LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
Data File : VX042051.D
Acq On : 26 Jun 2024 14:26
Operator : JC/MD
Sample : P3045-05
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
8AB

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: VX042051.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.647	1234	1240	1246	rBV	411670	629396	1.24%	0.796%
2	10.055	1466	1471	1481	rBV	414089	581870	1.14%	0.736%
3	10.299	1503	1511	1517	rBV	951485	1259692	2.48%	1.593%
4	10.640	1562	1567	1581	rVB	813775	1149699	2.26%	1.454%
5	11.079	1634	1639	1649	rBV	382404	532081	1.05%	0.673%
6	11.451	1695	1700	1710	rVB	713803	939041	1.85%	1.188%
7	11.750	1745	1749	1755	rBV	1346930	1626195	3.20%	2.057%
8	12.024	1789	1794	1800	rBV	550904	714193	1.41%	0.903%
9	12.085	1800	1804	1809	rVB	676727	825491	1.62%	1.044%
10	12.414	1848	1858	1863	rBV	1616620	2081511	4.10%	2.633%
11	12.963	1944	1948	1956	rVB2	451315	607539	1.20%	0.768%
12	13.286	1991	2001	2007	rBV3	329692	622066	1.22%	0.787%
13	13.786	2075	2083	2088	rBV2	31820989	50821898	100.00%	64.282%
14	13.871	2088	2097	2104	rVB	1068401	1361767	2.68%	1.722%
15	14.640	2218	2223	2232	rVB	6191561	7697625	15.15%	9.736%
16	14.780	2240	2246	2254	rVB	3501192	4346205	8.55%	5.497%
17	15.206	2307	2316	2321	rBV	725119	1003091	1.97%	1.269%
18	15.475	2355	2360	2373	rVV	521002	864093	1.70%	1.093%
19	15.615	2377	2383	2386	rVV	552609	888796	1.75%	1.124%
20	15.652	2386	2389	2397	rVB	355819	509070	1.00%	0.644%

Sum of corrected areas: 79061319

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
Data File : VX042051.D
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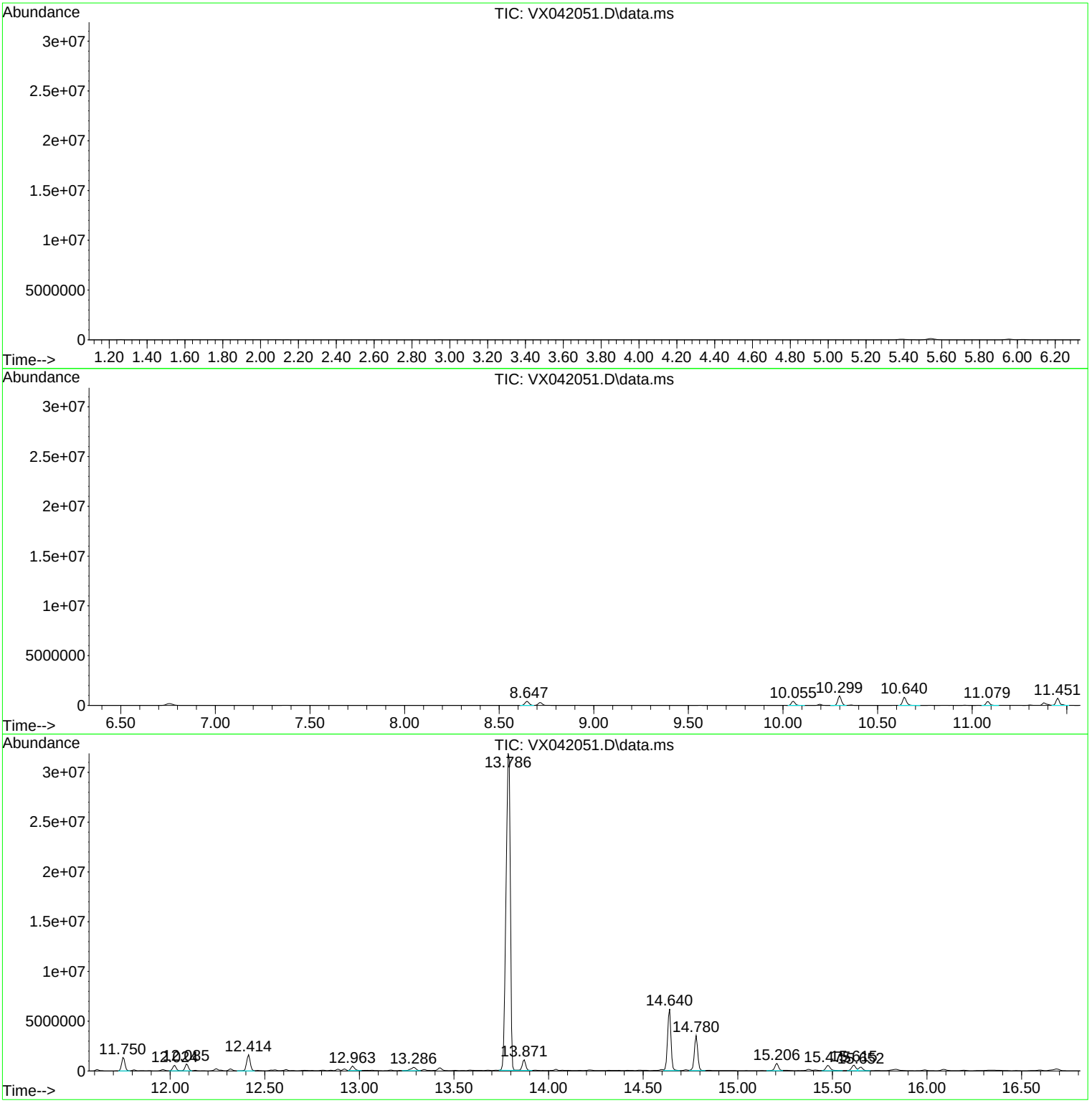
Operator : JC/MD
Sample : P3045-05
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
8AB

