LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : KTW-02

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\82X050721W.M
Title : SW846 8260

Signal : TIC: VX021969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.288	25	33	42	rBV2	168966	778416	5.43%	1.958%
2	2.514	227	234	263	rBV	3025519	5294141	36.93%	13.314%
3	5.391	696	706	718	rBV	70645	202874	1.42%	0.510%
4	5.562	723	734	745	rVB	90513	254368	1.77%	0.640%
5	5.964	790	800	806	rBV2	75650	202491	1.41%	0.509%
6	6.050	806	814	830	rVB	201618	543171	3.79%	1.366%
7	6.769	921	932	946	rBV	174486	414110	2.89%	1.041%
8	8.653	1232	1241	1247	rBV	415134	638905	4.46%	1.607%
9	8.720	1247	1252	1263	rVB	151556	238977	1.67%	0.601%
10	10.055	1465	1471	1485	rBV	413869	584619	4.08%	1.470%
11	10.195	1485	1494	1502	rVV	733605	970551	6.77%	2.441%
12	10.305	1502	1512	1525	rVB	1260065	1711436	11.94%	4.304%
13	10.646	1563	1568	1577	rVB	522126	671234	4.68%	1.688%
14	11.085	1634	1640	1646	rBV	393243	497252	3.47%	1.251%
15	11.305	1671	1676	1682	rVB	204449	256394	1.79%	0.645%
16	11.384	1682	1689	1691	rBV	576397	819336	5.71%	2.060%
17	11.457	1696	1701	1706	rVB	547564	695088	4.85%	1.748%
18	11.616	1722	1727	1738	rBV	430746	634435	4.43%	1.595%
19	11.756	1744	1750	1755	rBV	2101542	2462344	17.17%	6.192%
20	11.963	1779	1784	1789	rBV2	155723	221079	1.54%	0.556%
21	12.024	1789	1794	1800	rVB	491824	629696	4.39%	1.584%
22	12.091	1800	1805	1810	rBV	875036	1054611	7.36%	2.652%
23	12.244	1825	1830	1838	rBV	706248	937686	6.54%	2.358%
24	12.323	1838	1843	1850	rVB2	118703	169216	1.18%	0.426%
25	12.616	1886	1891	1894	rBV	125011	156679	1.09%	0.394%
26	12.707	1901	1906	1914	rBV4	97310	173149	1.21%	0.435%
27	12.969	1945	1949	1956	rVB	208640	271773	1.90%	0.683%
28	13.292	1998	2002	2008	rVB2	274983	374760	2.61%	0.942%
29	13.426	2019	2024	2033	rVB	283345	356916	2.49%	0.898%
30	13.670	2056	2064	2069	rVB2	93526	171797	1.20%	0.432%
31	13.786	2075	2083	2088	rBV	10736570	14337311	100.00%	36.056%
32	13.872	2091	2097	2102	rVV	444909	547738	3.82%	1.377%
33	14.640	2218	2223	2233	rVB	1219596	1546454	10.79%	3.889%
34	14.780	2241	2246	2255	rBV	606242	799070	5.57%	2.010%
35	15.207	2308	2316	2322	rBV	99364	146074	1.02%	0.367%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
KTW-02

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\82X050721W.M
Title : SW846 8260

Sum of corrected areas: 39764151

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
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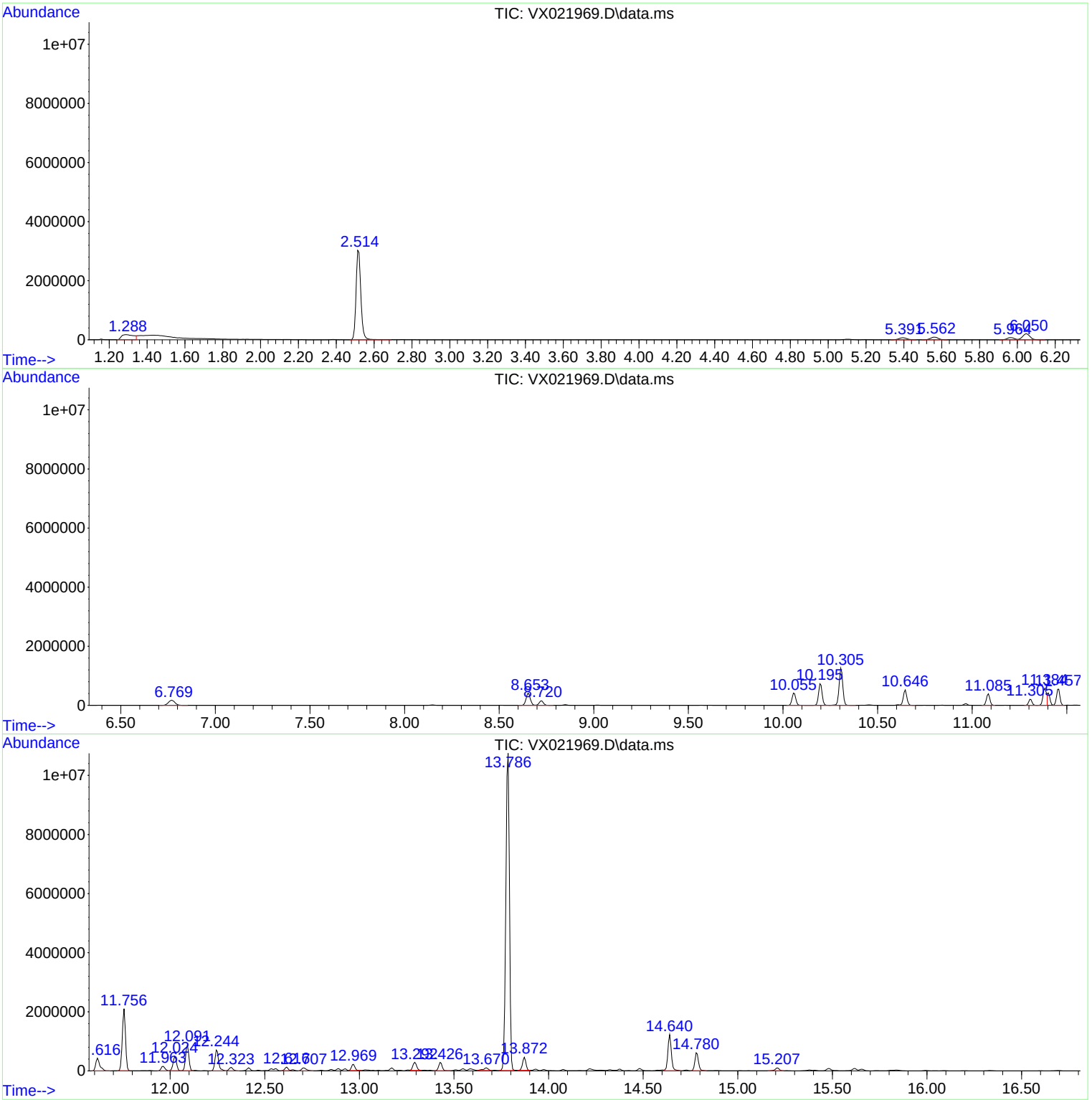
Instrument :
MSVOA_X
ClientSampleId :
KTW-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
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Instrument : MSVOA_X
ClientSampleId : KTW-02

