LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021580.D
Acq On : 29 Mar 2021 16:26
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-3R

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\82X032421W.M
Title : SW846 8260

Signal : TIC: VX021580.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.464	726	744	756	rBV	48465	135484	9.65%	1.944%
2	5.629	761	772	789	rVB	68613	193263	13.76%	2.773%
3	6.029	829	840	858	rBV	51718	135438	9.64%	1.943%
4	6.829	965	976	988	rBV	117898	277962	19.79%	3.988%
5	8.694	1287	1293	1303	rVB	255146	385112	27.42%	5.526%
6	10.094	1526	1531	1539	rBV	267237	356034	25.35%	5.108%
7	10.171	1539	1544	1548	rVB	9858	15772	1.12%	0.226%
8	10.235	1548	1555	1560	rBV	26976	39241	2.79%	0.563%
9	10.341	1560	1573	1579	rBV	95623	157639	11.23%	2.262%
10	10.624	1609	1621	1628	rBV5	20236	52660	3.75%	0.756%
11	10.682	1628	1631	1640	rVB4	8845	19719	1.40%	0.283%
12	10.818	1645	1654	1659	rVB2	43438	69422	4.94%	0.996%
13	10.894	1659	1667	1671	rBV3	39857	61213	4.36%	0.878%
14	11.000	1680	1685	1690	rBV	113501	142569	10.15%	2.046%
15	11.118	1700	1705	1710	rBV	223429	291246	20.74%	4.179%
16	11.165	1710	1713	1717	rVB	17913	23045	1.64%	0.331%
17	11.259	1721	1729	1738	rVV4	24210	38922	2.77%	0.558%
18	11.341	1738	1743	1752	rVV	195842	255081	18.16%	3.660%
19	11.418	1752	1756	1757	rVV	44440	51017	3.63%	0.732%
20	11.435	1757	1759	1763	rVV	51283	64173	4.57%	0.921%
21	11.488	1763	1768	1777	rVB	61206	96329	6.86%	1.382%
22	11.653	1791	1796	1803	rBV5	24652	43535	3.10%	0.625%
23	11.753	1809	1813	1815	rBV	40460	46549	3.31%	0.668%
24	11.788	1815	1819	1829	rVB	1160962	1404249	100.00%	20.148%
25	11.906	1829	1839	1840	rBV	54698	77934	5.55%	1.118%
26	11.930	1840	1843	1848	rVB	103654	125764	8.96%	1.804%
27	11.983	1848	1852	1853	rBV	13084	14043	1.00%	0.201%
28	12.006	1853	1856	1860	rVV	44702	52479	3.74%	0.753%
29	12.059	1860	1865	1871	rVB2	277919	371749	26.47%	5.334%
30	12.124	1871	1876	1887	rVB	236883	294995	21.01%	4.233%
31	12.218	1887	1892	1898	rVB	36639	50890	3.62%	0.730%
32	12.283	1898	1903	1910	rBV2	212928	313594	22.33%	4.500%
33	12.353	1910	1915	1923	rVB2	94680	183368	13.06%	2.631%
34	12.441	1924	1930	1937	rBV	41653	56886	4.05%	0.816%
35	12.571	1946	1952	1954	rBV	76651	106709	7.60%	1.531%
36	12.594	1954	1956	1960	rVV	80310	80913	5.76%	1.161%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021580.D
Acq On : 29 Mar 2021 16:26
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-3R

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\82X032421W.M
Title : SW846 8260

37	12.653	1961	1966	1969	rVV	163260	197806	14.09%	2.838%
38	12.683	1969	1971	1976	rVB	47914	53472	3.81%	0.767%
39	12.742	1976	1981	1989	rBV3	101423	185690	13.22%	2.664%
40	12.883	2001	2005	2010	rVB2	44020	61188	4.36%	0.878%
41	12.959	2010	2018	2022	rBV2	47328	73248	5.22%	1.051%
42	13.000	2022	2025	2032	rVB	74966	88692	6.32%	1.273%
43	13.065	2032	2036	2042	rBV3	17347	26701	1.90%	0.383%
44	13.130	2042	2047	2052	rBV	11329	15346	1.09%	0.220%
45	13.206	2057	2060	2063	rVB	13122	14756	1.05%	0.212%
46	13.330	2076	2081	2087	rVB2	79795	117445	8.36%	1.685%
47	13.459	2099	2103	2109	rVB	38459	50185	3.57%	0.720%

