

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX060220\
 Data File : VX016548.D
 Acq On : 02 Jun 2020 11:56
 Operator : JC/SP
 Sample : L2801-08
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SS050MW641-200528

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\82X052720W.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	2.416	211	218	236	rVB	1475922	2443075	53.23%	11.671%
2	2.575	236	244	256	rVB	236709	441135	9.61%	2.107%
3	4.629	561	581	601	rBV	1622981	4589867	100.00%	21.927%
4	5.074	643	654	676	rBV	199097	635549	13.85%	3.036%
5	5.464	706	718	730	rBV	199462	561426	12.23%	2.682%
6	5.629	733	745	761	rVB	351115	1000184	21.79%	4.778%
7	6.031	800	811	823	rBV	210871	570507	12.43%	2.725%
8	6.830	931	942	955	rBV	550493	1318451	28.73%	6.299%
9	7.513	1046	1054	1068	rBV	126109	255038	5.56%	1.218%
10	7.690	1078	1083	1091	rVB	45732	84594	1.84%	0.404%
11	8.622	1230	1236	1241	rBV	96225	157041	3.42%	0.750%
12	8.696	1241	1248	1255	rVV	1220837	1877814	40.91%	8.971%
13	10.098	1464	1478	1495	rBV	1205184	1676258	36.52%	8.008%
14	10.805	1587	1594	1600	rBV	103798	127711	2.78%	0.610%
15	11.122	1639	1646	1656	rBV	1060422	1351632	29.45%	6.457%
16	11.793	1752	1756	1763	rBV	43998	55202	1.20%	0.264%
17	11.878	1765	1770	1775	rBV	305097	376746	8.21%	1.800%
18	11.939	1775	1780	1788	rVB	46568	64588	1.41%	0.309%
19	12.061	1794	1800	1809	rBV	1427545	1736620	37.84%	8.296%
20	12.805	1917	1922	1925	rBV	678861	750056	16.34%	3.583%
21	12.835	1925	1927	1941	rVB	104936	142073	3.10%	0.679%
22	13.640	2051	2059	2067	rBV3	52810	75206	1.64%	0.359%
23	14.408	2179	2185	2196	rBV	575070	641501	13.98%	3.065%

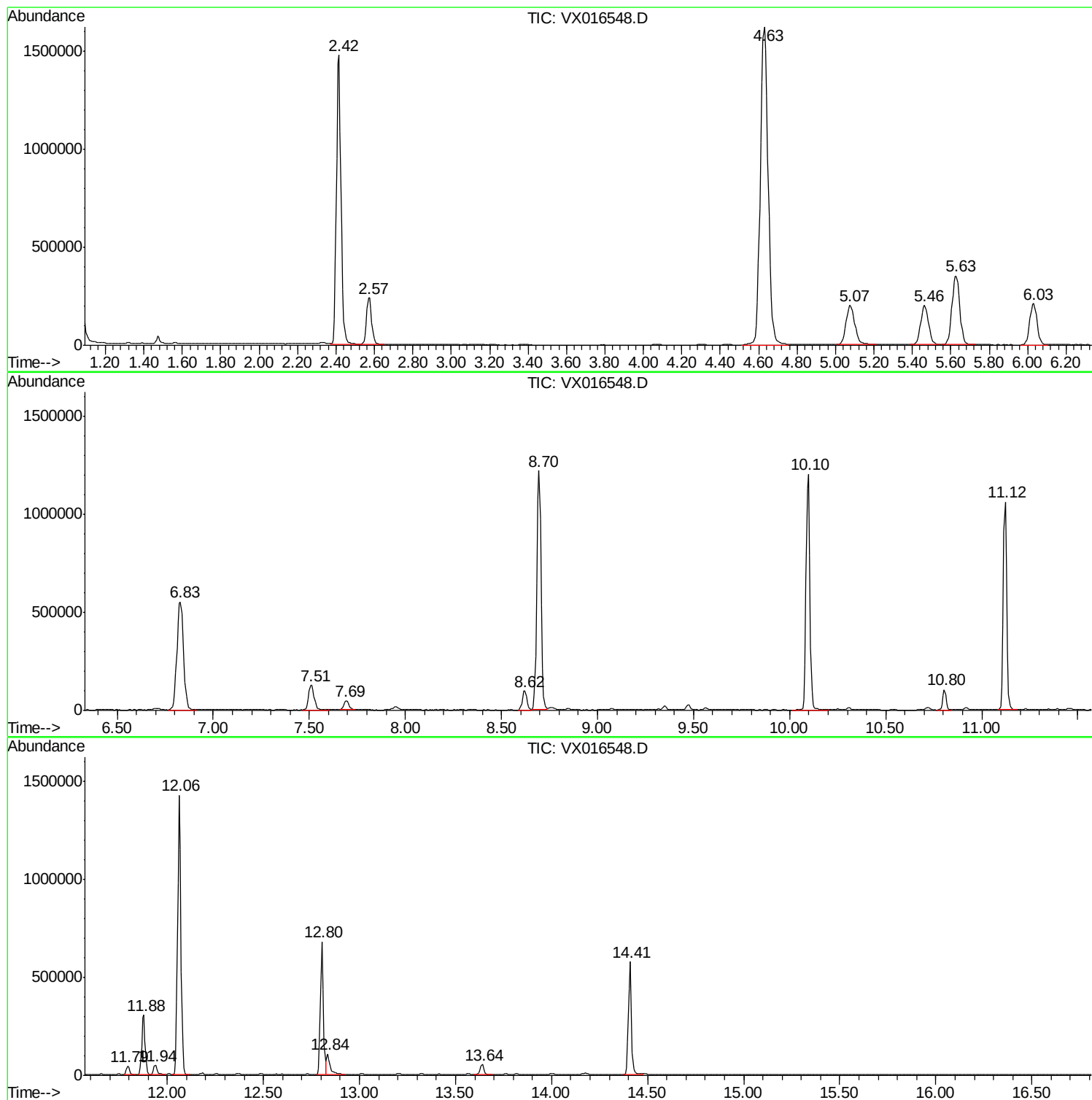
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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



