LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018769.D
Acq On : 05 Oct 2020 16:38
Operator : JC/SP
Sample : L4239-04DL2 400X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL2

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	1.392	46	50	55	rBV	67572	71747	2.10%	0.611%
2	1.697	95	100	107	rVB	59274	71520	2.09%	0.609%
3	2.343	199	206	218	rBV	131298	216923	6.34%	1.846%
4	3.154	328	339	348	rBV2	16160	40240	1.18%	0.342%
5	3.501	387	396	406	rVB2	19671	44693	1.31%	0.380%
6	4.373	528	539	551	rBV4	34592	104420	3.05%	0.889%
7	4.562	558	570	583	rBV2	181538	579403	16.94%	4.931%
8	5.135	649	664	678	rBV2	83334	263130	7.69%	2.239%
9	5.464	705	718	731	rBV2	285373	893957	26.13%	7.607%
10	6.044	802	813	825	rBV3	205852	599071	17.51%	5.098%
11	6.830	933	942	953	rBV	145386	355725	10.40%	3.027%
12	7.367	1022	1030	1042	rBV	128120	279116	8.16%	2.375%
13	8.373	1189	1195	1203	rBV	80664	134791	3.94%	1.147%
14	8.696	1239	1248	1253	rBV	321480	504763	14.75%	4.295%
15	8.763	1253	1259	1273	rVB	2234651	3421312	100.00%	29.115%
16	8.994	1289	1297	1308	rBV	59563	89190	2.61%	0.759%
17	9.427	1362	1368	1380	rBV	437130	608544	17.79%	5.179%
18	10.098	1471	1478	1488	rBV	301418	427419	12.49%	3.637%
19	10.342	1511	1518	1525	rBV	50851	71642	2.09%	0.610%
20	10.683	1569	1574	1581	rVB	34902	47582	1.39%	0.405%
21	11.232	1659	1664	1672	rVB2	130522	170259	4.98%	1.449%
22	11.421	1690	1695	1702	rBV	28881	52121	1.52%	0.444%
23	11.610	1720	1726	1731	rBV	1409626	1660403	48.53%	14.130%
24	11.793	1751	1756	1762	rVB	57284	72357	2.11%	0.616%
25	11.866	1762	1768	1775	rBV	62399	80880	2.36%	0.688%
26	12.061	1795	1800	1807	rBV	347631	420513	12.29%	3.579%
27	12.360	1844	1849	1856	rVB	375379	469356	13.72%	3.994%

Sum of corrected areas: 11751077

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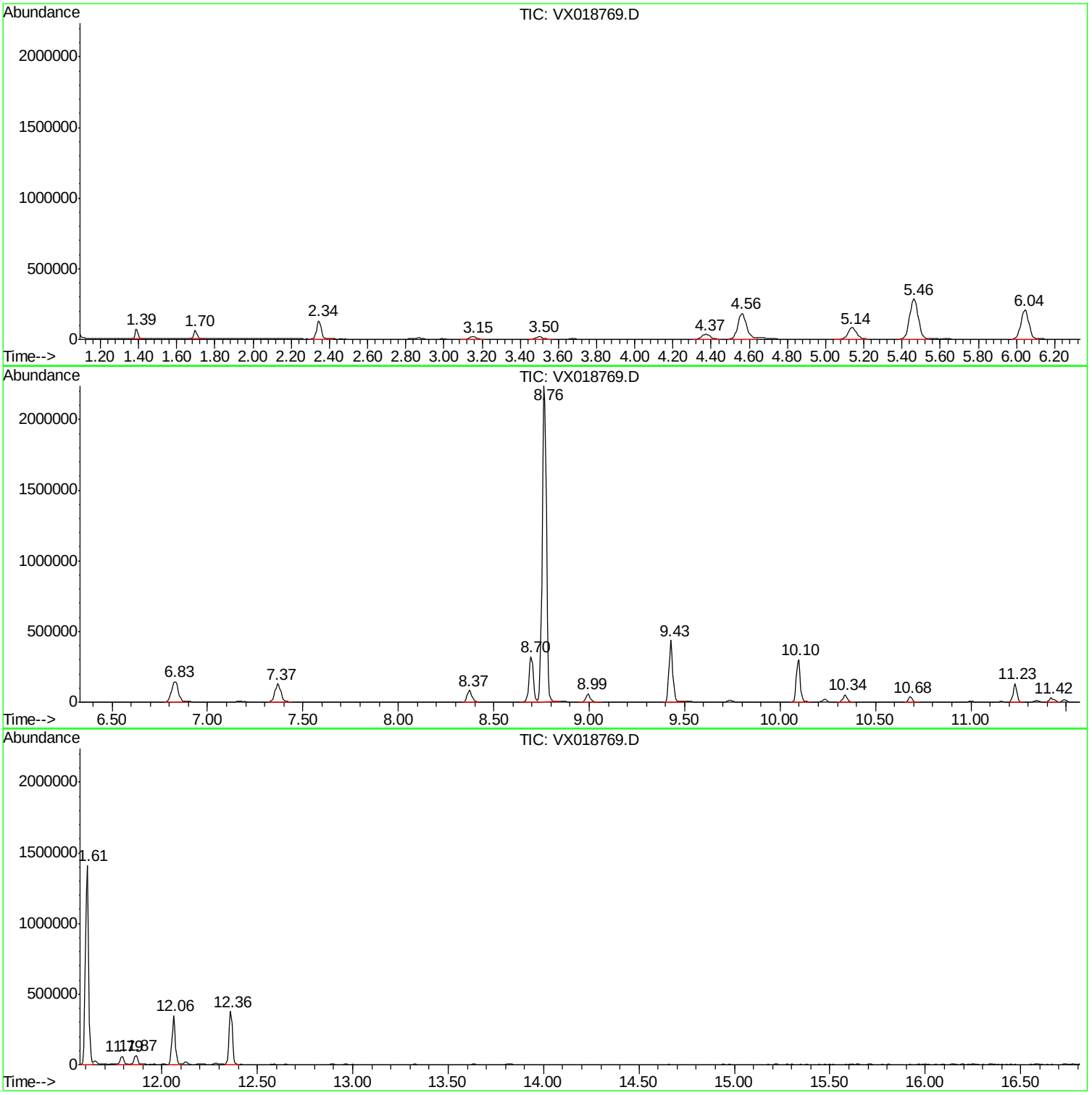
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3N3DL2