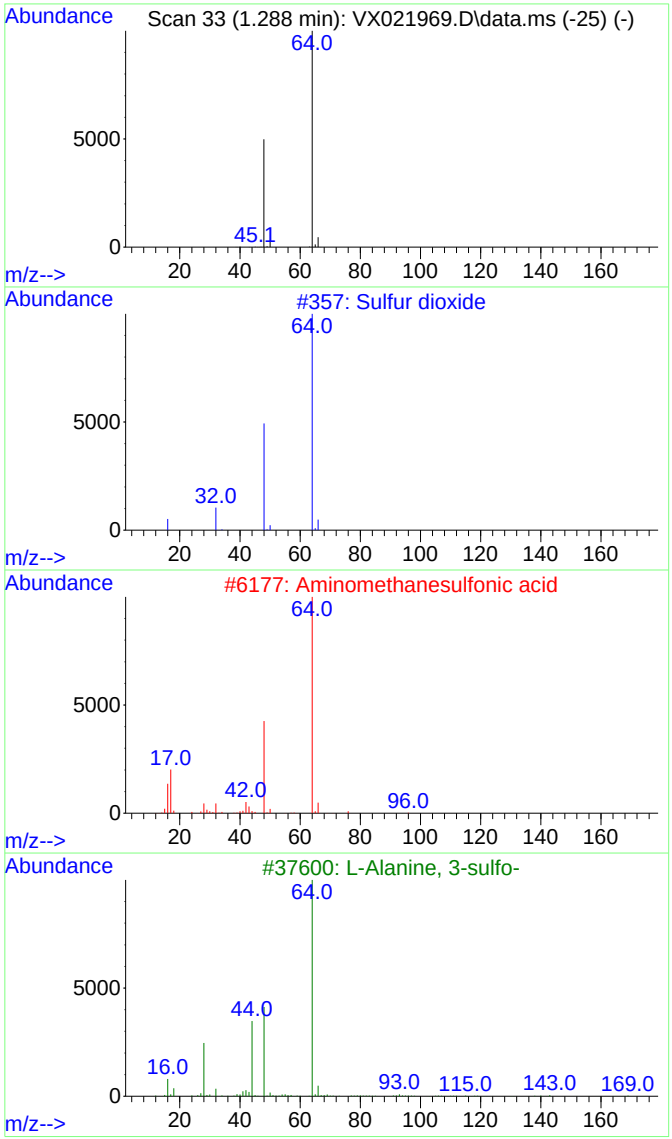
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

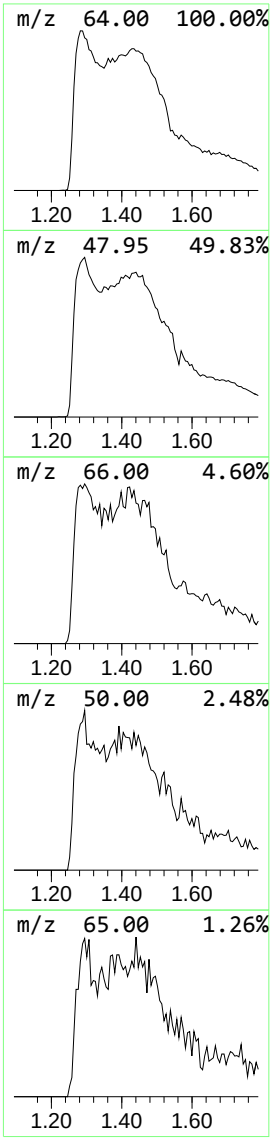
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.288	153.01 ug/l	778416	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : KTW-02

