LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
Data File : VX042052.D
Acq On : 26 Jun 2024 14:50
Operator : JC/MD
Sample : P3045-07
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
9AB

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_X\Method\82X061824W.M
Title : SW846 8260

Signal : TIC: VX042052.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% max.	% of total
1	6.757	921	930	945	rBV	190173	462314	1.06%	0.676%
2	8.647	1234	1240	1247	rBV	412506	639011	1.47%	0.934%
3	10.055	1466	1471	1480	rBV	428372	584151	1.34%	0.854%
4	10.299	1502	1511	1517	rBV	649900	869405	2.00%	1.271%
5	10.640	1562	1567	1583	rVB	602014	842398	1.93%	1.231%
6	11.085	1634	1640	1649	rBV	383793	534660	1.23%	0.781%
7	11.451	1695	1700	1709	rVB	553570	752790	1.73%	1.100%
8	11.750	1745	1749	1755	rBV	1040517	1301577	2.99%	1.902%
9	12.024	1789	1794	1800	rBV	559966	708277	1.63%	1.035%
10	12.085	1800	1804	1809	rVB	512210	661587	1.52%	0.967%
11	12.414	1849	1858	1864	rBV	1275253	1587471	3.64%	2.320%
12	12.963	1944	1948	1956	rVB2	358543	493743	1.13%	0.722%
13	13.286	1992	2001	2007	rBV3	268630	495373	1.14%	0.724%
14	13.786	2074	2083	2088	rBV	29292658	43577724	100.00%	63.683%
15	13.871	2088	2097	2104	rVB	884600	1130121	2.59%	1.652%
16	14.640	2218	2223	2233	rVB	5148206	6589660	15.12%	9.630%
17	14.780	2240	2246	2253	rVB	2957790	3738611	8.58%	5.463%
18	15.206	2308	2316	2321	rBV	640798	875090	2.01%	1.279%
19	15.475	2355	2360	2373	rVV	465704	777788	1.78%	1.137%
20	15.615	2377	2383	2386	rVV	493417	795488	1.83%	1.162%
21	15.652	2386	2389	2398	rVB	317738	465293	1.07%	0.680%
22	16.688	2549	2559	2572	rVB2	206841	547006	1.26%	0.799%

Sum of corrected areas: 68429538

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
Data File : VX042052.D
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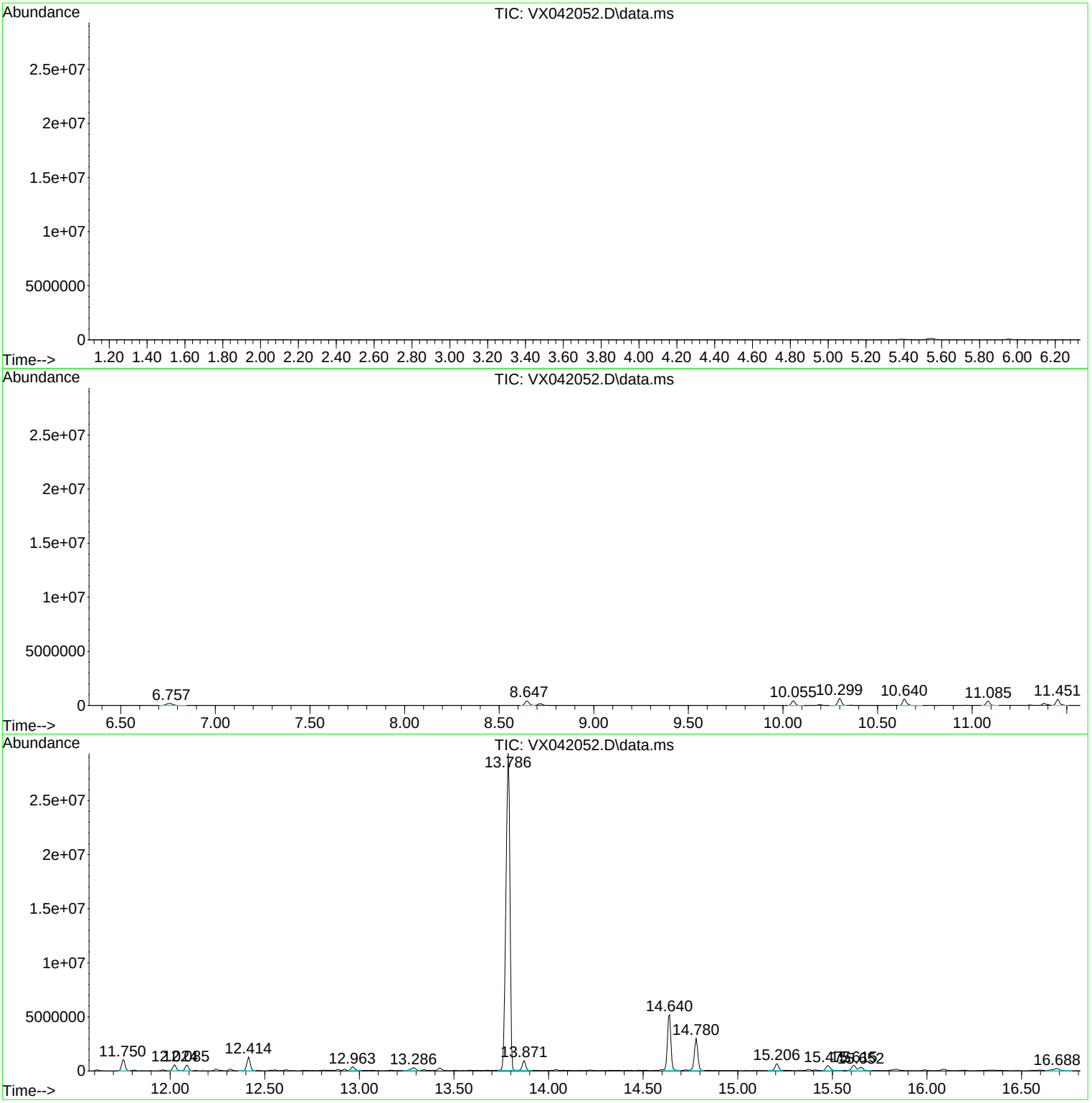
Sample : P3045-07
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
9AB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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



