LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033390.D
Acq On : 13 Dec 2022 14:21
Operator : JC/MD
Sample : N6001-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

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\82X120722W.M
Title : SW846 8260

Signal : TIC: VX033390.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.752	103	109	119	rBV	1537707	1974999	3.81%	1.410%
2	1.959	138	143	155	rVB	381252	543782	1.05%	0.388%
3	2.825	281	285	289	rVV	275177	597839	1.15%	0.427%
4	2.867	289	292	317	rVB2	359467	814016	1.57%	0.581%
5	4.306	518	528	540	rVB	559132	1586329	3.06%	1.132%
6	6.763	922	931	939	rBV	210560	527108	1.02%	0.376%
7	8.720	1245	1252	1259	rBV	6872909	10485493	20.22%	7.484%
8	10.055	1460	1471	1476	rBV	431193	624302	1.20%	0.446%
9	10.201	1489	1495	1501	rBV	18771306	28155236	54.30%	20.096%
10	10.317	1506	1514	1519	rBV	27710423	51849364	100.00%	37.008%
11	10.646	1562	1568	1574	rVB	14224994	18827291	36.31%	13.438%
12	10.963	1613	1620	1627	rVB	521498	649605	1.25%	0.464%
13	11.305	1667	1676	1682	rBV	1013667	1232612	2.38%	0.880%
14	11.378	1683	1688	1696	rVV	3768398	6587278	12.70%	4.702%
15	11.451	1696	1700	1706	rVB	1670081	1950803	3.76%	1.392%
16	11.616	1721	1727	1735	rVB	1718664	2199459	4.24%	1.570%
17	11.756	1744	1750	1755	rVB	4904178	6097977	11.76%	4.352%
18	12.024	1789	1794	1799	rVB	491625	621984	1.20%	0.444%
19	12.085	1799	1804	1810	rBV	1065367	1314493	2.54%	0.938%
20	12.244	1824	1830	1838	rBV2	2182982	2914987	5.62%	2.081%
21	12.317	1838	1842	1851	rVB2	379991	548085	1.06%	0.391%

