

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX052920\
 Data File : VX016506.D
 Acq On : 29 May 2020 13:24
 Operator : JC/SP
 Sample : L2795-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WATER-COMP-214-215

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	1.471	60	63	72	rBV	39367	46247	1.37%	0.215%
2	2.416	212	218	223	rVV	68365	112380	3.33%	0.523%
3	2.575	235	244	253	rBV2	86466	178551	5.28%	0.830%
4	4.306	518	528	538	rBV3	19502	54750	1.62%	0.255%
5	4.641	572	583	595	rBV2	25128	79112	2.34%	0.368%
6	5.471	706	719	732	rBV2	158396	460446	13.63%	2.141%
7	5.629	733	745	758	rVB	293808	822167	24.33%	3.823%
8	6.032	801	811	823	rBV	176373	478032	14.15%	2.223%
9	6.830	932	942	957	rBV	454258	1074690	31.80%	4.997%
10	7.513	1049	1054	1062	rBV	19480	38935	1.15%	0.181%
11	7.635	1068	1074	1081	rVB	21281	37530	1.11%	0.175%
12	8.623	1229	1236	1241	rBV2	21038	34509	1.02%	0.160%
13	8.696	1241	1248	1255	rVV	976544	1502735	44.47%	6.987%
14	8.763	1255	1259	1268	rVB	43289	76568	2.27%	0.356%
15	9.476	1370	1376	1383	rBV	28089	43627	1.29%	0.203%
16	9.561	1384	1390	1403	rVB	47624	74910	2.22%	0.348%
17	10.098	1468	1478	1492	rBV	1012237	1391879	41.19%	6.472%
18	10.342	1512	1518	1525	rVB	59984	83850	2.48%	0.390%
19	10.683	1569	1574	1578	rBV	45983	60935	1.80%	0.283%
20	10.805	1587	1594	1599	rBV	33704	47616	1.41%	0.221%
21	10.896	1599	1609	1619	rVB3	39332	73678	2.18%	0.343%
22	11.122	1638	1646	1657	rVB	882863	1123988	33.26%	5.226%
23	11.421	1688	1695	1700	rBV	42775	74405	2.20%	0.346%
24	11.652	1728	1733	1738	rBV	53308	71335	2.11%	0.332%
25	11.793	1752	1756	1761	rBV	120780	150178	4.44%	0.698%
26	11.878	1765	1770	1775	rBV	149272	191650	5.67%	0.891%
27	11.933	1775	1779	1782	rVV2	25460	44208	1.31%	0.206%
28	11.963	1782	1784	1788	rVB	46398	54738	1.62%	0.255%
29	12.061	1795	1800	1807	rVB	1124442	1442728	42.70%	6.708%
30	12.128	1807	1811	1820	rBV	56774	88303	2.61%	0.411%
31	12.256	1827	1832	1844	rBV	670979	1021907	30.24%	4.752%
32	12.360	1844	1849	1850	rVV3	39290	65527	1.94%	0.305%
33	12.384	1850	1853	1858	rVB2	51437	72511	2.15%	0.337%
34	12.506	1868	1873	1878	rVB3	43549	81780	2.42%	0.380%

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Integration Parameters: RTEINT.P

Integrator: RTE
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35	12.616	1885	1891	1895	rVV	224918	323976	9.59%	1.506%
36	12.732	1906	1910	1917	rBV3	40761	74007	2.19%	0.344%
37	12.805	1917	1922	1925	rVV2	144339	194518	5.76%	0.904%
38	12.890	1933	1936	1943	rVB2	43459	57746	1.71%	0.269%
39	13.006	1951	1955	1963	rBV2	237404	375751	11.12%	1.747%
40	13.110	1968	1972	1973	rBV	235621	260215	7.70%	1.210%
41	13.134	1973	1976	1992	rVB	2452573	3379051	100.00%	15.711%
42	13.298	2000	2003	2005	rBV3	42129	52545	1.56%	0.244%
43	13.335	2005	2009	2013	rVB2	89076	128390	3.80%	0.597%
44	13.463	2025	2030	2036	rVB	79110	108209	3.20%	0.503%
45	13.634	2053	2058	2064	rBV4	85295	136612	4.04%	0.635%
46	13.713	2066	2071	2076	rBV4	31697	61136	1.81%	0.284%
47	13.786	2076	2083	2090	rBV2	87491	248707	7.36%	1.156%
48	13.902	2095	2102	2103	rVV3	111363	185994	5.50%	0.865%
49	13.926	2103	2106	2118	rVB	1141285	1582703	46.84%	7.359%
50	14.268	2156	2162	2167	rVB2	56909	94848	2.81%	0.441%
51	14.414	2182	2186	2189	rBV2	25635	35618	1.05%	0.166%
52	14.524	2200	2204	2213	rVB4	54203	90259	2.67%	0.420%
53	14.609	2213	2218	2223	rBV	342900	534936	15.83%	2.487%
54	14.670	2223	2228	2233	rVV4	79385	205342	6.08%	0.955%
55	14.731	2233	2238	2246	rVV2	278503	477297	14.13%	2.219%
56	14.792	2246	2248	2251	rVV	54505	73347	2.17%	0.341%
57	14.835	2251	2255	2267	rVV5	88929	205514	6.08%	0.956%
58	14.938	2267	2272	2278	rVV3	61368	108857	3.22%	0.506%
59	15.054	2286	2291	2295	rBV2	54074	91702	2.71%	0.426%
60	15.201	2308	2315	2318	rBV	113816	216053	6.39%	1.005%
61	15.255	2318	2324	2329	rVV	265171	462243	13.68%	2.149%
62	15.414	2346	2350	2352	rBV2	44577	64819	1.92%	0.301%
63	15.444	2352	2355	2360	rVV	75855	115330	3.41%	0.536%
64	15.499	2360	2364	2368	rVV2	68079	115938	3.43%	0.539%
65	15.566	2372	2375	2380	rVB4	37254	57833	1.71%	0.269%
66	15.676	2390	2393	2401	rVB5	37067	88580	2.62%	0.412%
67	15.749	2401	2405	2409	rBV3	22191	42405	1.25%	0.197%

