LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

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\82X102622W.M
Title : SW846 8260

Signal : TIC: VX032682.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	69	rVB	16561	20219	4.96%	0.459%
2	1.752	105	109	124	rVB4	6999	11628	2.85%	0.264%
3	1.959	139	143	149	rVB2	5920	8608	2.11%	0.196%
4	2.050	152	158	165	rBV	14364	23665	5.80%	0.538%
5	2.380	206	212	221	rVB	24741	43461	10.66%	0.987%
6	2.831	281	286	296	rVB	9490	19481	4.78%	0.443%
7	3.111	322	332	341	rVB3	6174	14536	3.56%	0.330%
8	3.453	377	388	396	rVB3	5060	12112	2.97%	0.275%
9	4.306	522	528	537	rVB3	3138	8632	2.12%	0.196%
10	4.562	562	570	589	rBV	6935	20913	5.13%	0.475%
11	5.391	696	706	718	rBV2	16095	47014	11.53%	1.068%
12	5.562	718	734	759	rVB	69541	214154	52.52%	4.865%
13	5.836	771	779	787	rBV5	3189	9439	2.31%	0.214%
14	5.970	790	801	811	rBV3	11690	31997	7.85%	0.727%
15	6.257	839	848	856	rVB2	3932	11143	2.73%	0.253%
16	6.769	923	932	942	rBV	76225	184503	45.24%	4.191%
17	7.385	1023	1033	1040	rBV3	4443	10487	2.57%	0.238%
18	8.110	1145	1152	1157	rBV3	4026	9427	2.31%	0.214%
19	8.653	1235	1241	1247	rBV	149974	227288	55.74%	5.163%
20	8.720	1247	1252	1260	rVB	95246	149097	36.56%	3.387%
21	10.055	1466	1471	1480	rBV	93662	127361	31.23%	2.893%
22	10.195	1489	1494	1501	rBV	57373	73402	18.00%	1.667%
23	10.299	1506	1511	1520	rVV	241442	333877	81.87%	7.585%
24	10.640	1562	1567	1574	rVB	87667	115776	28.39%	2.630%
25	10.963	1615	1620	1626	rBV	19339	23905	5.86%	0.543%
26	11.085	1634	1640	1646	rBV	67584	89861	22.04%	2.041%
27	11.305	1669	1676	1682	rBV	56211	68819	16.88%	1.563%
28	11.378	1682	1688	1691	rBV	127723	194460	47.69%	4.418%
29	11.451	1696	1700	1709	rVB	90964	108734	26.66%	2.470%
30	11.616	1720	1727	1733	rBV	78755	108170	26.53%	2.457%
31	11.750	1744	1749	1756	rVB	319431	395853	97.07%	8.993%
32	11.969	1781	1785	1789	rBV	18963	23592	5.79%	0.536%
33	12.024	1789	1794	1800	rVV2	80477	118118	28.97%	2.683%
34	12.103	1800	1807	1816	rVB3	245098	407790	100.00%	9.264%
35	12.244	1822	1830	1833	rBV2	97297	137897	33.82%	3.133%
36	12.317	1838	1842	1850	rVB3	75949	119869	29.39%	2.723%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

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\82X102622W.M
Title : SW846 8260

37	12.402	1851	1856	1861	rBV3	7436	10440	2.56%	0.237%
38	12.463	1861	1866	1872	rVB	22738	28850	7.07%	0.655%
39	12.530	1872	1877	1879	rBV	41500	50812	12.46%	1.154%
40	12.555	1879	1881	1886	rVB	38745	42027	10.31%	0.955%
41	12.616	1886	1891	1894	rBV	77284	97222	23.84%	2.209%
42	12.646	1894	1896	1900	rVB	15712	15774	3.87%	0.358%
43	12.701	1900	1905	1913	rBV2	46509	73350	17.99%	1.666%
44	12.853	1925	1930	1936	rBV2	20274	34037	8.35%	0.773%
45	12.920	1936	1941	1945	rBV	41467	50409	12.36%	1.145%
46	12.963	1945	1948	1953	rVB	49661	57536	14.11%	1.307%
47	13.024	1955	1958	1960	rBV	7769	9655	2.37%	0.219%
48	13.170	1978	1982	1986	rVB	38660	49076	12.03%	1.115%
49	13.256	1992	1996	1998	rBV2	7464	9341	2.29%	0.212%
50	13.292	1998	2002	2008	rVB2	71876	95976	23.54%	2.180%
51	13.426	2019	2024	2028	rVB	8319	11309	2.77%	0.257%
52	13.512	2032	2038	2041	rBV2	28930	45097	11.06%	1.024%
53	13.542	2041	2043	2046	rVV2	13154	16113	3.95%	0.366%
54	13.579	2046	2049	2055	rVV2	15544	28224	6.92%	0.641%
55	13.664	2056	2063	2067	rVV3	11273	24598	6.03%	0.559%
56	13.707	2067	2070	2075	rVV	41341	46597	11.43%	1.059%
57	13.774	2075	2081	2089	rVB	32044	42430	10.40%	0.964%
58	14.213	2149	2153	2160	rBV4	4708	8359	2.05%	0.190%
59	14.408	2182	2185	2191	rVB	6411	8217	2.02%	0.187%
60	14.640	2212	2223	2226	rBV	9379	12966	3.18%	0.295%
61	14.780	2240	2246	2251	rBV	6885	8252	2.02%	0.187%

