LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018773.D
Acq On : 05 Oct 2020 18:20
Operator : JC/SP
Sample : L4239-04DL 100X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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\SOMXTR100220WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.343	200	206	216	rBV2	136068	228869	1.61%	0.681%
2	3.154	330	339	349	rBV	66271	152773	1.07%	0.454%
3	3.495	386	395	408	rBV2	76413	182273	1.28%	0.542%
4	4.373	528	539	552	rBV2	144846	423209	2.98%	1.259%
5	4.562	554	570	582	rBV2	592956	1722634	12.11%	5.123%
6	5.135	653	664	678	rBV	82136	248858	1.75%	0.740%
7	5.464	703	718	729	rBV	1209872	3747705	26.35%	11.145%
8	6.044	799	813	830	rBV2	199551	591485	4.16%	1.759%
9	6.830	932	942	952	rBV2	140634	339759	2.39%	1.010%
10	7.366	1019	1030	1040	rBV	120751	270402	1.90%	0.804%
11	8.696	1240	1248	1253	rBV	304628	482046	3.39%	1.434%
12	8.769	1253	1260	1279	rVB	9250894	14221258	100.00%	42.291%
13	9.427	1360	1368	1379	rBV	424015	587899	4.13%	1.748%
14	10.098	1470	1478	1492	rBV	289476	420865	2.96%	1.252%
15	10.342	1512	1518	1525	rBV	225037	307367	2.16%	0.914%
16	10.683	1568	1574	1579	rBV	156996	201120	1.41%	0.598%
17	11.232	1658	1664	1672	rBV	130994	167914	1.18%	0.499%
18	11.421	1689	1695	1702	rBV	132572	225884	1.59%	0.672%
19	11.610	1721	1726	1731	rVV	6639898	7535074	52.98%	22.408%
20	11.793	1751	1756	1762	rVB	251434	307269	2.16%	0.914%
21	11.866	1762	1768	1773	rBV	307786	371483	2.61%	1.105%
22	12.061	1795	1800	1806	rBV	323261	411284	2.89%	1.223%
23	12.359	1844	1849	1857	rVB	374489	479438	3.37%	1.426%

