LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040234.D
Acq On : 14 Feb 2024 20:31
Operator : JC/MD
Sample : P1427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50239

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\82X020924W.M
Title : SW846 8260

Signal : TIC: VX040234.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	41	47	53	rVV	1042283	1290463	6.74%	2.026%
2	1.447	57	59	65	rVV	1120625	1370540	7.16%	2.151%
3	1.752	103	109	122	rVB	452549	598975	3.13%	0.940%
4	1.953	138	142	152	rVB2	177868	289340	1.51%	0.454%
5	2.123	152	170	173	rBV	5644968	19154107	100.00%	30.065%
6	2.154	173	175	180	rVV	121060	192889	1.01%	0.303%
7	2.209	180	184	195	rVB	200072	311842	1.63%	0.489%
8	2.745	261	272	281	rBV	97531	213249	1.11%	0.335%
9	3.111	322	332	344	rBV	162306	380296	1.99%	0.597%
10	4.306	517	528	542	rVB3	69275	204936	1.07%	0.322%
11	4.708	584	594	610	rVB	190354	530630	2.77%	0.833%
12	5.556	725	733	755	rVB	72709	220544	1.15%	0.346%
13	6.044	802	813	832	rVB	2878279	7567085	39.51%	11.877%
14	6.763	922	931	953	rVB	116928	290385	1.52%	0.456%
15	8.647	1234	1240	1245	rBV	241180	393339	2.05%	0.617%
16	8.726	1245	1253	1282	rVB	9893469	15545472	81.16%	24.400%
17	10.055	1465	1471	1482	rVB	275978	382482	2.00%	0.600%
18	10.195	1488	1494	1505	rBV	1000679	1303829	6.81%	2.047%
19	10.299	1505	1511	1529	rVB	3218637	4380594	22.87%	6.876%
20	10.640	1561	1567	1578	rBV	1596766	2059159	10.75%	3.232%
21	11.079	1631	1639	1650	rVB	262846	339070	1.77%	0.532%
22	11.378	1682	1688	1696	rVV	681372	1151717	6.01%	1.808%
23	11.451	1696	1700	1711	rVB	325402	398708	2.08%	0.626%
24	11.610	1721	1726	1733	rVB	307224	371378	1.94%	0.583%
25	11.750	1744	1749	1756	rVB	1459063	1698753	8.87%	2.666%
26	12.018	1788	1793	1799	rVB	372289	485567	2.54%	0.762%
27	12.085	1799	1804	1810	rBV	421428	519456	2.71%	0.815%
28	12.244	1822	1830	1832	rBV2	280106	371669	1.94%	0.583%
29	12.317	1838	1842	1851	rVB3	209380	296701	1.55%	0.466%
30	12.609	1886	1890	1894	rBV	198133	230461	1.20%	0.362%
31	12.963	1944	1948	1954	rVB	224396	273413	1.43%	0.429%
32	13.292	1997	2002	2007	rVB2	275403	368463	1.92%	0.578%
33	13.774	2076	2081	2088	rBV	234395	297478	1.55%	0.467%
34	14.633	2214	2222	2227	rBV	155236	226728	1.18%	0.356%

Sum of corrected areas: 63709718

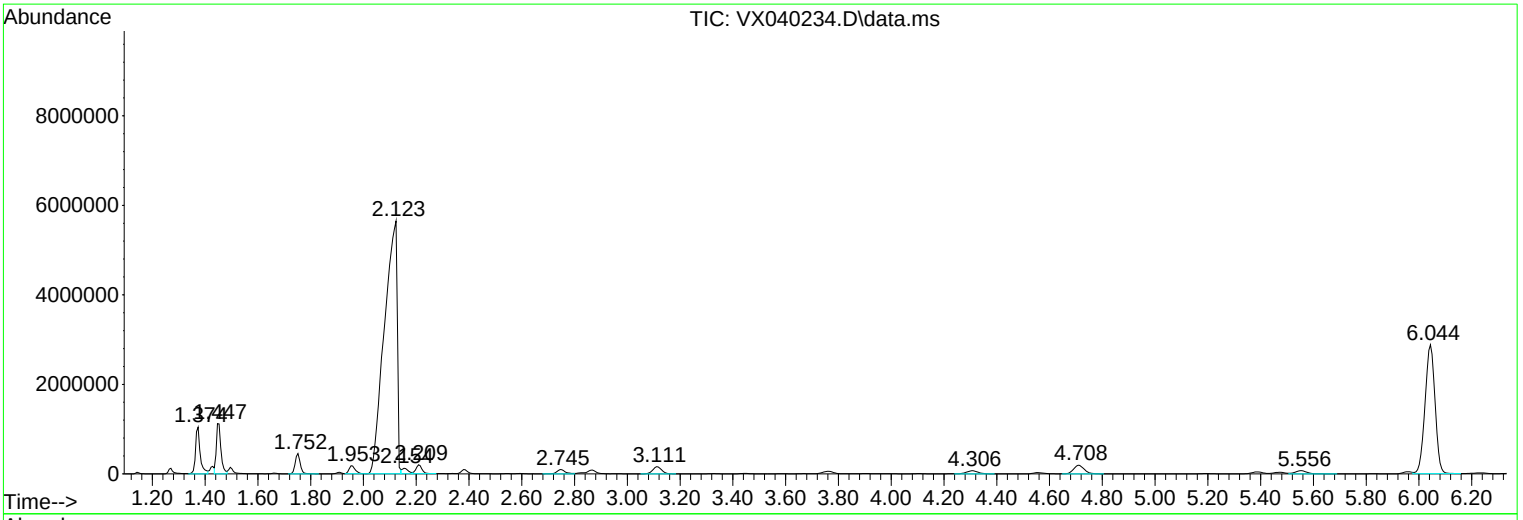
Instrument :
MSVOA_X
ClientSampleId :
50239