Sum of corrected areas: 4401955

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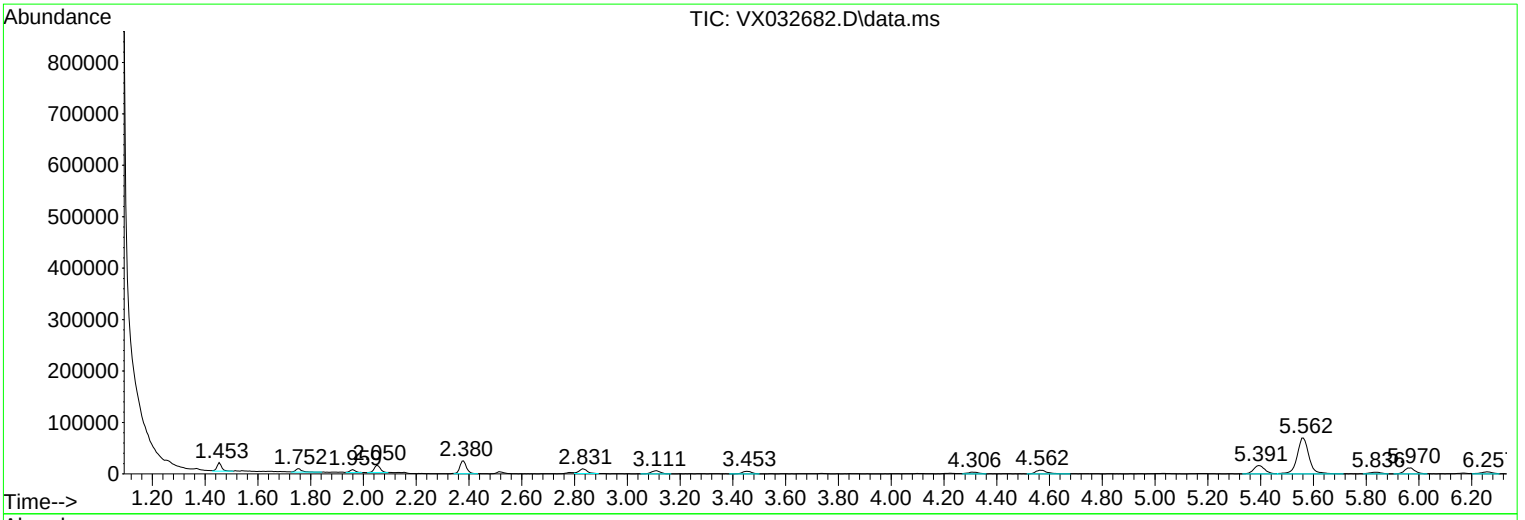
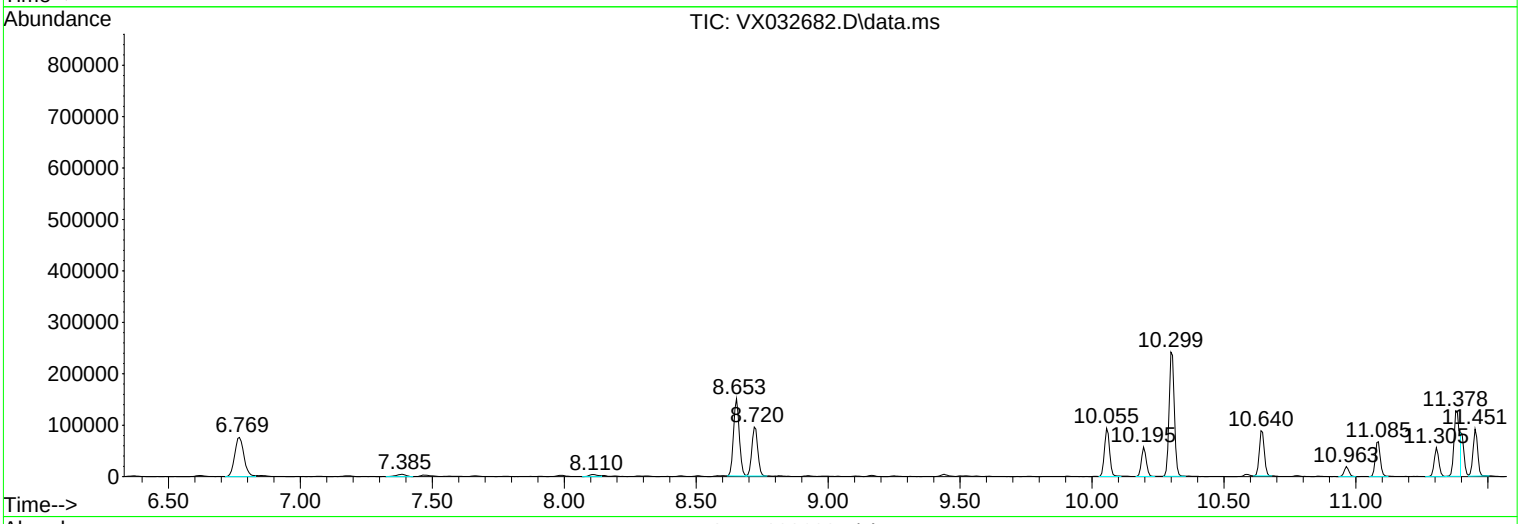
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

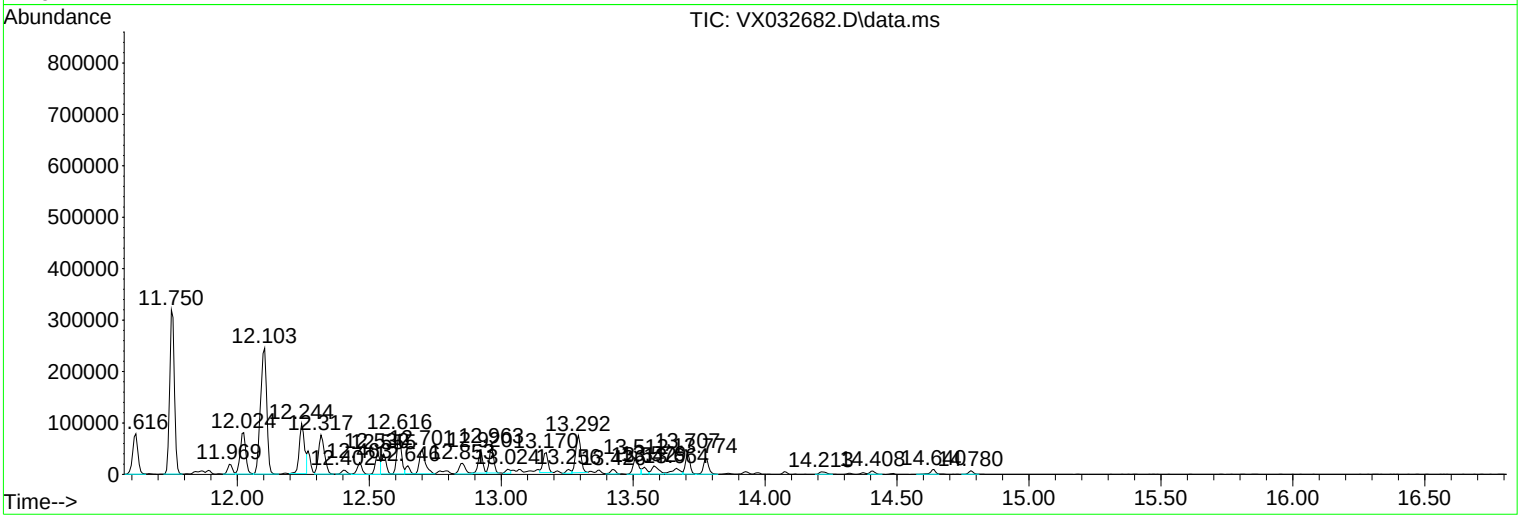
Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

