LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003133.D
Acq On : 02 Jul 2018 17:57
Operator : JC/MD
Sample : J3772-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

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\82X062518W.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	90	rBV	1124623	1489671	30.01%	4.054%
2	1.282	108	114	130	rBV	480718	1310955	26.41%	3.568%
3	1.398	131	133	141	rVB	59703	95534	1.92%	0.260%
4	1.995	227	231	239	rVB	162404	232597	4.69%	0.633%
5	2.209	261	266	271	rVB	34985	54193	1.09%	0.147%
6	2.447	300	305	309	rBV	83666	143780	2.90%	0.391%
7	2.623	328	334	343	rBV	74544	134741	2.71%	0.367%
8	4.605	649	659	669	rBV5	15258	50727	1.02%	0.138%
9	4.721	669	678	688	rVB	58980	164047	3.30%	0.446%
10	5.214	748	759	772	rBV	54945	167060	3.37%	0.455%
11	5.507	796	807	822	rBV2	198747	571919	11.52%	1.557%
12	5.665	822	833	846	rVB	297474	831462	16.75%	2.263%
13	6.074	886	900	909	rBV	209445	543346	10.94%	1.479%
14	6.482	958	967	975	rBV4	18588	51745	1.04%	0.141%
15	6.867	1021	1030	1044	rBV	421476	979112	19.72%	2.665%
16	7.232	1080	1090	1099	rBV3	40968	116335	2.34%	0.317%
17	7.342	1101	1108	1122	rVV	34259	78383	1.58%	0.213%
18	7.561	1137	1144	1155	rBV	408802	767125	15.45%	2.088%
19	7.671	1155	1162	1168	rVV2	127219	265398	5.35%	0.722%
20	7.738	1168	1173	1187	rVB	278381	507166	10.22%	1.380%