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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Data File : VX018769.D
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Instrument : MSVOA_X
ClientSampleId : BG3N3DL2

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

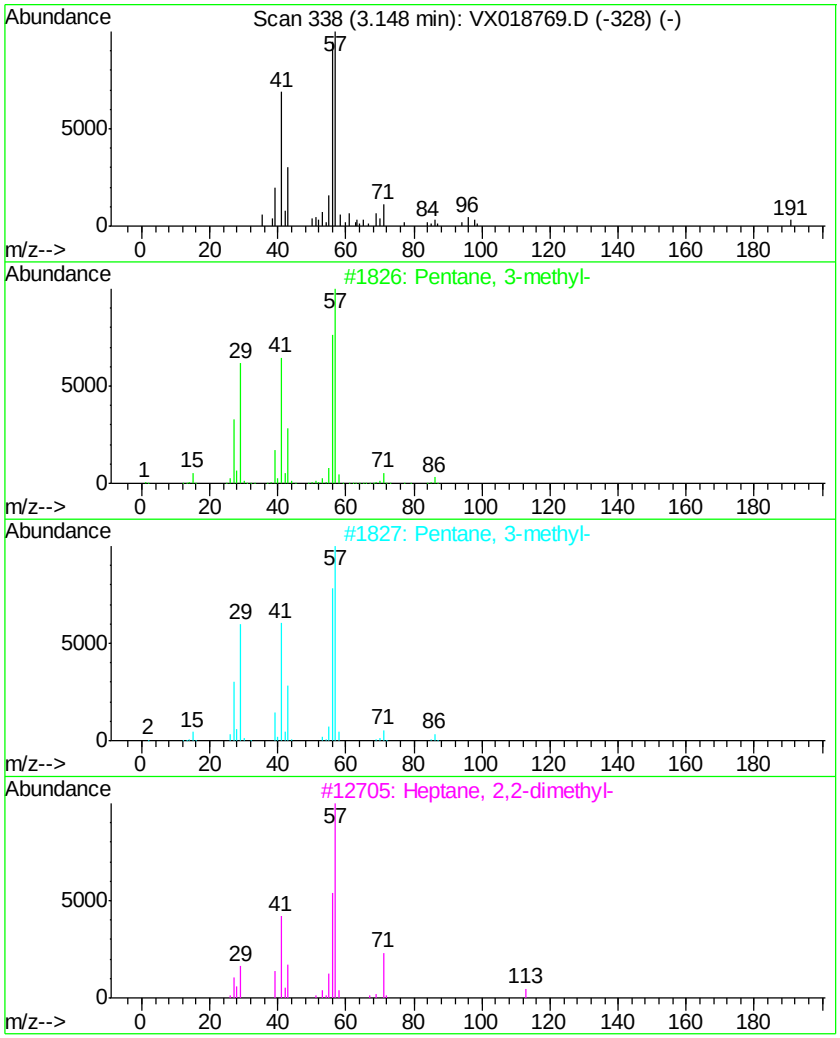
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

