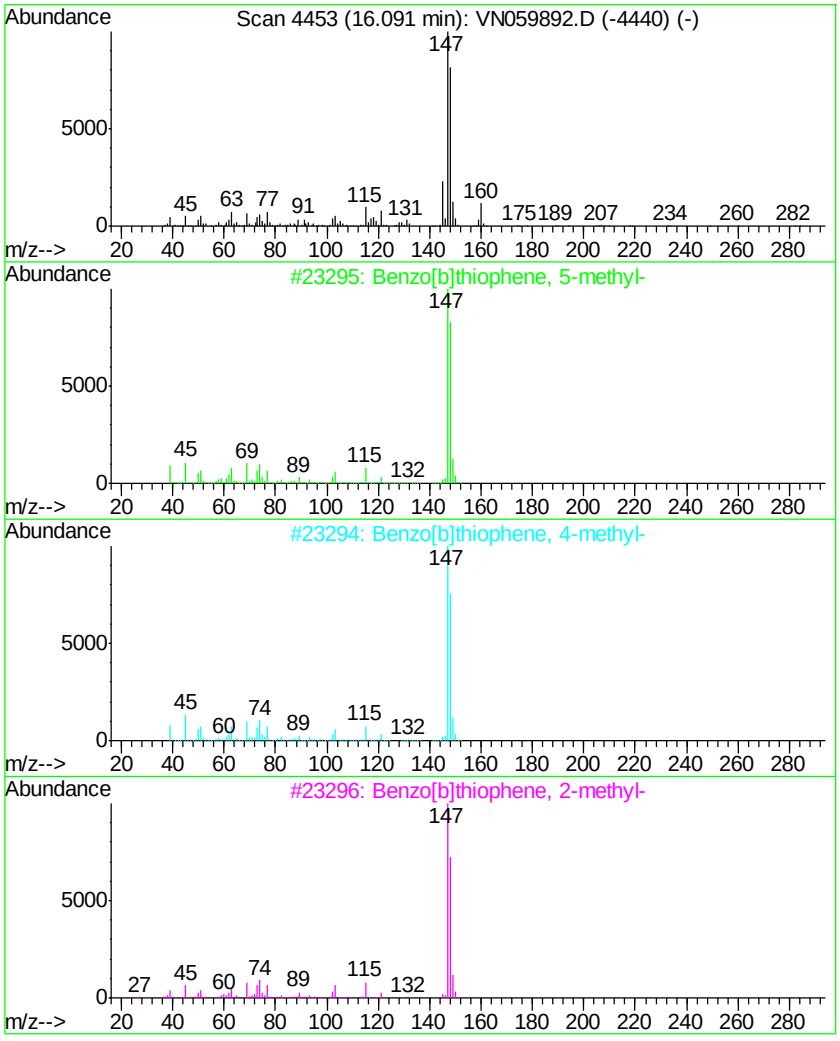
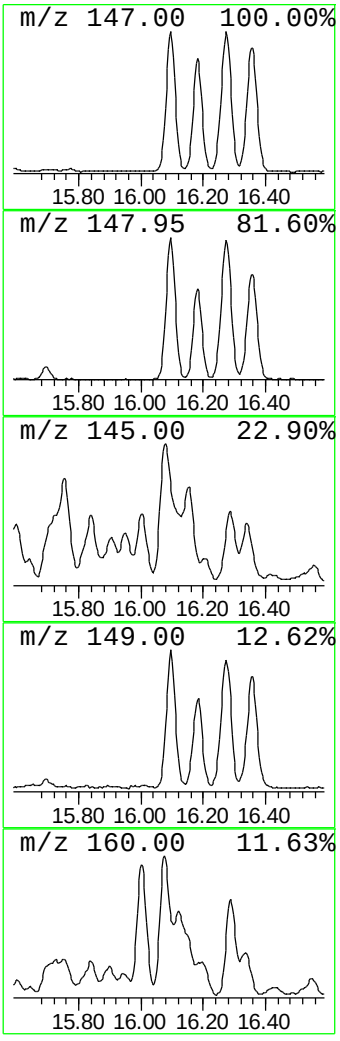
Peak Number 8 Benzo[b]thiophene, 5-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	32.61 ug/l	749902	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]thiophene, 5-methyl-	148	C9H8S	014315-14-1	81
2	Benzo[b]thiophene, 4-methyl-	148	C9H8S	014315-11-8	81
3	Benzo[b]thiophene, 2-methyl-	148	C9H8S	001195-14-8	81
4	3-Methylbenzothiophene	148	C9H8S	001455-18-1	81
5	1,2,4,5-Tetramethyl-3-neopentylb...	204	C15H24	033770-74-0	64





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Instrument : MSVOA_N
ClientSampleId : CLIFTON-POLES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

