LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003132.D
Acq On : 02 Jul 2018 17:30
Operator : JC/MD
Sample : J3772-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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	91	rBV	1187329	1573018	32.44%	4.141%
2	1.282	108	114	129	rBV	534892	1192872	24.60%	3.141%
3	1.398	131	133	142	rVV	76327	149718	3.09%	0.394%
4	1.489	144	148	159	rVB	49084	87288	1.80%	0.230%
5	1.995	227	231	244	rVB	178267	263969	5.44%	0.695%
6	2.123	246	252	260	rVB	31333	50828	1.05%	0.134%
7	2.209	260	266	273	rVB	36148	57822	1.19%	0.152%
8	2.355	285	290	297	rVB	46377	73276	1.51%	0.193%
9	2.446	300	305	309	rBV	85684	147665	3.05%	0.389%
10	2.623	329	334	341	rBV	79909	136992	2.83%	0.361%
11	4.361	609	619	630	rBV2	26702	74206	1.53%	0.195%
12	4.720	669	678	691	rVB	58745	168609	3.48%	0.444%
13	5.214	749	759	772	rBV	51598	158661	3.27%	0.418%
14	5.507	797	807	823	rBV2	173089	497060	10.25%	1.309%
15	5.665	823	833	850	rVB	258178	721844	14.89%	1.900%
16	6.074	889	900	909	rBV	177584	464263	9.58%	1.222%
17	6.482	958	967	975	rBV2	20100	52716	1.09%	0.139%
18	6.866	1020	1030	1041	rBV	369527	845043	17.43%	2.225%
19	7.226	1080	1089	1101	rVB4	37186	107085	2.21%	0.282%
20	7.342	1101	1108	1125	rBV2	32704	75683	1.56%	0.199%
21	7.561	1137	1144	1155	rBV	407006	756427	15.60%	1.991%
22	7.671	1155	1162	1168	rVV	247328	477099	9.84%	1.256%
23	7.738	1168	1173	1193	rVB	281542	515917	10.64%	1.358%
24	7.988	1208	1214	1230	rBV2	57126	156861	3.24%	0.413%
25	8.720	1327	1334	1342	rBV	889270	1358553	28.02%	3.577%
26	9.098	1388	1396	1411	rVB	31784	70621	1.46%	0.186%
27	9.226	1412	1417	1425	rBV	42556	66759	1.38%	0.176%
28	9.311	1425	1431	1439	rVV	614934	830768	17.13%	2.187%
29	9.378	1439	1442	1454	rVV	31158	64818	1.34%	0.171%
30	9.500	1457	1462	1468	rVV	234038	337184	6.95%	0.888%
31	9.585	1471	1476	1489	rVV	2058045	2905901	59.93%	7.651%
32	9.707	1492	1496	1512	rVB	40184	78203	1.61%	0.206%
33	10.061	1548	1554	1558	rBV	27306	57898	1.19%	0.152%
34	10.116	1558	1563	1583	rVB	789257	1095708	22.60%	2.885%

LSC Area Percent Report

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Sample : J3772-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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	10.542	1629	1633	1642	rVB	37555	55135	1.14%	0.145%
36	10.646	1645	1650	1661	rBV	4106812	4848534	100.00%	12.765%
37	10.744	1661	1666	1675	rVB	106032	172754	3.56%	0.455%
38	10.829	1675	1680	1686	rBV	1256098	1482686	30.58%	3.904%
39	10.914	1691	1694	1696	rVV	266561	349072	7.20%	0.919%
40	10.939	1696	1698	1708	rVB	309712	366611	7.56%	0.965%
41	11.140	1720	1731	1741	rBV	839640	1129569	23.30%	2.974%
42	11.646	1809	1814	1817	rBV	237125	288170	5.94%	0.759%
43	11.676	1817	1819	1822	rVV	83282	103208	2.13%	0.272%
44	11.713	1822	1825	1830	rVV	577312	686028	14.15%	1.806%
45	11.780	1830	1836	1839	rVV	364256	539612	11.13%	1.421%
46	11.817	1839	1842	1847	rVV	1146577	1285515	26.51%	3.384%
47	11.896	1851	1855	1861	rVV2	2719877	3594245	74.13%	9.463%
48	11.957	1861	1865	1869	rVV	1553388	1823604	37.61%	4.801%
49	11.987	1869	1870	1876	rVV2	177043	165367	3.41%	0.435%
50	12.054	1876	1881	1883	rVV	359988	528964	10.91%	1.393%
51	12.079	1883	1885	1891	rVB	995444	1214293	25.04%	3.197%
52	12.207	1900	1906	1911	rVB	101882	140259	2.89%	0.369%
53	12.274	1913	1917	1923	rVB	61918	82256	1.70%	0.217%
54	12.646	1966	1978	1991	rBV	692306	1168153	24.09%	3.075%
55	12.749	1991	1995	2000	rVV	67520	99846	2.06%	0.263%
56	12.829	2002	2008	2010	rVV	345752	445297	9.18%	1.172%
57	12.853	2010	2012	2015	rVV	251497	291934	6.02%	0.769%
58	12.914	2019	2022	2031	rVB	139569	176738	3.65%	0.465%
59	13.170	2059	2064	2068	rBV	46643	55520	1.15%	0.146%
60	13.219	2068	2072	2080	rBV	61926	90951	1.88%	0.239%
61	13.481	2108	2115	2119	rBV	244050	326408	6.73%	0.859%
62	13.524	2119	2122	2127	rVB	126379	150720	3.11%	0.397%
63	13.664	2140	2145	2155	rVB2	158024	232423	4.79%	0.612%
64	14.322	2248	2253	2260	rBV	82725	108882	2.25%	0.287%
65	15.066	2370	2375	2381	rBV2	40138	55391	1.14%	0.146%
66	15.212	2395	2399	2408	rVB	39987	50915	1.05%	0.134%
67	15.535	2446	2452	2467	rBV	118927	202722	4.18%	0.534%