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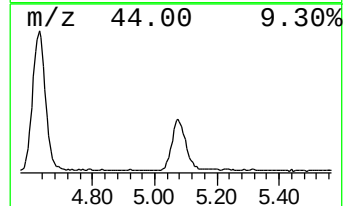
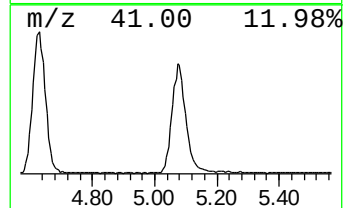
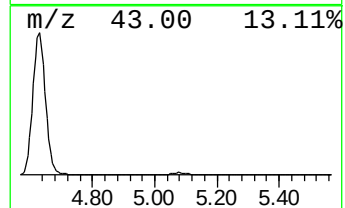
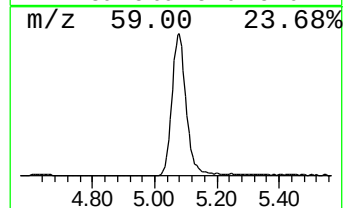
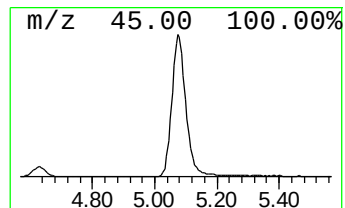
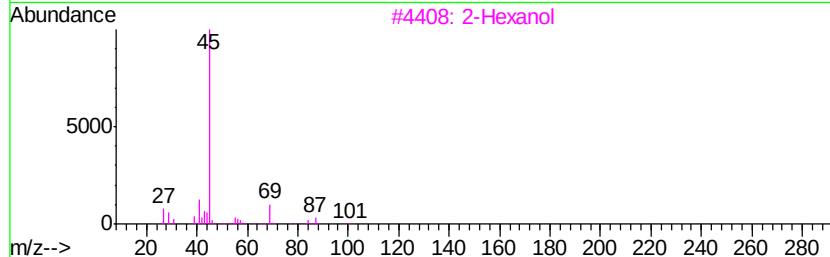
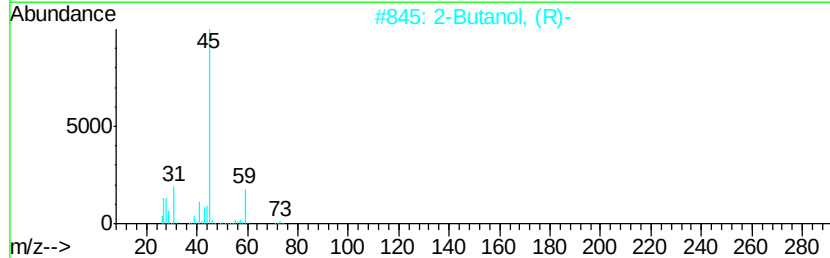
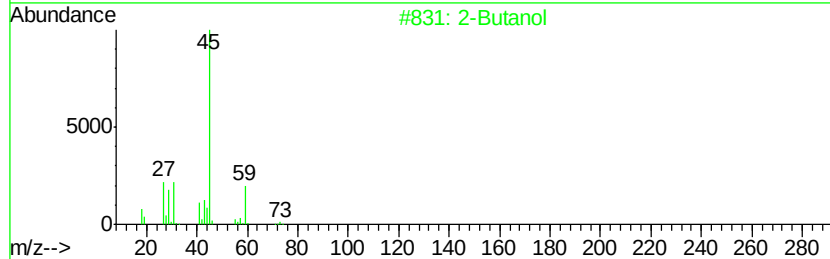
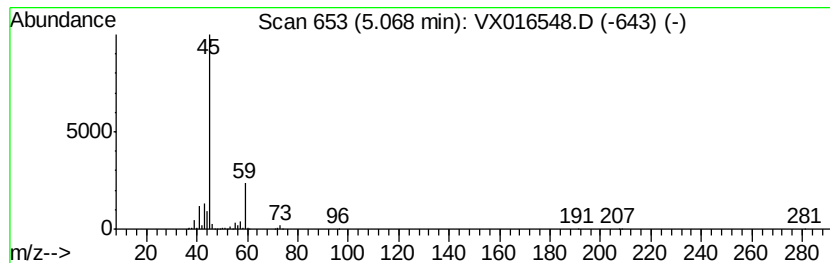
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Butanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	31.77 ug/l	635549	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butanol	74	C4H10O	000078-92-2	83
2		2-Butanol, (R)-	74	C4H10O	014898-79-4	78
3		2-Hexanol	102	C6H14O	000626-93-7	38
4		2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	36
5		Isopropyl Alcohol	60	C3H8O	000067-63-0	9



