LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043594.D
Acq On : 06 May 2021 19:26
Operator : SY/MD
Sample : M2295-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DRUM-B-C-E

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_U\Method\82U050621W.M
Title : SW846 8260

Signal : TIC: VU043594.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.629	386	401	430	rBV	349683	589257	6.25%	3.091%
2	5.382	1243	1257	1277	rVB	178765	361569	3.83%	1.896%
3	5.710	1343	1359	1374	rBV	159358	321455	3.41%	1.686%
4	6.256	1513	1529	1546	rBV	287546	534180	5.66%	2.802%
5	7.906	2027	2042	2056	rBV	480493	815317	8.64%	4.276%
6	9.423	2501	2514	2534	rBV	419532	673503	7.14%	3.532%
7	9.578	2549	2562	2579	rVB	104515	164295	1.74%	0.862%
8	9.700	2586	2600	2612	rBV	199320	327263	3.47%	1.716%
9	10.108	2716	2727	2744	rVB	124336	201970	2.14%	1.059%
10	10.639	2880	2892	2912	rVB	355551	557682	5.91%	2.925%
11	11.475	3131	3152	3165	rBV	161953	251691	2.67%	1.320%
12	11.735	3224	3233	3244	rVB	62973	100989	1.07%	0.530%
13	11.819	3244	3259	3274	rVB	447360	690455	7.32%	3.621%
14	11.902	3274	3285	3294	rBV	65676	101230	1.07%	0.531%
15	12.102	3325	3347	3358	rBV	1224063	2045968	21.69%	10.731%
16	12.317	3405	3414	3429	rVB	103465	164818	1.75%	0.864%
17	13.034	3626	3637	3648	rBV2	146709	280734	2.98%	1.472%
18	14.095	3950	3967	3985	rBV	5957031	9432111	100.00%	49.469%
19	14.214	3993	4004	4021	rVB	176752	296431	3.14%	1.555%
20	15.230	4309	4320	4345	rVB	315036	486140	5.15%	2.550%
21	15.417	4364	4378	4396	rBV	324771	521360	5.53%	2.734%
22	17.105	4891	4903	4916	rBV	89158	148288	1.57%	0.778%

Sum of corrected areas: 19066706

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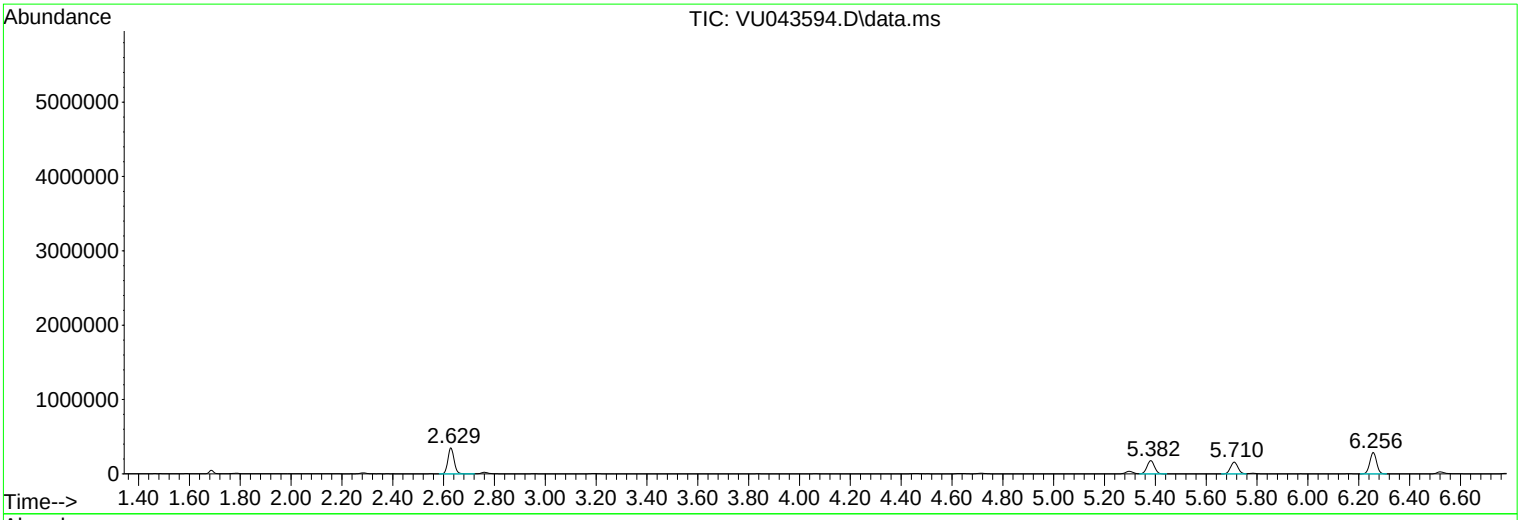
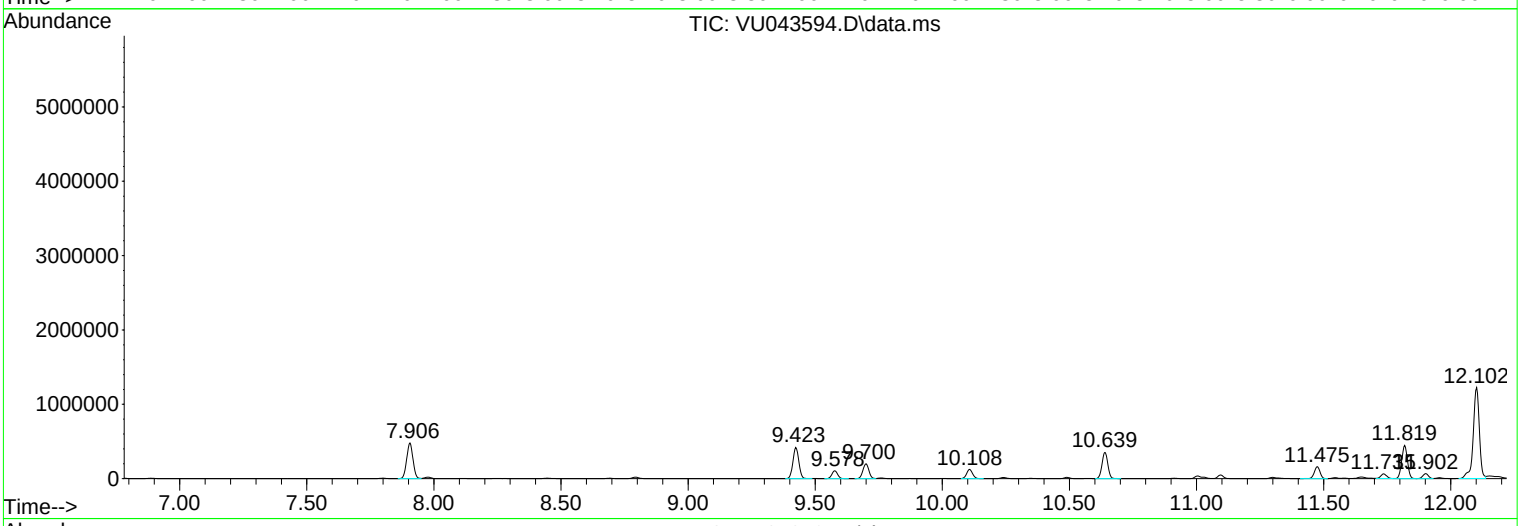
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

