LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

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\82X031023W.M
Title : SW846 8260

Signal : TIC: VX034811.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	53	rBV	6484600	7170457	5.45%	1.377%
2	1.752	103	109	123	rBV	10253386	13858004	10.53%	2.661%
3	1.959	138	143	156	rVV2	5487836	9653385	7.33%	1.854%
4	2.069	156	161	169	rVV	2305942	3216377	2.44%	0.618%
5	2.166	169	177	181	rVV	1434127	2166970	1.65%	0.416%
6	2.215	181	185	198	rVB	5145870	7843783	5.96%	1.506%
7	2.751	257	273	281	rBV2	1585369	5039596	3.83%	0.968%
8	2.825	281	285	289	rVV	2440768	5213339	3.96%	1.001%
9	2.867	289	292	316	rVB2	2821921	5925058	4.50%	1.138%
10	3.105	318	331	353	rVB	1679738	3840298	2.92%	0.738%
11	3.325	355	367	378	rBV3	516684	1324900	1.01%	0.254%
12	3.446	378	387	400	rVB	1347079	2984524	2.27%	0.573%
13	3.733	428	434	443	rVB	768651	1814282	1.38%	0.348%
14	4.105	485	495	504	rVB	643072	1683026	1.28%	0.323%
15	4.306	518	528	541	rVB	2703561	7709690	5.86%	1.481%
16	5.196	662	674	690	rVB	952591	2989396	2.27%	0.574%
17	5.477	710	720	730	rBV3	1039768	3948963	3.00%	0.758%
18	5.830	765	778	790	rBV2	595841	1813099	1.38%	0.348%
19	6.044	803	813	824	rVV	10631796	28891146	21.95%	5.548%
20	6.196	824	838	844	rVV3	489700	2271014	1.73%	0.436%
21	6.763	923	931	936	rBV	535123	1332778	1.01%	0.256%
22	7.379	1019	1032	1044	rBV4	1279585	3327536	2.53%	0.639%
23	8.653	1236	1241	1246	rBV	878149	1520610	1.16%	0.292%
24	8.744	1246	1256	1262	rVV3	50926402	131607697	100.00%	25.274%
25	10.055	1466	1471	1475	rBV	1152312	1498241	1.14%	0.288%
26	10.195	1488	1494	1500	rVB	18196625	25733869	19.55%	4.942%
27	10.311	1504	1513	1518	rBV	44567635	72501951	55.09%	13.924%
28	10.646	1562	1568	1580	rVB	23731241	31841227	24.19%	6.115%
29	11.305	1668	1676	1681	rBV	2807366	3489164	2.65%	0.670%
30	11.384	1681	1689	1696	rVV	13295173	24352697	18.50%	4.677%
31	11.451	1696	1700	1706	rVB	7769643	9512066	7.23%	1.827%
32	11.610	1721	1726	1737	rVB	6639196	8640155	6.57%	1.659%
33	11.756	1744	1750	1755	rBV	22379010	28042350	21.31%	5.385%
34	12.018	1789	1793	1799	rVB2	1317399	1824337	1.39%	0.350%
35	12.085	1799	1804	1809	rBV	7219634	9004283	6.84%	1.729%
36	12.244	1824	1830	1838	rBV2	7485717	11324367	8.60%	2.175%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

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\82X031023W.M
Title : SW846 8260

37	12.317	1838	1842	1849	rVV2	3359655	4638605	3.52%	0.891%
38	12.530	1872	1877	1879	rBV	1853250	2278605	1.73%	0.438%
39	12.555	1879	1881	1886	rVB	1693103	1736260	1.32%	0.333%
40	12.616	1886	1891	1894	rBV	3036080	3861836	2.93%	0.742%
41	12.701	1900	1905	1912	rBV2	2148709	3061973	2.33%	0.588%
42	12.920	1934	1941	1944	rBV	1933773	2336794	1.78%	0.449%
43	12.963	1944	1948	1953	rVB	2425734	2921606	2.22%	0.561%
44	13.170	1978	1982	1986	rVB	1827794	2207582	1.68%	0.424%
45	13.292	1998	2002	2007	rVB2	3553013	4591085	3.49%	0.882%
46	13.774	2074	2081	2091	rBV	5102782	6578440	5.00%	1.263%
47	14.633	2218	2222	2233	rVB	1217826	1591491	1.21%	0.306%