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
Data File : VX042051.D
Acq On : 26 Jun 2024 14:26
Operator : JC/MD
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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

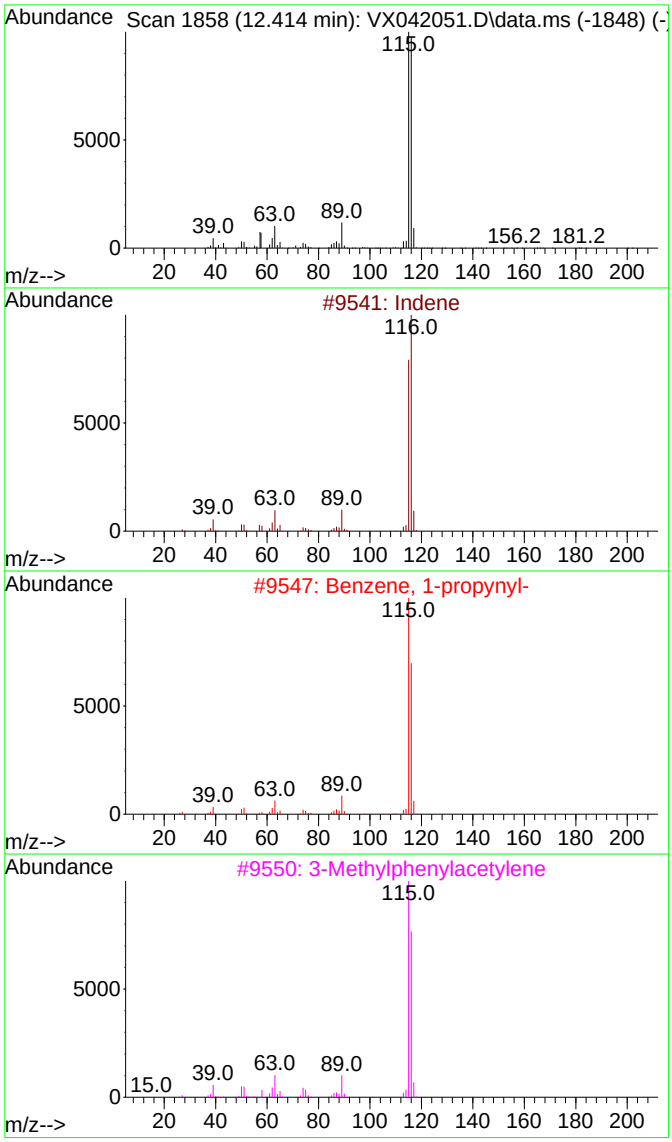
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

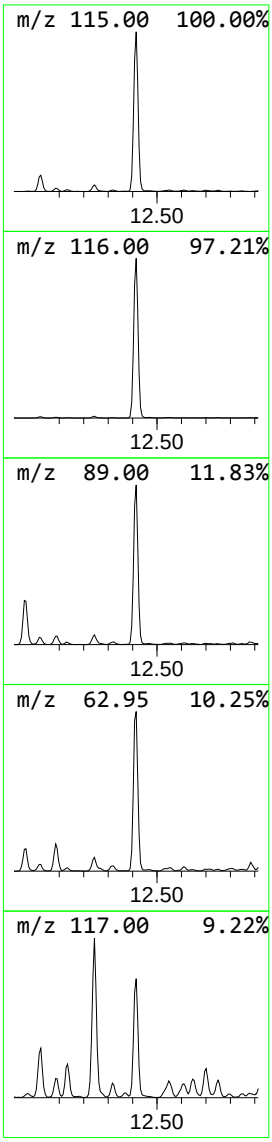
****

Peak Number 2 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	145.72 ug/l	2081510	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	90
5	2-Methylphenylacetylene	116	C9H8	000766-47-2	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
Data File : VX042051.D
Acq On : 26 Jun 2024 14:26
Operator : JC/MD
Sample : P3045-05
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
8AB

