

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051822\
 Data File : VX028806.D
 Acq On : 18 May 2022 15:19
 Operator : JC/MD
 Sample : N2902-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WASTE-WATER-5/16/22

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
 Title : SW846 8260

Signal : TIC: VX028806.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	34	rBV2	7892	20699	1.37%	0.162%
2	1.563	69	78	83	rBV8	9299	21999	1.46%	0.173%
3	2.380	205	212	222	rBV	22378	37952	2.52%	0.298%
4	5.099	643	658	670	rBV2	18337	55690	3.70%	0.437%
5	5.385	690	705	720	rBV	211634	623524	41.39%	4.894%
6	5.556	722	733	752	rVB	336276	936020	62.13%	7.347%
7	5.958	788	799	816	rBV	203059	514623	34.16%	4.040%
8	6.763	921	931	946	rBV	469335	1107876	73.54%	8.696%
9	8.653	1233	1241	1250	rBV	939462	1506432	100.00%	11.825%
10	9.525	1376	1384	1395	rBV	95209	146597	9.73%	1.151%
11	10.055	1465	1471	1481	rBV	1048490	1369234	90.89%	10.748%
12	10.768	1582	1588	1598	rBV	142008	192454	12.78%	1.511%
13	10.860	1598	1603	1614	rVV	117024	164378	10.91%	1.290%
14	11.079	1634	1639	1646	rBV	811404	1057334	70.19%	8.300%
15	11.219	1654	1662	1671	rVB6	8318	17059	1.13%	0.134%
16	11.622	1723	1728	1733	rVB6	7922	16673	1.11%	0.131%
17	11.756	1746	1750	1759	rVB8	12205	24135	1.60%	0.189%
18	11.841	1759	1764	1770	rBV	785151	971009	64.46%	7.622%
19	11.902	1770	1774	1784	rVB2	141379	224431	14.90%	1.762%
20	12.024	1789	1794	1801	rVV	1096215	1333823	88.54%	10.470%
21	12.103	1801	1807	1811	rVB6	11088	23412	1.55%	0.184%
22	12.219	1822	1826	1829	rBV	82929	116484	7.73%	0.914%
23	12.317	1838	1842	1848	rVB7	13698	28724	1.91%	0.225%
24	12.408	1853	1857	1861	rVB2	10556	16184	1.07%	0.127%
25	12.561	1875	1882	1883	rBV6	13075	24691	1.64%	0.194%
26	12.616	1885	1891	1894	rVB	43022	70837	4.70%	0.556%
27	12.701	1900	1905	1909	rBV2	25373	46113	3.06%	0.362%
28	12.768	1913	1916	1920	rVV	76959	100376	6.66%	0.788%
29	12.817	1921	1924	1931	rVB4	35711	63500	4.22%	0.498%
30	12.890	1932	1936	1938	rBV4	13725	20273	1.35%	0.159%
31	12.920	1938	1941	1945	rVB	53603	64628	4.29%	0.507%
32	12.987	1949	1952	1955	rBV4	23314	27185	1.80%	0.213%
33	13.091	1965	1969	1974	rBV5	20437	37681	2.50%	0.296%
34	13.140	1974	1977	1984	rVB6	19171	26583	1.76%	0.209%
35	13.207	1984	1988	1992	rBV3	23710	35192	2.34%	0.276%
36	13.286	1997	2001	2008	rVB2	115454	184274	12.23%	1.446%

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Integration Parameters: RTEINT.P

