

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
 Data File : VX003134.D
 Acq On : 02 Jul 2018 18:24
 Operator : JC/MD
 Sample : J3772-08
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SP18-CHY05

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	94	rBV	1042076	1400575	44.05%	5.370%
2	1.270	108	112	119	rBV	149271	197568	6.21%	0.758%
3	1.404	129	134	142	rVB4	51661	76198	2.40%	0.292%
4	1.995	227	231	245	rVB	147569	222125	6.99%	0.852%
5	2.355	285	290	298	rVB	31038	50901	1.60%	0.195%
6	2.452	300	306	309	rVV	47058	80679	2.54%	0.309%
7	2.483	309	311	322	rVB	25936	40501	1.27%	0.155%
8	2.623	329	334	343	rVB	39155	71232	2.24%	0.273%
9	4.361	610	619	632	rBV2	17998	50795	1.60%	0.195%
10	4.604	647	659	669	rBV2	68827	199939	6.29%	0.767%
11	4.726	671	679	686	rVB2	15795	45755	1.44%	0.175%
12	5.220	746	760	767	rBV	11174	35880	1.13%	0.138%
13	5.507	796	807	819	rBV	168602	483403	15.20%	1.853%
14	5.665	823	833	847	rVB	251935	709948	22.33%	2.722%
15	6.074	889	900	909	rBV	175813	459761	14.46%	1.763%
16	6.866	1020	1030	1041	rBV	360491	838473	26.37%	3.215%
17	7.220	1079	1088	1101	rBV2	45661	116039	3.65%	0.445%
18	7.561	1137	1144	1155	rBV	111466	218842	6.88%	0.839%
19	7.671	1155	1162	1168	rVV	147084	278860	8.77%	1.069%
20	7.738	1168	1173	1181	rVB	117343	208724	6.56%	0.800%
21	7.988	1206	1214	1224	rBV3	48286	122245	3.84%	0.469%
22	8.719	1327	1334	1341	rBV	880243	1348622	42.42%	5.171%
23	9.225	1412	1417	1425	rBV	48976	72728	2.29%	0.279%
24	9.311	1426	1431	1438	rBV	75461	109765	3.45%	0.421%
25	9.500	1457	1462	1469	rBV	104279	146758	4.62%	0.563%
26	9.585	1470	1476	1489	rVV	1489463	2097577	65.97%	8.042%
27	9.707	1492	1496	1511	rVB	30026	57367	1.80%	0.220%
28	10.116	1557	1563	1580	rVB	760888	1054757	33.17%	4.044%
29	10.542	1630	1633	1643	rVB	23907	34972	1.10%	0.134%
30	10.640	1644	1649	1662	rBV	425541	580290	18.25%	2.225%
31	10.743	1662	1666	1675	rVV	58829	83054	2.61%	0.318%
32	10.829	1675	1680	1686	rVV	643884	765428	24.07%	2.935%
33	10.914	1690	1694	1696	rVV	161725	230310	7.24%	0.883%
34	10.939	1696	1698	1707	rVB	267688	305145	9.60%	1.170%

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35	11.140	1721	1731	1742	rBV	833149	1084314	34.10%	4.157%
36	11.646	1807	1814	1817	rBV	118219	145247	4.57%	0.557%
37	11.676	1817	1819	1822	rVV2	50122	60778	1.91%	0.233%
38	11.713	1822	1825	1830	rVV	159988	196923	6.19%	0.755%
39	11.780	1830	1836	1839	rVV3	88813	160102	5.04%	0.614%
40	11.816	1839	1842	1850	rVV	670951	778403	24.48%	2.985%
41	11.896	1850	1855	1861	rVV	2489233	3179537	100.00%	12.191%
42	11.957	1861	1865	1876	rVV	2060643	2511546	78.99%	9.630%
43	12.048	1876	1880	1882	rVV	224229	299747	9.43%	1.149%
44	12.079	1882	1885	1892	rVB	996578	1268931	39.91%	4.865%
45	12.207	1900	1906	1912	rVV	99292	131632	4.14%	0.505%
46	12.274	1913	1917	1924	rVB	32356	42066	1.32%	0.161%
47	12.646	1966	1978	1990	rBV2	367669	643831	20.25%	2.469%
48	12.749	1990	1995	1999	rVV	55304	72683	2.29%	0.279%
49	12.829	2002	2008	2010	rVV	360651	485831	15.28%	1.863%
50	12.853	2010	2012	2015	rVV	334269	371399	11.68%	1.424%
51	12.889	2015	2018	2020	rVV	171485	223920	7.04%	0.859%
52	12.914	2020	2022	2031	rVB	109569	128712	4.05%	0.494%
53	13.219	2068	2072	2080	rBV	75271	103230	3.25%	0.396%
54	13.481	2108	2115	2119	rBV	201271	273857	8.61%	1.050%
55	13.524	2119	2122	2126	rVB	67607	80278	2.52%	0.308%
56	13.664	2140	2145	2155	rVB2	257829	358079	11.26%	1.373%
57	14.237	2234	2239	2246	rBV3	33602	69235	2.18%	0.265%
58	14.316	2248	2252	2259	rBV	95646	126870	3.99%	0.486%
59	14.395	2260	2265	2268	rBV2	53864	65345	2.06%	0.251%
60	14.956	2352	2357	2361	rBV	24930	37381	1.18%	0.143%
61	15.066	2369	2375	2387	rVB2	45246	69463	2.18%	0.266%
62	15.535	2445	2452	2465	rBV	193734	316621	9.96%	1.214%