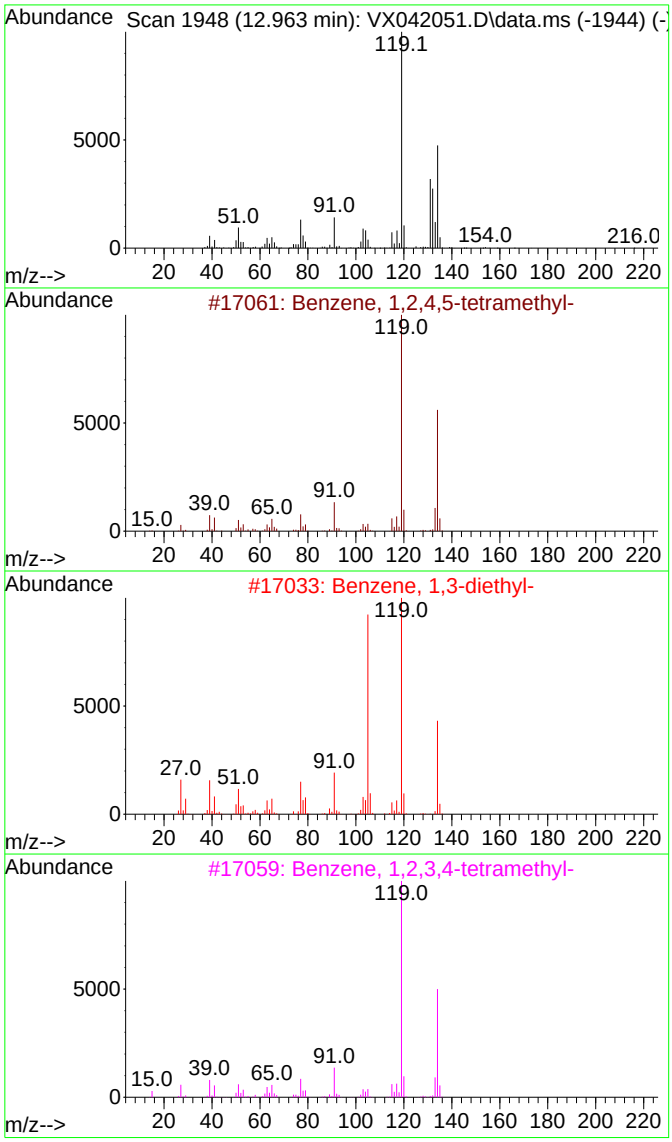
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

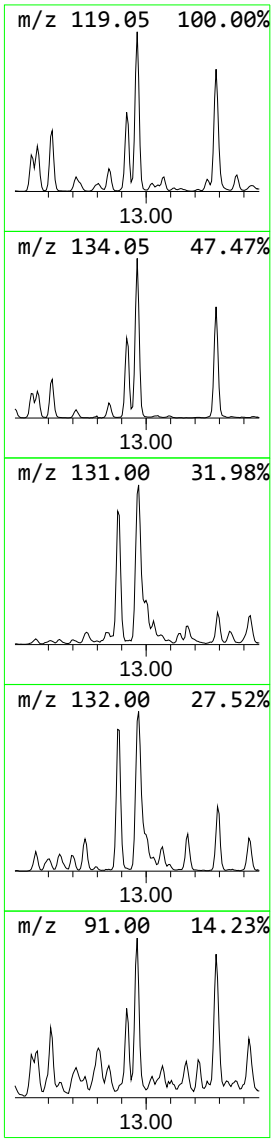
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	42.53 ug/l	607539	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	76
2	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	76
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	76
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	76
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	76





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Data File : VX042051.D
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Operator : JC/MD
Sample : P3045-05
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
8AB

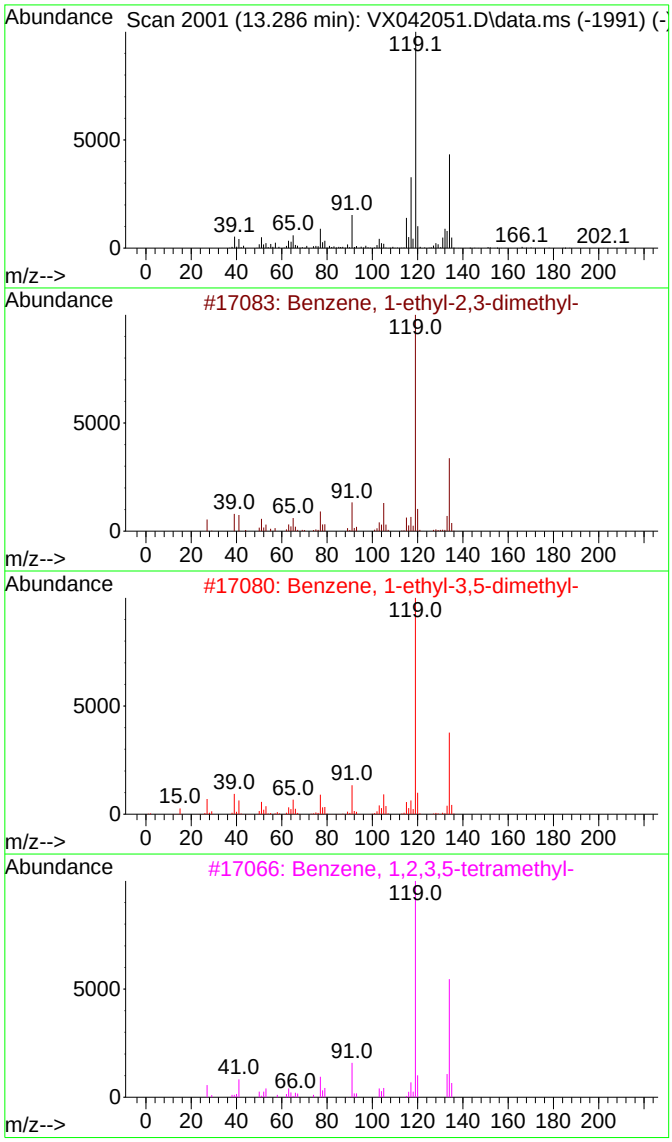
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

