LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020824\
Data File : VN080972.D
Acq On : 08 Feb 2024 18:34
Operator : JC\MD
Sample : P1372-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CG-MW-17-ch5

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\82N020624W.M
Title : SW846 8260

Signal : TIC: VN080972.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.171	1048	1057	1061	rBV	325879	782802	1.42%	0.863%
2	8.230	1061	1067	1079	rVB	624222	1394853	2.54%	1.537%
3	8.612	1118	1132	1149	rBV2	24004004	54937064	100.00%	60.533%
4	9.106	1207	1216	1225	rBV	905002	1846460	3.36%	2.035%
5	10.571	1456	1465	1472	rBV	1119183	2083844	3.79%	2.296%
6	11.871	1676	1686	1694	rBV	1155694	2075467	3.78%	2.287%
7	11.965	1694	1702	1711	rVV	2845796	4801813	8.74%	5.291%
8	12.082	1711	1722	1729	rVB	300714	553630	1.01%	0.610%
9	12.400	1769	1776	1784	rVB	413962	712461	1.30%	0.785%
10	12.641	1789	1817	1823	rBV3	146393	789530	1.44%	0.870%
11	12.853	1844	1853	1863	rVB	829519	1439497	2.62%	1.586%
12	13.341	1927	1936	1951	rVB	264090	574323	1.05%	0.633%
13	13.670	1973	1992	2007	rBV6	187483	1050374	1.91%	1.157%
14	13.794	2007	2013	2024	rVB2	1084227	1995530	3.63%	2.199%
15	14.000	2037	2048	2061	rBV2	1271765	3045429	5.54%	3.356%
16	15.070	2217	2230	2234	rBV4	238703	788974	1.44%	0.869%
17	15.206	2246	2253	2262	rVB	413831	781387	1.42%	0.861%
18	15.523	2287	2307	2319	rBV3	475973	1878704	3.42%	2.070%
19	15.647	2319	2328	2338	rVV	4069175	8153388	14.84%	8.984%
20	15.747	2338	2345	2354	rVB	512284	1070086	1.95%	1.179%

Sum of corrected areas: 90755616

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020824\
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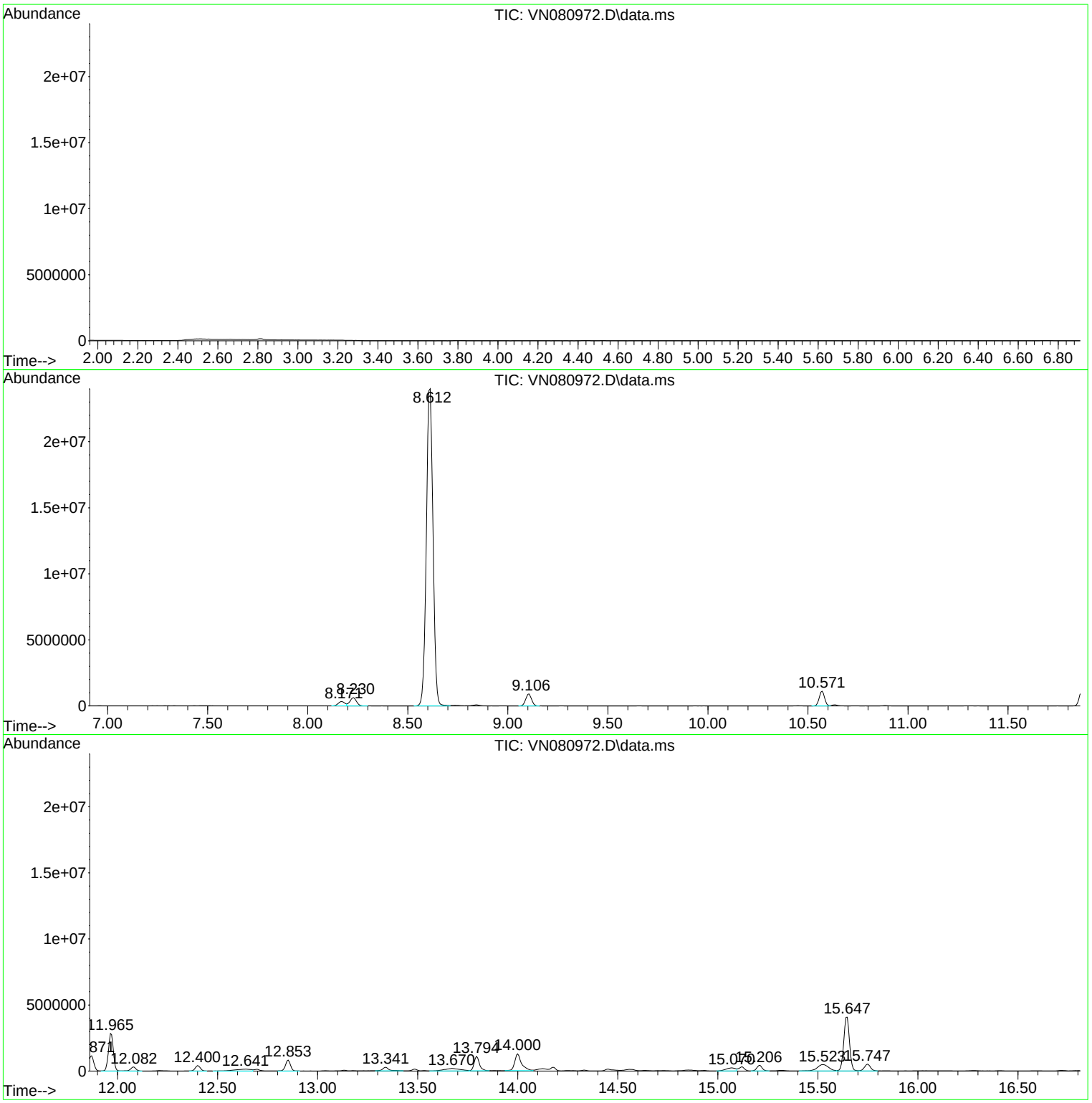
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CG-MW-17-ch5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