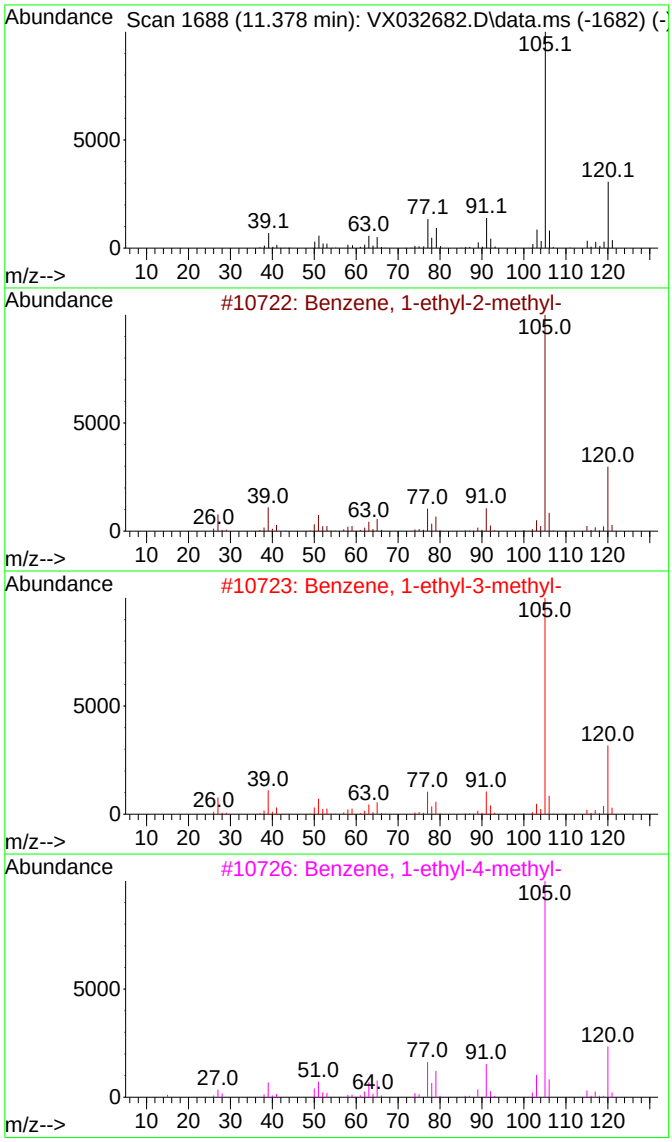
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

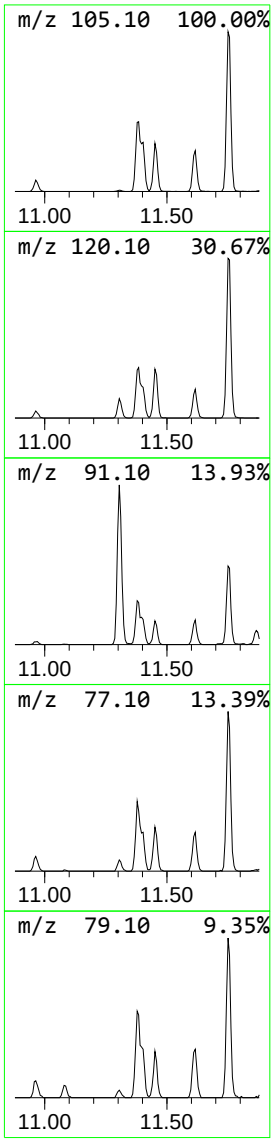
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	82.32 ug/l	194460	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	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

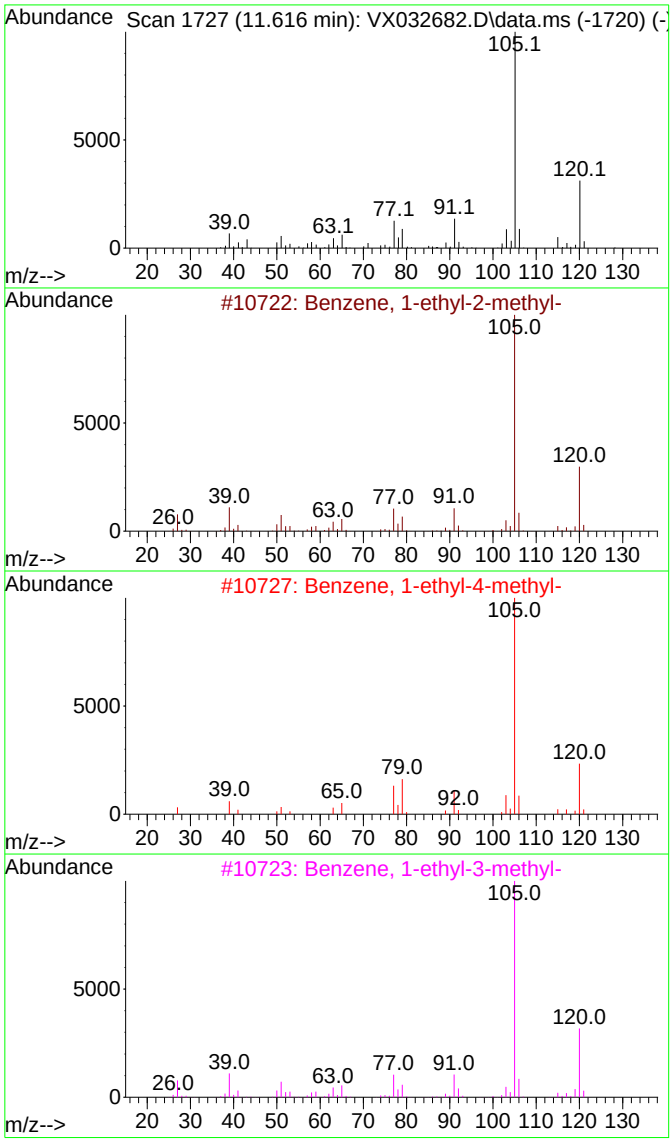
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