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Data File : VX042052.D
Acq On : 26 Jun 2024 14:50
Operator : JC/MD
Sample : P3045-07
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
9AB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

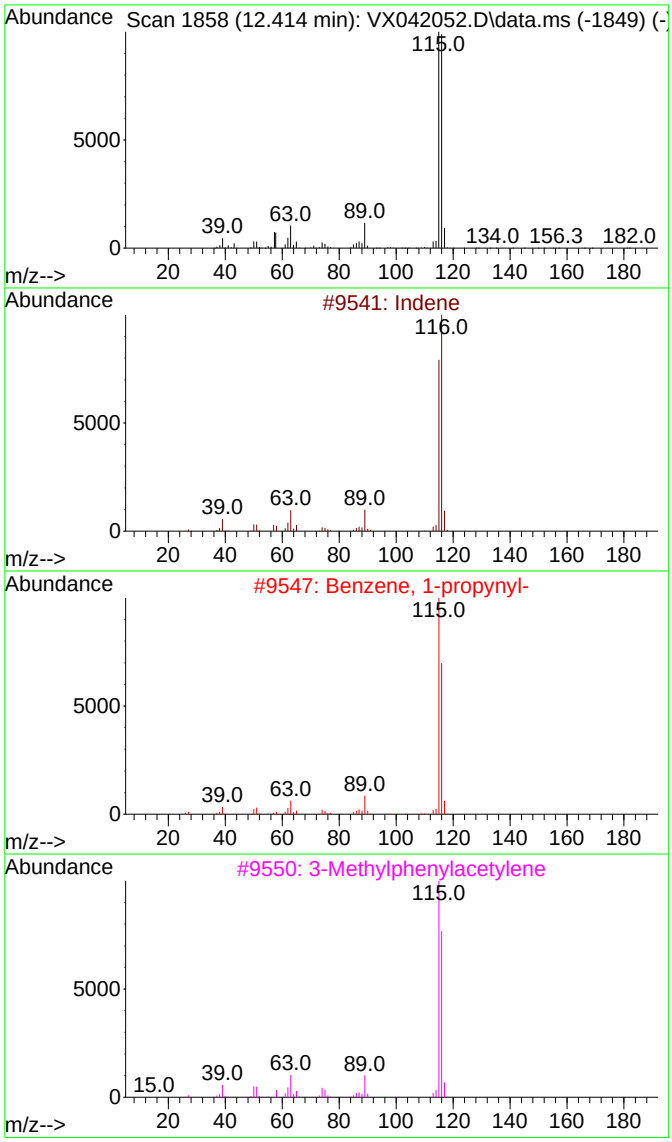
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

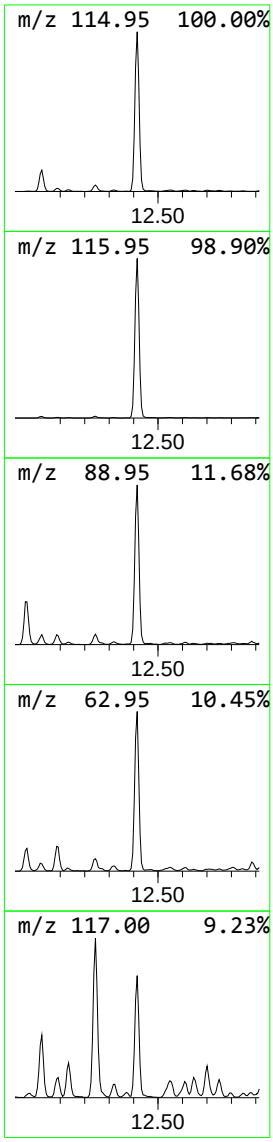
****

Peak Number 2 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	112.07 ug/l	1587470	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5	2-Methylphenylacetylene	116	C9H8	000766-47-2	90





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Data File : VX042052.D
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Operator : JC/MD
Sample : P3045-07
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
9AB