Sum of corrected areas: 6969527

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021580.D
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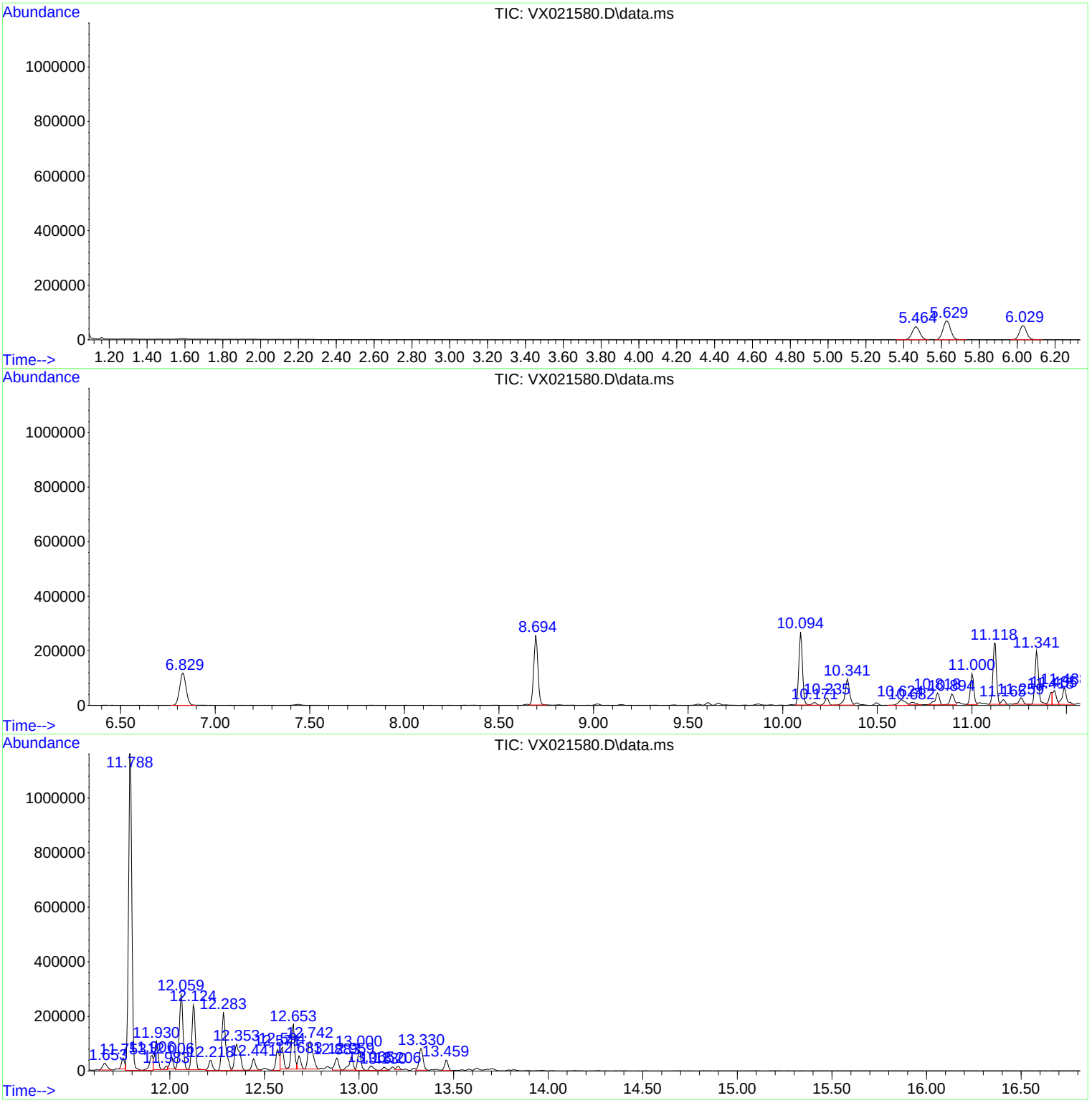
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021580.D
Acq On : 29 Mar 2021 16:26
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3R

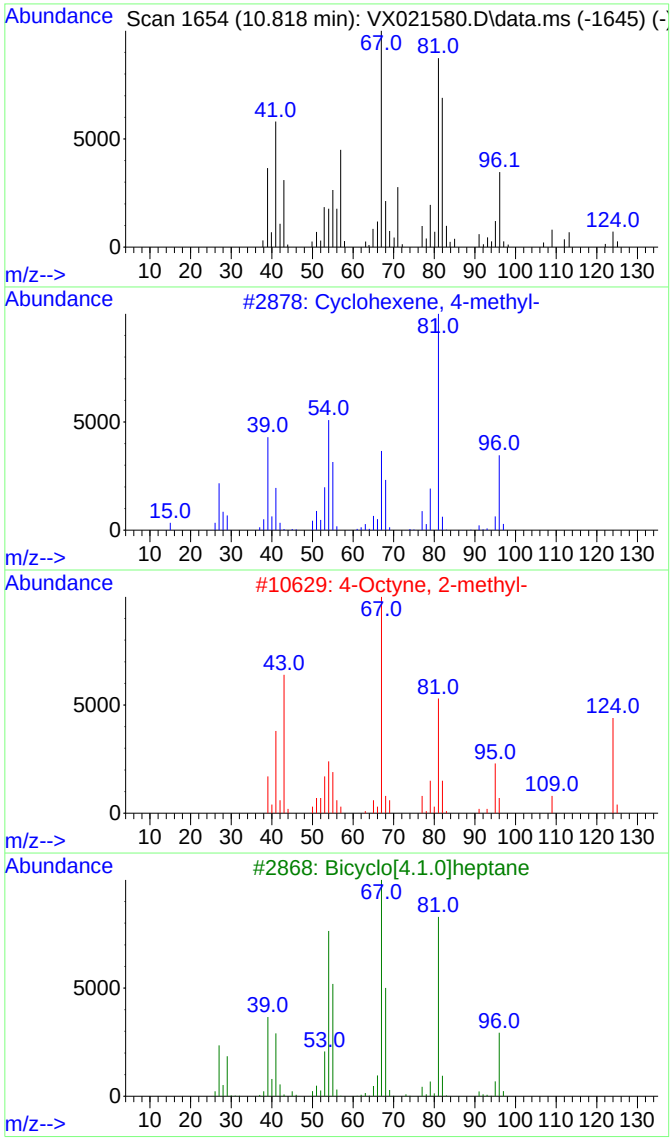
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

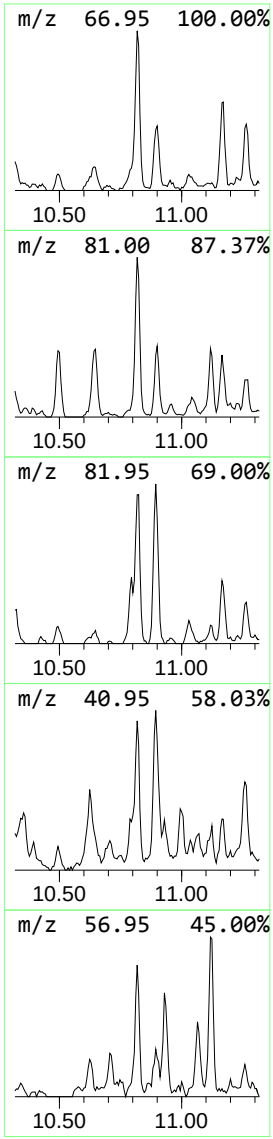
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclohexene, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.818	9.75 ug/l	69422	Chlorobenzene-d5	10.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	55
2	4-Octyne, 2-methyl-	124	C9H16	010306-94-2	52
3	Bicyclo[4.1.0]heptane	96	C7H12	000286-08-8	52
4	1,4-Hexadiene, 2-methyl-	96	C7H12	001119-14-8	46
5	Ethylidenecycloheptane	124	C9H16	010494-87-8	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021580.D
Acq On : 29 Mar 2021 16:26
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3R