21	7.988	1207	1214	1228	rBV2	56589	158989	3.20%	0.433%
22	8.720	1327	1334	1342	rBV	993532	1554340	31.31%	4.230%
23	9.098	1388	1396	1407	rVB	42537	79181	1.59%	0.216%
24	9.226	1412	1417	1425	rBV	55321	83192	1.68%	0.226%
25	9.311	1425	1431	1439	rBV	627281	857837	17.28%	2.335%
26	9.378	1439	1442	1454	rVB2	29587	51369	1.03%	0.140%
27	9.500	1457	1462	1468	rBV	243204	334699	6.74%	0.911%
28	9.586	1471	1476	1487	rBV	933055	1293752	26.06%	3.521%
29	9.707	1492	1496	1511	rVB	40298	73233	1.48%	0.199%
30	10.061	1548	1554	1558	rBV2	45611	101211	2.04%	0.275%
31	10.116	1558	1563	1581	rVB	897608	1264967	25.48%	3.443%
32	10.543	1629	1633	1644	rVB	45544	65374	1.32%	0.178%
33	10.646	1644	1650	1661	rBV	4071326	4964463	100.00%	13.511%
34	10.744	1661	1666	1675	rVB	110897	181213	3.65%	0.493%

LSC Area Percent Report

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Data File : VX003133.D
Acq On : 02 Jul 2018 17:57
Operator : JC/MD
Sample : J3772-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

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\82X062518W.M
Title : SW846 8260

35	10.829	1675	1680	1686	rBV	1265626	1498303	30.18%	4.078%
36	10.939	1695	1698	1707	rVB	309574	410114	8.26%	1.116%
37	11.140	1720	1731	1741	rBV	949060	1304343	26.27%	3.550%
38	11.646	1809	1814	1818	rBV	286317	348362	7.02%	0.948%