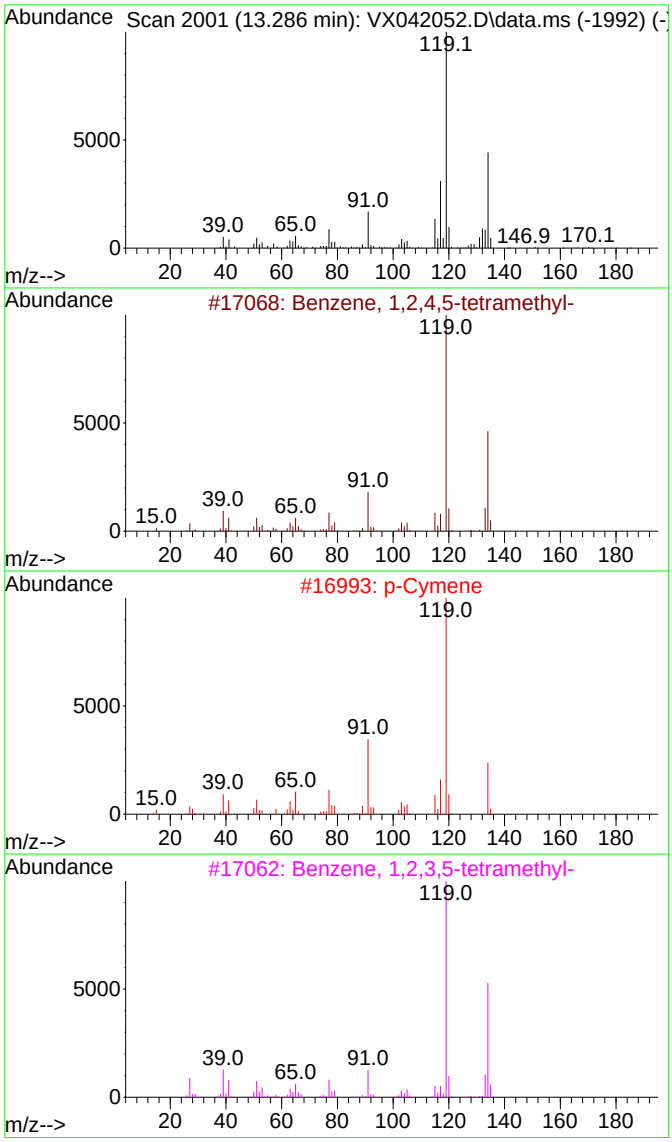
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

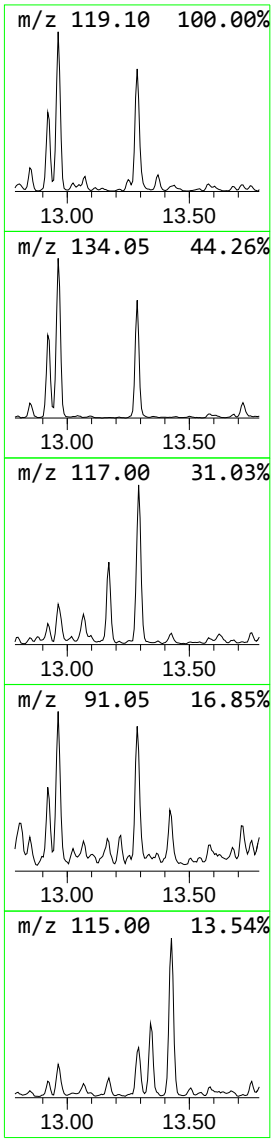
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	34.97 ug/l	495373	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	81
2	p-Cymene	134	C10H14	000099-87-6	81
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	81
5	o-Cymene	134	C10H14	000527-84-4	81