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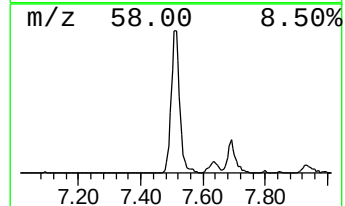
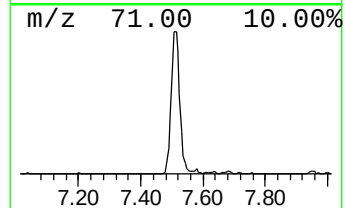
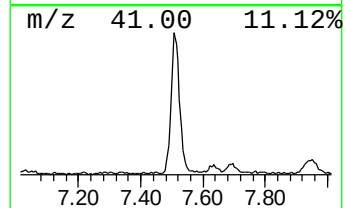
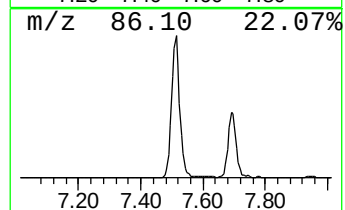
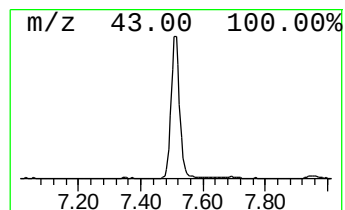
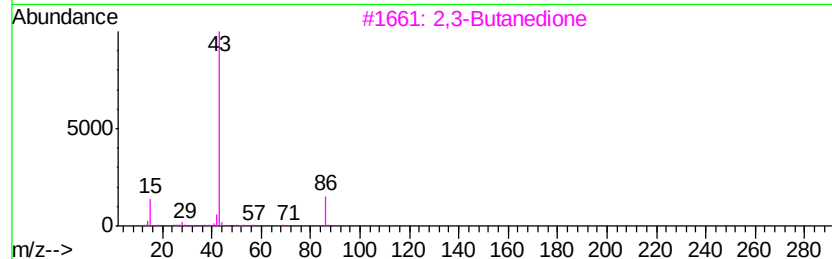
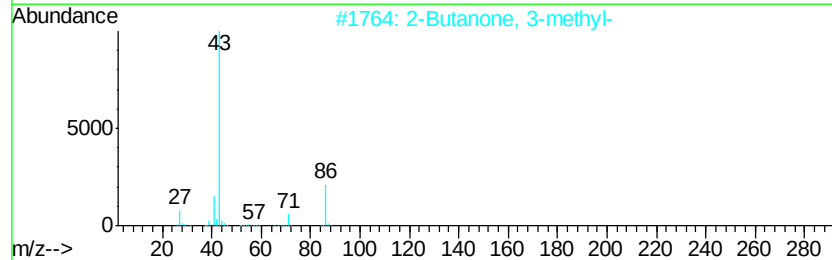
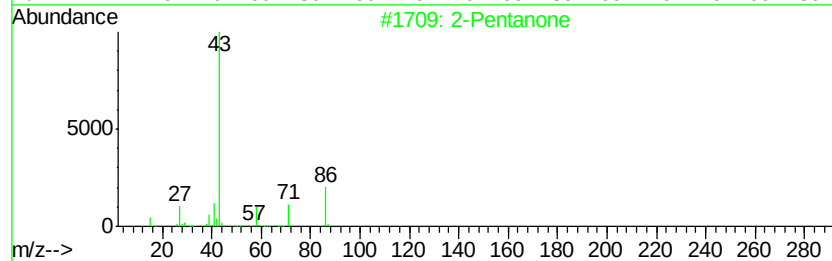
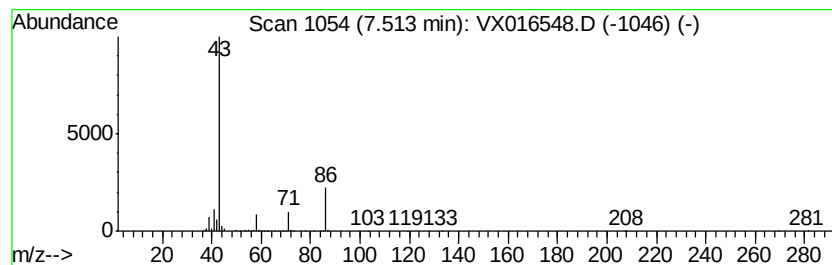
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.51	9.67 ug/l	255038	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone	86	C5H10O	000107-87-9	90
2		2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3		2,3-Butanedione	86	C4H6O2	000431-03-8	50
4		2,3-Pentanedione, 4-methyl-	114	C6H10O2	007493-58-5	25
5		3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9