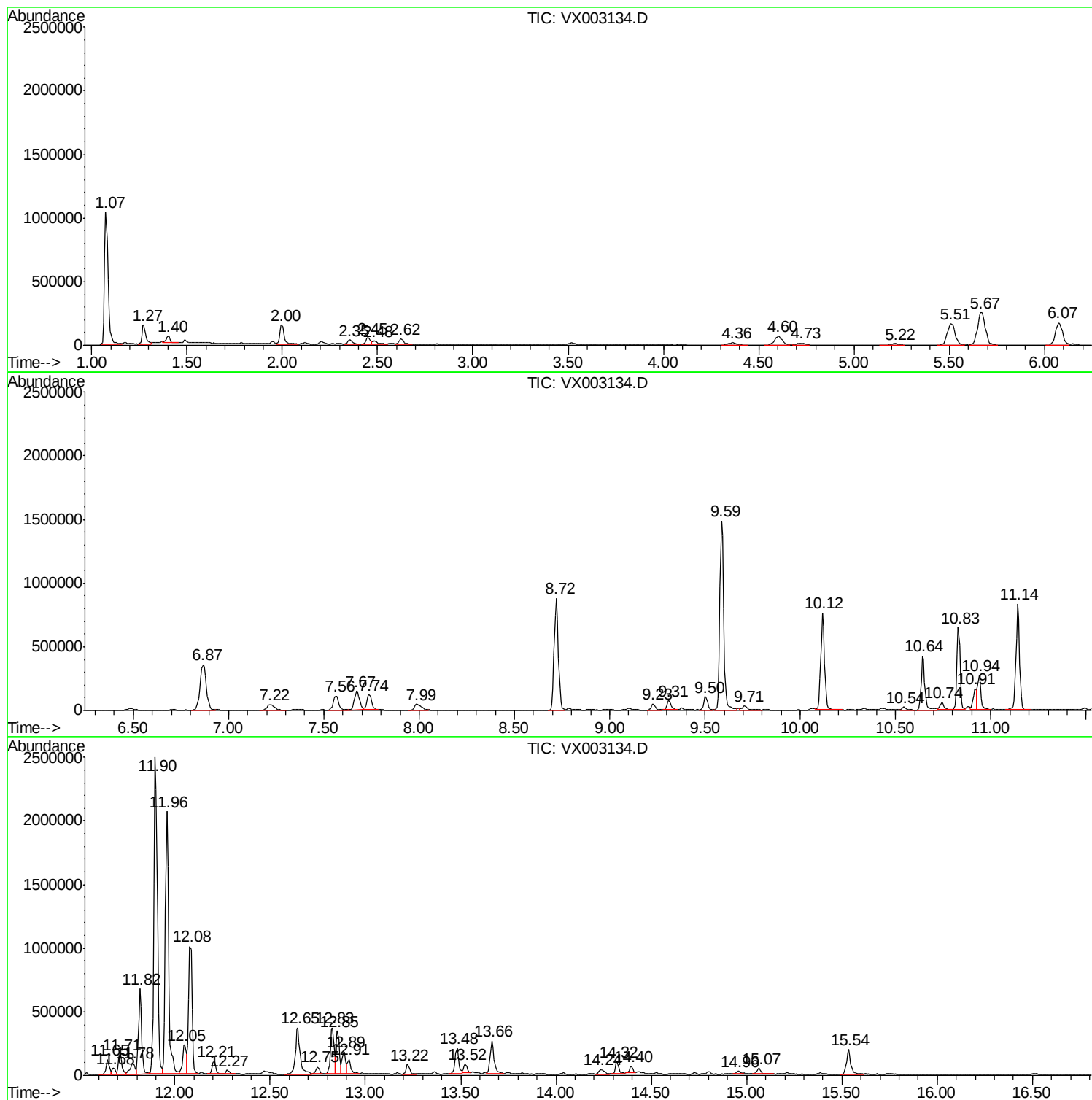
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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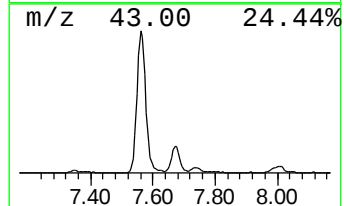
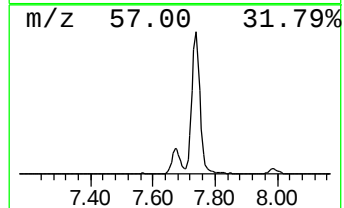
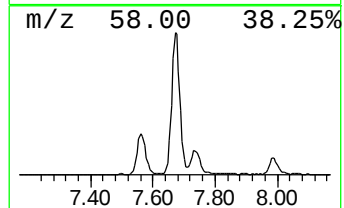
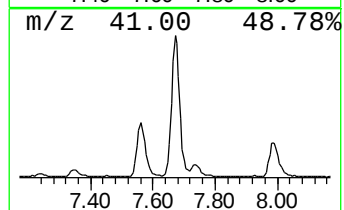
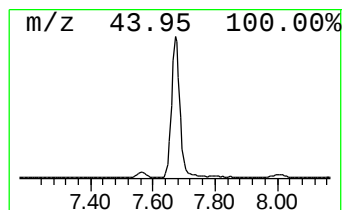
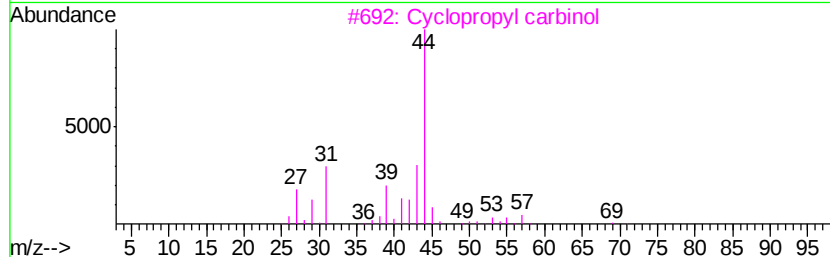
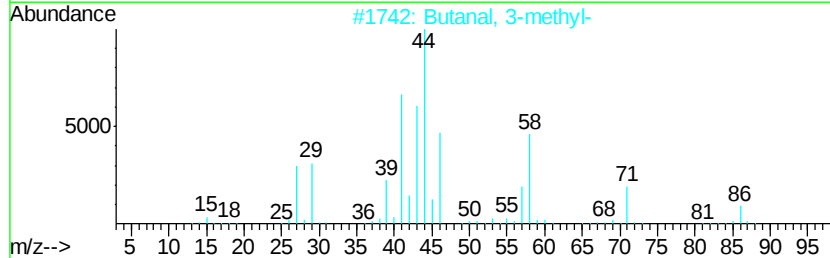
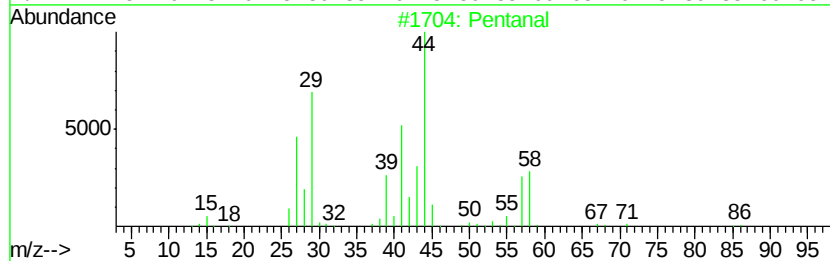
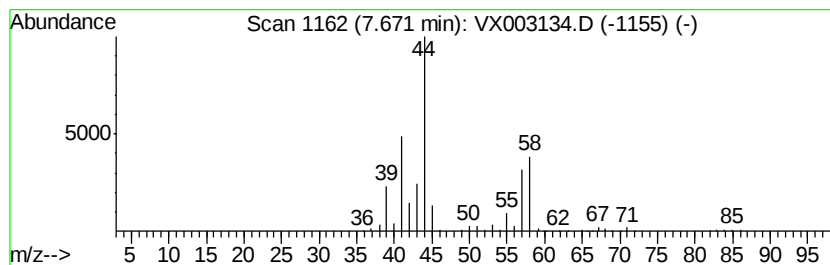
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	16.63 ug/l	278860	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanal	86	C5H10O	000110-62-3	90
2		Butanal, 3-methyl-	86	C5H10O	000590-86-3	64
3		Cyclopropyl carbinol	72	C4H8O	002516-33-8	40
4		2-Formylhistamine	139	C6H9N3O	1000132-95-8	28
5		Ethylene oxide	44	C2H4O	000075-21-8	9