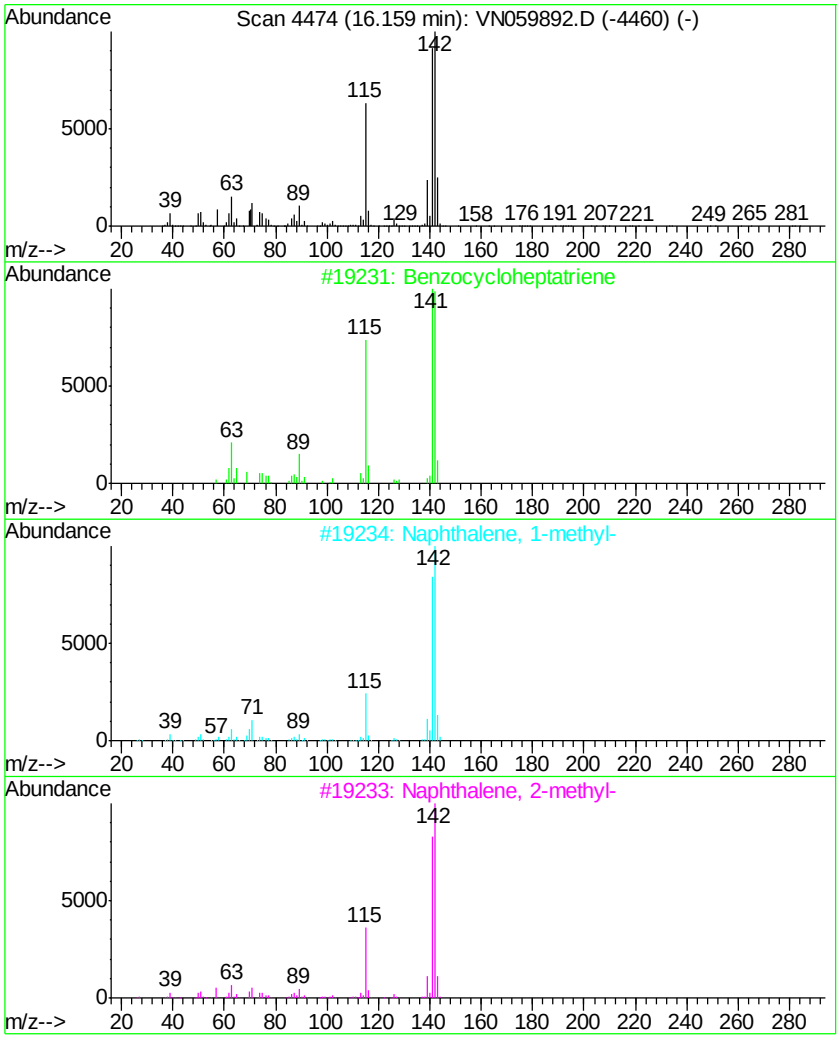
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

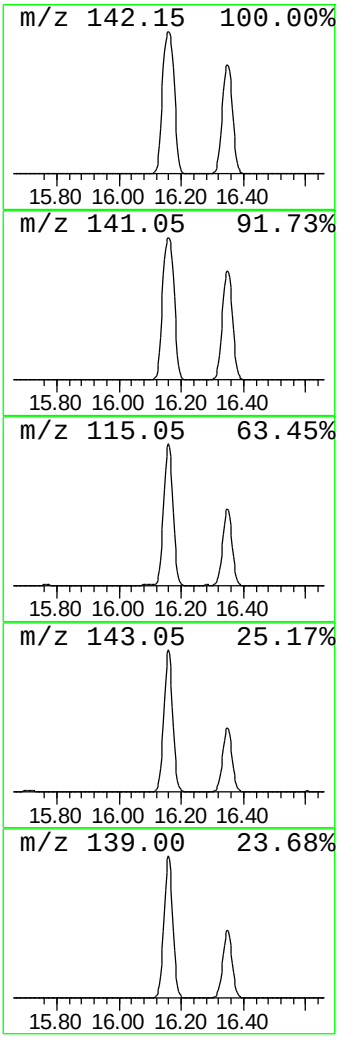
****

Peak Number 9 Benzocycloheptatriene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	1400.96 ug/l	32215900	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzocycloheptatriene	142	C11H10	000264-09-5	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	90
4	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	90
5	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	87





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Data File : VN059892.D
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Operator : JC/MD
Sample : L1238-01 5X
Misc : 3.33g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CLIFTON-POLES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