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



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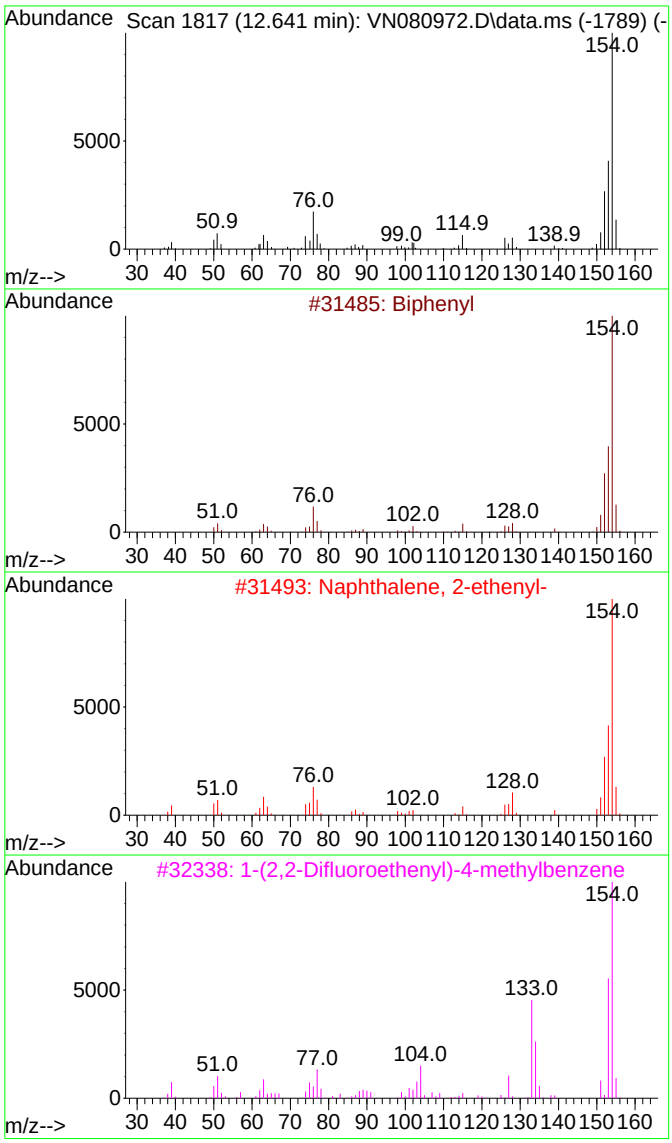
Quant Title : SW846 8260

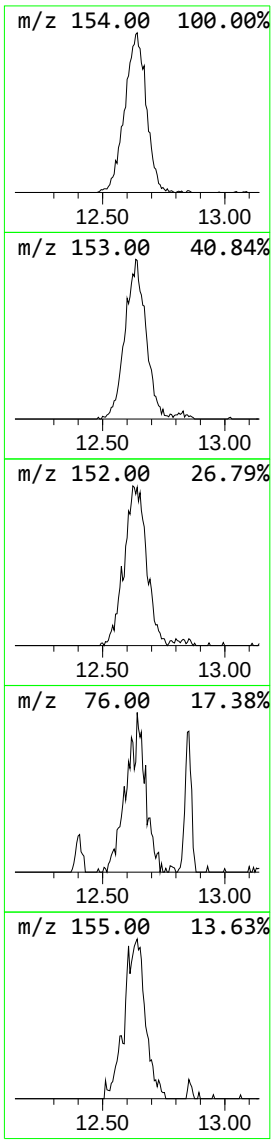
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Naphthalene, 2-ethenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.641	19.02 ug/l	789530	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Biphenyl	154	C12H10	000092-52-4	93
2	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	74
3	1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	59
4	3-Quinolinecarbonitrile	154	C10H6N2	034846-64-5	47
5	Propanedinitrile, 2,4,6-cyclohep...	154	C10H6N2	002860-54-0	43





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ClientSampleId :
CG-MW-17-ch5