39	11.713	1821	1825	1830	rBV	560777	632366	12.74%	1.721%
40	11.780	1830	1836	1839	rBV	345476	442394	8.91%	1.204%
41	11.817	1839	1842	1847	rVB	1114083	1226338	24.70%	3.338%
42	11.896	1850	1855	1861	rBV2	2834792	3495481	70.41%	9.513%
43	11.957	1861	1865	1869	rBV	1459024	1620775	32.65%	4.411%
44	12.079	1876	1885	1894	rVB2	1158332	2199233	44.30%	5.985%
45	12.207	1899	1906	1911	rVB	102415	150582	3.03%	0.410%
46	12.274	1913	1917	1923	rVB	62436	78517	1.58%	0.214%
47	12.463	1945	1948	1954	rBV2	38776	64848	1.31%	0.176%
48	12.640	1965	1977	1991	rBV	655941	1079926	21.75%	2.939%
49	12.750	1991	1995	1999	rVV	68356	95052	1.91%	0.259%
50	12.829	2002	2008	2010	rVV	330810	441499	8.89%	1.202%
51	12.853	2010	2012	2015	rVV	238072	270119	5.44%	0.735%
52	12.890	2015	2018	2020	rVV	201466	259360	5.22%	0.706%
53	12.914	2020	2022	2031	rVB	107413	125593	2.53%	0.342%
54	13.164	2059	2063	2067	rVB	70408	81912	1.65%	0.223%
55	13.219	2067	2072	2078	rBV2	69748	97147	1.96%	0.264%
56	13.481	2108	2115	2119	rBV	231208	316124	6.37%	0.860%
57	13.524	2119	2122	2127	rVB2	59445	76030	1.53%	0.207%
58	13.664	2140	2145	2155	rVB2	245640	338710	6.82%	0.922%
59	14.524	2282	2286	2293	rVB	38559	53979	1.09%	0.147%
60	15.213	2394	2399	2404	rVB	52295	65627	1.32%	0.179%
61	15.536	2446	2452	2468	rBV	220926	351032	7.07%	0.955%

Sum of corrected areas: 36742882