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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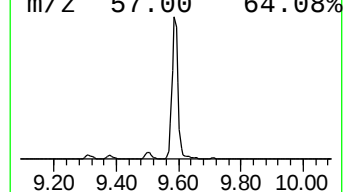
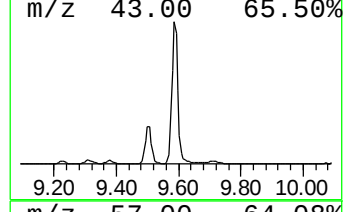
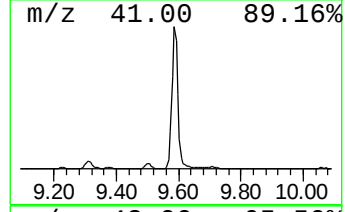
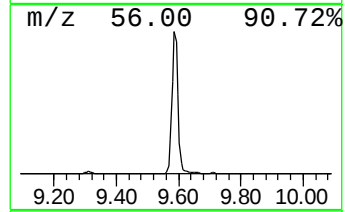
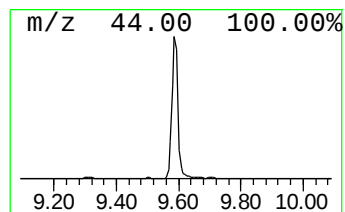
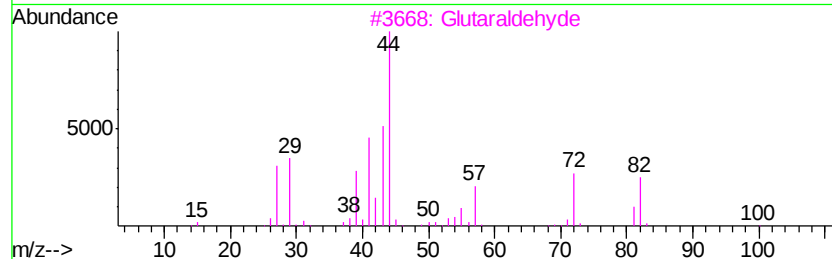
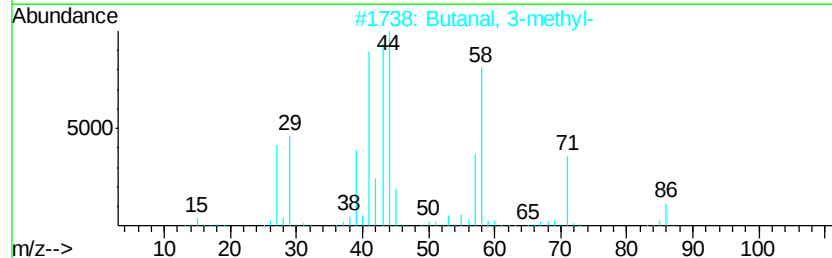
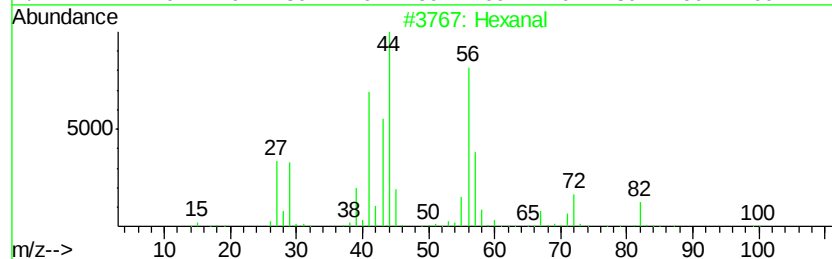
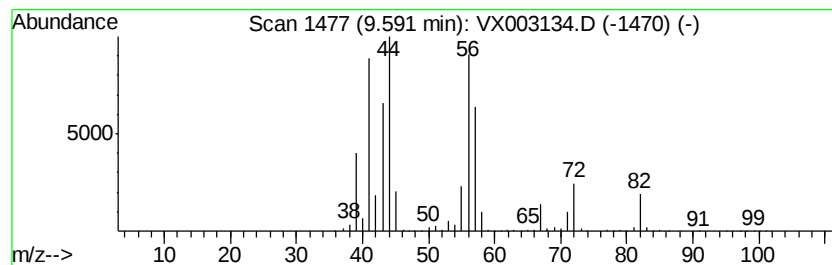
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 3 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.59	99.43 ug/l	2097580	Chlorobenzene-d5	10.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal		100	C6H12O	000066-25-1	80
2	Butanal, 3-methyl-		86	C5H10O	000590-86-3	32
3	Glutaraldehyde		100	C5H8O2	000111-30-8	30
4	Cyclobutane		56	C4H8	000287-23-0	14
5	Butanal		72	C4H8O	000123-72-8	12