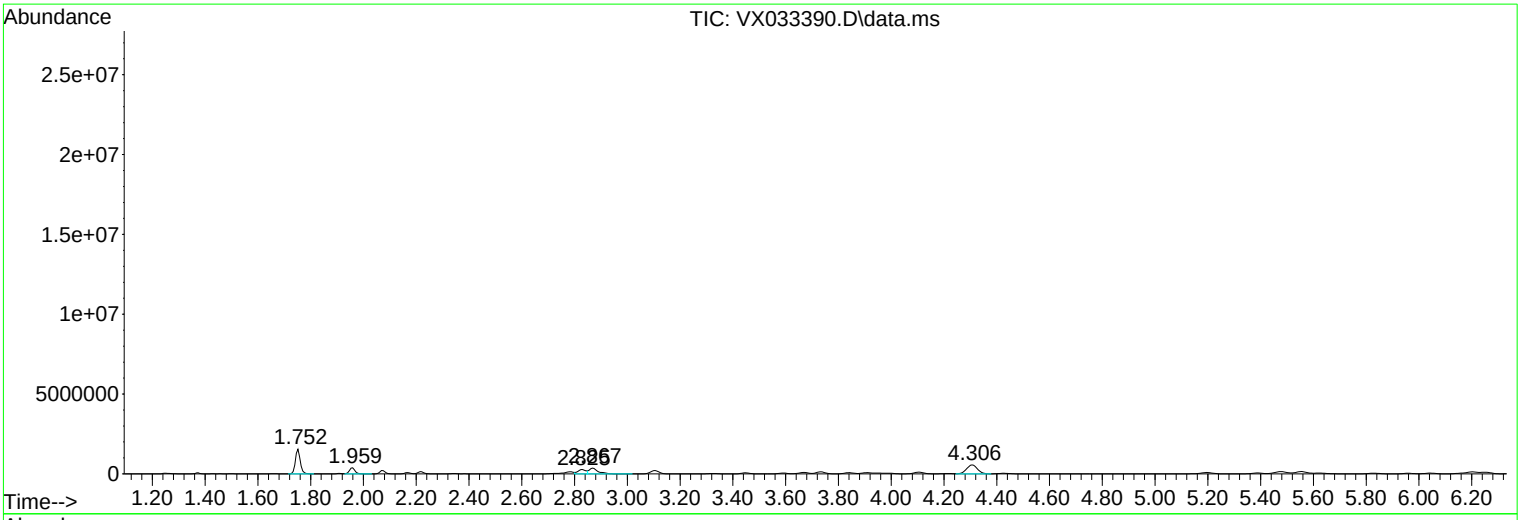
Sum of corrected areas: 140103042

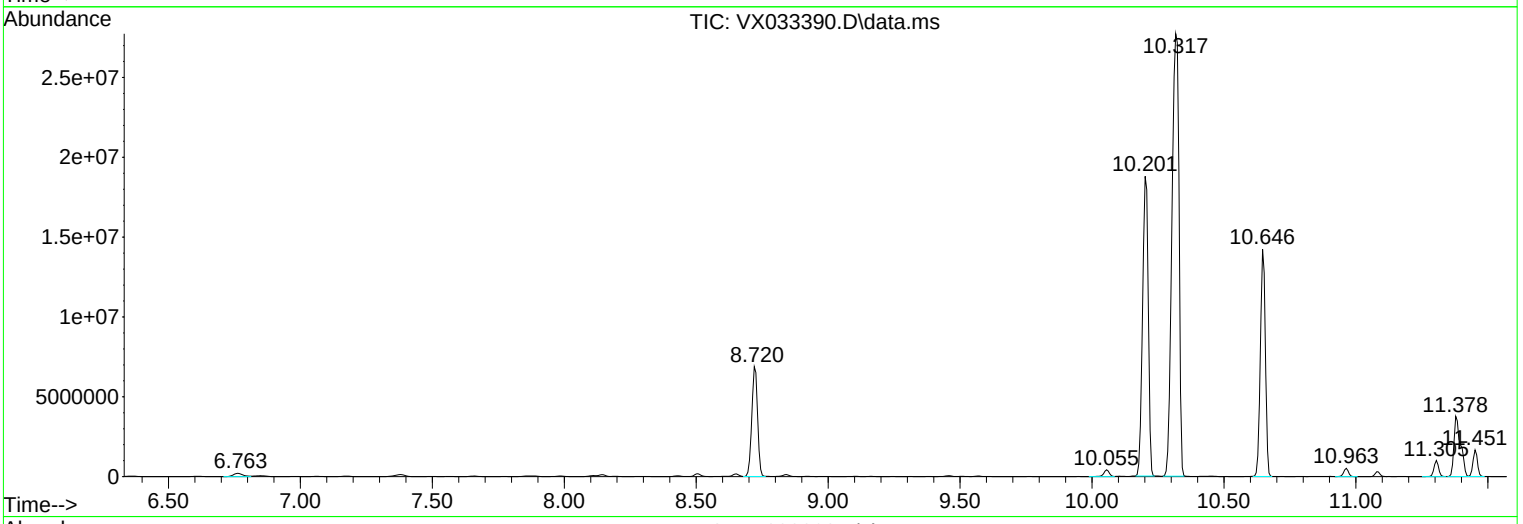
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033390.D
Acq On : 13 Dec 2022 14:21
Operator : JC/MD
Sample : N6001-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

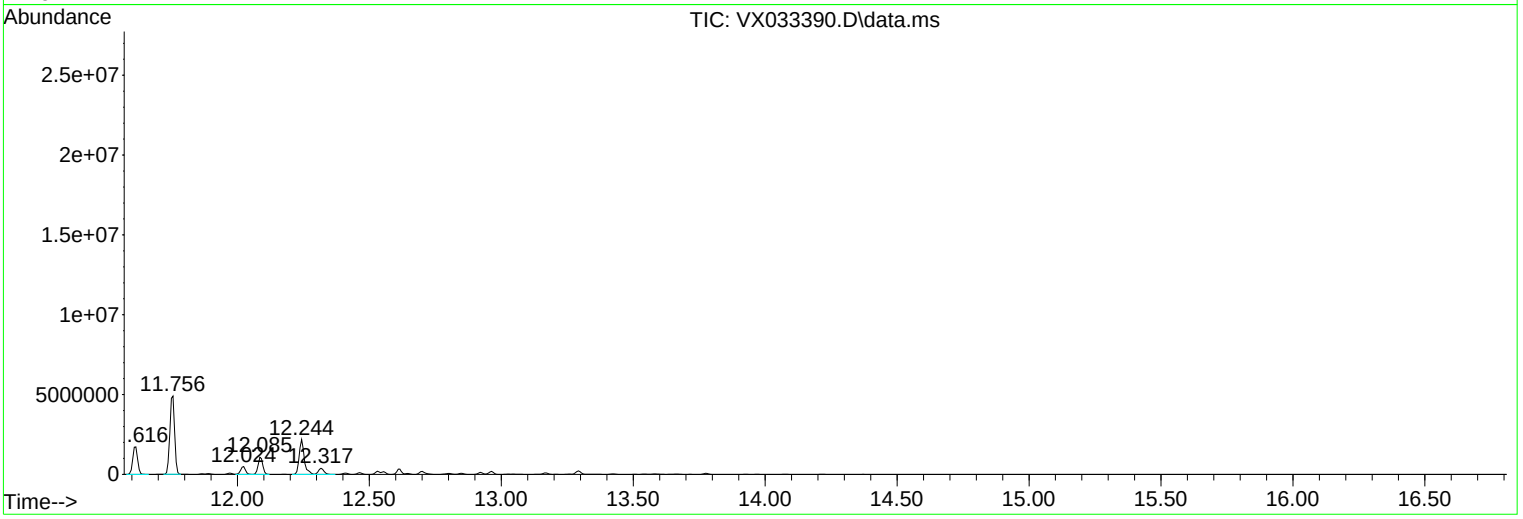
Instrument :
MSVOA_X
ClientSampleId :
MW-6R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033390.D
Acq On : 13 Dec 2022 14:21
Operator : JC/MD
Sample : N6001-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