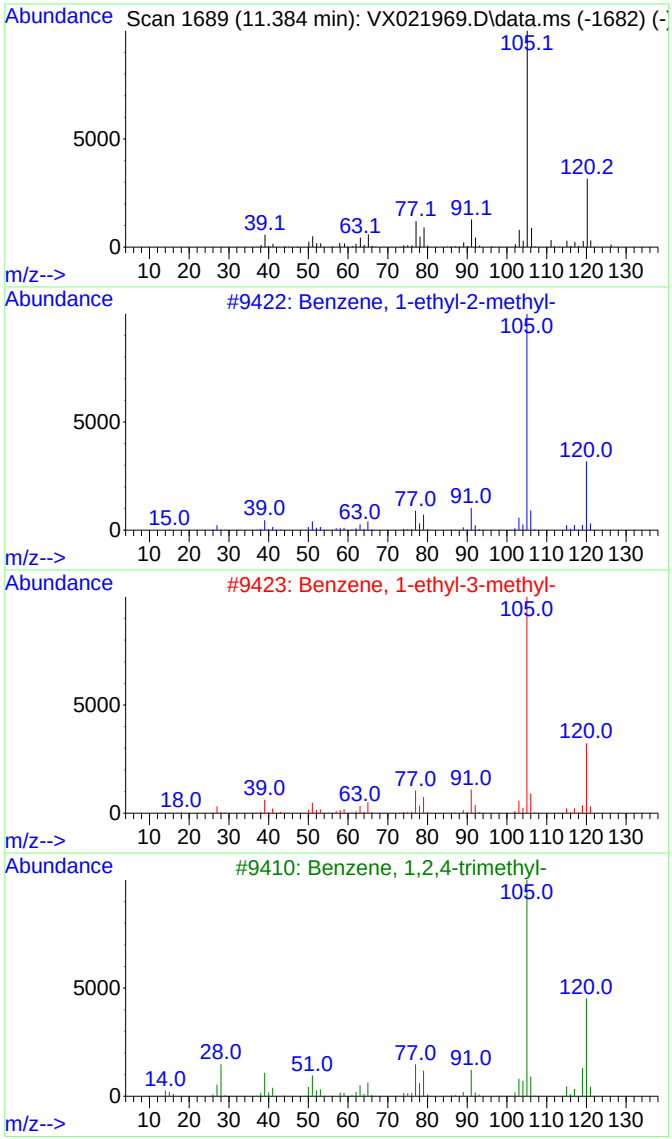
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

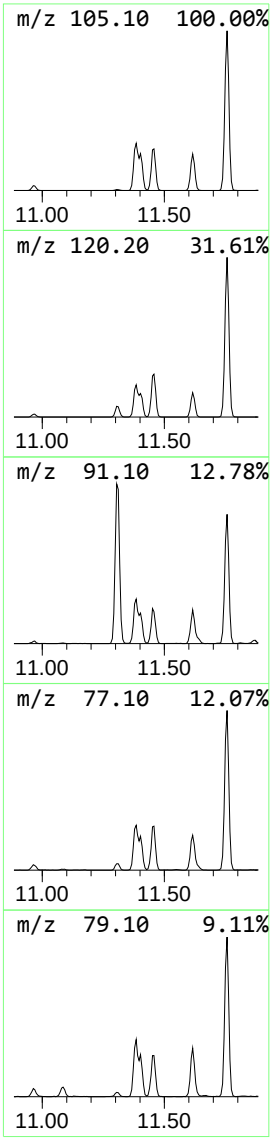
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	65.06 ug/l	819336	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : KTW-02

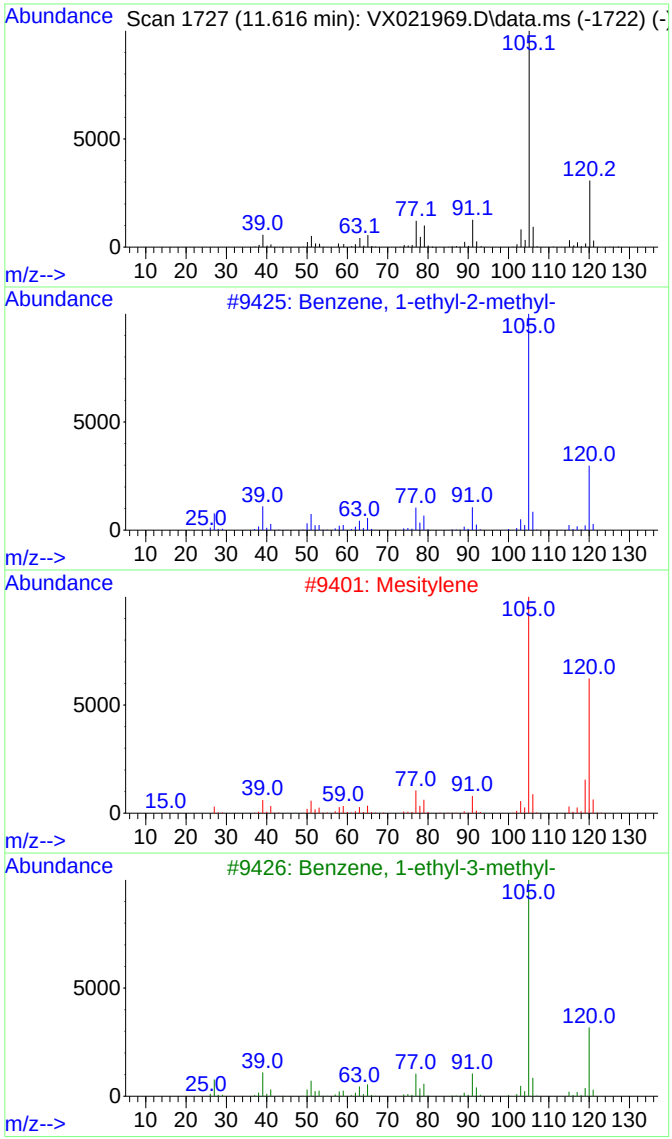
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