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Data File : VX042052.D
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Operator : JC/MD
Sample : P3045-07
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
9AB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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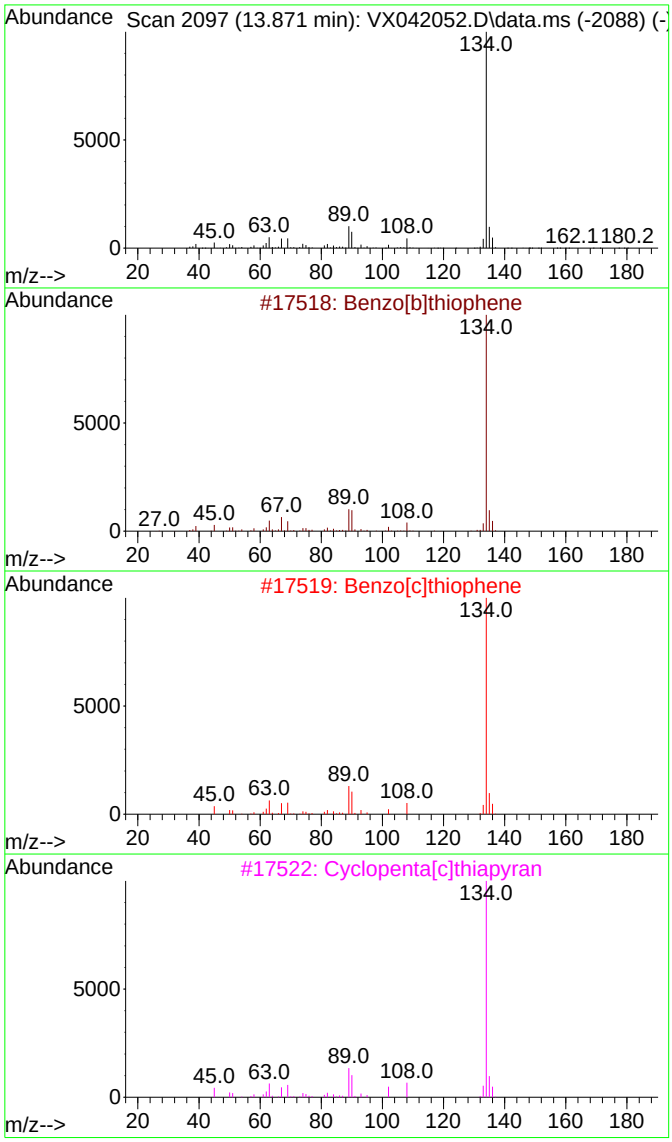
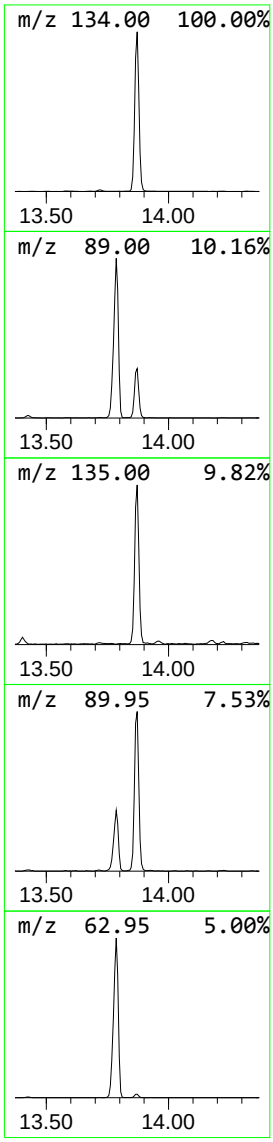
****

Peak Number 4 Benzo[b]thiophene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	79.78 ug/l	1130120	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]thiophene	134	C8H6S	000095-15-8	95
2	Benzo[c]thiophene	134	C8H6S	000270-82-6	94
3	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
4	Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	50
5	3-Deazaadenine	134	C6H6N4	006811-77-4	50





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Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
9AB

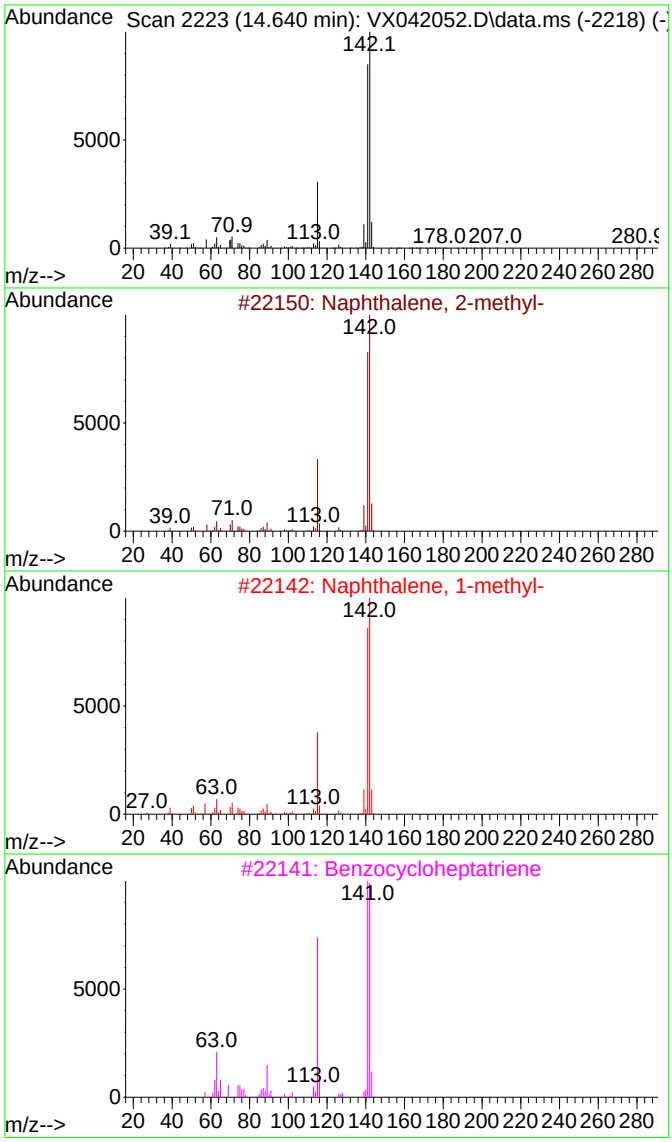
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