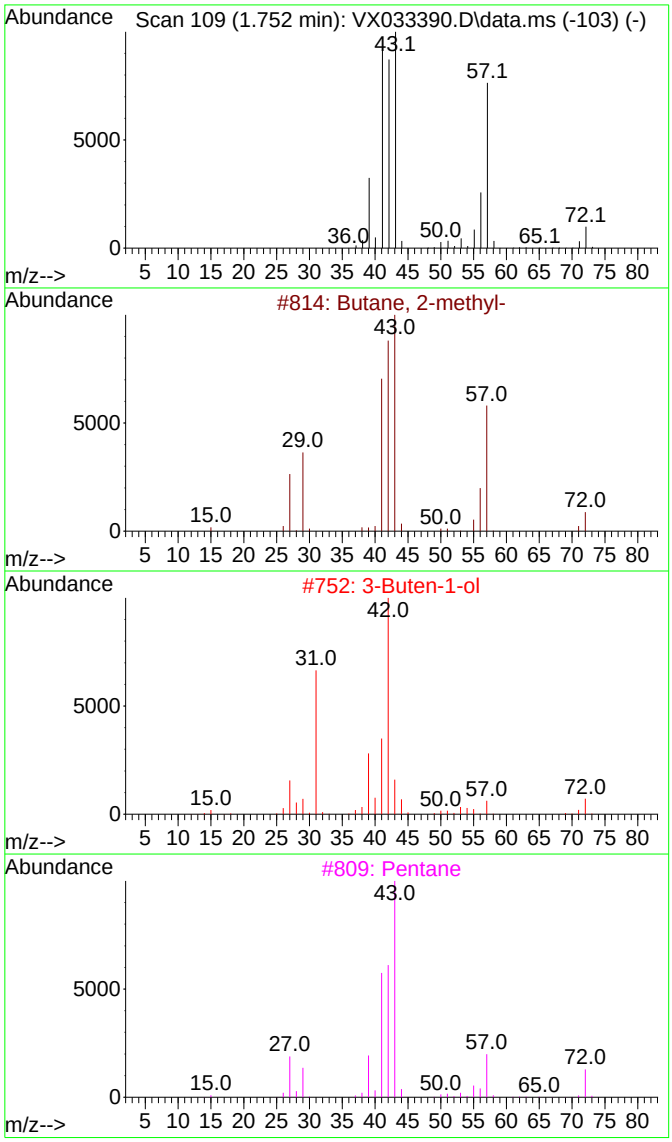
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

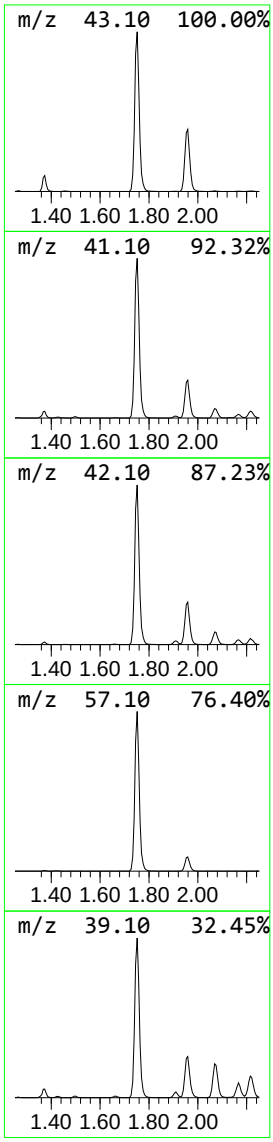
****

Peak Number 1 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	187.34 ug/l	1975000	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Pentane	72	C5H12	000109-66-0	32
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	10
5	1-Butene	56	C4H8	000106-98-9	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033390.D
Acq On : 13 Dec 2022 14:21
Operator : JC/MD
Sample : N6001-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

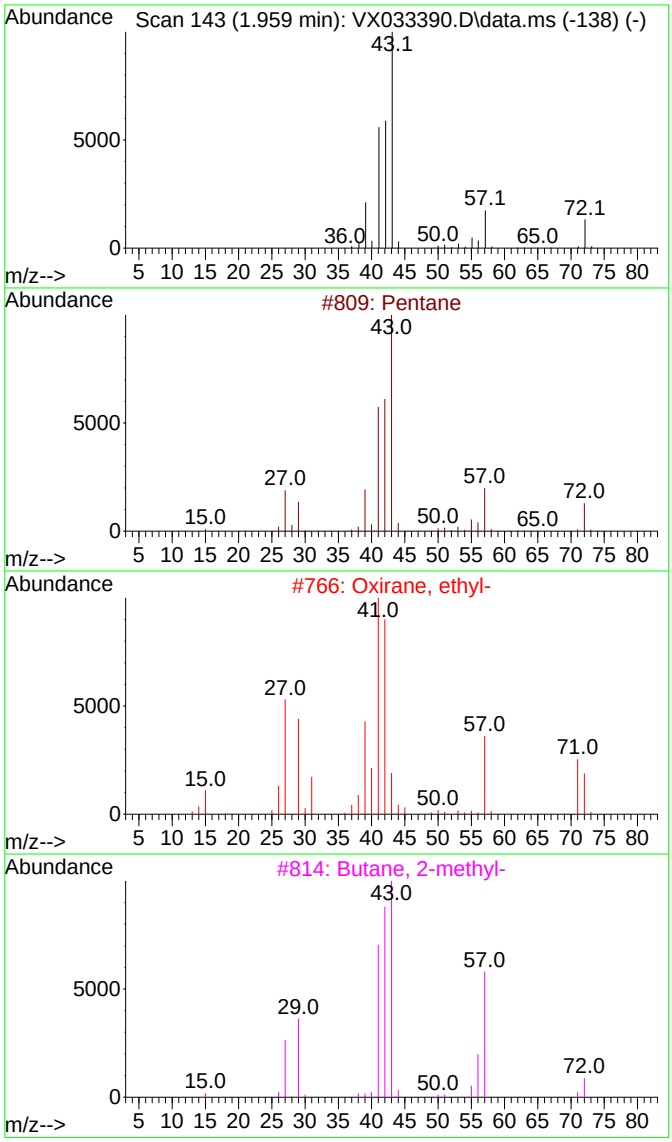
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