Sum of corrected areas: 33626868

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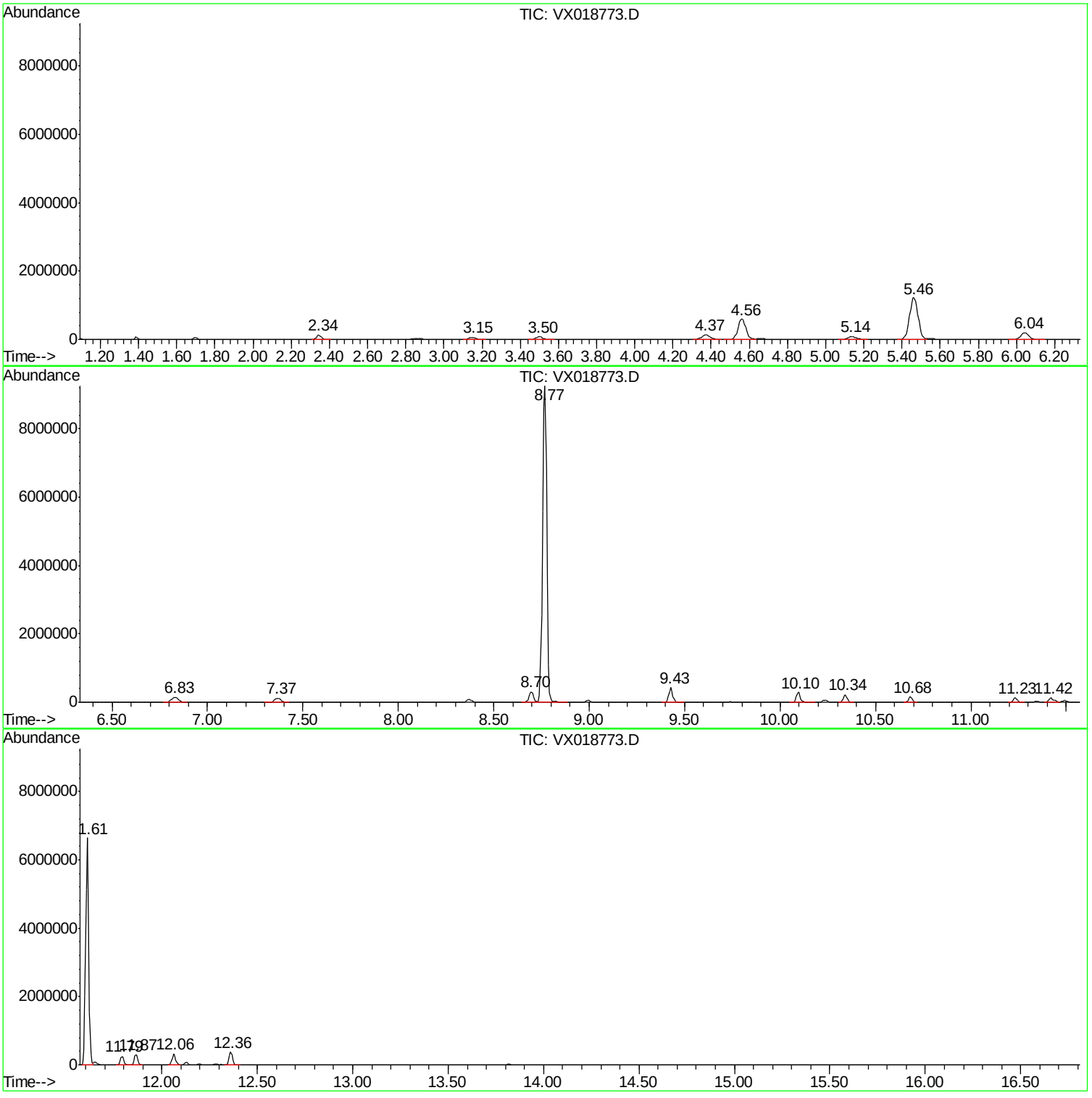
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3N3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018773.D
Acq On : 05 Oct 2020 18:20
Operator : JC/SP
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Misc : 25.0mL/MSVOA X/WATER
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Instrument : MSVOA_X
ClientSampleId : BG3N3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

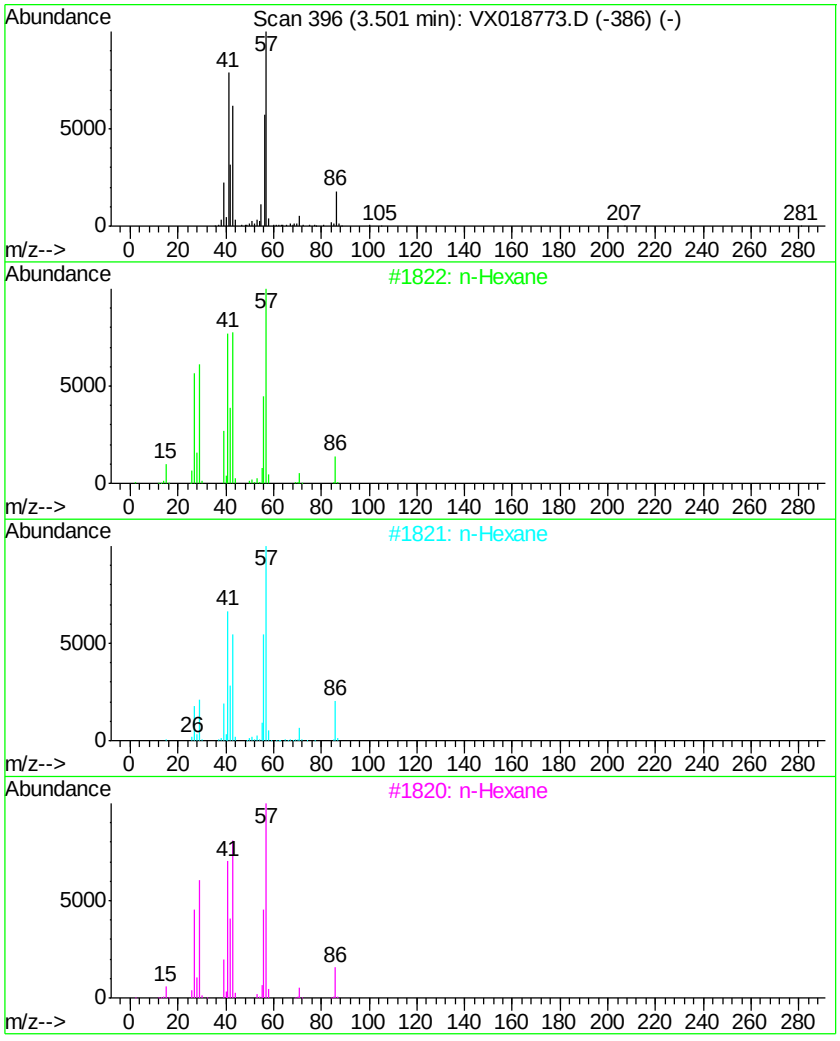
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