Integrator: RTE

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Peak separation: 5

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37	13.347	2008	2011	2013	rBV3	13577	15283	1.01%	0.120%
38	13.390	2013	2018	2019	rBV3	12804	20891	1.39%	0.164%
39	13.420	2020	2023	2026	rVB3	20627	24740	1.64%	0.194%
40	13.506	2033	2037	2040	rBV4	14515	24239	1.61%	0.190%
41	13.585	2046	2050	2053	rBV2	26058	37289	2.48%	0.293%
42	13.664	2061	2063	2067	rVB2	23834	28758	1.91%	0.226%
43	13.707	2067	2070	2075	rVB4	23302	25214	1.67%	0.198%
44	13.798	2081	2085	2089	rVB4	44651	54146	3.59%	0.425%
45	13.847	2089	2093	2099	rBV2	101763	147393	9.78%	1.157%
46	13.926	2099	2106	2110	rVB4	53460	125778	8.35%	0.987%
47	13.993	2111	2117	2119	rBV4	19902	44335	2.94%	0.348%
48	14.073	2126	2130	2132	rBV5	23421	32380	2.15%	0.254%
49	14.103	2132	2135	2138	rVV4	20860	25941	1.72%	0.204%
50	14.140	2138	2141	2143	rVV2	16850	16853	1.12%	0.132%
51	14.213	2151	2153	2160	rVB2	37410	54176	3.60%	0.425%
52	14.371	2176	2179	2185	rVB5	29351	41680	2.77%	0.327%
53	14.481	2193	2197	2201	rBV3	56023	78722	5.23%	0.618%
54	14.615	2215	2219	2225	rBV2	126221	166836	11.07%	1.310%
55	14.670	2225	2228	2233	rVB4	34437	45830	3.04%	0.360%
56	14.755	2239	2242	2244	rBV2	20308	20696	1.37%	0.162%
57	14.792	2244	2248	2252	rVV4	38283	52719	3.50%	0.414%
58	14.847	2254	2257	2261	rVB4	30243	42316	2.81%	0.332%
59	15.182	2310	2312	2314	rBV3	20127	24102	1.60%	0.189%
60	15.213	2314	2317	2321	rVB	89029	101424	6.73%	0.796%
61	15.377	2341	2344	2347	rBV3	14965	18020	1.20%	0.141%
62	15.414	2347	2350	2356	rVB4	33113	50895	3.38%	0.400%
63	15.481	2357	2361	2367	rBV	39179	60703	4.03%	0.476%
64	15.615	2379	2383	2388	rVB	61085	97692	6.48%	0.767%
65	16.084	2457	2460	2467	rVB6	19693	32525	2.16%	0.255%

