

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
 Data File : VX014426.D
 Acq On : 06 Jan 2020 14:45
 Operator : JC/SP
 Sample : K6484-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30628

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\82X121319W.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	1.070	26	30	43	rBV	642210	804389	4.94%	0.672%
2	1.168	43	46	52	rVV	373395	333431	2.05%	0.278%
3	1.491	94	99	140	rBV	5726542	16279937	100.00%	13.594%
4	4.332	551	565	594	rBV	928025	3155421	19.38%	2.635%
5	5.490	745	755	766	rBV	287557	804143	4.94%	0.671%
6	5.648	771	781	797	rVB	526780	1468059	9.02%	1.226%
7	5.965	824	833	840	rBV	64174	224608	1.38%	0.188%
8	6.057	840	848	855	rVV	329298	895454	5.50%	0.748%
9	6.136	855	861	869	rVB3	70171	188011	1.15%	0.157%
10	6.849	960	978	987	rBV2	1191148	4883960	30.00%	4.078%
11	7.374	1051	1064	1092	rBV	266825	1488086	9.14%	1.243%
12	8.709	1277	1283	1290	rBV	1707328	2606947	16.01%	2.177%
13	8.782	1290	1295	1300	rVB	116445	177378	1.09%	0.148%
14	9.136	1349	1353	1364	rVB	123383	184954	1.14%	0.154%
15	9.306	1375	1381	1396	rVB	191214	397564	2.44%	0.332%
16	10.050	1495	1503	1507	rBV2	139250	347922	2.14%	0.291%
17	10.105	1507	1512	1524	rVV	1680447	2433585	14.95%	2.032%
18	10.209	1524	1529	1545	rVV	345527	572576	3.52%	0.478%
19	10.367	1547	1555	1564	rVB2	445421	739093	4.54%	0.617%
20	10.800	1622	1626	1635	rBV	329375	448638	2.76%	0.375%
21	11.129	1675	1680	1686	rBV	1362925	1791363	11.00%	1.496%
22	11.684	1767	1771	1776	rVV	560313	815462	5.01%	0.681%
23	11.733	1776	1779	1786	rVB	314143	363149	2.23%	0.303%
24	11.800	1786	1790	1797	rBV	542877	735696	4.52%	0.614%
25	11.916	1806	1809	1818	rVB2	308111	419476	2.58%	0.350%
26	12.038	1824	1829	1831	rBV2	238817	311541	1.91%	0.260%
27	12.074	1831	1835	1842	rVB	1840465	2331665	14.32%	1.947%
28	12.263	1861	1866	1877	rBV	4379524	5304492	32.58%	4.429%
29	12.355	1877	1881	1887	rVB2	198153	311572	1.91%	0.260%
30	12.464	1895	1899	1904	rBV2	251945	339859	2.09%	0.284%
31	12.635	1916	1927	1932	rBV4	358800	869325	5.34%	0.726%
32	12.733	1939	1943	1947	rBV	375476	453652	2.79%	0.379%
33	12.787	1947	1952	1954	rBV	130325	199379	1.22%	0.166%
34	12.867	1954	1965	1971	rBV4	1085586	2353158	14.45%	1.965%

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35	12.940	1971	1977	1983	rBV3	1350871	3199849	19.66%	2.672%
36	12.995	1983	1986	1988	rBV2	906531	1008650	6.20%	0.842%
37	13.025	1988	1991	1998	rVB3	2032809	3069550	18.85%	2.563%
38	13.092	1998	2002	2006	rVB	1764667	1947844	11.96%	1.627%
39	13.141	2006	2010	2016	rBV4	481350	992193	6.09%	0.829%
40	13.208	2018	2021	2022	rBV3	195396	206760	1.27%	0.173%
41	13.257	2027	2029	2031	rBV	272761	297844	1.83%	0.249%
42	13.348	2037	2044	2049	rBV2	2803748	4466773	27.44%	3.730%
43	13.397	2049	2052	2055	rBV	1236107	1682662	10.34%	1.405%
44	13.434	2055	2058	2061	rBV	4798907	5530872	33.97%	4.618%
45	13.470	2061	2064	2066	rVB4	1166027	1365400	8.39%	1.140%
46	13.549	2073	2077	2082	rVB5	839160	1490206	9.15%	1.244%
47	13.604	2083	2086	2089	rVB2	371794	356142	2.19%	0.297%
48	13.653	2089	2094	2098	rBV6	668196	1598507	9.82%	1.335%
49	13.732	2103	2107	2108	rVV	1843715	2363290	14.52%	1.973%
50	13.751	2108	2110	2113	rVV2	2181978	3038667	18.67%	2.537%
51	13.787	2113	2116	2119	rVV2	3590722	4868895	29.91%	4.066%
52	13.818	2119	2121	2124	rVV3	2987685	3338401	20.51%	2.788%
53	13.854	2124	2127	2130	rVV	5948965	7872531	48.36%	6.574%
54	13.891	2130	2133	2137	rVV2	4850865	7233272	44.43%	6.040%
55	13.958	2141	2144	2151	rVB6	1382381	2793220	17.16%	2.332%
56	14.043	2156	2158	2160	rBV2	378148	415898	2.55%	0.347%
57	14.122	2168	2171	2173	rBV3	531392	653246	4.01%	0.545%
58	14.153	2173	2176	2179	rVB3	813610	1010189	6.21%	0.844%
59	14.238	2188	2190	2193	rVB	569733	529168	3.25%	0.442%
60	14.458	2223	2226	2228	rBV2	251413	331210	2.03%	0.277%
61	14.494	2229	2232	2235	rVB	551768	633483	3.89%	0.529%
62	14.549	2238	2241	2243	rBV2	370261	450480	2.77%	0.376%
63	14.610	2248	2251	2257	rVB2	450833	737329	4.53%	0.616%
64	14.665	2257	2260	2272	rVB2	425948	752197	4.62%	0.628%
65	14.891	2295	2297	2311	rVB8	126698	316882	1.95%	0.265%
66	15.951	2466	2471	2477	rBV4	72310	169423	1.04%	0.141%