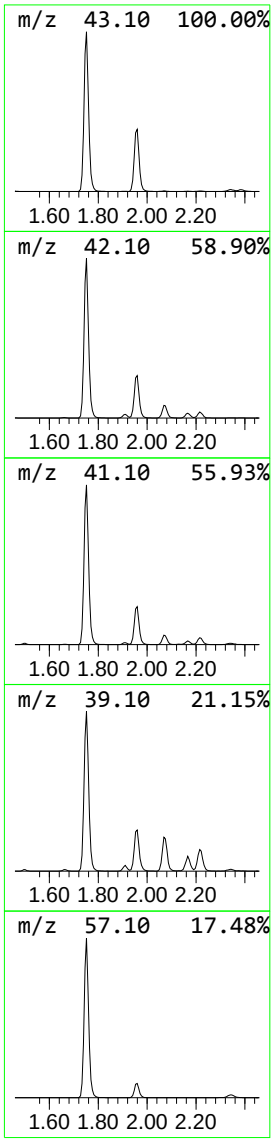
****

Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	51.58 ug/l	543782	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3	Butane, 2-methyl-	72	C5H12	000078-78-4	38
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
5	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033390.D
Acq On : 13 Dec 2022 14:21
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

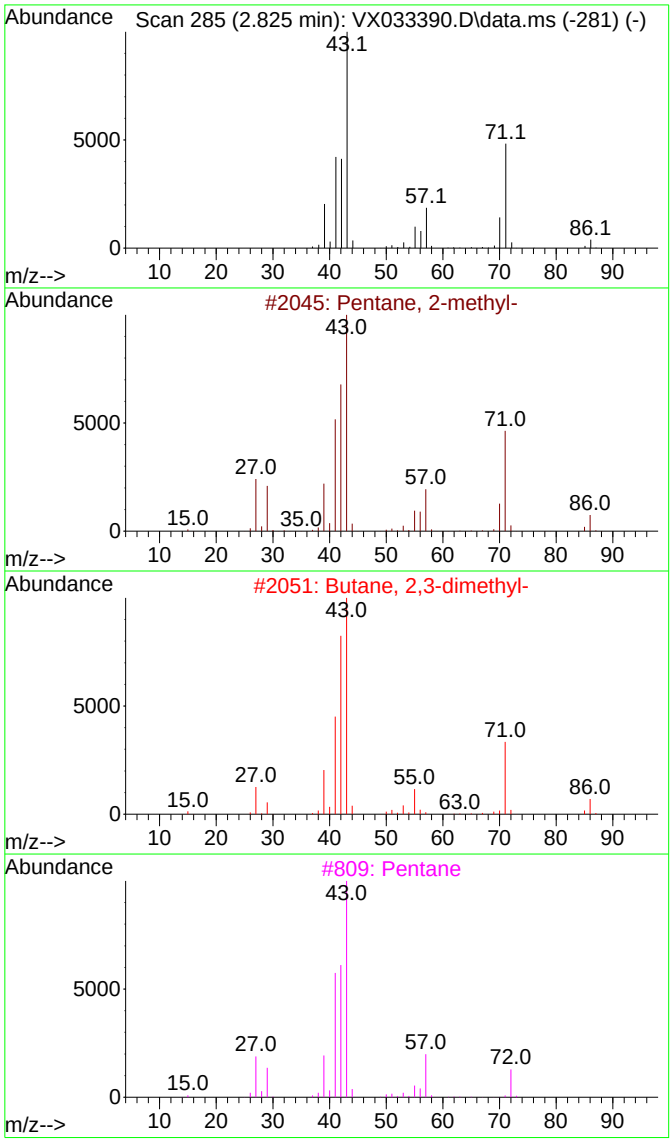
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

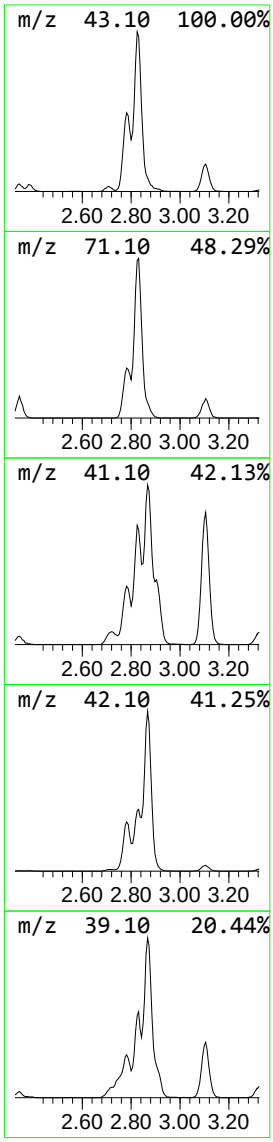
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	56.71 ug/l	597839	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	50
3	Pentane	72	C5H12	000109-66-0	43
4	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38
5	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033390.D
Acq On : 13 Dec 2022 14:21
Operator : JC/MD
Sample : N6001-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