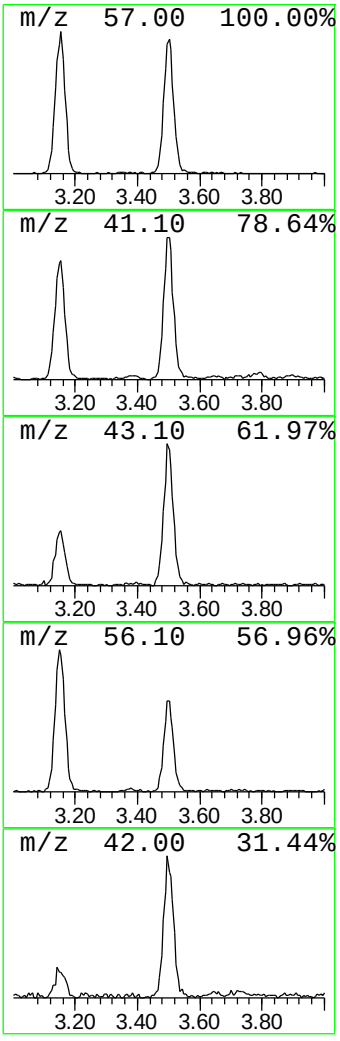
****

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	2.68 ug/L	182273	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	86
2	n-Hexane	86	C6H14	000110-54-3	72
3	n-Hexane	86	C6H14	000110-54-3	58
4	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	42
5	Pentane, 3-methyl-	86	C6H14	000096-14-0	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100520\
Data File : VX018773.D
Acq On : 05 Oct 2020 18:20
Operator : JC/SP
Sample : L4239-04DL 100X
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL

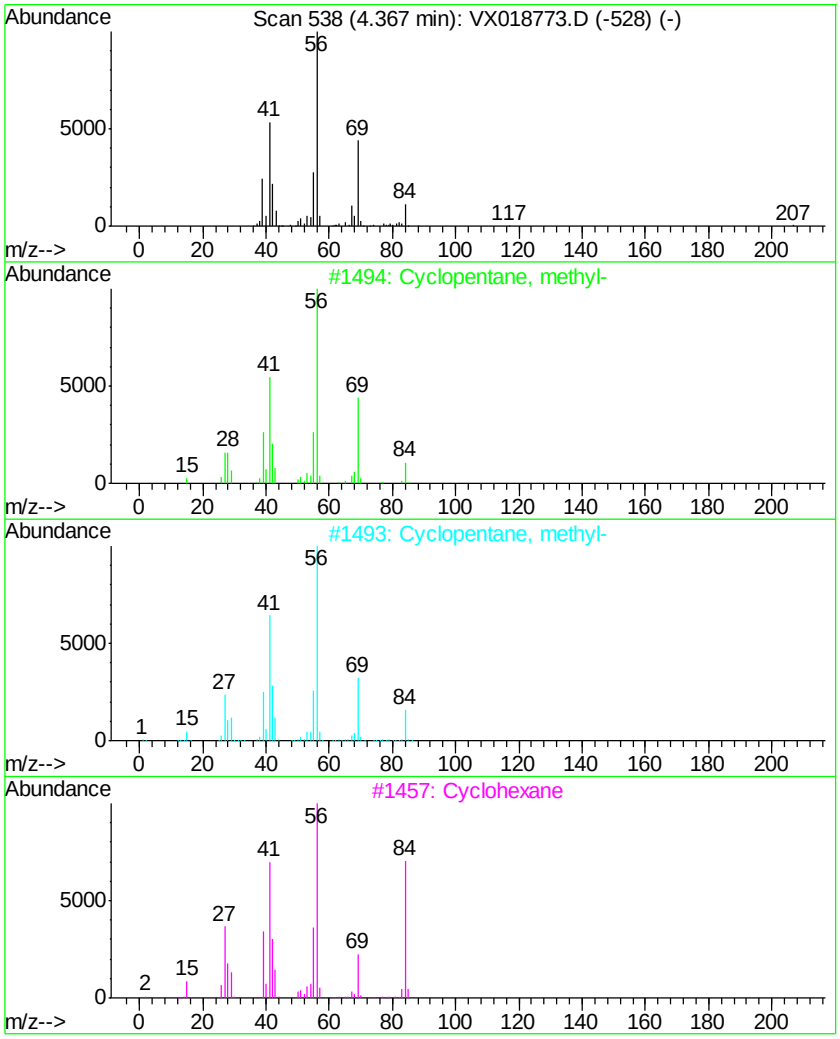
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