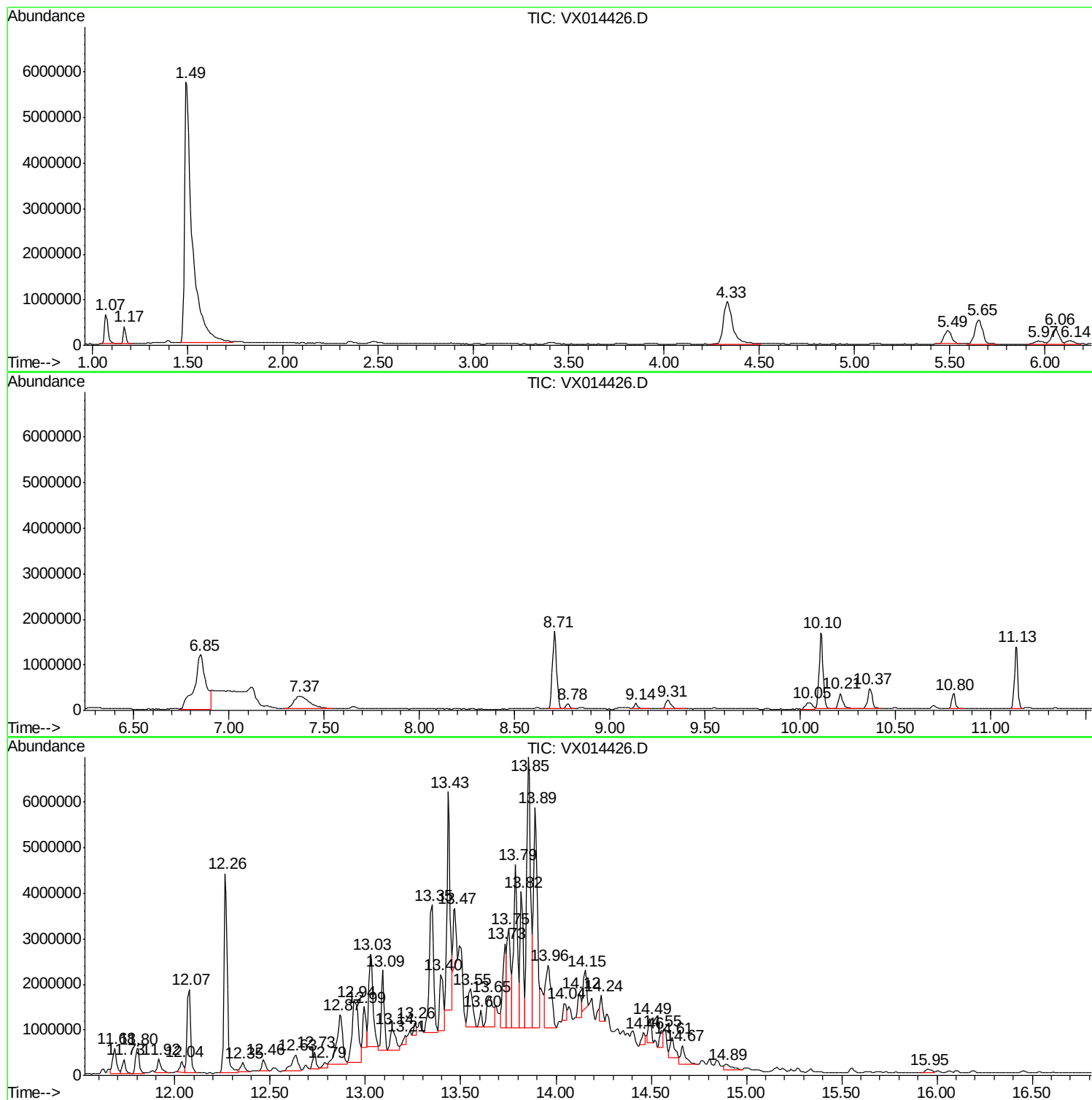
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Quant Title : SW846 8260

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



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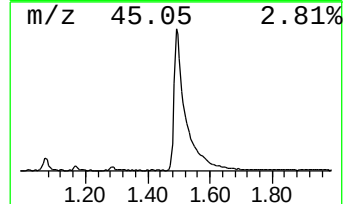
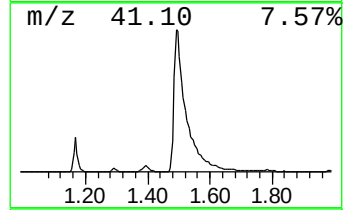
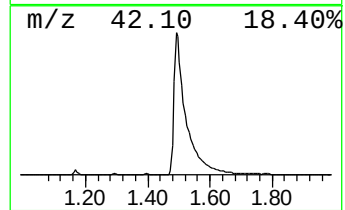
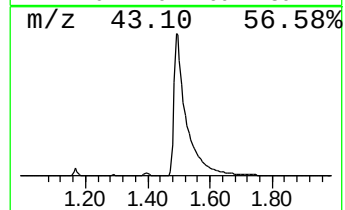
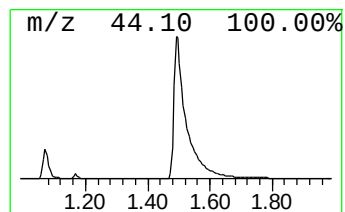
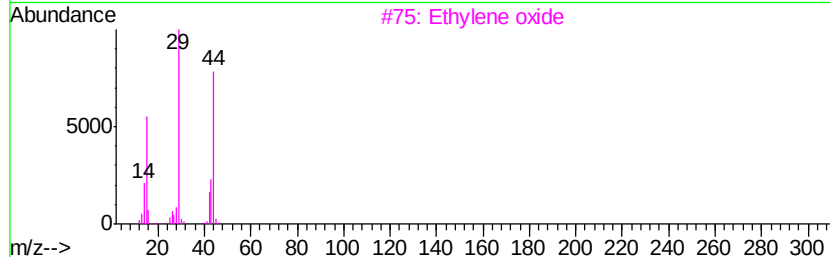
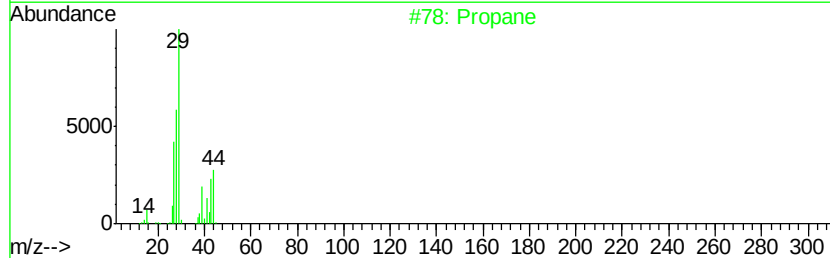
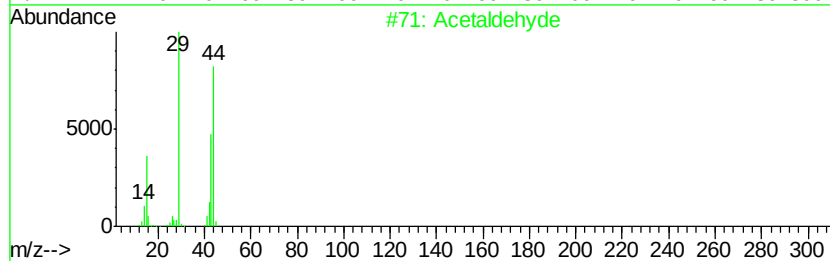
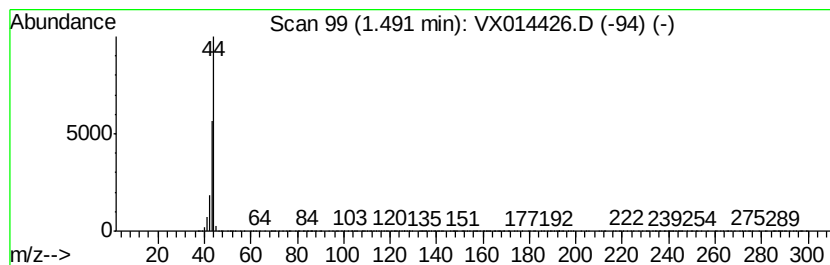
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
1.49	554.47 ug/l	16279900	Pentafluorobenzene	5.65		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde		44	C2H4O	000075-07-0	64
2	Propane		44	C3H8	000074-98-6	5
3	Ethylene oxide		44	C2H4O	000075-21-8	5
4	Alanine		89	C3H7NO2	000056-41-7	4
5	1,2-Propanediamine		74	C3H10N2	000078-90-0	4