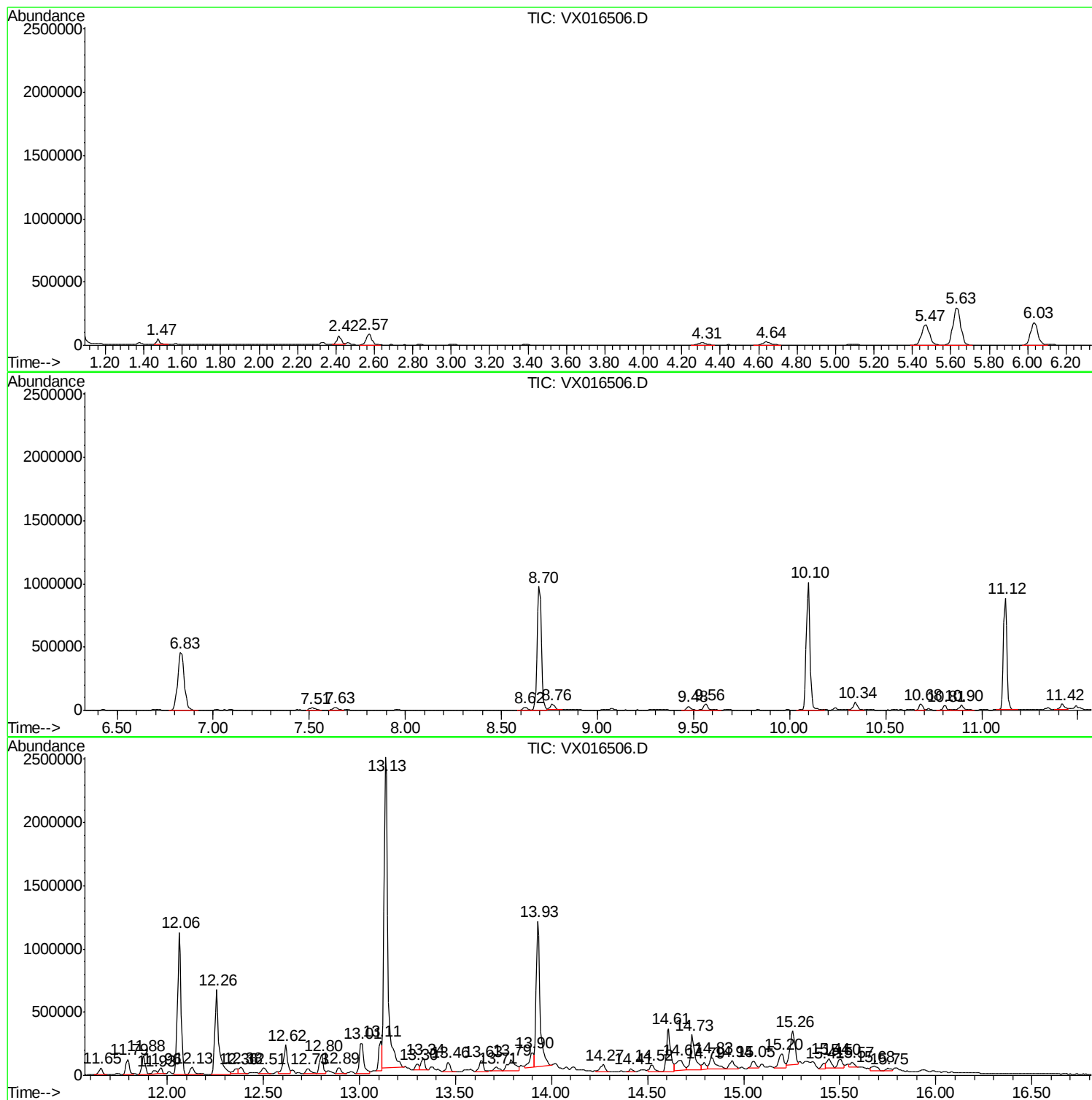
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Instrument :
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ClientSampleId :
WATER-COMP-214-215

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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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

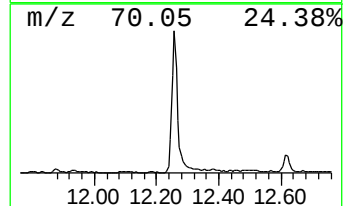
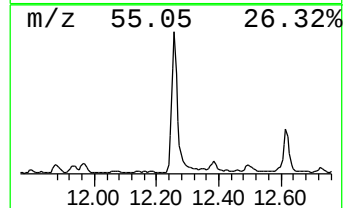
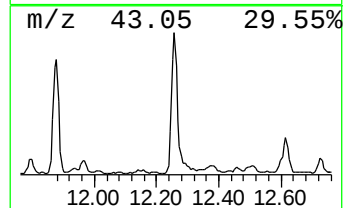
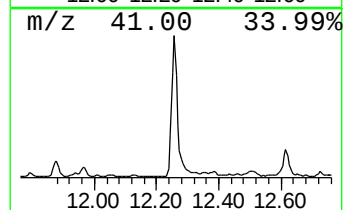
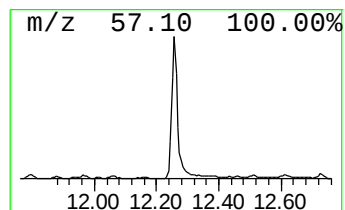
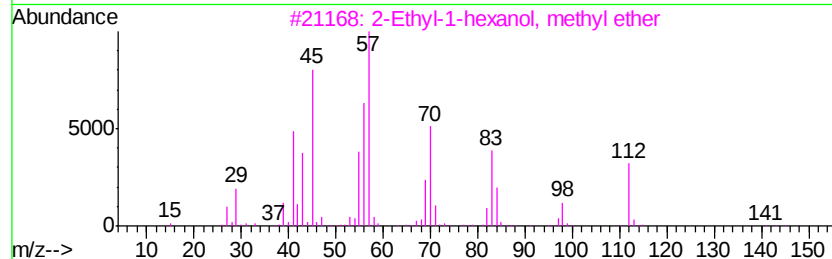
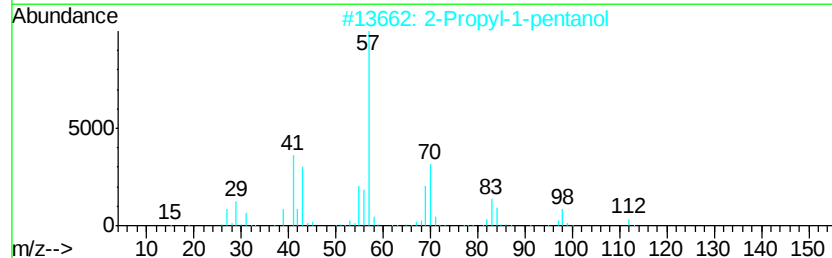
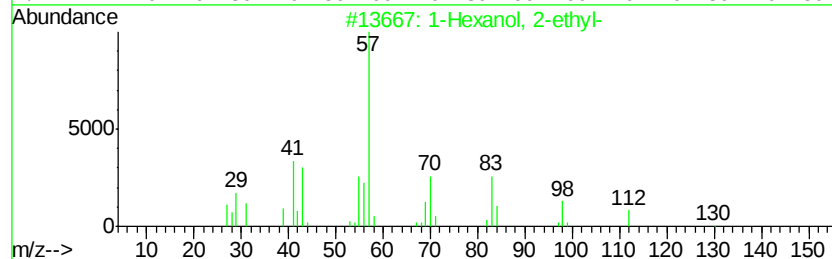
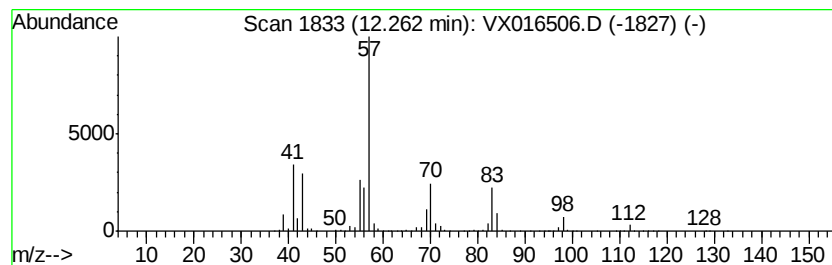
Instrument :
MSVOA_X
ClientSampleId :
WATER-COMP-214-215