Sum of corrected areas: 37983117

LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
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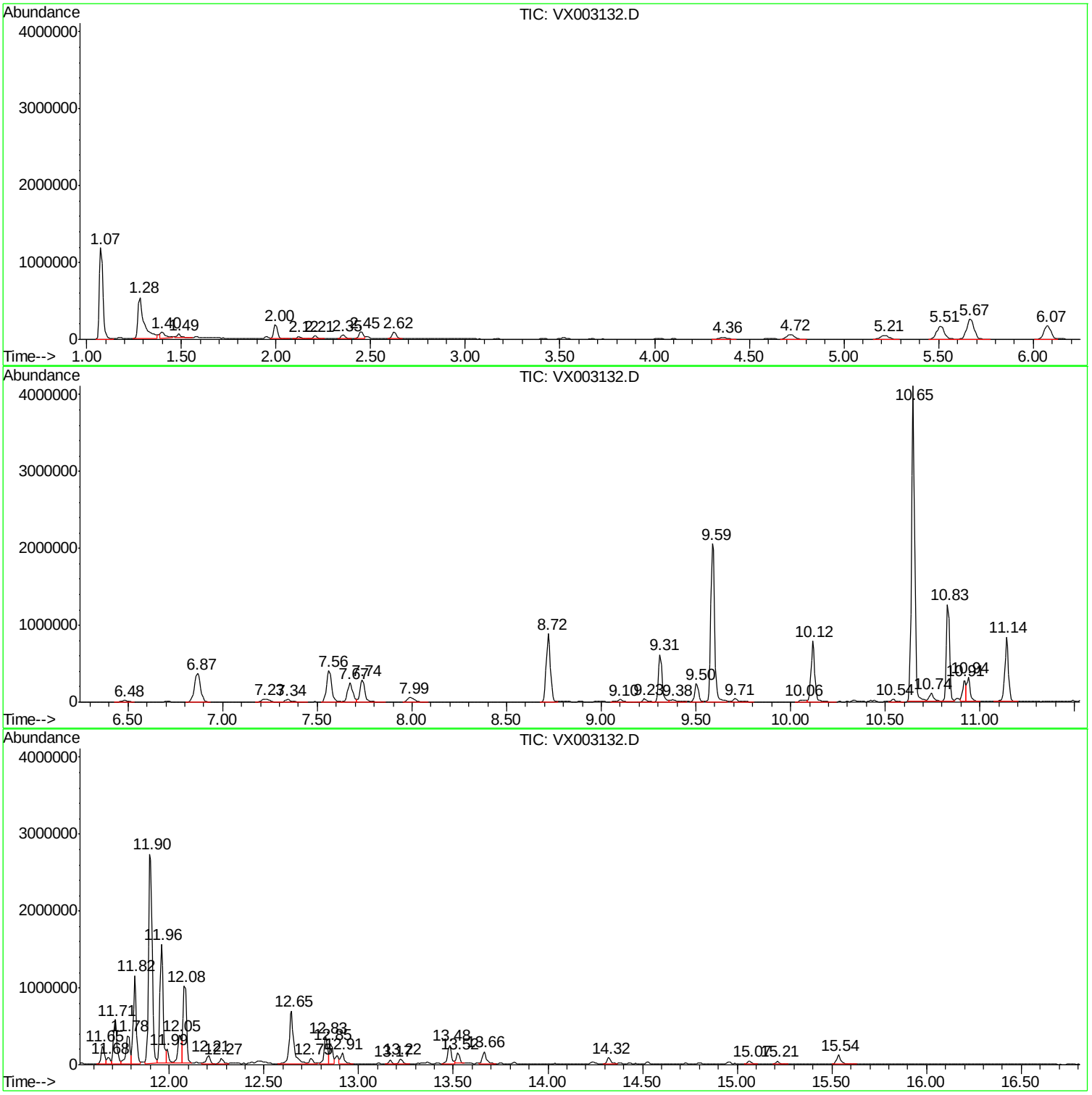
Sample : J3772-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP18-CHY02