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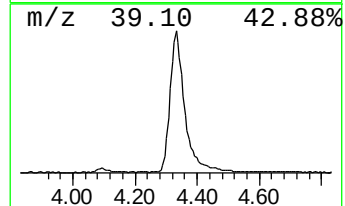
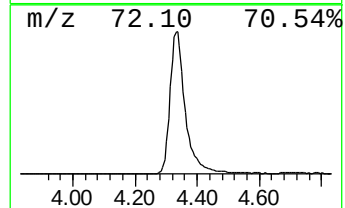
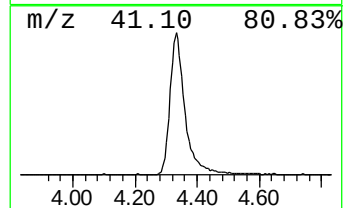
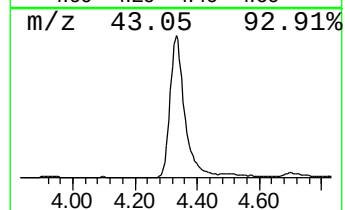
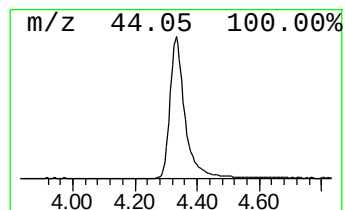
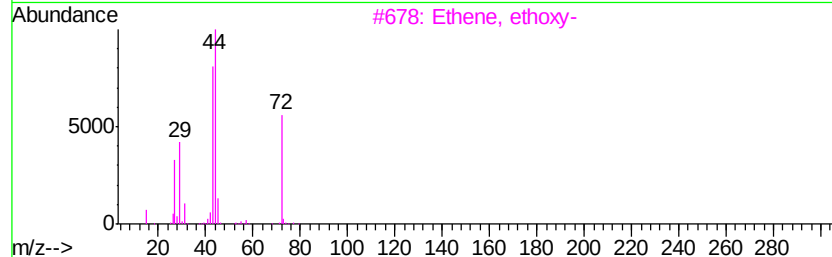
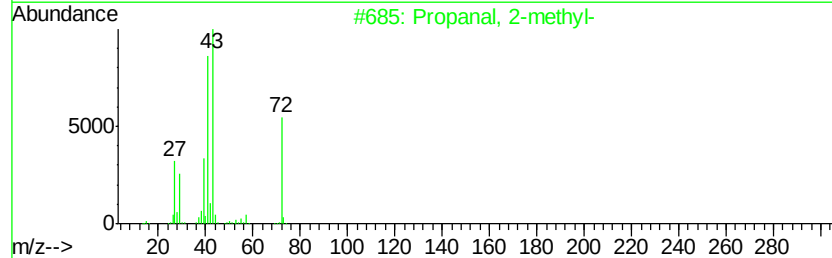
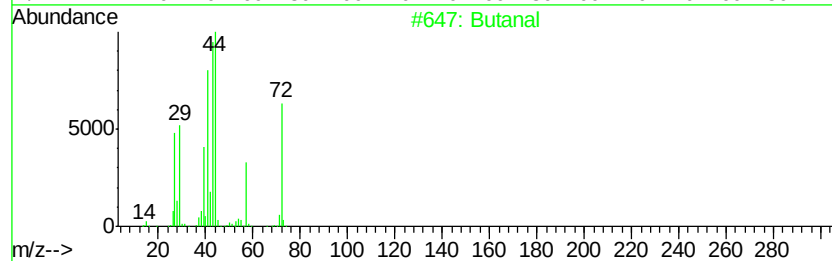
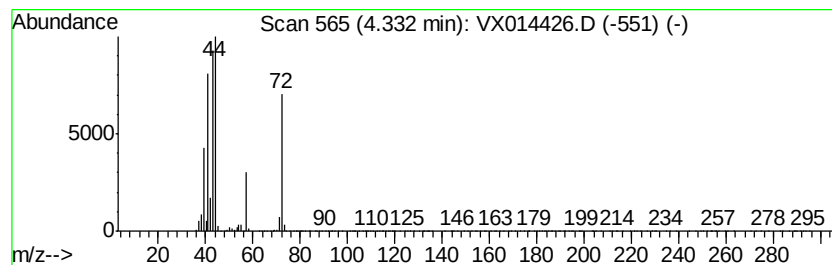
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	107.47 ug/l	3155420	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal		72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-		72	C4H8O	000078-84-2	52
3	Ethene, ethoxy-		72	C4H8O	000109-92-2	52
4	1-Propene, 3-methoxy-		72	C4H8O	000627-40-7	32
5	Methacrolein		70	C4H6O	000078-85-3	22



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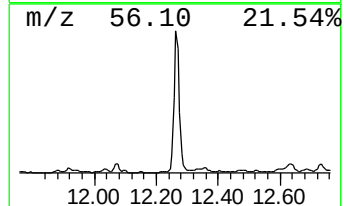
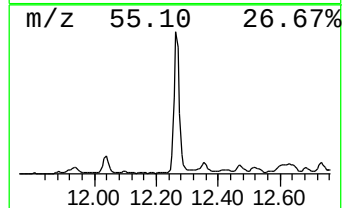
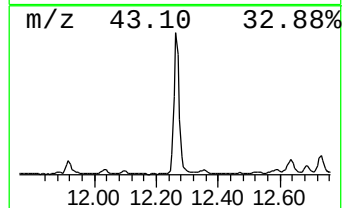
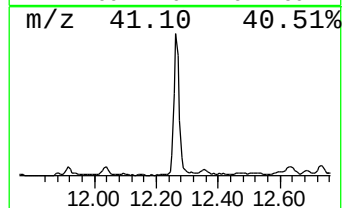
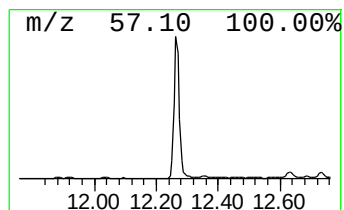
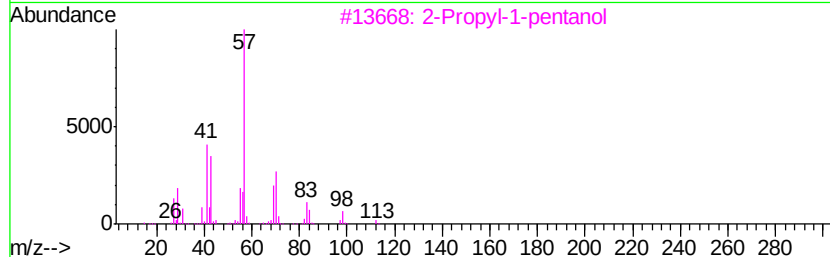
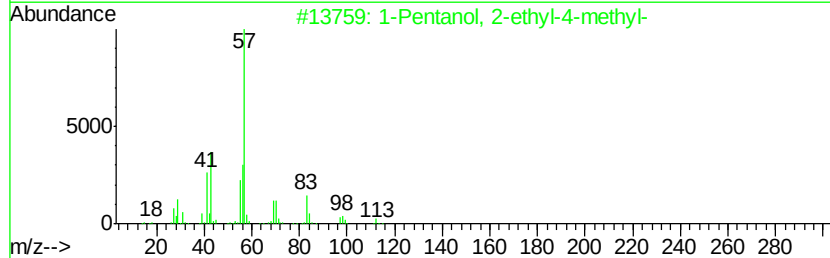
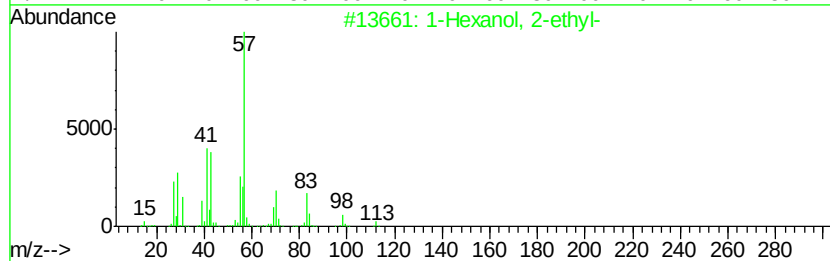
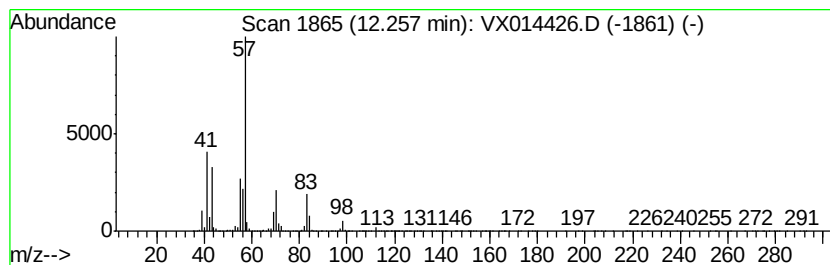
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	113.75 ug/l	5304490	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4		1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47
5		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