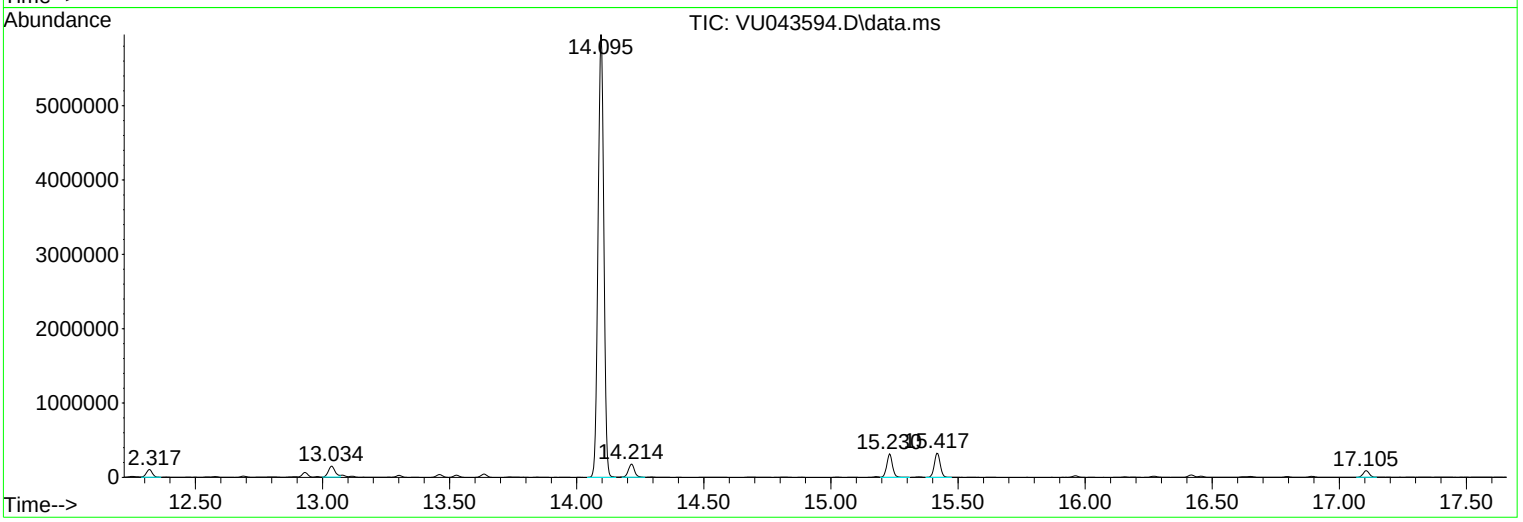
Instrument :
MSVOA_U
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

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







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Data File : VU043594.D
Acq On : 06 May 2021 19:26
Operator : SY/MD
Sample : M2295-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DRUM-B-C-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