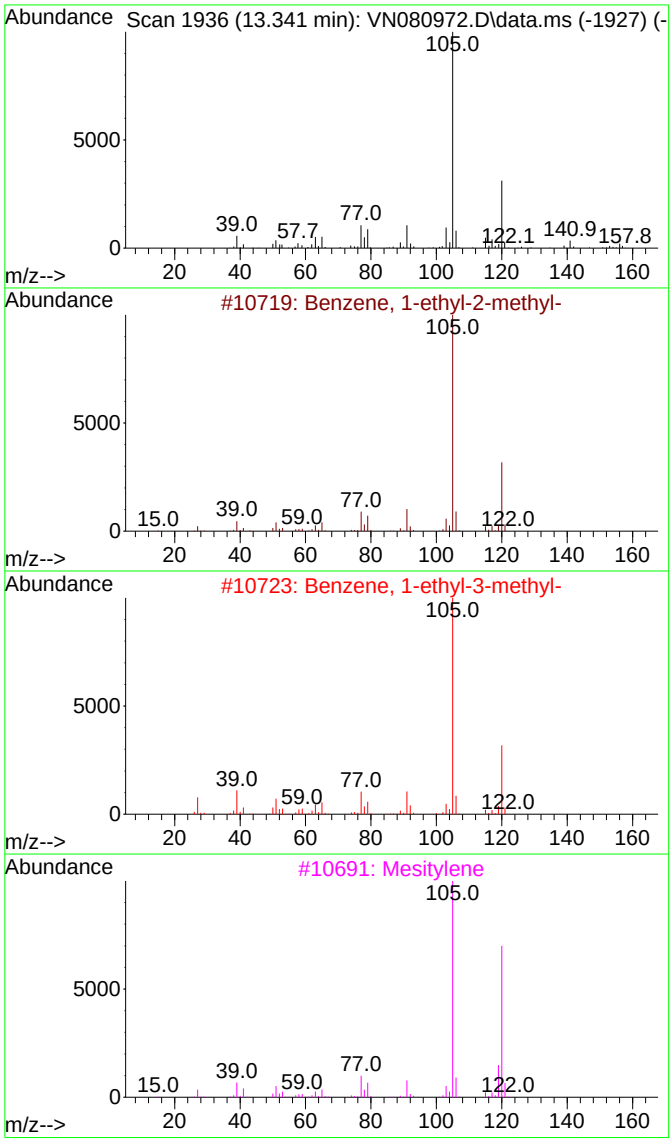
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

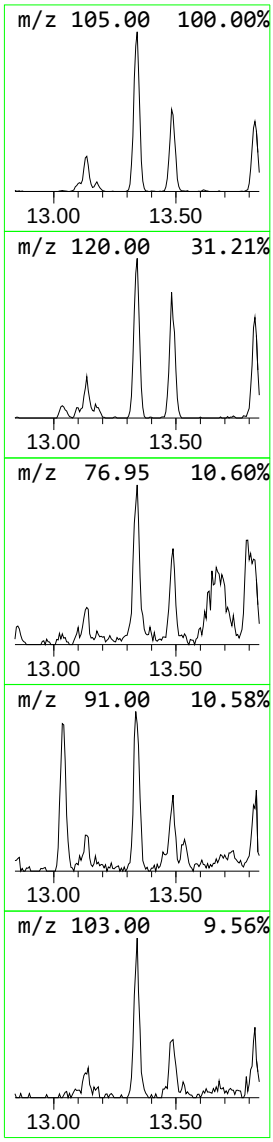
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	14.39 ug/l	574323	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87
3	Mesitylene	120	C9H12	000108-67-8	87
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	87





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CG-MW-17-ch5

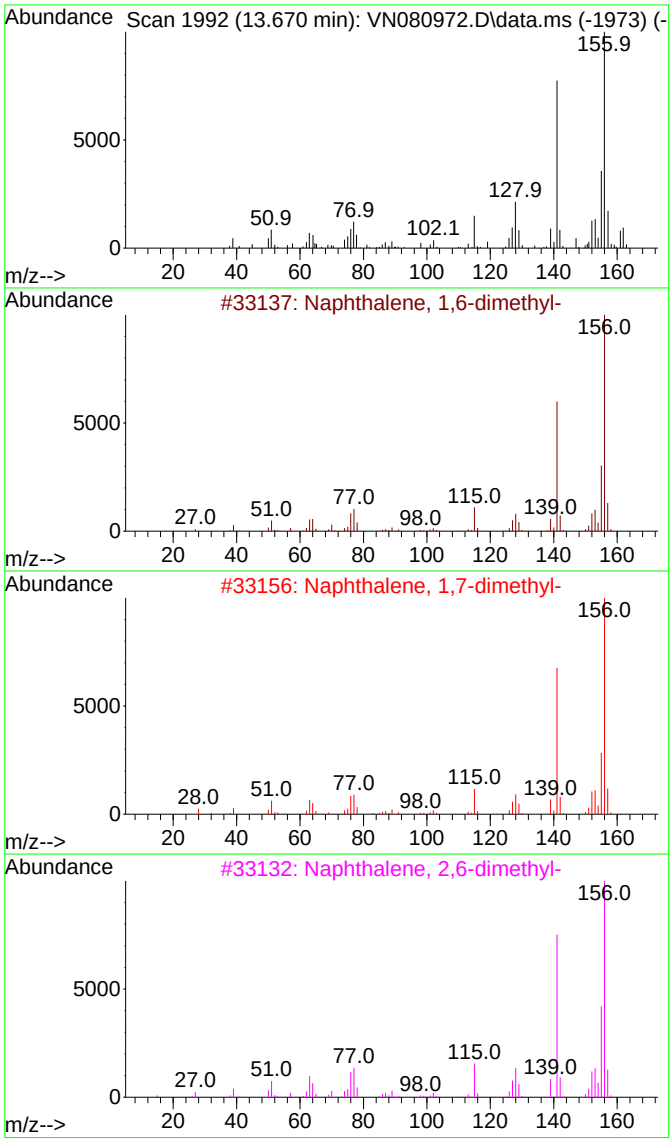
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

