LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000615.D
Acq On : 01 Apr 2018 01:30
Operator : JC/MD
Sample : J2150-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 36 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	76	80	93	rBV	368909	443448	4.85%	2.043%
2	3.087	395	410	421	rBV	4076960	9137496	100.00%	42.100%
3	3.215	421	431	449	rVB	3271410	7348870	80.43%	33.859%
4	5.513	799	808	821	rVB	71429	197380	2.16%	0.909%
5	5.672	821	834	851	rBV2	112429	317179	3.47%	1.461%
6	6.080	891	901	914	rBV2	79423	202997	2.22%	0.935%
7	6.360	934	947	948	rBV2	73908	179940	1.97%	0.829%
8	6.403	949	954	957	rVV	114506	276884	3.03%	1.276%
9	6.458	958	963	974	rVB2	219198	587102	6.43%	2.705%
10	6.873	1021	1031	1043	rBV	181576	431810	4.73%	1.990%
11	8.061	1218	1226	1236	rVB	85571	163077	1.78%	0.751%
12	8.183	1239	1246	1255	rVB	80275	156960	1.72%	0.723%
13	8.726	1323	1335	1343	rBV	394575	632720	6.92%	2.915%
14	10.122	1558	1564	1569	rVB	417427	548993	6.01%	2.529%
15	11.146	1726	1732	1738	rBV	363852	453844	4.97%	2.091%
16	12.085	1880	1886	1894	rBV	512317	625420	6.84%	2.882%

Sum of corrected areas: 21704120

LSC Report - Integrated Chromatogram

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
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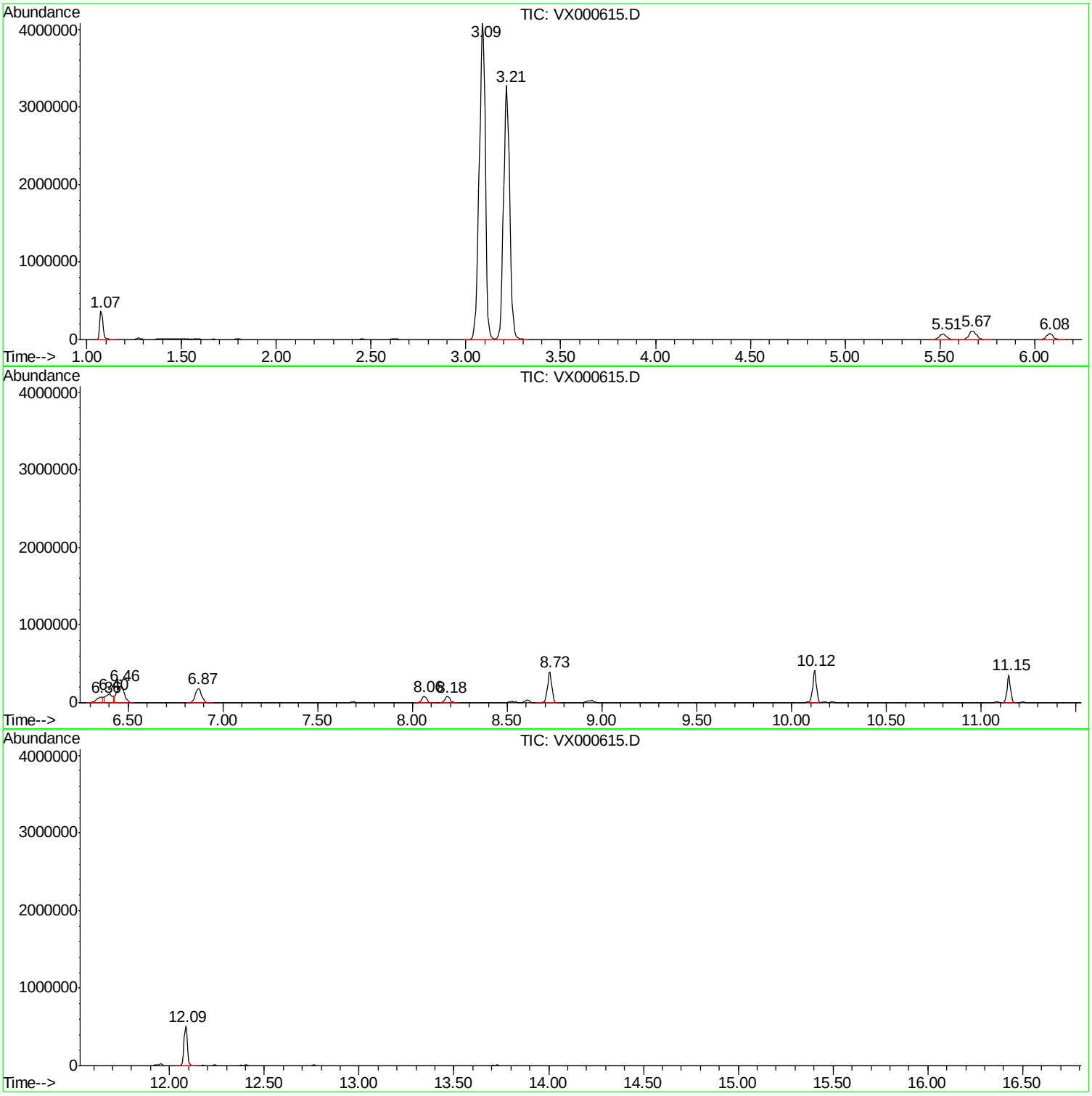