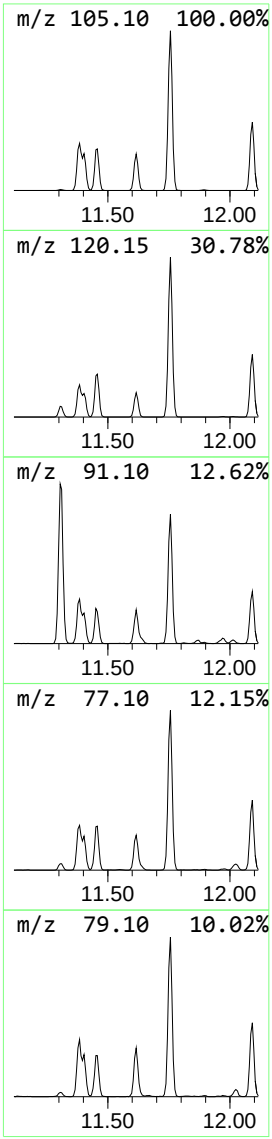
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Mesitylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	50.38 ug/l	634435	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : KTW-02

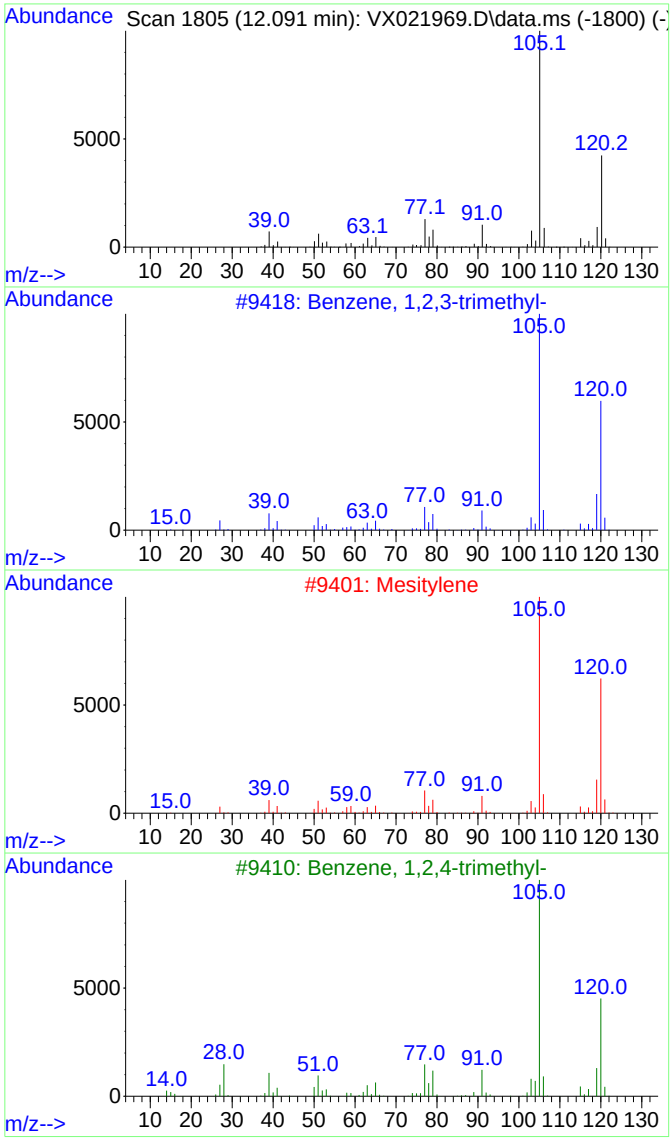
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

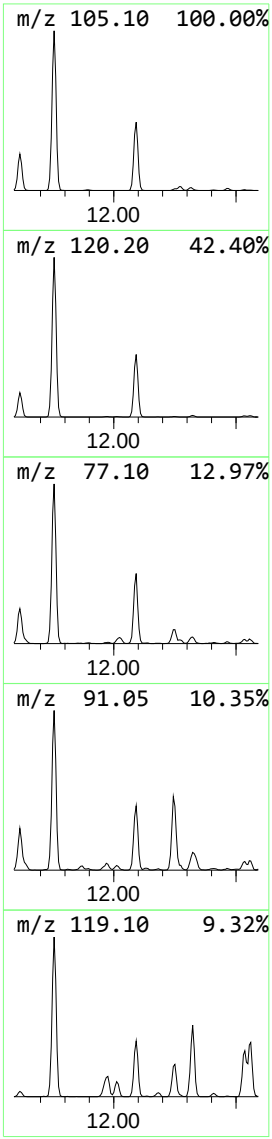
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	83.74 ug/l	1054610	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Mesitylene	120	C9H12	000108-67-8	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : KTW-02