Sum of corrected areas: 520714912

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
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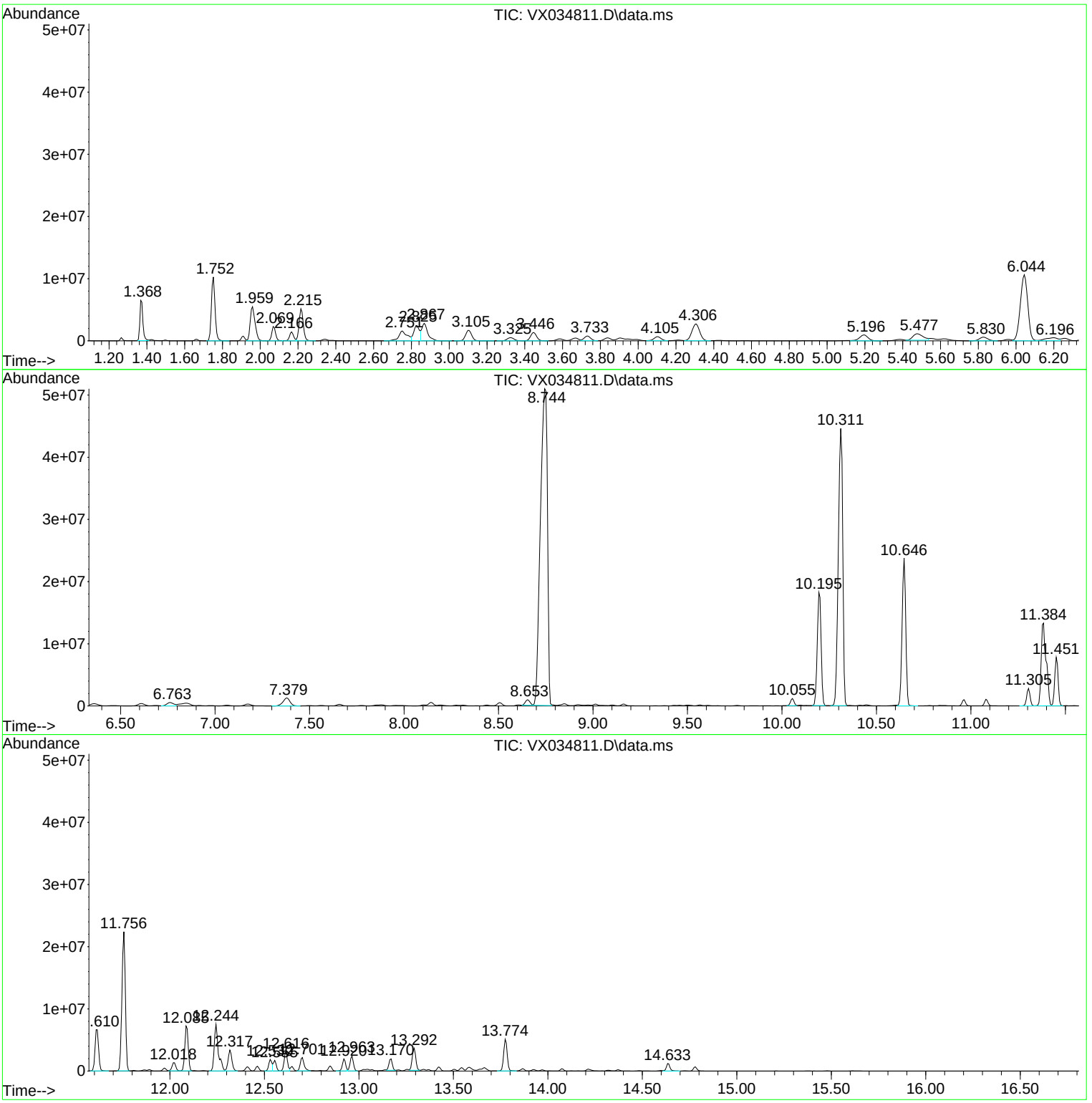
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

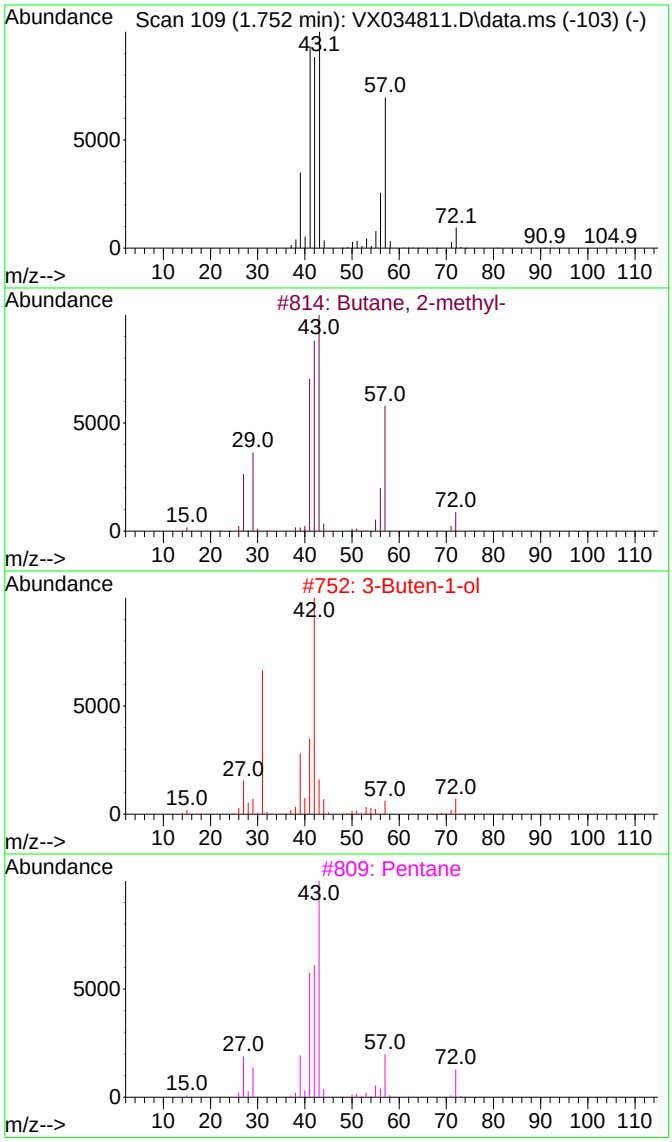
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

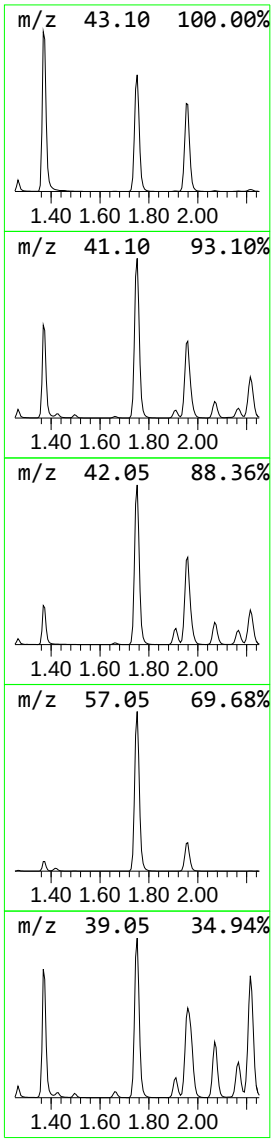
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	175.46 ug/l	13858000	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	42
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