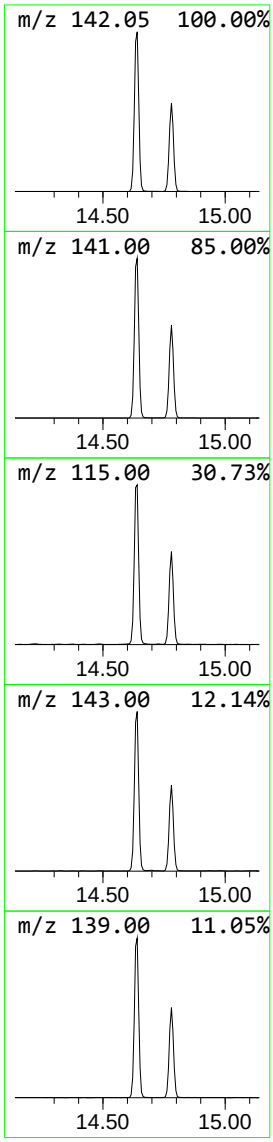
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	465.19 ug/l	6589660	1,4-Dichlorobenzene-d4	12.024

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	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
Data File : VX042052.D
Acq On : 26 Jun 2024 14:50
Operator : JC/MD
Sample : P3045-07
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
9AB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

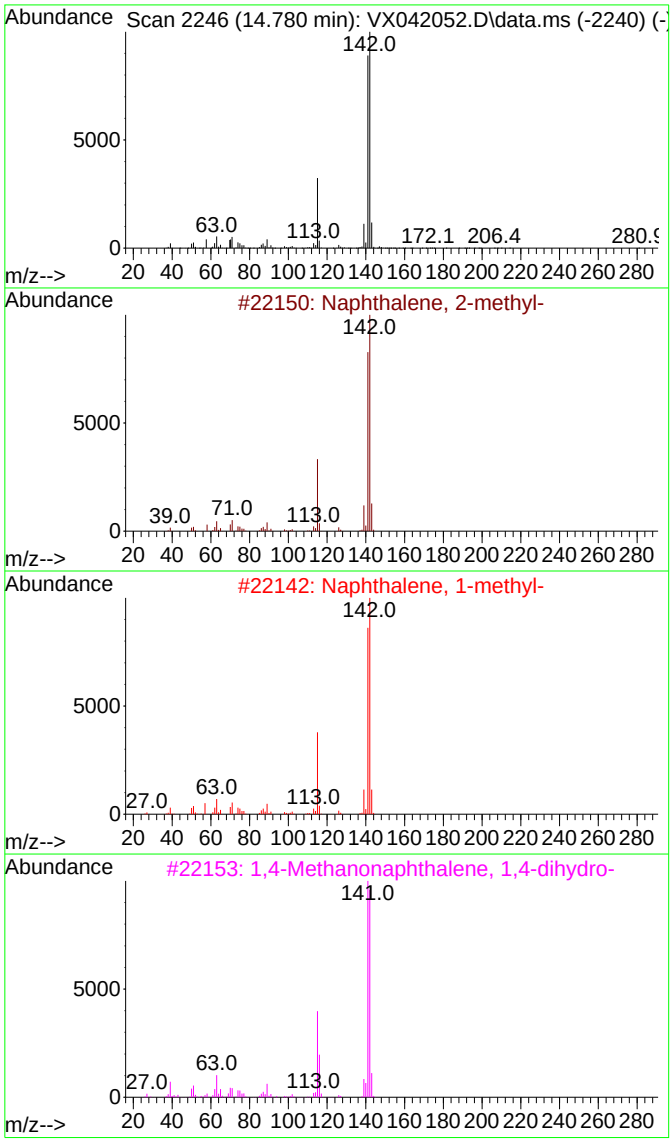
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

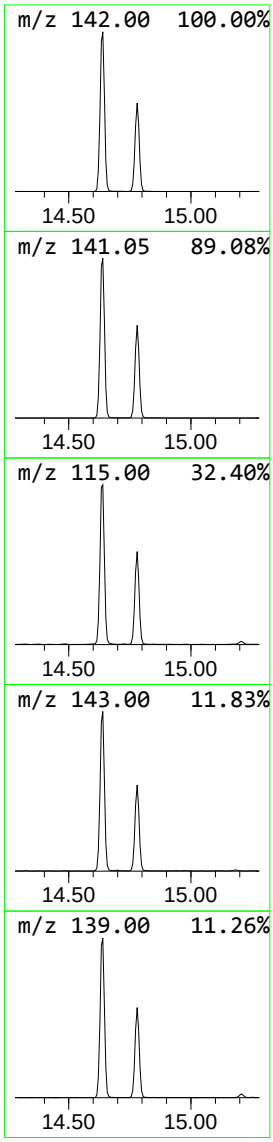
****

Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	263.92 ug/l	3738610	1,4-Dichlorobenzene-d4	12.024

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	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	50





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Operator : JC/MD
Sample : P3045-07
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
9AB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