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

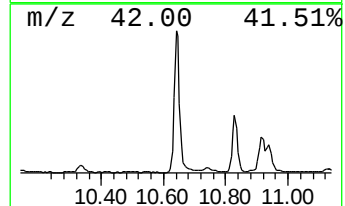
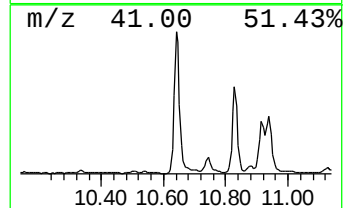
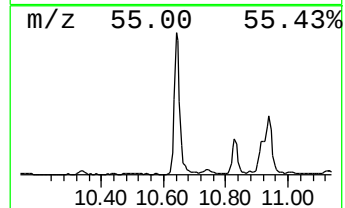
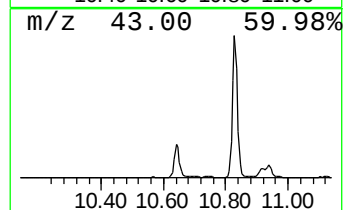
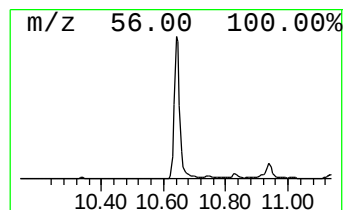
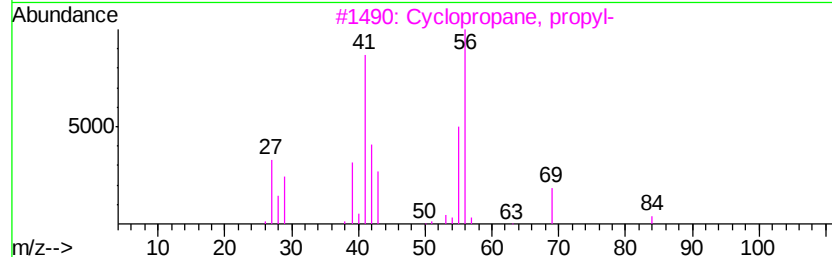
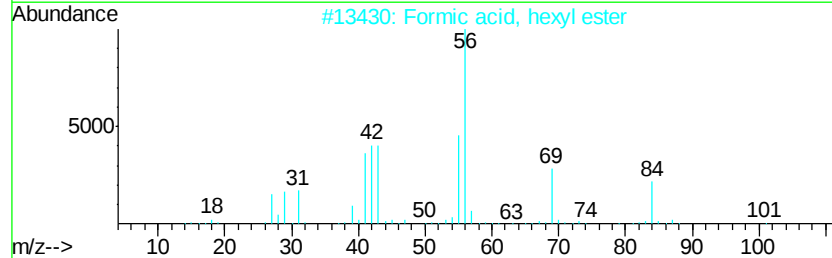
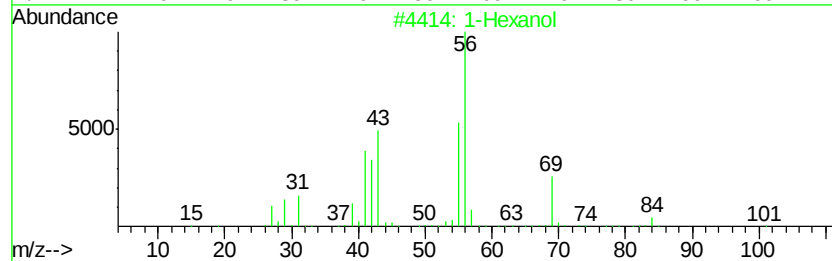
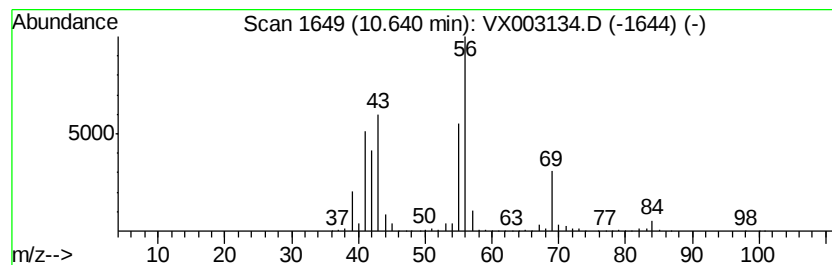
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ClientSampled :
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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.64	27.51 ug/l	580290	Chlorobenzene-d5	10.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol	102	C6H14O	000111-27-3	83
2		Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
3		Cyclopropane, propyl-	84	C6H12	002415-72-7	64
4		Hexyl chloroformate	164	C7H13ClO2	006092-54-2	64
5		1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	64



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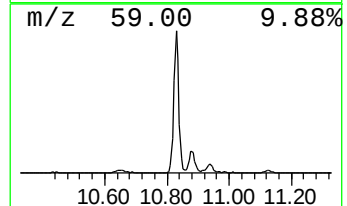
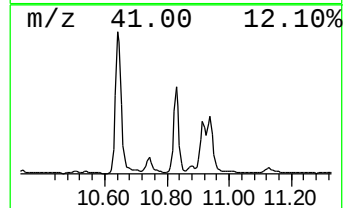
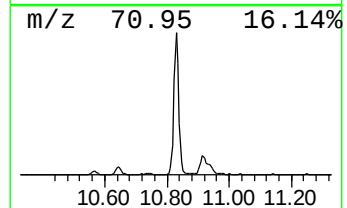
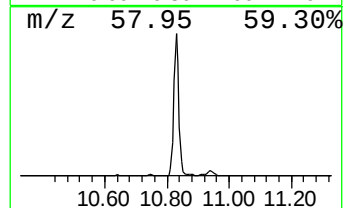
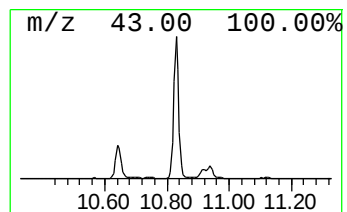
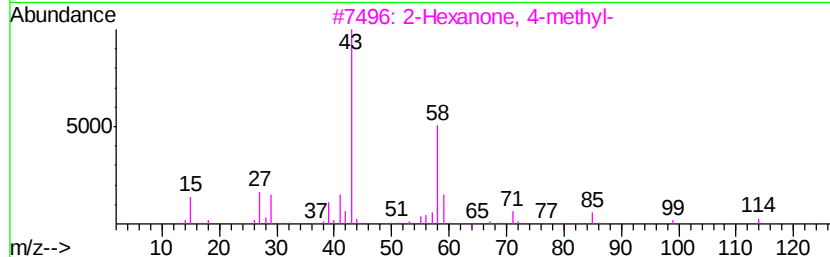
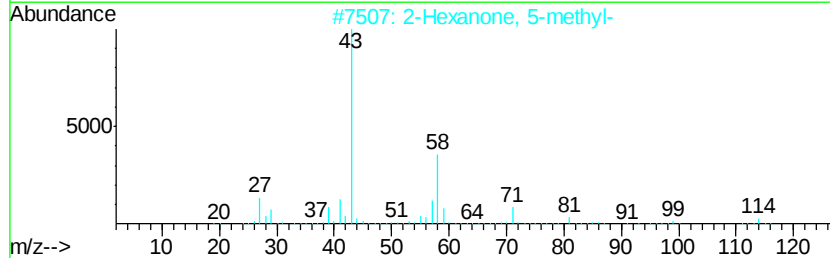
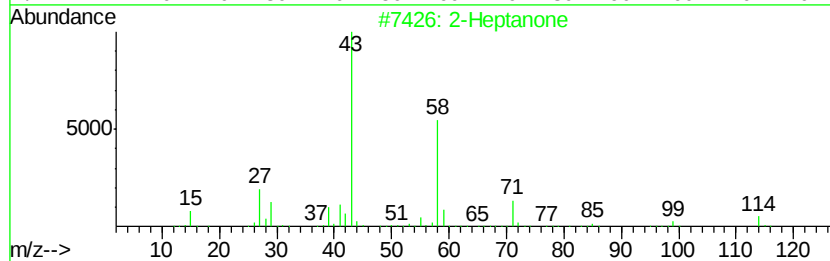
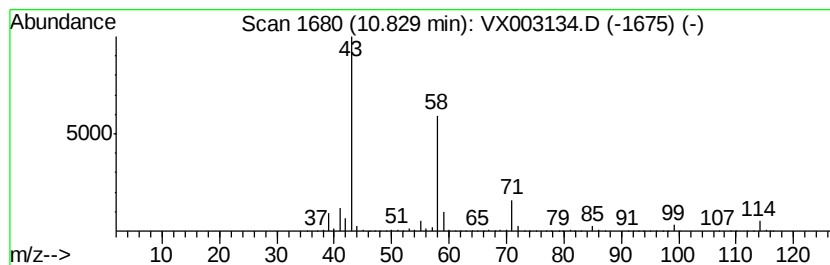
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Quant Title : SW846 8260