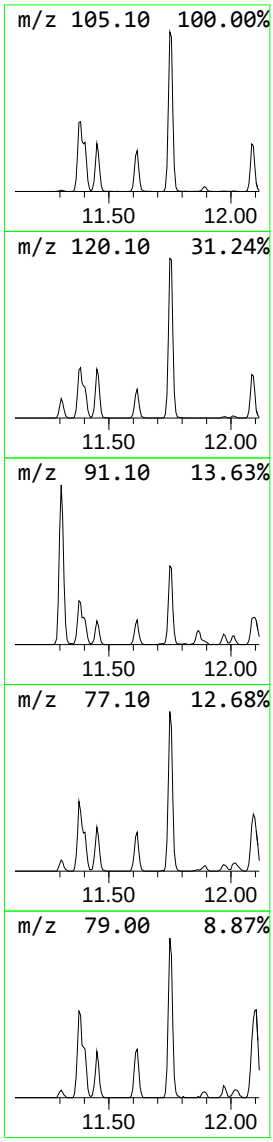
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-ethyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	45.79 ug/l	108170	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	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
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\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

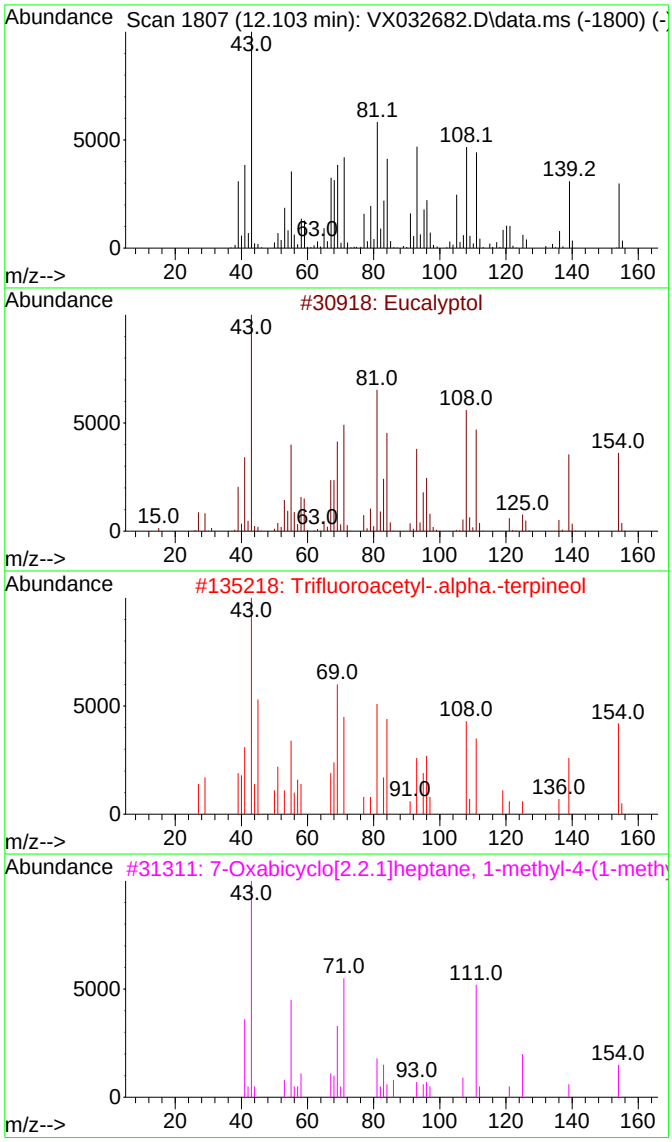
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

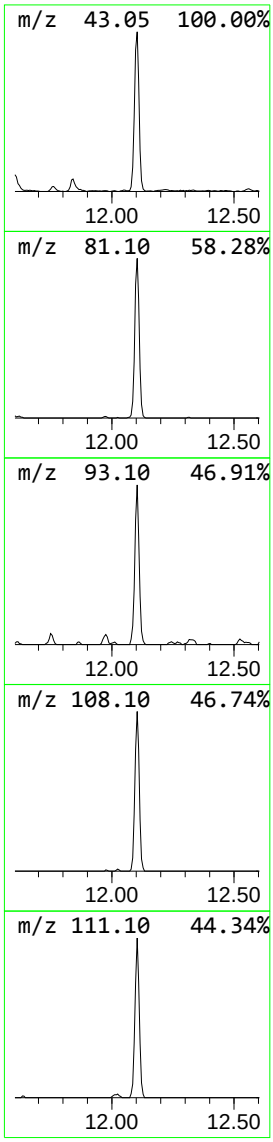
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Eucalyptol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	172.62 ug/l	407790	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	98
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	52
3	7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	35
4	2-Cyclohexen-1-ol, 1-methyl-4-(1...	154	C10H18O	029803-82-5	16
5	3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	15