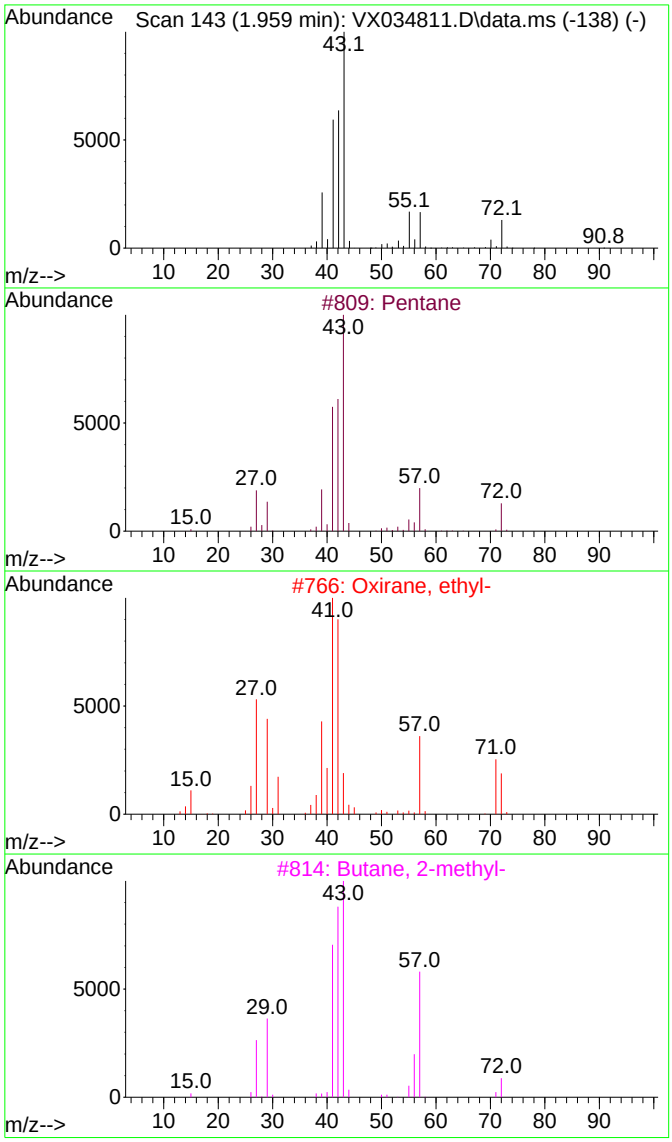
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

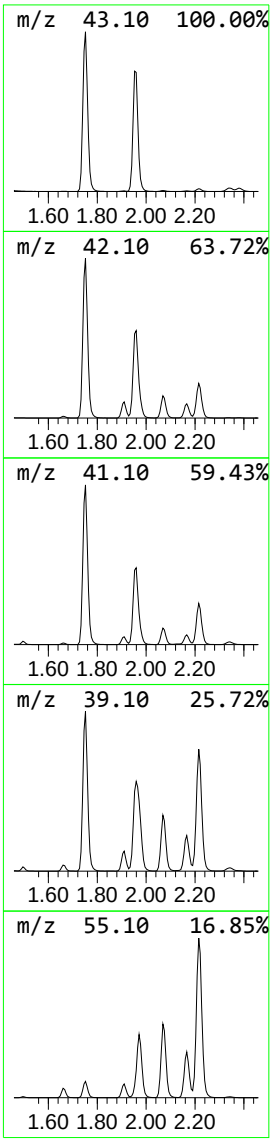
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	122.23 ug/l	9653390	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	87
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	43
3	Butane, 2-methyl-	72	C5H12	000078-78-4	42
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

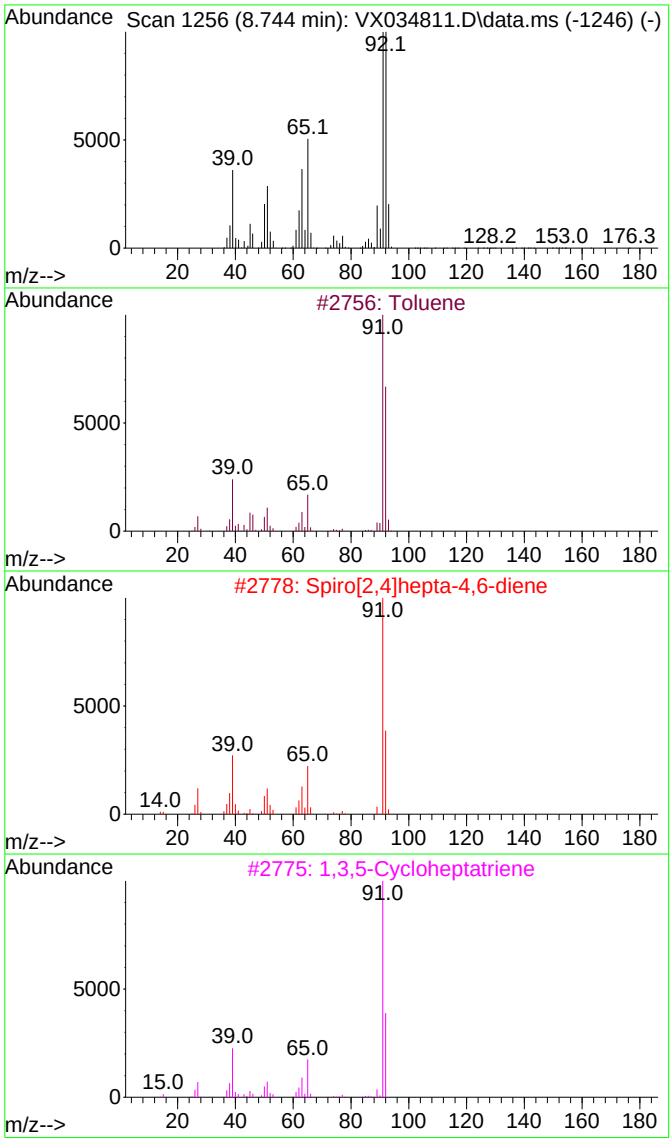
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