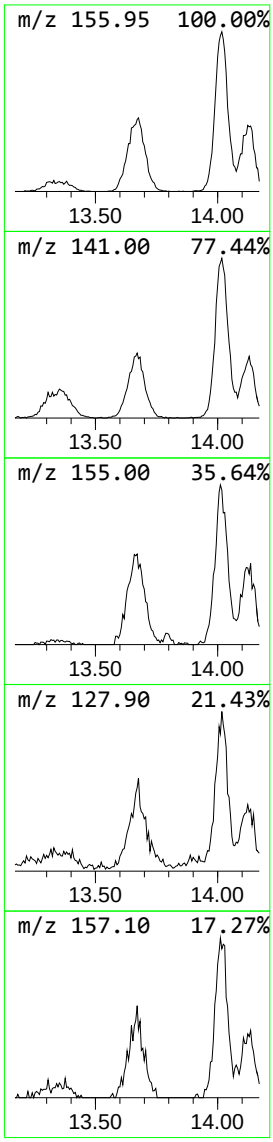
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Naphthalene, 1,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.670	26.32 ug/l	1050370	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
3	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
5	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	95





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CG-MW-17-ch5

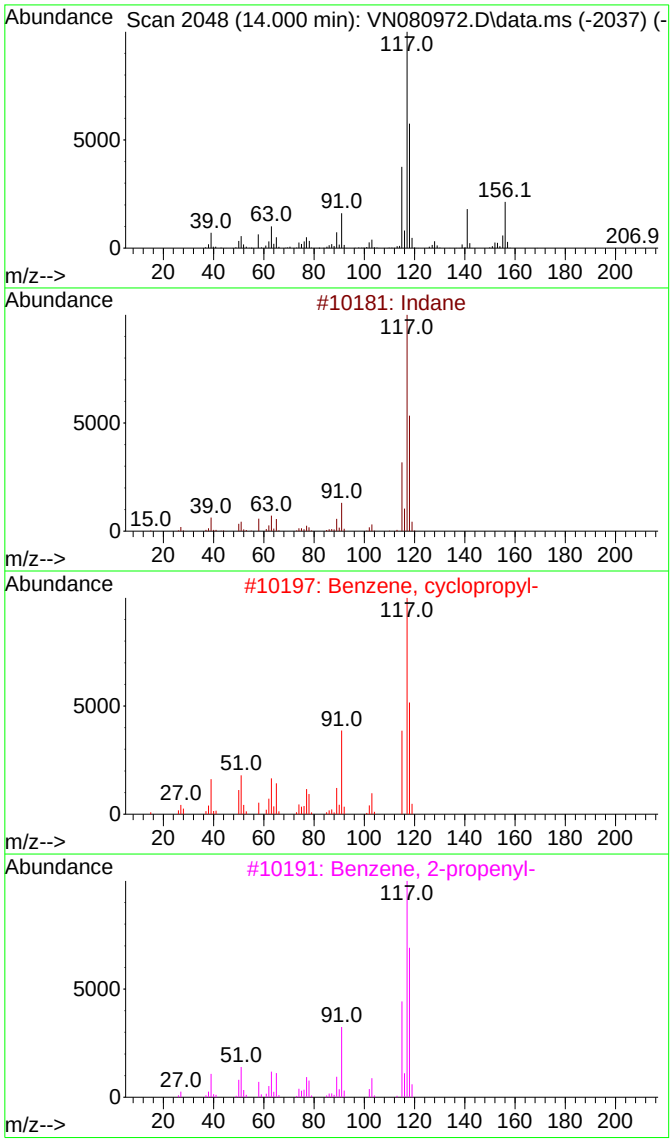
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

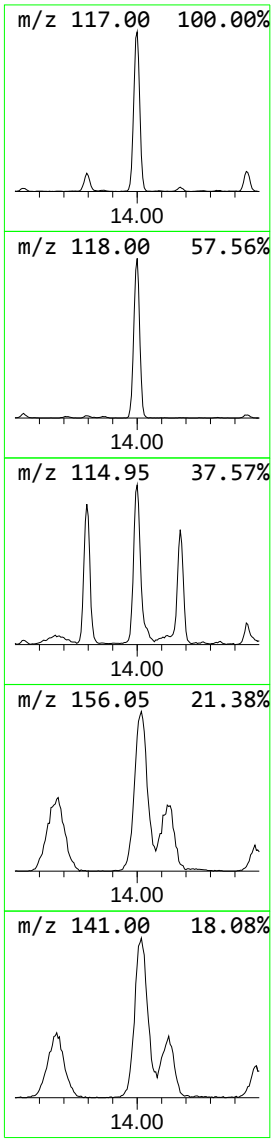
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	76.31 ug/l	3045430	1,4-Dichlorobenzene-d4	13.794