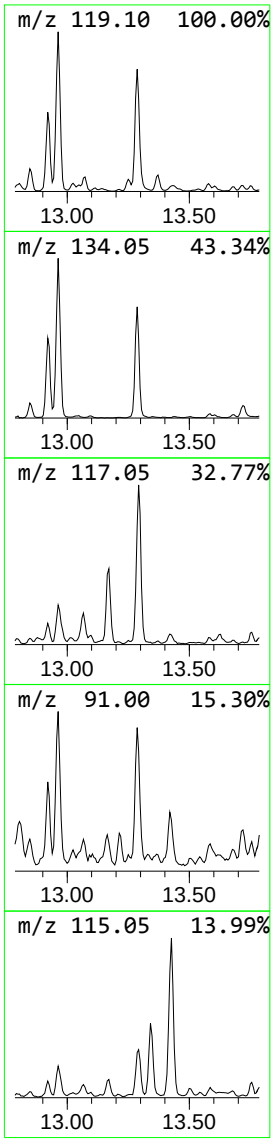
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	43.55 ug/l	622066	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	87
2	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	87
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	87
4	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	83
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	83





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Data File : VX042051.D
Acq On : 26 Jun 2024 14:26
Operator : JC/MD
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Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
8AB

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

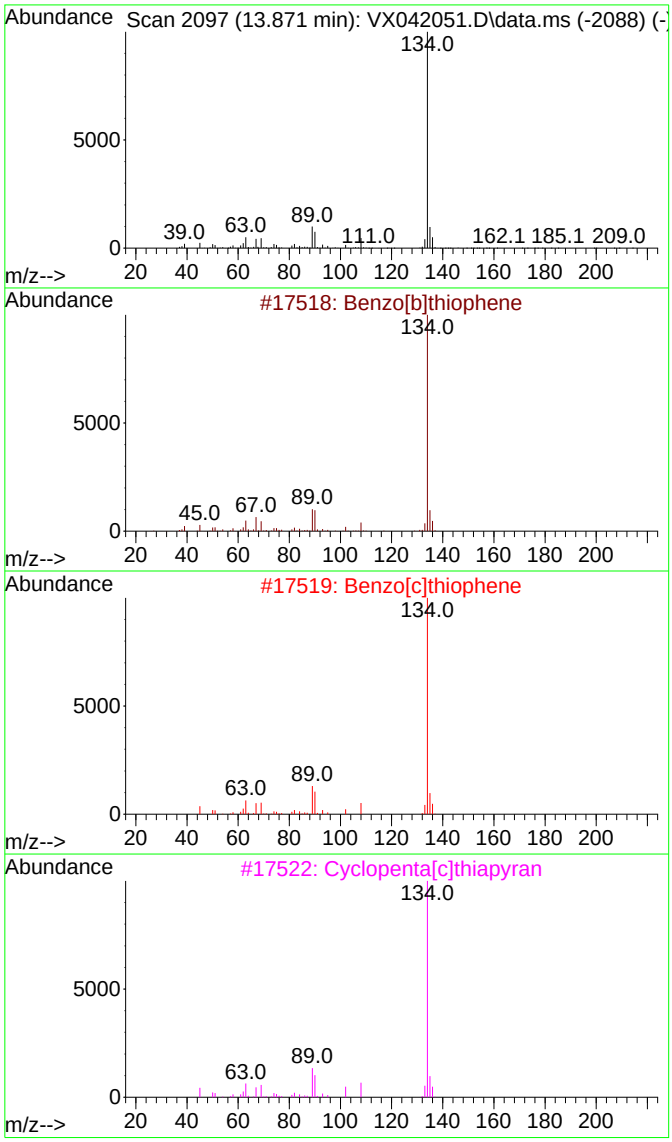
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