Operator : JC/MD
Sample : J2150-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000615.D
Acq On : 01 Apr 2018 01:30
Operator : JC/MD
Sample : J2150-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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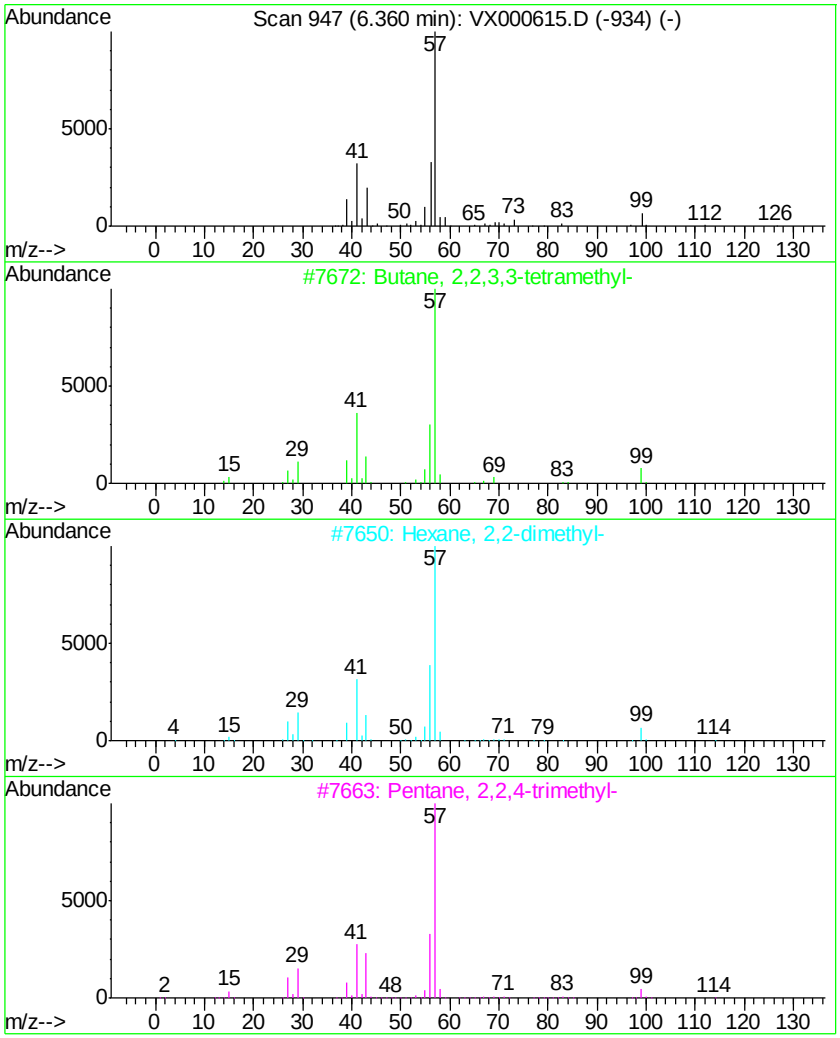
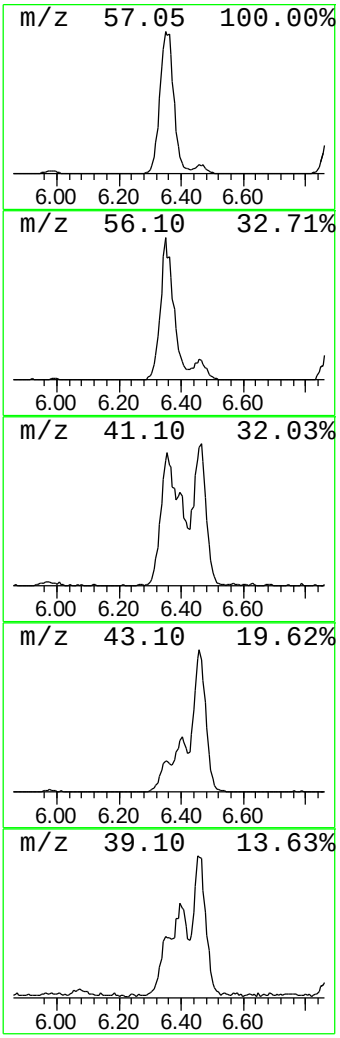
Peak Number 2 Butane, 2,2,3,3-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	20.84 ug/l	179940	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	59
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	50
5	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	40