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

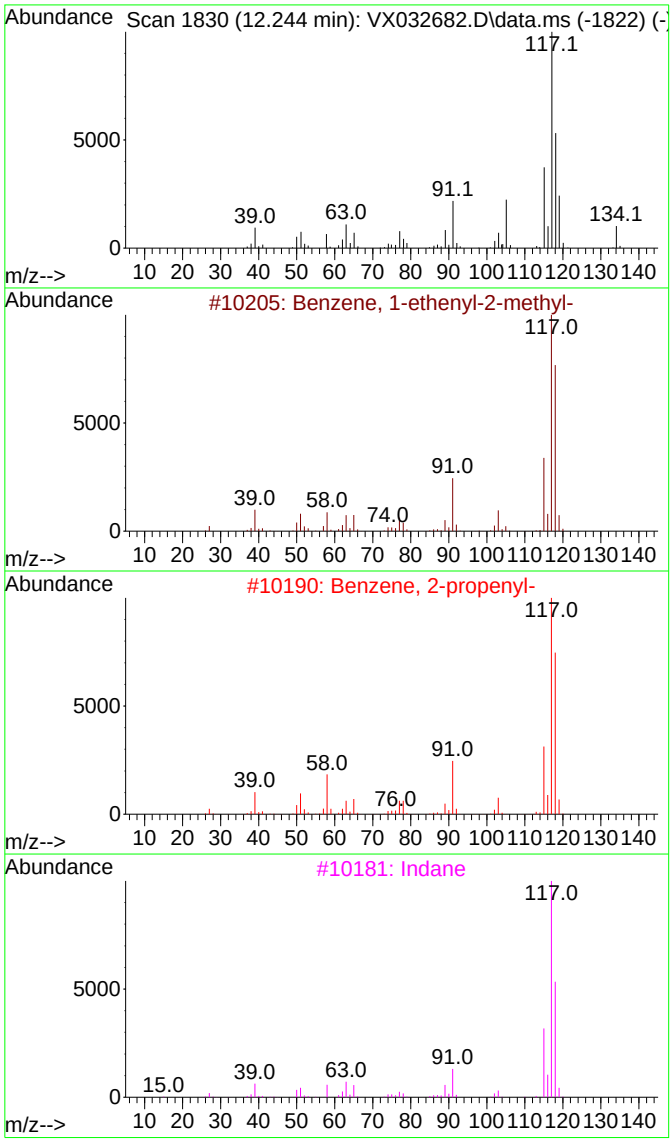
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

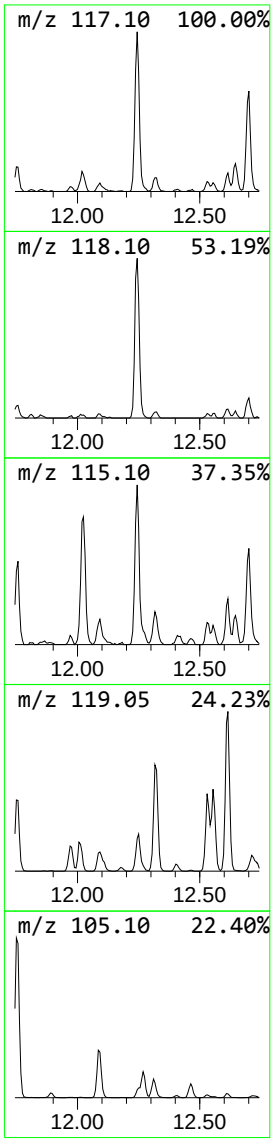
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	58.37 ug/l	137897	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
3	Indane	118	C9H10	000496-11-7	64
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

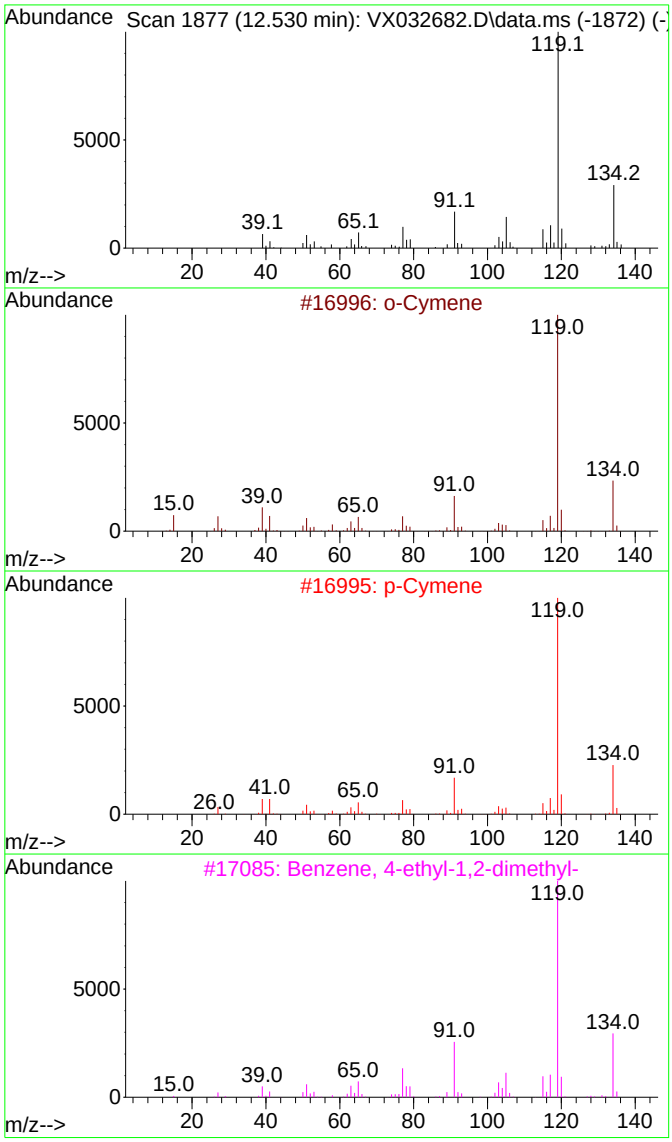
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

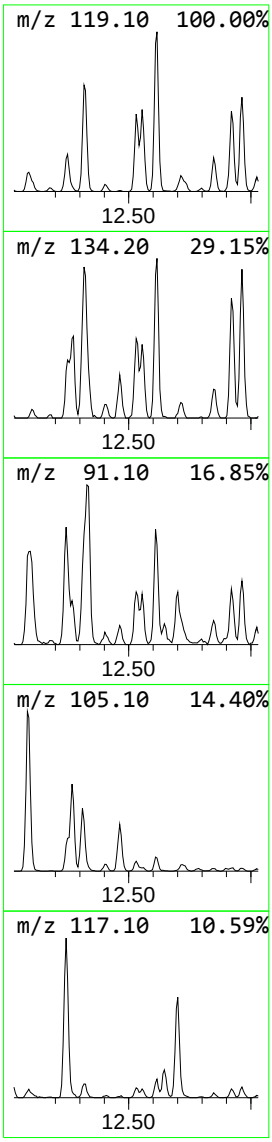
****

Peak Number 5 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.530	21.51 ug/l	50812	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	95
2	p-Cymene	134	C10H14	000099-87-6	95
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