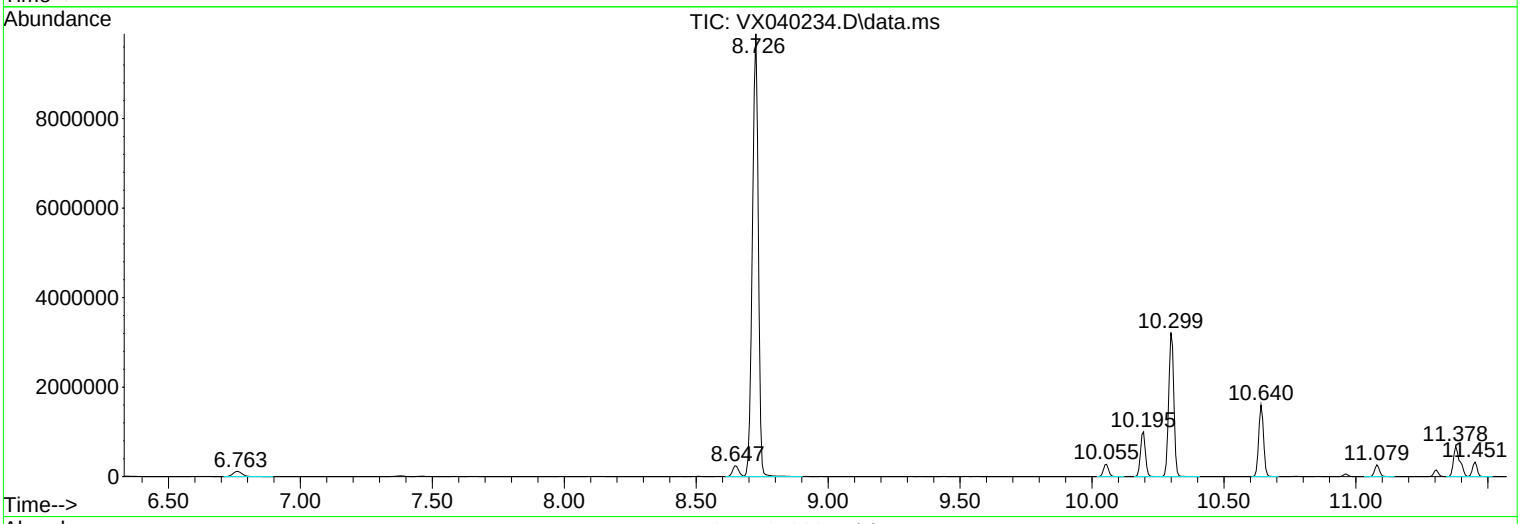
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040234.D
Acq On : 14 Feb 2024 20:31
Operator : JC/MD
Sample : P1427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

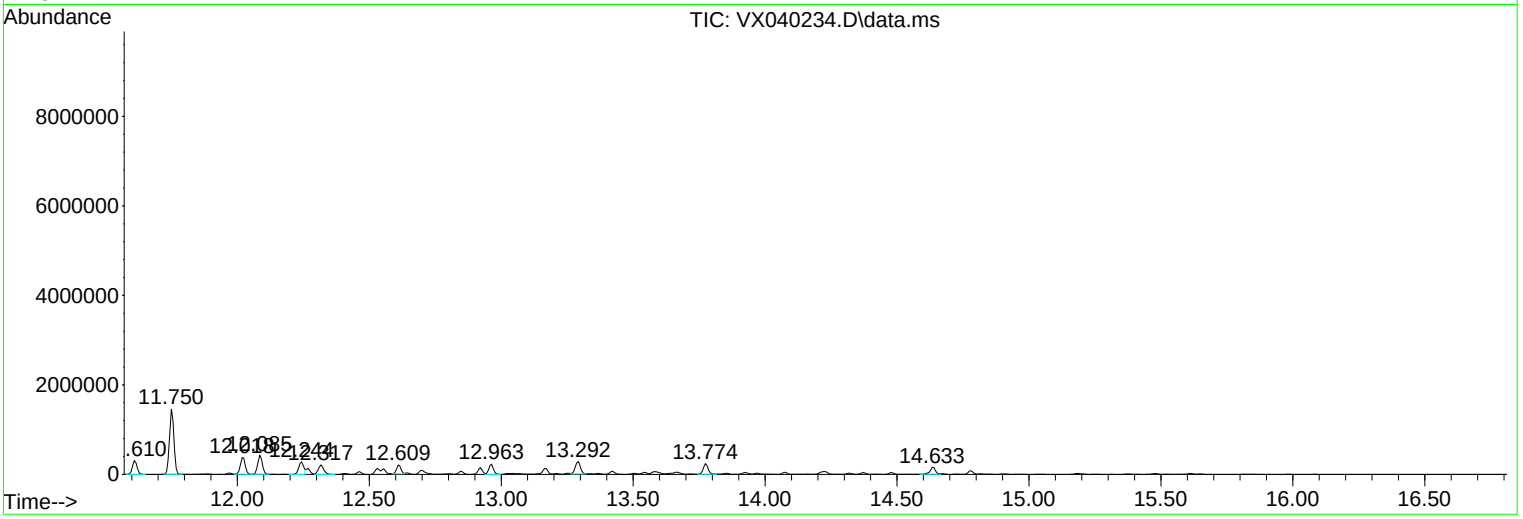
Instrument :
MSVOA_X
ClientSampleId :
50239