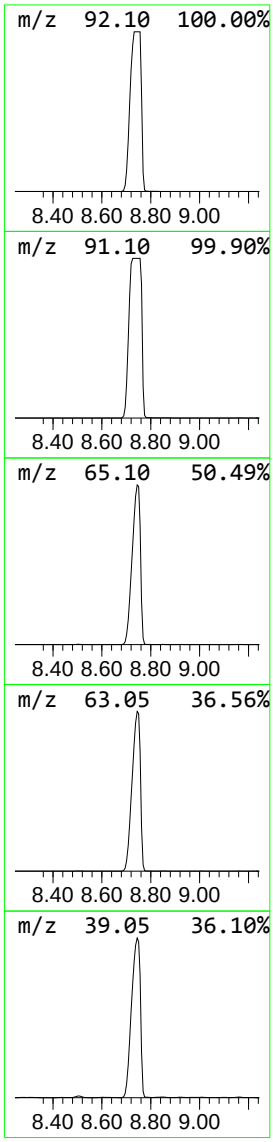
****

Peak Number 3 Toluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.744	4392.07 ug/l	131608000	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	83
2	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	72
3	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	64
4	1,5-Hexadien-3-yne, 2-methyl-	92	C7H8	000820-54-2	64
5	1,6-Heptadien-3-yne	92	C7H8	005150-80-1	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

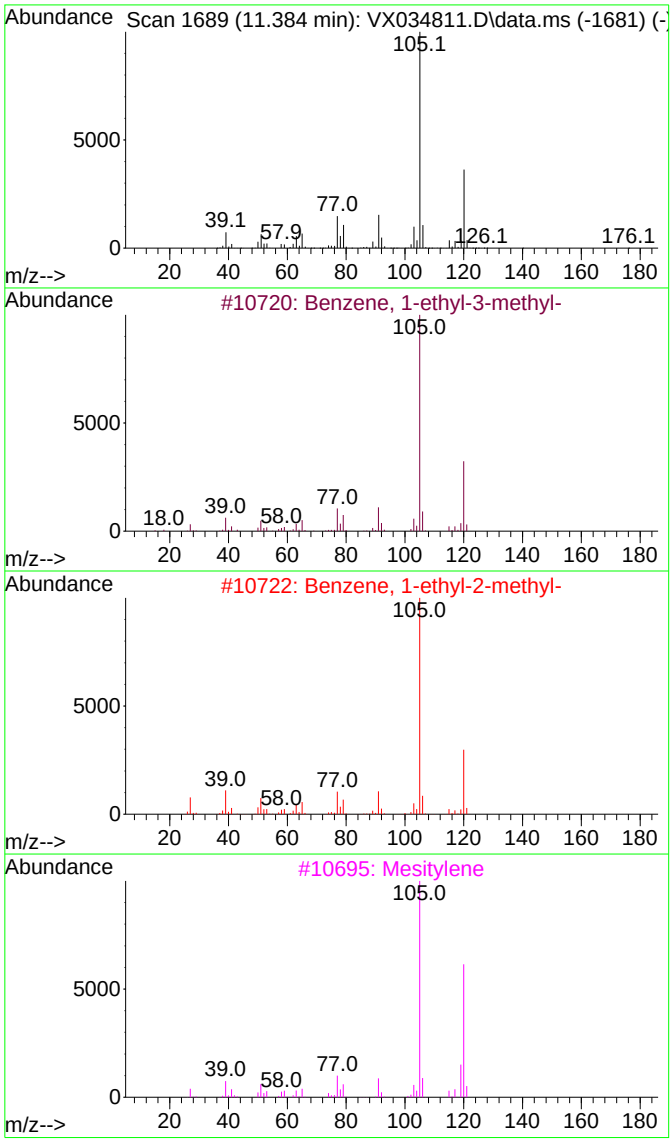
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

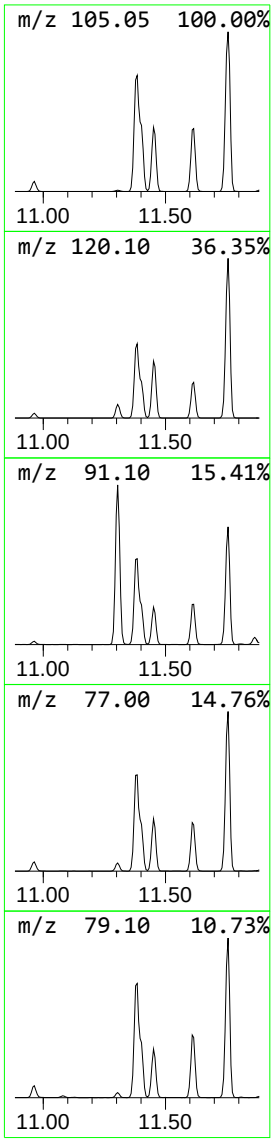
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	667.44 ug/l	24352700	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