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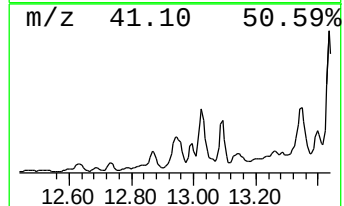
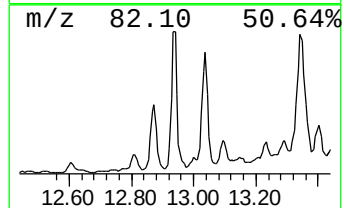
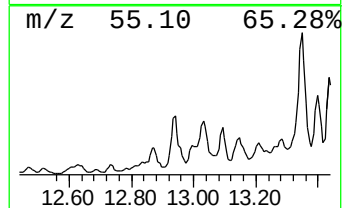
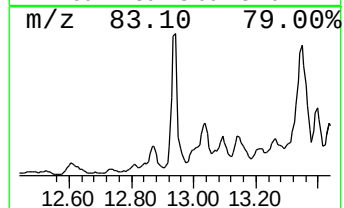
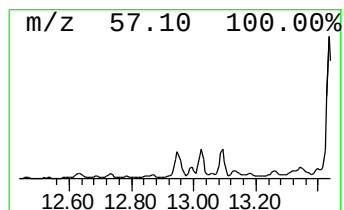
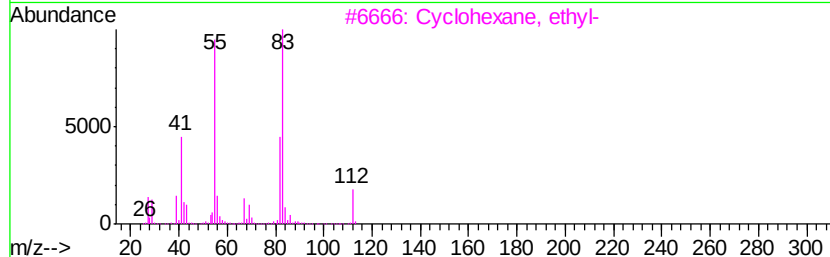
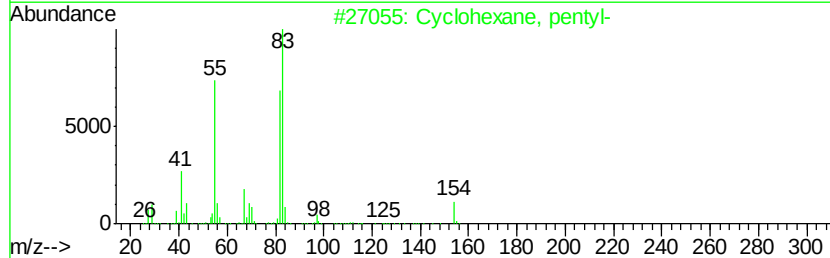
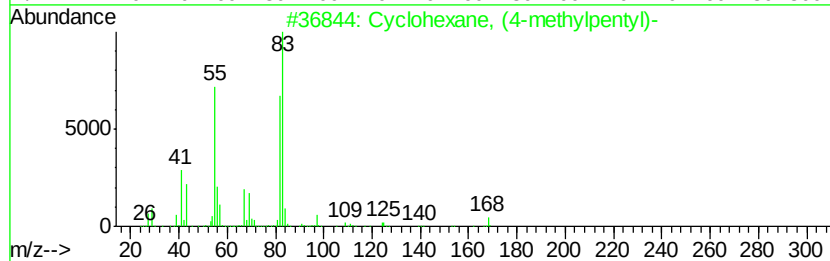
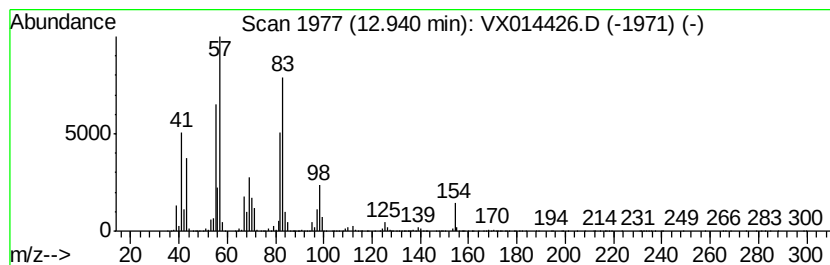
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexane, (4-methylpentyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.94	68.62 ug/l	3199850	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	64
2		Cyclohexane, pentyl-	154	C11H22	004292-92-6	52
3		Cyclohexane, ethyl-	112	C8H16	001678-91-7	52
4		Cyclohexane, (3-methylpentyl)-	168	C12H24	061142-38-9	47
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	43