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 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.26	35.42 ug/l	1021910	1,4-Dichlorobenzene-d4	12.06		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5		Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45



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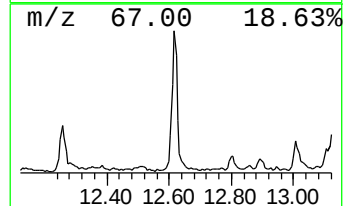
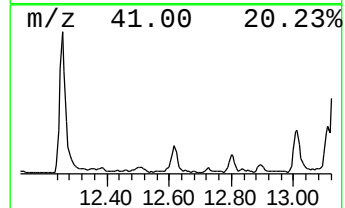
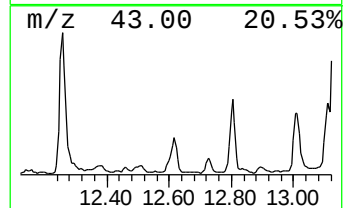
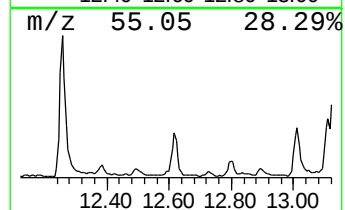
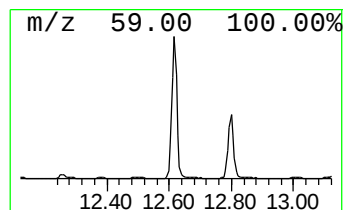
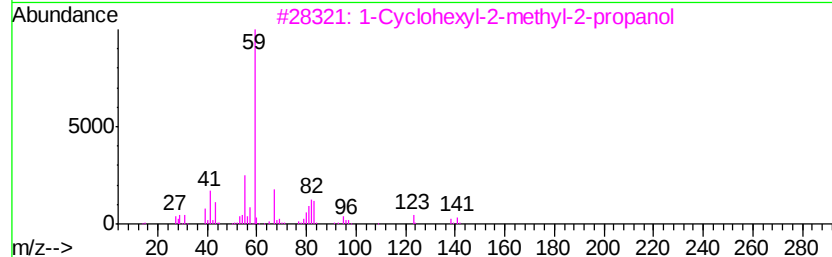
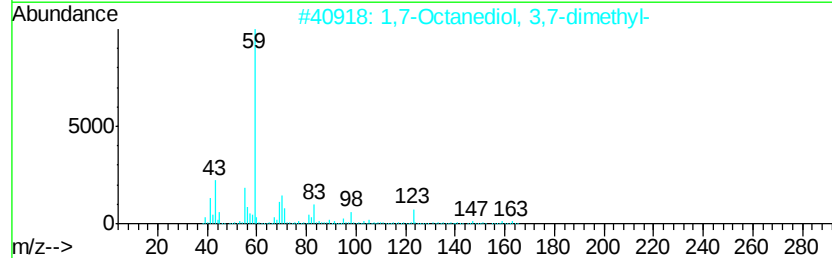
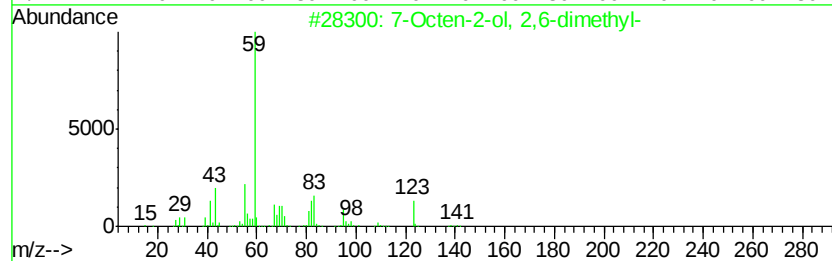
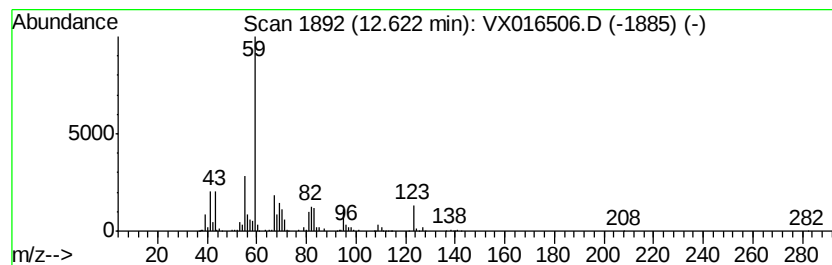
Instrument :
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ClientSampleID :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	11.23 ug/l	323976	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	7-Octen-2-ol, 2,6-dimethyl-	156 C10H20O	018479-58-8	86
2	1,7-Octanediol, 3,7-dimethyl-	174 C10H22O2	000107-74-4	72
3	1-Cyclohexyl-2-methyl-2-propanol	156 C10H20O	005531-30-6	56
4	2-Octanol, 2-methyl-6-methylene-	156 C10H20O	018479-59-9	50
5	1,8-Nonanediol, 8-methyl-	174 C10H22O2	054725-73-4	50