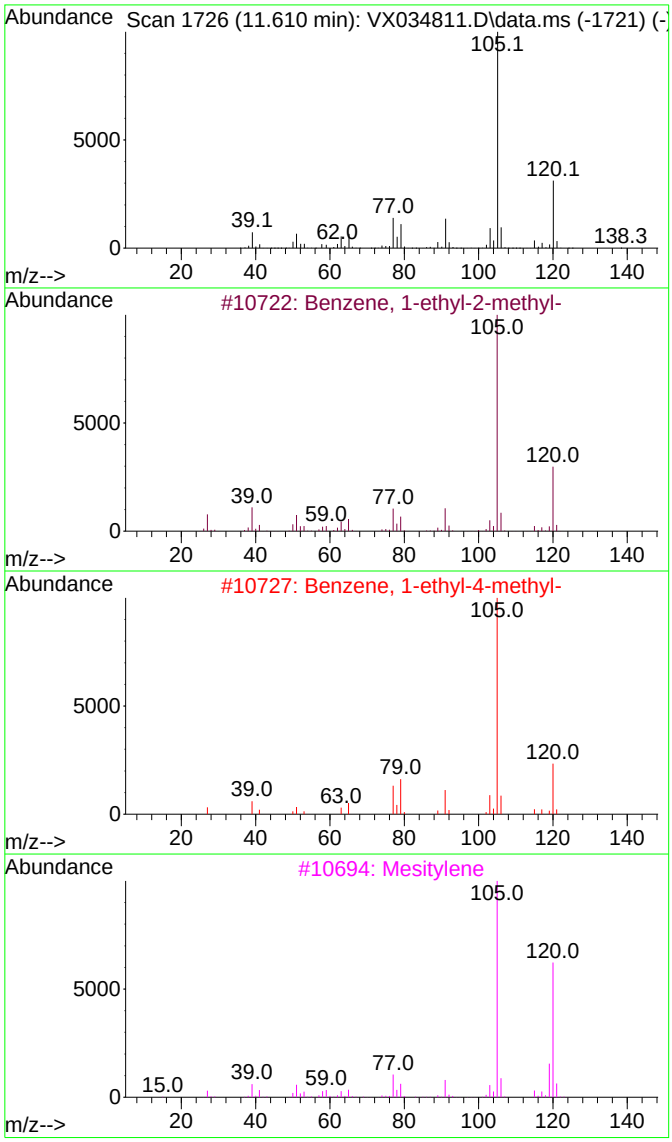
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

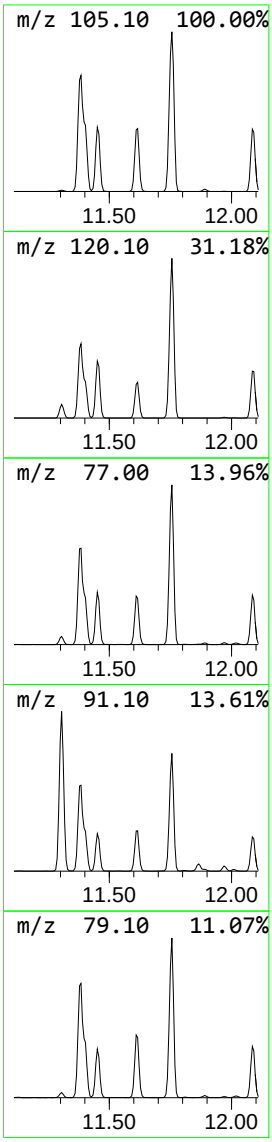
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	236.80 ug/l	8640160	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	93
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

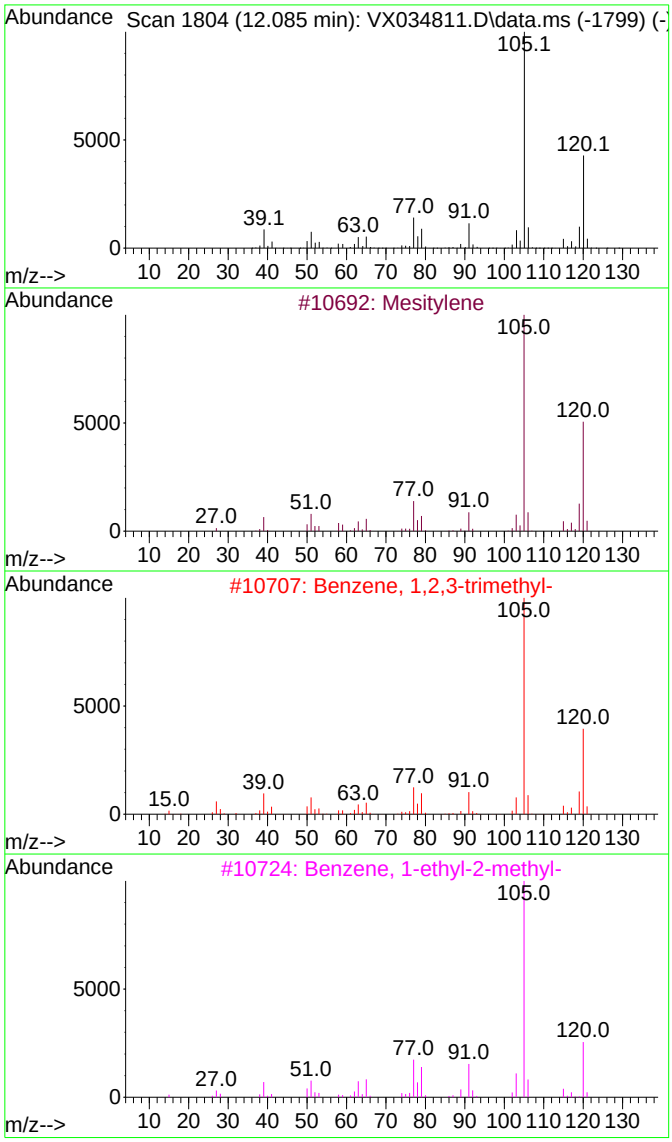
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