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040234.D
Acq On : 14 Feb 2024 20:31
Operator : JC/MD
Sample : P1427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50239

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

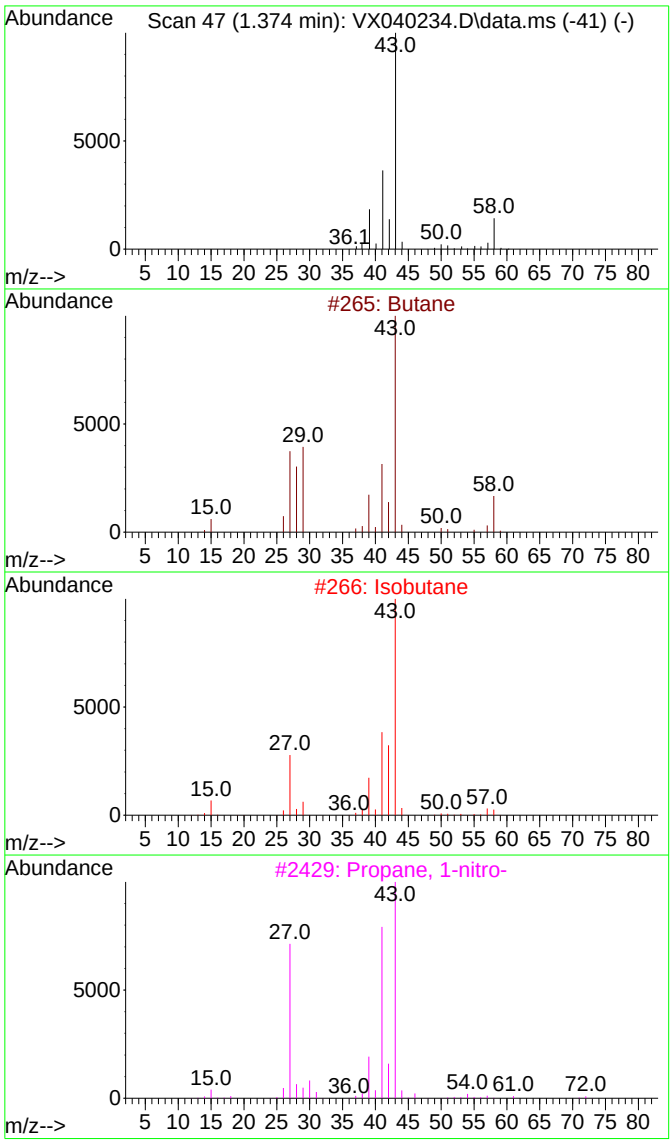
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

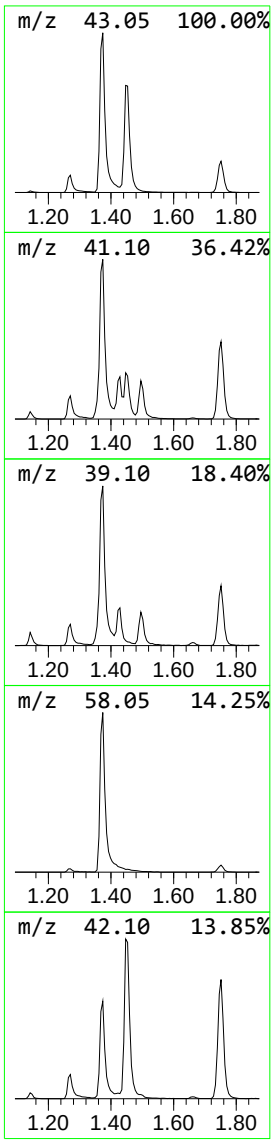
****

Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	292.56 ug/l	1290460	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Isobutane	58	C4H10	000075-28-5	9
3	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
4	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5	Acetone	58	C3H6O	000067-64-1	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040234.D
Acq On : 14 Feb 2024 20:31
Operator : JC/MD
Sample : P1427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50239