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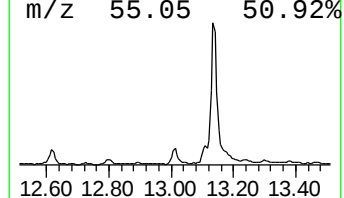
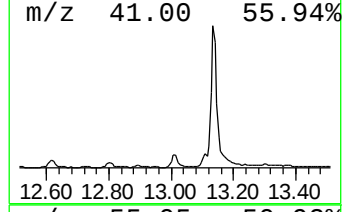
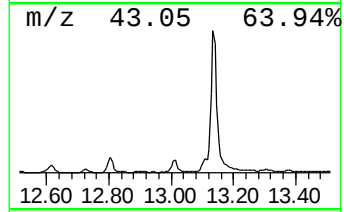
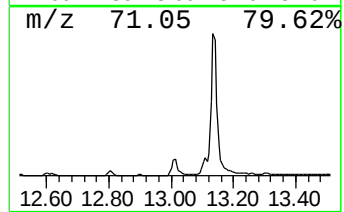
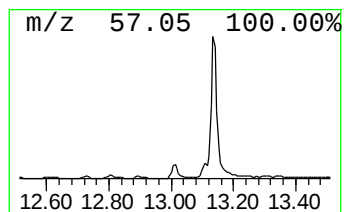
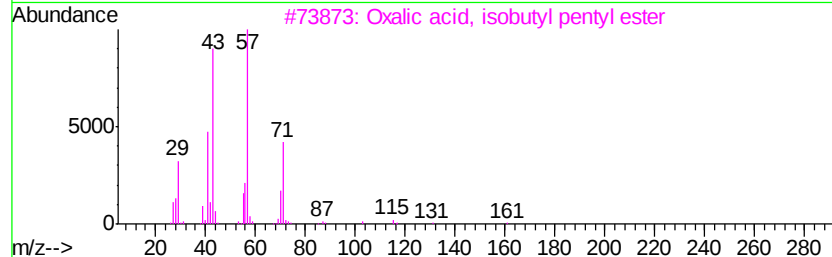
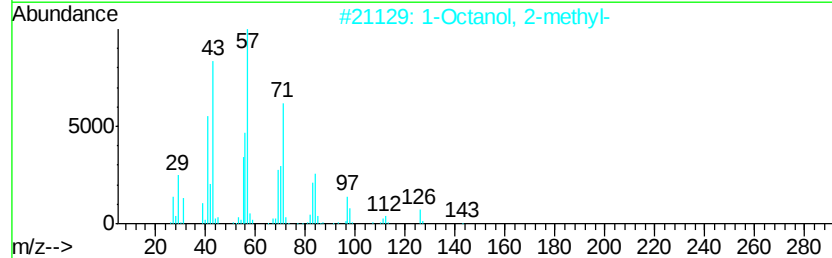
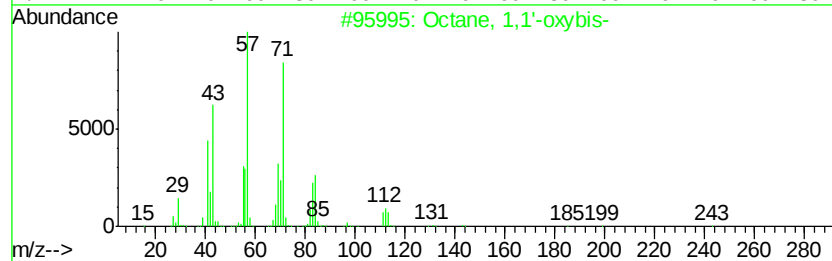
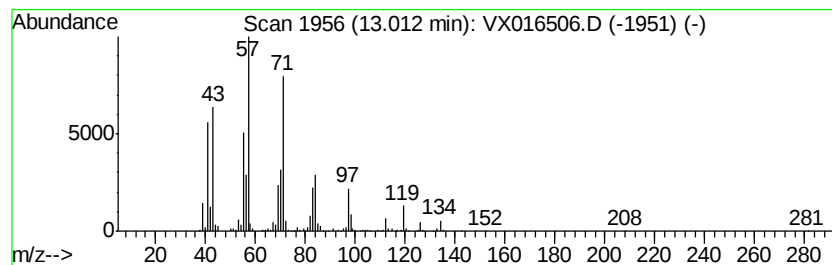
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octane, 1,1'-oxybis- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.01	13.02 ug/l	375751	1,4-Dichlorobenzene-d4	12.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	59
2	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	47
3	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	47
4	Oxalic acid, octyl propyl ester	244	C13H24O4	1000309-26-1	47
5	Isobutyl 3-methylbutan-2-yl carb...	188	C10H20O3	1000372-77-0	43



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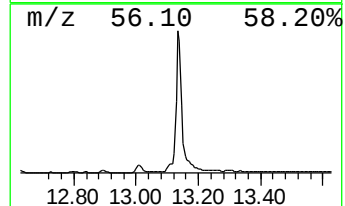
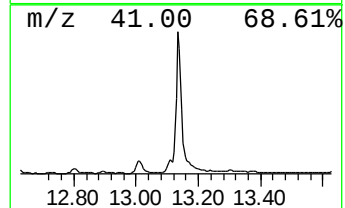
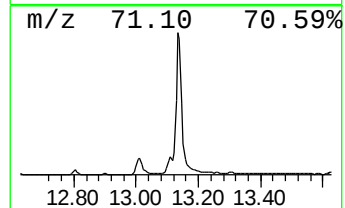
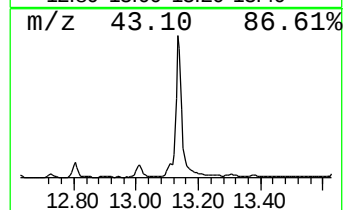
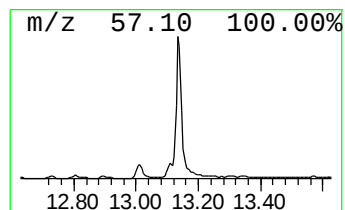
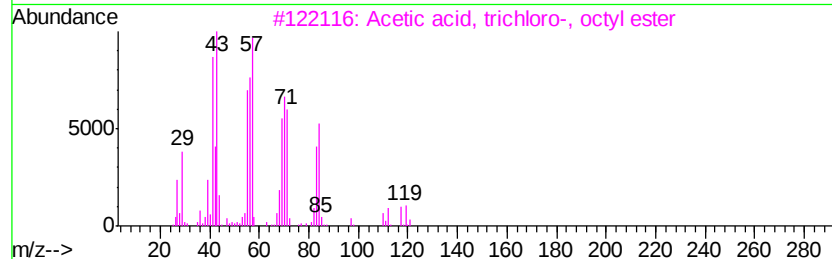
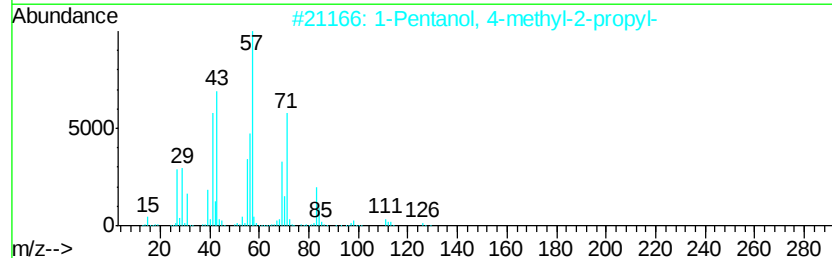
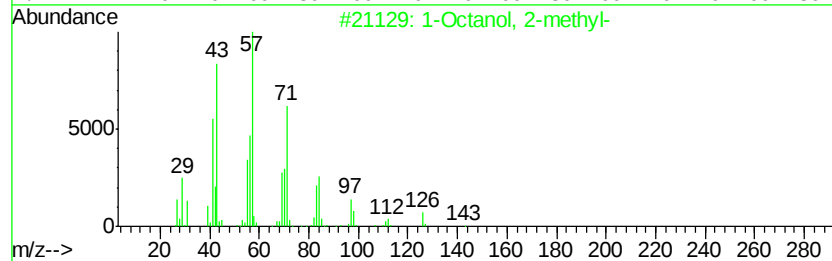
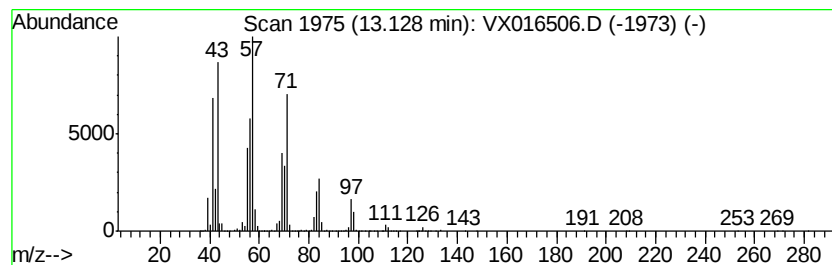
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 5 1-Octanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	117.11 ug/l	3379050	1,4-Dichlorobenzene-d4	12.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	90
2			1-Pentanol, 4-methyl-2-propyl-	144	C9H20O	054004-41-0	59
3			Acetic acid, trichloro-, octyl e...	274	C10H17Cl3O2	016958-78-4	59
4			1-Nonene	126	C9H18	000124-11-8	58
5			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX052920\
Data File : VX016506.D
Acq On : 29 May 2020 13:24
Operator : JC/SP
Sample : L2795-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