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ClientSampled :
30628

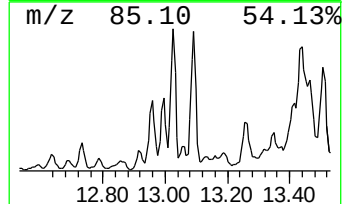
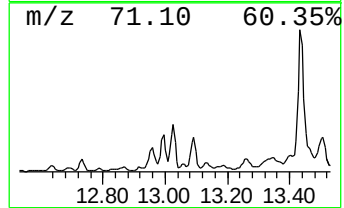
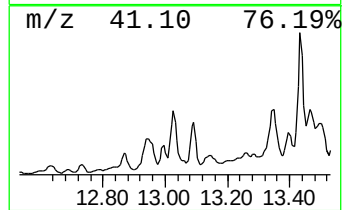
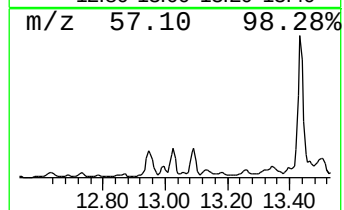
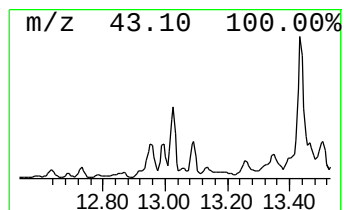
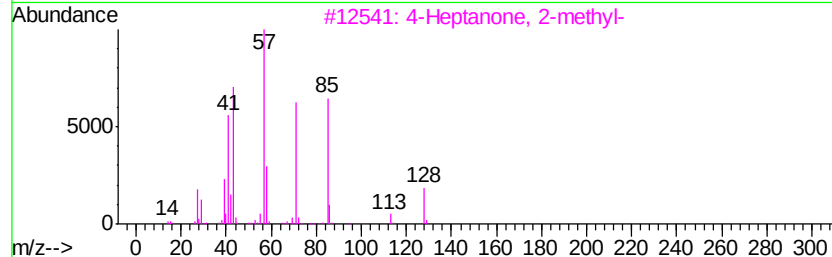
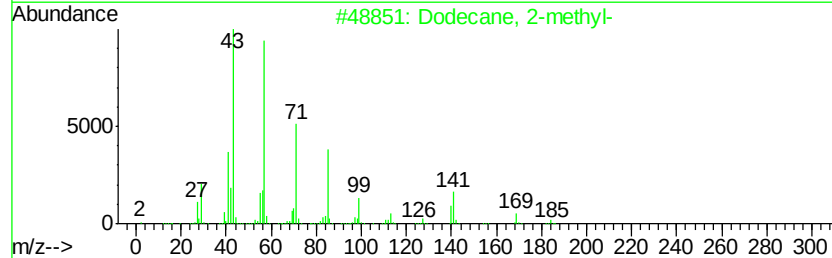
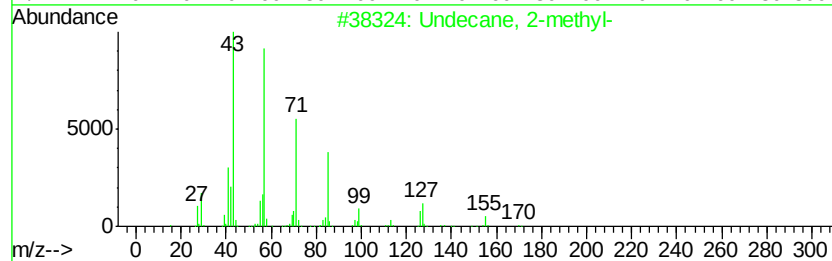
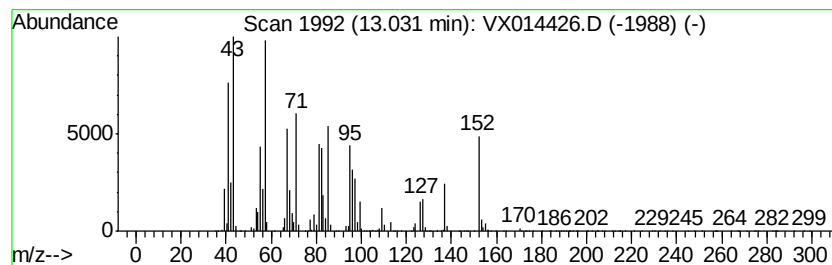
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Quant Title : SW846 8260

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

Peak Number 5 Undecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.03	65.82 ug/l	3069550	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane, 2-methyl-	170	C12H26	007045-71-8	91
2		Dodecane, 2-methyl-	184	C13H28	001560-97-0	68
3		4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	53
4		Undecane, 4-methyl-	170	C12H26	002980-69-0	49
5		Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	49



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014426.D
Acq On : 06 Jan 2020 14:45
Operator : JC/SP
Sample : K6484-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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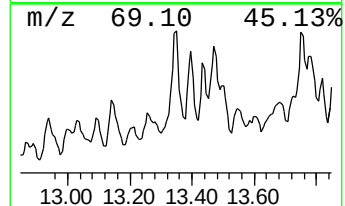
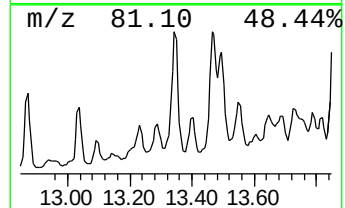
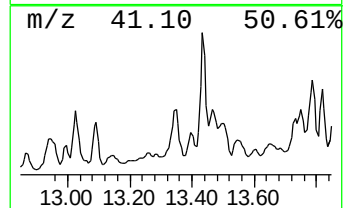
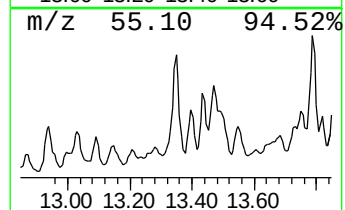
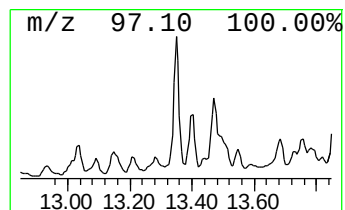
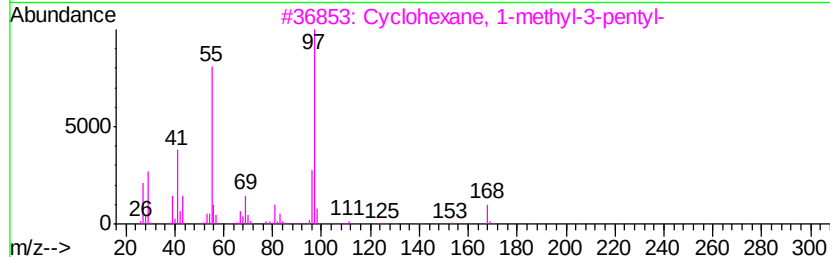
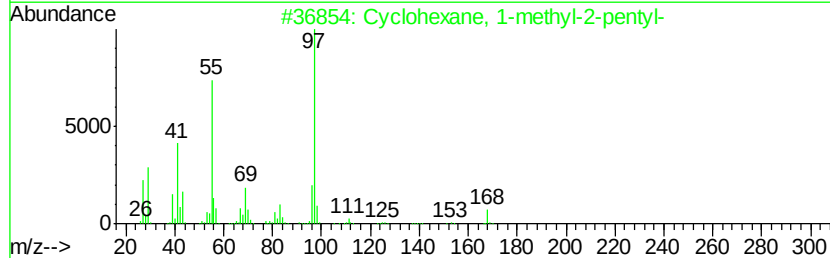
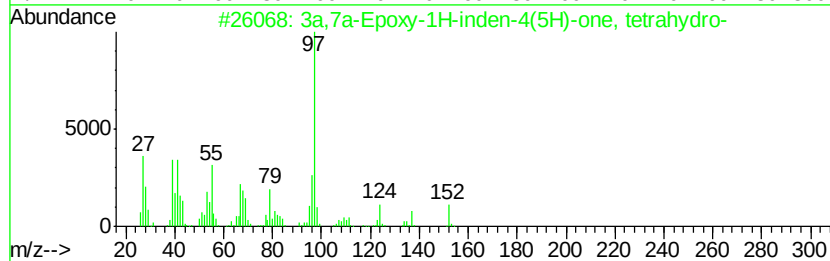
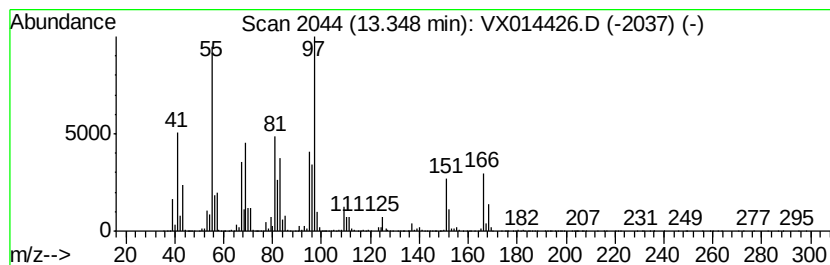
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Quant Title : SW846 8260