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	64
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	58
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	52
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	52





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Acq On : 08 Feb 2024 18:34
Operator : JC\MD
Sample : P1372-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CG-MW-17-ch5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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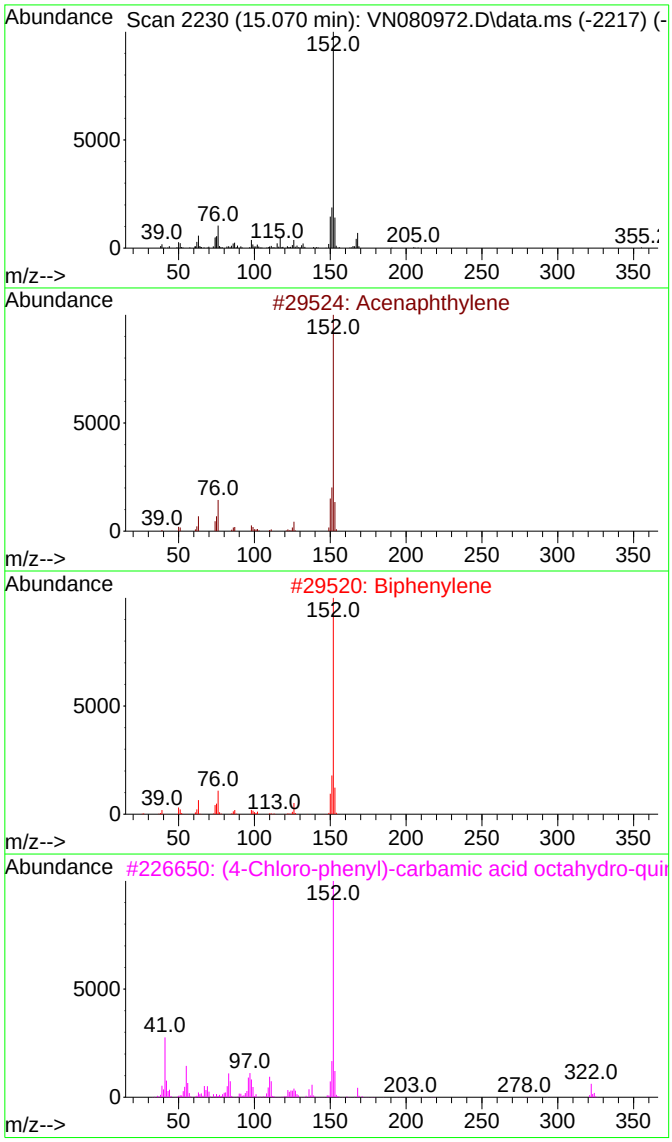
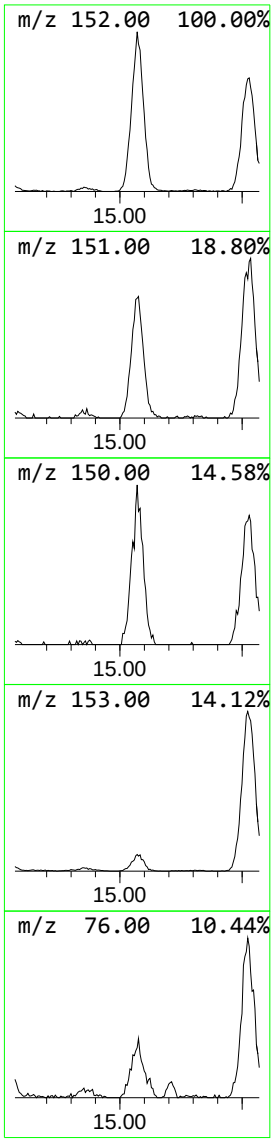
****
Peak Number 5 Biphenylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.070	19.77 ug/l	788974	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthylene	152	C12H8	000208-96-8	95
2	Biphenylene	152	C12H8	000259-79-0	91
3	(4-Chloro-phenyl)-carbamic acid ...	322	C17H23ClN2O2	1000275-38-8	72
4	Benzaldehyde, 2-hydroxy-3-methoxy-	152	C8H8O3	000148-53-8	59
5	(6Balpha,7beta,11alpha,11aalpha)...	334	C25H18O	1000241-69-8	56