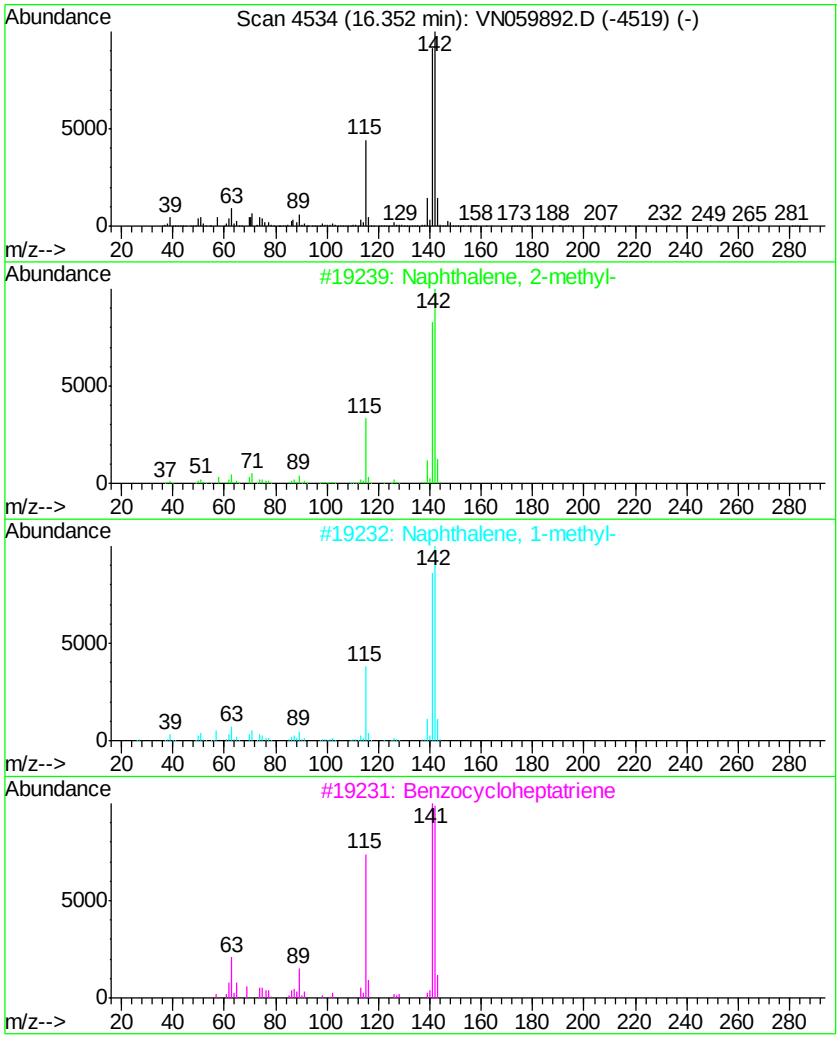
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

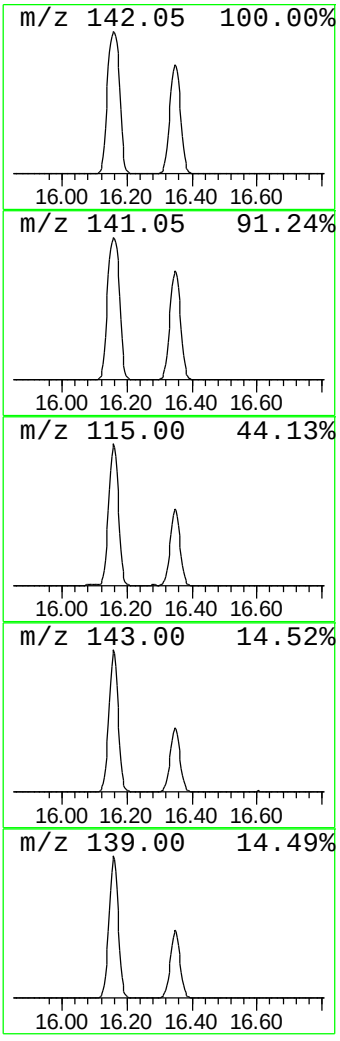
****

Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	837.69 ug/l	19263300	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	93
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN012820\
Data File : VN059892.D
Acq On : 28 Jan 2020 13:09
Operator : JC/MD
Sample : L1238-01 5X
Misc : 3.33g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CLIFTON-POLES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.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
Indane	13.54	144.4	ug/l	3321260	4	13.34	1149780	50.0
1H-Indene, 2,3-di...	14.47	36.3	ug/l	834072	4	13.34	1149780	50.0
Benzene, 2-etheny...	14.59	76.5	ug/l	1759580	4	13.34	1149780	50.0
1,4-Dihydronaphth...	14.65	45.7	ug/l	1051740	4	13.34	1149780	50.0
2-Methylindene	14.74	56.5	ug/l	1298350	4	13.34	1149780	50.0
Benzene, 2-etheny...	14.85	29.5	ug/l	678253	4	13.34	1149780	50.0
Benzo[c]thiophene	15.22	126.2	ug/l	2902800	4	13.34	1149780	50.0
Benzo[b]thiophene...	16.09	32.6	ug/l	749902	4	13.34	1149780	50.0
Benzocycloheptatr...	16.16	1401.0	ug/l	32215900	4	13.34	1149780	50.0
Naphthalene, 2-me...	16.35	837.7	ug/l	19263300	4	13.34	1149780	50.0