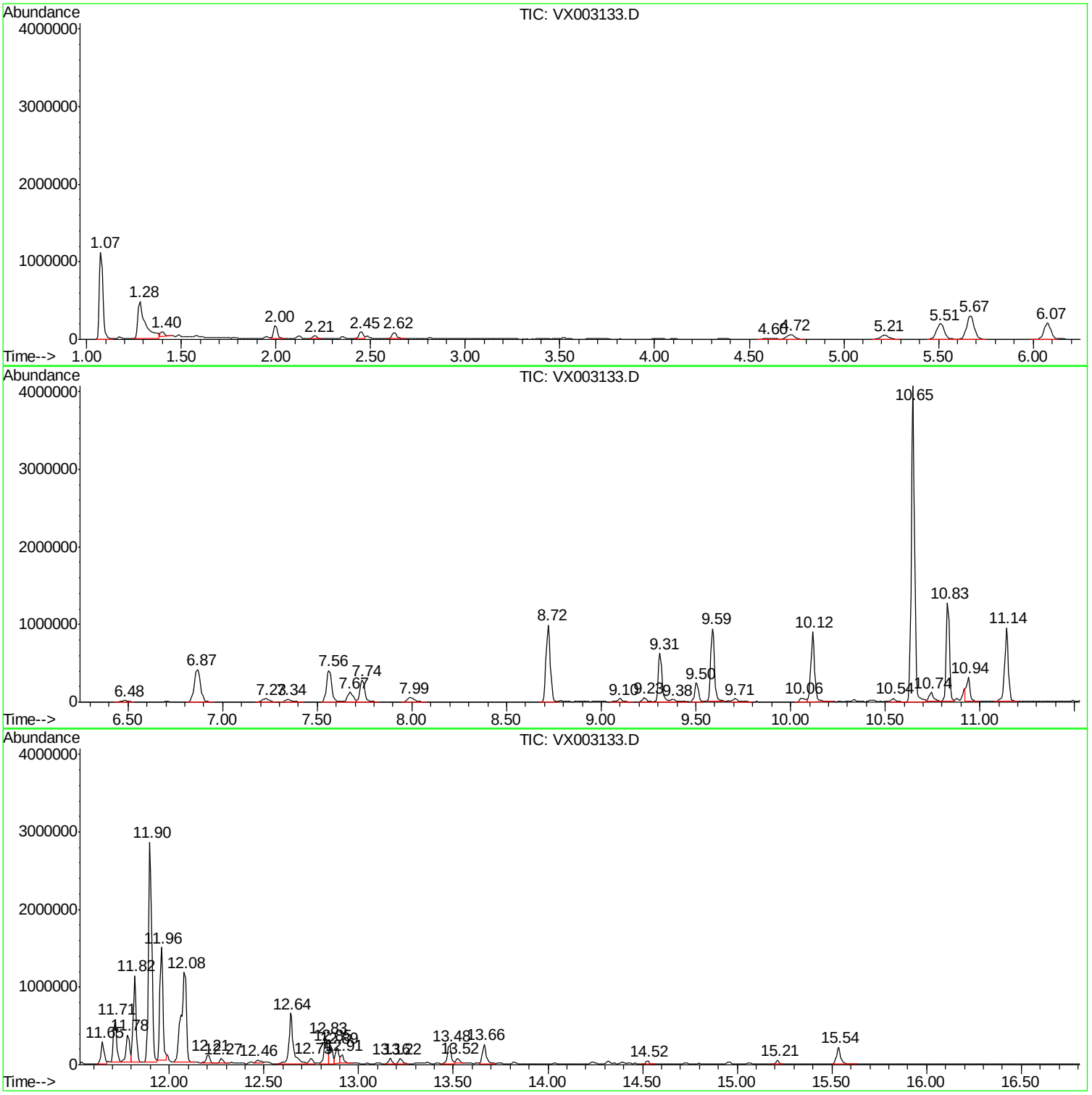
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003133.D
Acq On : 02 Jul 2018 17:57
Operator : JC/MD
Sample : J3772-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003133.D
Acq On : 02 Jul 2018 17:57
Operator : JC/MD
Sample : J3772-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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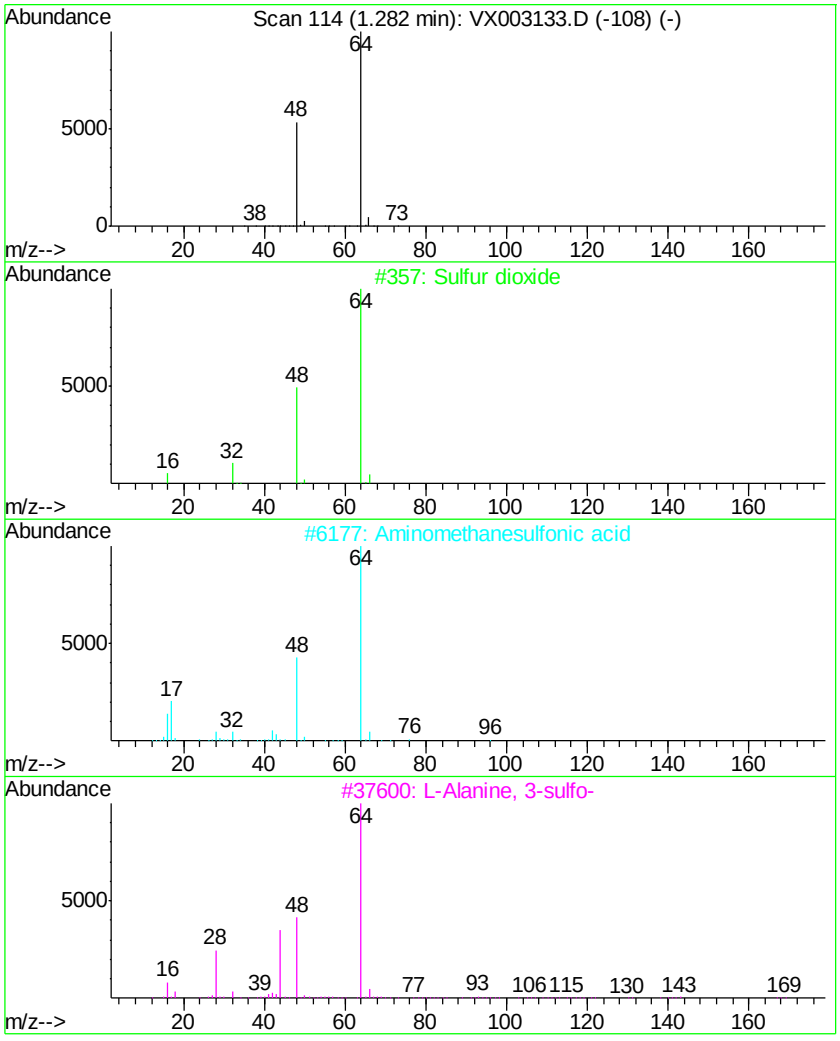
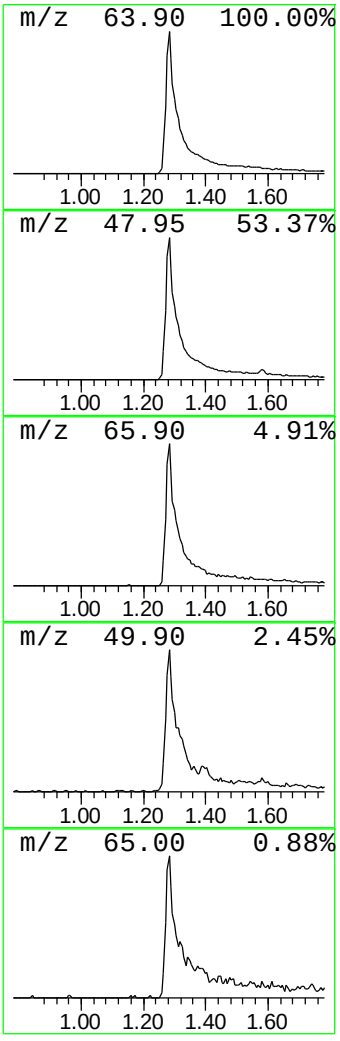
Peak Number 2 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	78.83 ug/l	1310960	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003133.D
Acq On : 02 Jul 2018 17:57
Operator : JC/MD
Sample : J3772-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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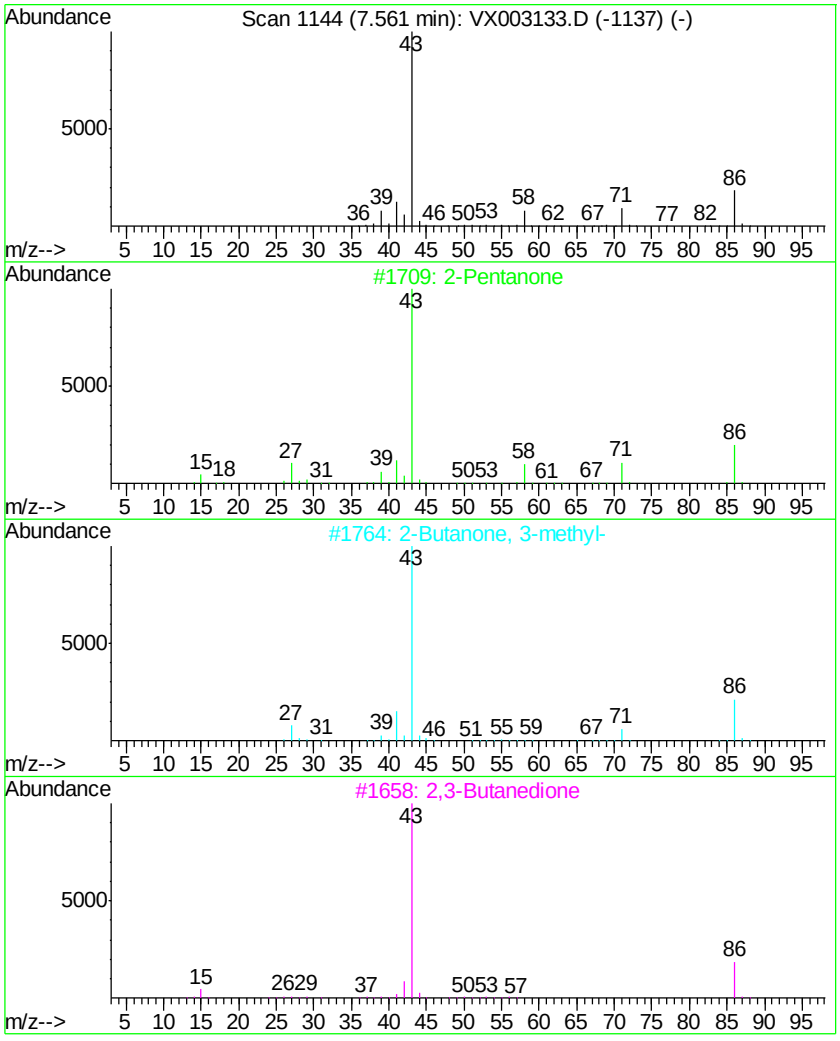
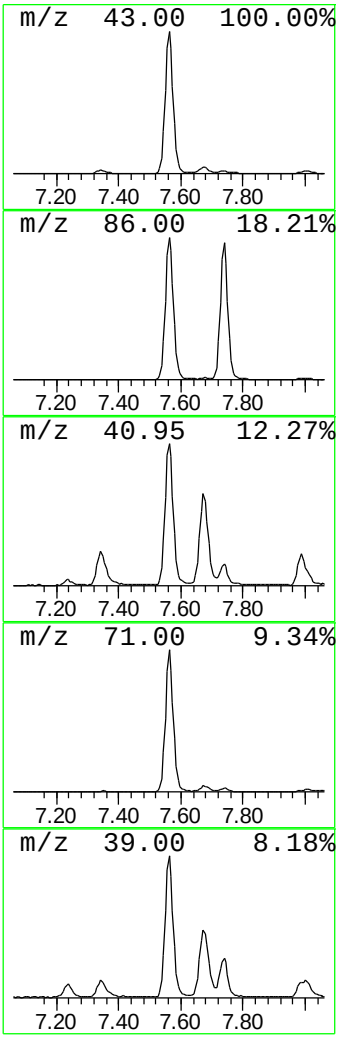
Peak Number 3 2-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	39.17 ug/l	767125	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	90
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
3	2,3-Butanedione	86	C4H6O2	000431-03-8	47
4	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	38
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003133.D
Acq On : 02 Jul 2018 17:57
Operator : JC/MD