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CG-MW-17-ch5

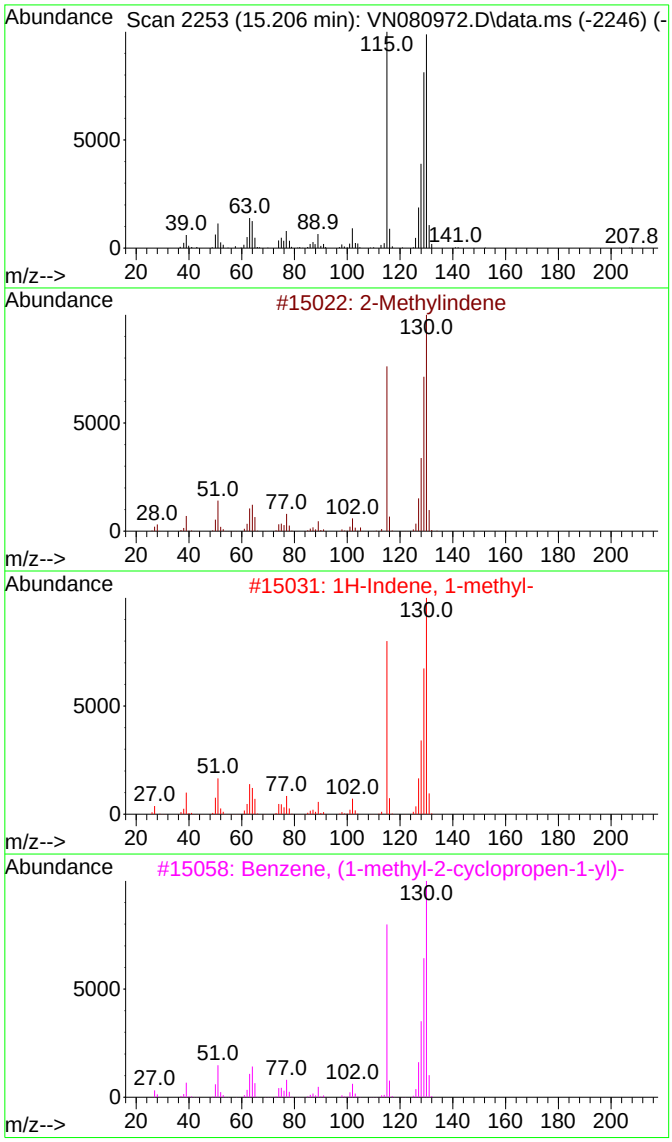
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

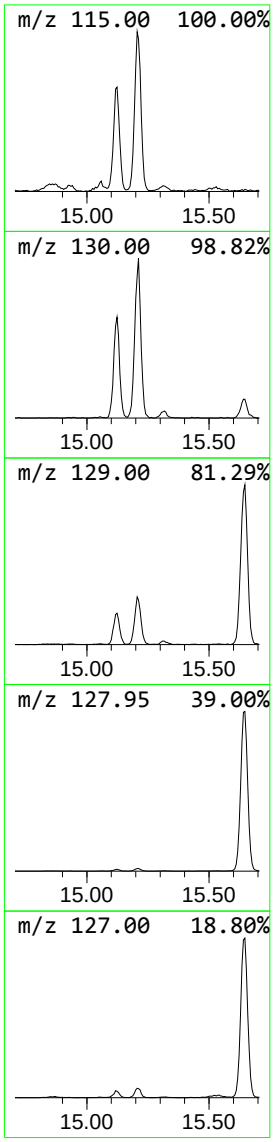
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Methylindene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.206	19.58 ug/l	781387	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	95
2	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	95
3	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	94
4	Benzene, 1-butynyl-	130	C10H10	000622-76-4	94
5	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93





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ClientSampleId :
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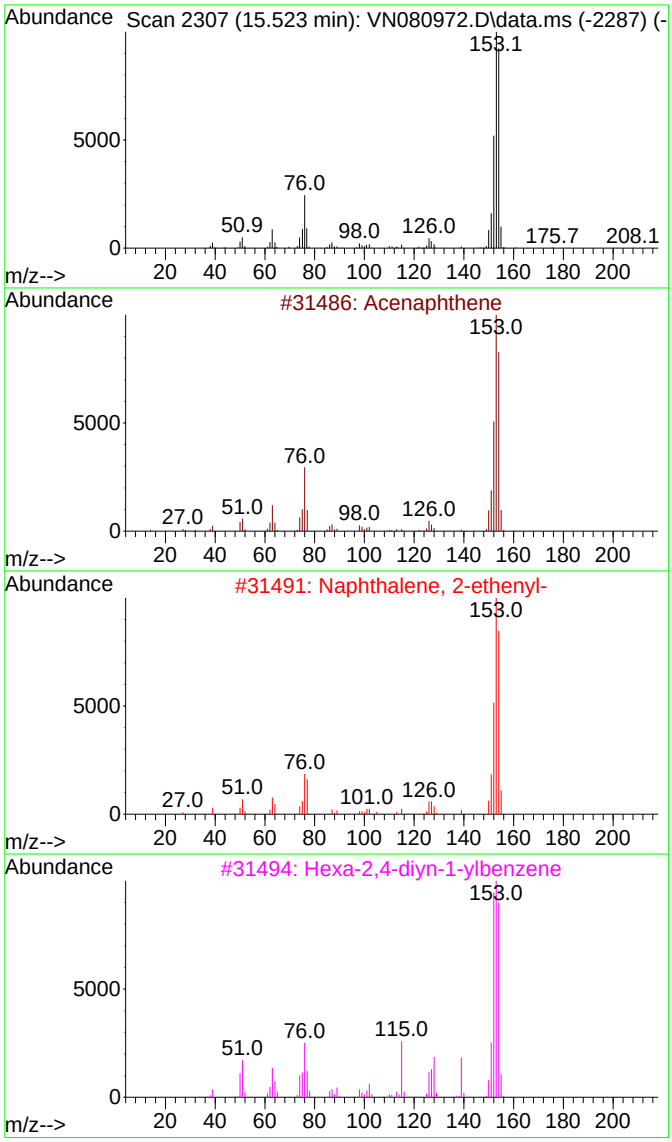
Quant Title : SW846 8260