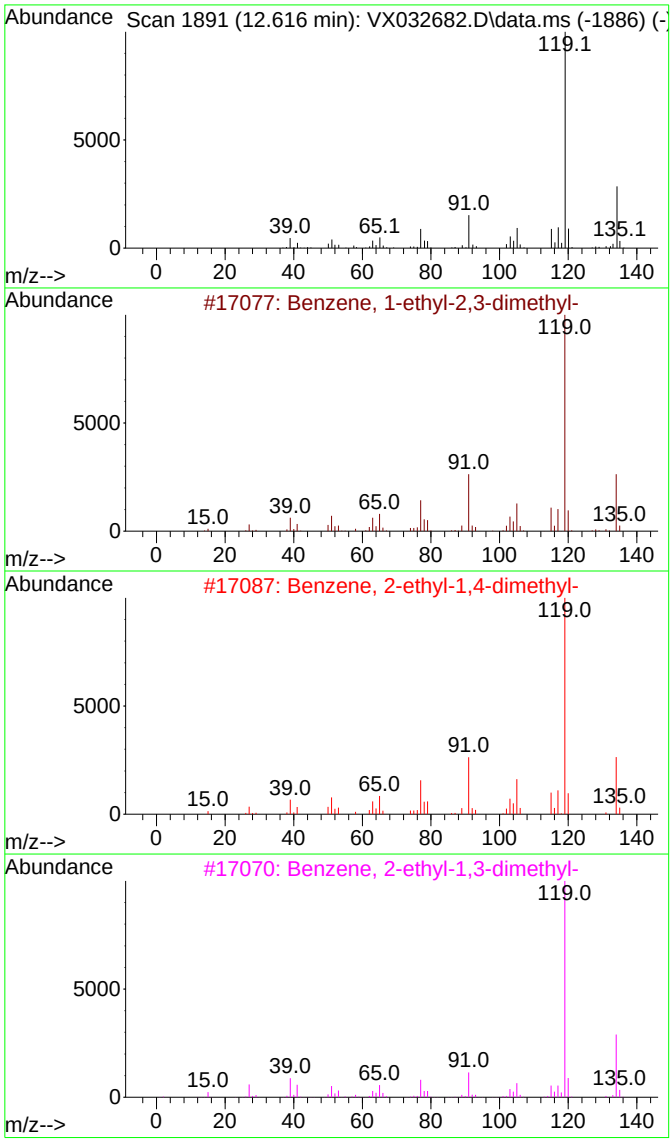
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

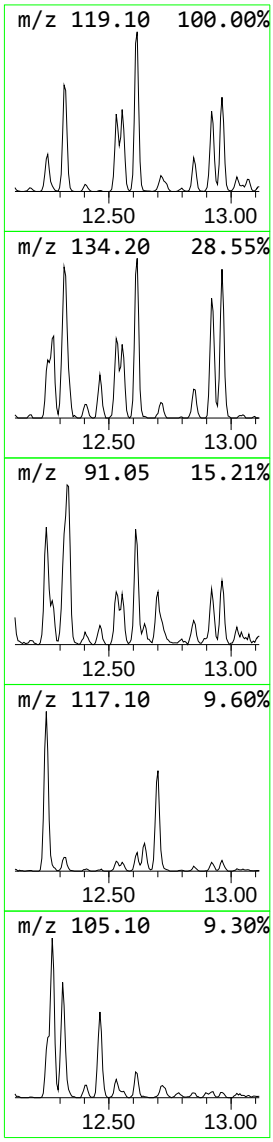
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	41.15 ug/l	97222	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	96
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

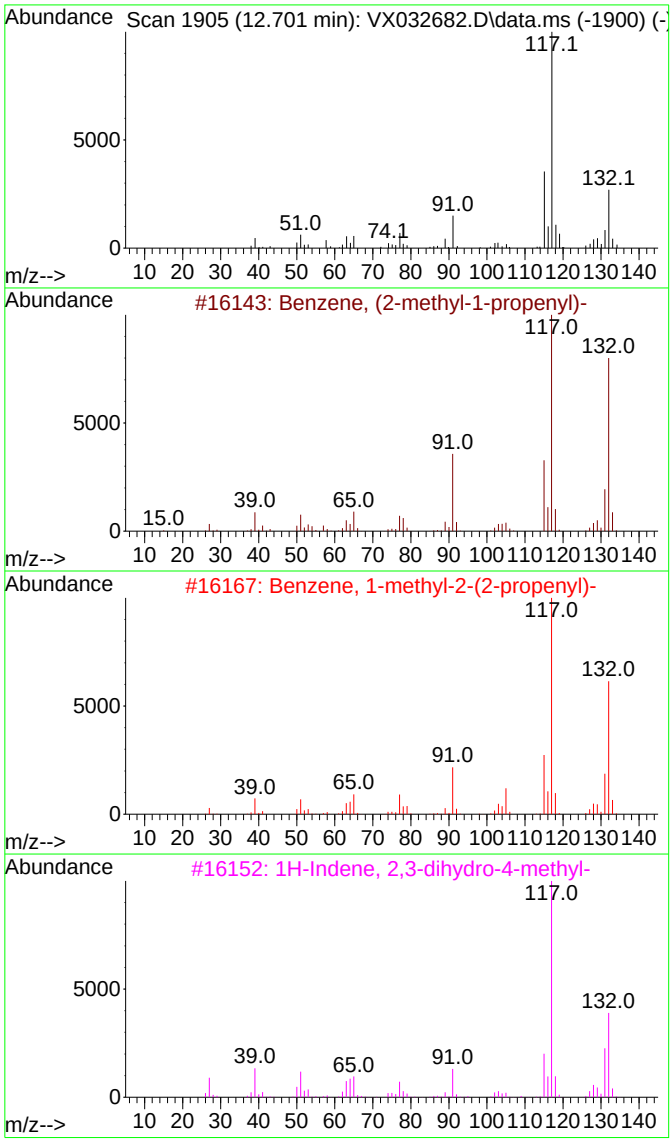
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