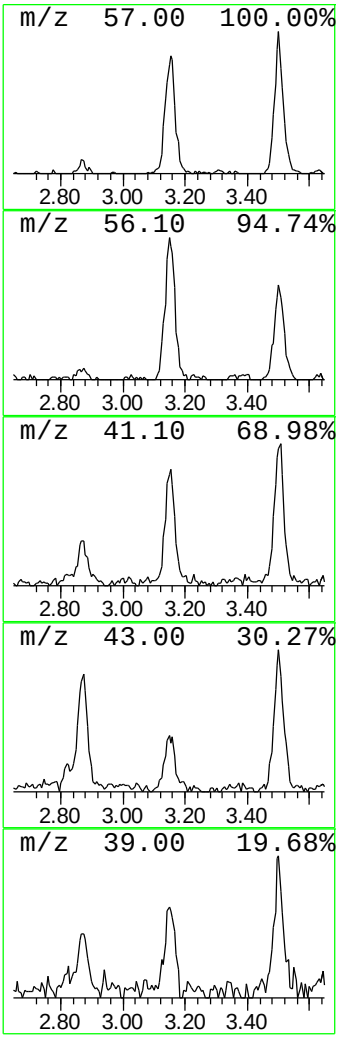
****

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	0.57 ug/L	40240	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	80
2	Pentane, 3-methyl-	86	C6H14	000096-14-0	72
3	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	72
4	Pentane, 3-methyl-	86	C6H14	000096-14-0	72
5	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	56





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Data File : VX018769.D
Acq On : 05 Oct 2020 16:38
Operator : JC/SP
Sample : L4239-04DL2 400X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL2

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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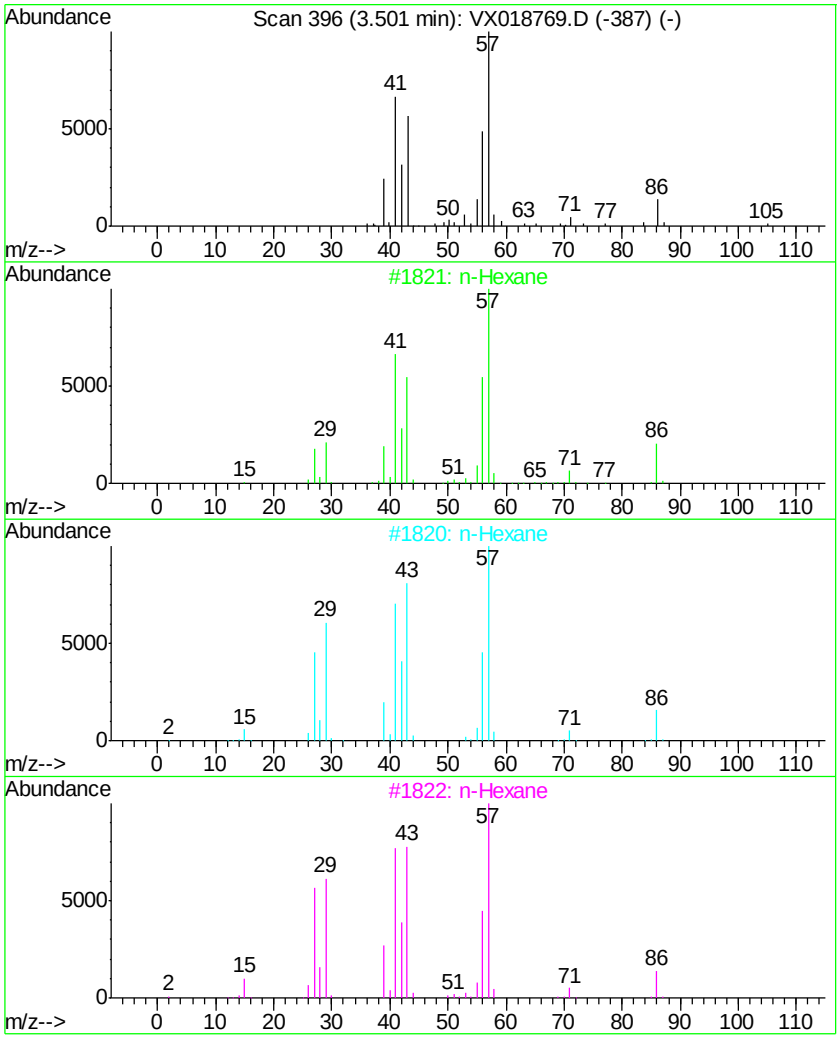
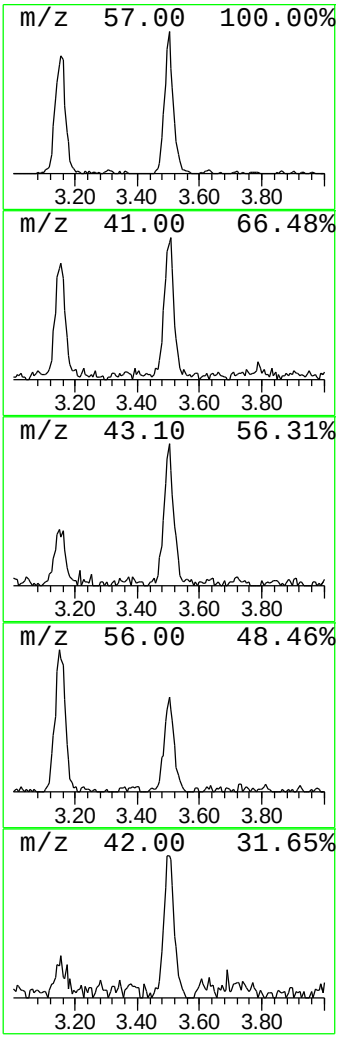
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	0.63 ug/L	44693	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	72
2	n-Hexane	86	C6H14	000110-54-3	58
3	n-Hexane	86	C6H14	000110-54-3	58
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	37
5	1-Butene	56	C4H8	000106-98-9	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018769.D
Acq On : 05 Oct 2020 16:38
Operator : JC/SP
Sample : L4239-04DL2 400X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL2