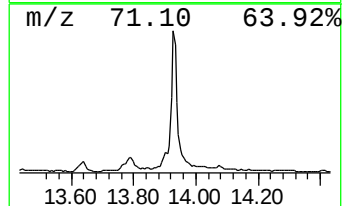
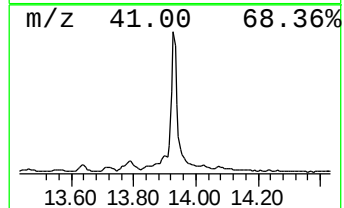
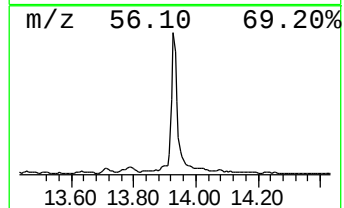
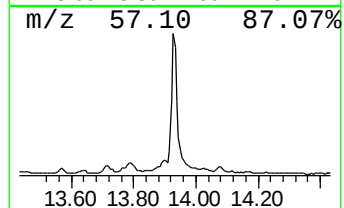
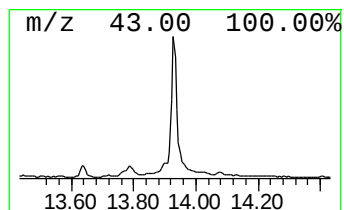
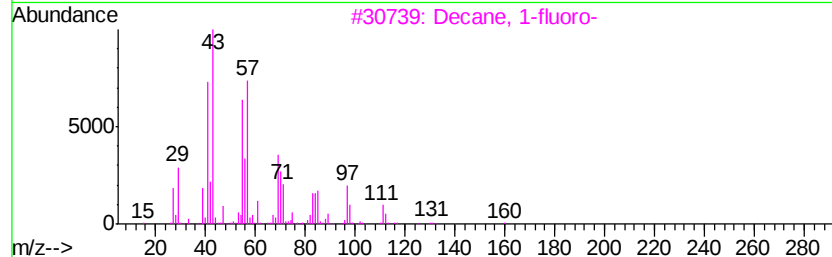
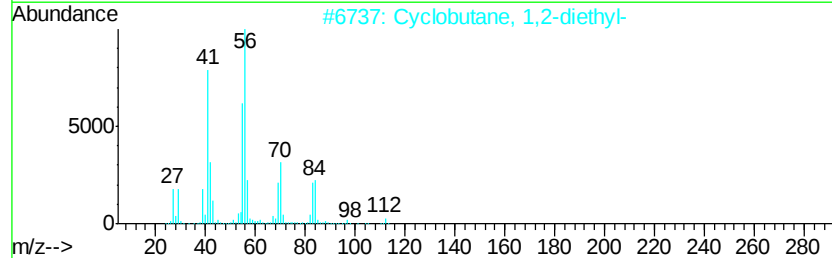
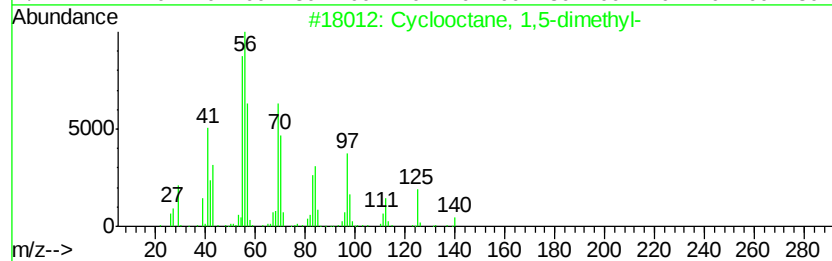
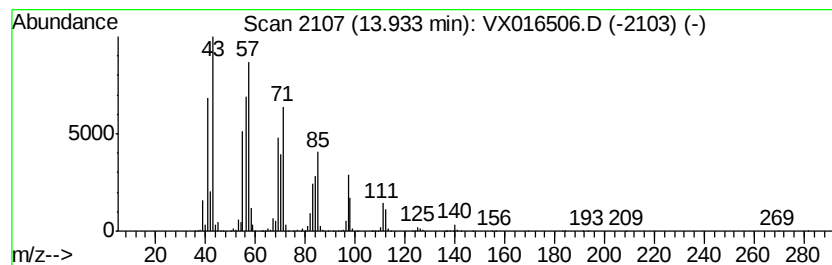
Instrument :
MSVOA_X
ClientSampleId :
WATER-COMP-214-215

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 6 Cyclooctane, 1,5-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.93	54.85 ug/l	1582700	1,4-Dichlorobenzene-d4	12.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane, 1,5-dimethyl-	140	C10H20	021328-57-4	93
2	Cyclobutane, 1,2-diethyl-	112	C8H16	061141-83-1	53
3	Decane, 1-fluoro-	160	C10H21F	000334-56-5	50
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	43
5	Cyclopropane, 1,2-dimethyl-3-pen...	140	C10H20	062238-10-2	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX052920\
Data File : VX016506.D
Acq On : 29 May 2020 13:24
Operator : JC/SP
Sample : L2795-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WATER-COMP-214-215