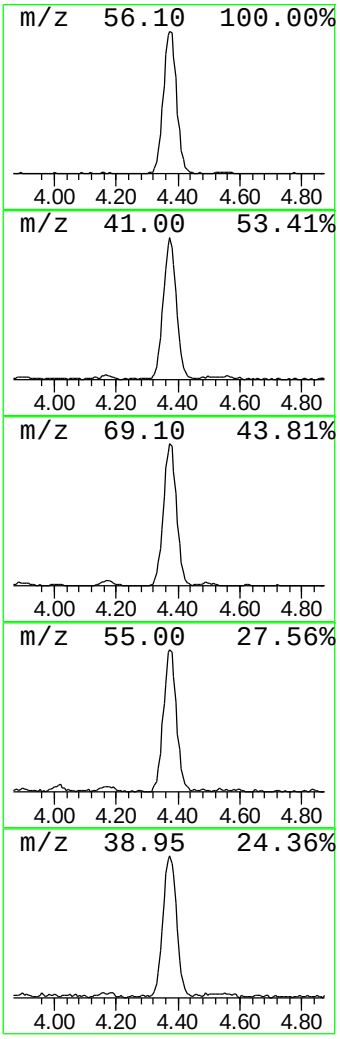
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Cyclic4.37 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	6.23 ug/L	423209	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	80
3	Cyclohexane	84	C6H12	000110-82-7	80
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018773.D
Acq On : 05 Oct 2020 18:20
Operator : JC/SP
Sample : L4239-04DL 100X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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