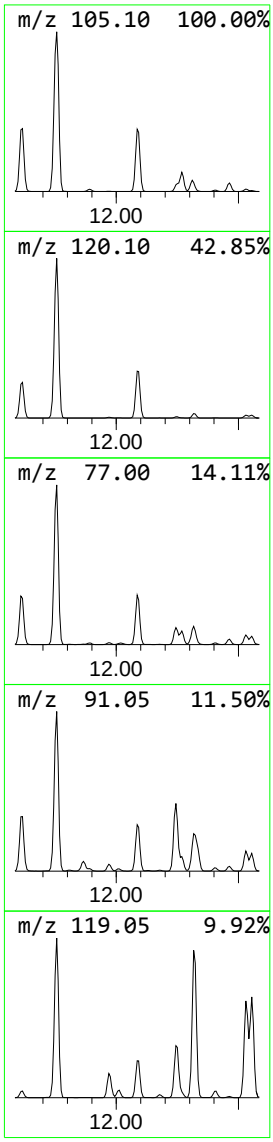
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	246.78 ug/l	9004280	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





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Data File : VX034811.D
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Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

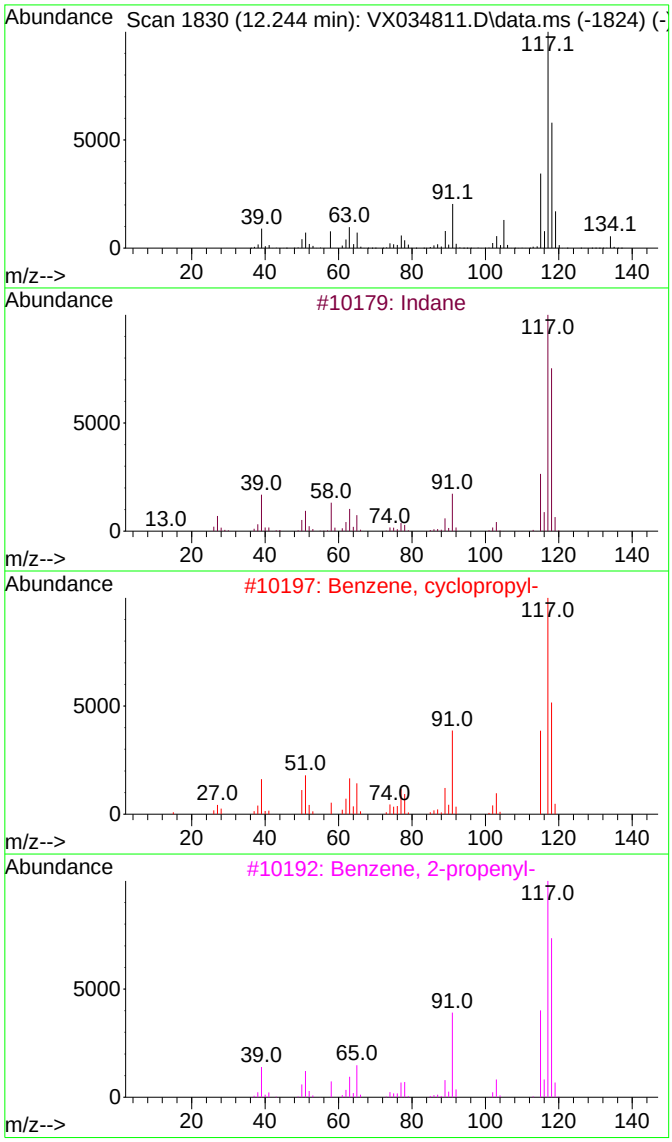
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

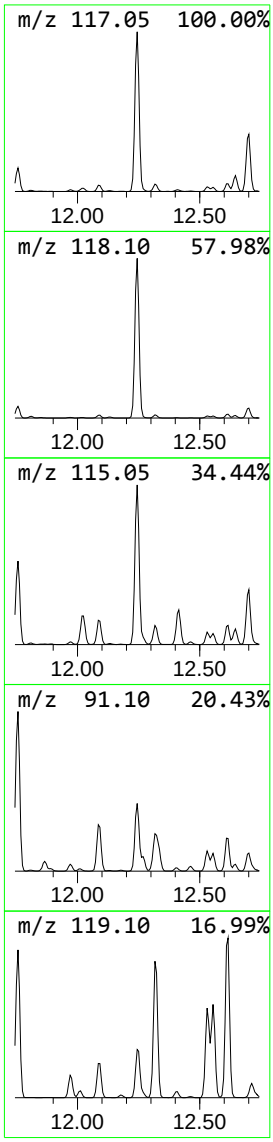
****

Peak Number 7 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	310.37 ug/l	11324400	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	70
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	55