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

Peak Number 5 2-Heptanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	36.28 ug/l	765428	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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-Hexanone	100	C6H12O	000591-78-6	56
5		2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	52



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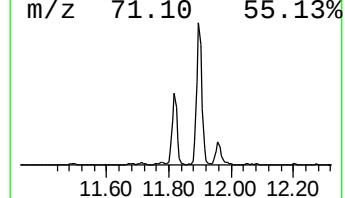
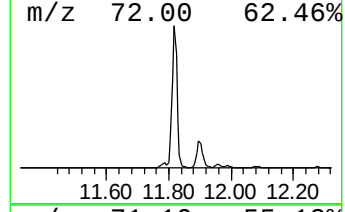
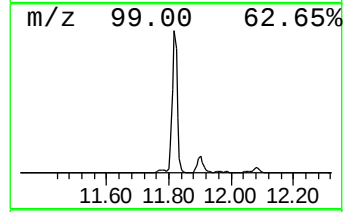
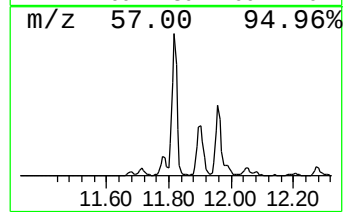
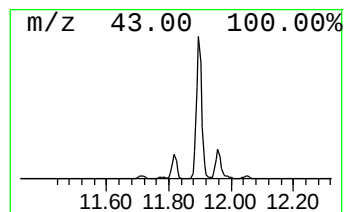
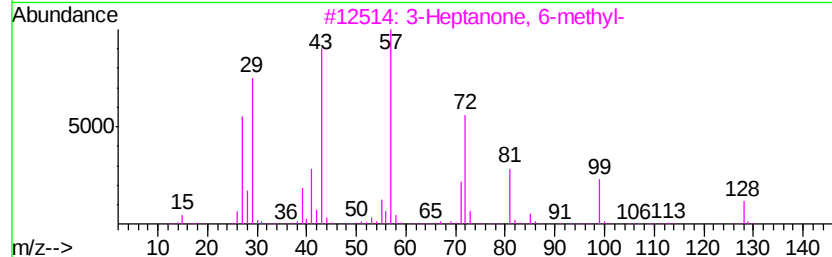
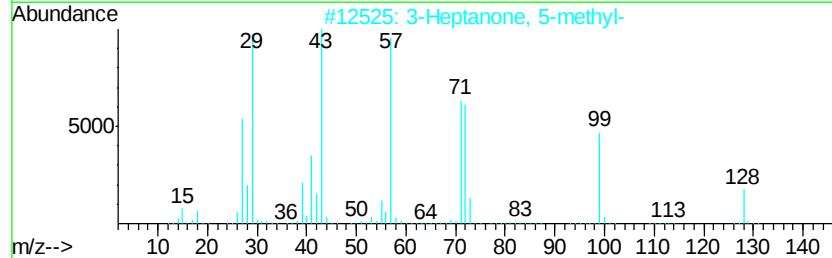
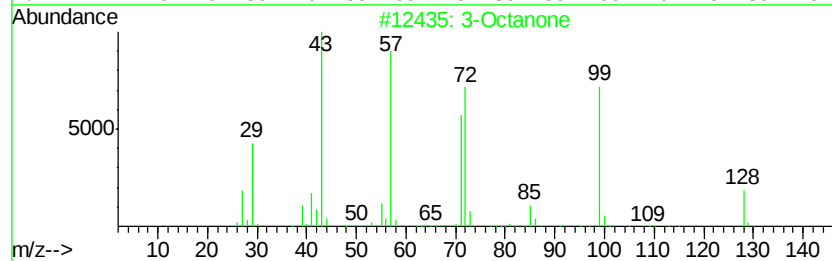
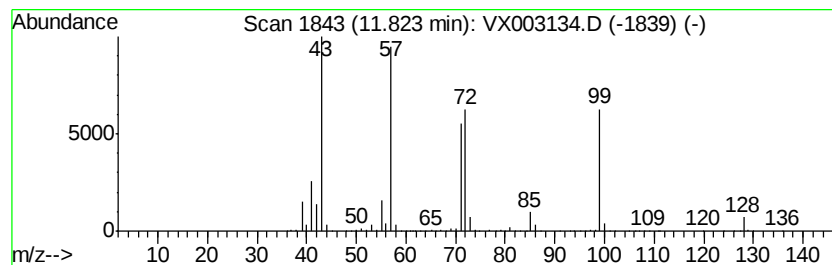
Instrument :
MSVOA_X
ClientSampleId :
SP18-CHY05

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 6 3-Octanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	30.67 ug/l	778403	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	52
4	Ethanone, 1-(3,3-dimethyloxiranyl)-	114 C6H10O2	004478-63-1	50
5	n-Caproic acid vinyl ester	142 C8H14O2	003050-69-9	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003134.D
Acq On : 02 Jul 2018 18:24
Operator : JC/MD
Sample : J3772-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP18-CHY05