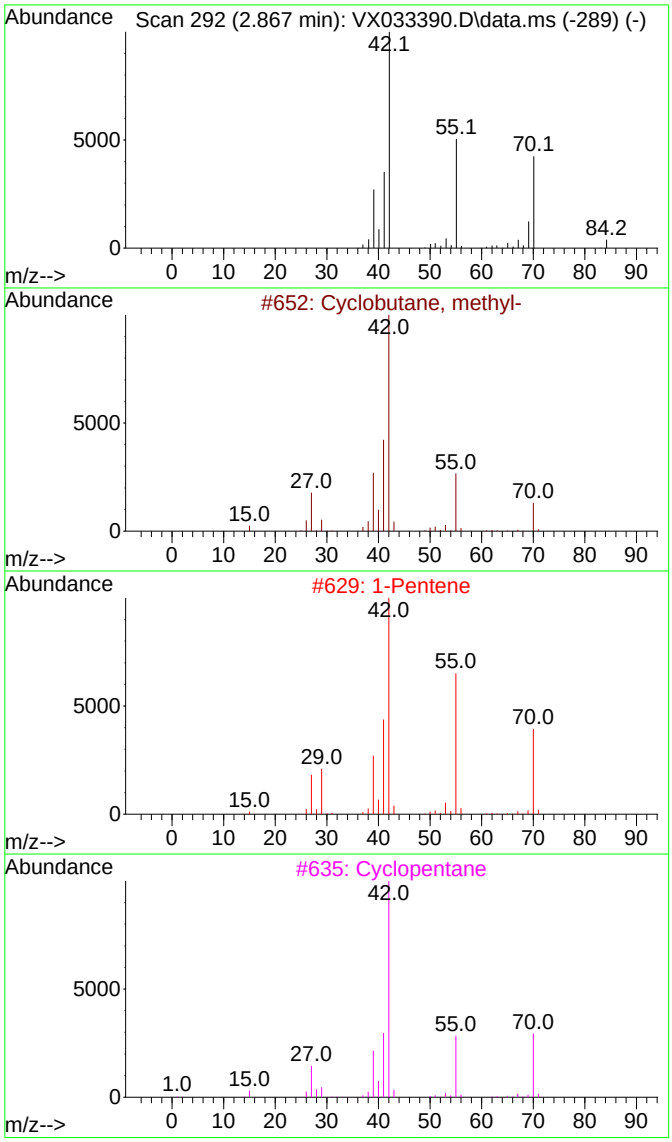
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

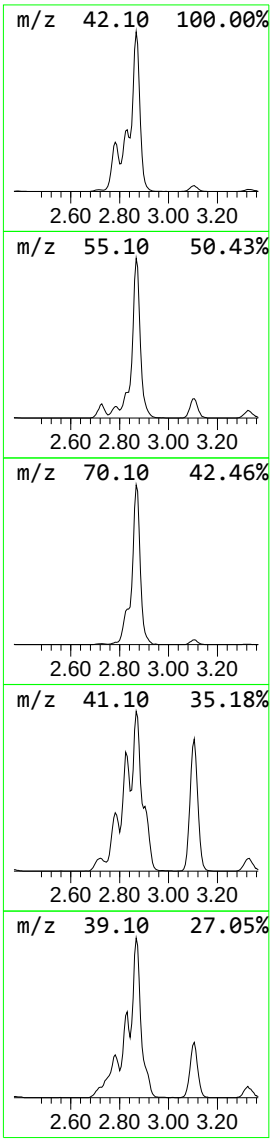
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclobutane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	77.22 ug/l	814016	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, methyl-	70	C5H10	000598-61-8	80
2	1-Pentene	70	C5H10	000109-67-1	80
3	Cyclopentane	70	C5H10	000287-92-3	78
4	2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	56
5	1-Pentanol	88	C5H12O	000071-41-0	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033390.D
Acq On : 13 Dec 2022 14:21
Operator : JC/MD
Sample : N6001-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

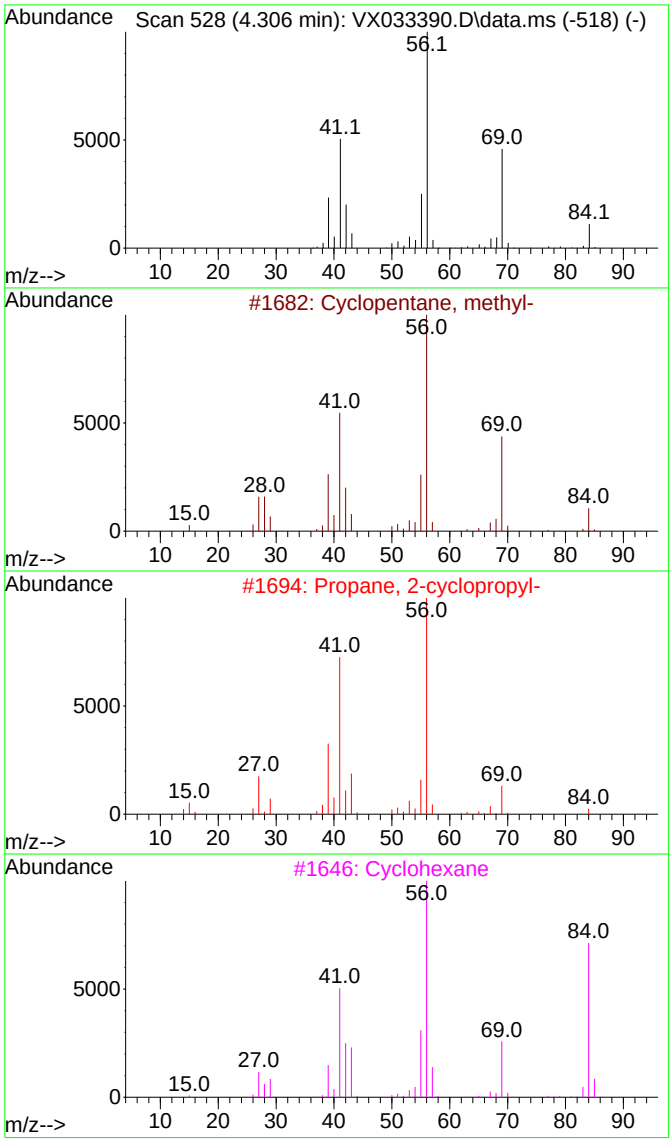
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