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000615.D
Acq On : 01 Apr 2018 01:30
Operator : JC/MD
Sample : J2150-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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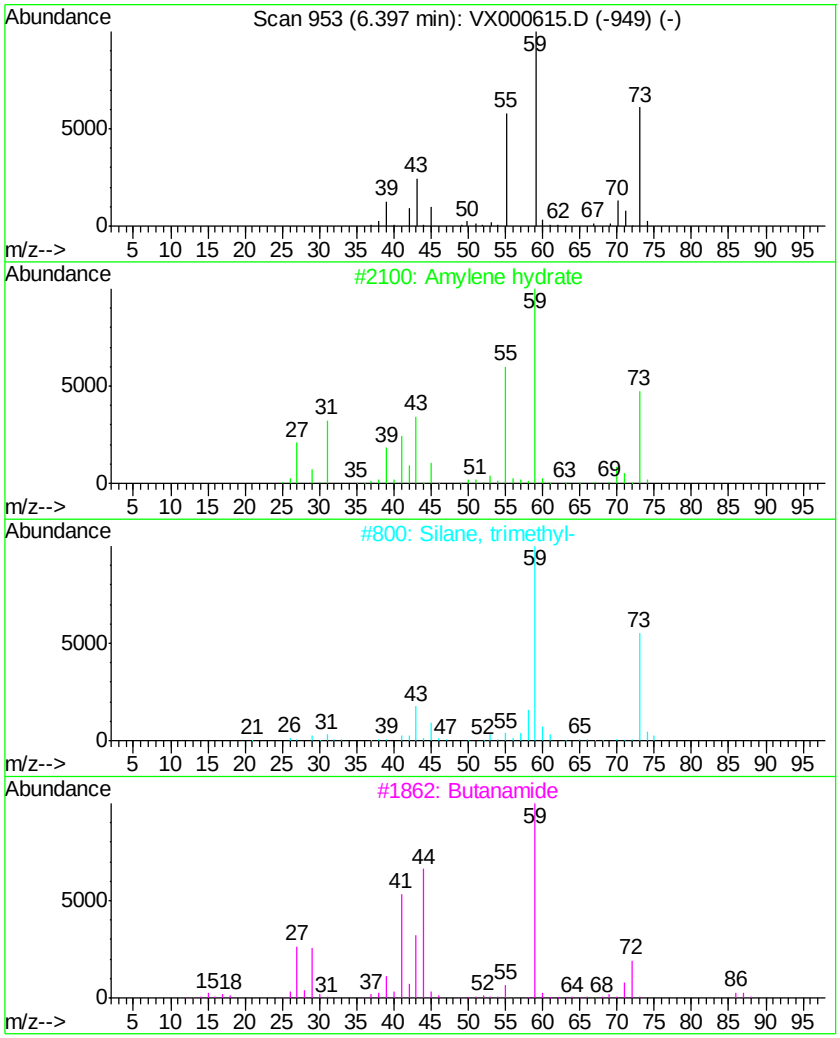
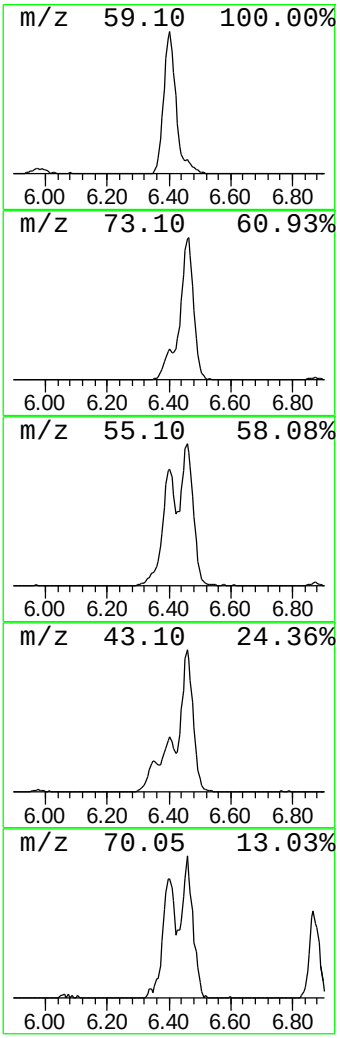
Peak Number 3 Amylene hydrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	32.06 ug/l	276884	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	83
2	Silane, trimethyl-	74	C3H10Si	000993-07-7	9
3	Butanamide	87	C4H9NO	000541-35-5	9
4	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9