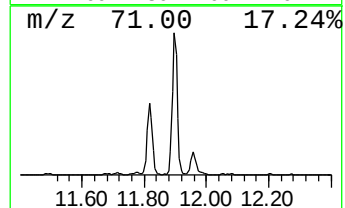
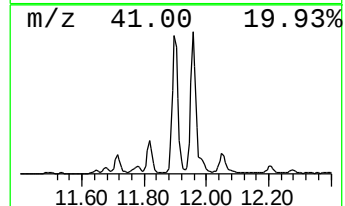
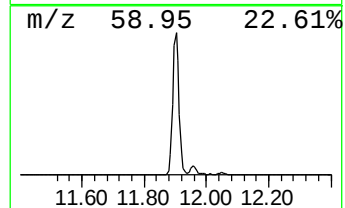
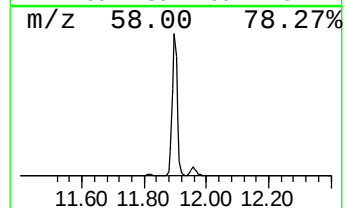
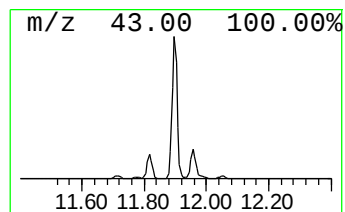
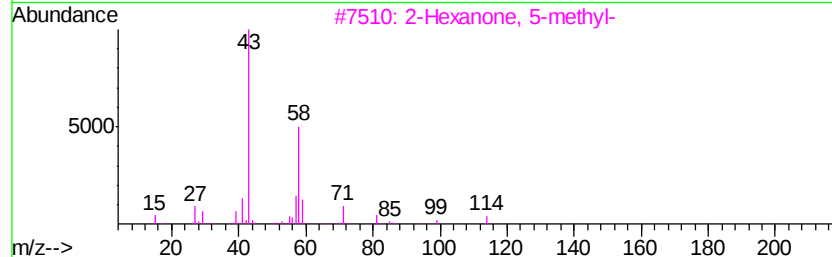
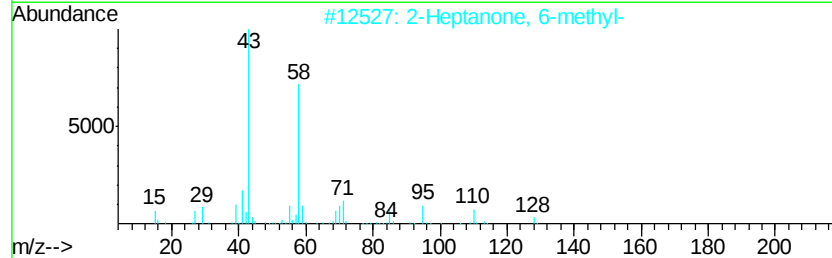
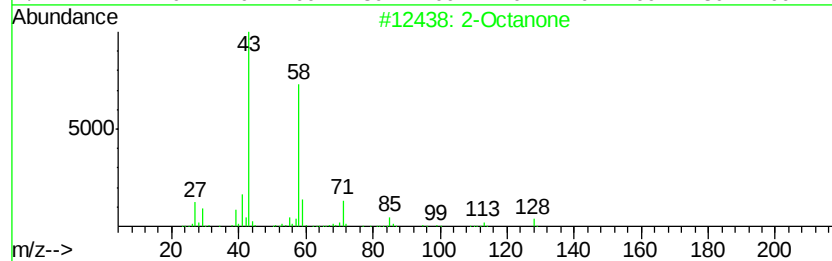
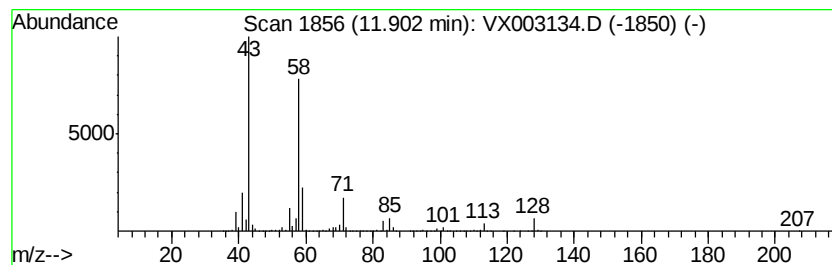
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Quant Title : SW846 8260

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

Peak Number 7 2-Octanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	125.28 ug/l	3179540	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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-Heptanone	114	C7H14O	000110-43-0	72
5		2-Nonanone	142	C9H18O	000821-55-6	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003134.D
Acq On : 02 Jul 2018 18:24
Operator : JC/MD
Sample : J3772-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP18-CHY05

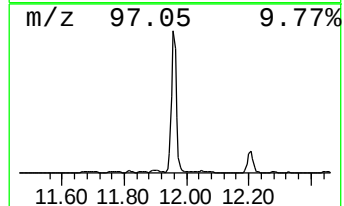
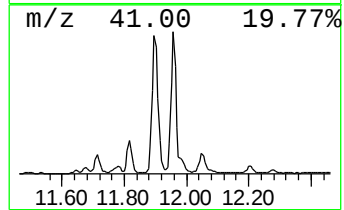
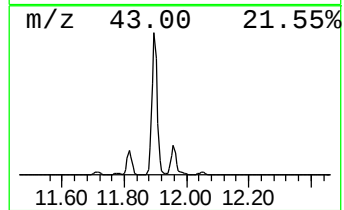
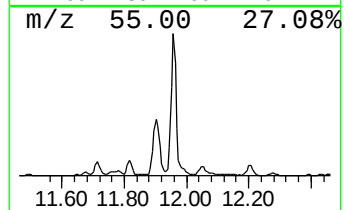
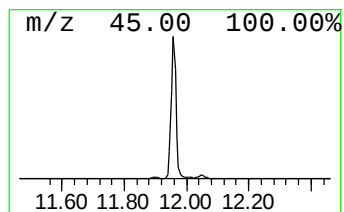
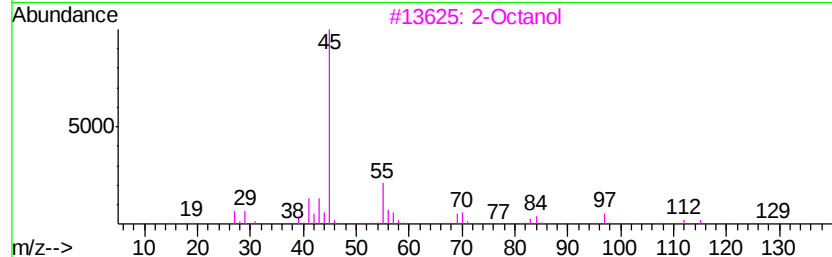
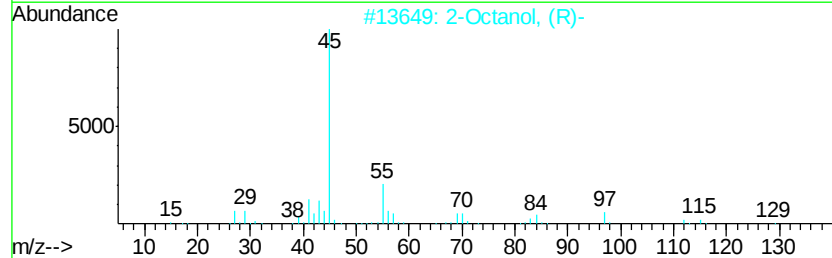
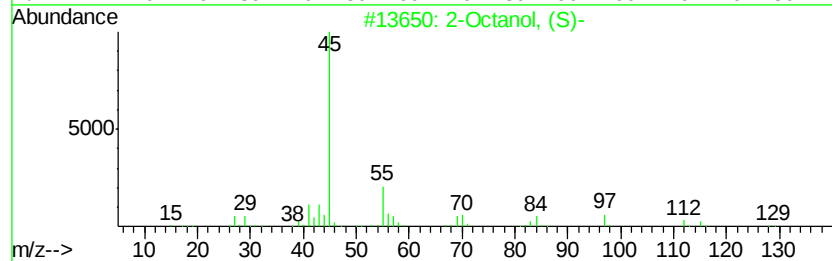
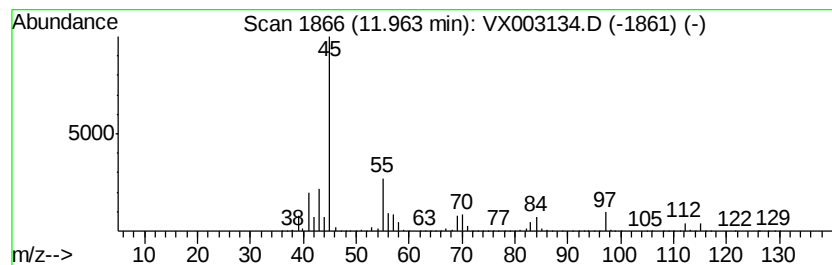
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Quant Title : SW846 8260