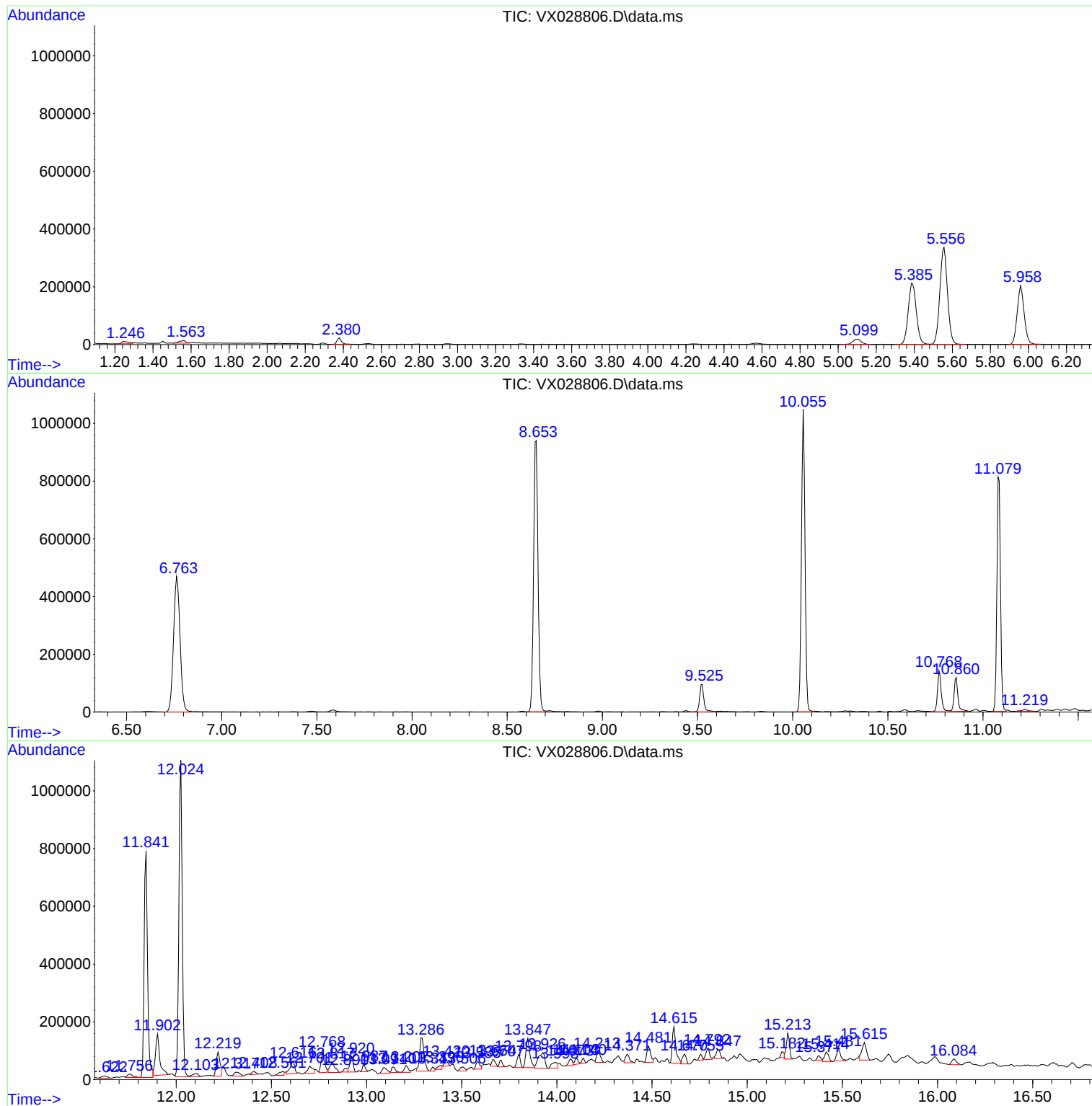
Sum of corrected areas: 12739655

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Instrument :
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ClientSampleId :
WASTE-WATER-5/16/22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_X
ClientSampleId :
WASTE-WATER-5/16/22

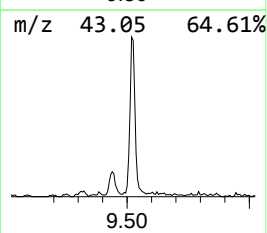
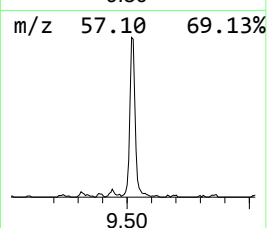
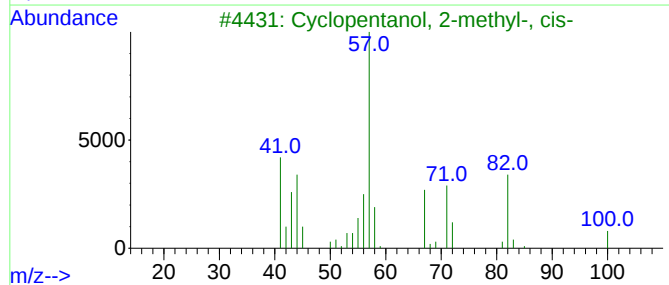
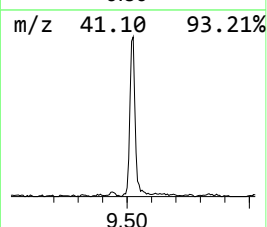
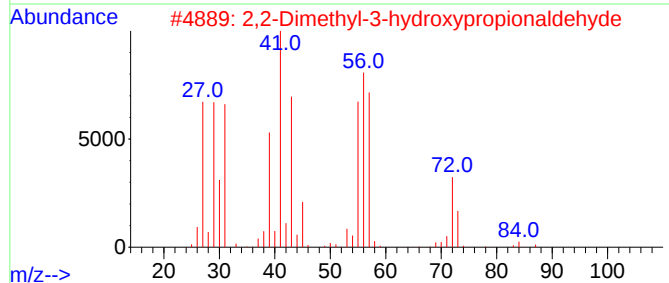
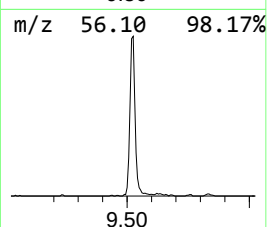
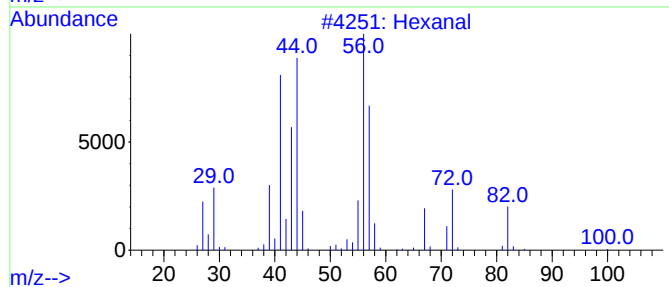
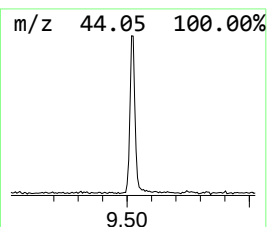
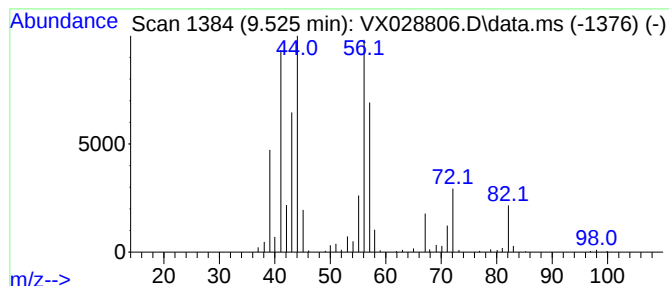
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.525	5.35 ug/l	146597	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	90
2			2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	37
3			Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	35
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	32
5			Glutaraldehyde	100	C5H8O2	000111-30-8	30