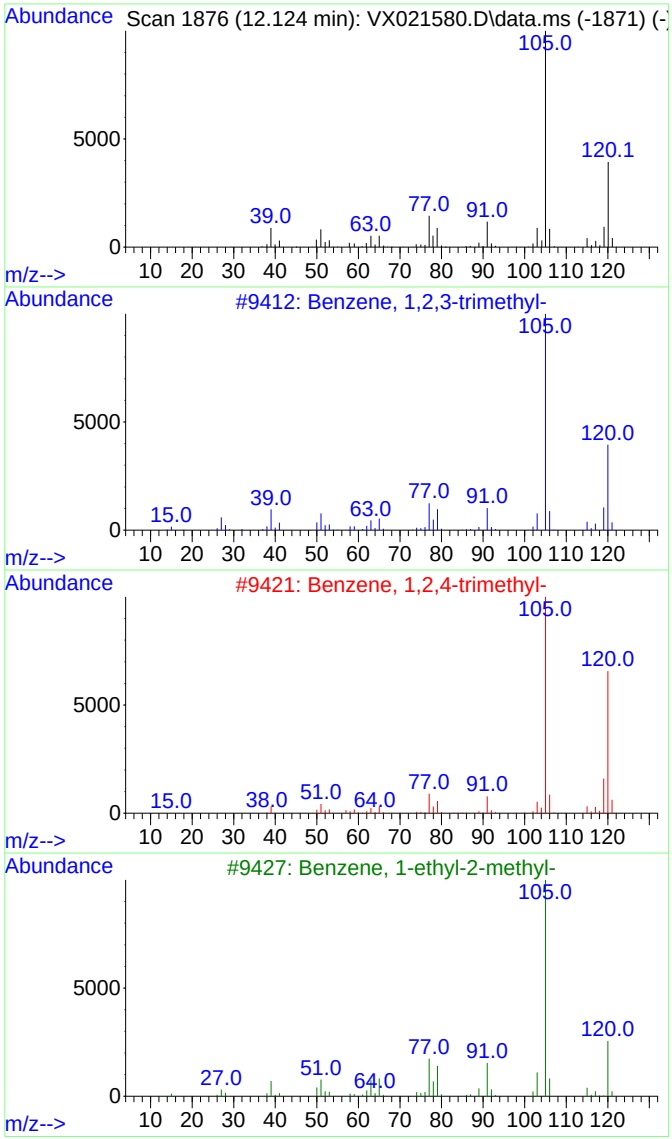
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

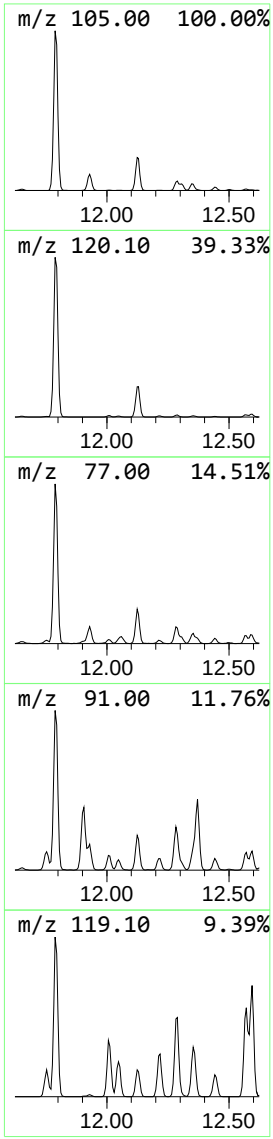
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.124	39.68 ug/l	294995	1,4-Dichlorobenzene-d4	12.065

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-3-methyl-	120	C9H12	000620-14-4	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021580.D
Acq On : 29 Mar 2021 16:26
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3R

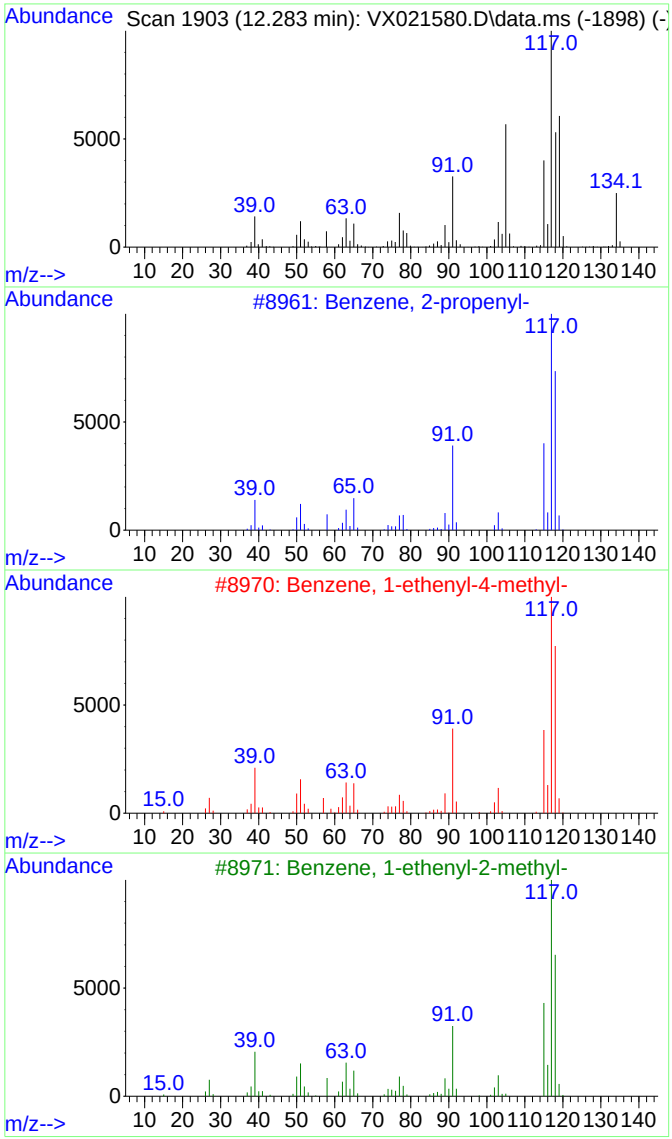
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