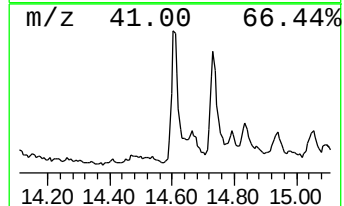
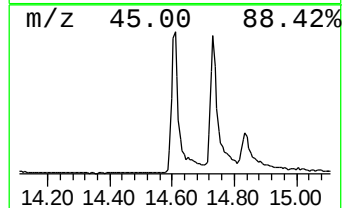
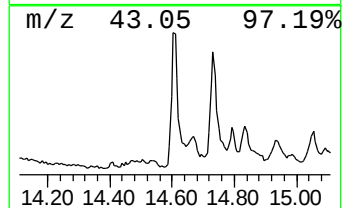
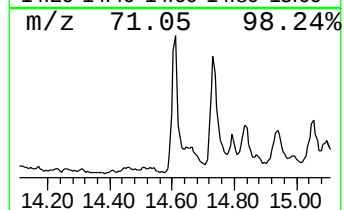
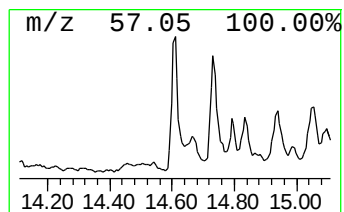
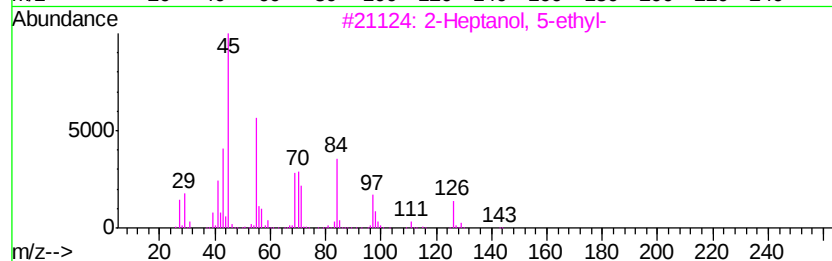
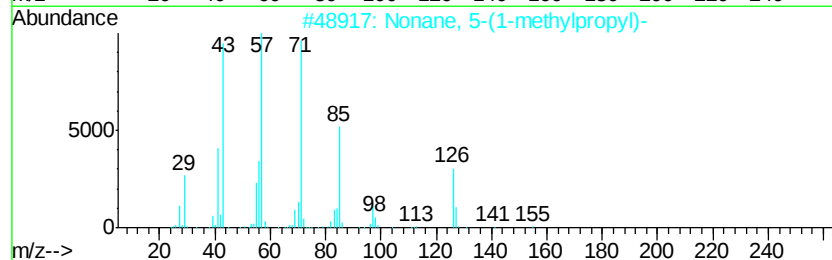
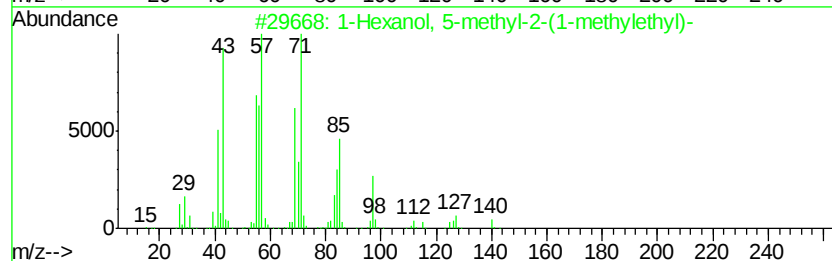
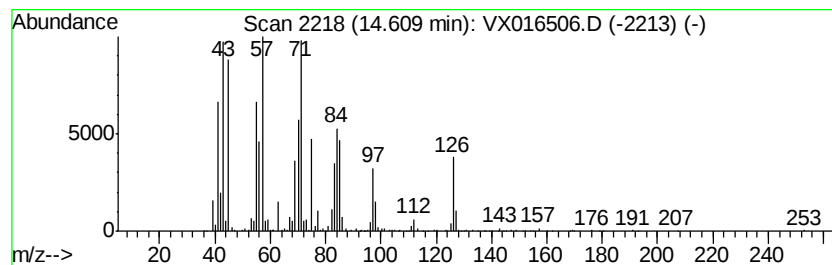
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.61 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	18.54 ug/l	534936	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 5-methyl-2-(1-methyle...	158	C10H22O	002051-33-4	43
2		Nonane, 5-(1-methylpropyl)-	184	C13H28	062185-54-0	38
3		2-Heptanol, 5-ethyl-	144	C9H20O	019780-40-6	38
4		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	38
5		Decane, 3-methyl-	156	C11H24	013151-34-3	35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX052920\
Data File : VX016506.D
Acq On : 29 May 2020 13:24
Operator : JC/SP
Sample : L2795-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WATER-COMP-214-215