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

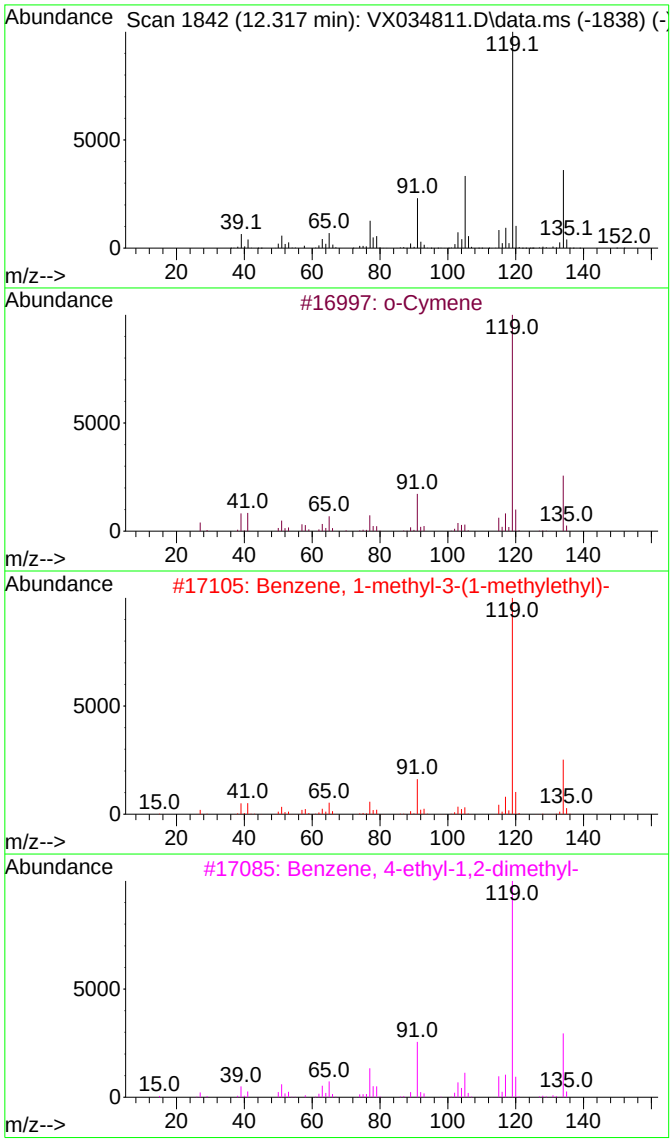
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

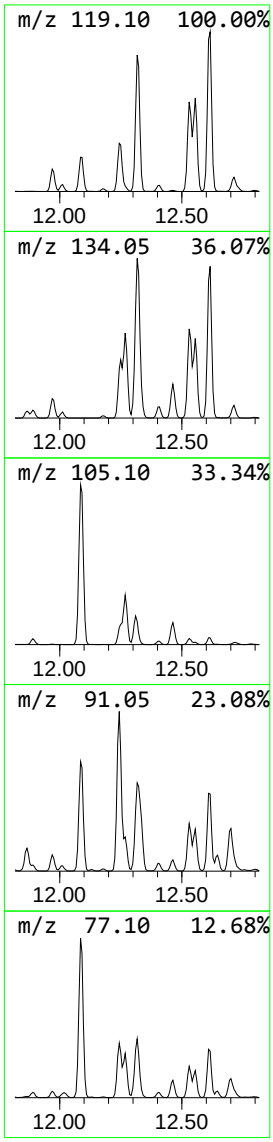
****

Peak Number 8 o-Cymene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	127.13 ug/l	4638610	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	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
4	p-Cymene	134	C10H14	000099-87-6	94
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	93





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Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

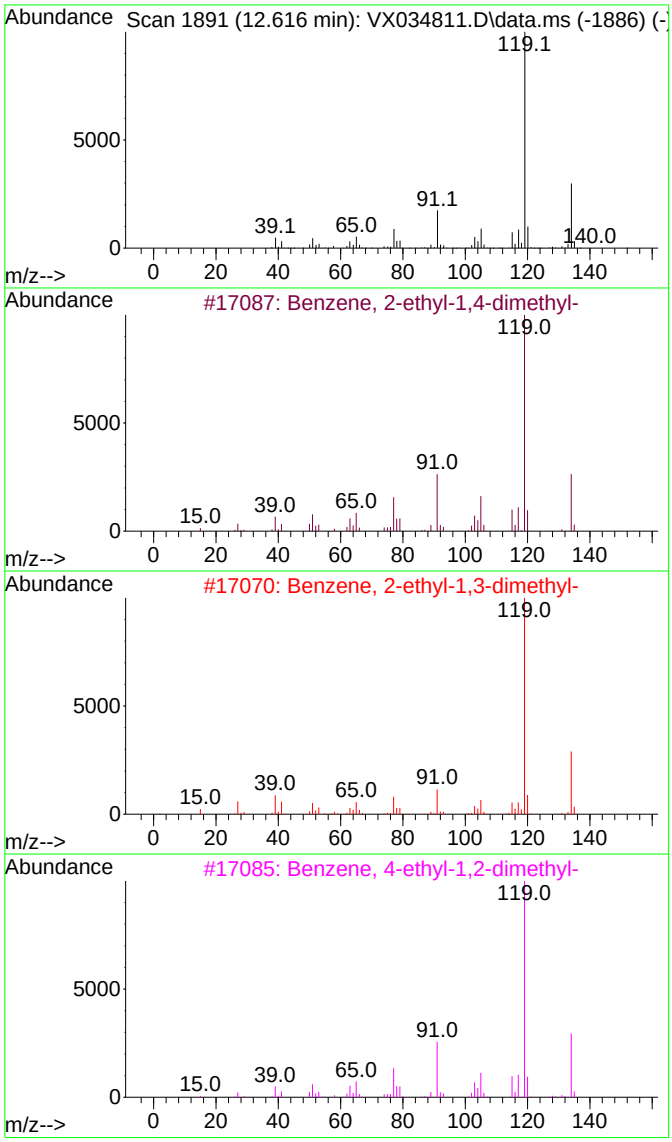
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