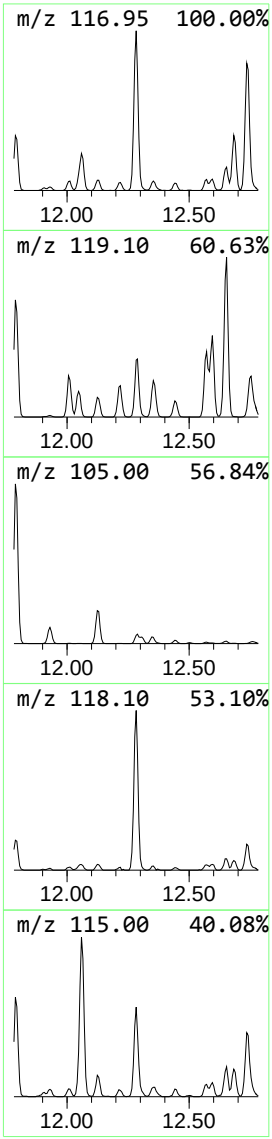
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 2-propenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.283	42.18 ug/l	313594	1,4-Dichlorobenzene-d4	12.065

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	91
2	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	86
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	83
4	Indane	118	C9H10	000496-11-7	70
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021580.D
Acq On : 29 Mar 2021 16:26
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3R

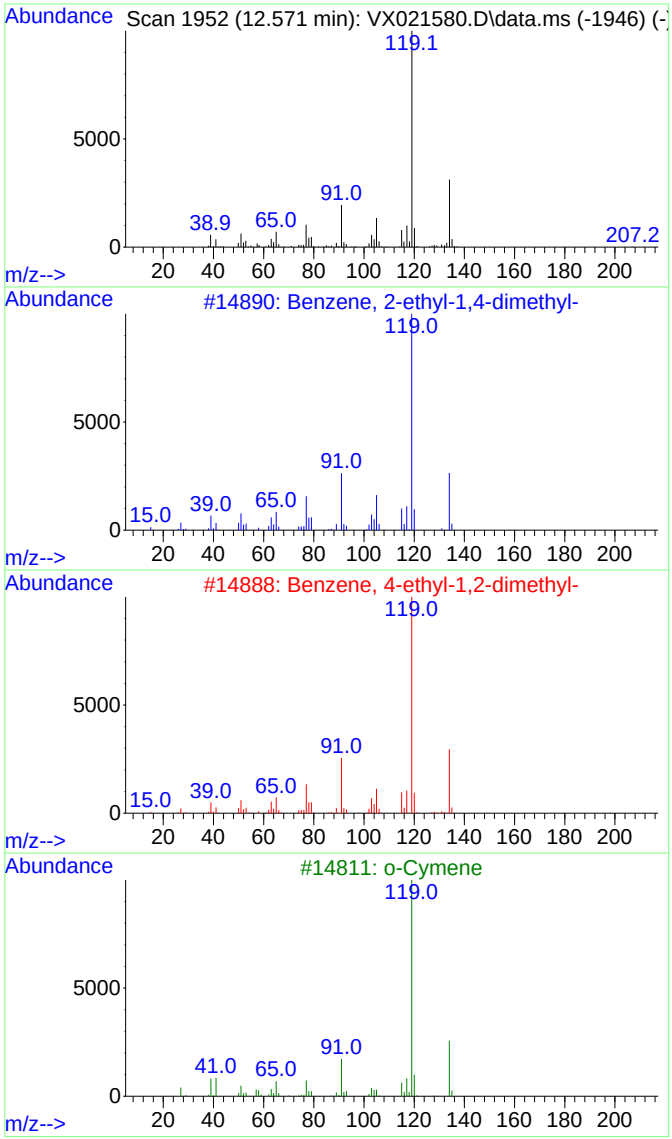
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

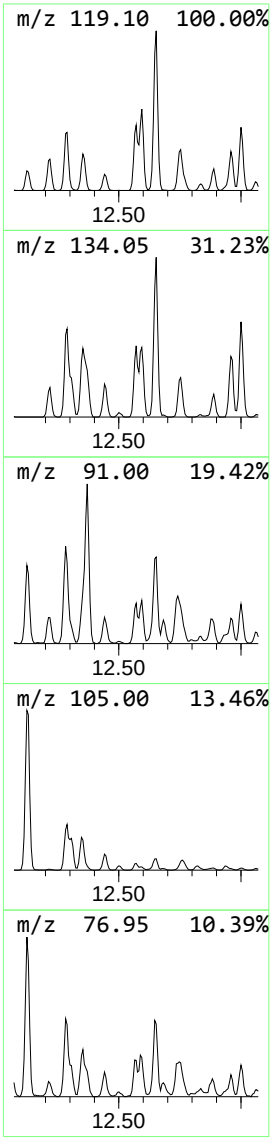
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.571	14.35 ug/l	106709	1,4-Dichlorobenzene-d4	12.065