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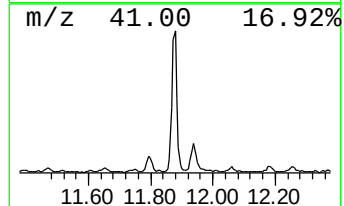
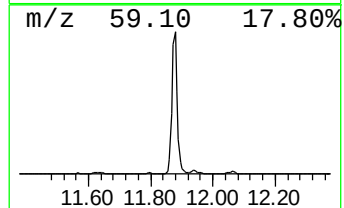
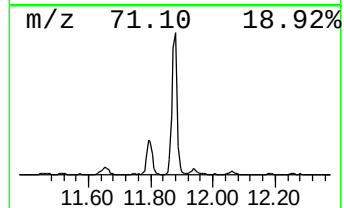
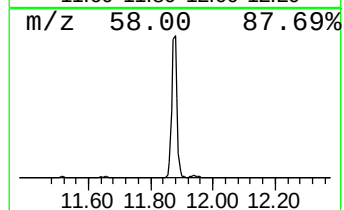
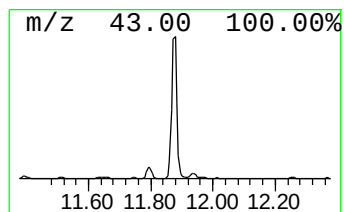
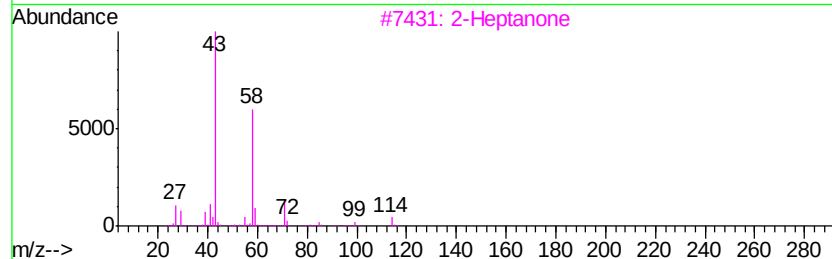
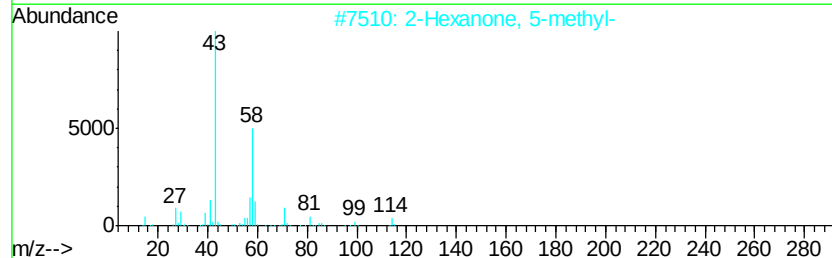
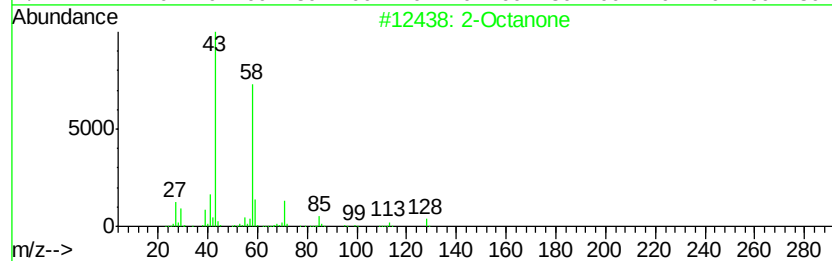
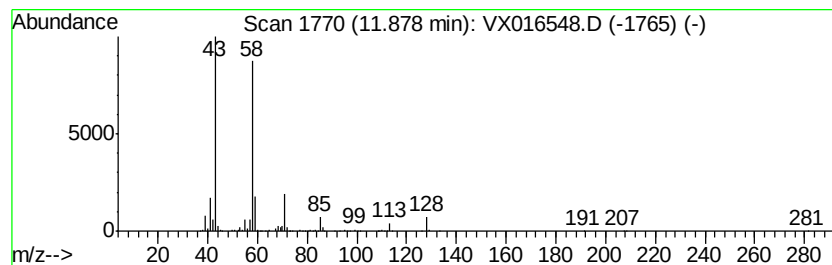
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 Quant Title : SW846 8260