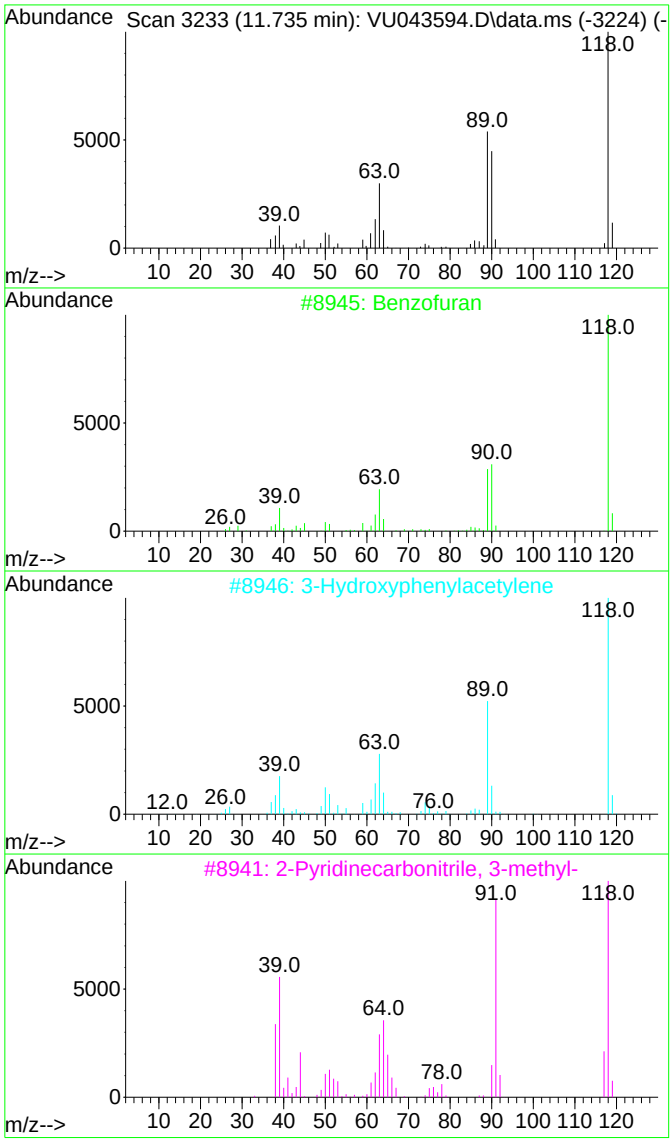
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

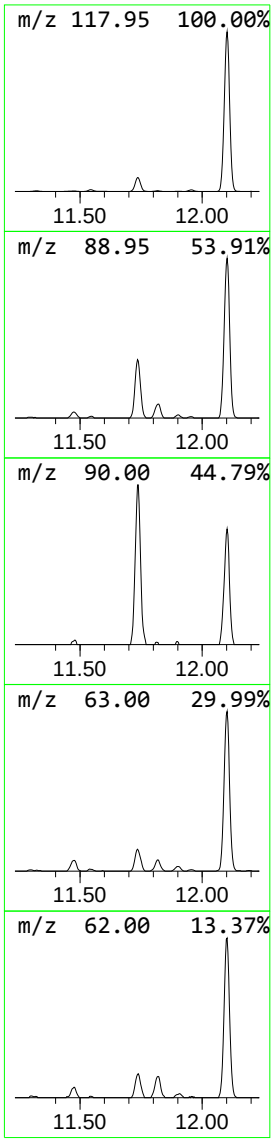
****

Peak Number 1 Benzofuran Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.735	7.31 ug/l	100989	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran	118	C8H6O	000271-89-6	91
2	3-Hydroxyphenylacetylene	118	C8H6O	010401-11-3	87
3	2-Pyridinecarbonitrile, 3-methyl-	118	C7H6N2	1000318-76-9	28
4	1H-Benzimidazole	118	C7H6N2	000051-17-2	25
5	2-Pyridylacetonitrile	118	C7H6N2	002739-97-1	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043594.D
Acq On : 06 May 2021 19:26
Operator : SY/MD
Sample : M2295-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DRUM-B-C-E