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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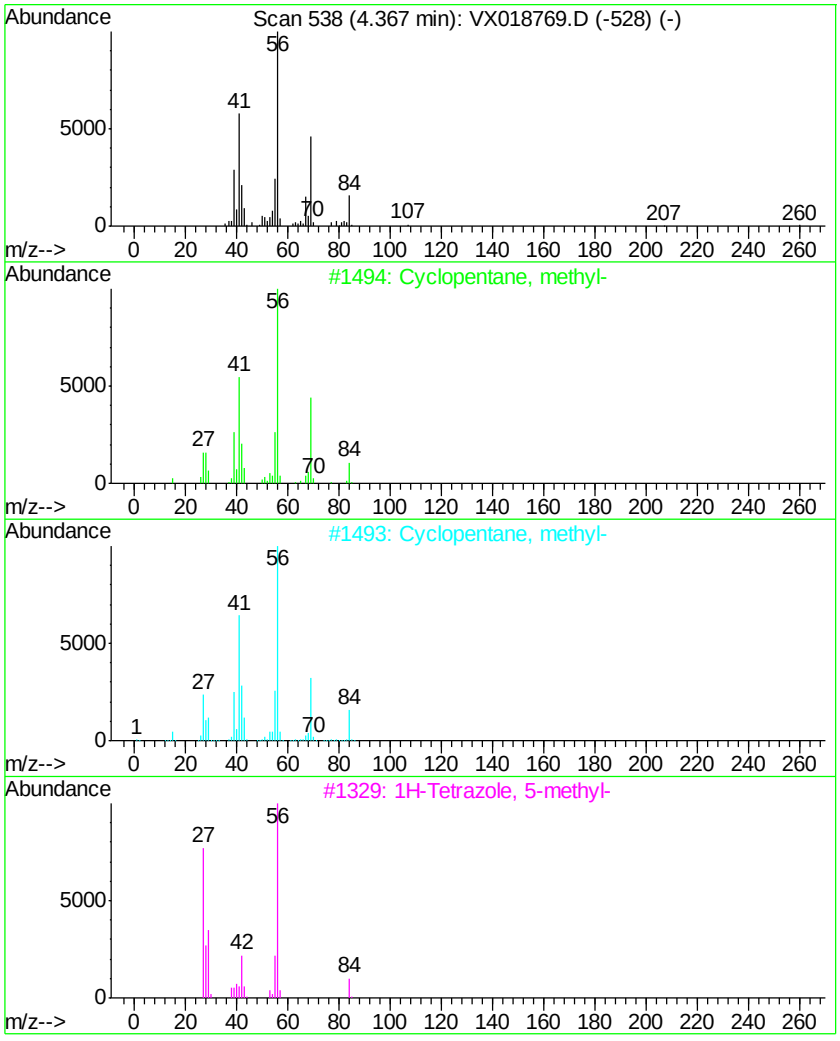
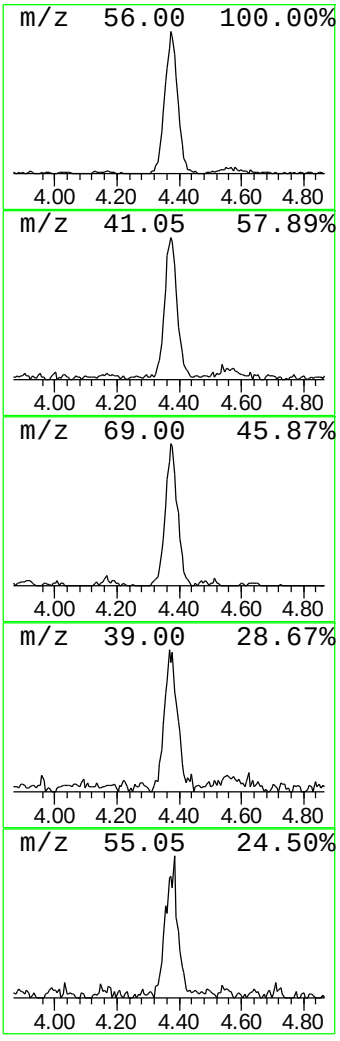
Peak Number 3 (DEL) Alkane: Cyclic4.37 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	1.47 ug/L	104420	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	74
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	50
5	Cyclobutane	56	C4H8	000287-23-0	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018769.D
Acq On : 05 Oct 2020 16:38
Operator : JC/SP
Sample : L4239-04DL2 400X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL2