5	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9





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Data File : VX000615.D
Acq On : 01 Apr 2018 01:30
Operator : JC/MD
Sample : J2150-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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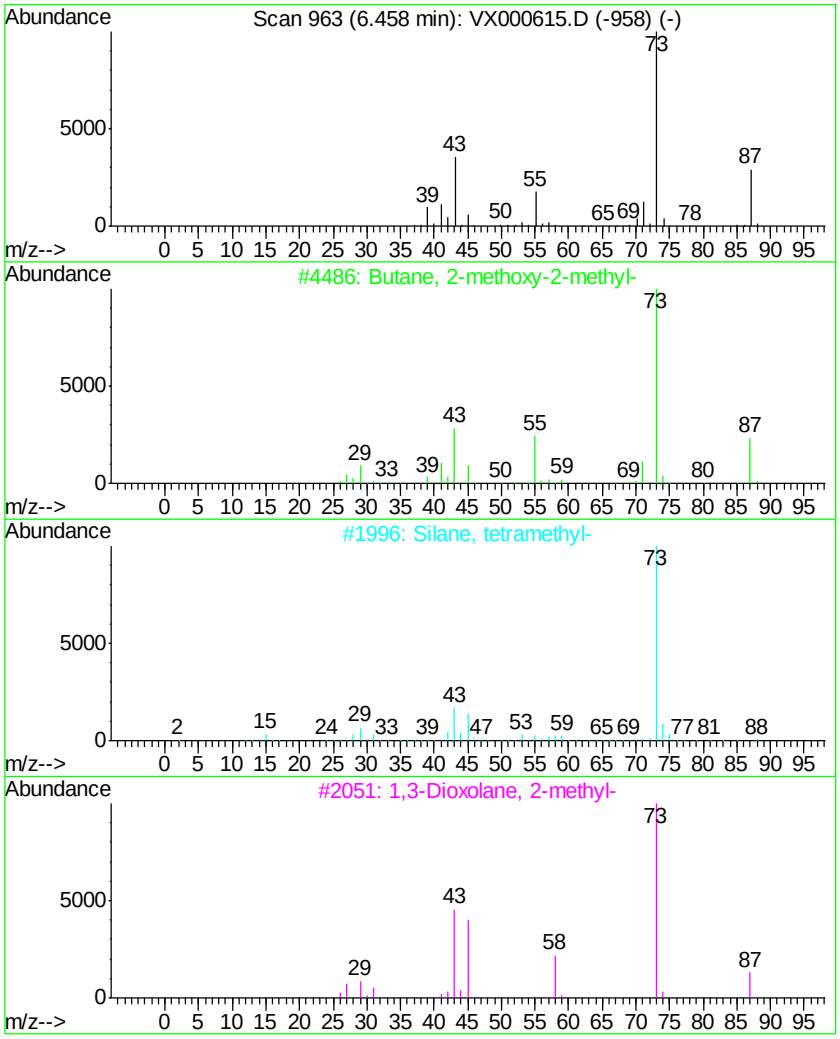
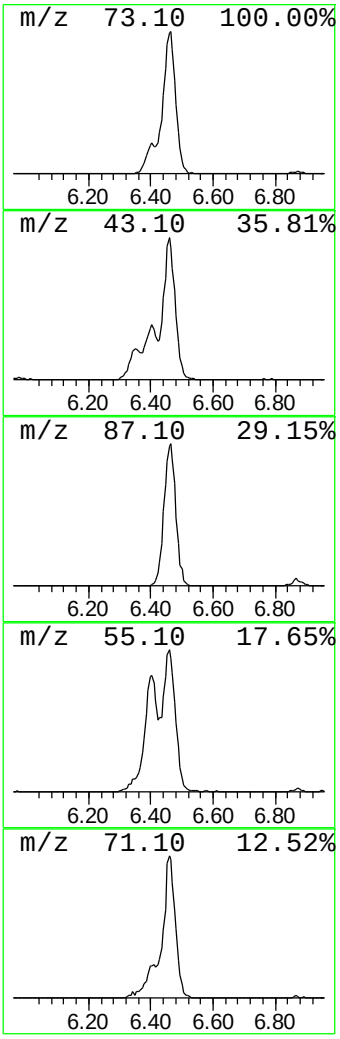
Peak Number 4 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	67.98 ug/l	587102	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
5	1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	9