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

Peak Number 8 2-Octanol, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	98.96 ug/l	2511550	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Octanol, (S)-	130	C8H18O	006169-06-8	90
2		2-Octanol, (R)-	130	C8H18O	005978-70-1	90
3		2-Octanol	130	C8H18O	000123-96-6	90
4		2-Decanol	158	C10H22O	001120-06-5	72
5		2-Nonanol	144	C9H20O	000628-99-9	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003134.D
Acq On : 02 Jul 2018 18:24
Operator : JC/MD
Sample : J3772-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

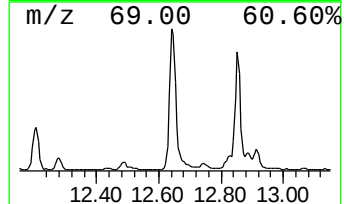
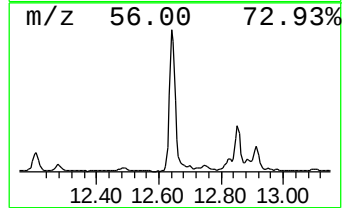
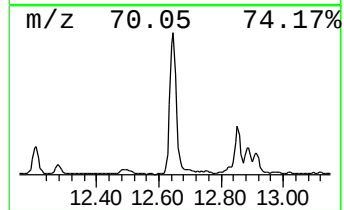
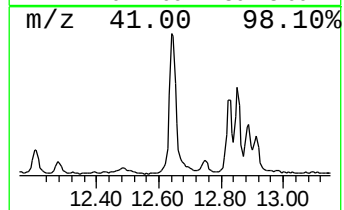
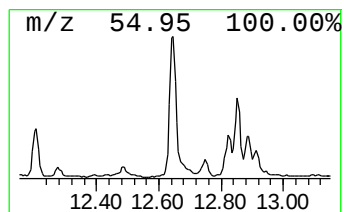
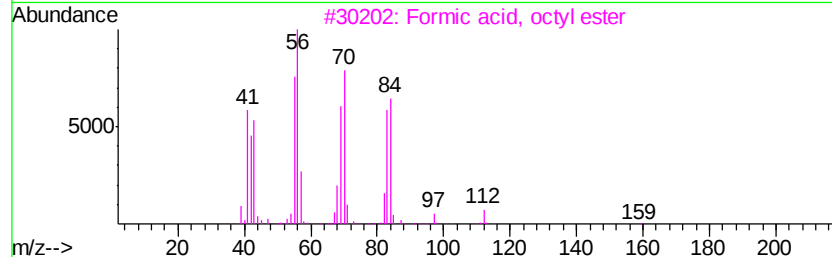
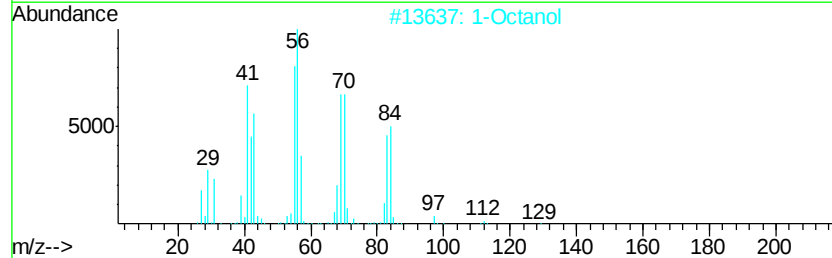
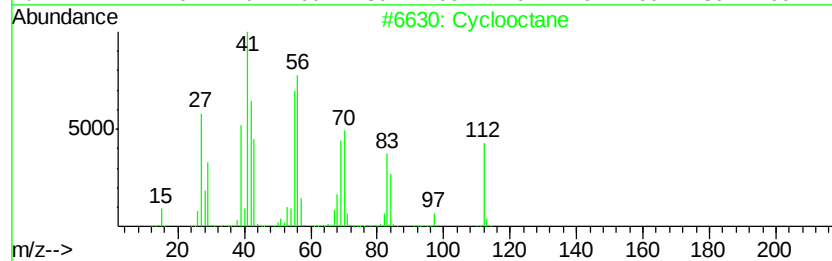
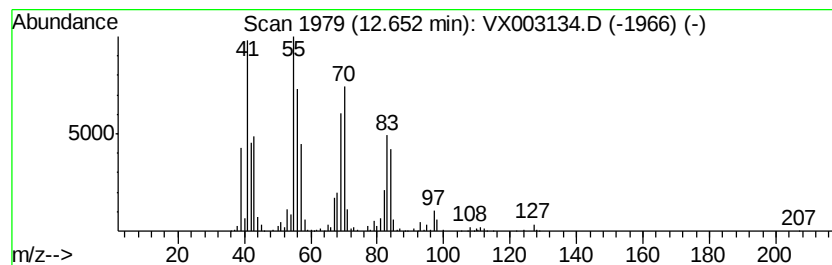
Instrument :
MSVOA_X
ClientSampleId :
SP18-CHY05