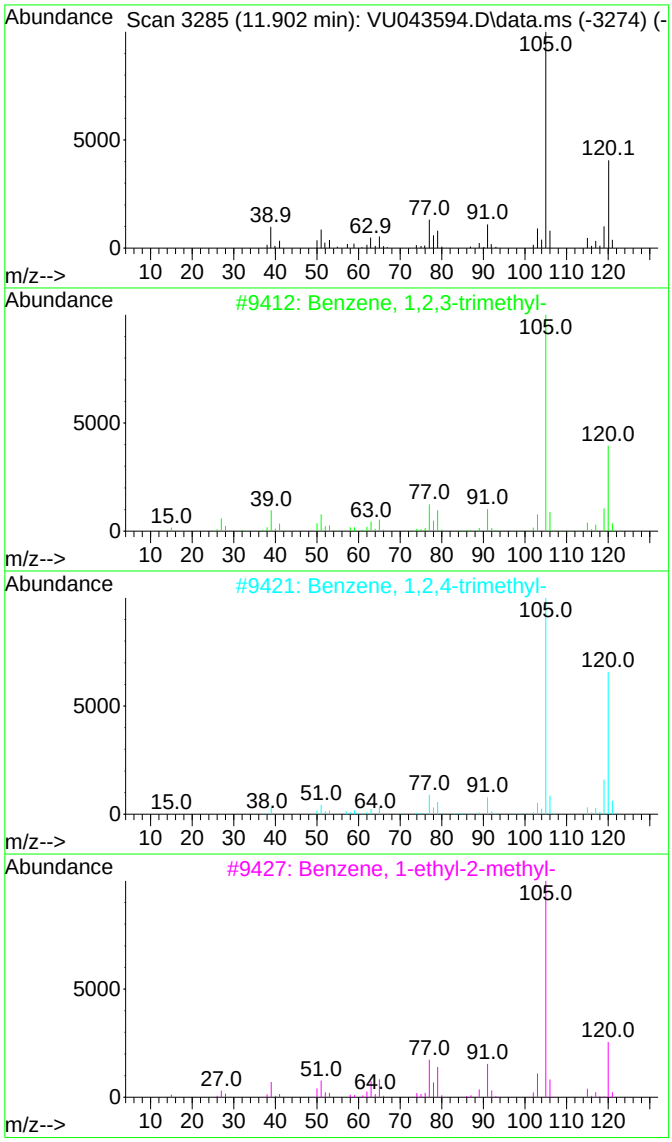
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

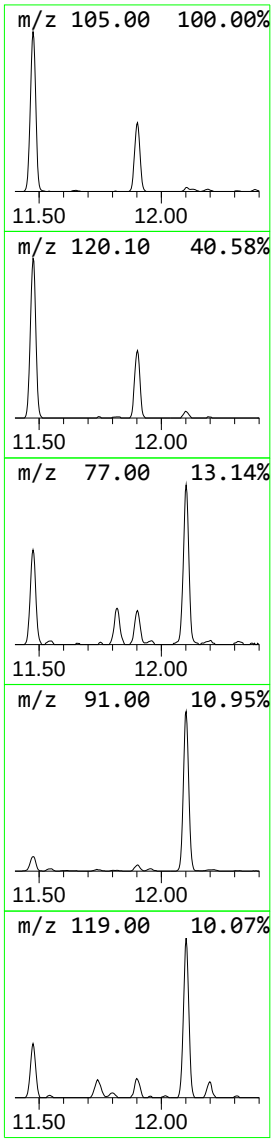
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.902	7.33 ug/l	101230	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043594.D
Acq On : 06 May 2021 19:26
Operator : SY/MD
Sample : M2295-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

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

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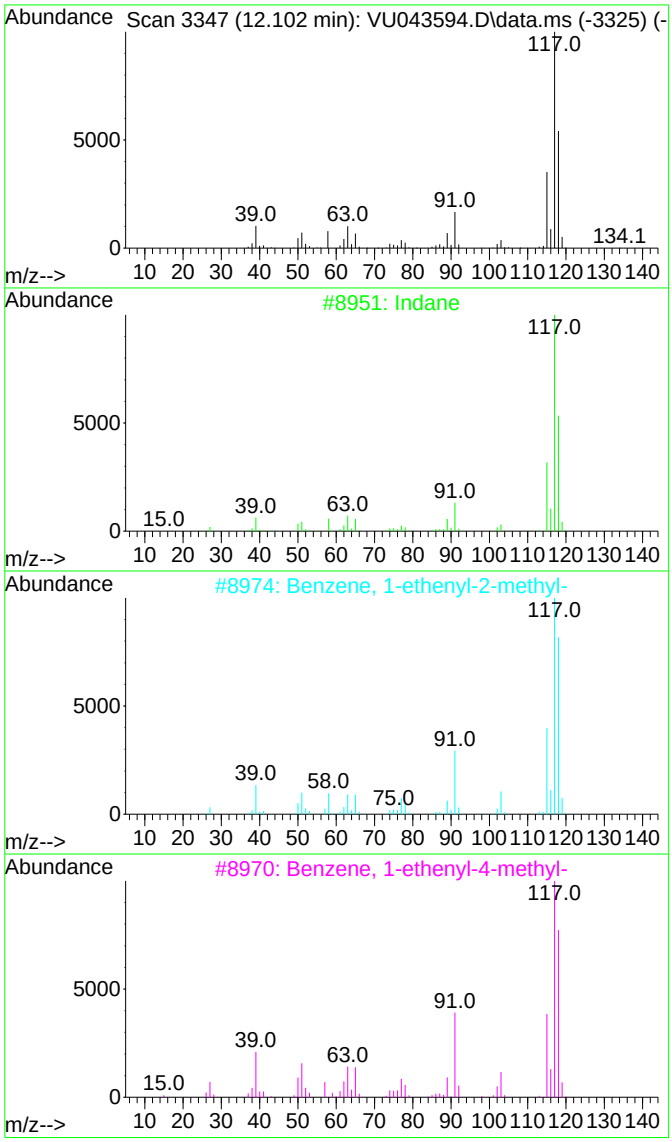
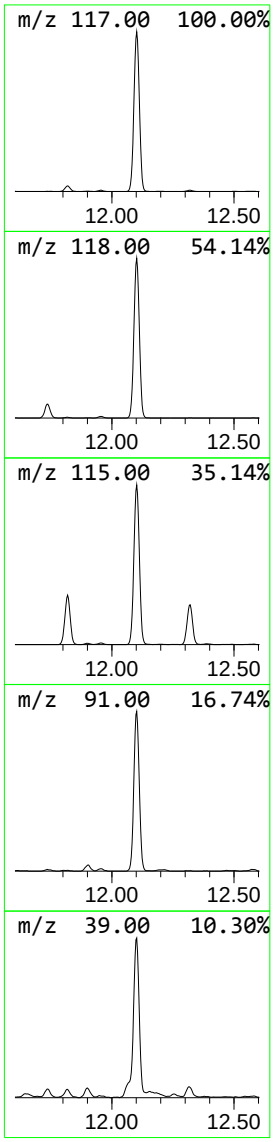
Peak Number 3 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.102	148.16 ug/l	2045970	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	83
3	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	83
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	72
5	Deltacyclene	118	C9H10	007785-10-6	68