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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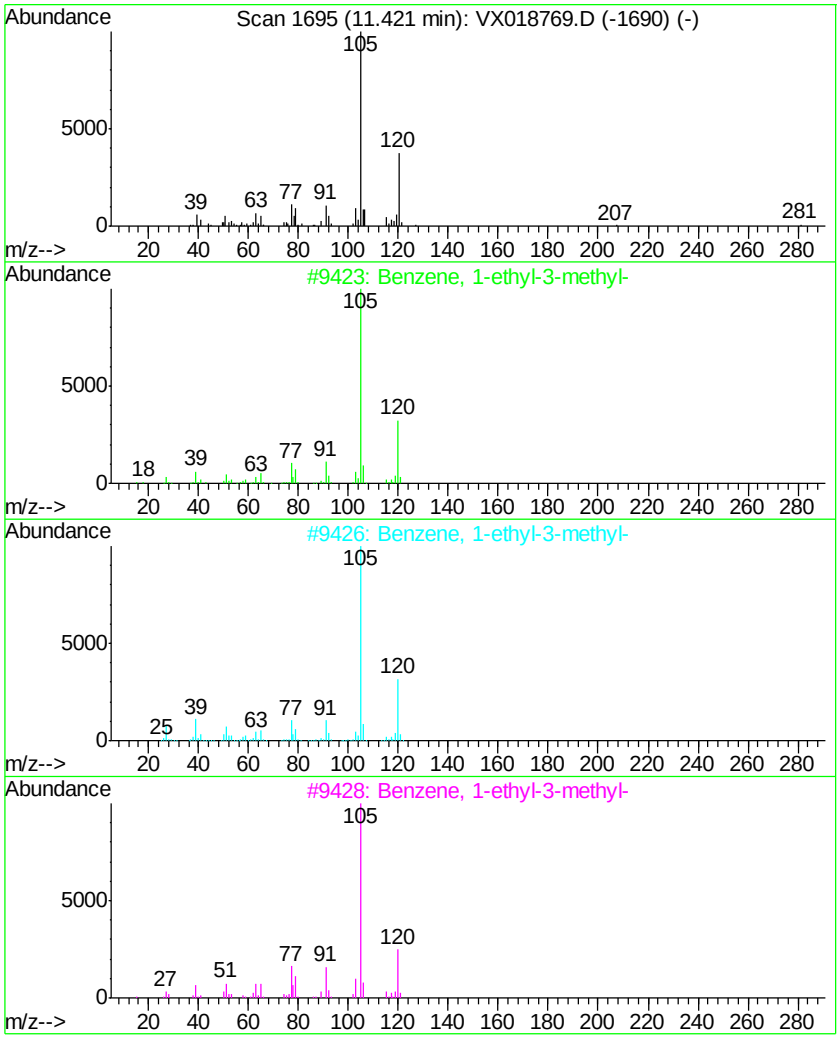
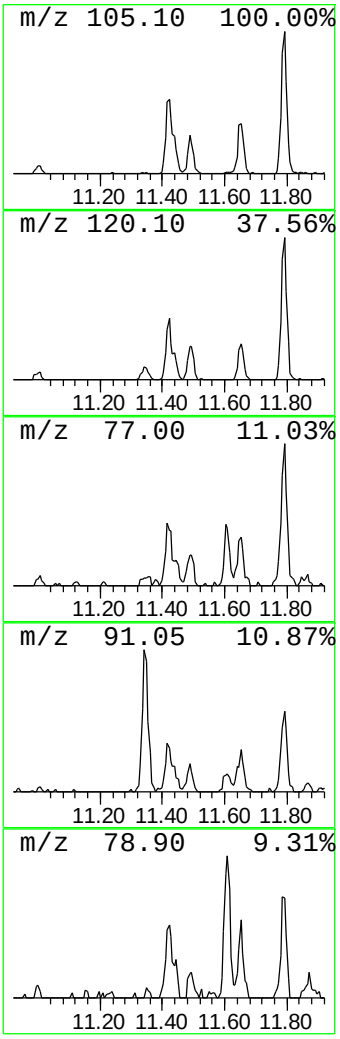
Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	0.62 ug/L	52121	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-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018769.D
Acq On : 05 Oct 2020 16:38
Operator : JC/SP
Sample : L4239-04DL2 400X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL2