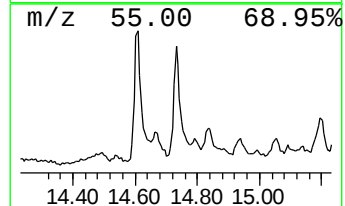
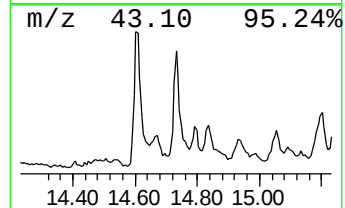
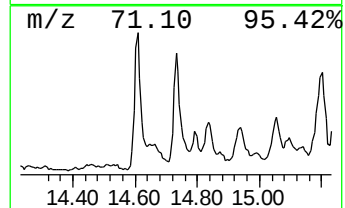
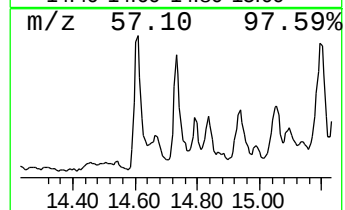
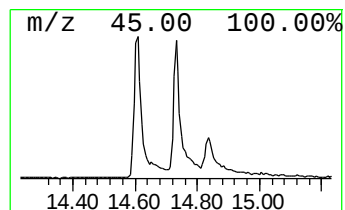
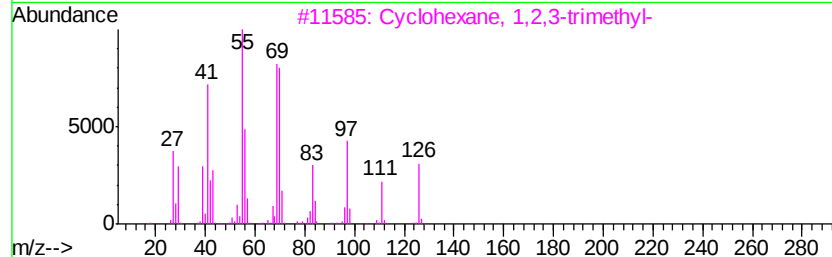
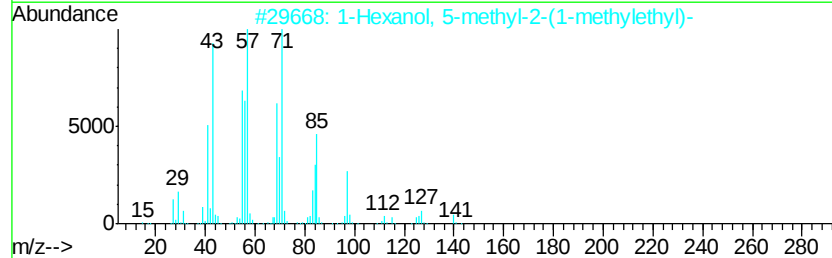
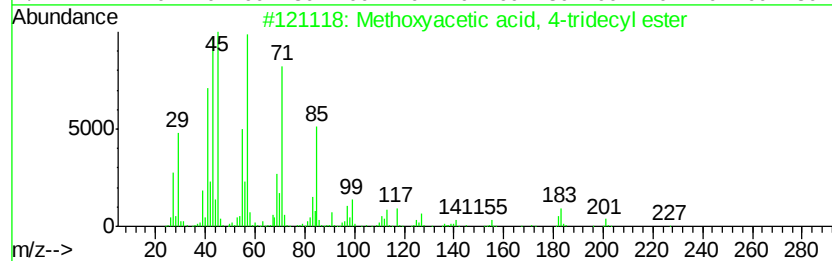
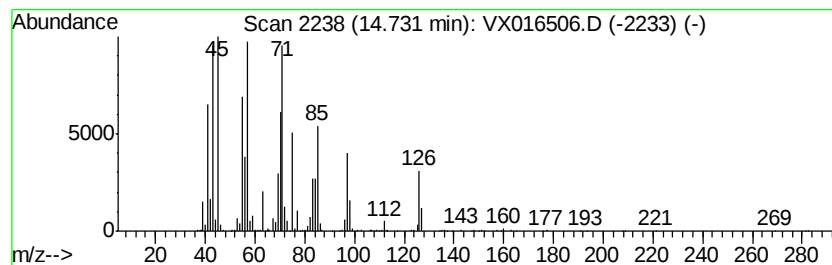
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Quant Title : SW846 8260

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

Peak Number 8 unknown14.73 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	16.54 ug/l	477297	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methoxyacetic acid, 4-tridecyl e...	272	C16H32O3	1000282-04-7	43
2		1-Hexanol, 5-methyl-2-(1-methyle...	158	C10H22O	002051-33-4	43
3		Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	38
4		Nonane, 5-(1-methylpropyl)-	184	C13H28	062185-54-0	38
5		2,3-Dimethyldecane	170	C12H26	017312-44-6	35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX052920\
Data File : VX016506.D
Acq On : 29 May 2020 13:24
Operator : JC/SP
Sample : L2795-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WATER-COMP-214-215

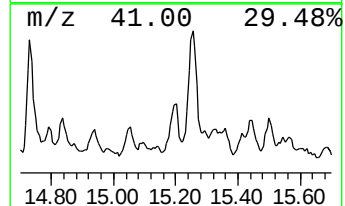
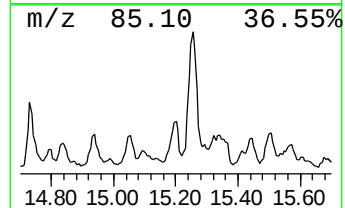
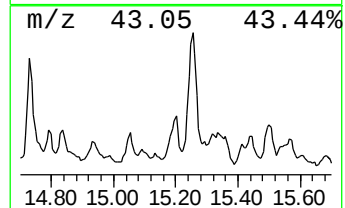
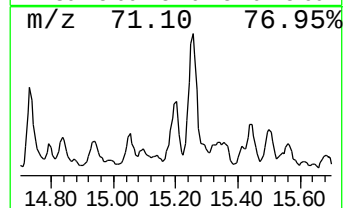
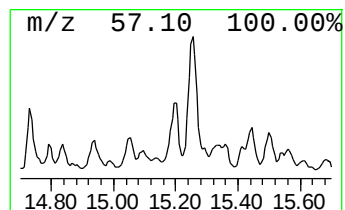
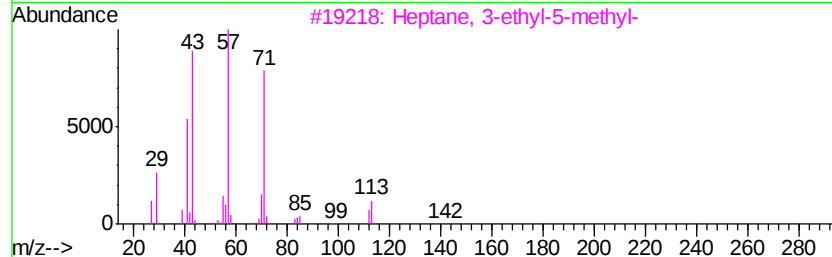
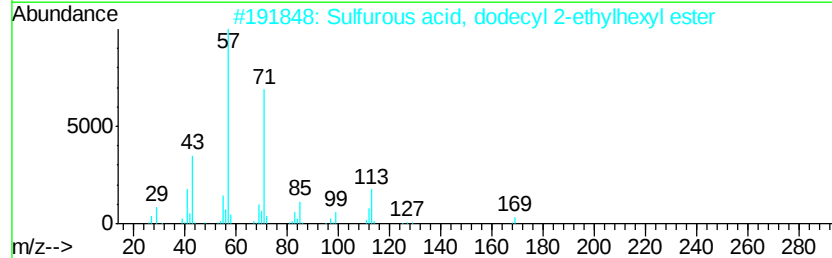
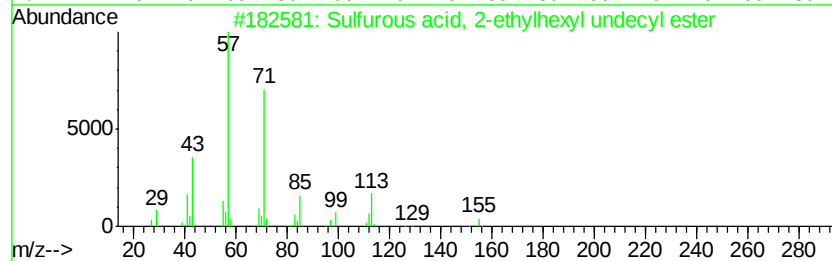
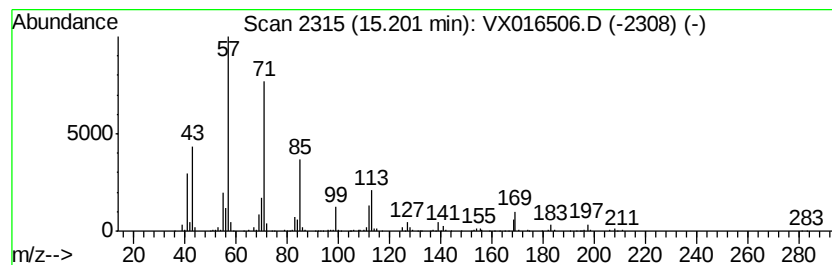
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Quant Title : SW846 8260