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 : VX003132.D
Acq On : 02 Jul 2018 17:30
Operator : JC/MD
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Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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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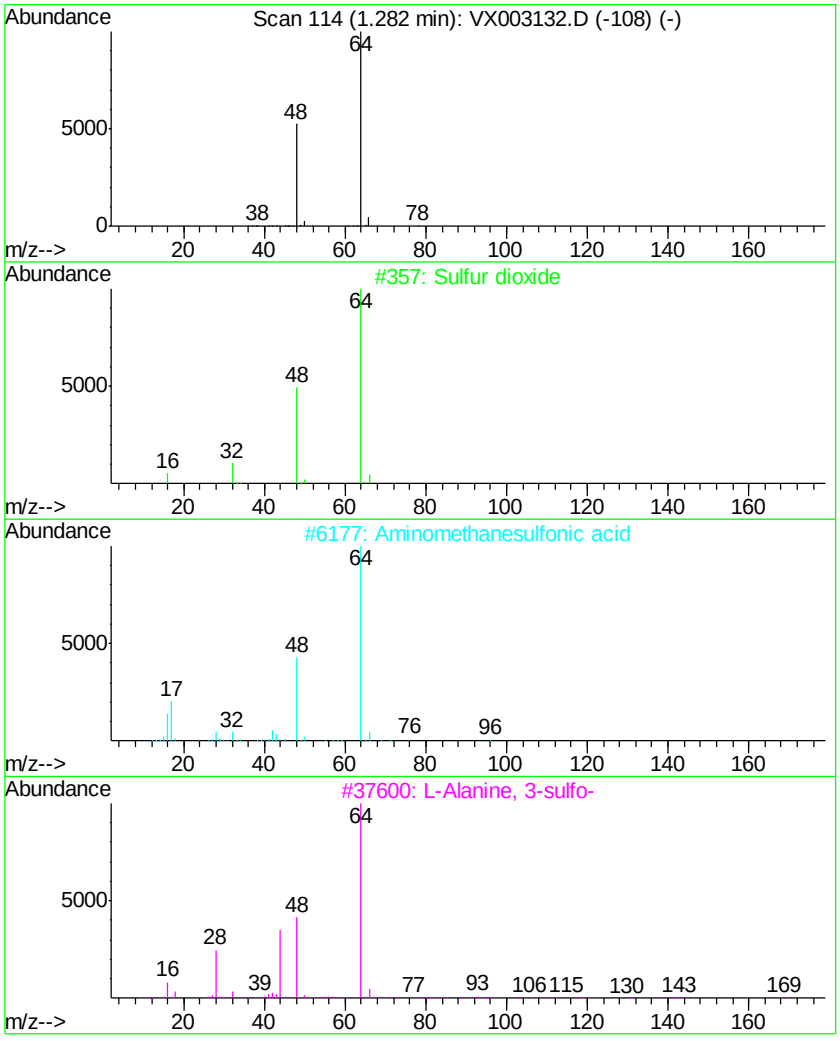
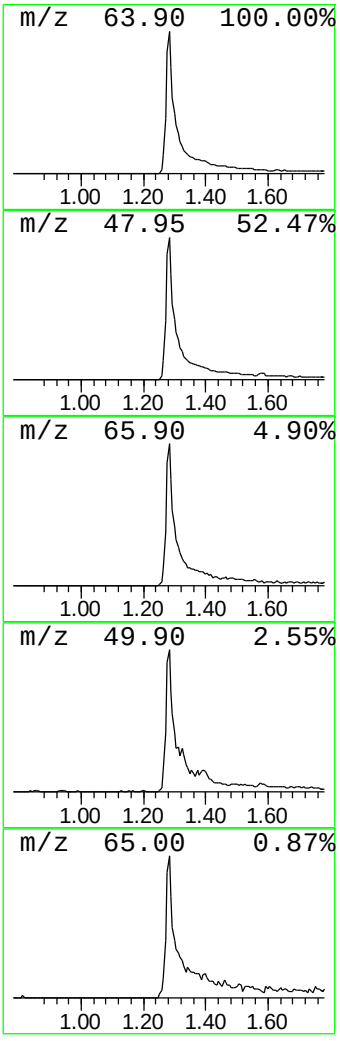
Peak Number 2 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	82.63 ug/l	1192870	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 : VX003132.D
Acq On : 02 Jul 2018 17:30
Operator : JC/MD
Sample : J3772-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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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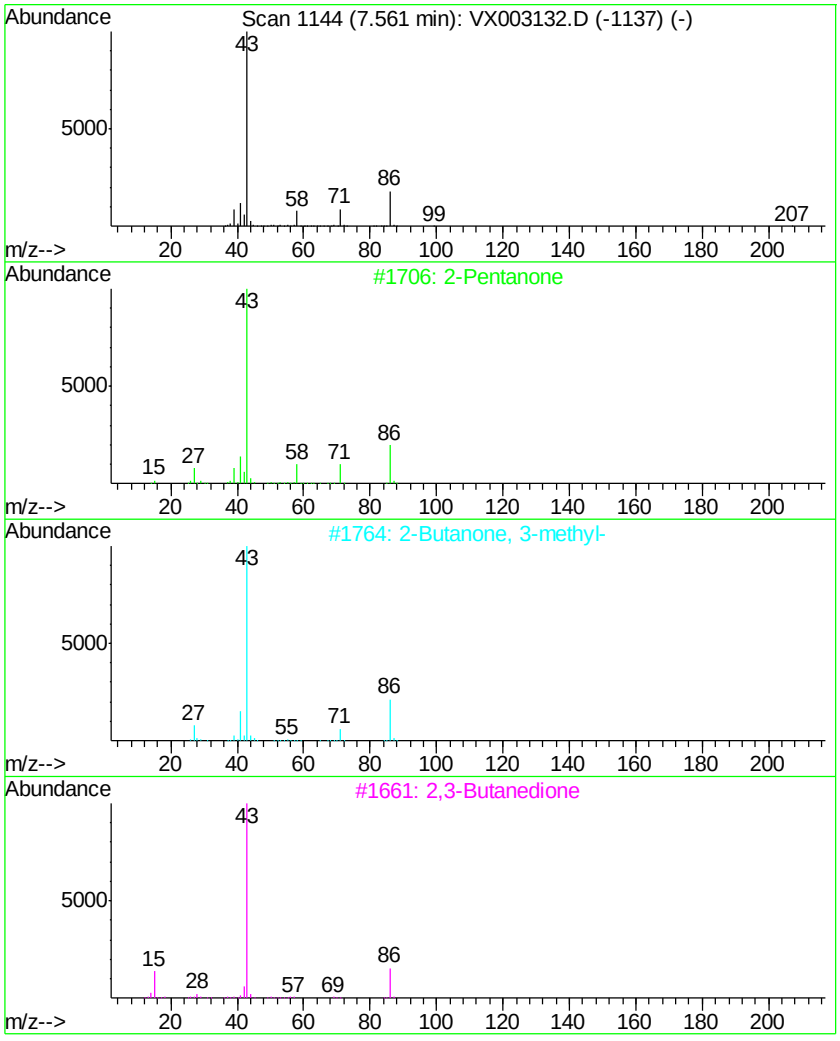
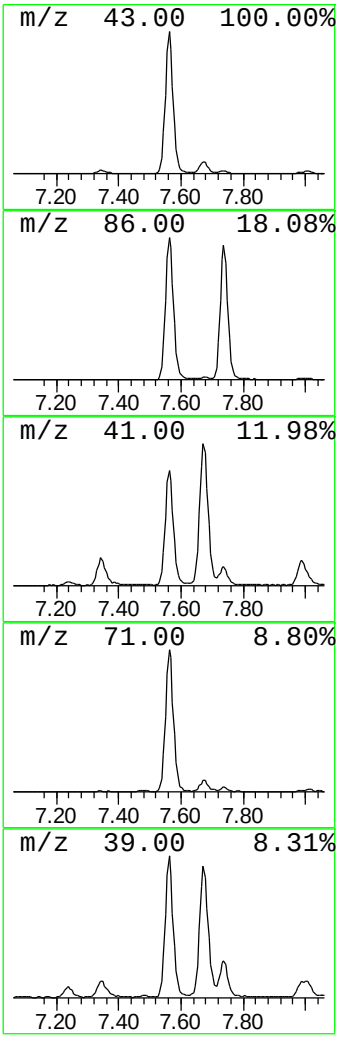
Peak Number 3 2-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	44.76 ug/l	756427	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	91
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
3	2,3-Butanedione	86	C4H6O2	000431-03-8	50
4	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	9
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX070218\
Data File : VX003132.D
Acq On : 02 Jul 2018 17:30
Operator : JC/MD
Sample : J3772-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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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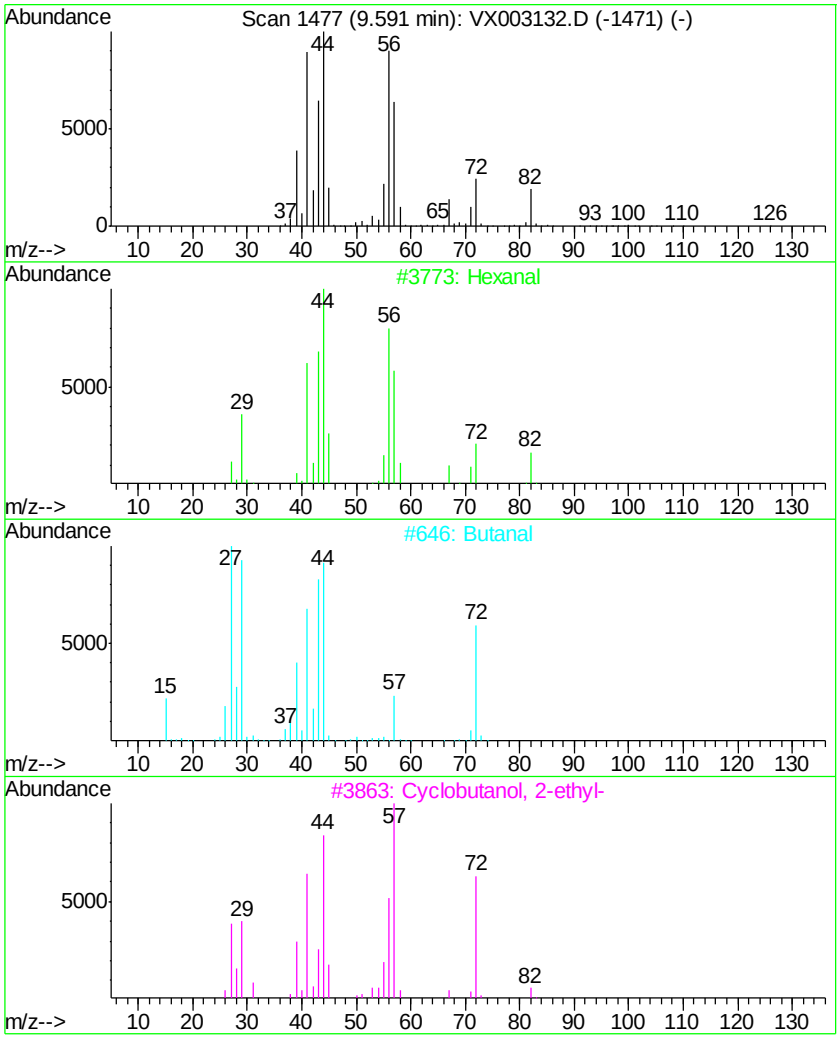
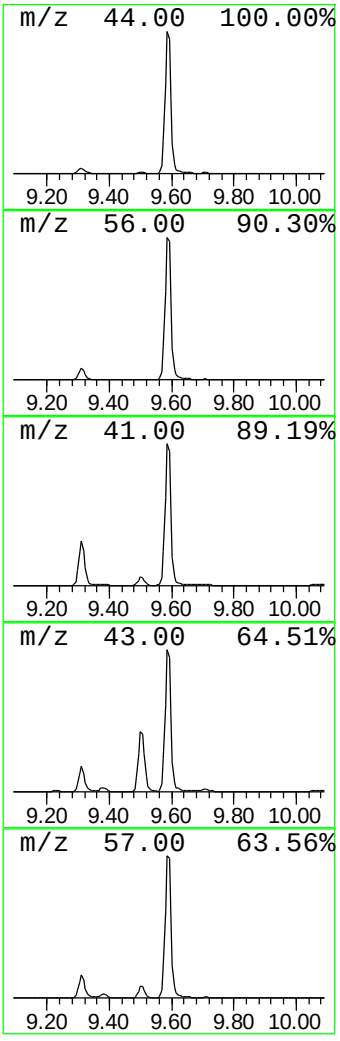
Peak Number 4 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.59	132.60 ug/l	2905900	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	80
2	Butanal	72	C4H8O	000123-72-8	43
3	Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	42
4	Glutaraldehyde	100	C5H8O2	000111-30-8	30
5	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	25





