

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
 Data File : VX032276.D
 Acq On : 20 Oct 2022 20:20
 Operator : JC/MD
 Sample : N5185-19 40X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PZ-3R

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\82X101922W.M
 Title : SW846 8260

Signal : TIC: VX032276.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	34	rBV	10746	10217	1.40%	0.132%
2	1.368	43	46	52	rBV	69556	71671	9.85%	0.929%
3	1.752	103	109	118	rBV	283589	375224	51.59%	4.864%
4	1.953	137	142	154	rVB2	73302	112296	15.44%	1.456%
5	2.069	156	161	166	rVV	9705	13140	1.81%	0.170%
6	2.215	181	185	192	rVB	19743	30052	4.13%	0.390%
7	2.343	199	206	211	rBV2	6022	11720	1.61%	0.152%
8	2.782	268	278	281	rBV3	17725	40090	5.51%	0.520%
9	2.825	281	285	290	rVV	38846	84936	11.68%	1.101%
10	2.867	290	292	303	rVV3	20247	42114	5.79%	0.546%
11	3.099	322	330	343	rBV	29120	66116	9.09%	0.857%
12	3.324	359	367	374	rVB2	4249	9273	1.27%	0.120%
13	3.446	379	387	395	rVB	10616	22876	3.15%	0.297%
14	3.733	427	434	443	rVB2	9021	21354	2.94%	0.277%
15	3.837	443	451	458	rBV3	5554	13769	1.89%	0.178%
16	4.105	487	495	504	rVB3	6332	16960	2.33%	0.220%
17	4.215	504	513	519	rBV3	4100	13190	1.81%	0.171%
18	4.306	519	528	541	rVV2	46558	135212	18.59%	1.753%
19	4.568	558	571	588	rBV2	3492	12629	1.74%	0.164%
20	5.196	666	674	684	rVB4	4415	13191	1.81%	0.171%
21	5.385	694	705	714	rBV	83343	244192	33.57%	3.166%
22	5.556	715	733	759	rVB	158248	524417	72.10%	6.798%
23	5.830	768	778	789	rVB3	8236	24095	3.31%	0.312%
24	5.958	789	799	807	rBV2	95238	248678	34.19%	3.224%
25	6.043	807	813	823	rVV2	18331	51038	7.02%	0.662%
26	6.159	823	832	838	rVV6	5361	17974	2.47%	0.233%
27	6.257	838	848	857	rVV5	14379	47464	6.53%	0.615%
28	6.354	857	864	875	rVB4	4604	12210	1.68%	0.158%
29	6.610	899	906	915	rVB5	2954	7295	1.00%	0.095%
30	6.763	921	931	941	rBV	228631	545329	74.98%	7.070%
31	7.373	1021	1031	1042	rVB3	13115	36369	5.00%	0.471%
32	7.982	1122	1131	1139	rVB2	6786	14075	1.94%	0.182%
33	8.104	1143	1151	1156	rBV2	9916	21908	3.01%	0.284%
34	8.506	1212	1217	1225	rVB4	5427	10391	1.43%	0.135%
35	8.653	1229	1241	1249	rBV	455532	727344	100.00%	9.429%
36	10.055	1465	1471	1482	rVB	464771	615642	84.64%	7.981%

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37	10.195	1488	1494	1504	rVB	322852	408763	56.20%	5.299%
38	10.305	1506	1512	1519	rVB	150454	209046	28.74%	2.710%
39	10.646	1563	1568	1576	rVB	17349	24074	3.31%	0.312%
40	10.963	1615	1620	1626	rBV	29878	36433	5.01%	0.472%
41	11.079	1634	1639	1652	rBV	389270	494738	68.02%	6.414%
42	11.305	1667	1676	1684	rBV	79095	94842	13.04%	1.230%
43	11.402	1684	1692	1696	rVV	88883	121934	16.76%	1.581%
44	11.451	1696	1700	1711	rVB	25749	33270	4.57%	0.431%
45	11.616	1720	1727	1734	rBV	54462	69112	9.50%	0.896%
46	11.750	1744	1749	1756	rVB	398855	480705	66.09%	6.232%
47	12.024	1788	1794	1800	rBV	487384	590857	81.23%	7.660%
48	12.085	1800	1804	1810	rVB	128103	162278	22.31%	2.104%
49	12.244	1825	1830	1837	rBV2	120607	153371	21.09%	1.988%
50	12.317	1837	1842	1851	rVV3	25535	41931	5.76%	0.544%
51	12.463	1862	1866	1872	rVV	16754	20841	2.87%	0.270%
52	12.530	1872	1877	1880	rVV	30141	41695	5.73%	0.541%
53	12.555	1880	1881	1886	rVV	22683	19298	2.65%	0.250%
54	12.615	1886	1891	1894	rVV	58820	69890	9.61%	0.906%
55	12.646	1894	1896	1900	rVV	7489	7725	1.06%	0.100%
56	12.701	1900	1905	1916	rVB2	24552	36278	4.99%	0.470%
57	12.847	1925	1929	1934	rBV	13844	16444	2.26%	0.213%
58	12.920	1934	1941	1945	rBV	27651	34815	4.79%	0.451%
59	12.963	1945	1948	1953	rVB	36187	40866	5.62%	0.530%
60	13.170	1975	1982	1986	rBV	26156	30569	4.20%	0.396%
61	13.292	1998	2002	2008	rVB2	52785	67103	9.23%	0.870%
62	13.426	2020	2024	2029	rVB2	6914	8208	1.13%	0.106%
63	13.579	2046	2049	2055	rVB3	5125	9110	1.25%	0.118%
64	13.774	2076	2081	2087	rBV	63265	81899	11.26%	1.062%
65	14.640	2218	2223	2231	rVB	20825	25980	3.57%	0.337%
66	14.780	2242	2246	2257	rVB	13654	17254	2.37%	0.224%