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ALS Vial : 36 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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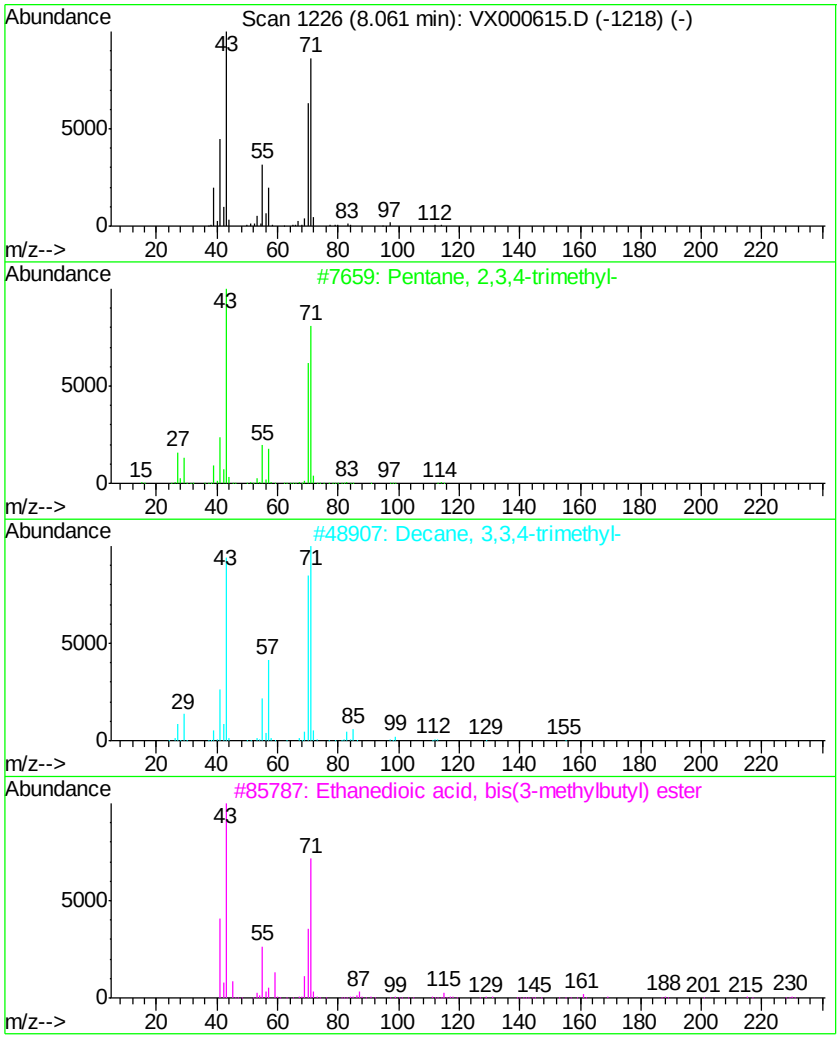
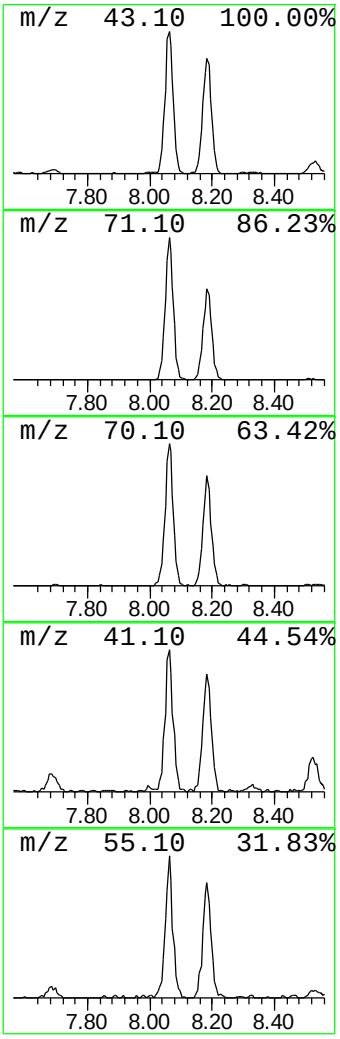
Peak Number 5 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	18.88 ug/l	163077	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	83
3	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	83
4	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	78





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Quant Title : SW846 8260

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