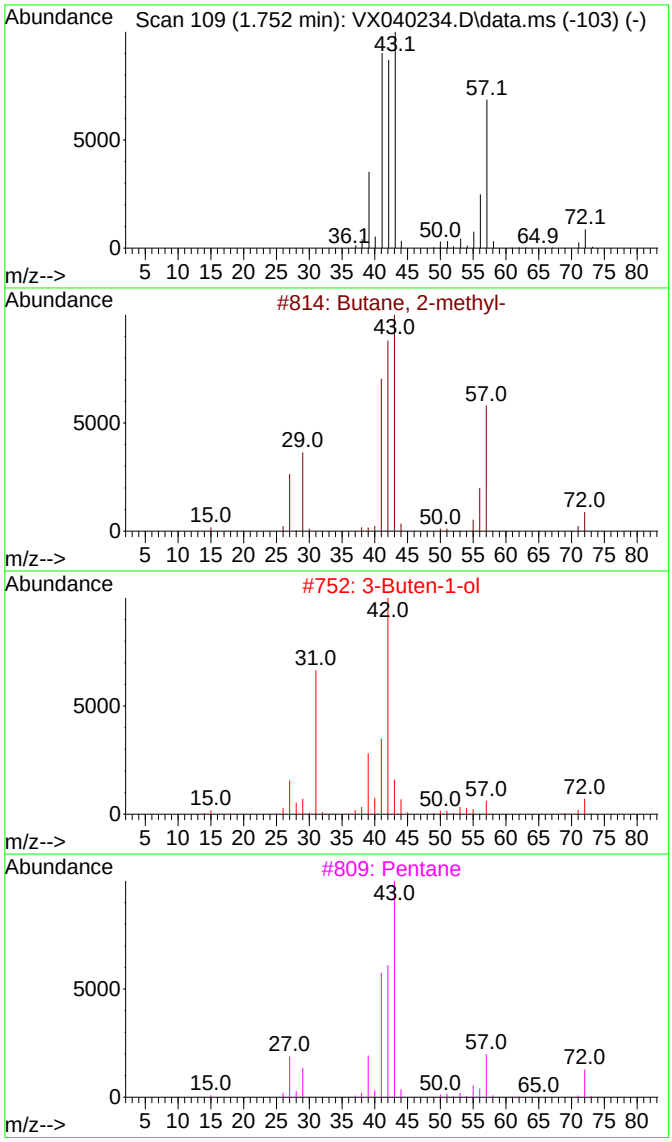
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

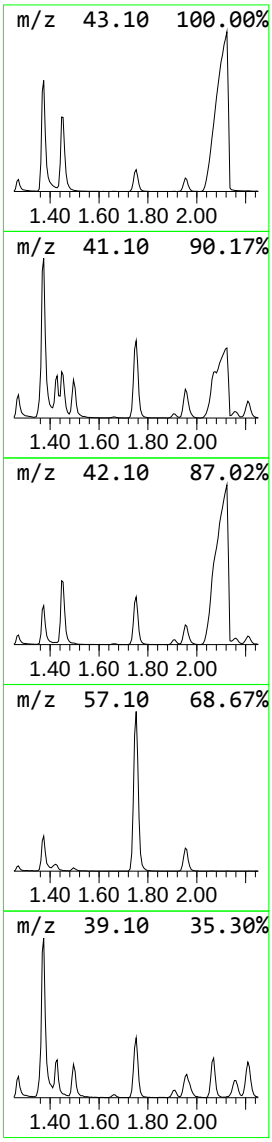
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	135.79 ug/l	598975	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	Azetidine	57	C3H7N	000503-29-7	9
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040234.D
Acq On : 14 Feb 2024 20:31
Operator : JC/MD
Sample : P1427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50239

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

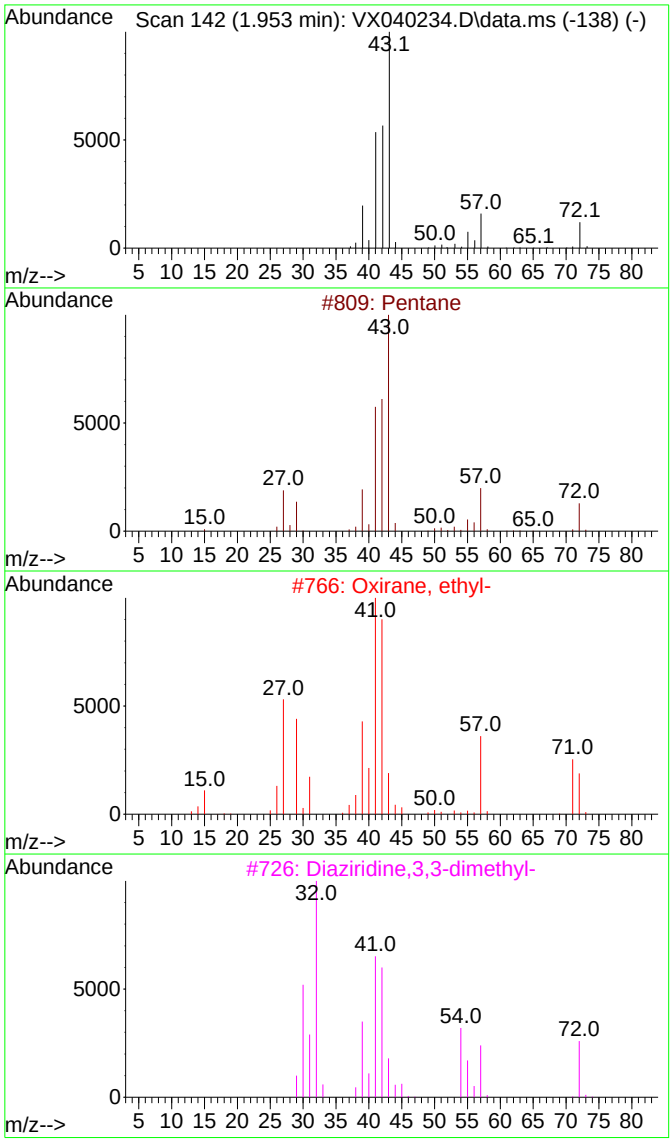
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