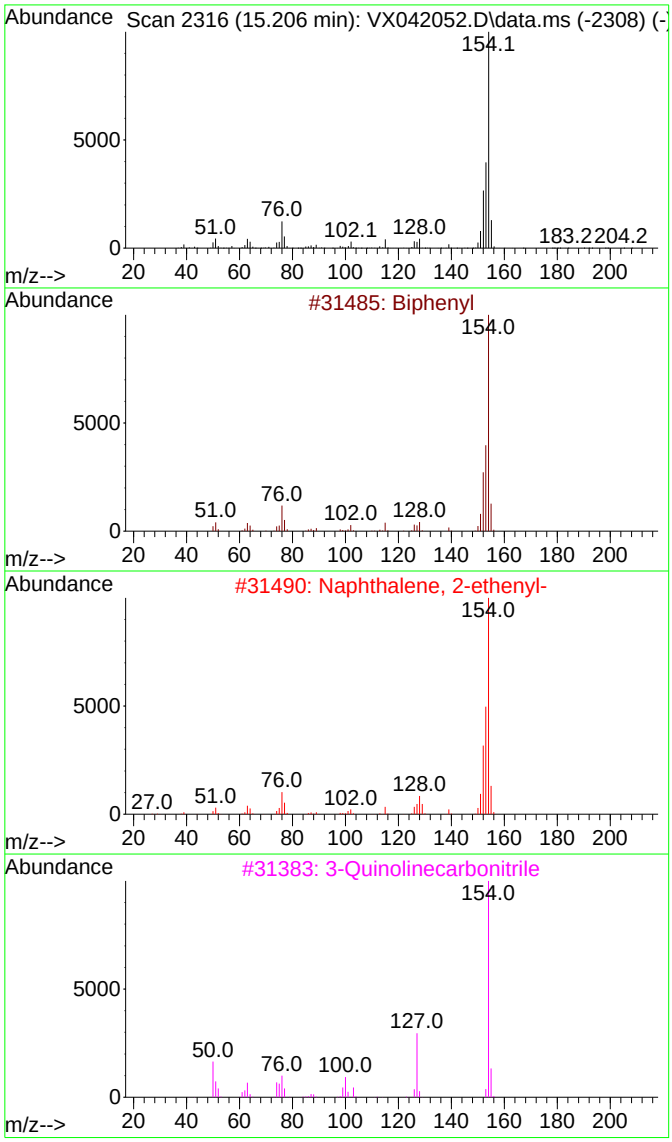
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

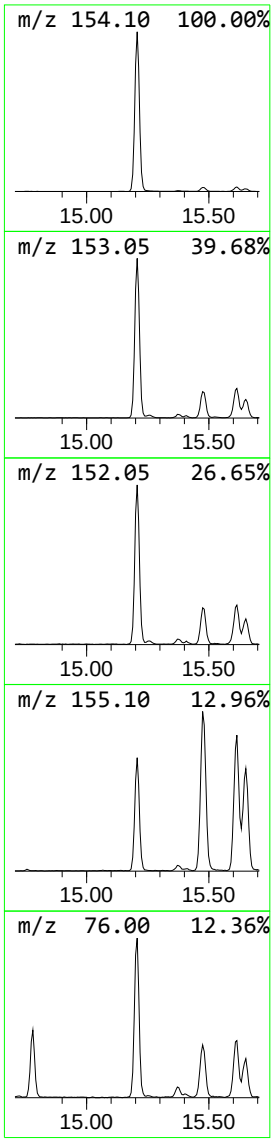
****

Peak Number 7 Biphenyl Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.207	61.78 ug/l	875090	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Biphenyl	154	C12H10	000092-52-4	95
2	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	87
3	3-Quinolinecarbonitrile	154	C10H6N2	034846-64-5	47
4	Acenaphthene	154	C12H10	000083-32-9	47
5	1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	45





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Instrument :
MSVOA_X
ClientSampleId :
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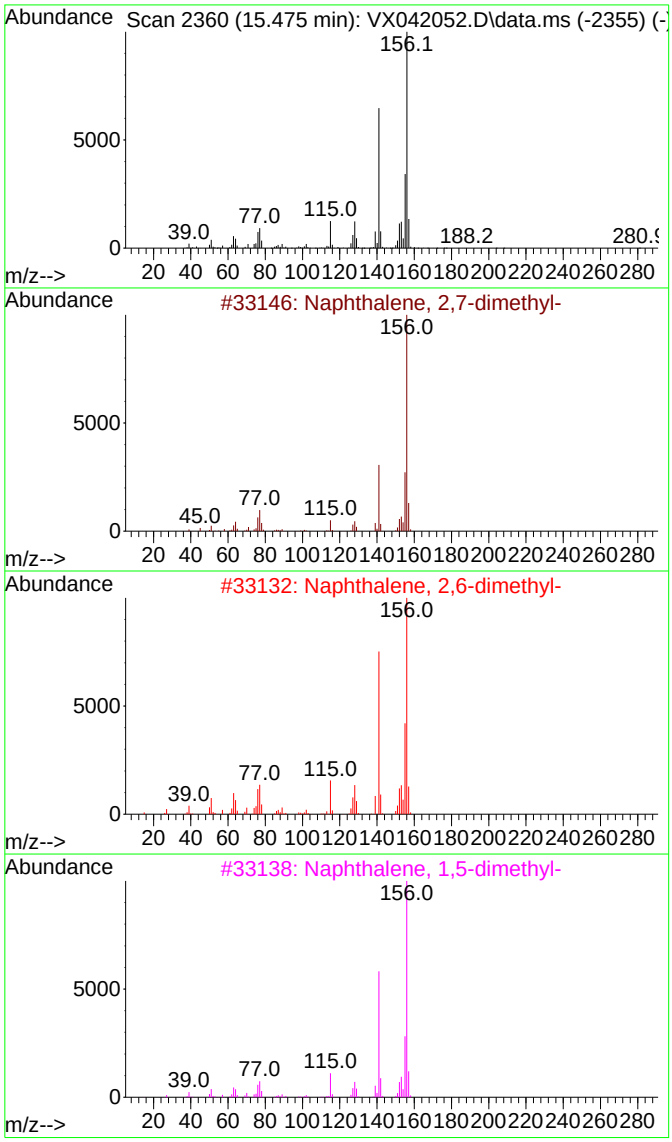
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