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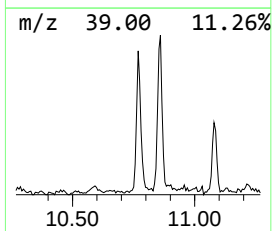
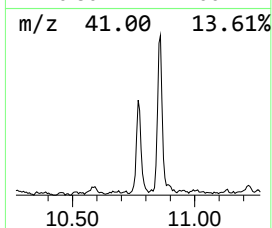
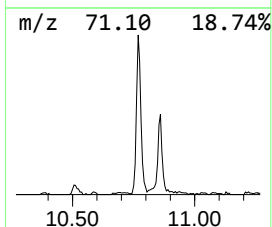
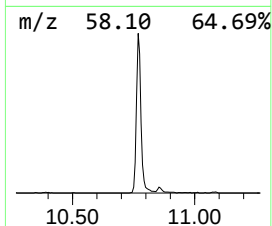
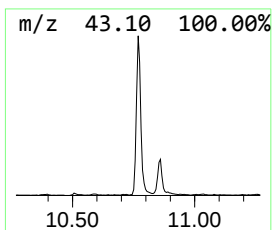
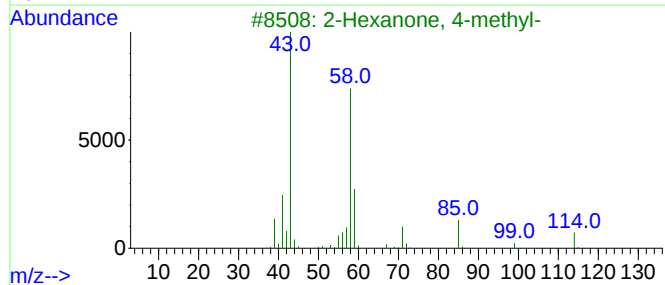
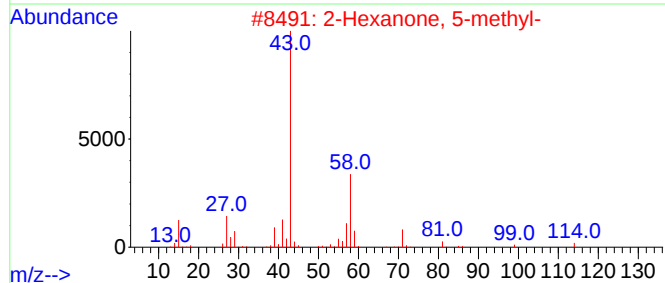
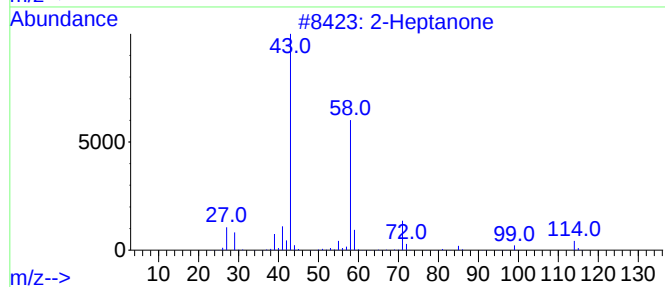
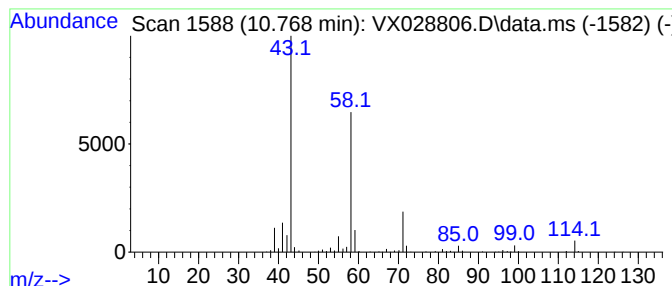
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Heptanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.768	7.03 ug/l	192454	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone	114	C7H14O	000110-43-0	91
2			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78
3			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	50
4			2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	50
5			N-Cyclohexyl-N'-[2-(dimethylamin...	213	C11H23N3O	097943-37-8	38