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

Peak Number 6 unknown13.35 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	95.79 ug/l	4466770	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3a,7a-Epoxy-1H-inden-4(5H)-one, ...	152	C9H12O2	039746-31-1	46
2		Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	46
3		Cyclohexane, 1-methyl-3-pentyl-	168	C12H24	054411-02-8	43
4		Trans-1-methyl-2-nonyl-cyclohexane	224	C16H32	1000371-47-8	38
5		Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014426.D
Acq On : 06 Jan 2020 14:45
Operator : JC/SP
Sample : K6484-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
30628

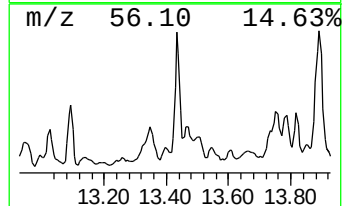
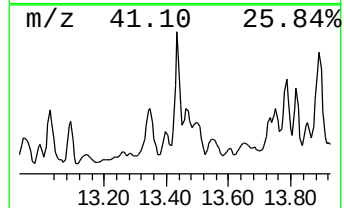
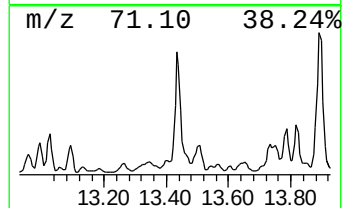
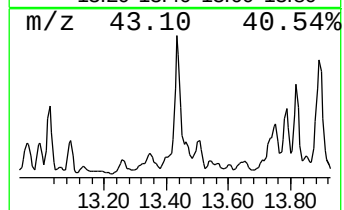
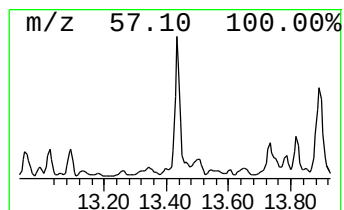
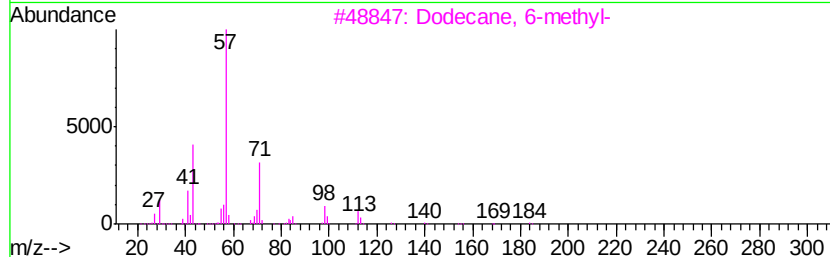
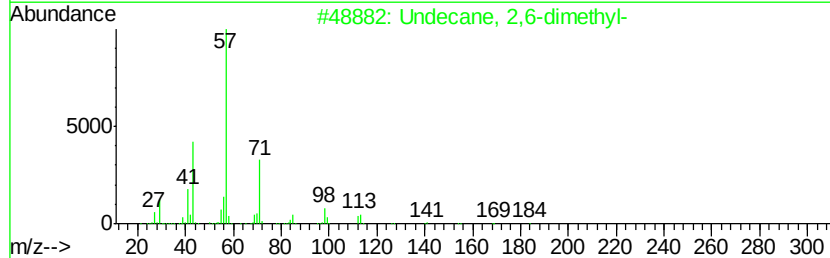
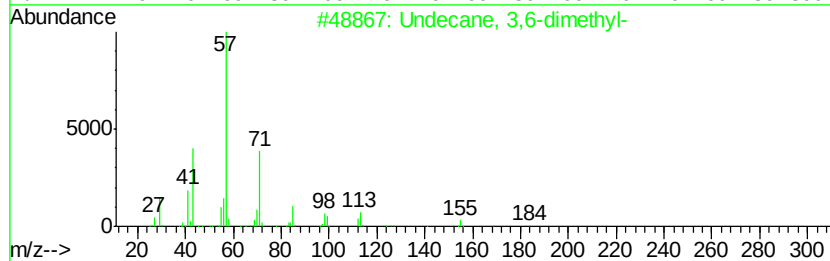
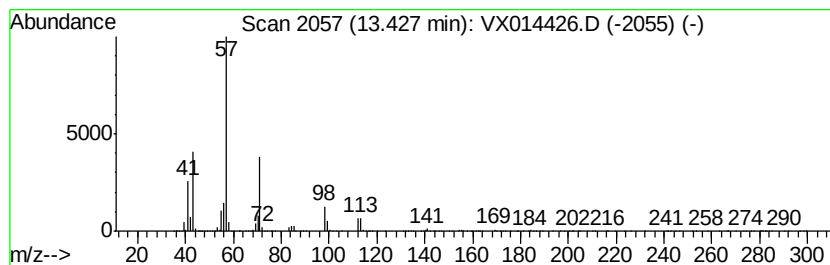
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Quant Title : SW846 8260