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

Peak Number 9 Sulfurous acid, 2-ethylhexy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	7.49 ug/l	216053	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	72
2		Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	72
3		Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	70
4		Tridecane	184	C13H28	000629-50-5	68
5		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX052920\
Data File : VX016506.D
Acq On : 29 May 2020 13:24
Operator : JC/SP
Sample : L2795-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleID :
WATER-COMP-214-215

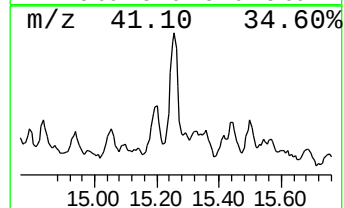
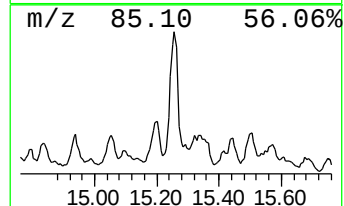
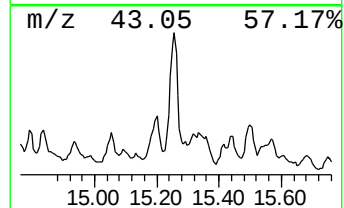
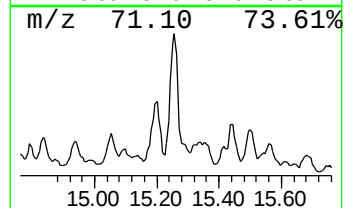
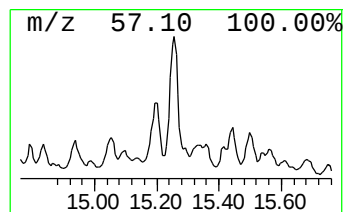
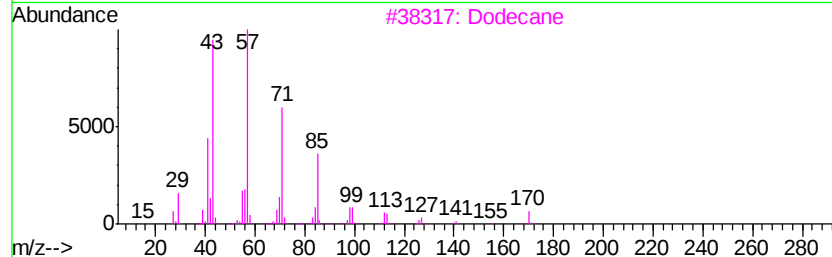
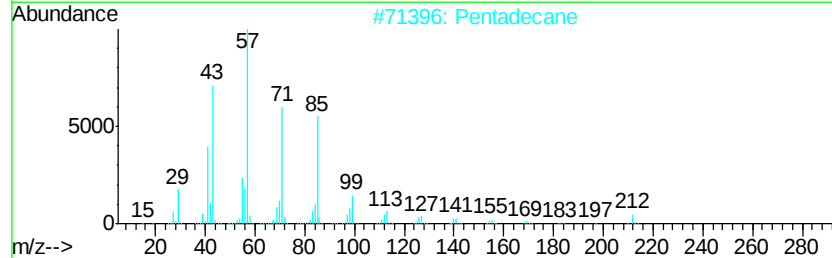
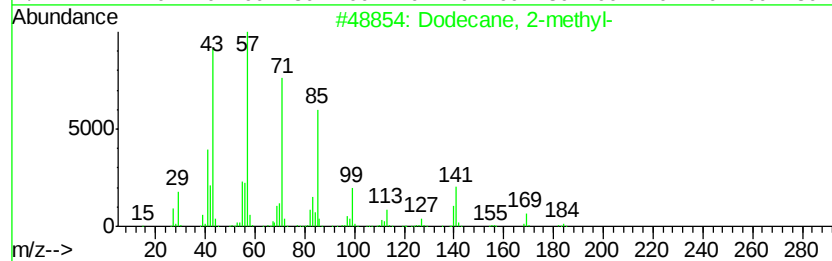
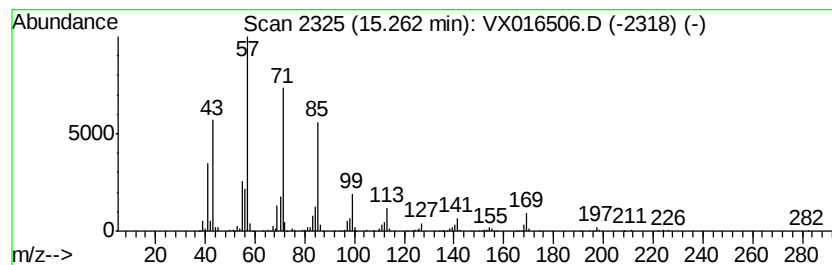
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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

Peak Number 10 Dodecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	16.02 ug/l	462243	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
2		Pentadecane	212	C15H32	000629-62-9	87
3		Dodecane	170	C12H26	000112-40-3	86
4		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86
5		Pentadecane, 2-methyl-	226	C16H34	001560-93-6	86



Data Path : Z:\V0ASRV\HPCHEM1\MSV0A_X\DATA\VX052920\
Data File : VX016506.D
Acq On : 29 May 2020 13:24
Operator : JC/SP
Sample : L2795-05
Misc : 5.0mL/MSV0A_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSV0A_X
ClientSampleId :
WATER-COMP-214-215

Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_X\METHOD\82X052720W.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
1-Hexanol, 2-ethyl-	12.26	35.4	ug/l	1021910	4	12.06	1442730	50.0
7-Octen-2-ol, 2,6...	12.62	11.2	ug/l	323976	4	12.06	1442730	50.0
Octane, 1,1'-oxybis-	13.01	13.0	ug/l	375751	4	12.06	1442730	50.0
1-Octanol, 2-methyl-	13.13	117.1	ug/l	3379050	4	12.06	1442730	50.0
Cyclooctane, 1,5-...	13.93	54.9	ug/l	1582700	4	12.06	1442730	50.0
unknown14.61	14.61	18.5	ug/l	534936	4	12.06	1442730	50.0
unknown14.73	14.73	16.5	ug/l	477297	4	12.06	1442730	50.0
Sulfurous acid, 2...	15.20	7.5	ug/l	216053	4	12.06	1442730	50.0
Dodecane, 2-methyl-	15.26	16.0	ug/l	462243	4	12.06	1442730	50.0