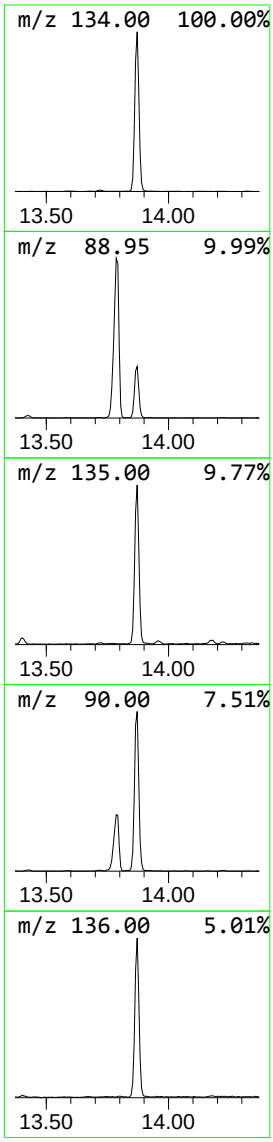
****

Peak Number 5 Benzo[b]thiophene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	95.34 ug/l	1361770	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]thiophene	134	C8H6S	000095-15-8	94
2	Benzo[c]thiophene	134	C8H6S	000270-82-6	94
3	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	78
4	[1]Benzothieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	64
5	Benzaldehyde, 4-ethyl-	134	C9H10O	004748-78-1	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
Data File : VX042051.D
Acq On : 26 Jun 2024 14:26
Operator : JC/MD
Sample : P3045-05
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
8AB

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

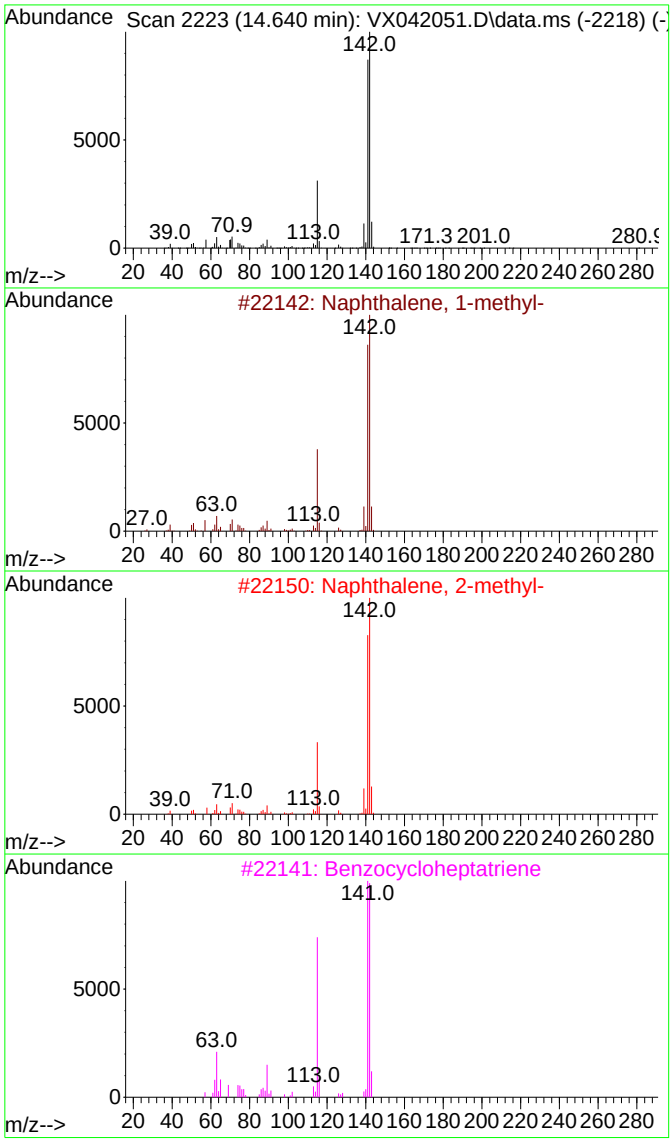
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

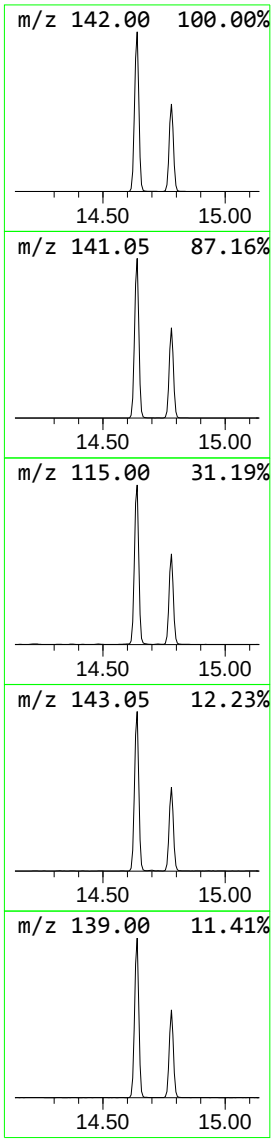
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	538.90 ug/l	7697630	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	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





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Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
8AB