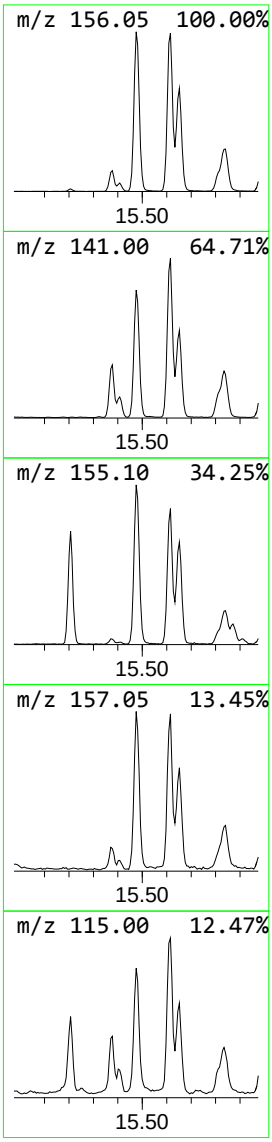
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 2,7-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	54.91 ug/l	777788	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

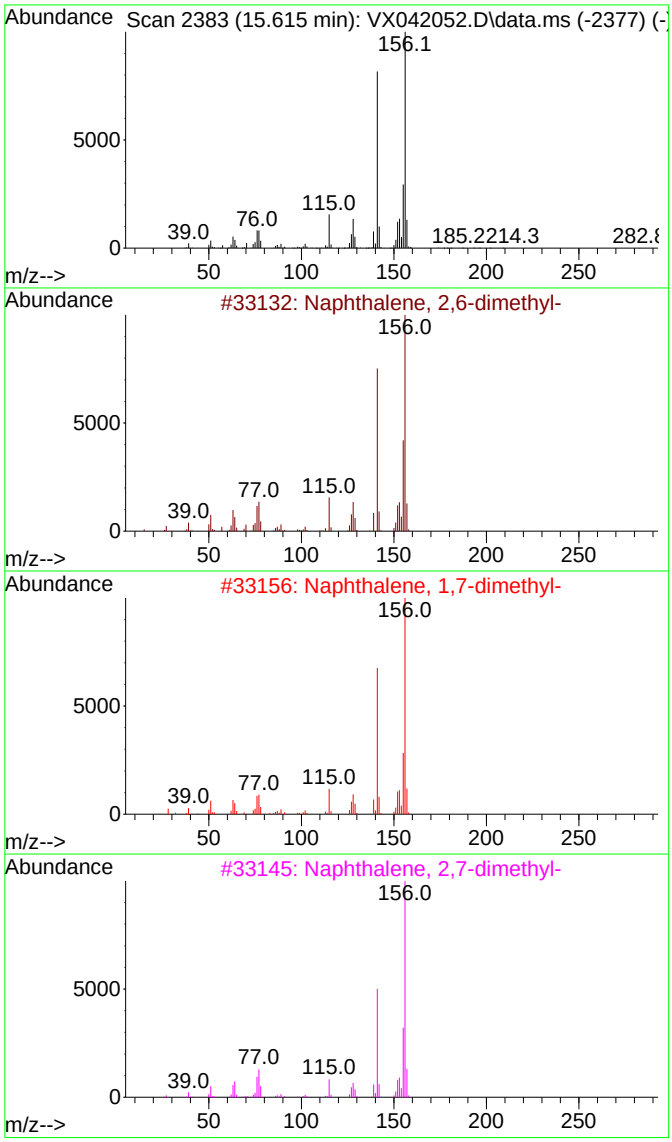
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

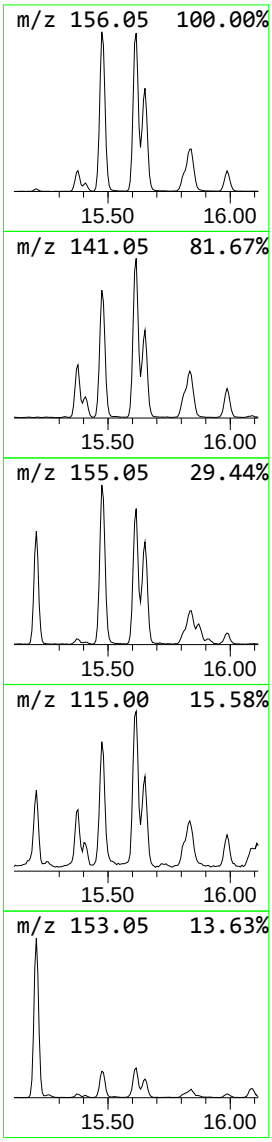
****

Peak Number 9 Naphthalene, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	56.16 ug/l	795488	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
4	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
9AB