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	o-Cymene	134	C10H14	000527-84-4	95
4	p-Cymene	134	C10H14	000099-87-6	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021580.D
Acq On : 29 Mar 2021 16:26
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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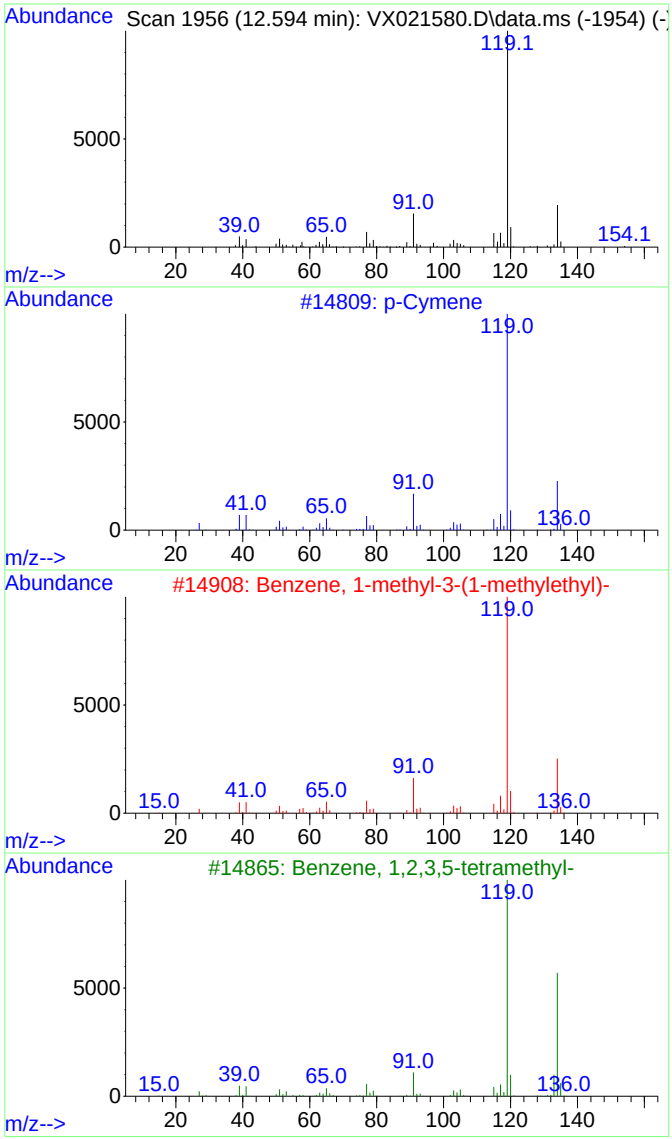
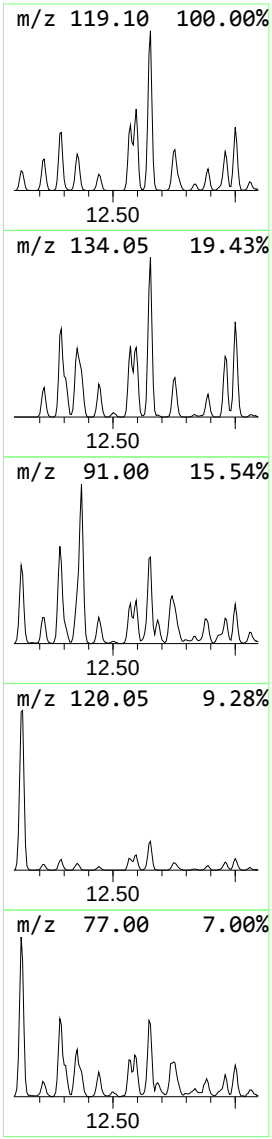
****

Peak Number 5 p-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.595	10.88 ug/l	80913	1,4-Dichlorobenzene-d4	12.065

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Cymene	134	C10H14	000099-87-6	95
2	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

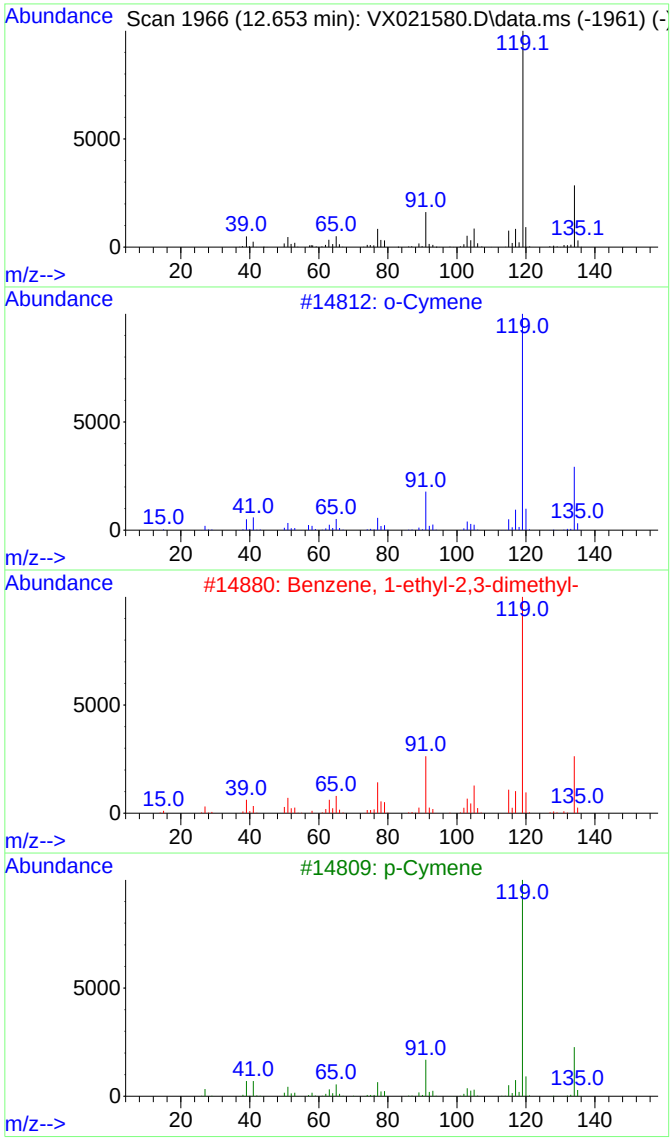
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