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003132.D
Acq On : 02 Jul 2018 17:30
Operator : JC/MD
Sample : J3772-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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

TIC Library : C:\DATABASE\NIST11.L
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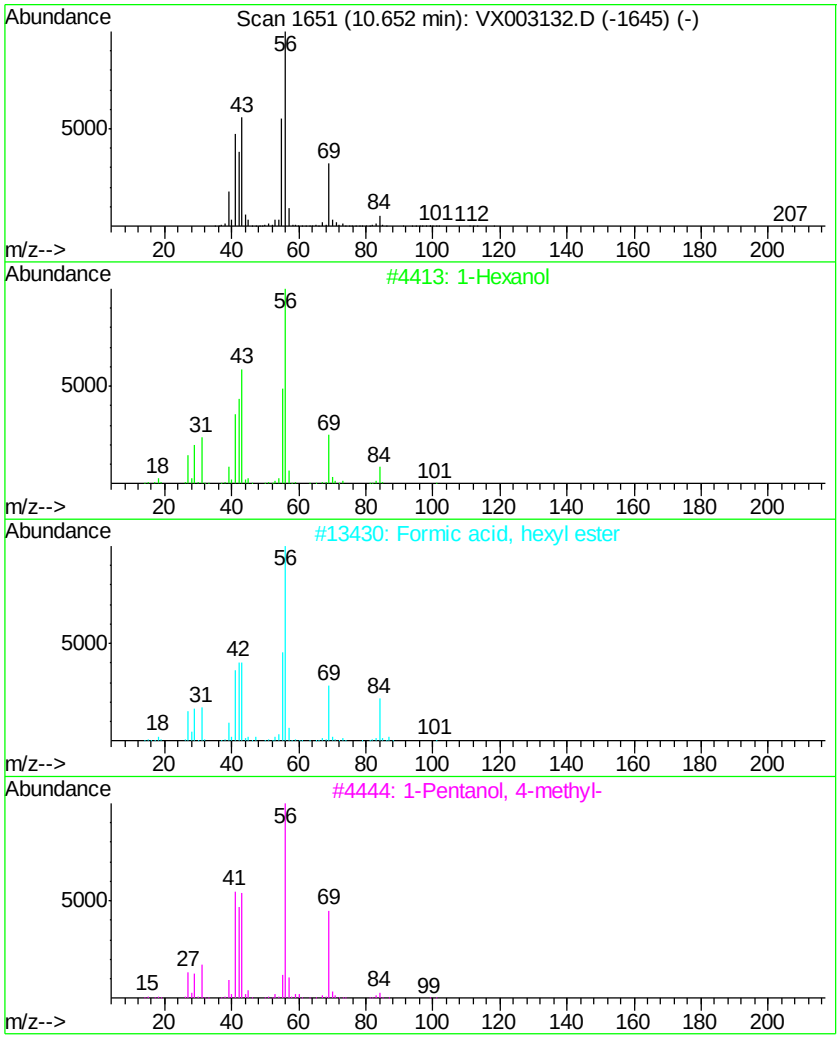
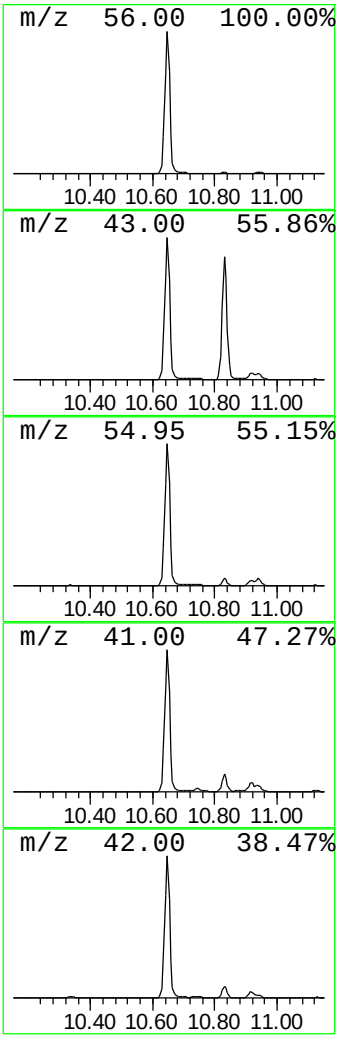
****