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

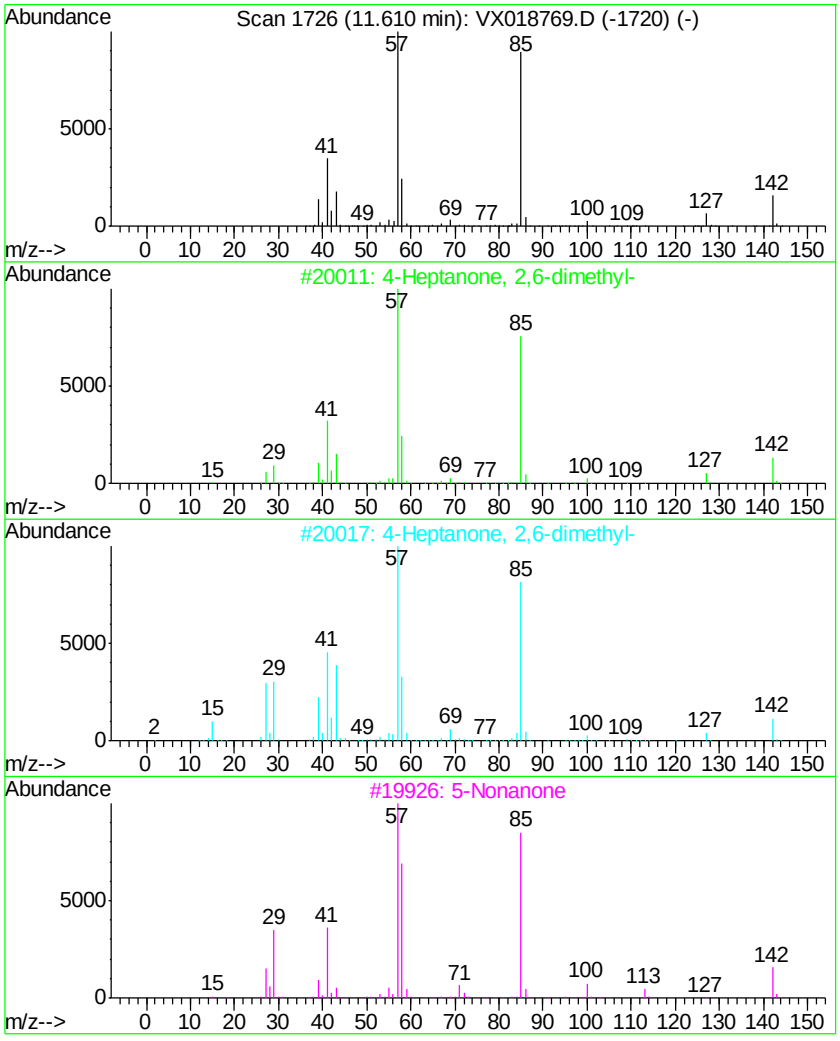
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

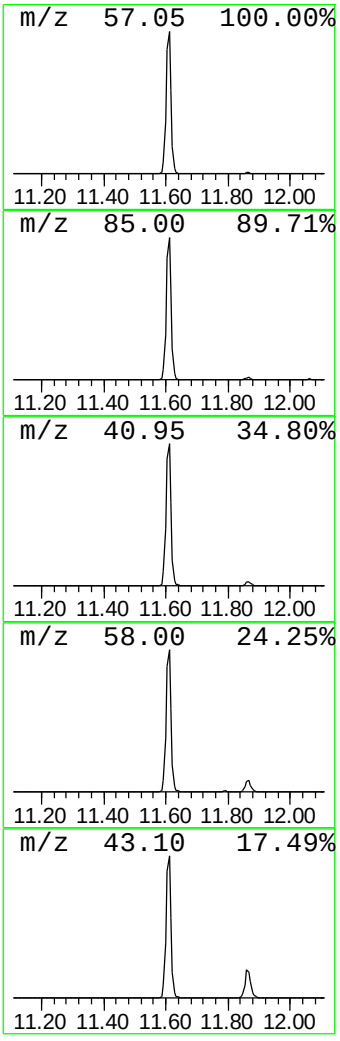
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.61	19.74 ug/L	1660400	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-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	64
3	5-Nonanone	142	C9H18O	000502-56-7	59
4	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	50
5	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100520\
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ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3N3DL2