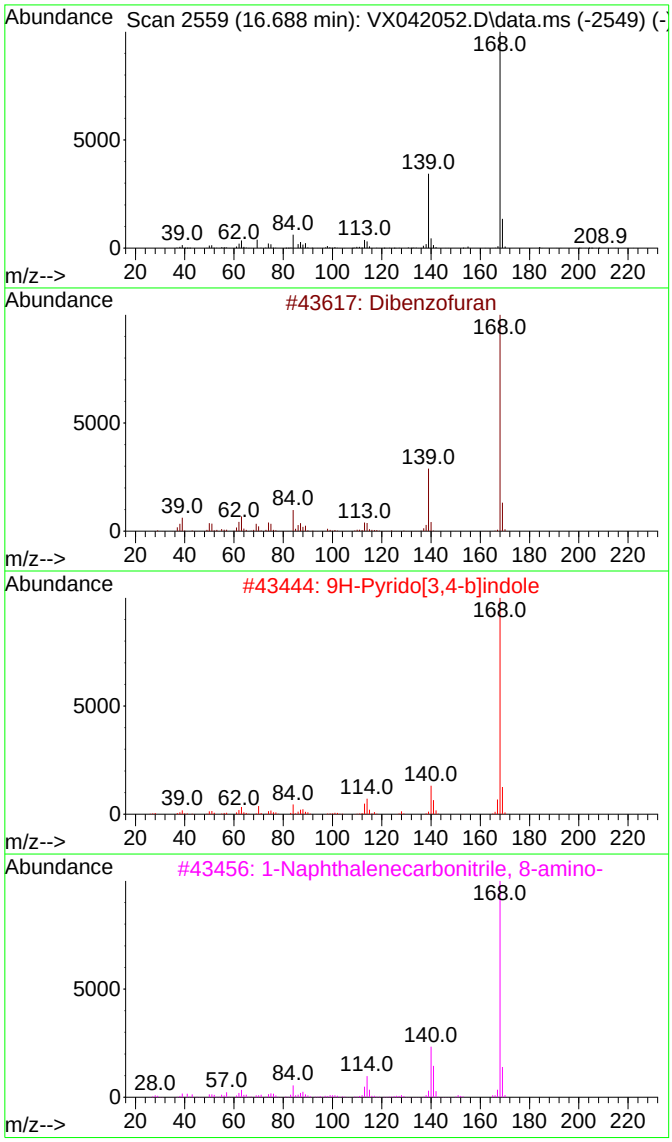
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

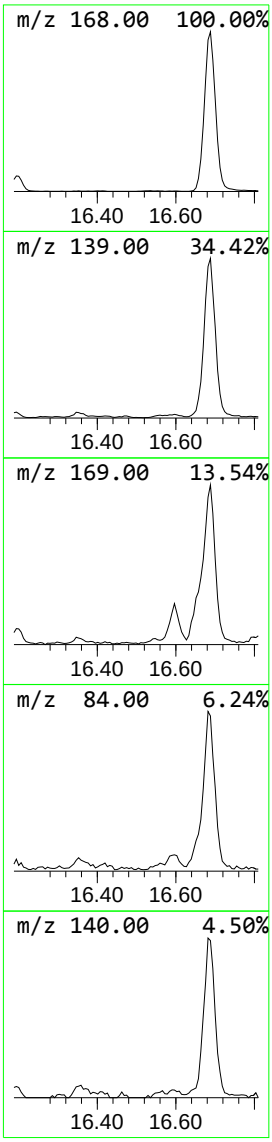
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Dibenzofuran Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.688	38.62 ug/l	547006	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzofuran	168	C12H8O	000132-64-9	87
2	9H-Pyrido[3,4-b]indole	168	C11H8N2	000244-63-3	64
3	1-Naphthalenecarbonitrile, 8-amino-	168	C11H8N2	038515-13-8	59
4	3,5-Dimethoxybenzyl alcohol	168	C9H12O3	000705-76-0	56
5	Naphtho[2,1-d]imidazole	168	C11H8N2	000233-53-4	53





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
Indene	12.414	112.1	ug/l	1587470	4	12.024	708277	50.0
Benzene, 1,2,4,...	13.286	35.0	ug/l	495373	4	12.024	708277	50.0
Benzo[b]thiophene	13.871	79.8	ug/l	1130120	4	12.024	708277	50.0
Naphthalene, 2-...	14.640	465.2	ug/l	6589660	4	12.024	708277	50.0
Naphthalene, 1-...	14.780	263.9	ug/l	3738610	4	12.024	708277	50.0
Biphenyl	15.207	61.8	ug/l	875090	4	12.024	708277	50.0
Naphthalene, 2,...	15.475	54.9	ug/l	777788	4	12.024	708277	50.0
Naphthalene, 2,...	15.615	56.2	ug/l	795488	4	12.024	708277	50.0
Dibenzofuran	16.688	38.6	ug/l	547006	4	12.024	708277	50.0