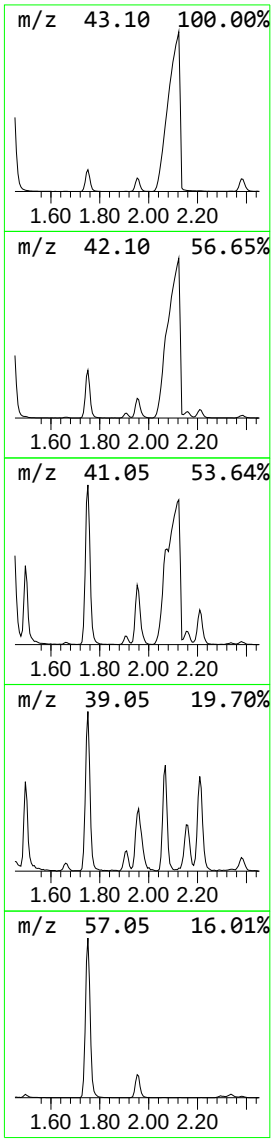
****

Peak Number 4 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	65.60 ug/l	289340	Pentafluorobenzene	5.550

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	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4	Butane, 2-methyl-	72	C5H12	000078-78-4	36
5	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040234.D
Acq On : 14 Feb 2024 20:31
Operator : JC/MD
Sample : P1427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50239

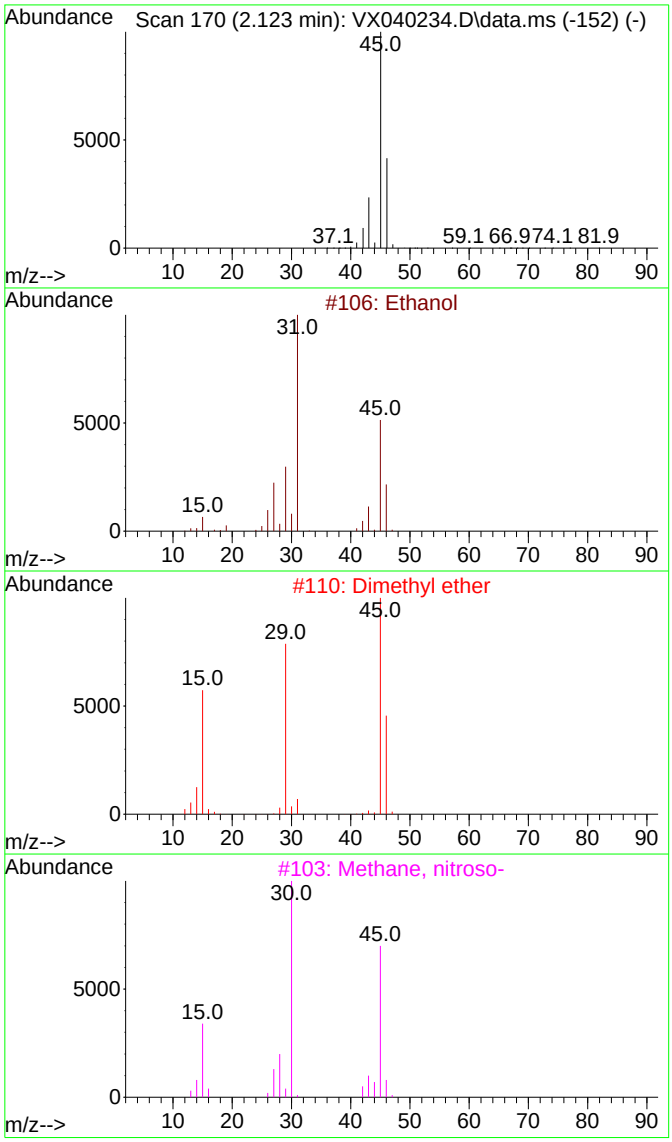
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

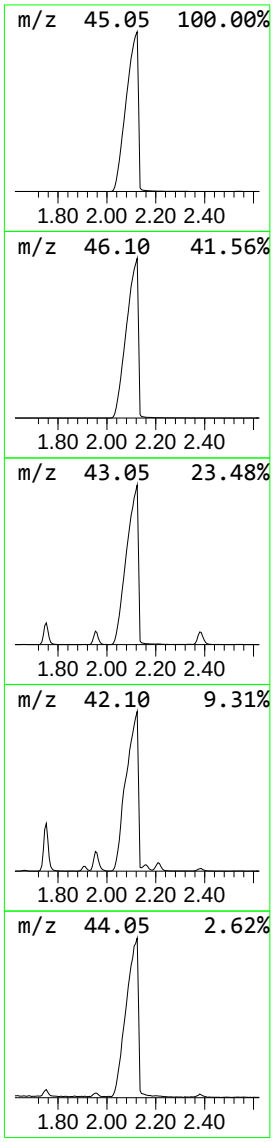
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.123	4342.47 ug/l	19154100	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	86
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	4-Penten-2-ol	86	C5H10O	000625-31-0	2





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040234.D
Acq On : 14 Feb 2024 20:31
Operator : JC/MD
Sample : P1427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50239