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

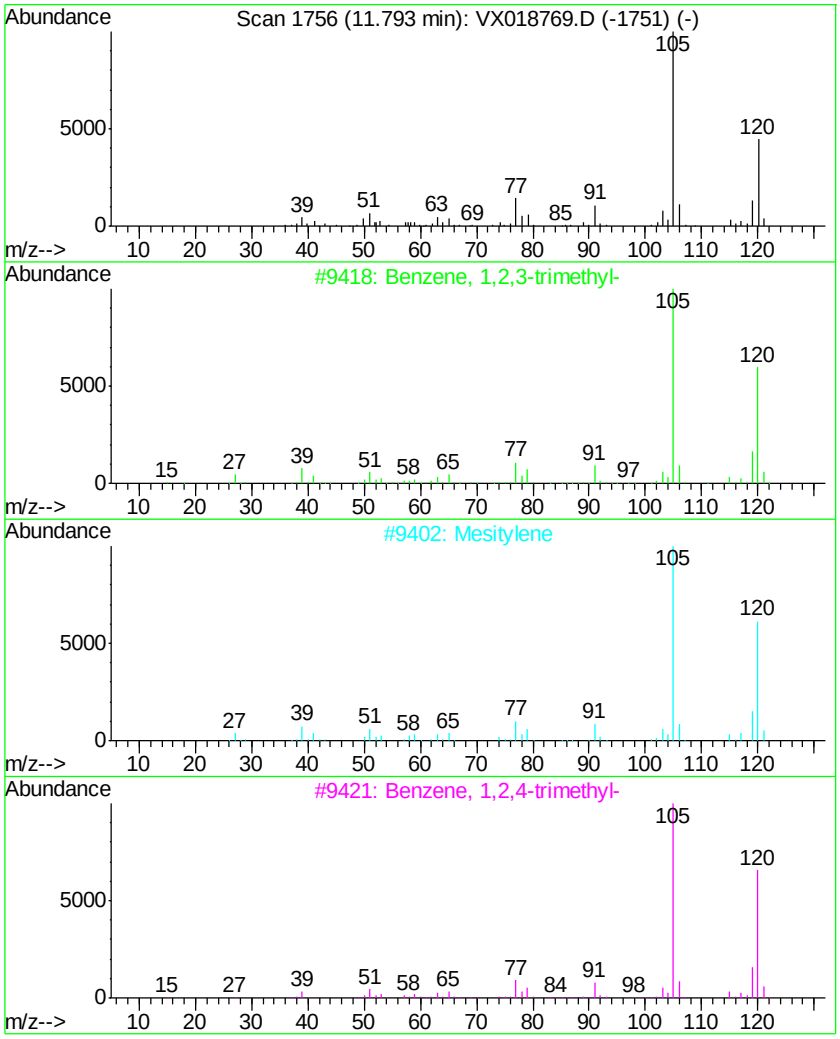
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

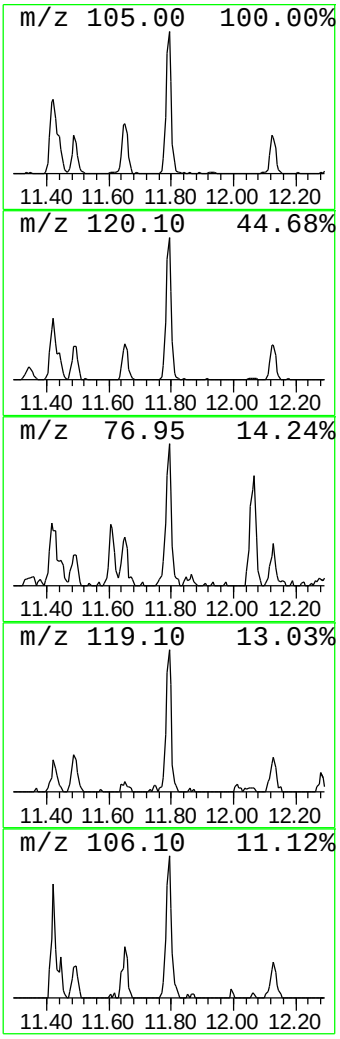
****

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	0.86 ug/L	72357	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	95
2	Mesitylene	120	C9H12	000108-67-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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Quant Title : TRACE VOA SOM01.0