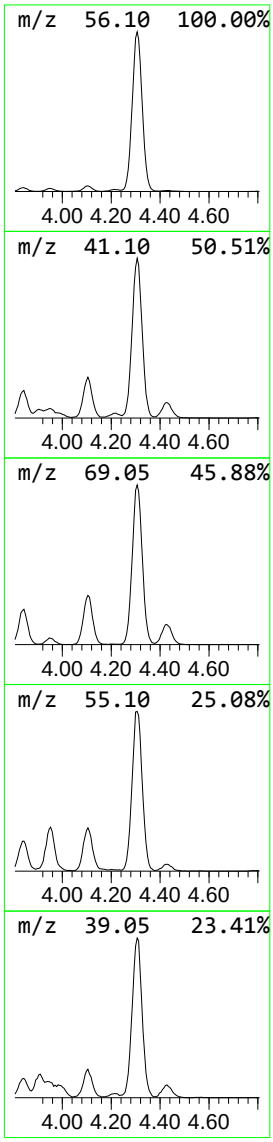
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	150.47 ug/l	1586330	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
3	Cyclohexane	84	C6H12	000110-82-7	78
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033390.D
Acq On : 13 Dec 2022 14:21
Operator : JC/MD
Sample : N6001-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

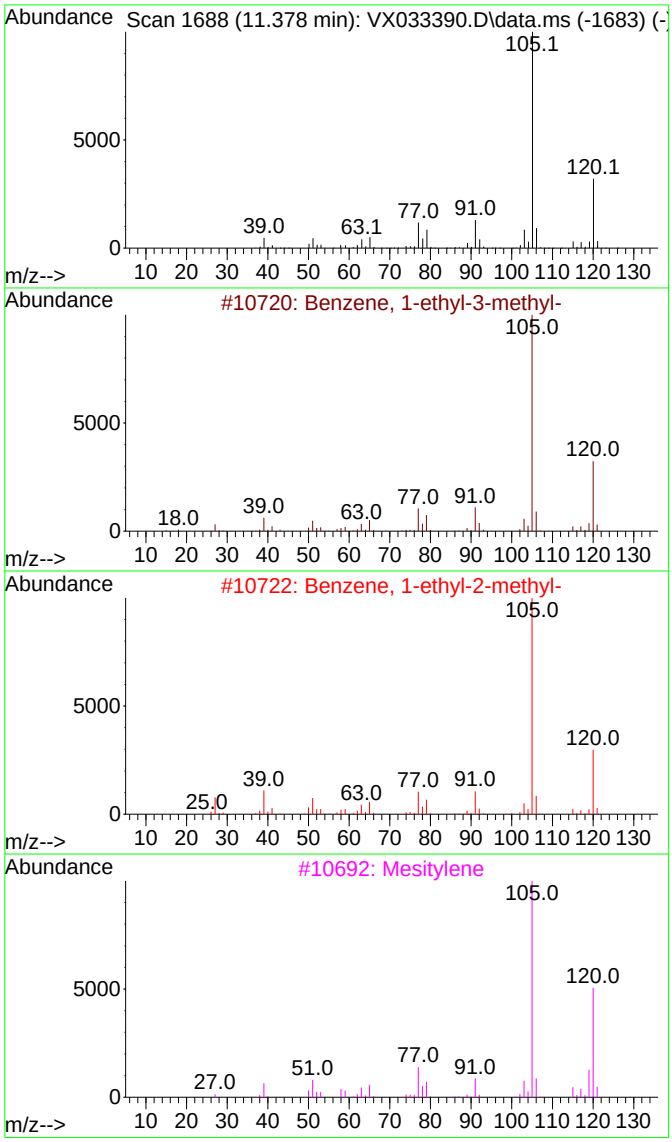
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

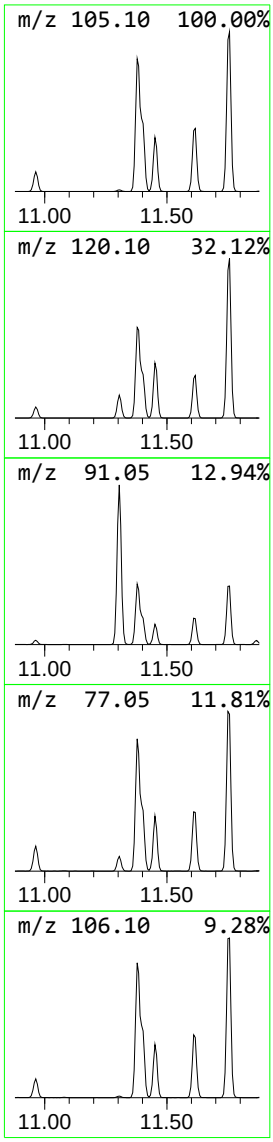
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	529.54 ug/l	6587280	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	95
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	91