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

Peak Number 7 Undecane, 3,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	118.60 ug/l	5530870	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	87	
2	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	87	
3	Dodecane, 6-methyl-	184	C13H28	006044-71-9	76	
4	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	72	
5	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	64	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014426.D
Acq On : 06 Jan 2020 14:45
Operator : JC/SP
Sample : K6484-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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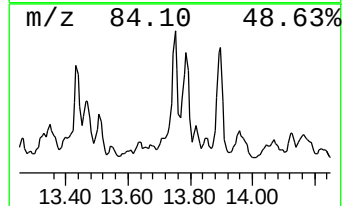
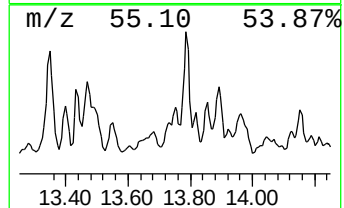
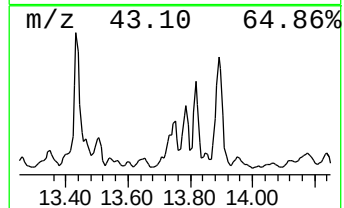
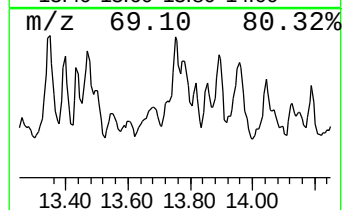
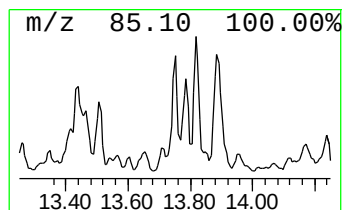
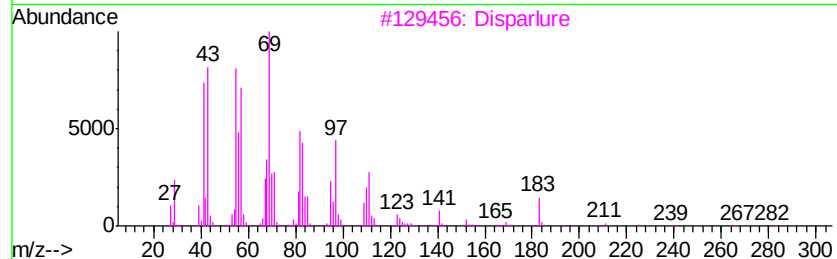
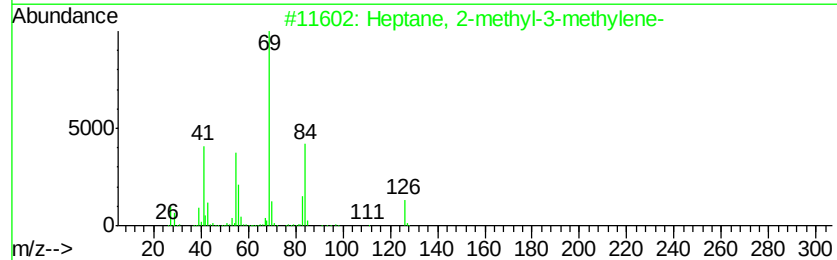
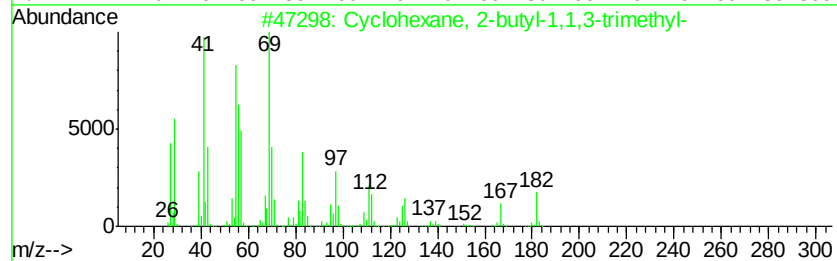
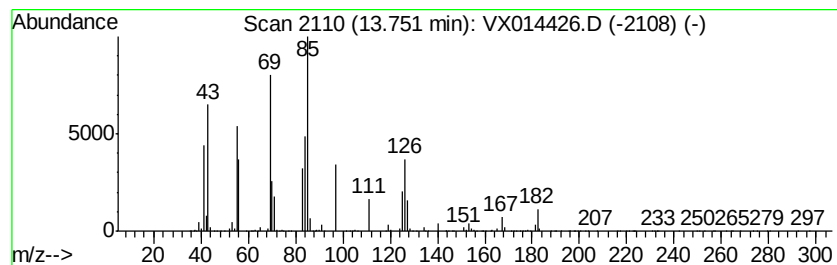
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 8 unknown13.75 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	65.16 ug/l	3038670	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 2-butyl-1,1,3-trime...	182	C13H26	054676-39-0	46
2		Heptane, 2-methyl-3-methylene-	126	C9H18	062187-11-5	38
3		Disparlure	282	C19H38O	029804-22-6	35
4		Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	35
5		Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	001839-88-9	35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014426.D
Acq On : 06 Jan 2020 14:45
Operator : JC/SP
Sample : K6484-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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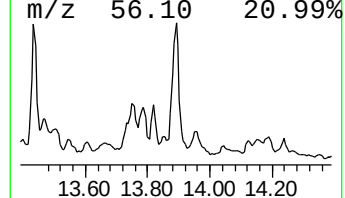
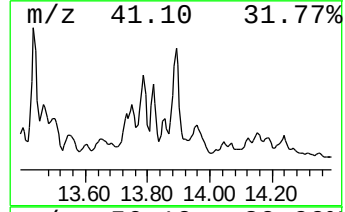
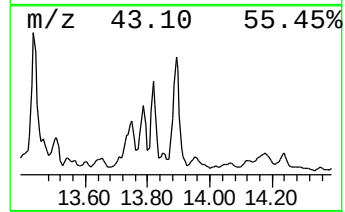
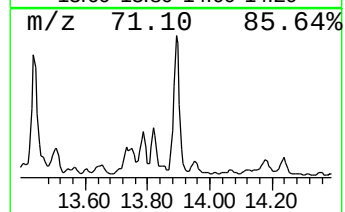
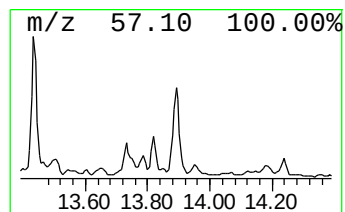
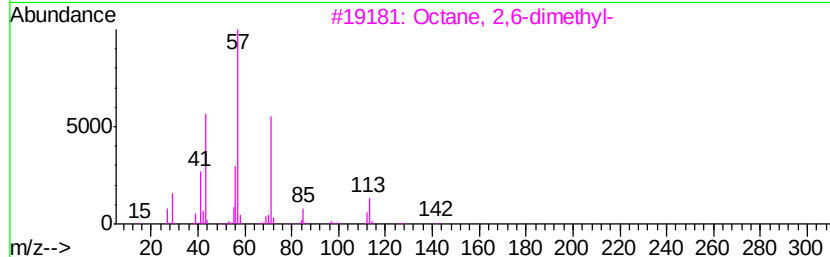
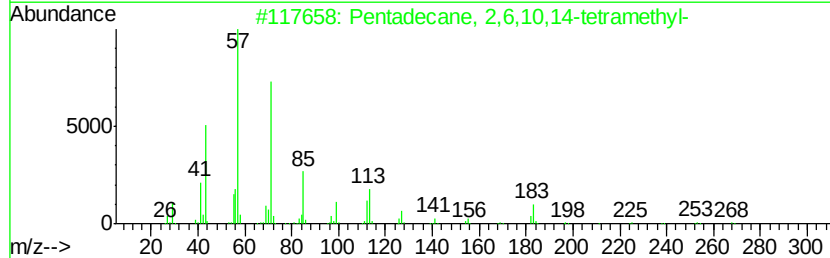
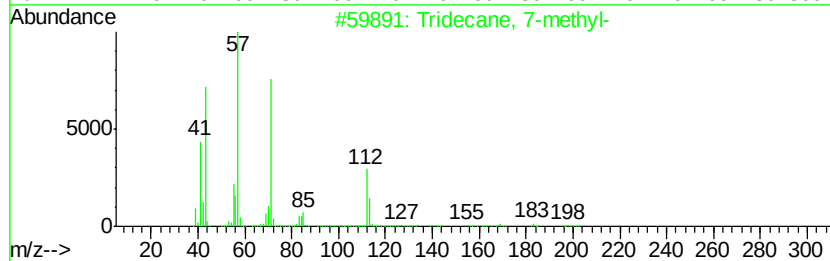
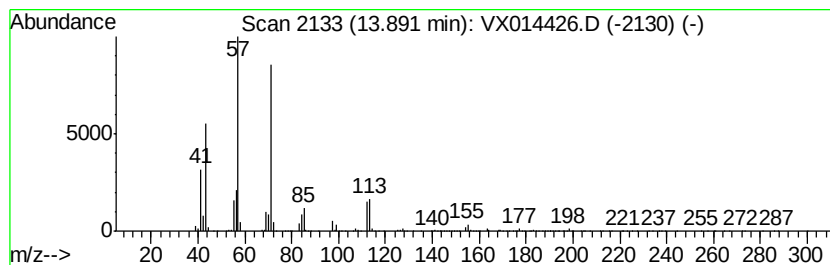
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 9 Tridecane, 7-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	155.11 ug/l	7233270	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 7-methyl-	198	C14H30	026730-14-3	90
2		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	86
3		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	78
4		Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	72
5		Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014426.D
Acq On : 06 Jan 2020 14:45
Operator : JC/SP
Sample : K6484-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
30628