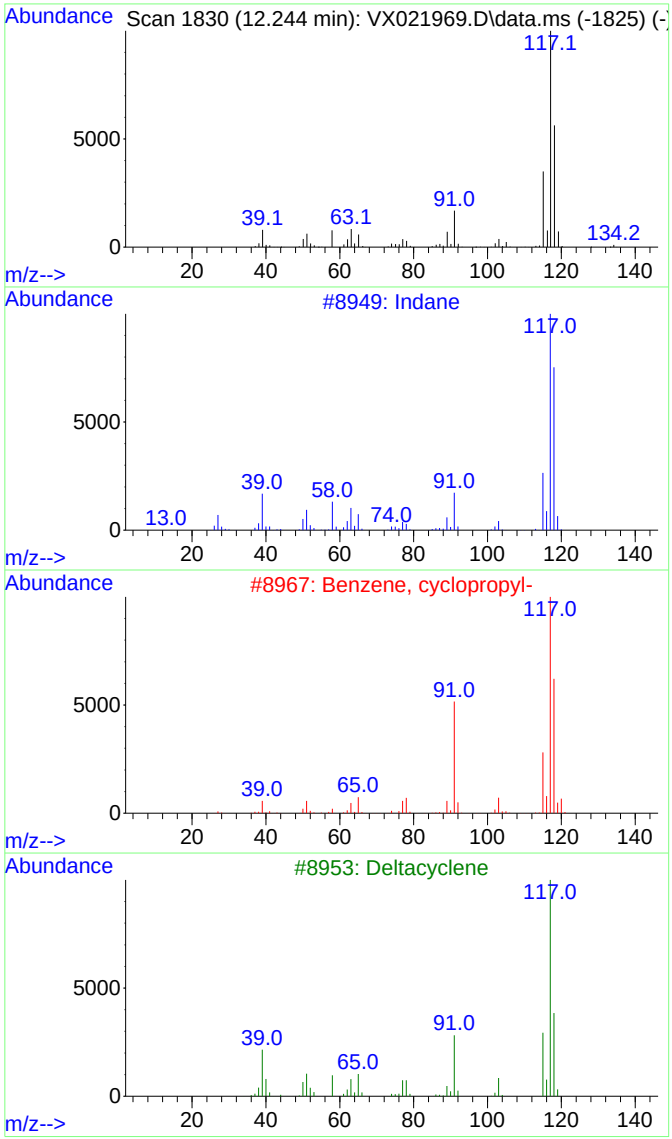
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

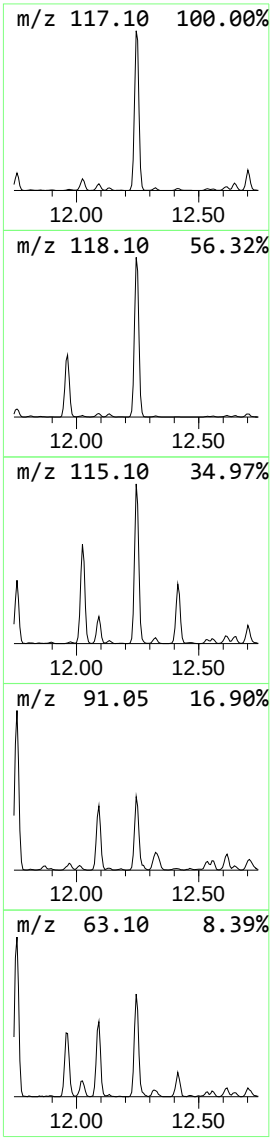
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	74.46 ug/l	937686	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3	Deltacyclene	118	C9H10	007785-10-6	74
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60





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Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
KTW-02

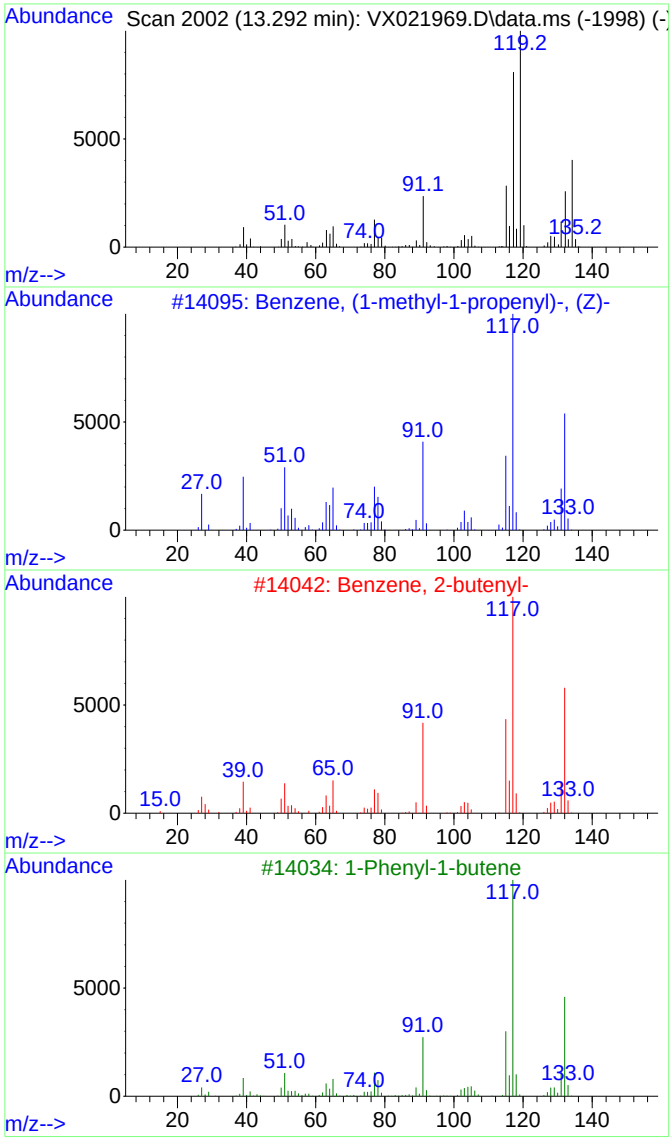
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