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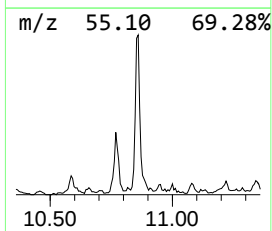
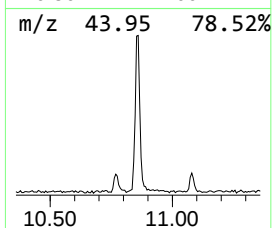
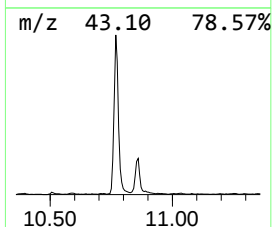
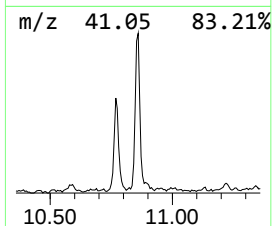
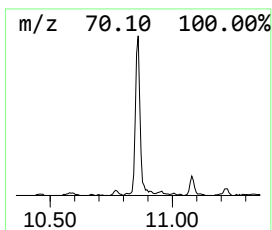
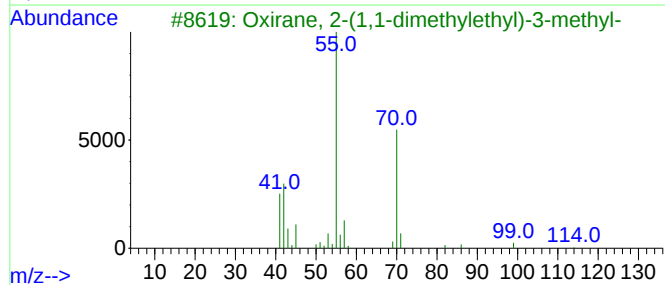
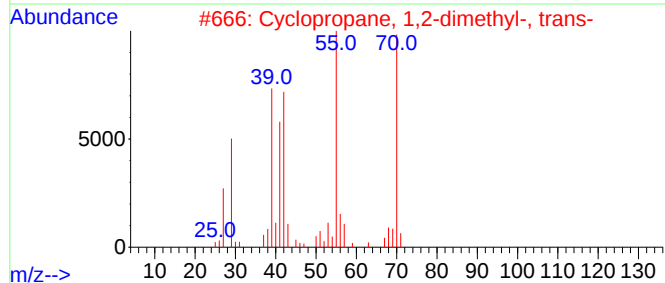
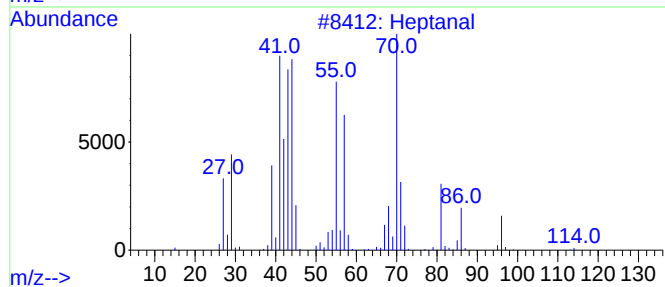
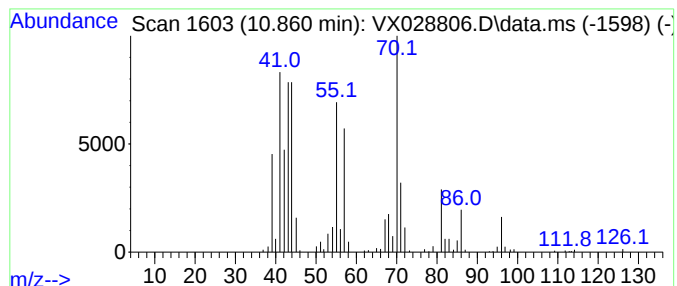
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.860	6.00 ug/l	164378	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	96
2			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	38
3			Oxirane, 2-(1,1-dimethylethyl)-3-methyl-	114	C7H14O	053897-30-6	38
4			2-Butene, 2-methyl-	70	C5H10	000513-35-9	38
5			Hexanal, 3-methyl-	114	C7H14O	019269-28-4	32