Peak Number 5 1-Hexanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	221.25 ug/l	4848530	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	86
2	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	72
3	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	72
4	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	64
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX070218\
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Acq On : 02 Jul 2018 17:30
Operator : JC/MD
Sample : J3772-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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

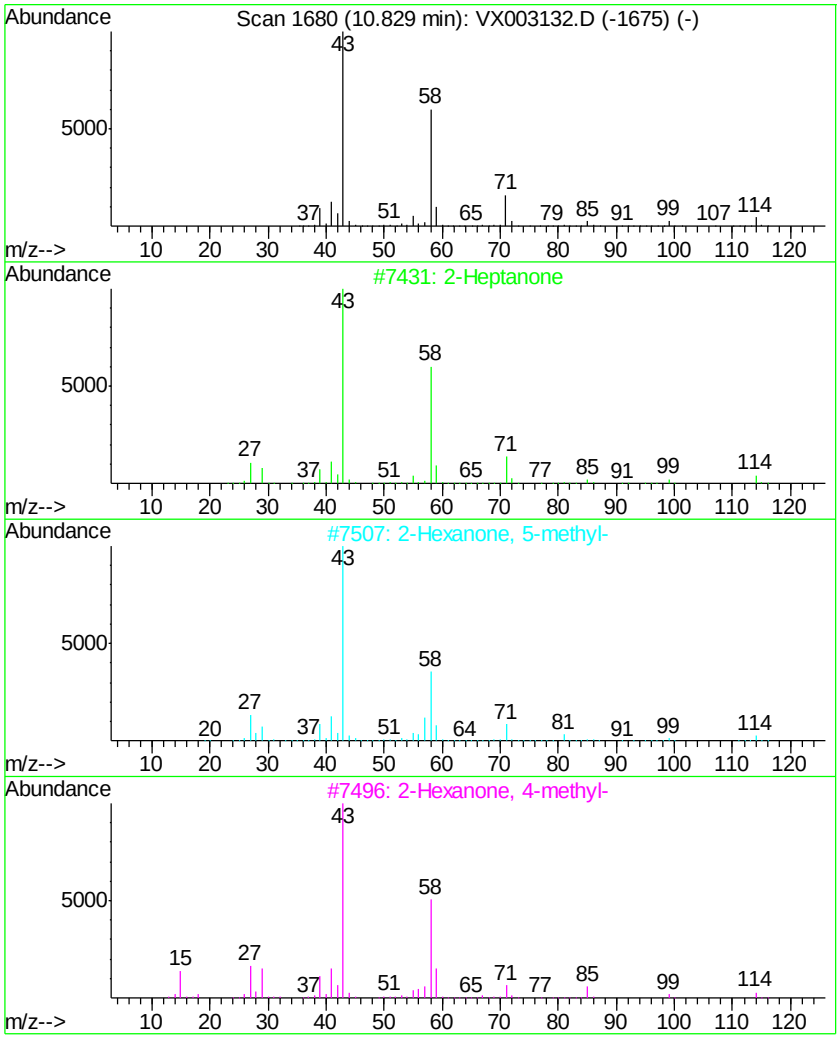
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

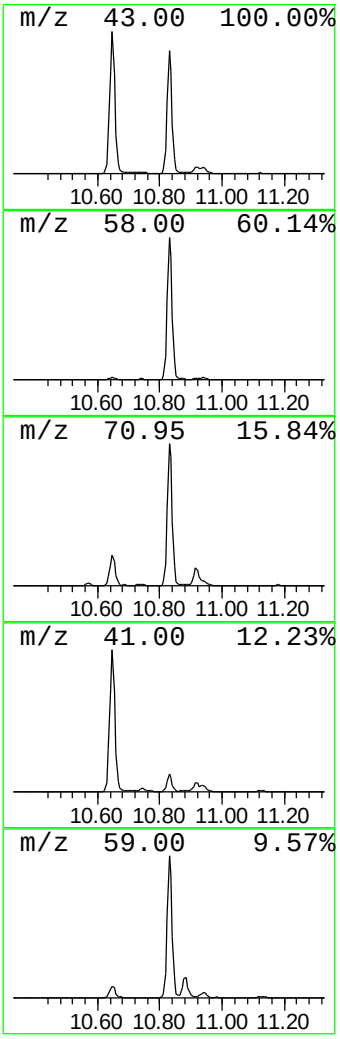
****

Peak Number 6 2-Heptanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	67.66 ug/l	1482690	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	40
5	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	39