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
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Acq On : 06 May 2021 19:26
Operator : SY/MD
Sample : M2295-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

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

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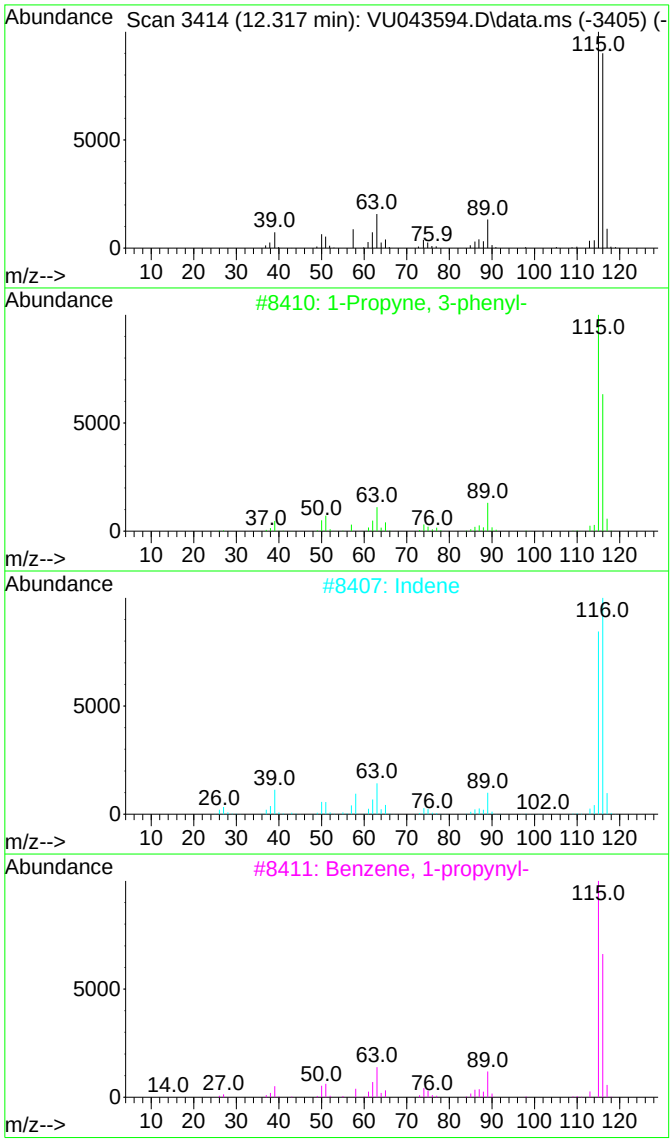
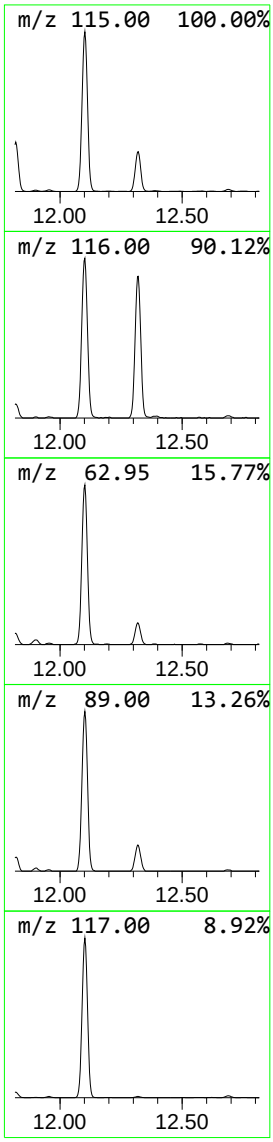
Peak Number 4 1-Propyne, 3-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	11.94 ug/l	164818	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	95
2	Indene	116	C9H8	000095-13-6	95
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
4	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5	3-Methylphenylacetylene	116	C9H8	000766-82-5	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
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Operator : SY/MD
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ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DRUM-B-C-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