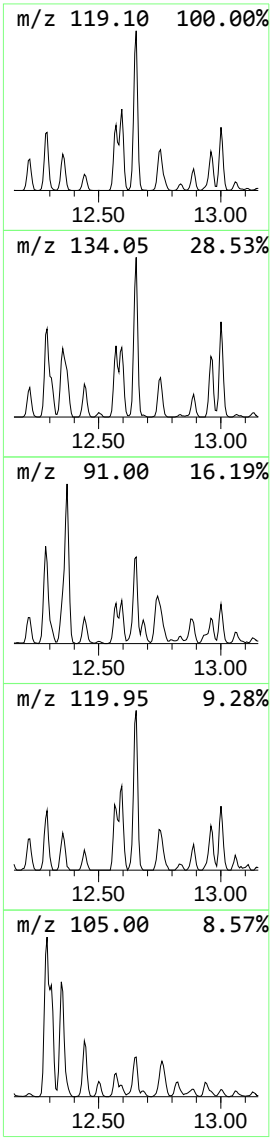
****

Peak Number 6 o-Cymene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.653	26.60 ug/l	197806	1,4-Dichlorobenzene-d4	12.065

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3	p-Cymene	134	C10H14	000099-87-6	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3R

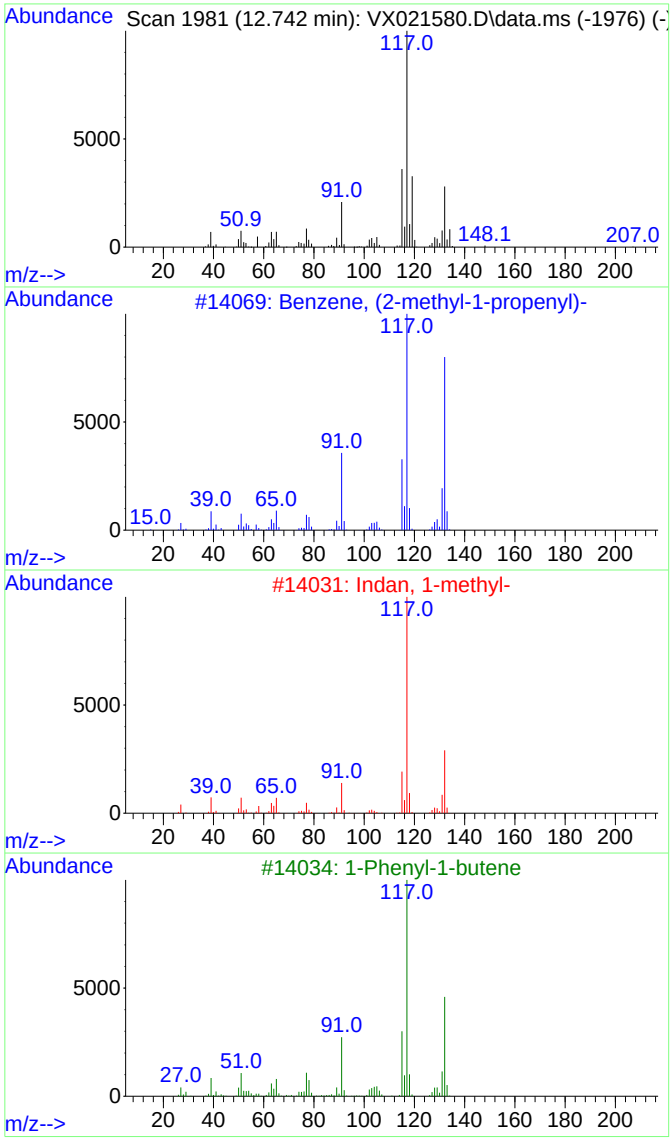
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

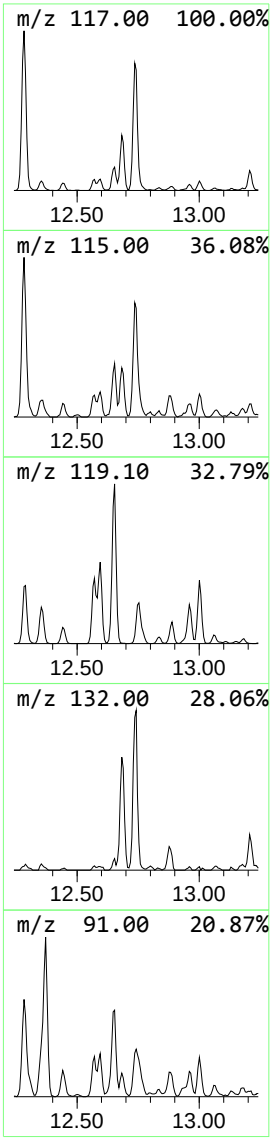
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (2-methyl-1-propen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.742	24.98 ug/l	185690	1,4-Dichlorobenzene-d4	12.065

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
2	Indan, 1-methyl-	132	C10H12	000767-58-8	87
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021580.D
Acq On : 29 Mar 2021 16:26
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3R