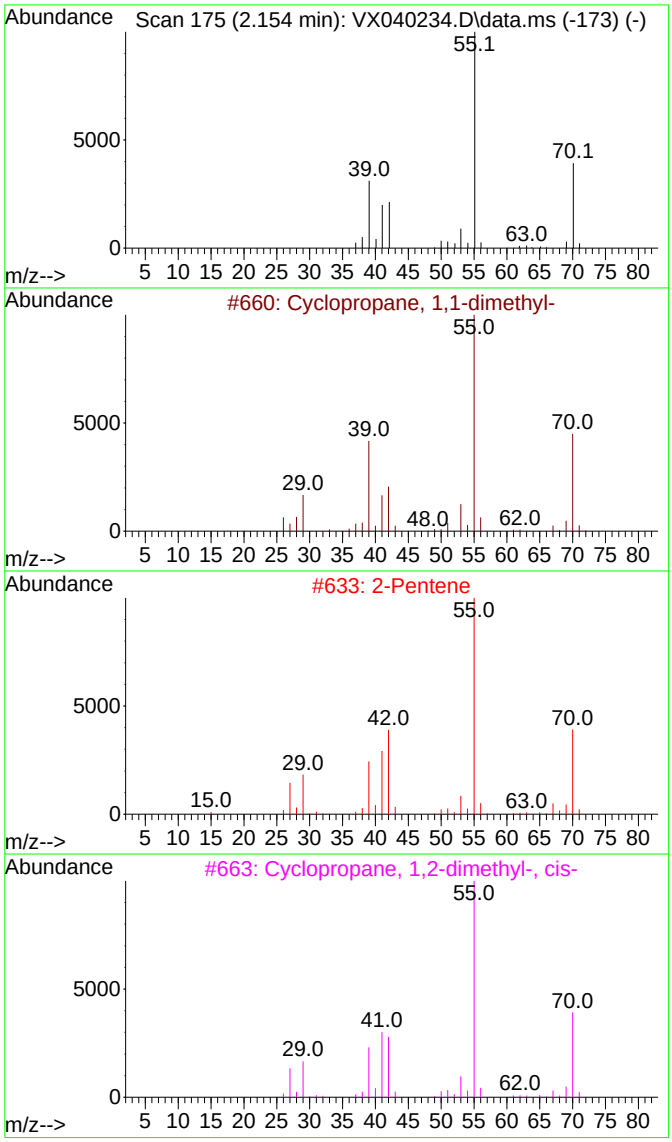
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

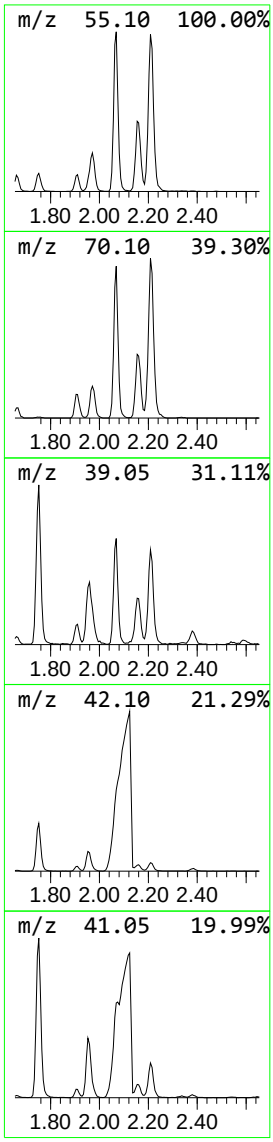
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopropane, 1,1-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.154	43.73 ug/l	192889	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	86
2	2-Pentene	70	C5H10	000109-68-2	72
3	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	72
4	2-Butene, 2-methyl-	70	C5H10	000513-35-9	72
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040234.D
Acq On : 14 Feb 2024 20:31
Operator : JC/MD
Sample : P1427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50239

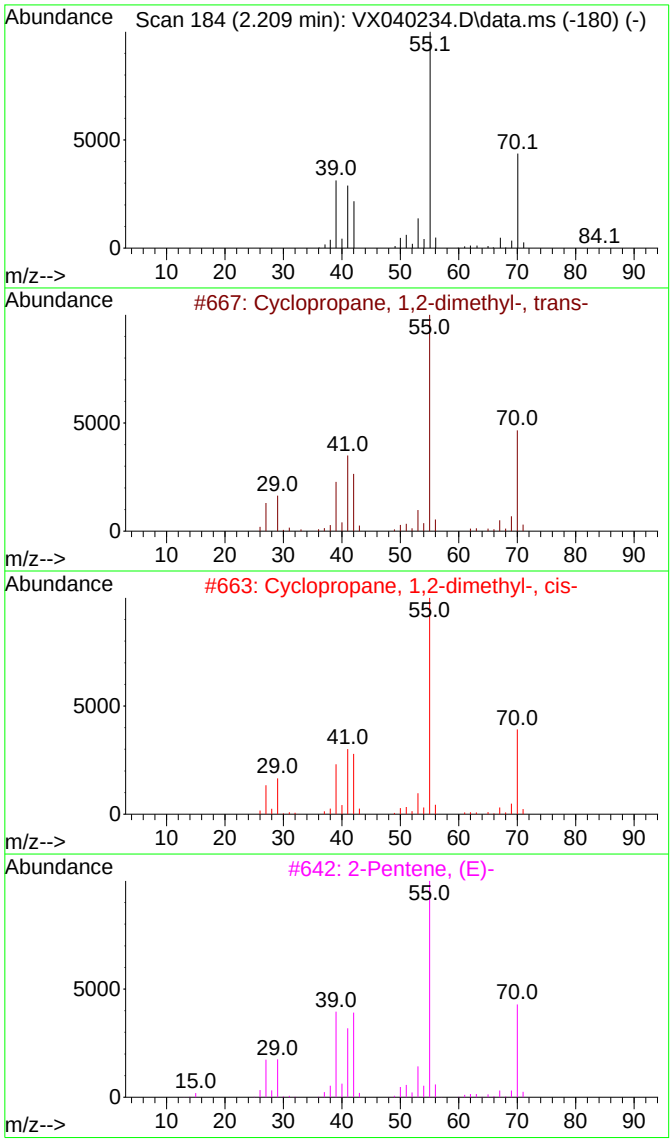
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