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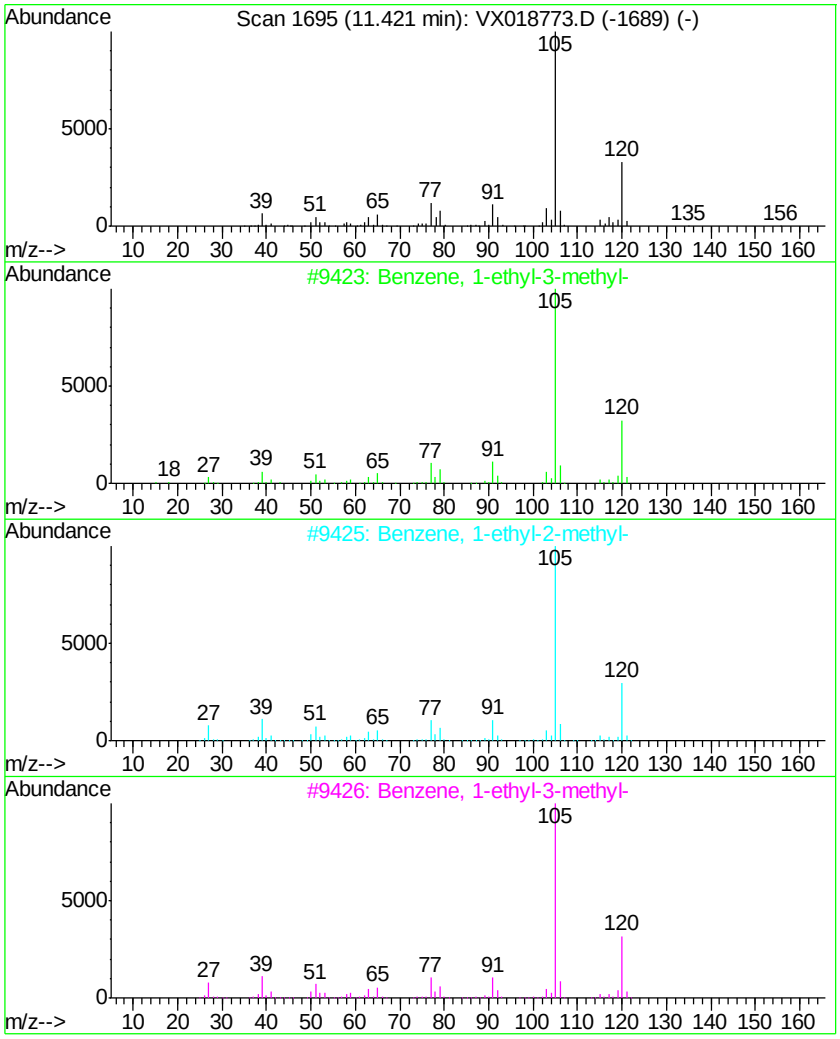
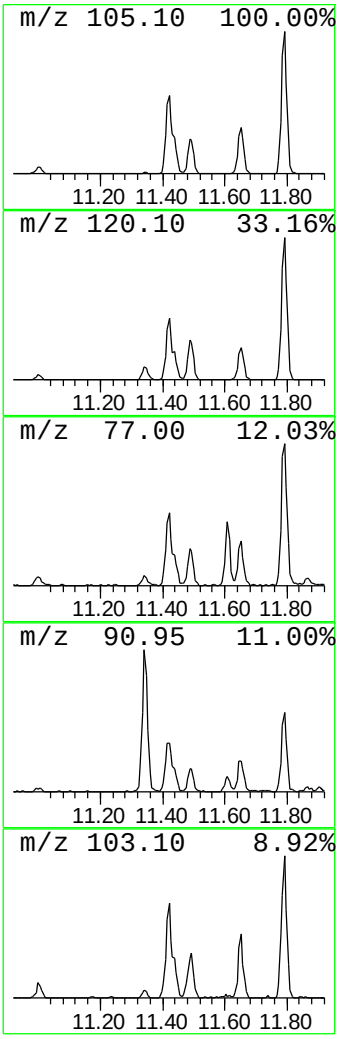
Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	2.75 ug/L	225884	1,4-Dichlorobenzene-d4	12.06

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	94
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100520\
Data File : VX018773.D
Acq On : 05 Oct 2020 18:20
Operator : JC/SP
Sample : L4239-04DL 100X
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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