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 9 Cyclooctane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	25.37 ug/l	643831	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclooctane	112 C8H16	000292-64-8 91
2		1-Octanol	130 C8H18O	000111-87-5 91
3		Formic acid, octyl ester	158 C9H18O2	000112-32-3 90
4		Octyl chloroformate	192 C9H17ClO2	007452-59-7 86
5		Nonyl chloroformate	206 C10H19ClO2	057045-82-6 83



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX070218\
Data File : VX003134.D
Acq On : 02 Jul 2018 18:24
Operator : JC/MD
Sample : J3772-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP18-CHY05

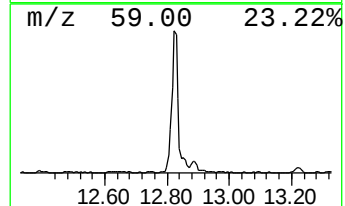
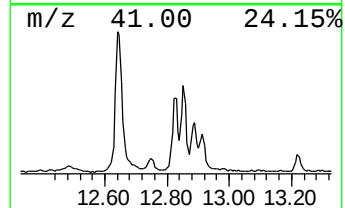
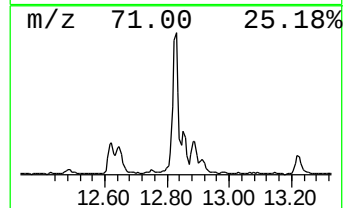
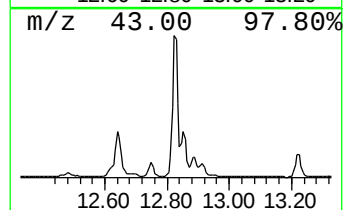
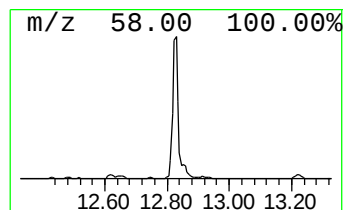
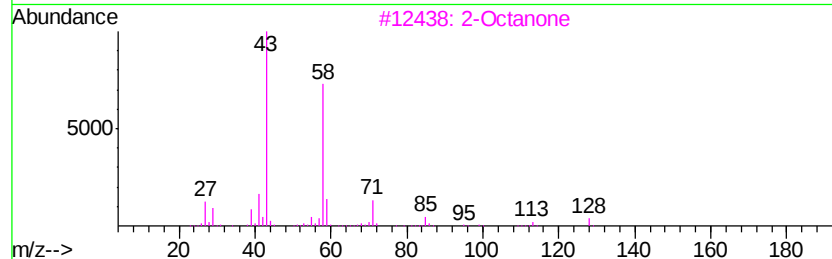
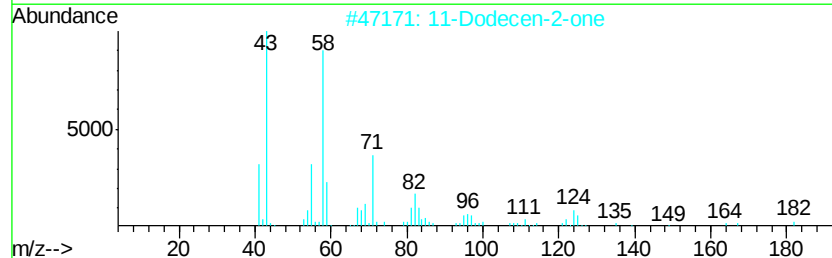
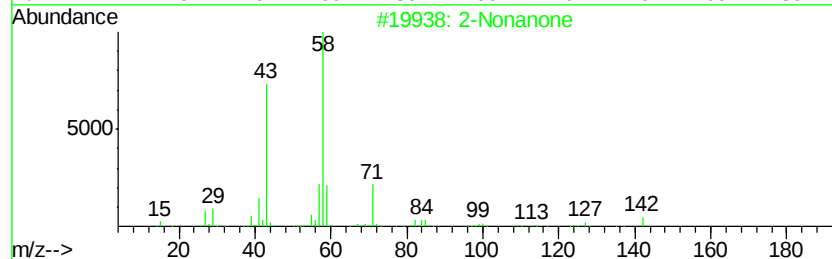
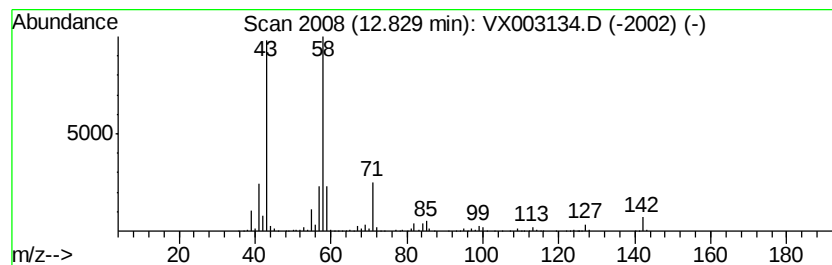
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 10 2-Nonanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	19.14 ug/l	485831	1,4-Dichlorobenzene-d4	12.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Nonanone	142	C9H18O	000821-55-6	97
2			11-Dodecen-2-one	182	C12H22O	005009-33-6	78
3			2-Octanone	128	C8H16O	000111-13-7	72
4			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	59
5			Silacyclohexan-4-one, 1,1-dimethyl-	142	C7H14OSi	018276-42-1	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX070218\
Data File : VX003134.D
Acq On : 02 Jul 2018 18:24
Operator : JC/MD
Sample : J3772-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP18-CHY05

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentanal	7.67	16.6	ug/l	278860	2	6.87	838473	50.0
Hexanal	9.59	99.4	ug/l	2097580	3	10.12	1054760	50.0
1-Hexanol	10.64	27.5	ug/l	580290	3	10.12	1054760	50.0
2-Heptanone	10.83	36.3	ug/l	765428	3	10.12	1054760	50.0
3-Octanone	11.82	30.7	ug/l	778403	4	12.08	1268930	50.0
2-Octanone	11.90	125.3	ug/l	3179540	4	12.08	1268930	50.0
2-Octanol, (S)-	11.96	99.0	ug/l	2511550	4	12.08	1268930	50.0
Cyclooctane	12.65	25.4	ug/l	643831	4	12.08	1268930	50.0
2-Nonanone	12.83	19.1	ug/l	485831	4	12.08	1268930	50.0