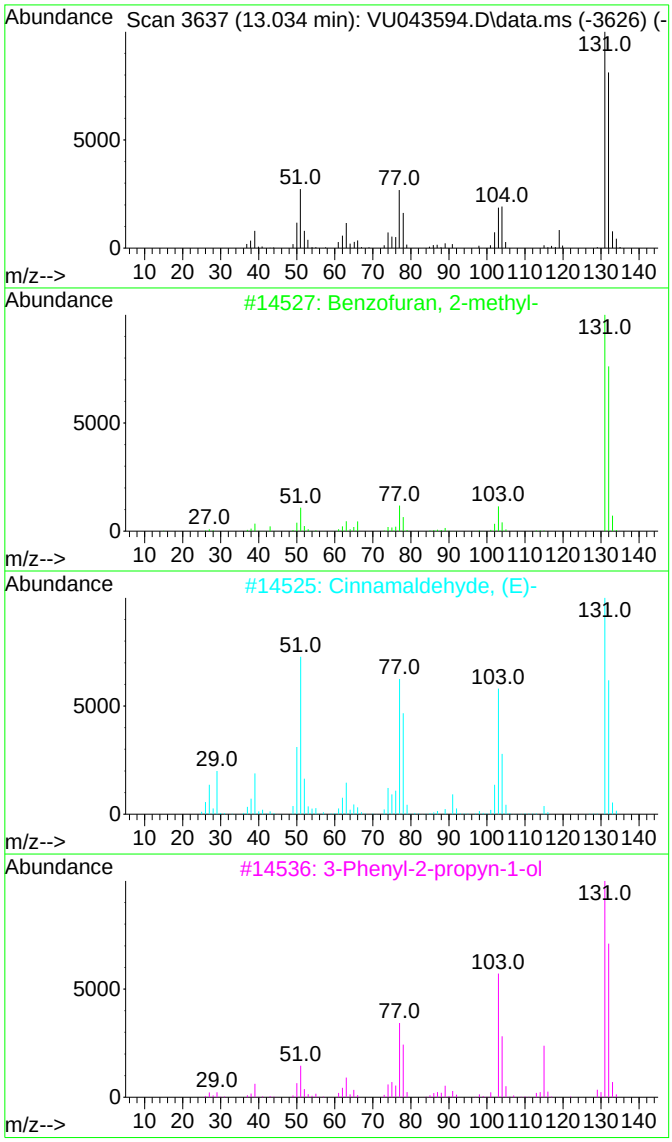
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

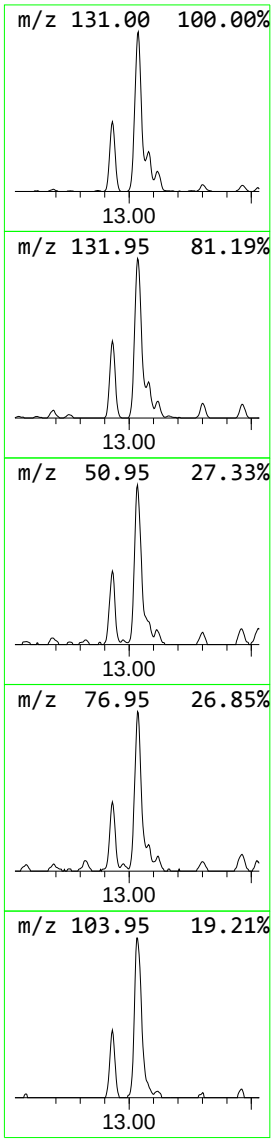
****

Peak Number 5 Benzofuran, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.034	20.33 ug/l	280734	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	94
2	Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	90
3	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	87
4	2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	87
5	Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043594.D
Acq On : 06 May 2021 19:26
Operator : SY/MD
Sample : M2295-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DRUM-B-C-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

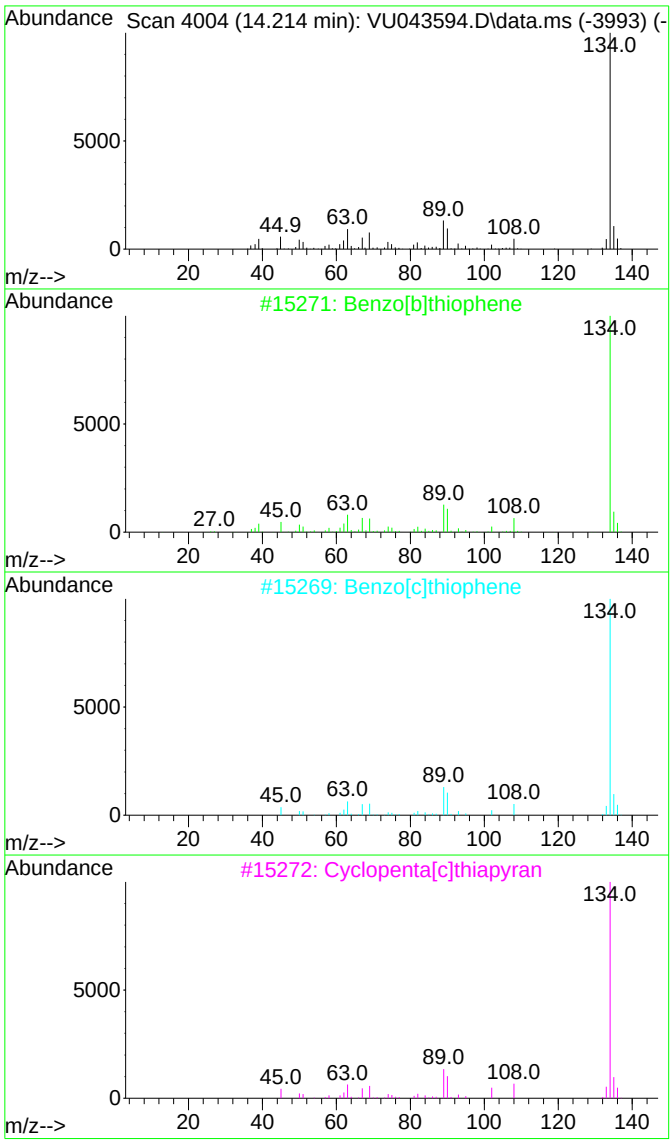
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