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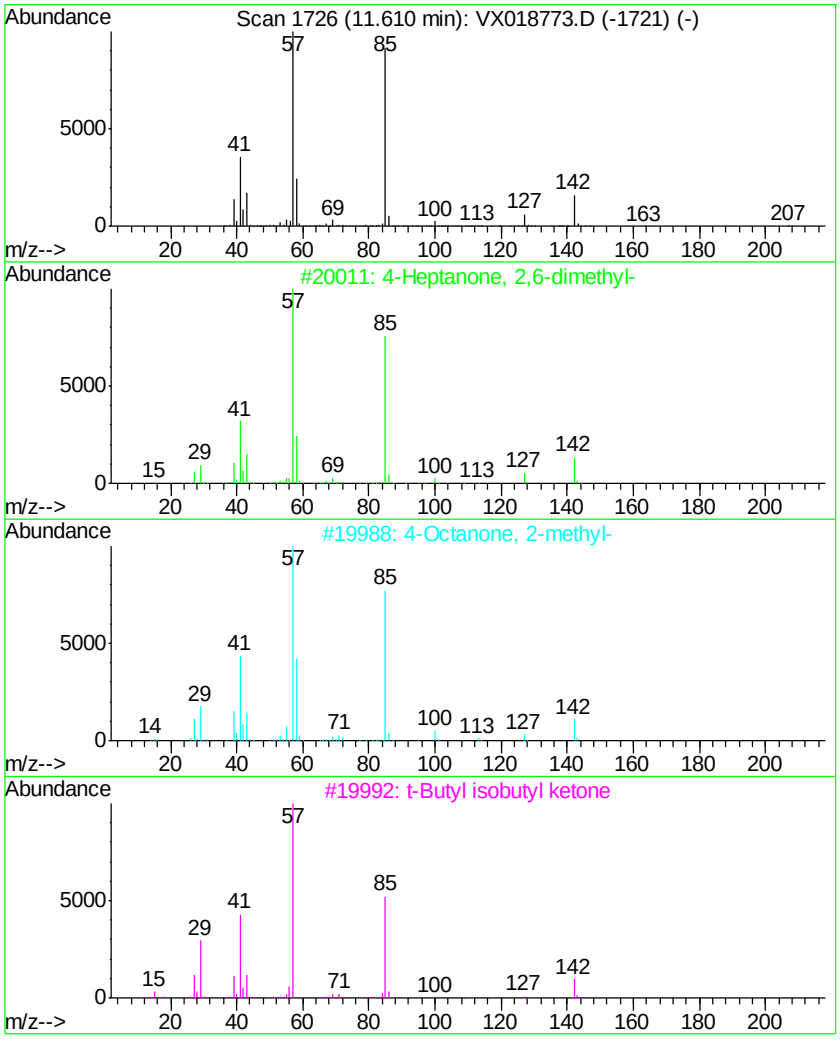
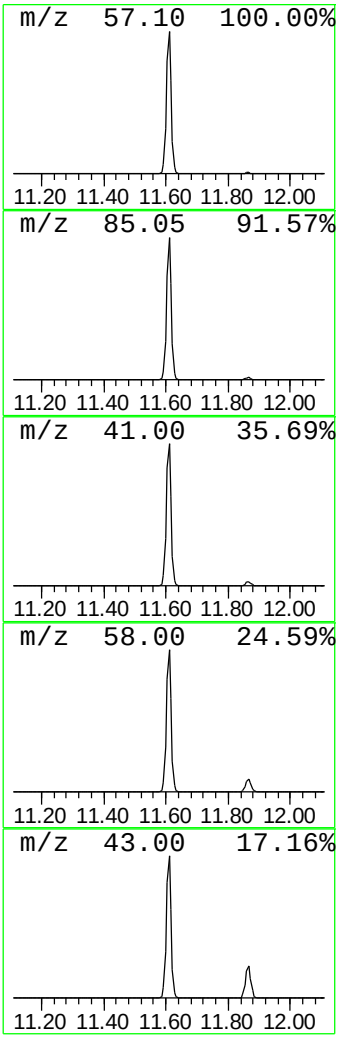
Peak Number 4 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.61	91.60 ug/L	7535070	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	64
3	t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	59
4	5-Nonanone	142	C9H18O	000502-56-7	59
5	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	52





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018773.D
Acq On : 05 Oct 2020 18:20
Operator : JC/SP
Sample : L4239-04DL 100X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