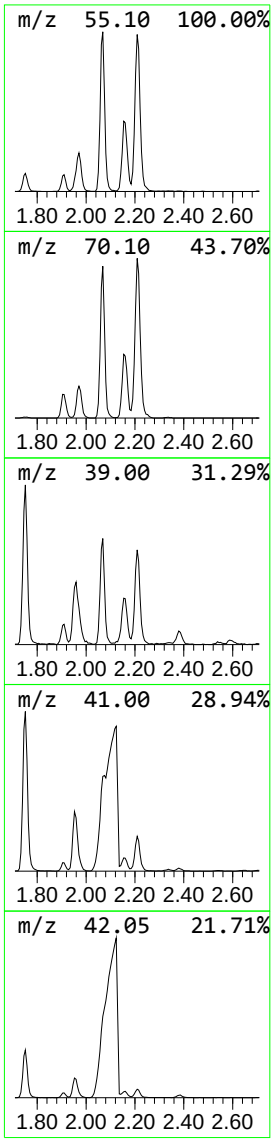
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopropane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.209	70.70 ug/l	311842	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
2	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87
3	2-Pentene, (E)-	70	C5H10	000646-04-8	87
4	2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040234.D
Acq On : 14 Feb 2024 20:31
Operator : JC/MD
Sample : P1427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50239

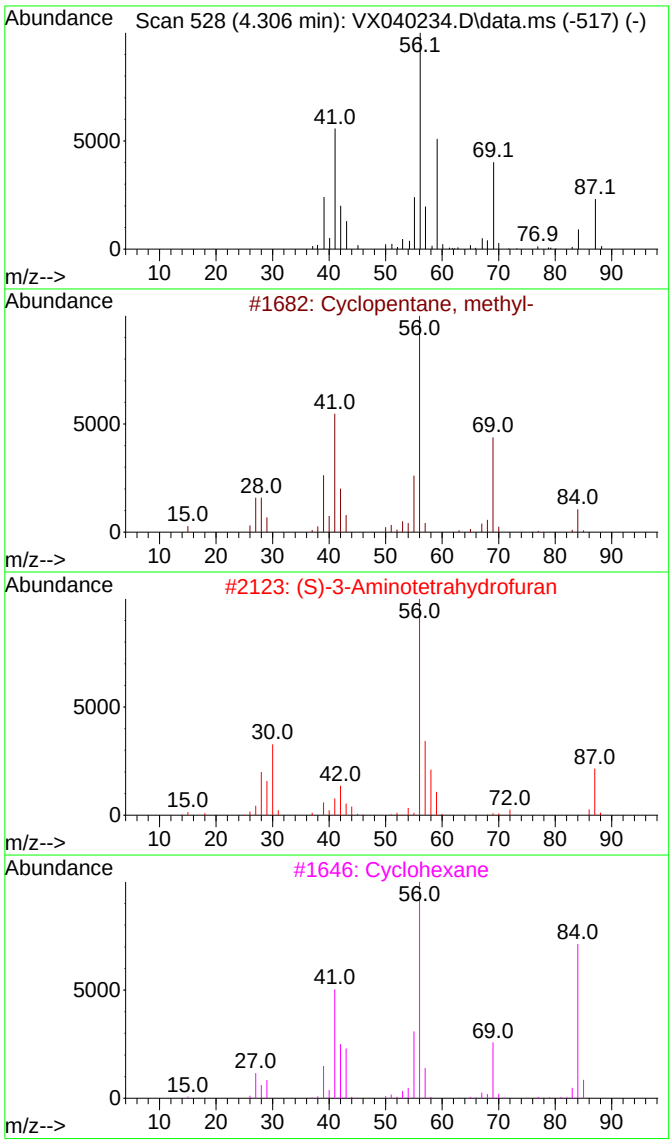
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