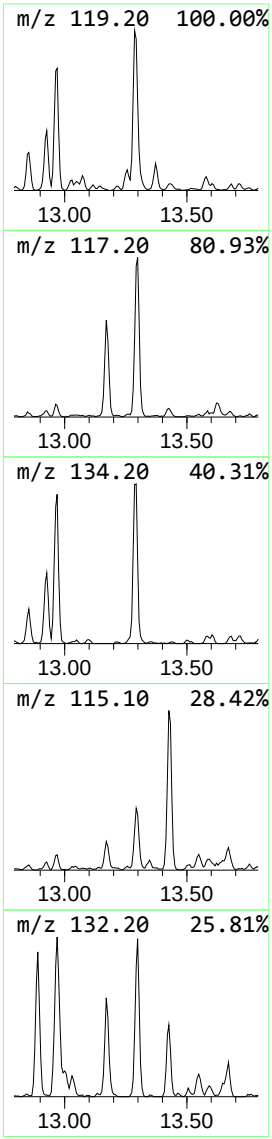
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, (1-methyl-1-propen... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	29.76 ug/l	374760	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	90
2	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	83
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	64
5	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
KTW-02

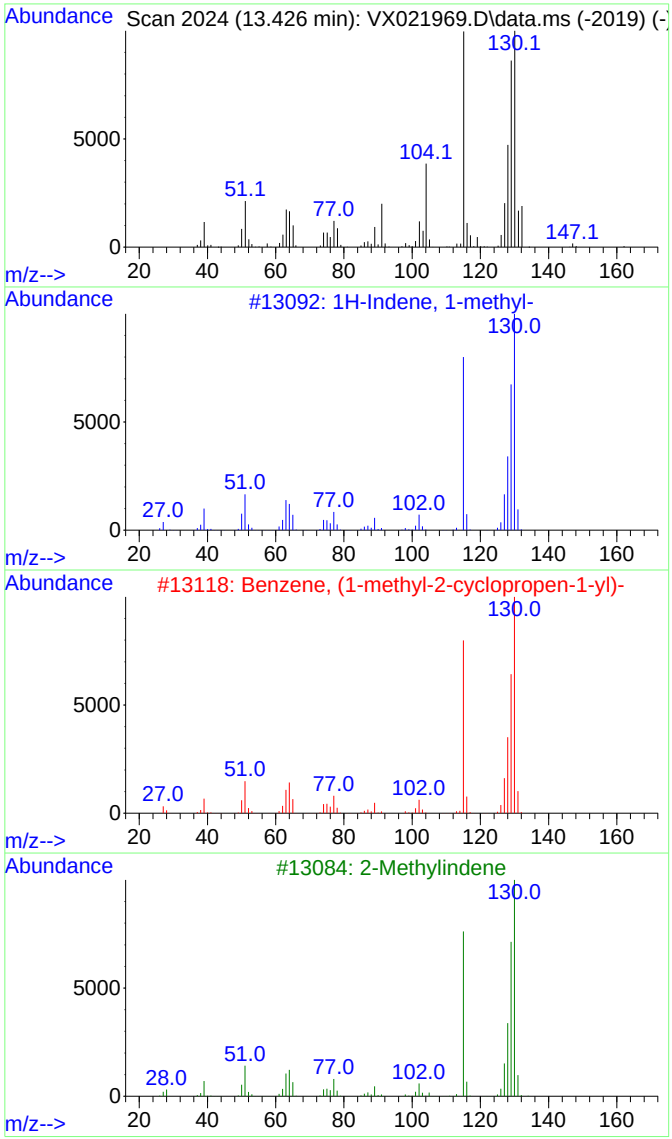
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

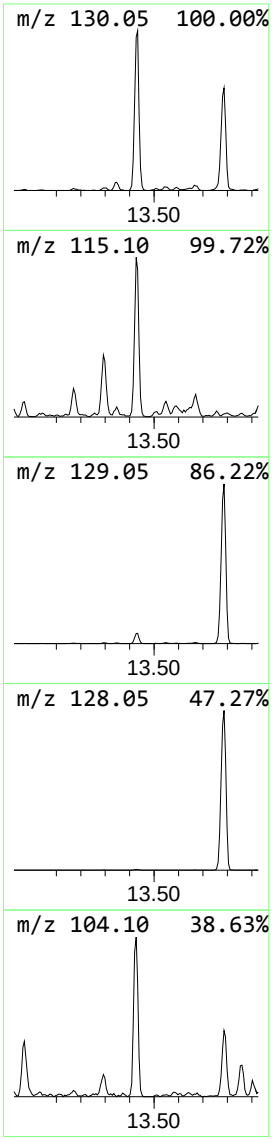
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	28.34 ug/l	356916	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
2	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	95
3	2-Methylindene	130	C10H10	002177-47-1	94
4	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	91
5	Benzene, 1-butynyl-	130	C10H10	000622-76-4	89





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Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : KTW-02