Sample : J3772-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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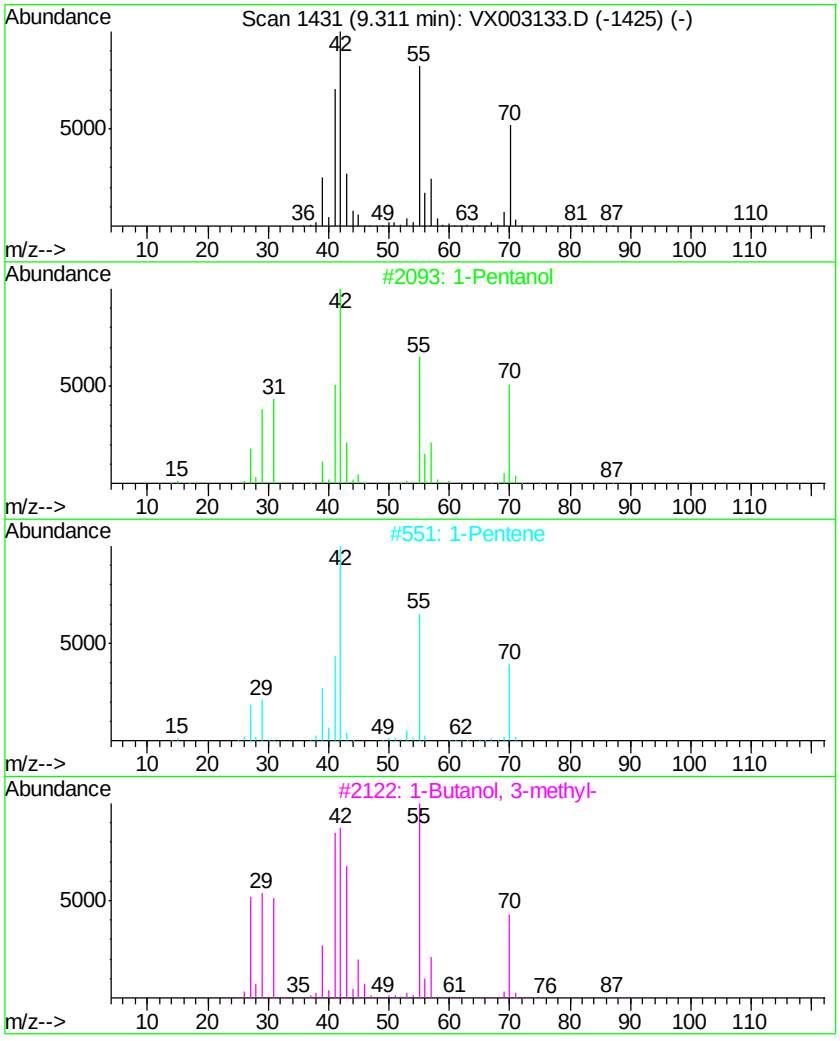
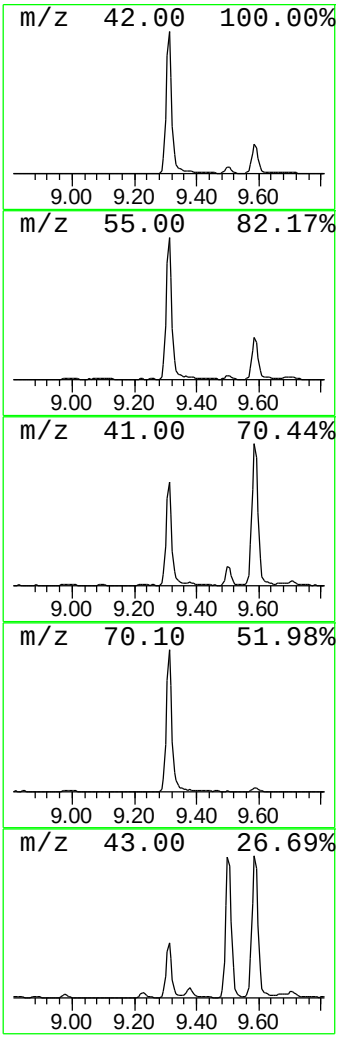
Peak Number 4 1-Pentanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.31	33.91 ug/l	857837	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	90
2	1-Pentene	70	C5H10	000109-67-1	80
3	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	59
4	Carbonochloridic acid, pentyl ester	150	C6H11ClO2	000638-41-5	40
5	Formic acid, pentyl ester	116	C6H12O2	000638-49-3	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003133.D
Acq On : 02 Jul 2018 17:57
Operator : JC/MD
Sample : J3772-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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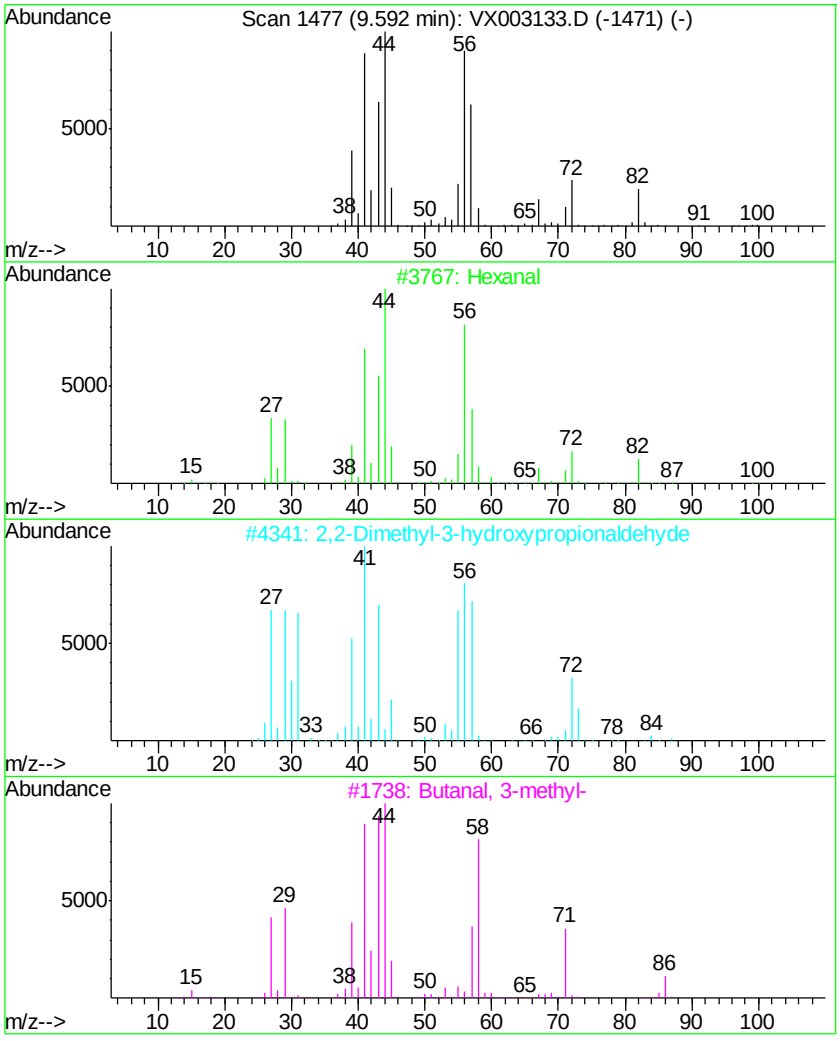
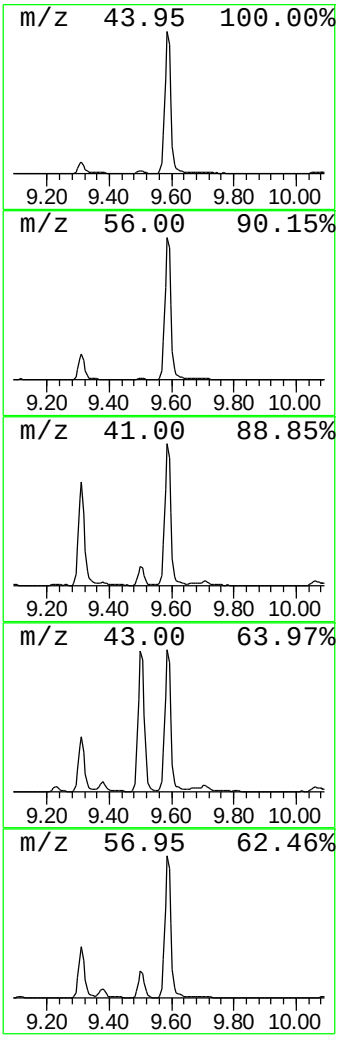
Peak Number 5 Hexanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.59	51.14 ug/l	1293750	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	87
2	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	37
3	Butanal, 3-methyl-	86	C5H10O	000590-86-3	25
4	Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	22
5	Cyclobutane	56	C4H8	000287-23-0	14





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Sample : J3772-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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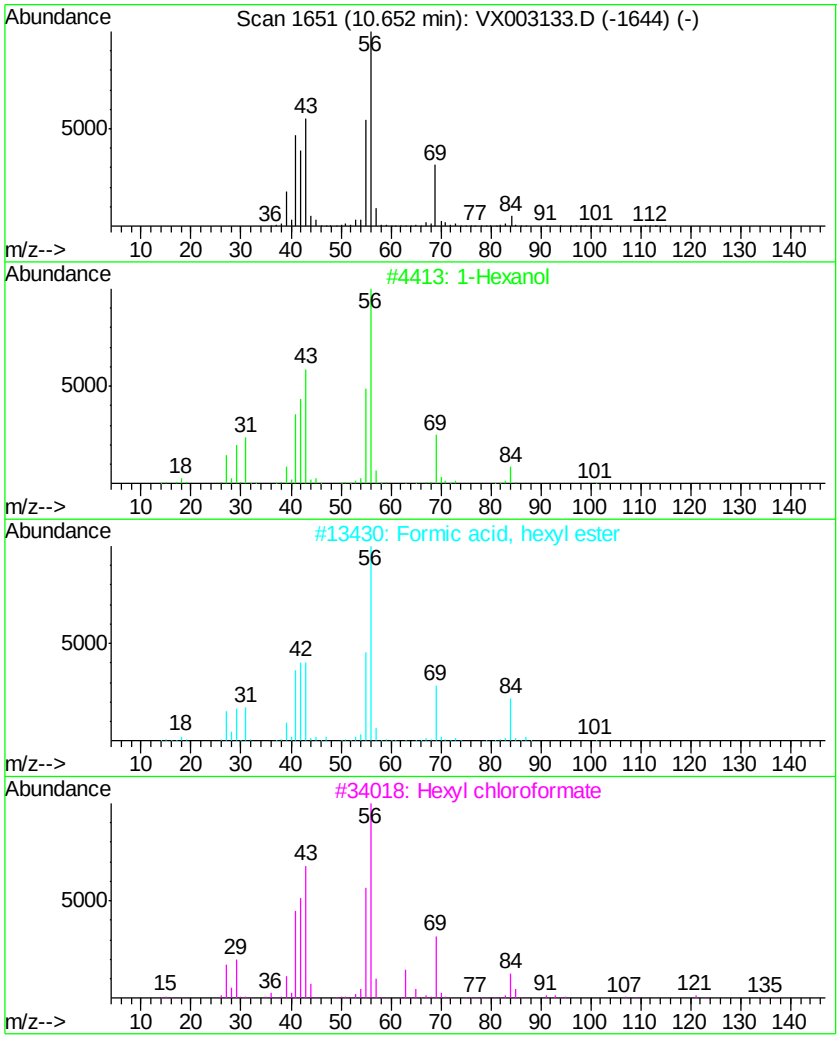