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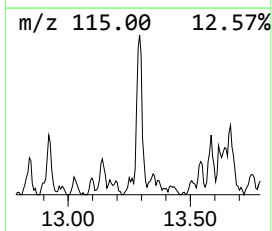
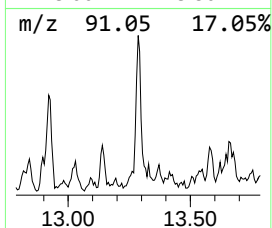
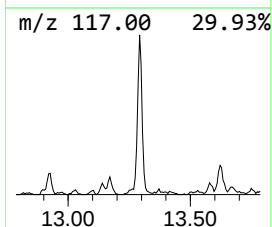
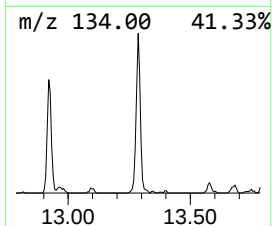
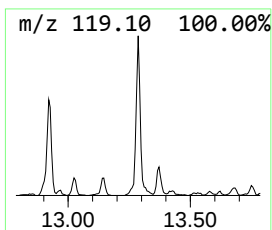
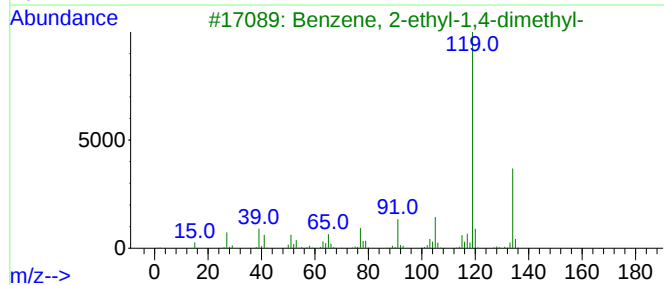
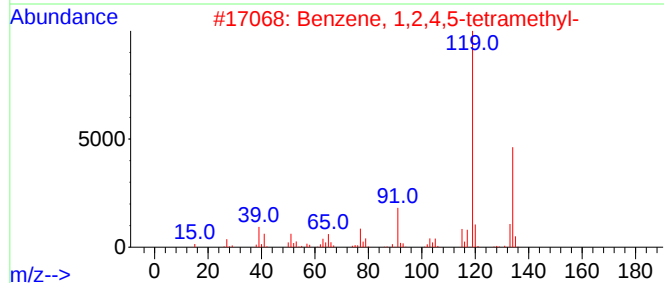
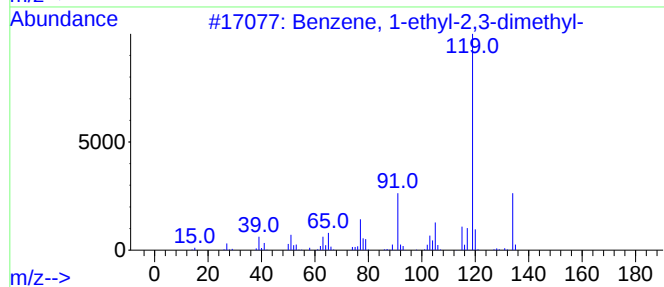
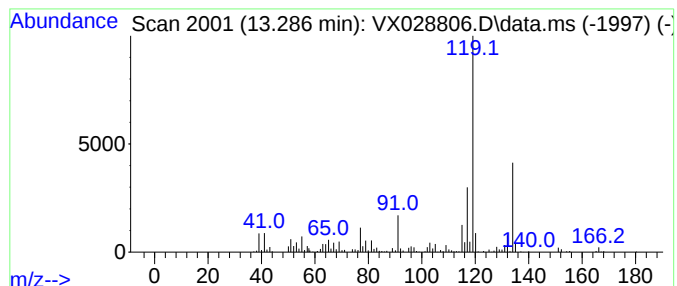
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	6.91 ug/l	184274	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	87
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	87
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	87
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	87
5			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	87



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Acq On : 18 May 2022 15:19
Operator : JC/MD
Sample : N2902-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASTE-WATER-5/16/22