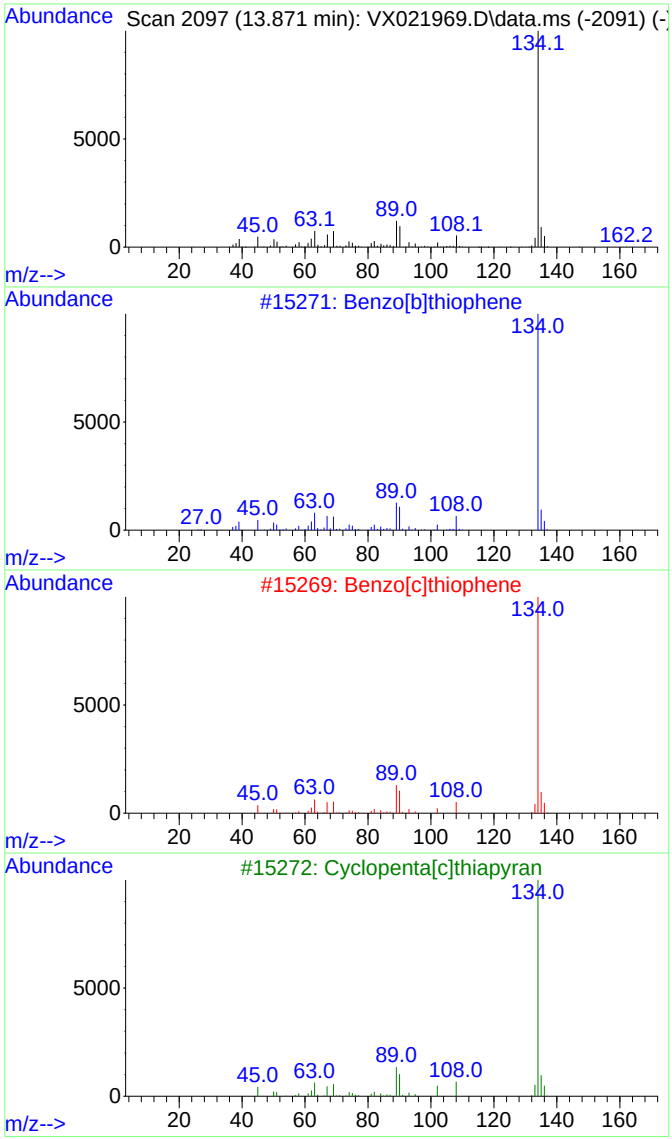
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

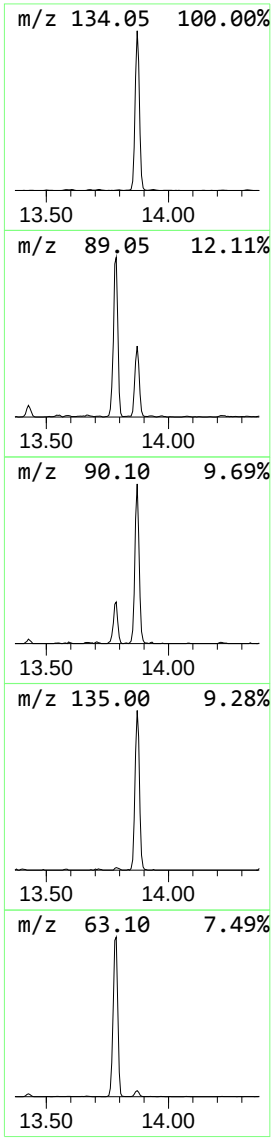
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzo[b]thiophene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	43.49 ug/l	547738	1,4-Dichlorobenzene-d4	12.024

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	97
3	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4	Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	50
5	2H-Benzimidazol-2-one, 1,3-dihydro-	134	C7H6N2O	000615-16-7	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : KTW-02

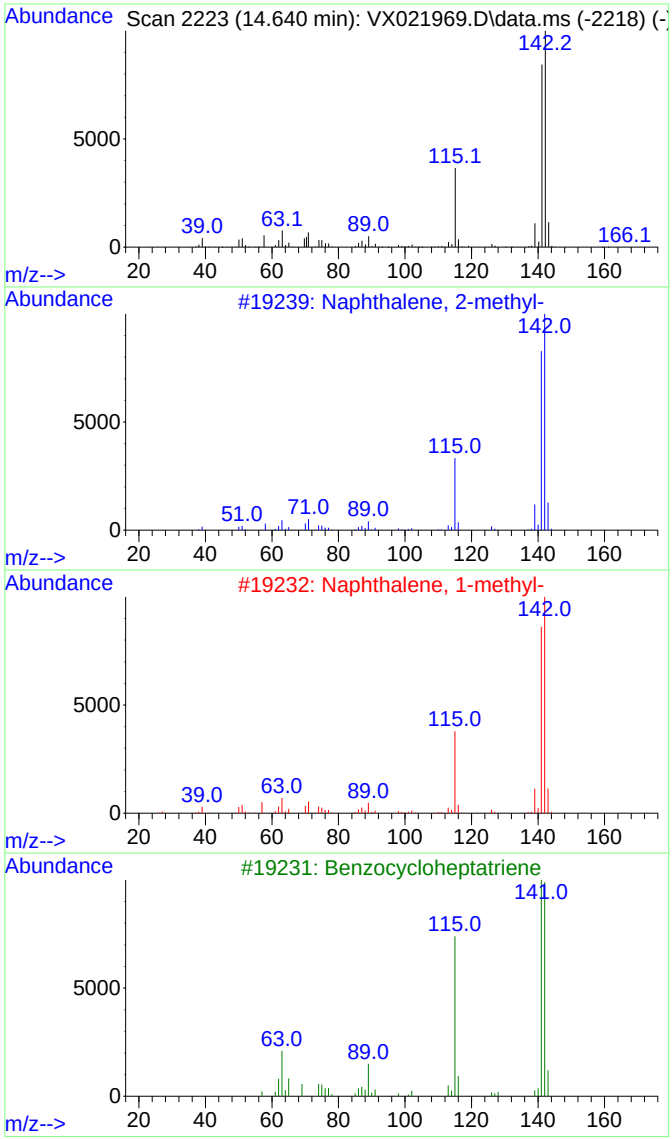
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