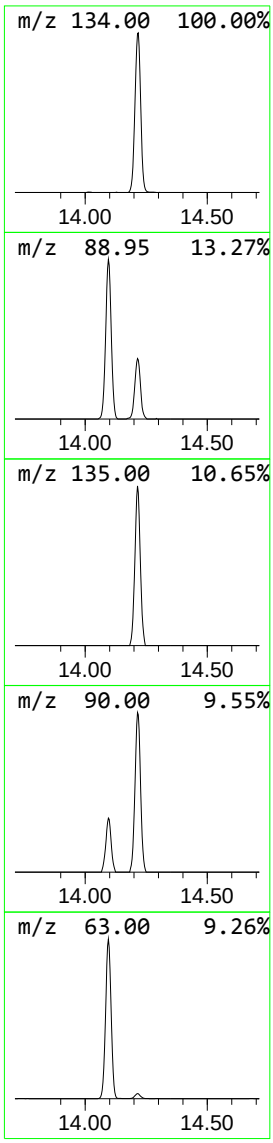
****

Peak Number 6 Benzo[b]thiophene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.214	21.47 ug/l	296431	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]thiophene	134	C8H6S	000095-15-8	97
2	Benzo[c]thiophene	134	C8H6S	000270-82-6	95
3	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4	2-Benzoxazolamine	134	C7H6N2O	004570-41-6	53
5	[1]Benzothieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043594.D
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Operator : SY/MD
Sample : M2295-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DRUM-B-C-E

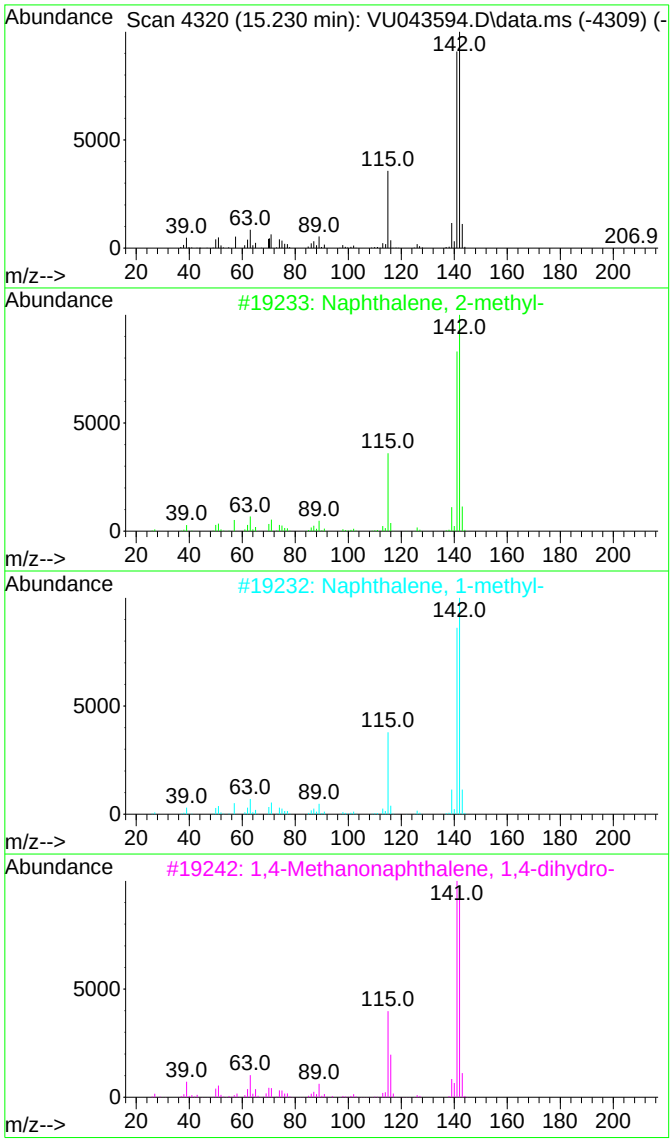
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