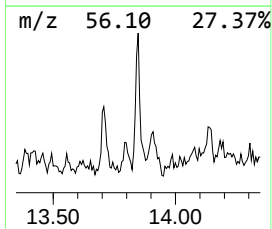
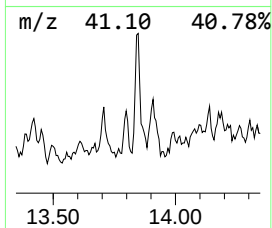
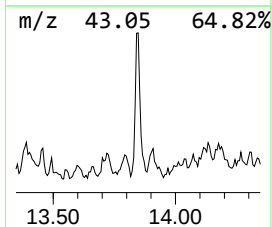
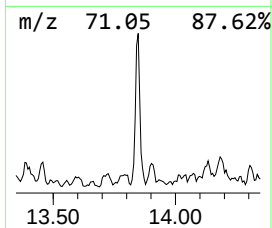
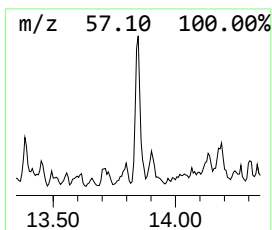
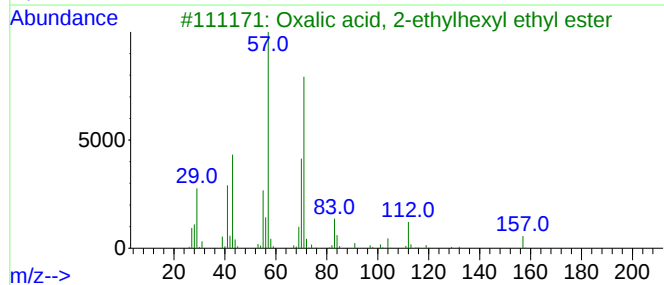
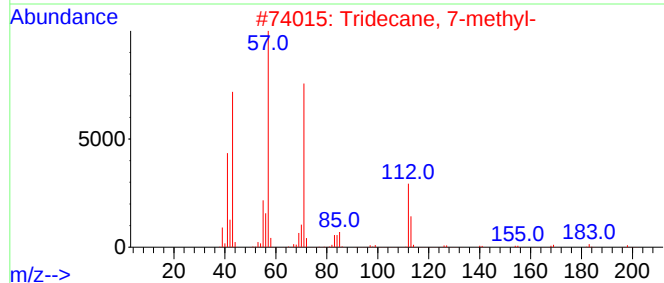
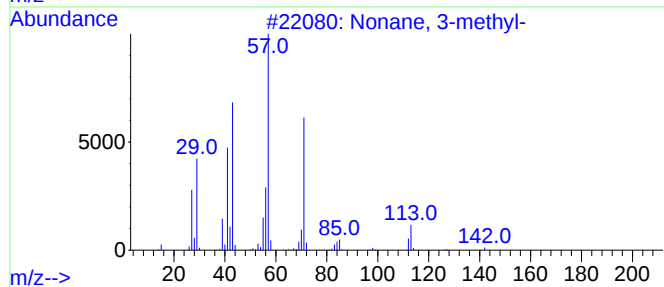
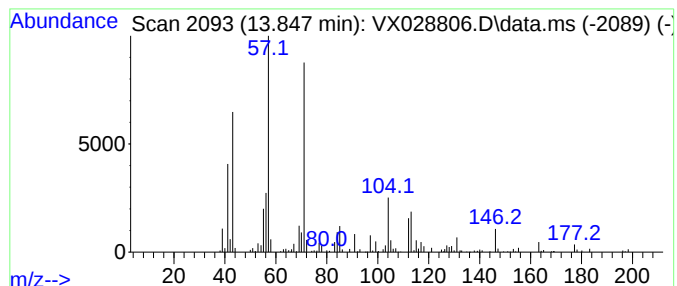
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Nonane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.847	5.53 ug/l	147393	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 3-methyl-	142	C10H22	005911-04-6	59
2			Tridecane, 7-methyl-	198	C14H30	026730-14-3	58
3			Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	53
4			Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	50
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051822\
Data File : VX028806.D
Acq On : 18 May 2022 15:19
Operator : JC/MD
Sample : N2902-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASTE-WATER-5/16/22