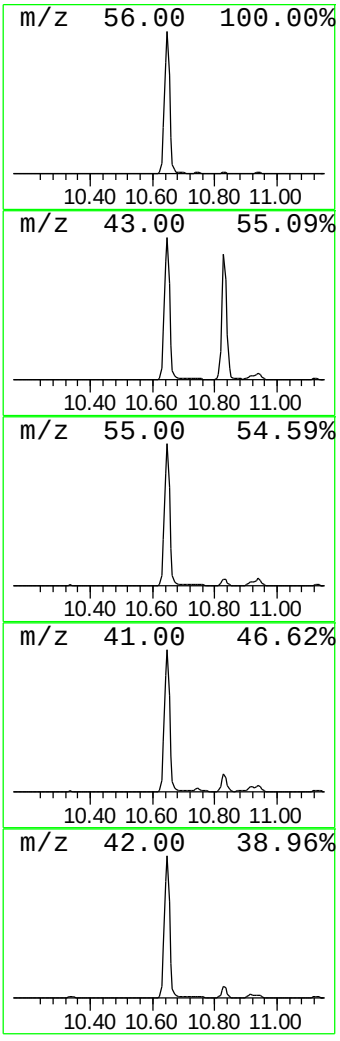
Peak Number 6 1-Hexanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	196.23 ug/l	4964460	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	90
2	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
3	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
4	2H-Pyran-2-one, tetrahydro-5,6-d...	128	C7H12O2	024405-16-1	72
5	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX070218\
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Operator : JC/MD
Sample : J3772-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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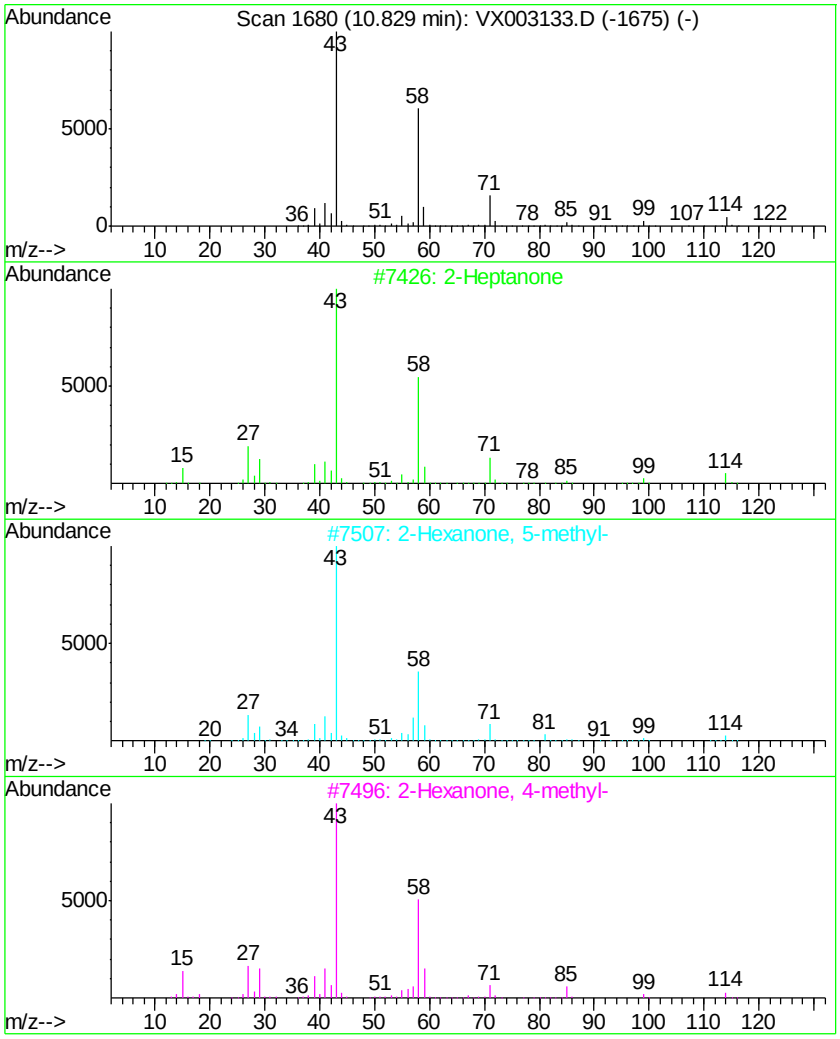
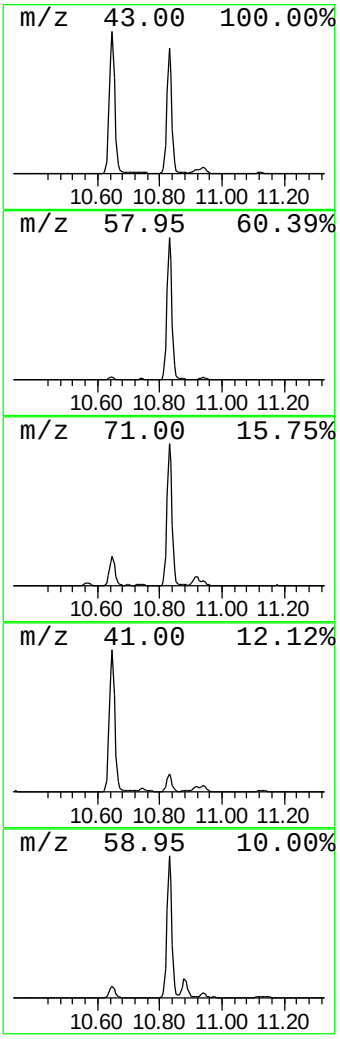
Peak Number 7 2-Heptanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	59.22 ug/l	1498300	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	91
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	90
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	64
4	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	50
5	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	39





Library Search Compound Report

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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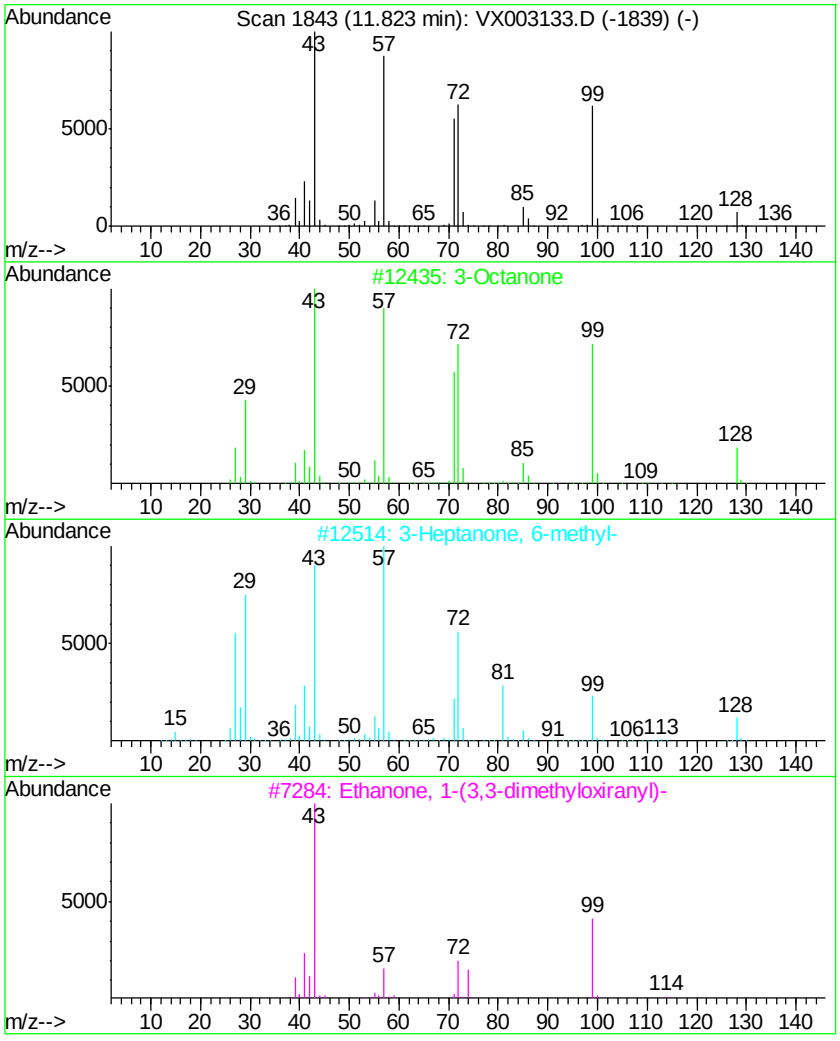