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Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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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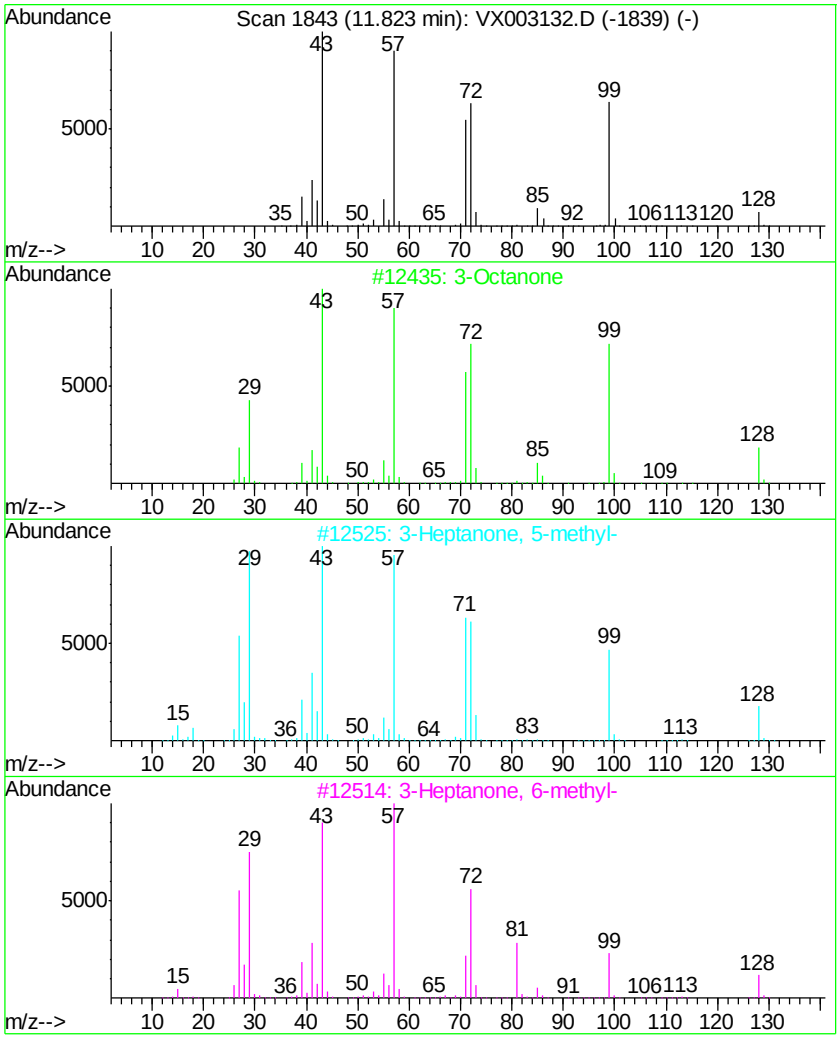
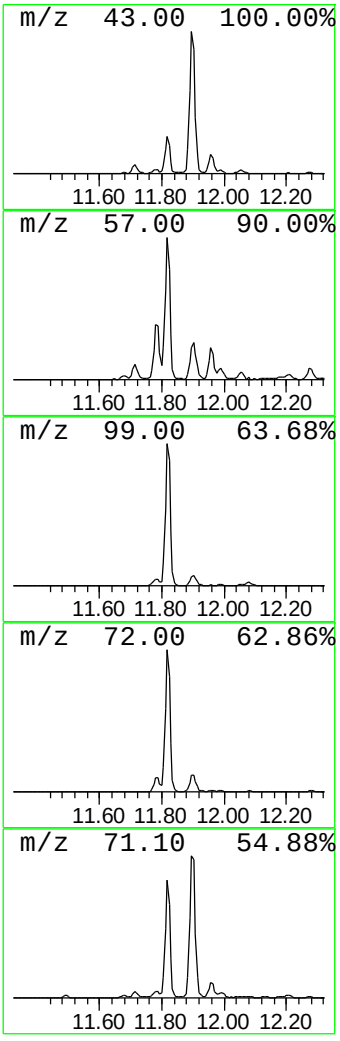
Peak Number 7 3-Octanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	52.93 ug/l	1285520	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone	128	C8H16O	000106-68-3	94
2	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	64
3	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	58
4	Ethanone, 1-(3,3-dimethyloxiranyl)-	114	C6H10O2	004478-63-1	50
5	4-Methylthiazole	99	C4H5NS	000693-95-8	49