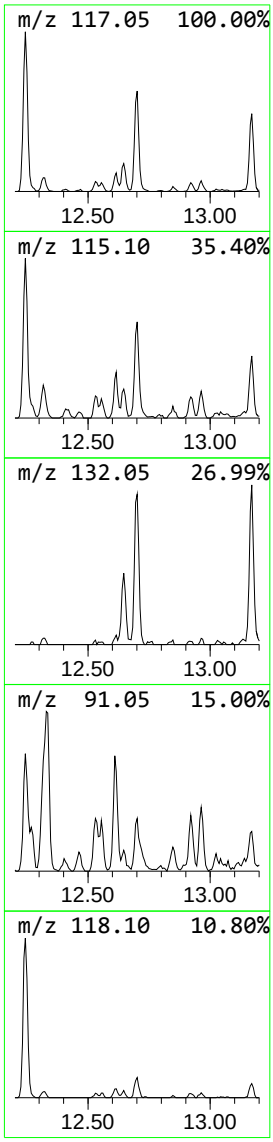
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (2-methyl-1-propen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	31.05 ug/l	73350	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	91
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	90
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
5	Indan, 1-methyl-	132	C10H12	000767-58-8	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

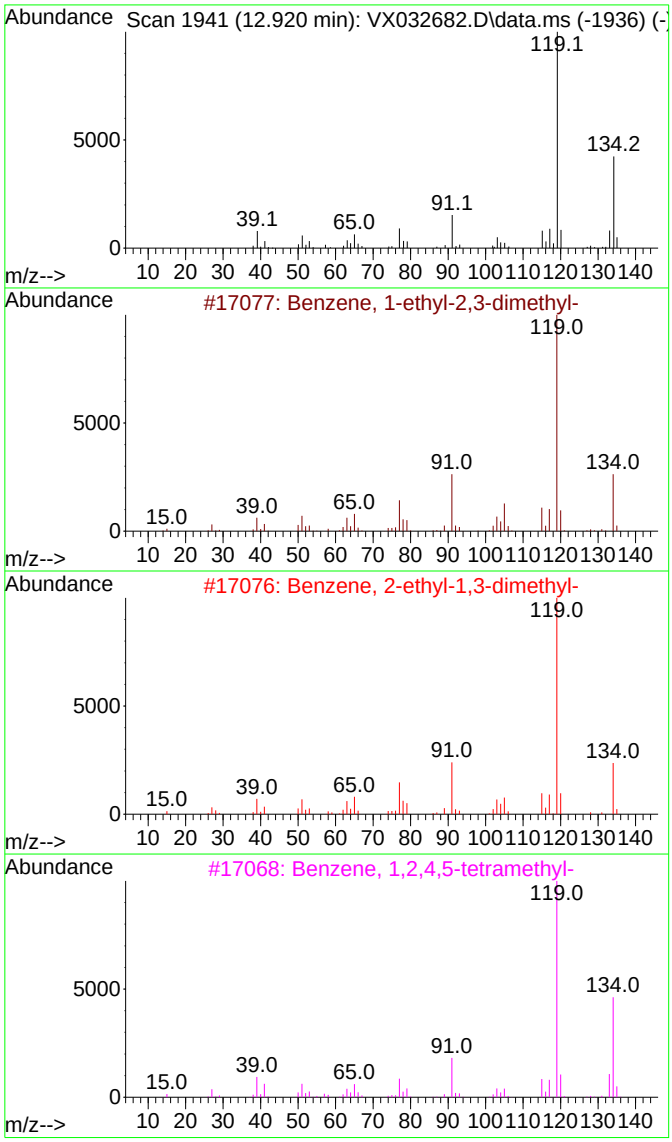
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

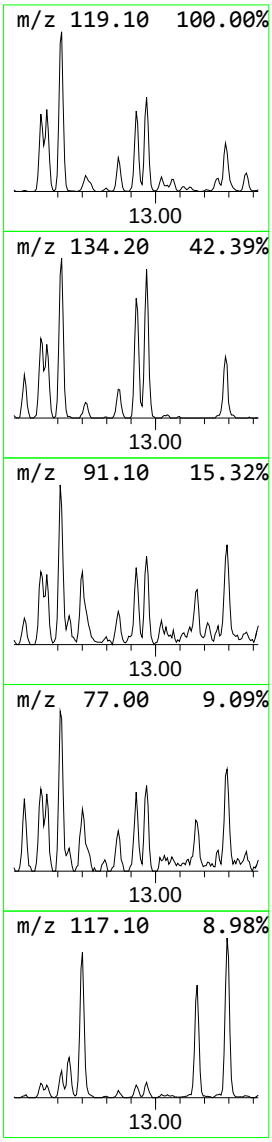
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethyl-1,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	21.34 ug/l	50409	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	95
2	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

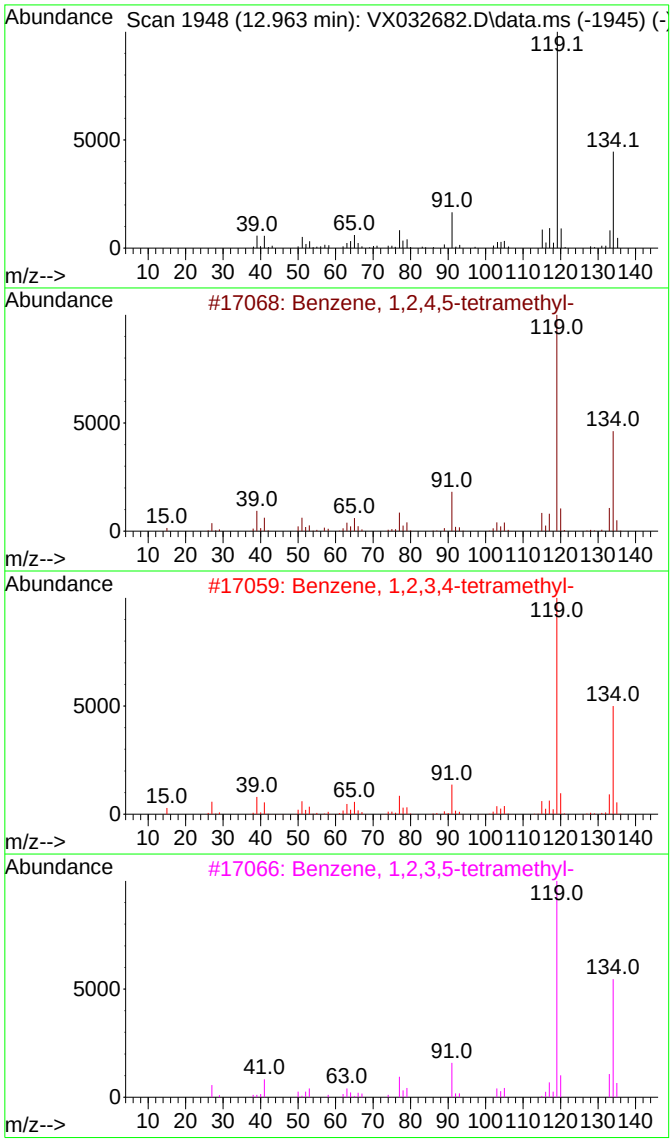
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