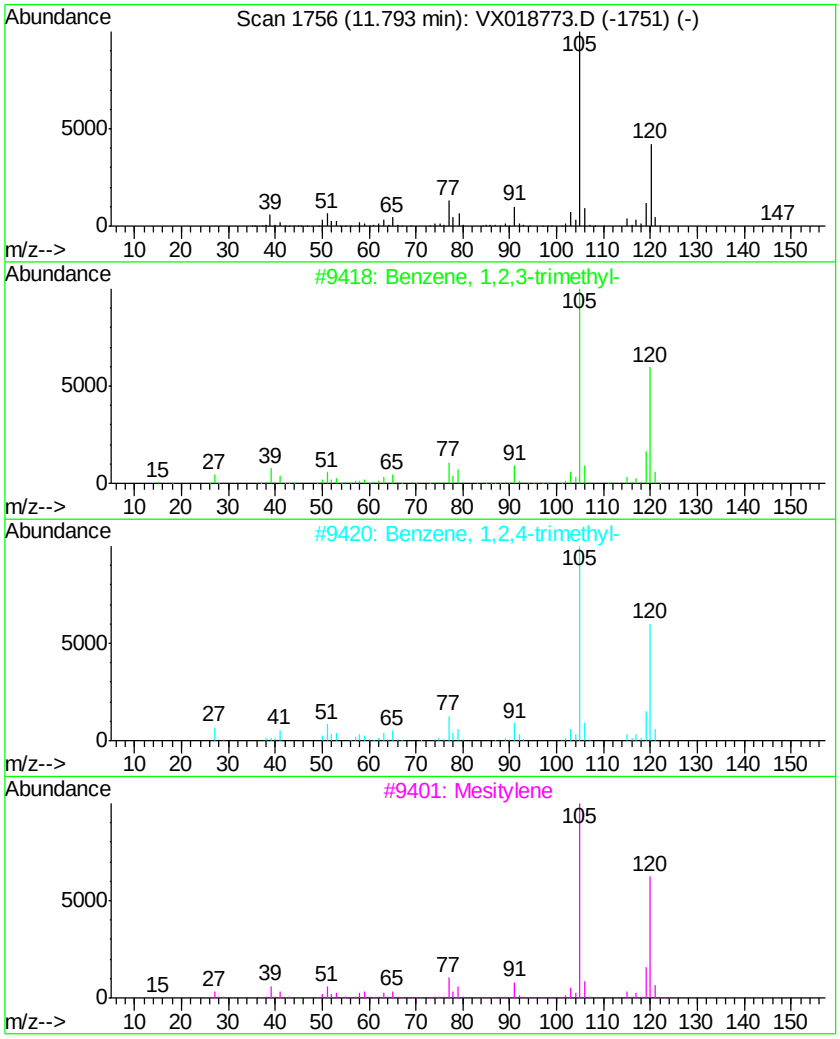
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

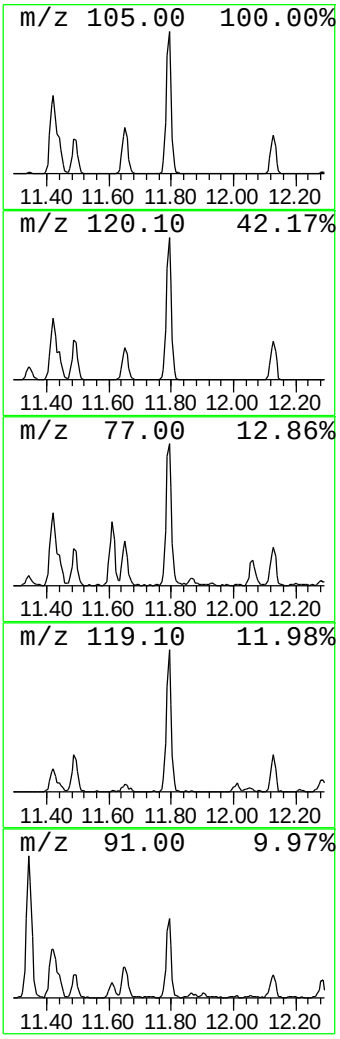
****

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	3.74 ug/L	307269	1,4-Dichlorobenzene-d4	12.06

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





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Sample : L4239-04DL 100X
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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