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003132.D
Acq On : 02 Jul 2018 17:30
Operator : JC/MD
Sample : J3772-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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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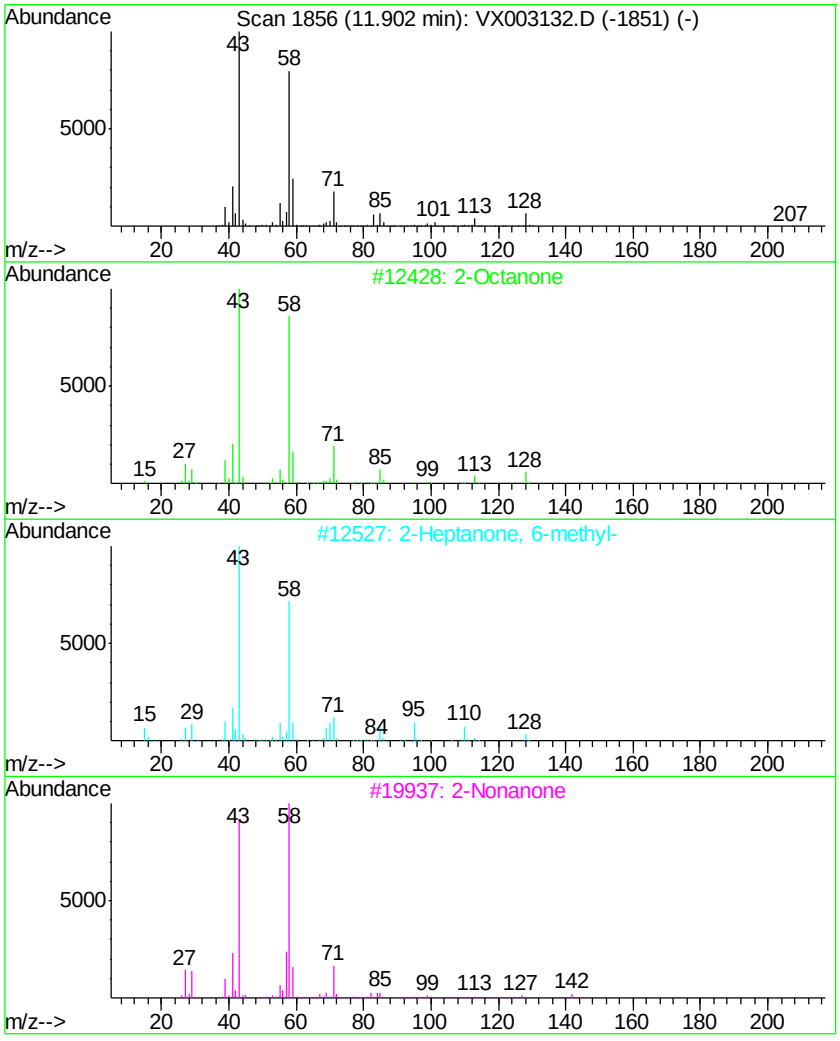
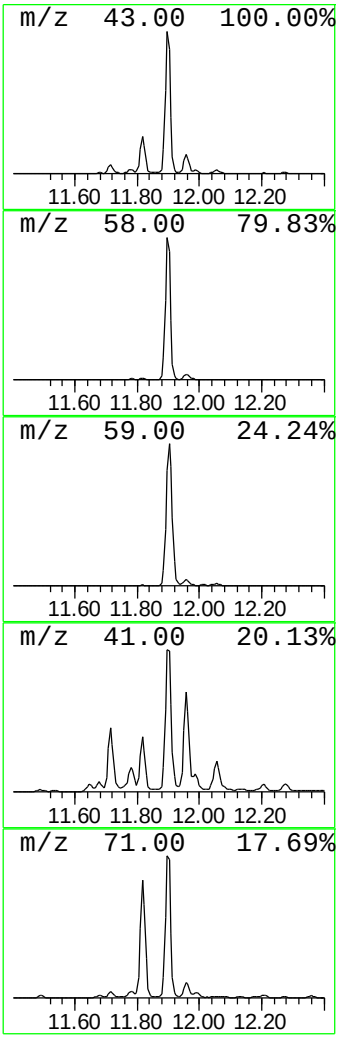
Peak Number 8 2-Octanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	148.00 ug/l	3594250	1,4-Dichlorobenzene-d4	12.08

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	74
3	2-Nonanone	142	C9H18O	000821-55-6	72
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64
5	2-Hexanone	100	C6H12O	000591-78-6	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX070218\
Data File : VX003132.D
Acq On : 02 Jul 2018 17:30
Operator : JC/MD
Sample : J3772-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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

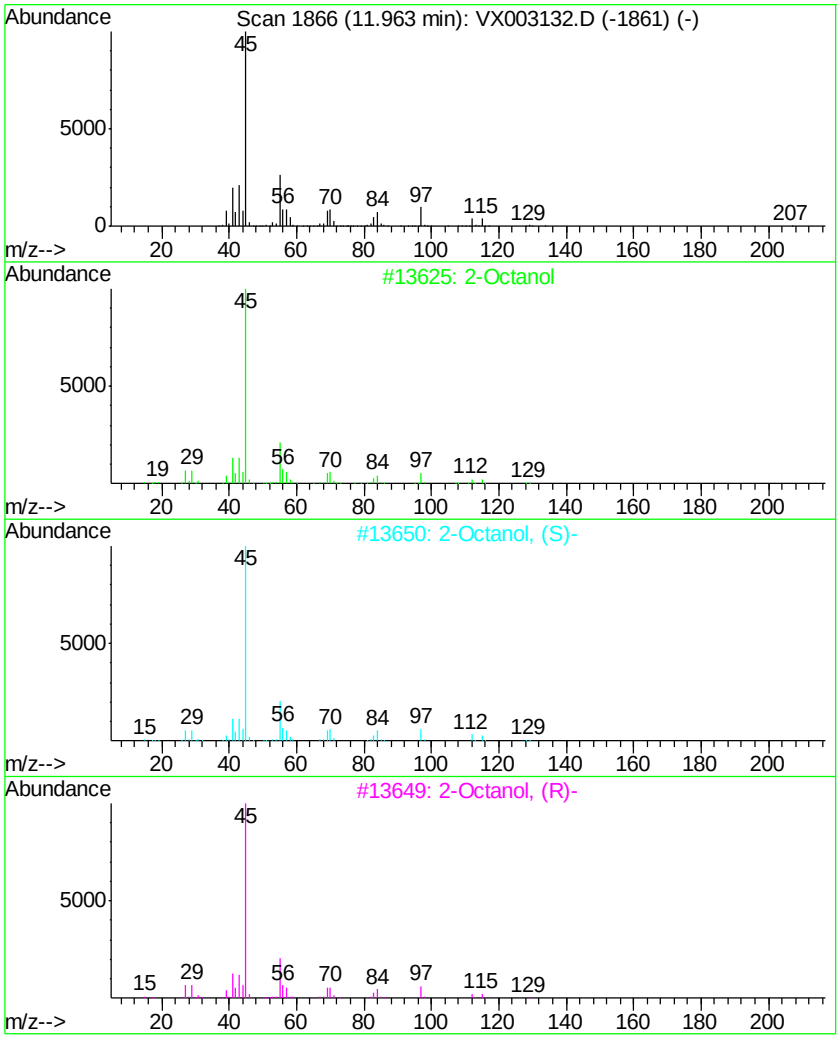
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