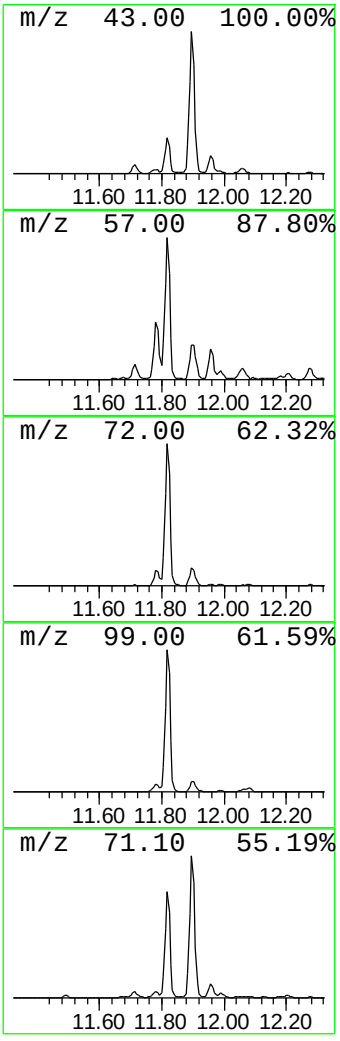
Peak Number 8 3-Octanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	27.88 ug/l	1226340	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone	128	C8H16O	000106-68-3	94
2	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	58
3	Ethanone, 1-(3,3-dimethyloxiranyl)-	114	C6H10O2	004478-63-1	50
4	4-Methylthiazole	99	C4H5NS	000693-95-8	49
5	n-Caproic acid vinyl ester	142	C8H14O2	003050-69-9	47





Library Search Compound Report

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Data File : VX003133.D
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Operator : JC/MD
Sample : J3772-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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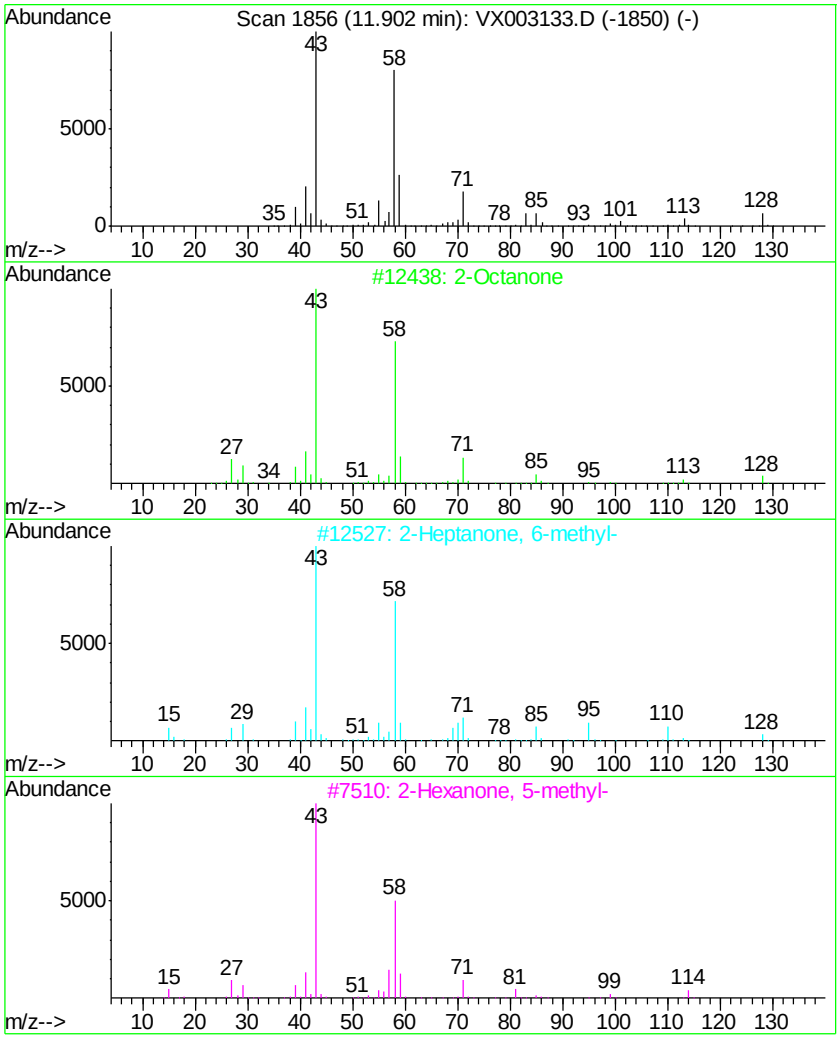
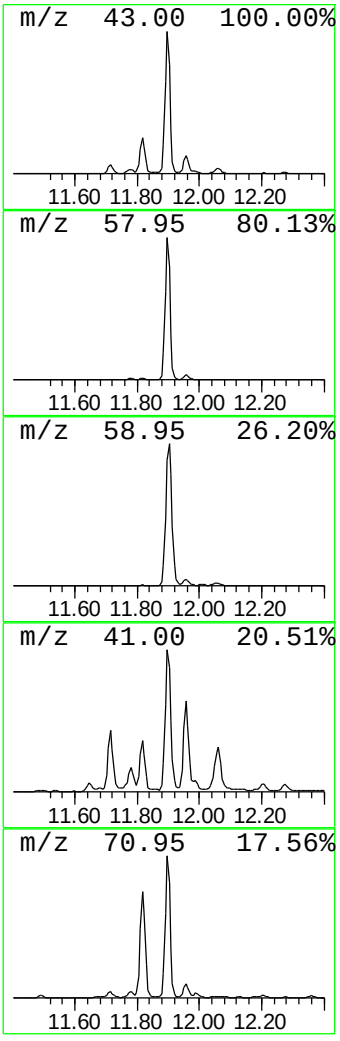
Peak Number 9 2-Octanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	79.47 ug/l	3495480	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	94
2	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	83
3	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78
4	2-Nonanone	142	C9H18O	000821-55-6	72
5	2-Heptanone	114	C7H14O	000110-43-0	56





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003133.D
Acq On : 02 Jul 2018 17:57
Operator : JC/MD