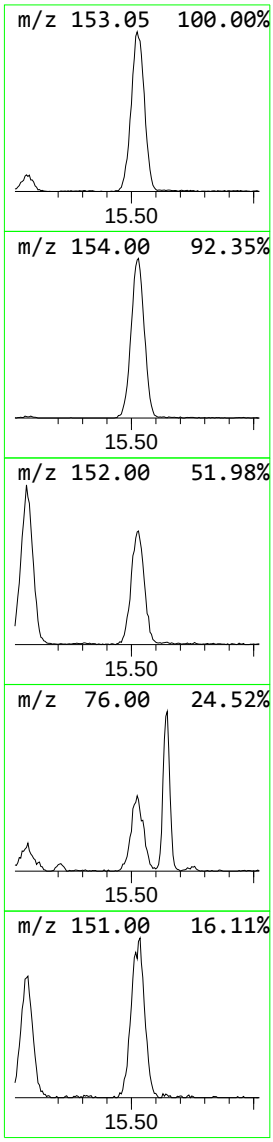
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.523	47.07 ug/l	1878700	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	89
2	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	68
3	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
4	3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	53
5	2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50





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Instrument :
MSVOA_N
ClientSampleId :
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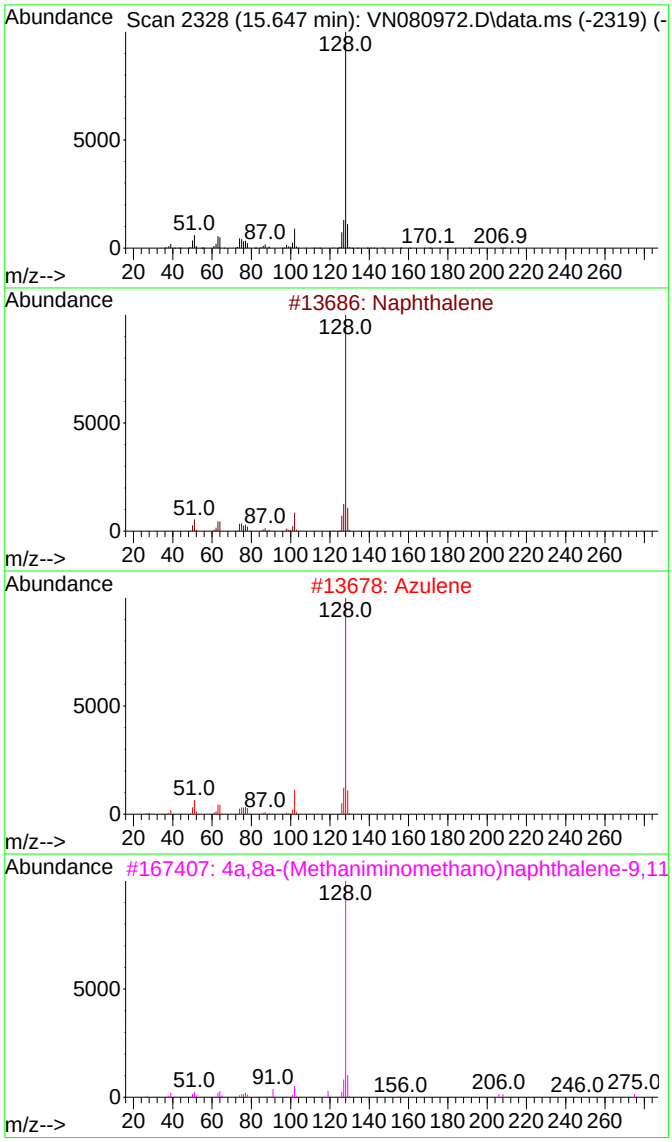
Quant Title : SW846 8260

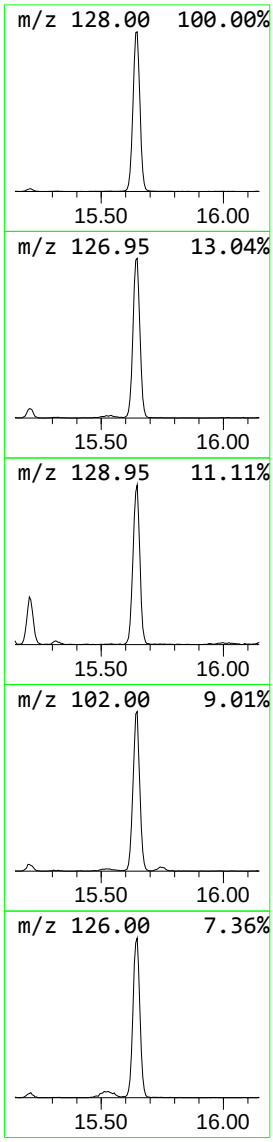
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	204.29 ug/l	8153390	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	94
3	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
4	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	53
5	[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	50