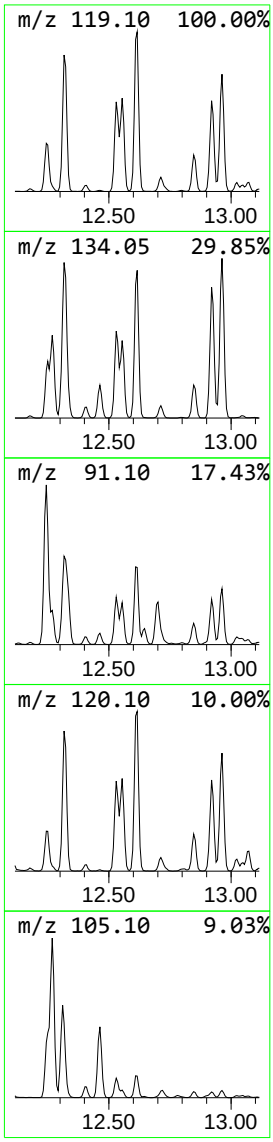
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	105.84 ug/l	3861840	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
5	o-Cymene	134	C10H14	000527-84-4	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

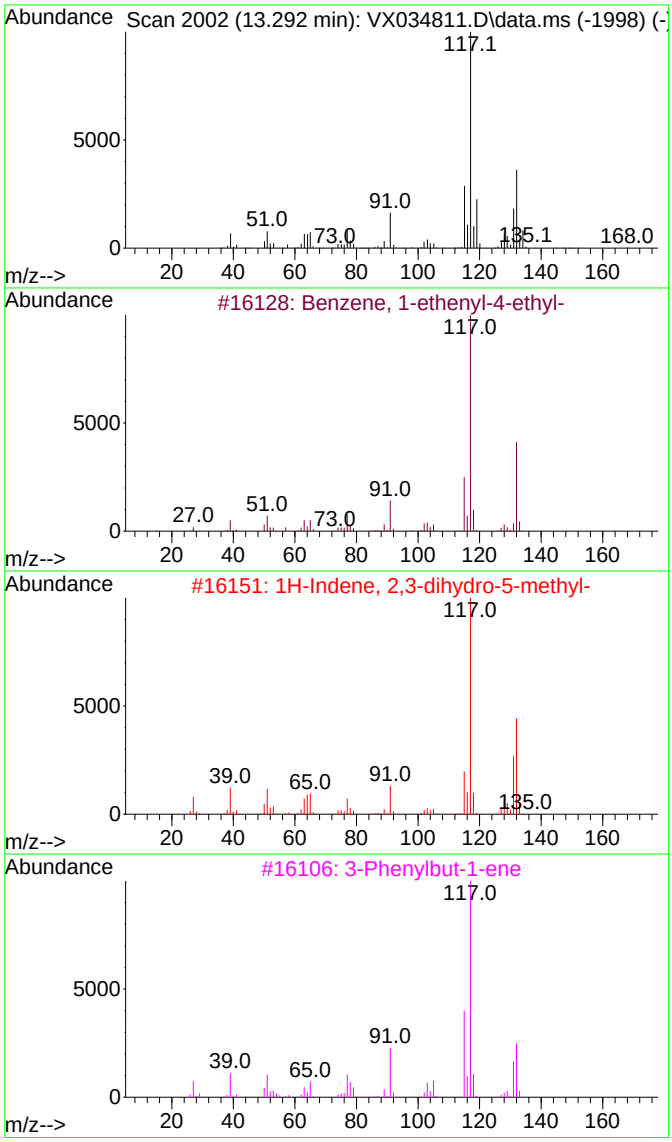
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

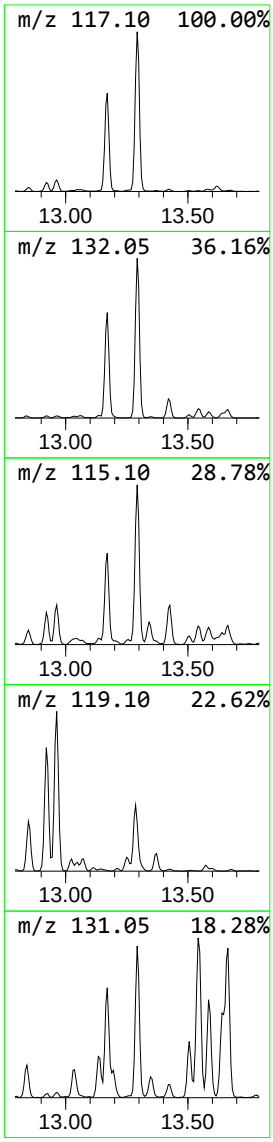
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	125.83 ug/l	4591090	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4	Indan, 1-methyl-	132	C10H12	000767-58-8	87
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034811.D
Acq On : 28 Mar 2023 22:14
Operator : JC/MD
Sample : 02084-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.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
Butane, 2-methyl-	1.752	175.5	ug/l	13858000	1	5.550	3948960	50.0
Pentane	1.959	122.2	ug/l	9653390	1	5.550	3948960	50.0
Toluene	8.744	4392.1	ug/l	131608000	3	10.055	1498240	50.0
Benzene, 1-ethy...	11.384	667.4	ug/l	24352700	4	12.024	1824340	50.0
Benzene, 1-ethy...	11.610	236.8	ug/l	8640160	4	12.024	1824340	50.0
Benzene, 1,2,3-...	12.085	246.8	ug/l	9004280	4	12.024	1824340	50.0
Indane	12.244	310.4	ug/l	11324400	4	12.024	1824340	50.0
o-Cymene	12.317	127.1	ug/l	4638610	4	12.024	1824340	50.0
Benzene, 2-ethy...	12.616	105.8	ug/l	3861840	4	12.024	1824340	50.0
Benzene, 1-ethe...	13.292	125.8	ug/l	4591090	4	12.024	1824340	50.0