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

 Peak Number 3 2-Octanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	10.85 ug/l	376746	1,4-Dichlorobenzene-d4	12.06

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



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 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 5 Sample Multiplier: 1

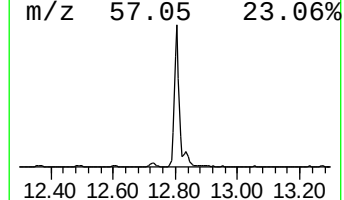
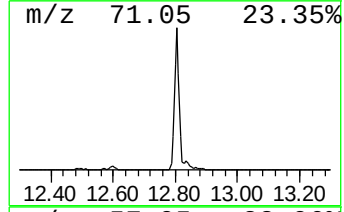
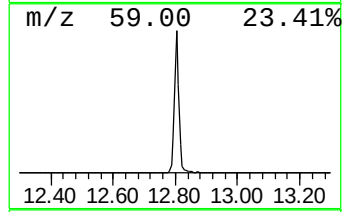
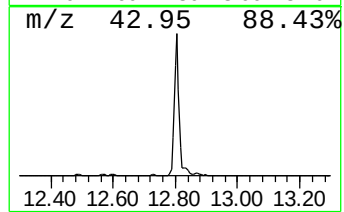
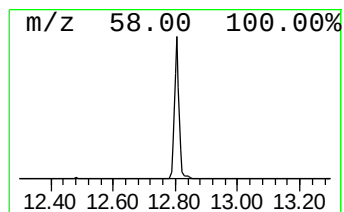
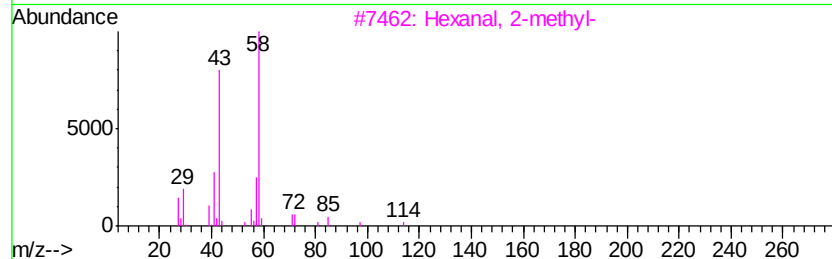
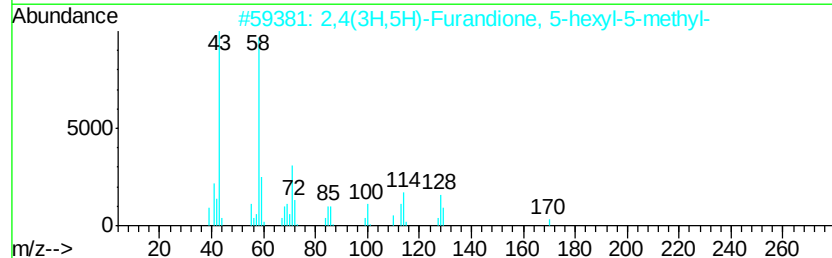
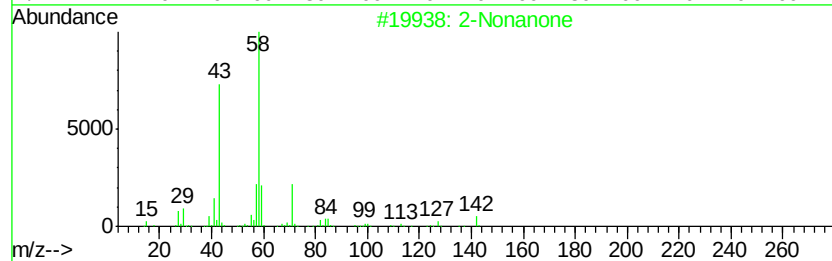
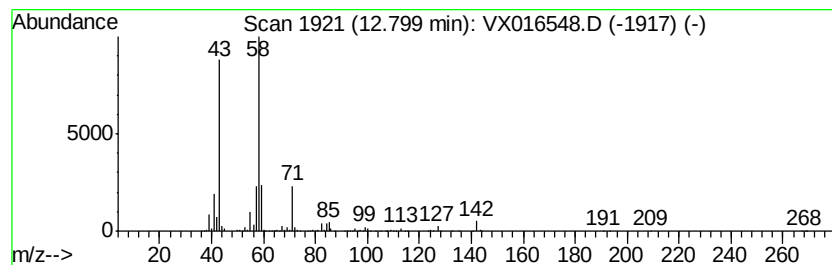
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 ClientSampleId :
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 Quant Title : SW846 8260

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

 Peak Number 4 2-Nonanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	21.60 ug/l	750056	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Nonanone		142 C9H18O	000821-55-6 97
2	2,4(3H,5H)-Furandione, 5-hexyl-5-methyl-		198 C11H18O3	054852-79-8 64
3	Hexanal, 2-methyl-		114 C7H14O	000925-54-2 53
4	Pentanal, 2-methyl-		100 C6H12O	000123-15-9 53
5	2-Heptanone		114 C7H14O	000110-43-0 50