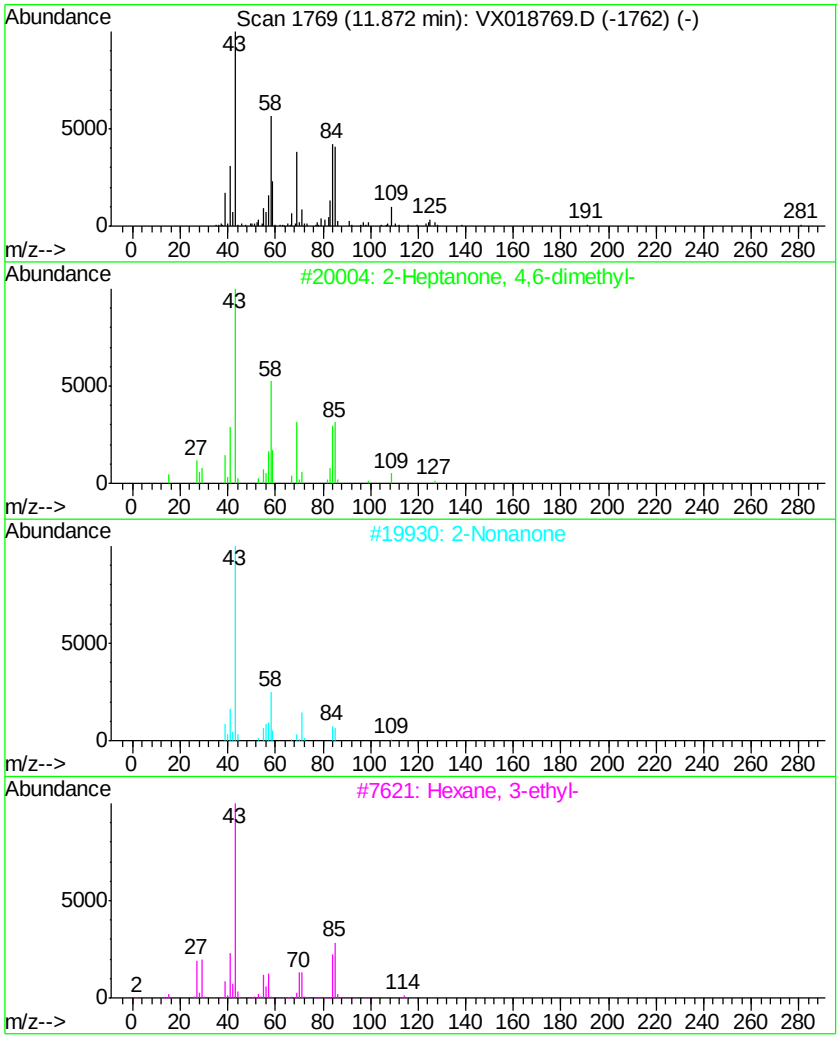
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

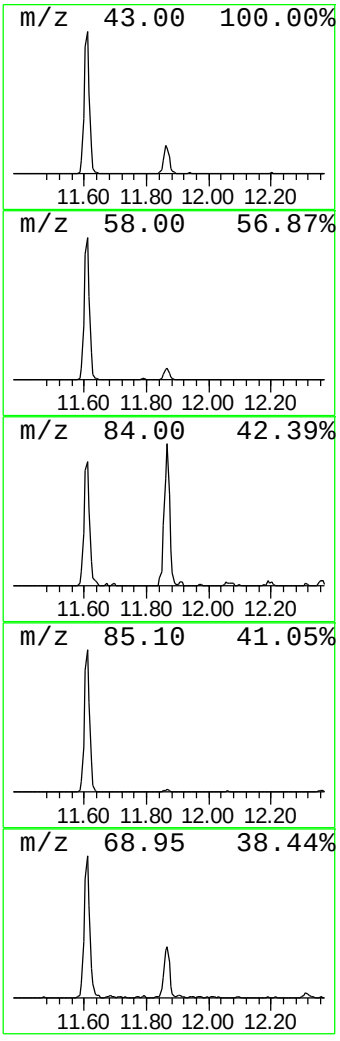
****

Peak Number 8 2-Heptanone, 4,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	0.96 ug/L	80880	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	2-Nonanone	142	C9H18O	000821-55-6	53
3	Hexane, 3-ethyl-	114	C8H18	000619-99-8	43
4	trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	38
5	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	38





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...	3.15	0.6	ug/L	40240	1	6.83	355725	5.0
(DEL) Alkane: Str...	3.50	0.6	ug/L	44693	1	6.83	355725	5.0
(DEL) Alkane: Cyc...	4.37	1.5	ug/L	104420	1	6.83	355725	5.0
Benzene, 1-ethyl-...	11.42	0.6	ug/L	52121	3	12.06	420513	5.0
4-Heptanone, 2,6-...	11.61	19.7	ug/L	1660400	3	12.06	420513	5.0
Benzene, 1,2,3-tr...	11.79	0.9	ug/L	72357	3	12.06	420513	5.0
2-Heptanone, 4,6-...	11.87	1.0	ug/L	80880	3	12.06	420513	5.0