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

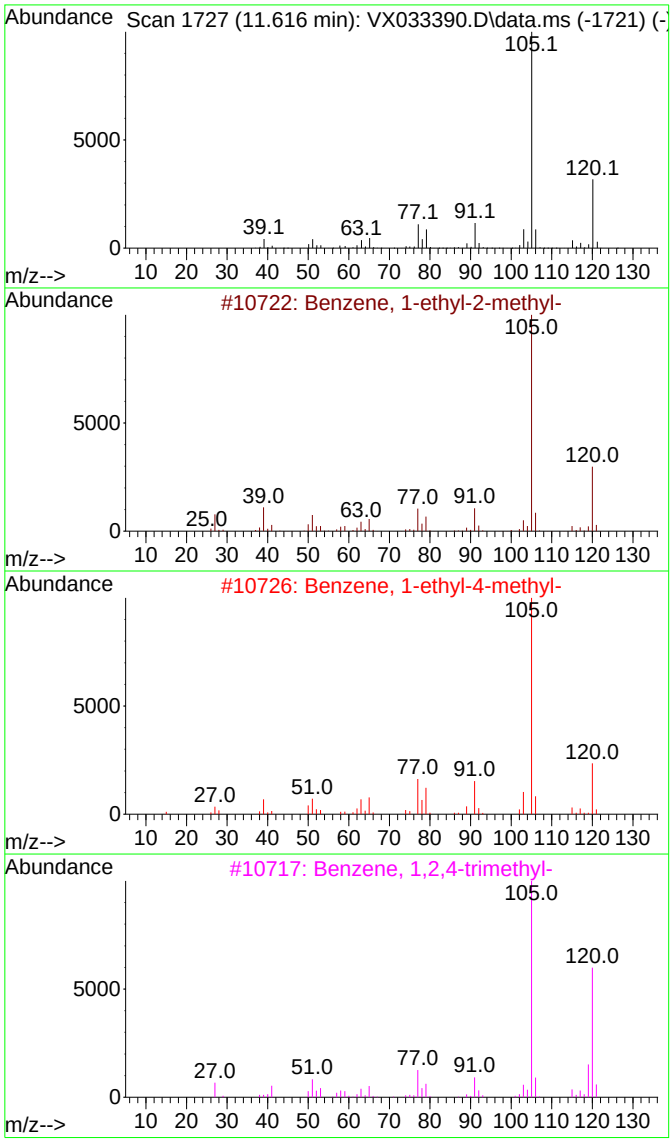
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

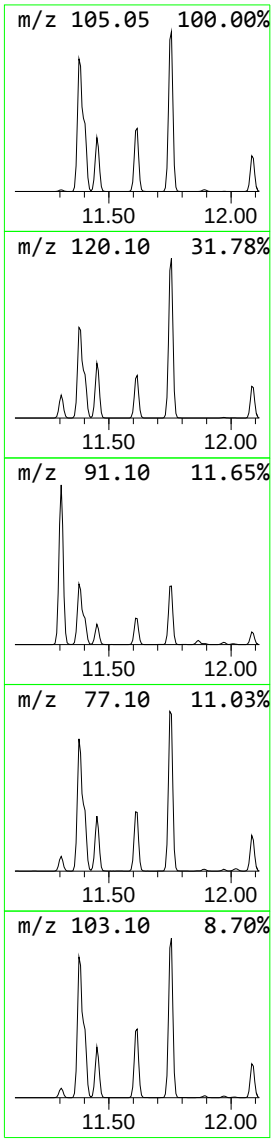
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	176.81 ug/l	2199460	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	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Mesitylene	120	C9H12	000108-67-8	90





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

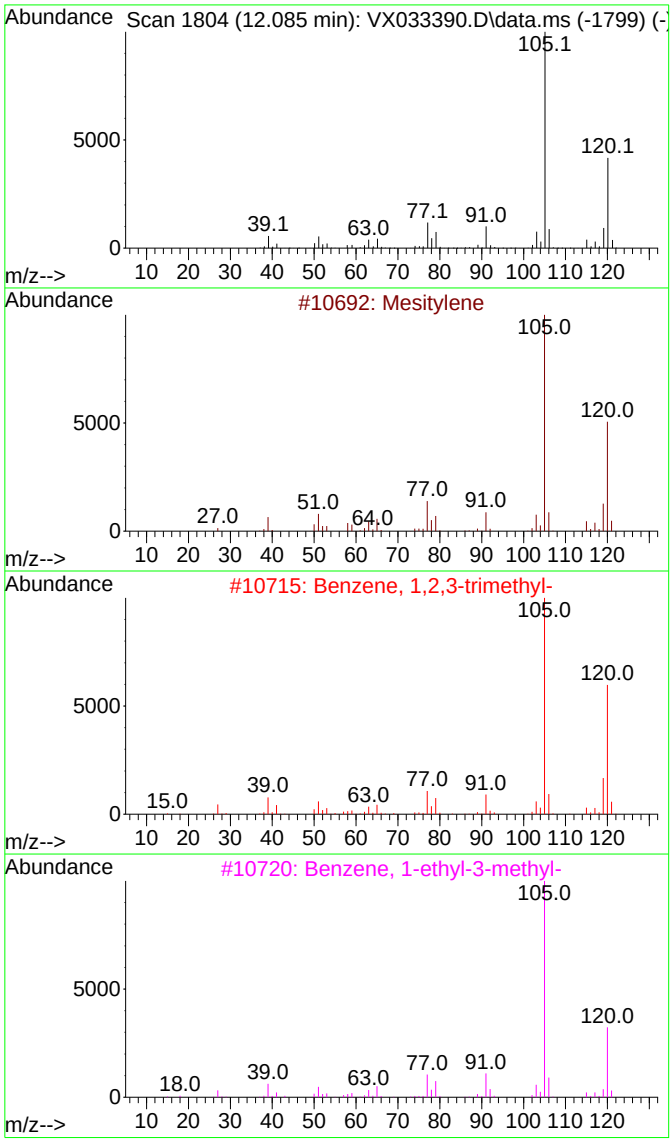
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