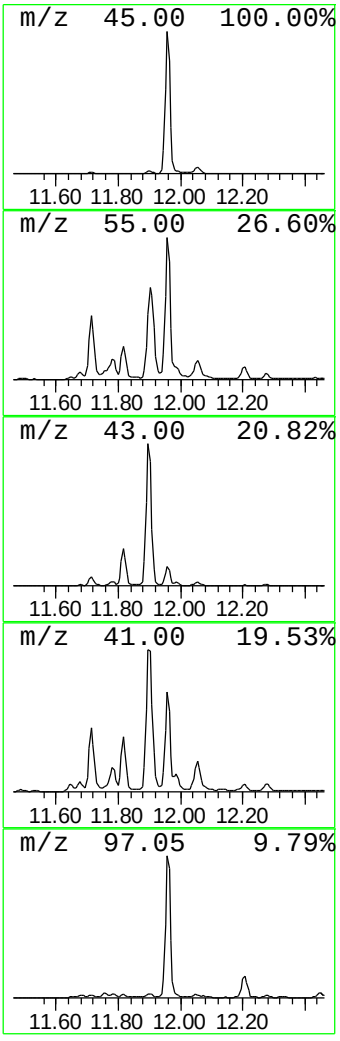
****

Peak Number 9 2-Octanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	75.09 ug/l	1823600	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanol	130	C8H18O	000123-96-6	86
2	2-Octanol, (S)-	130	C8H18O	006169-06-8	86
3	2-Octanol, (R)-	130	C8H18O	005978-70-1	86
4	2-Decanol	158	C10H22O	001120-06-5	72
5	2-Hexanol, 5-methyl-	116	C7H16O	000627-59-8	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003132.D
Acq On : 02 Jul 2018 17:30
Operator : JC/MD
Sample : J3772-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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

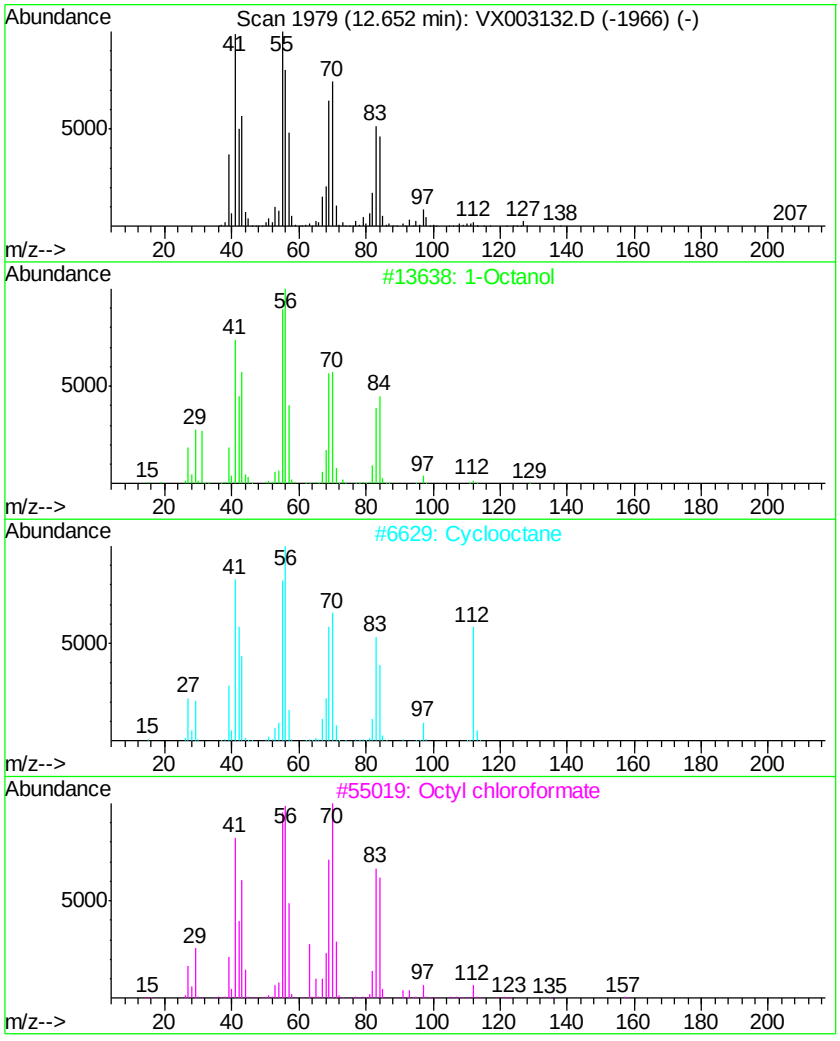
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

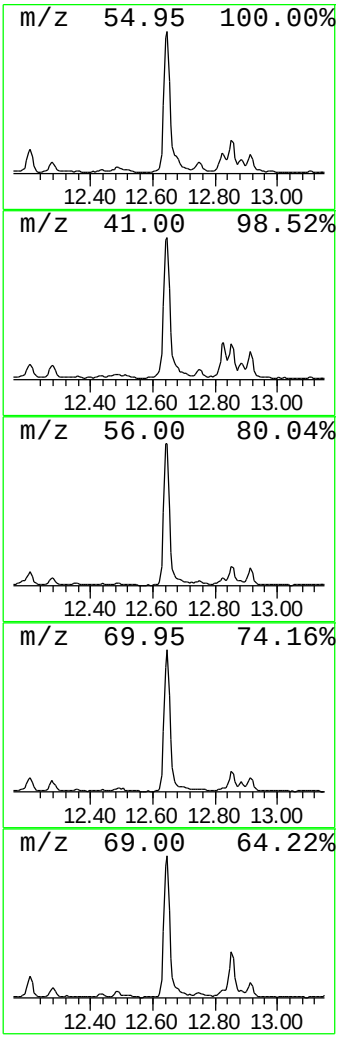
****

Peak Number 10 1-Octanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	48.10 ug/l	1168150	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol	130	C8H18O	000111-87-5	91
2	Cyclooctane	112	C8H16	000292-64-8	90
3	Octyl chloroformate	192	C9H17ClO2	007452-59-7	90
4	Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
5	1-Nonanol	144	C9H20O	000143-08-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX070218\
Data File : VX003132.D
Acq On : 02 Jul 2018 17:30
Operator : JC/MD
Sample : J3772-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP18-CHY02

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	82.6	ug/l	1192870	1	5.67	721844	50.0
2-Pentanone	7.56	44.8	ug/l	756427	2	6.87	845043	50.0
Hexanal	9.59	132.6	ug/l	2905900	3	10.12	1095710	50.0
1-Hexanol	10.65	221.3	ug/l	4848530	3	10.12	1095710	50.0
2-Heptanone	10.83	67.7	ug/l	1482690	3	10.12	1095710	50.0
3-Octanone	11.82	52.9	ug/l	1285520	4	12.08	1214290	50.0
2-Octanone	11.90	148.0	ug/l	3594250	4	12.08	1214290	50.0
2-Octanol	11.96	75.1	ug/l	1823600	4	12.08	1214290	50.0
1-Octanol	12.65	48.1	ug/l	1168150	4	12.08	1214290	50.0