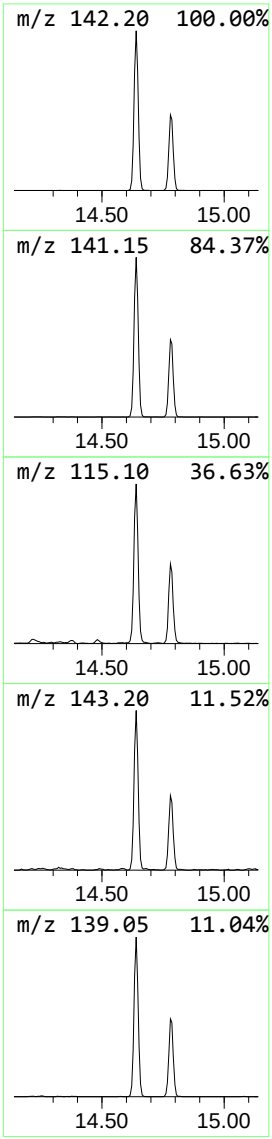
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	122.79 ug/l	1546450	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	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : KTW-02

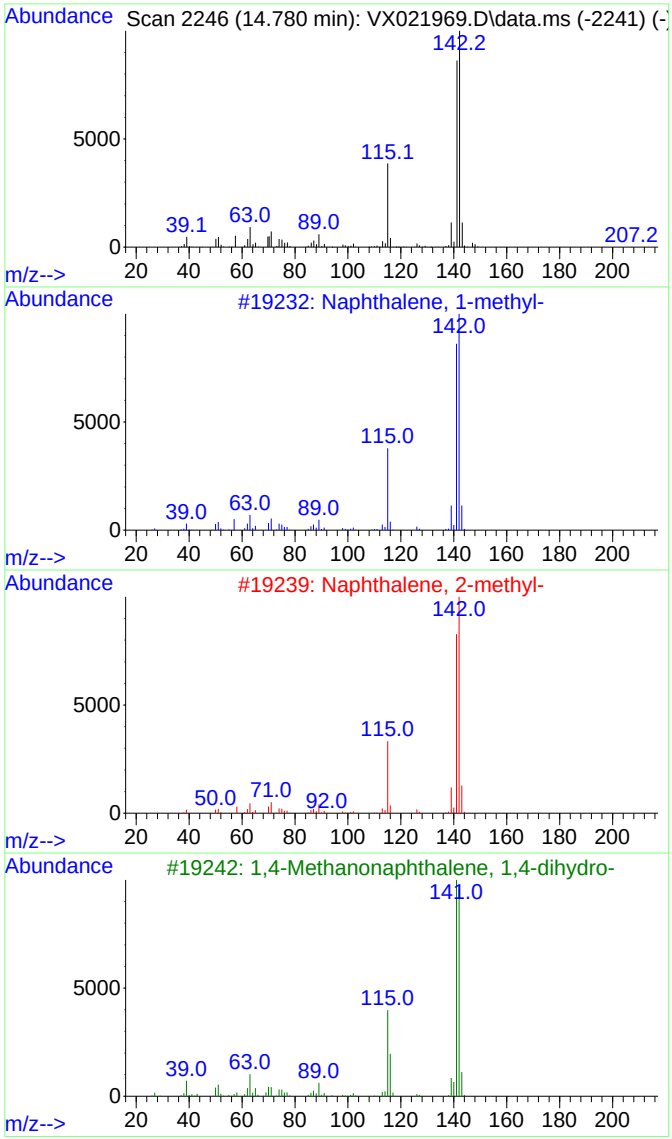
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

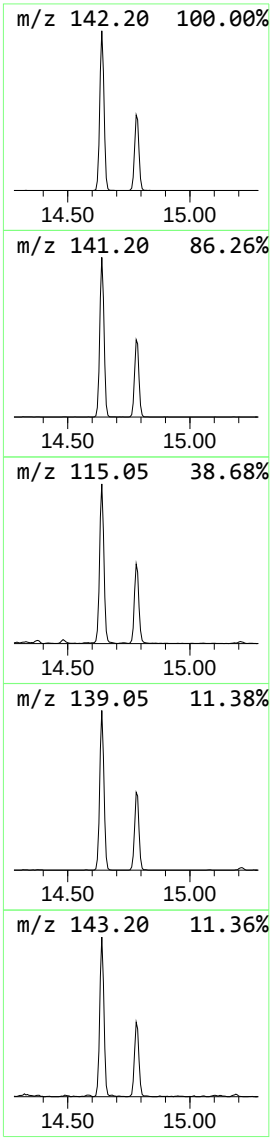
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	63.45 ug/l	799070	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	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
Data File : VX021969.D
Acq On : 13 May 2021 15:57
Operator : JC/MD
Sample : M2383-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : KTW-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.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
Sulfur dioxide	1.288	153.0	ug/l	778416	1	5.556	254368	50.0
Benzene, 1-ethy...	11.384	65.1	ug/l	819336	4	12.024	629696	50.0
Mesitylene	11.616	50.4	ug/l	634435	4	12.024	629696	50.0
Benzene, 1,2,3-...	12.091	83.7	ug/l	1054610	4	12.024	629696	50.0
Indane	12.244	74.5	ug/l	937686	4	12.024	629696	50.0
Benzene, (1-met...	13.292	29.8	ug/l	374760	4	12.024	629696	50.0
1H-Indene, 1-me...	13.427	28.3	ug/l	356916	4	12.024	629696	50.0
Benzo[b]thiophene	13.871	43.5	ug/l	547738	4	12.024	629696	50.0
Naphthalene, 1-...	14.640	122.8	ug/l	1546450	4	12.024	629696	50.0
1,4-Methanonaph...	14.780	63.5	ug/l	799070	4	12.024	629696	50.0