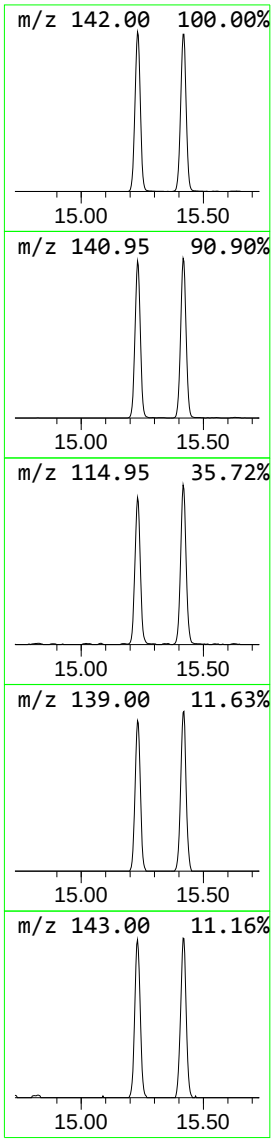
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.230	35.20 ug/l	486140	1,4-Dichlorobenzene-d4	11.819

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	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	64





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ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DRUM-B-C-E

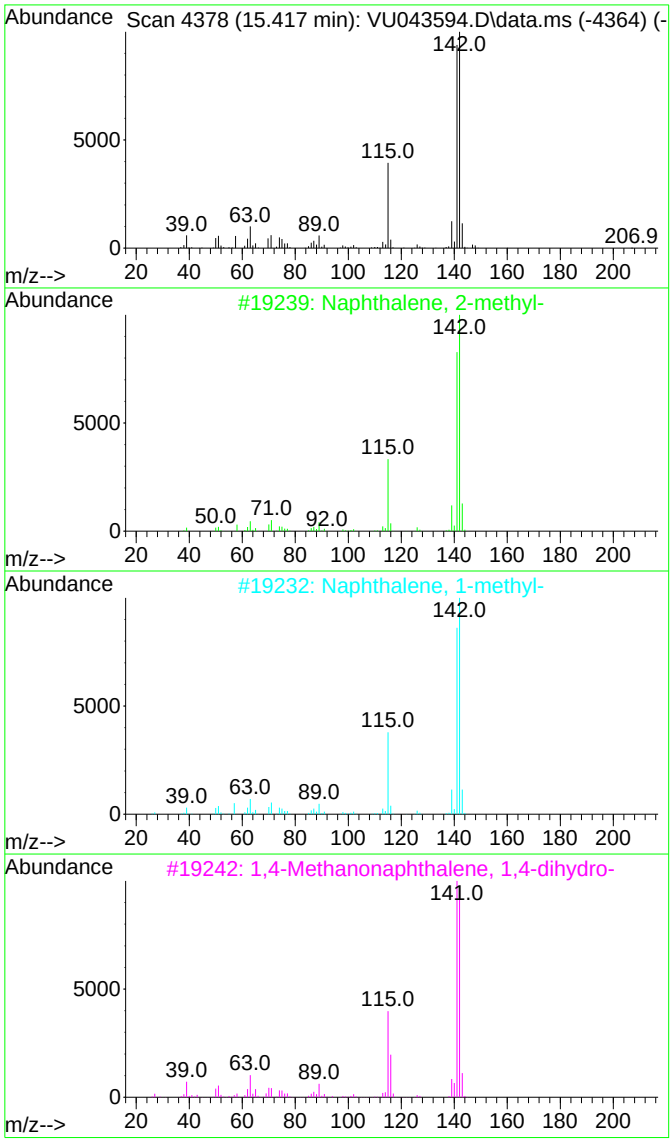
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

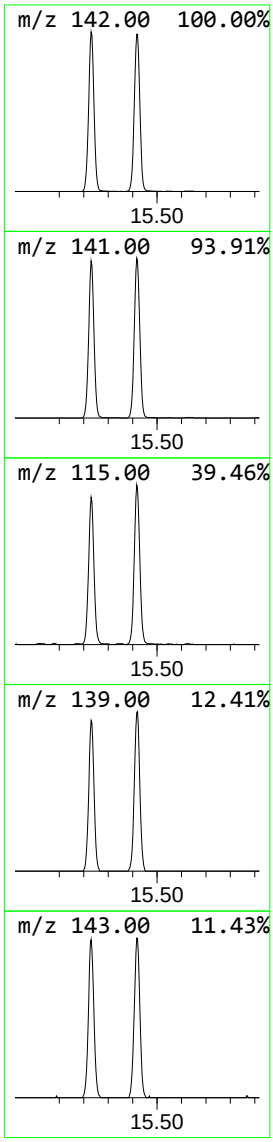
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.417	37.75 ug/l	521360	1,4-Dichlorobenzene-d4	11.819

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	94
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	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043594.D
Acq On : 06 May 2021 19:26
Operator : SY/MD
Sample : M2295-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DRUM-B-C-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.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
Benzofuran	11.735	7.3	ug/l	100989	4	11.819	690455	50.0
Benzene, 1,2,3-...	11.902	7.3	ug/l	101230	4	11.819	690455	50.0
Indane	12.102	148.2	ug/l	2045970	4	11.819	690455	50.0
1-Propyne, 3-ph...	12.317	11.9	ug/l	164818	4	11.819	690455	50.0
Benzofuran, 2-m...	13.034	20.3	ug/l	280734	4	11.819	690455	50.0
Benzo[b]thiophene	14.214	21.5	ug/l	296431	4	11.819	690455	50.0
Naphthalene, 1-...	15.230	35.2	ug/l	486140	4	11.819	690455	50.0
1,4-Methanonaph...	15.417	37.8	ug/l	521360	4	11.819	690455	50.0