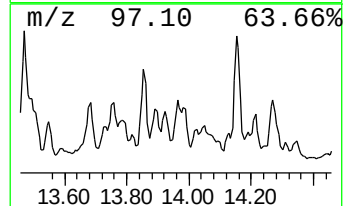
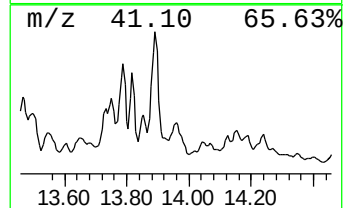
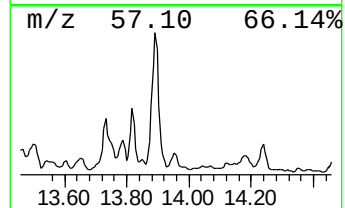
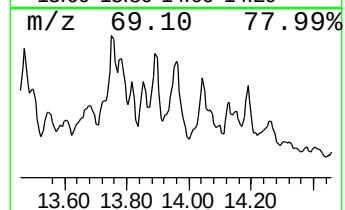
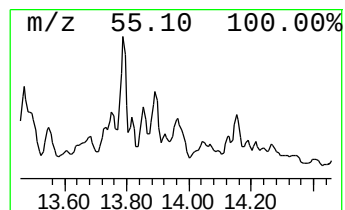
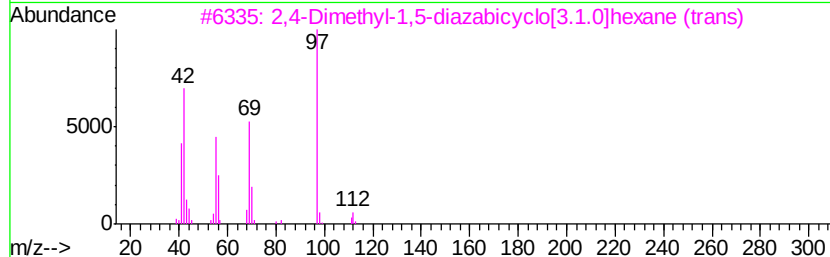
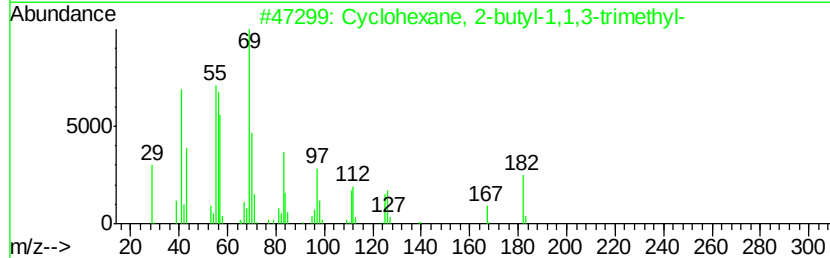
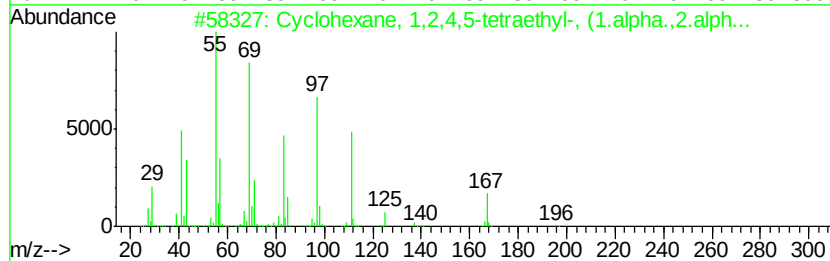
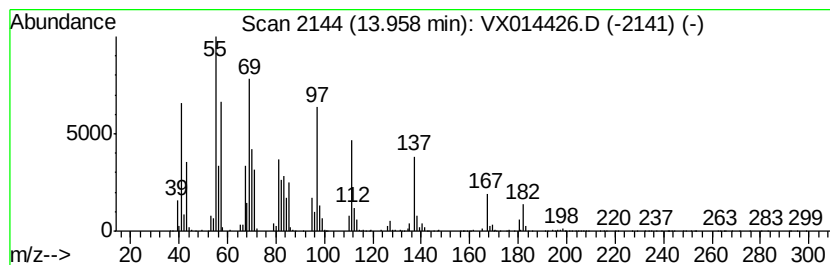
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclohexane, 1,2,4,5-tetrae... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	59.90 ug/l	2793220	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,2,4,5-tetraethyl-...	196	C14H28	061142-24-3	70
2		Cyclohexane, 2-butyl-1,1,3-trime...	182	C13H26	054676-39-0	49
3		2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	1000283-20-9	38
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	30
5		Cyclooctane, ethyl-	140	C10H20	013152-02-8	27



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014426.D
Acq On : 06 Jan 2020 14:45
Operator : JC/SP
Sample : K6484-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30628

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.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
Acetaldehyde	1.49	554.5	ug/l	16279900	1	5.65	1468060	50.0
Butanal	4.33	107.5	ug/l	3155420	1	5.65	1468060	50.0
1-Hexanol, 2-ethyl-	12.26	113.8	ug/l	5304490	4	12.07	2331670	50.0
Cyclohexane, (4-m...	12.94	68.6	ug/l	3199850	4	12.07	2331670	50.0
Undecane, 2-methyl-	13.03	65.8	ug/l	3069550	4	12.07	2331670	50.0
unknown13.35	13.35	95.8	ug/l	4466770	4	12.07	2331670	50.0
Undecane, 3,6-dim...	13.43	118.6	ug/l	5530870	4	12.07	2331670	50.0
unknown13.75	13.75	65.2	ug/l	3038670	4	12.07	2331670	50.0
Tridecane, 7-methyl-	13.89	155.1	ug/l	7233270	4	12.07	2331670	50.0
Cyclohexane, 1,2,...	13.96	59.9	ug/l	2793220	4	12.07	2331670	50.0