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

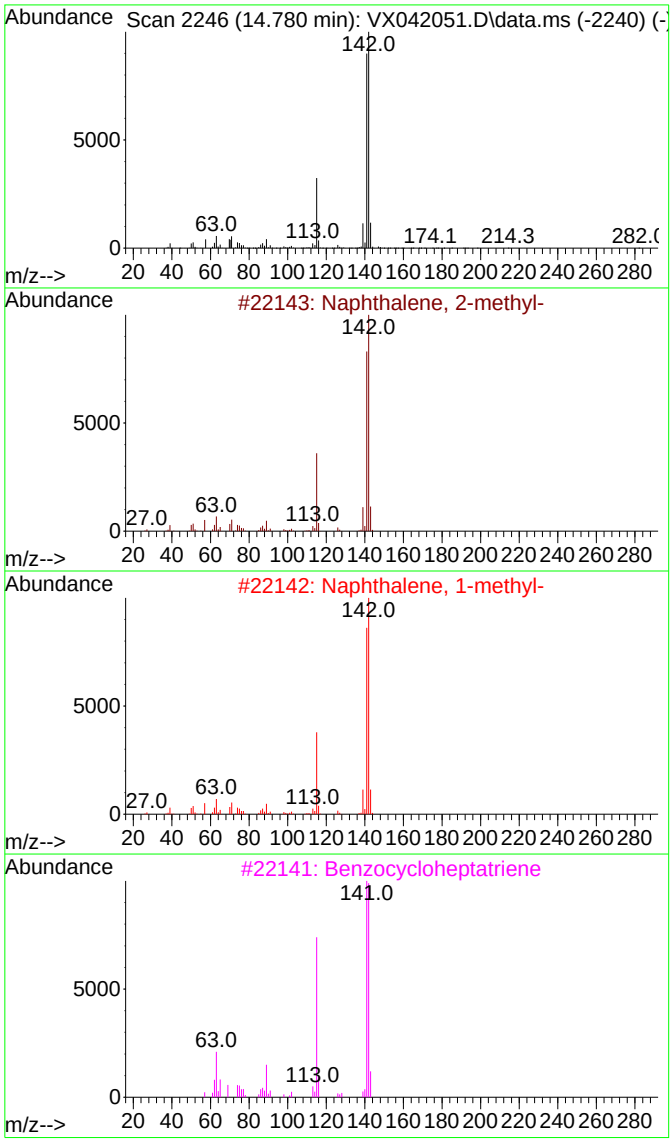
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

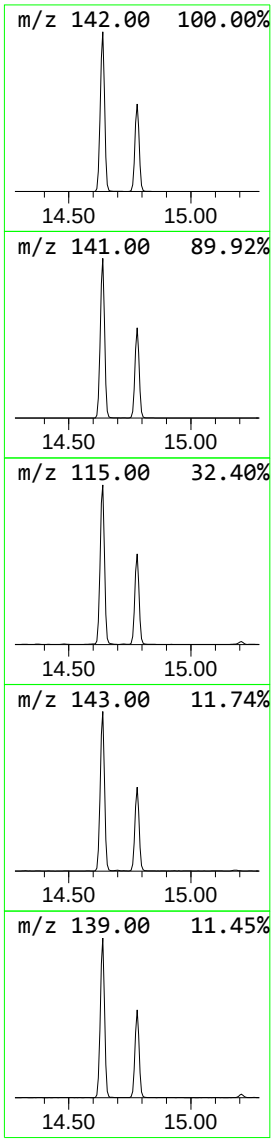
****

Peak Number 7 Naphthalene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	304.27 ug/l	4346210	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	49





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

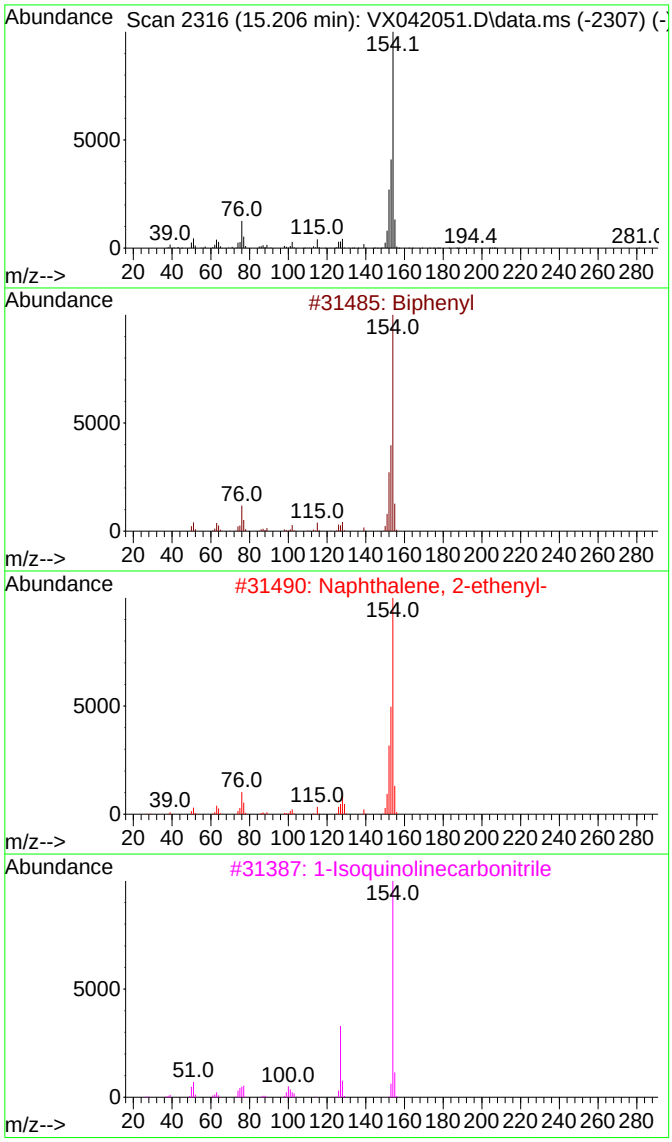
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