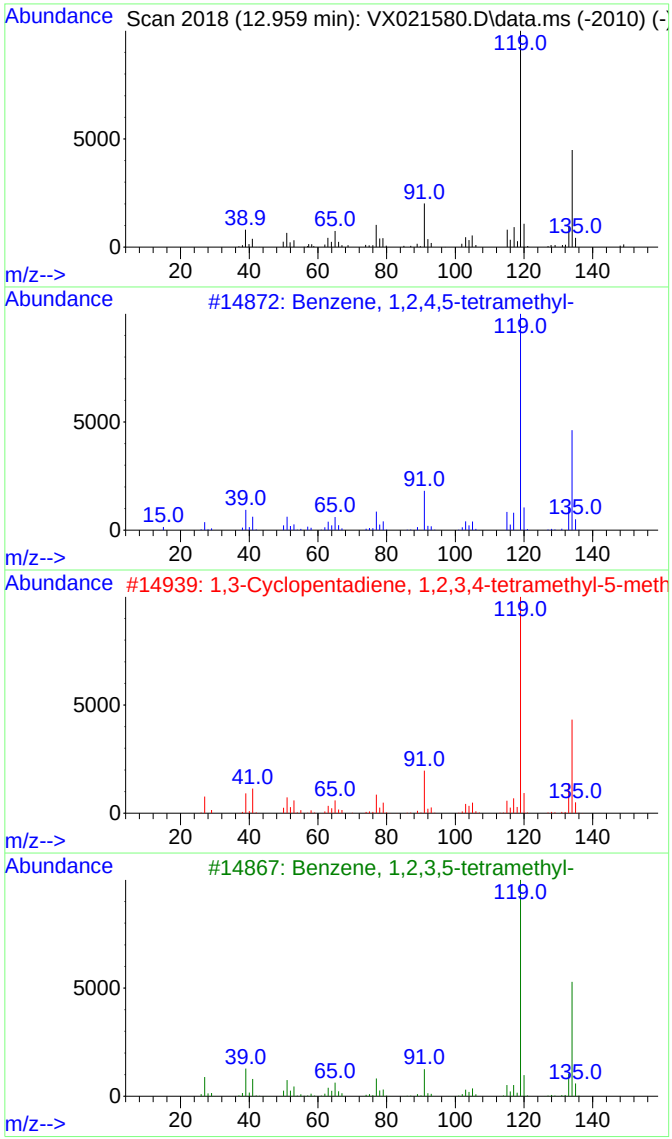
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

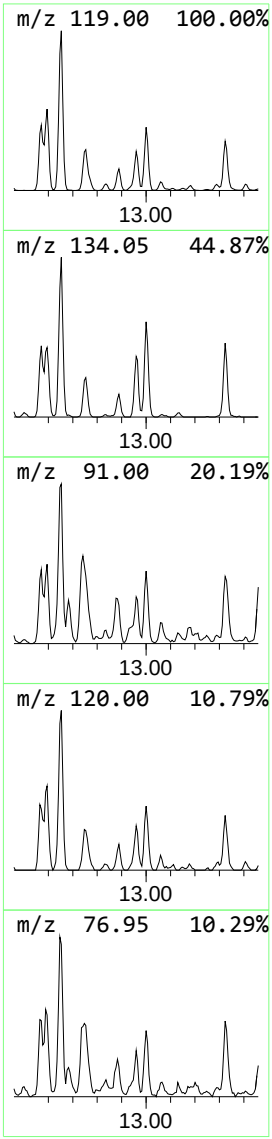
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.959	9.85 ug/l	73248	1,4-Dichlorobenzene-d4	12.065

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
2	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	94
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	93
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93





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Data File : VX021580.D
Acq On : 29 Mar 2021 16:26
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3R

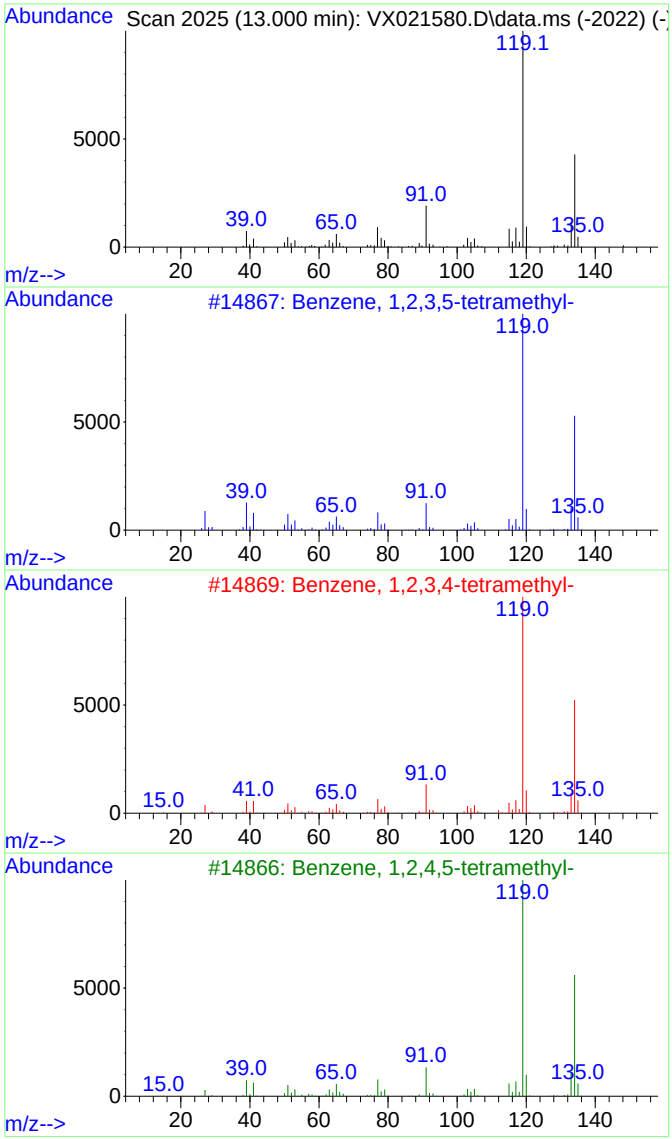
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