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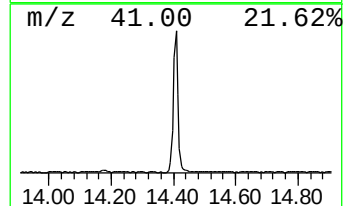
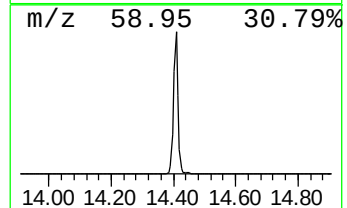
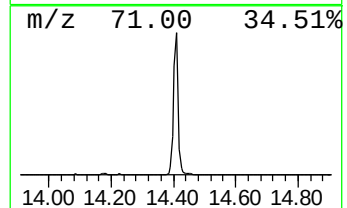
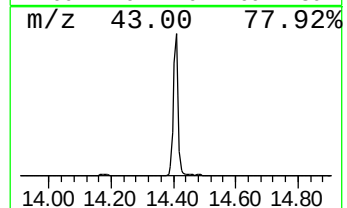
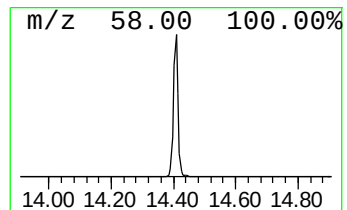
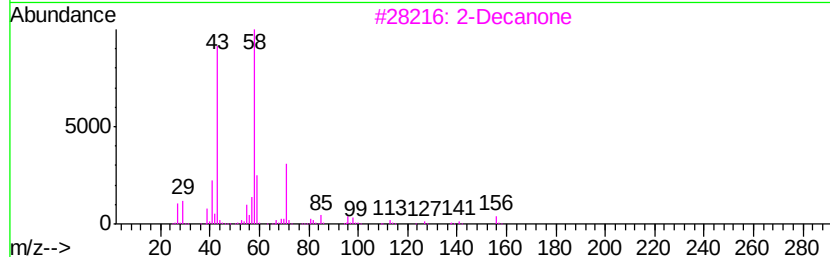
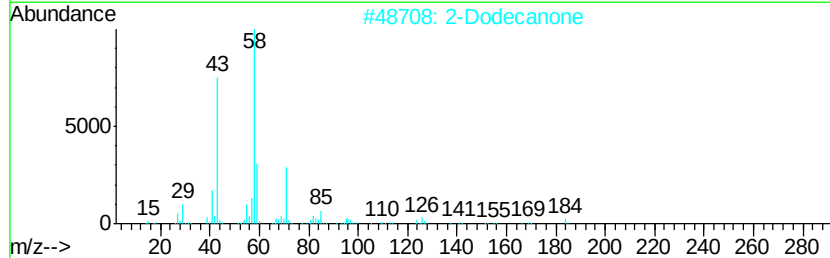
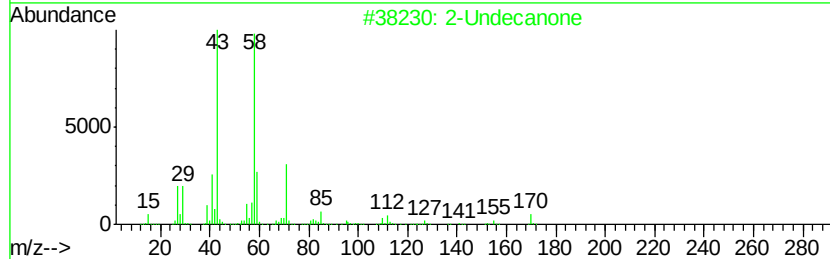
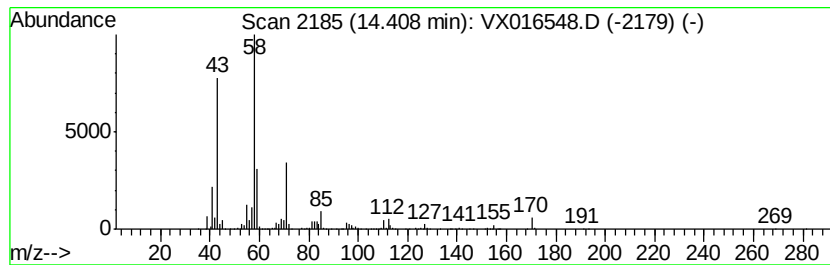
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Quant Title : SW846 8260

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

Peak Number 5 2-Undecanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	18.47 ug/l	641501	1,4-Dichlorobenzene-d4	12.06

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Undecanone	170	C11H22O	000112-12-9	94
2	2-Dodecanone	184	C12H24O	006175-49-1	78
3	2-Decanone	156	C10H20O	000693-54-9	72
4	2-Octanone	128	C8H16O	000111-13-7	59
5	1-Propene, 2-(1-methylethoxy)	100	C6H12O	004188-63-0	53



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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
2-Butanol	5.07	31.8	ug/l	635549	1	5.63	1000180	50.0
2-Pentanone	7.51	9.7	ug/l	255038	2	6.83	1318450	50.0
2-Octanone	11.88	10.9	ug/l	376746	4	12.06	1736620	50.0
2-Nonanone	12.80	21.6	ug/l	750056	4	12.06	1736620	50.0
2-Undecanone	14.41	18.5	ug/l	641501	4	12.06	1736620	50.0