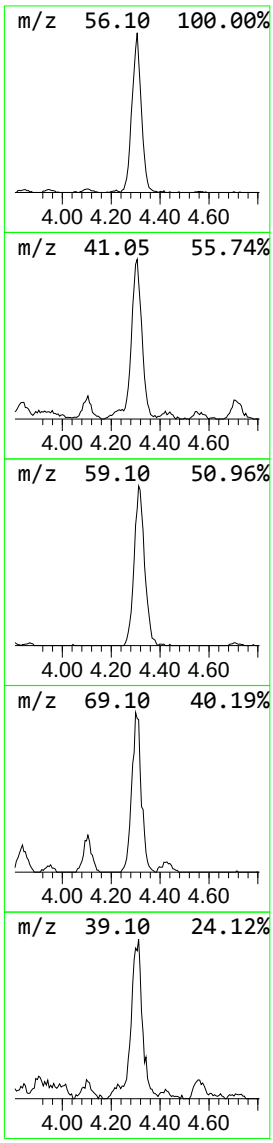
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	46.46 ug/l	204936	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	64
2	(S)-3-Aminotetrahydrofuran	87	C4H9NO	204512-95-8	50
3	Cyclohexane	84	C6H12	000110-82-7	50
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	43
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	43





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Data File : VX040234.D
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Operator : JC/MD
Sample : P1427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50239

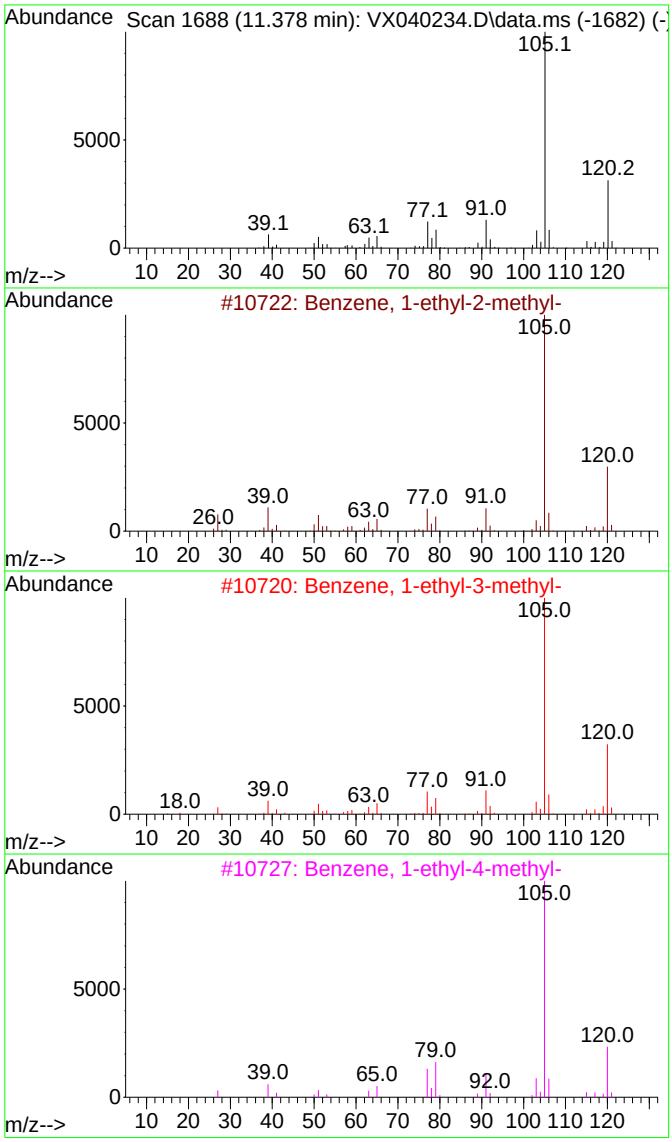
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

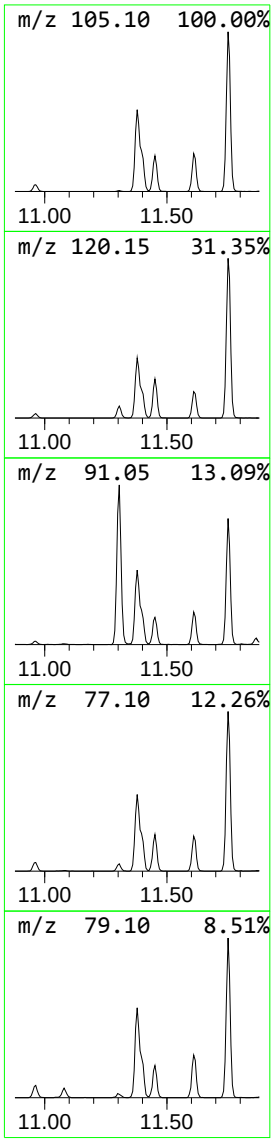
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	118.60 ug/l	1151720	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-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040234.D
Acq On : 14 Feb 2024 20:31
Operator : JC/MD
Sample : P1427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50239

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.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	1.374	292.6	ug/l	1290460	1	5.550	220544	50.0
Butane, 2-methyl-	1.752	135.8	ug/l	598975	1	5.550	220544	50.0
Pentane	1.953	65.6	ug/l	289340	1	5.550	220544	50.0
Ethanol	2.123	4342.5	ug/l	19154100	1	5.550	220544	50.0
Cyclopropane, 1...	2.154	43.7	ug/l	192889	1	5.550	220544	50.0
Cyclopropane, 1...	2.209	70.7	ug/l	311842	1	5.550	220544	50.0
Cyclopentane, m...	4.306	46.5	ug/l	204936	1	5.550	220544	50.0
Benzene, 1-ethy...	11.378	118.6	ug/l	1151720	4	12.024	485567	50.0