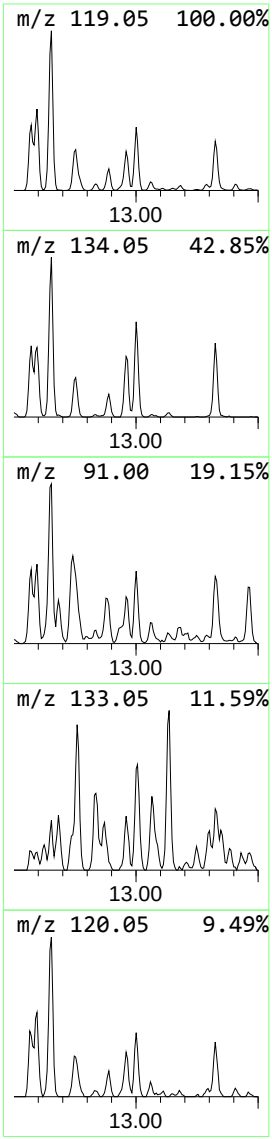
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.000	11.93 ug/l	88692	1,4-Dichlorobenzene-d4	12.065

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	94
5	o-Cymene	134	C10H14	000527-84-4	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021580.D
Acq On : 29 Mar 2021 16:26
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3R

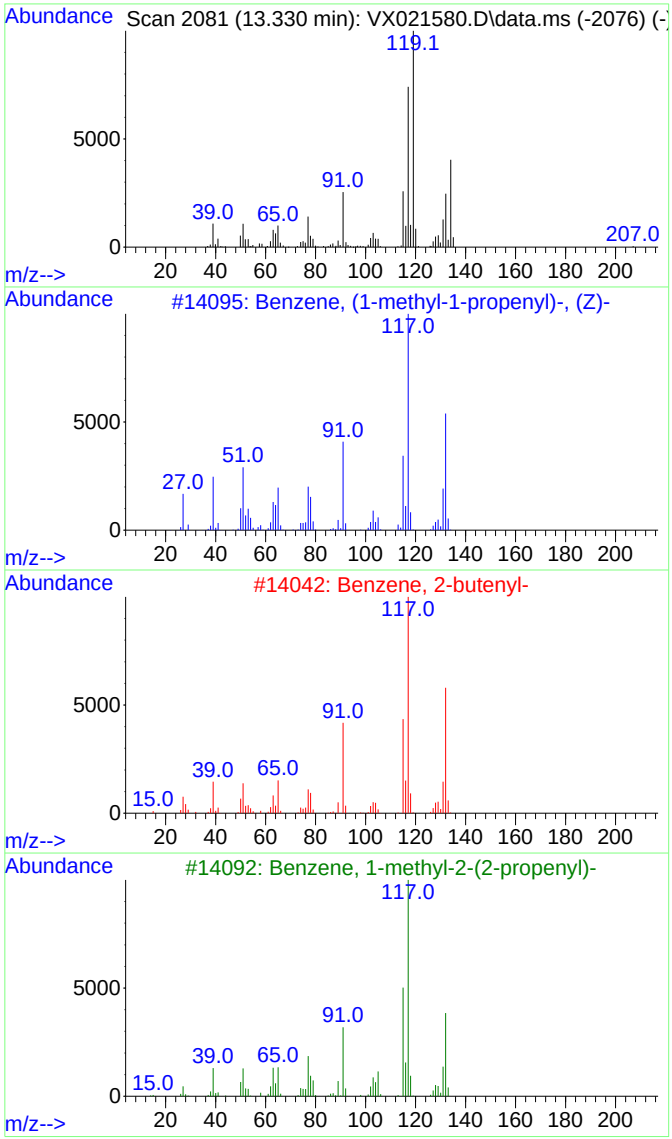
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

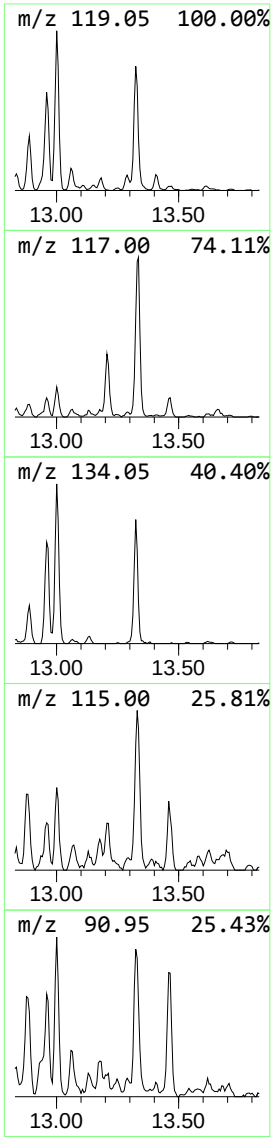
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, (1-methyl-1-propen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.330	15.80 ug/l	117445	1,4-Dichlorobenzene-d4	12.065

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	70
3	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	55
5	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	55





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021580.D
Acq On : 29 Mar 2021 16:26
Operator : JC/MD
Sample : M1785-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.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
Cyclohexene, 4-...	10.818	9.8	ug/l	69422	3	10.094	356034	50.0
Benzene, 1,2,3-...	12.124	39.7	ug/l	294995	4	12.065	371749	50.0
Benzene, 2-prop...	12.283	42.2	ug/l	313594	4	12.065	371749	50.0
Benzene, 2-ethy...	12.571	14.4	ug/l	106709	4	12.065	371749	50.0
p-Cymene	12.595	10.9	ug/l	80913	4	12.065	371749	50.0
o-Cymene	12.653	26.6	ug/l	197806	4	12.065	371749	50.0
Benzene, (2-met...	12.742	25.0	ug/l	185690	4	12.065	371749	50.0
Benzene, 1,2,4,...	12.959	9.8	ug/l	73248	4	12.065	371749	50.0
Benzene, 1,2,3,...	13.000	11.9	ug/l	88692	4	12.065	371749	50.0
Benzene, (1-met...	13.330	15.8	ug/l	117445	4	12.065	371749	50.0