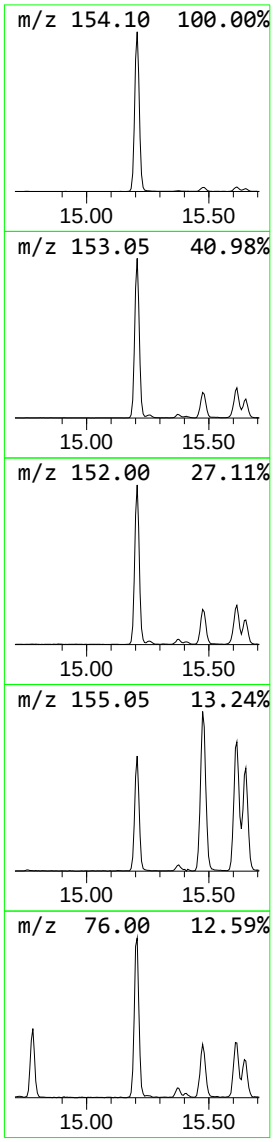
****

Peak Number 8 Biphenyl Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.207	70.23 ug/l	1003090	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	1-Isoquinolinecarbonitrile	154	C10H6N2	001198-30-7	47
4	3-Quinolinecarbonitrile	154	C10H6N2	034846-64-5	47
5	1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	45





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Instrument :
MSVOA_X
ClientSampleId :
8AB

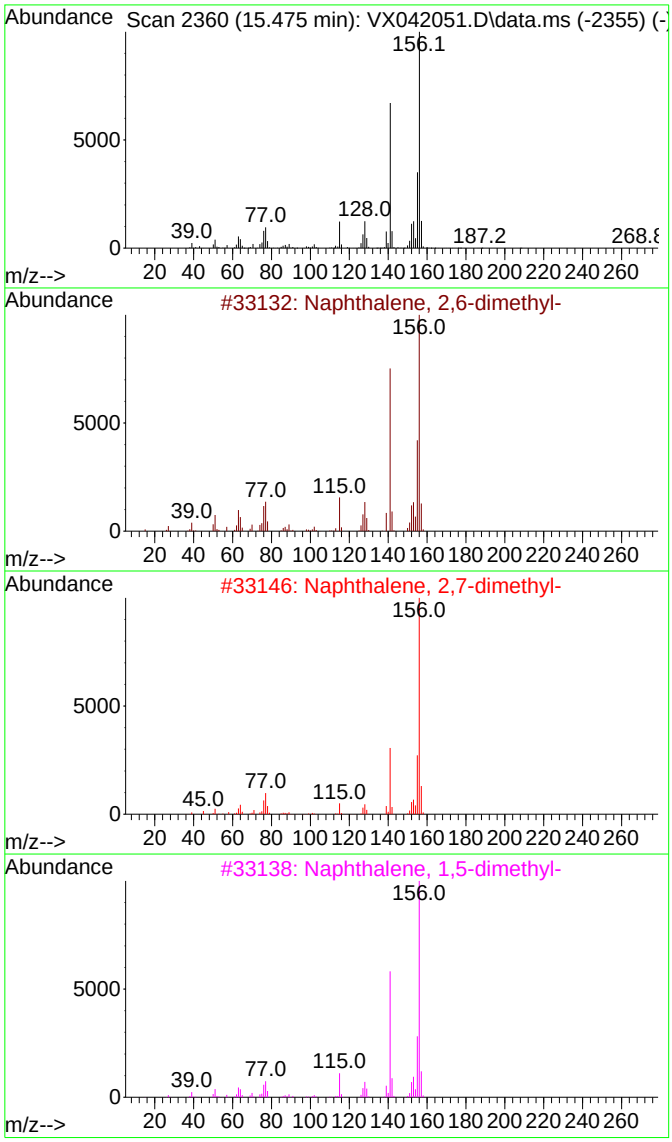
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

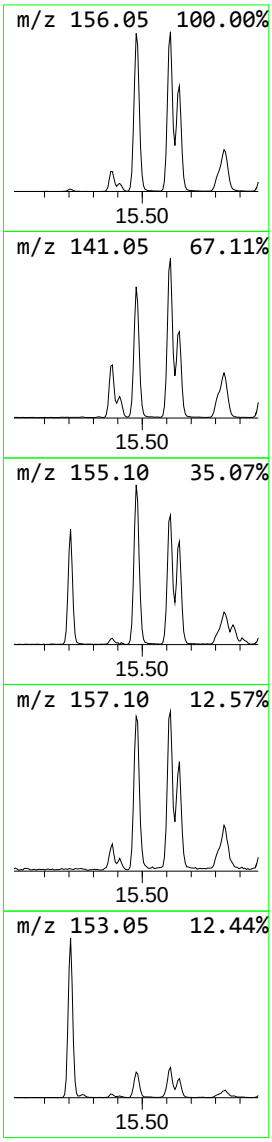
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	60.49 ug/l	864093	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	98
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97