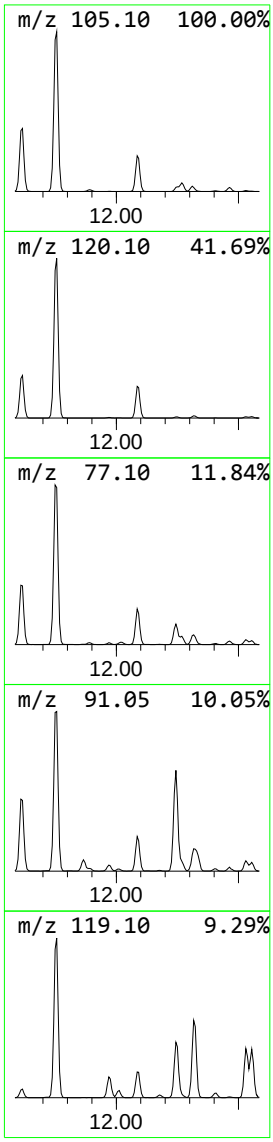
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	105.67 ug/l	1314490	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-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

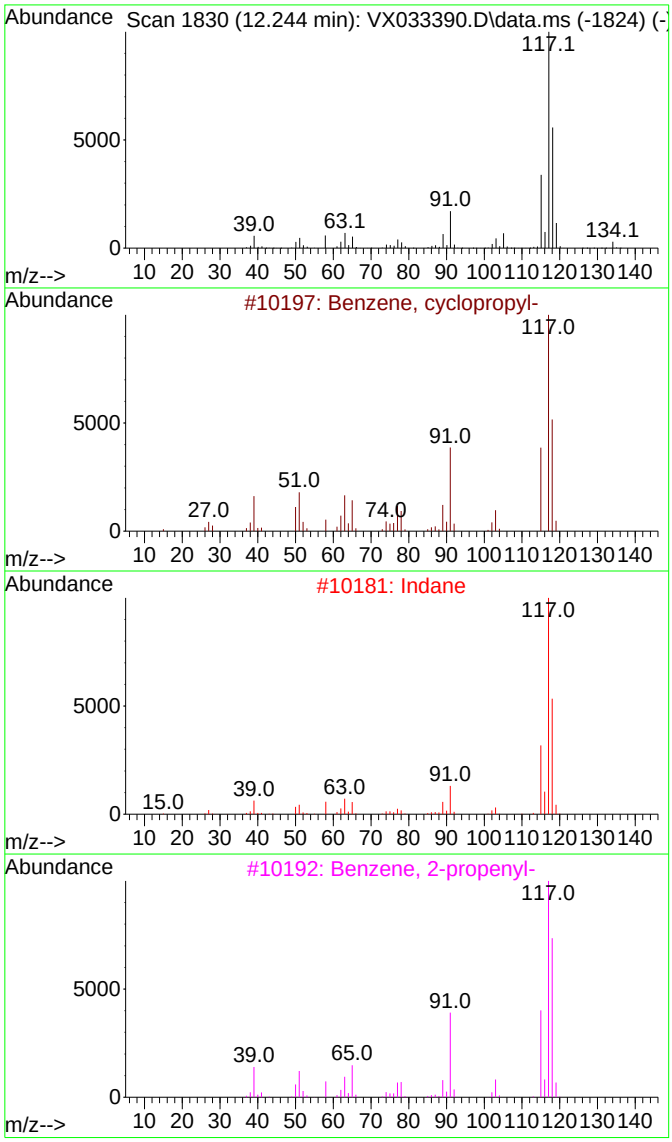
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

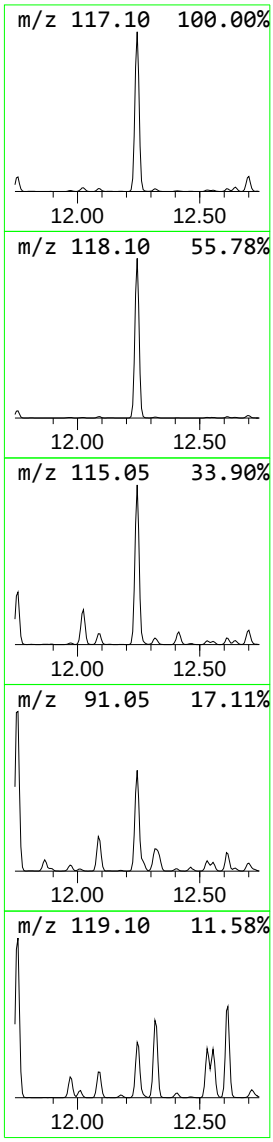
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, cyclopropyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	234.33 ug/l	2914990	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
2	Indane	118	C9H10	000496-11-7	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53
5	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033390.D
Acq On : 13 Dec 2022 14:21
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.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	187.3	ug/l	1975000	1	5.556	527108	50.0
Pentane	1.959	51.6	ug/l	543782	1	5.556	527108	50.0
Pentane, 2-methyl-	2.825	56.7	ug/l	597839	1	5.556	527108	50.0
Cyclobutane, me...	2.867	77.2	ug/l	814016	1	5.556	527108	50.0
Cyclopentane, m...	4.306	150.5	ug/l	1586330	1	5.556	527108	50.0
Benzene, 1-ethy...	11.378	529.5	ug/l	6587280	4	12.024	621984	50.0
Benzene, 1-ethy...	11.616	176.8	ug/l	2199460	4	12.024	621984	50.0
Benzene, 1,2,3-...	12.085	105.7	ug/l	1314490	4	12.024	621984	50.0
Benzene, cyclop...	12.244	234.3	ug/l	2914990	4	12.024	621984	50.0