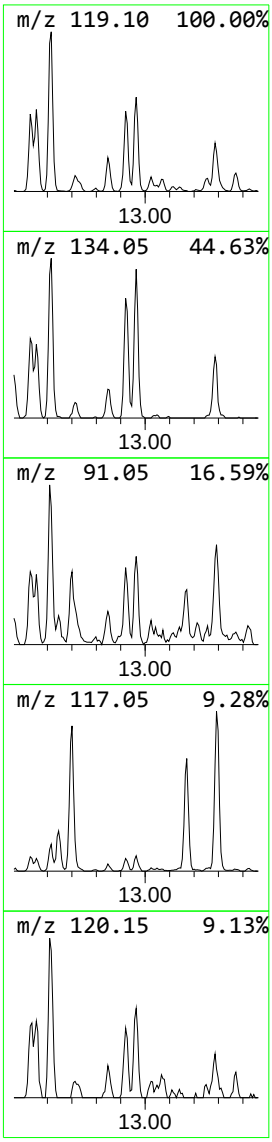
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	24.36 ug/l	57536	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	95
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4	o-Cymene	134	C10H14	000527-84-4	94
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

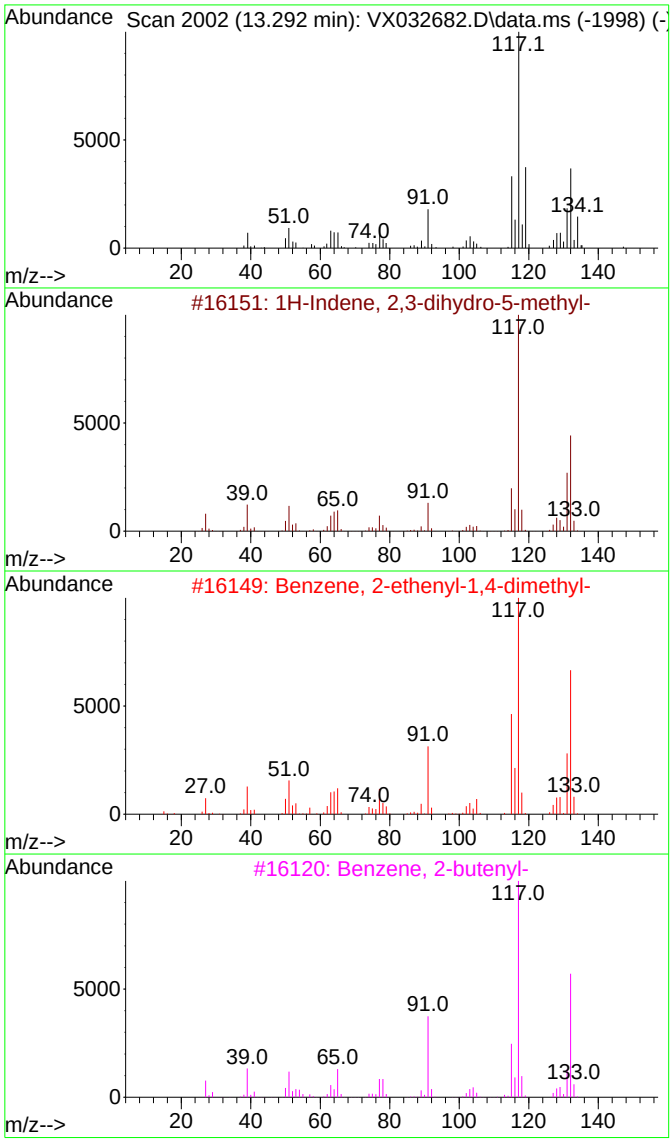
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

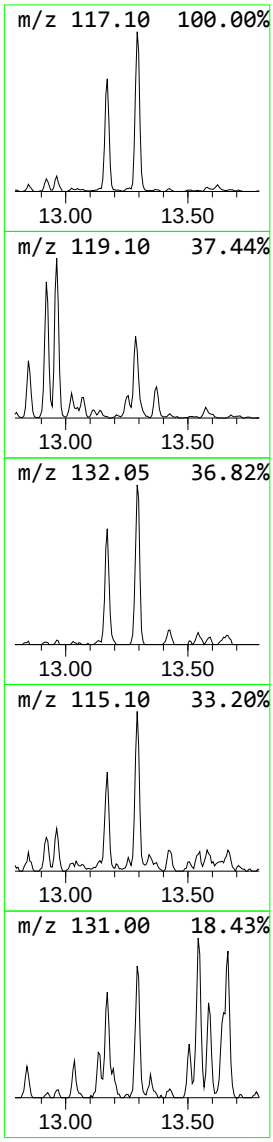
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	40.63 ug/l	95976	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	95
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	83
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81
5	Indan, 1-methyl-	132	C10H12	000767-58-8	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032682.D
Acq On : 09 Nov 2022 16:15
Operator : JC/MD
Sample : N5500-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1851

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
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
Benzene, 1-ethy...	11.378	82.3	ug/l	194460	4	12.024	118118	50.0
Benzene, 1-ethy...	11.616	45.8	ug/l	108170	4	12.024	118118	50.0
Eucalyptol	12.103	172.6	ug/l	407790	4	12.024	118118	50.0
Benzene, 1-ethe...	12.244	58.4	ug/l	137897	4	12.024	118118	50.0
o-Cymene	12.530	21.5	ug/l	50812	4	12.024	118118	50.0
Benzene, 1-ethy...	12.616	41.1	ug/l	97222	4	12.024	118118	50.0
Benzene, (2-met...	12.701	31.1	ug/l	73350	4	12.024	118118	50.0
Benzene, 2-ethy...	12.920	21.3	ug/l	50409	4	12.024	118118	50.0
Benzene, 1,2,4,...	12.963	24.4	ug/l	57536	4	12.024	118118	50.0
1H-Indene, 2,3-...	13.292	40.6	ug/l	95976	4	12.024	118118	50.0