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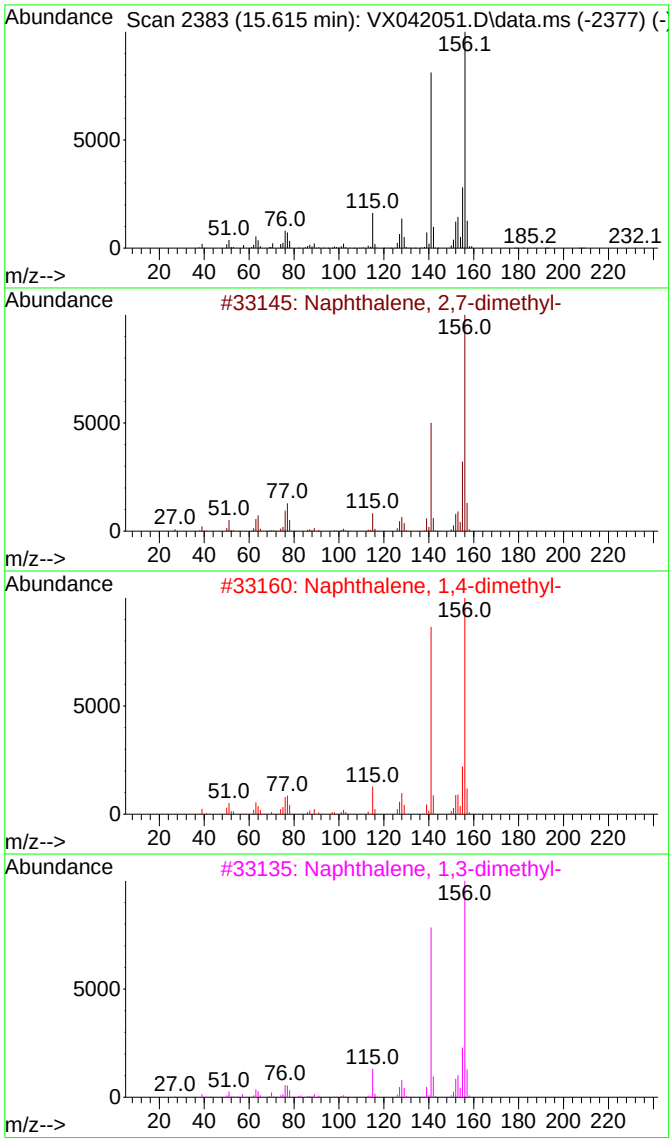
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

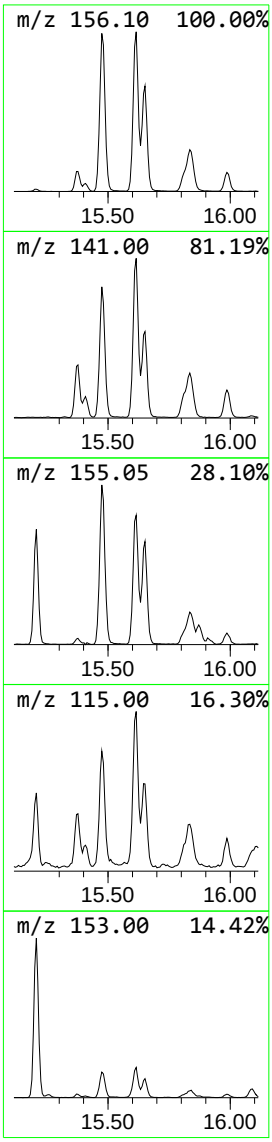
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 2,7-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	62.22 ug/l	888796	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, 1,4-dimethyl-	156	C12H12	000571-58-4	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Indene	12.414	145.7	ug/l	2081510	4	12.024	714193	50.0
Benzene, 1,2,4,...	12.963	42.5	ug/l	607539	4	12.024	714193	50.0
Benzene, 1-ethy...	13.286	43.5	ug/l	622066	4	12.024	714193	50.0
Benzo[b]thiophene	13.871	95.3	ug/l	1361770	4	12.024	714193	50.0
Naphthalene, 1-...	14.640	538.9	ug/l	7697630	4	12.024	714193	50.0
Naphthalene, 2-...	14.780	304.3	ug/l	4346210	4	12.024	714193	50.0
Biphenyl	15.207	70.2	ug/l	1003090	4	12.024	714193	50.0
Naphthalene, 2,...	15.475	60.5	ug/l	864093	4	12.024	714193	50.0
Naphthalene, 2,...	15.615	62.2	ug/l	888796	4	12.024	714193	50.0