Sample : J3772-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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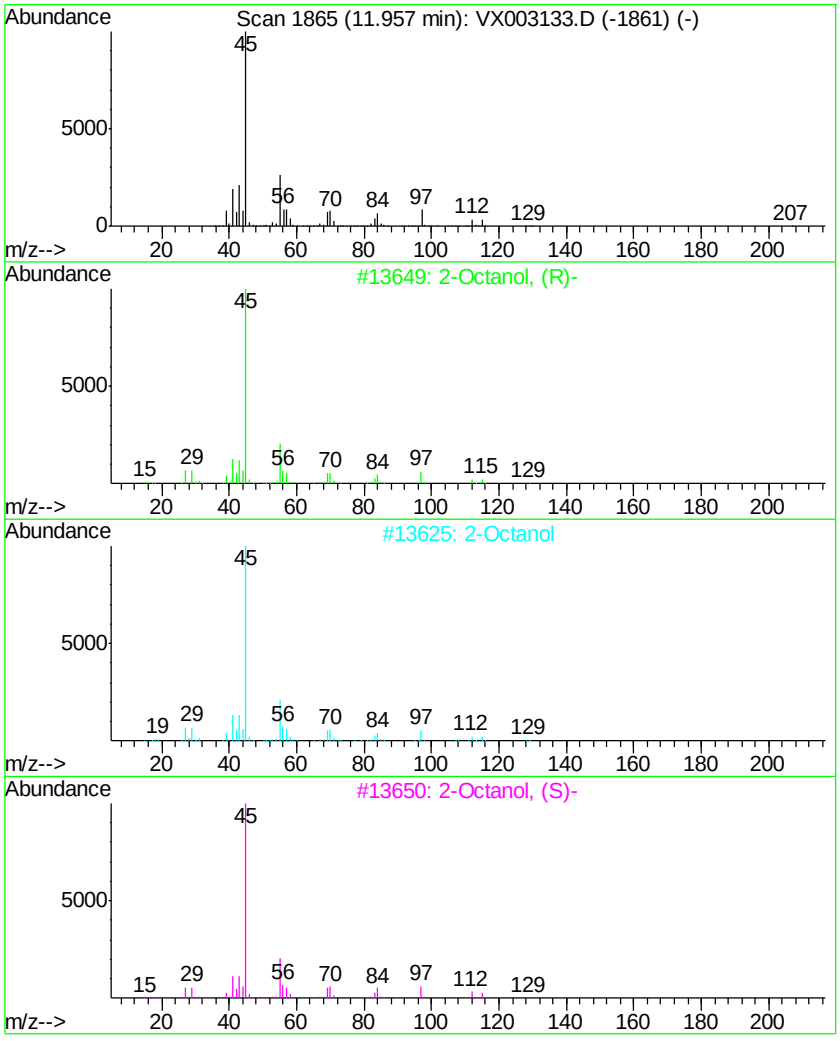
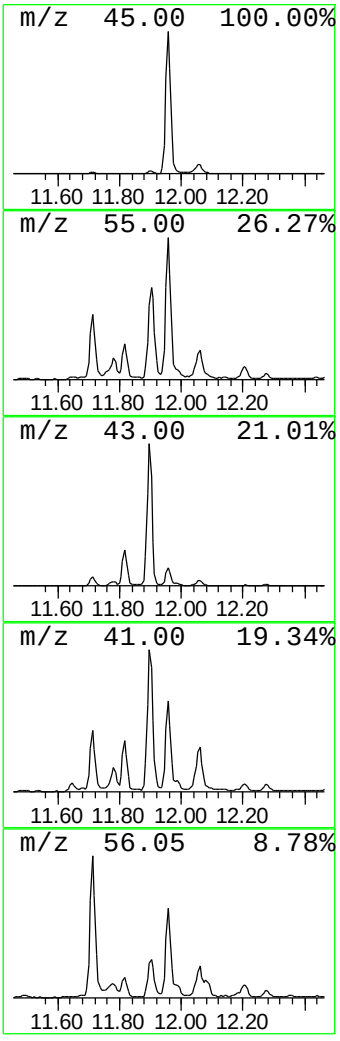
Peak Number 10 2-Octanol, (R)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	36.85 ug/l	1620780	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanol, (R)-	130	C8H18O	005978-70-1	86
2	2-Octanol	130	C8H18O	000123-96-6	86
3	2-Octanol, (S)-	130	C8H18O	006169-06-8	86
4	2-Heptanol, 6-methyl-	130	C8H18O	004730-22-7	78
5	2-Decanol	158	C10H22O	001120-06-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX070218\
Data File : VX003133.D
Acq On : 02 Jul 2018 17:57
Operator : JC/MD
Sample : J3772-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02-9001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
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
Sulfur dioxide	1.28	78.8	ug/l	1310960	1	5.67	831462	50.0
2-Pentanone	7.56	39.2	ug/l	767125	2	6.87	979112	50.0
1-Pentanol	9.31	33.9	ug/l	857837	3	10.12	1264970	50.0
Hexanal	9.59	51.1	ug/l	1293750	3	10.12	1264970	50.0
1-Hexanol	10.65	196.2	ug/l	4964460	3	10.12	1264970	50.0
2-Heptanone	10.83	59.2	ug/l	1498300	3	10.12	1264970	50.0
3-Octanone	11.82	27.9	ug/l	1226340	4	12.09	2199230	50.0
2-Octanone	11.90	79.5	ug/l	3495480	4	12.09	2199230	50.0
2-Octanol, (R)-	11.96	36.9	ug/l	1620780	4	12.09	2199230	50.0