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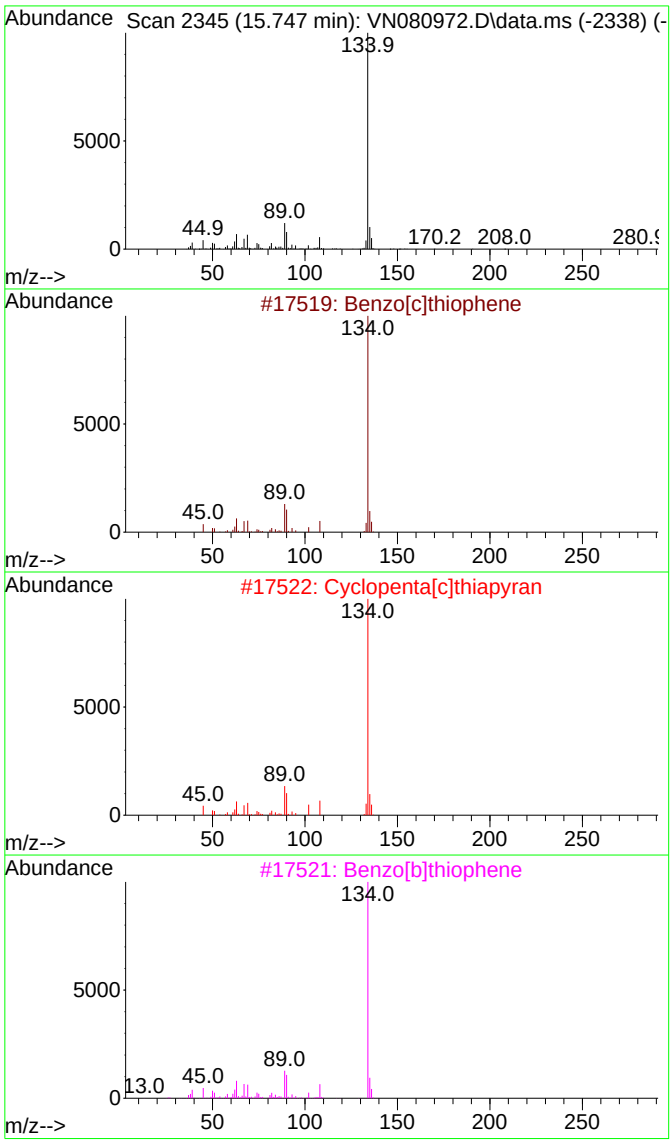
Quant Title : SW846 8260

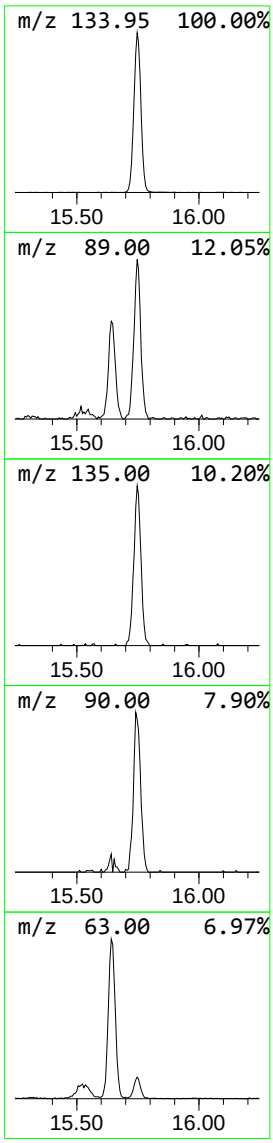
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzo[c]thiophene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.747	26.81 ug/l	1070090	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
3	Benzo[b]thiophene	134	C8H6S	000095-15-8	94
4	[1]Benzothieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	56
5	5H-Pyrrolo(3,2-d)pyrimidin-4-amine	134	C6H6N4	002227-98-7	45





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Naphthalene, 2-...	12.641	19.0	ug/l	789530	3	11.871	2075470	50.0
Benzene, 1-ethy...	13.341	14.4	ug/l	574323	4	13.794	1995530	50.0
Naphthalene, 1,...	13.670	26.3	ug/l	1050370	4	13.794	1995530	50.0
Indane	14.000	76.3	ug/l	3045430	4	13.794	1995530	50.0
Biphenylene	15.070	19.8	ug/l	788974	4	13.794	1995530	50.0
2-Methylindene	15.206	19.6	ug/l	781387	4	13.794	1995530	50.0
Hexa-2,4-diyn-1...	15.523	47.1	ug/l	1878700	4	13.794	1995530	50.0
Azulene	15.647	204.3	ug/l	8153390	4	13.794	1995530	50.0
Benzo[c]thiophene	15.747	26.8	ug/l	1070090	4	13.794	1995530	50.0