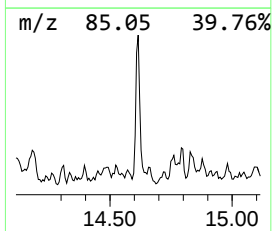
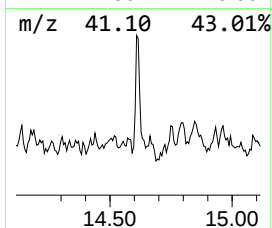
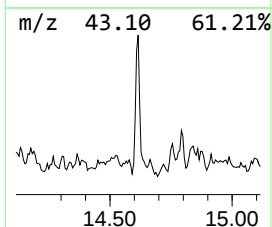
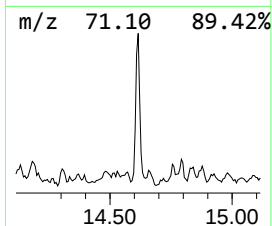
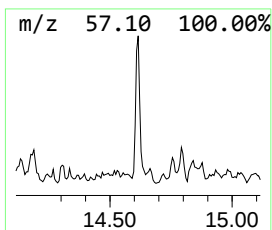
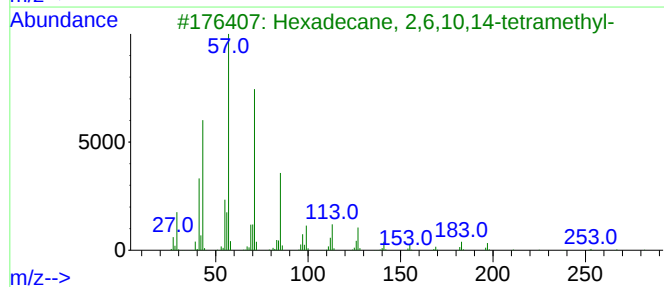
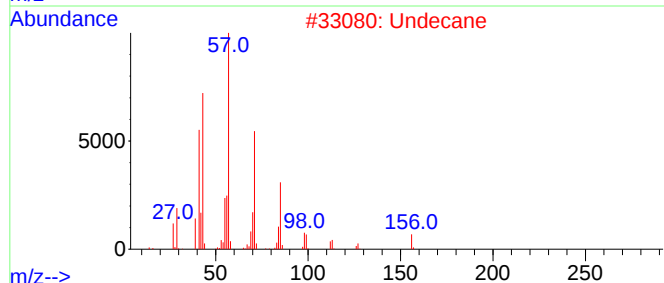
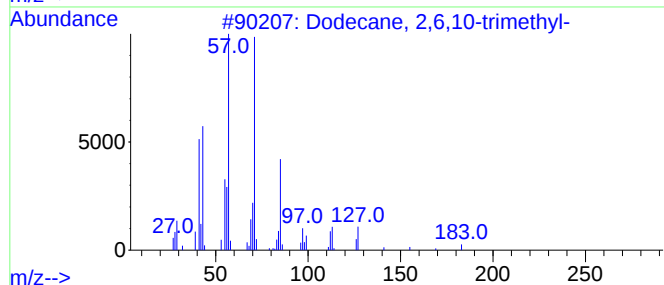
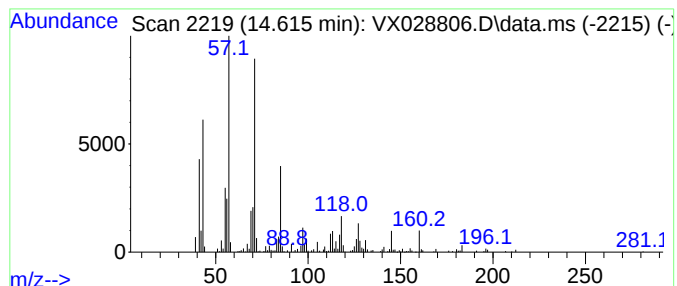
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Dodecane, 2,6,10-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	6.25 ug/l	166836	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	87
2			Undecane	156	C11H24	001120-21-4	64
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	59
5			Tetradecane, 4-methyl-	212	C15H32	025117-24-2	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051822\
Data File : VX028806.D
Acq On : 18 May 2022 15:19
Operator : JC/MD
Sample : N2902-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASTE-WATER-5/16/22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	9.525	5.3	ug/l	146597	3	10.055	1369230	50.0
2-Heptanone	10.768	7.0	ug/l	192454	3	10.055	1369230	50.0
Heptanal	10.860	6.0	ug/l	164378	3	10.055	1369230	50.0
Benzene, 1-ethy...	13.286	6.9	ug/l	184274	4	12.024	1333820	50.0
Nonane, 3-methyl-	13.847	5.5	ug/l	147393	4	12.024	1333820	50.0
Dodecane, 2,6,1...	14.615	6.3	ug/l	166836	4	12.024	1333820	50.0