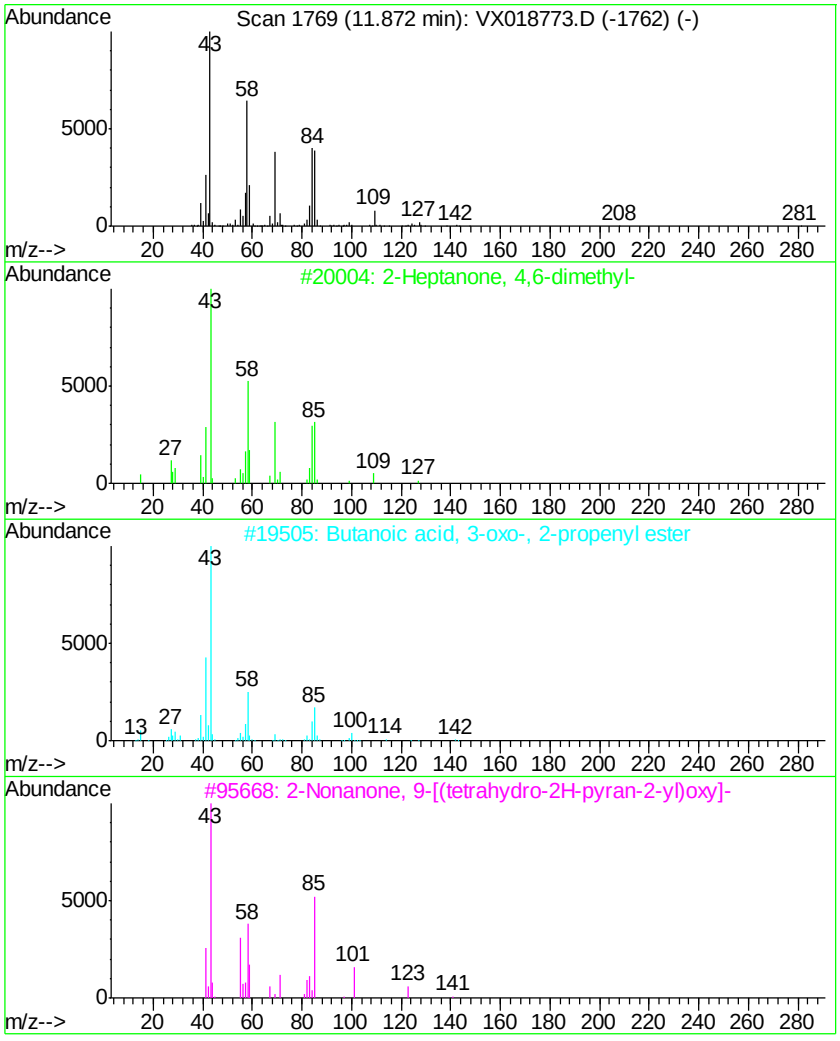
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

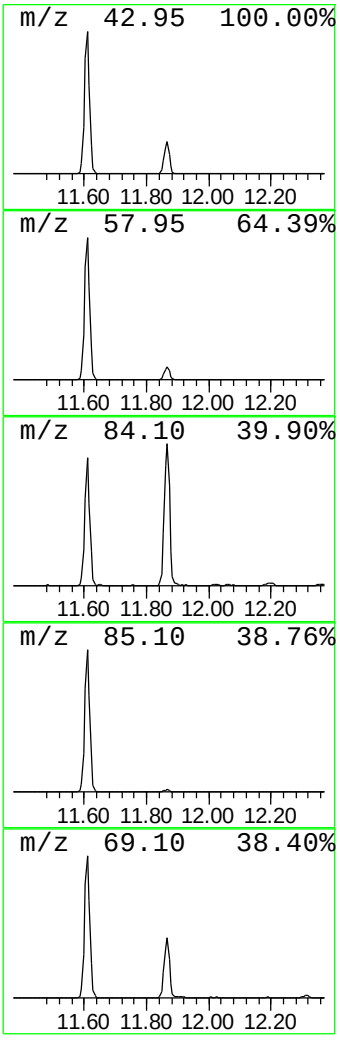
****

Peak Number 6 2-Heptanone, 4,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	4.52 ug/L	371483	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	90
2	Butanoic acid, 3-oxo-, 2-propenyl...	142	C7H10O3	001118-84-9	53
3	2-Nonanone, 9-[(tetrahydro-2H-py...	242	C14H26O3	054699-41-1	45
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	43
5	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	43





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SOM01.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Str...	3.50	2.7	ug/L	182273	1	6.83	339759	5.0
(DEL) Alkane: Cyc...	4.37	6.2	ug/L	423209	1	6.83	339759	5.0
Benzene, 1-ethyl-...	11.42	2.8	ug/L	225884	3	12.06	411284	5.0
4-Heptanone, 2,6-...	11.61	91.6	ug/L	7535070	3	12.06	411284	5.0
Benzene, 1,2,3-tr...	11.79	3.7	ug/L	307269	3	12.06	411284	5.0
2-Heptanone, 4,6-...	11.87	4.5	ug/L	371483	3	12.06	411284	5.0