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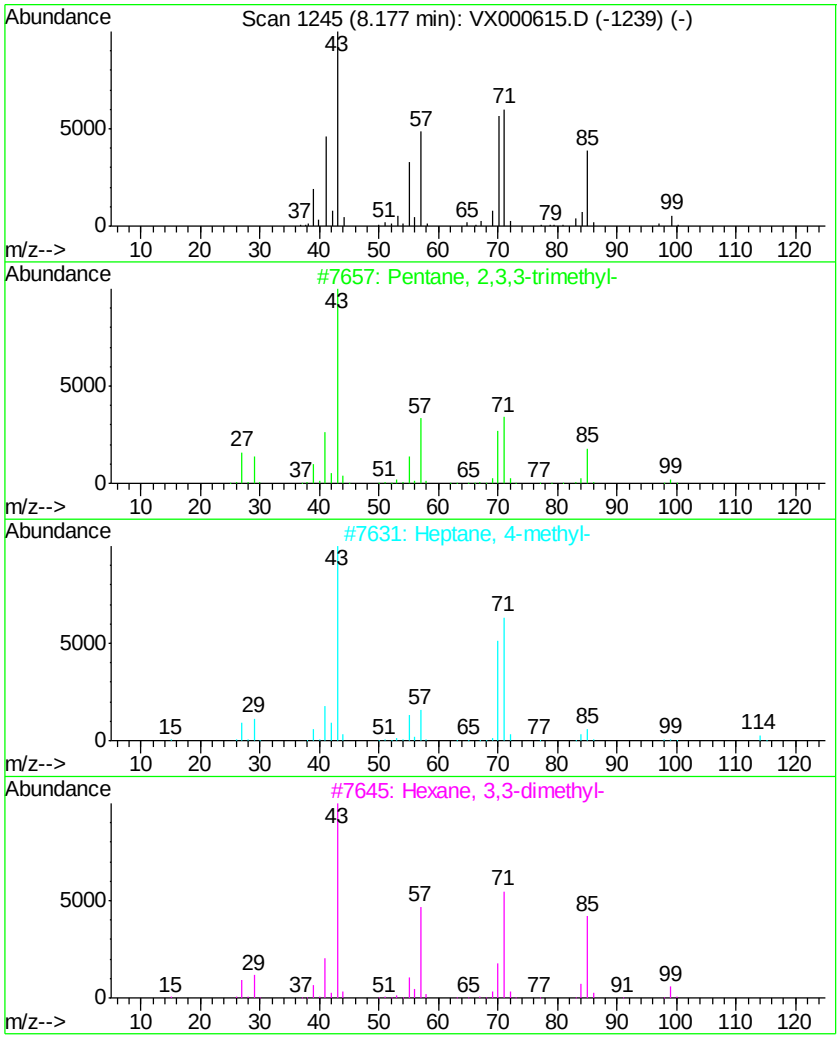
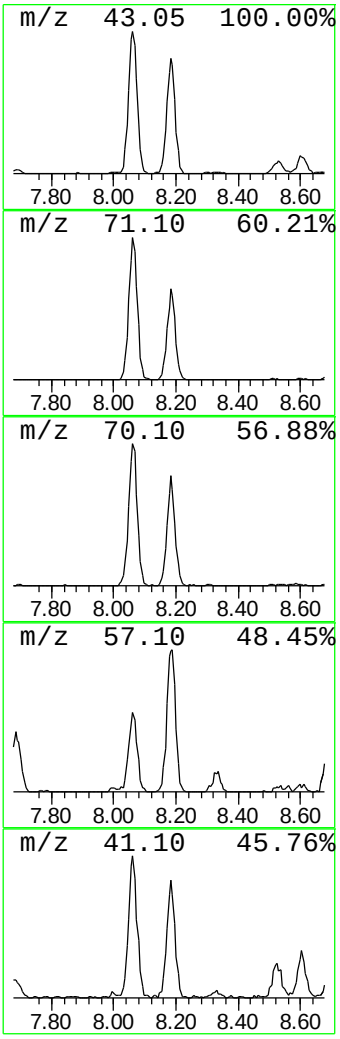
Peak Number 6 Pentane, 2,3,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	18.17 ug/l	156960	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4	Pentane, 3-ethyl-	100	C7H16	000617-78-7	53
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2,2,3,3-t...	6.36	20.8	ug/l	179940	2	6.87	431810	50.0
Amylene hydrate	6.40	32.1	ug/l	276884	2	6.87	431810	50.0
unknown6.46	6.46	68.0	ug/l	587102	2	6.87	431810	50.0
Pentane, 2,3,4-tr...	8.06	18.9	ug/l	163077	2	6.87	431810	50.0
Pentane, 2,3,3-tr...	8.18	18.2	ug/l	156960	2	6.87	431810	50.0