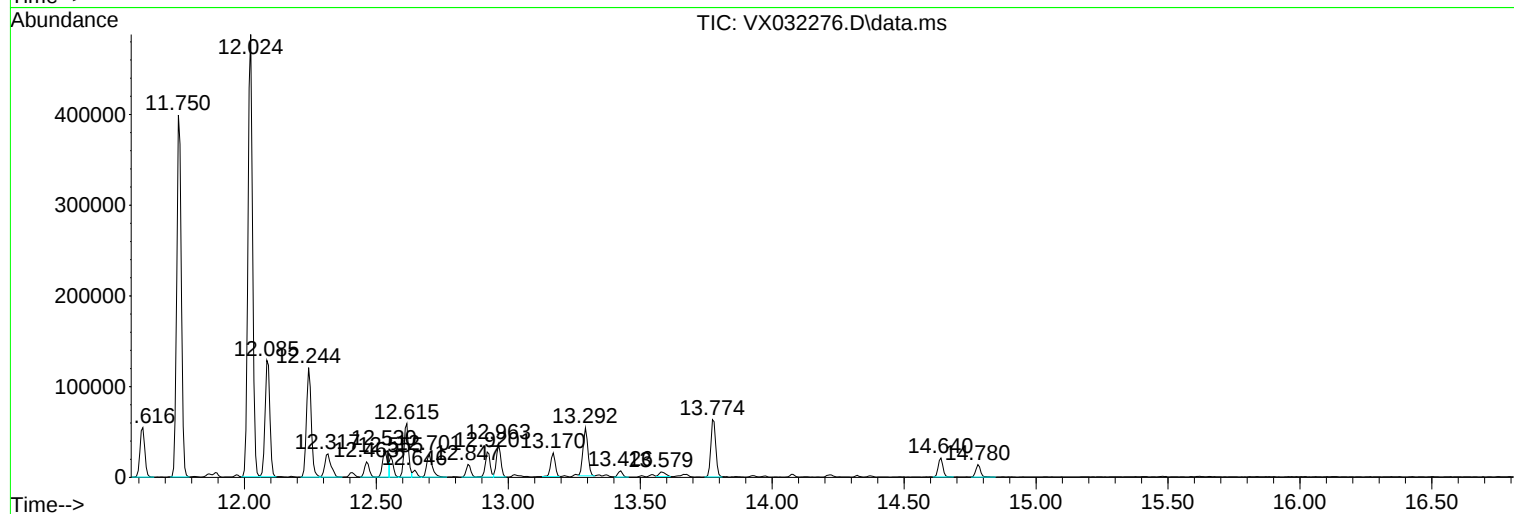
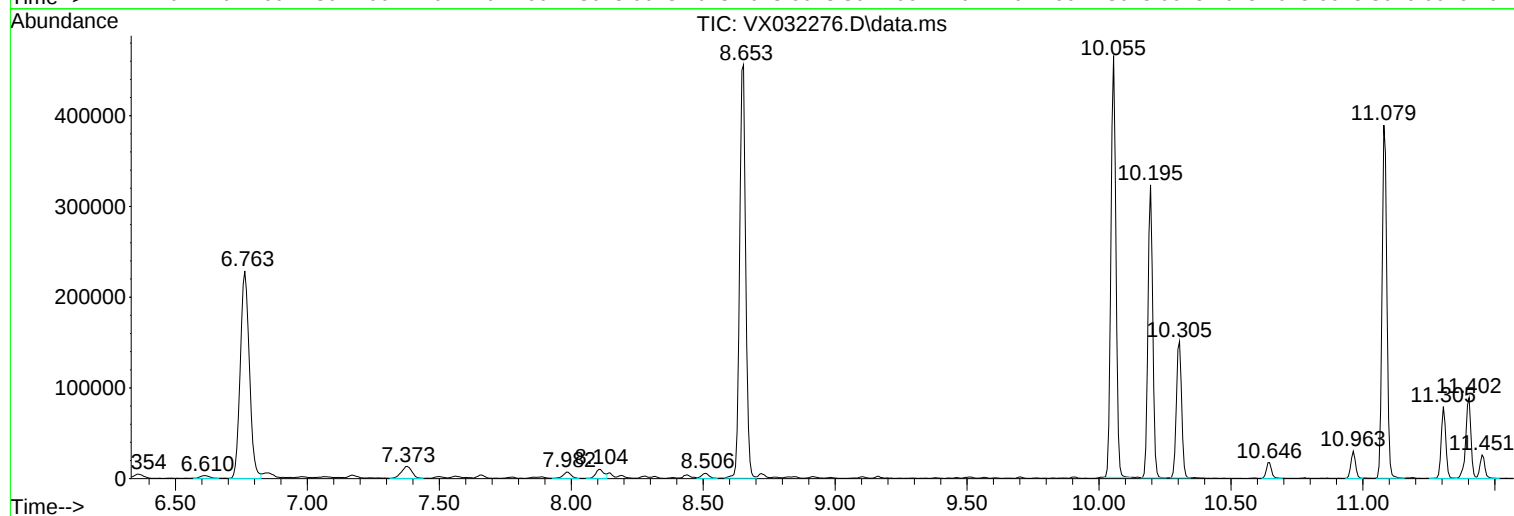
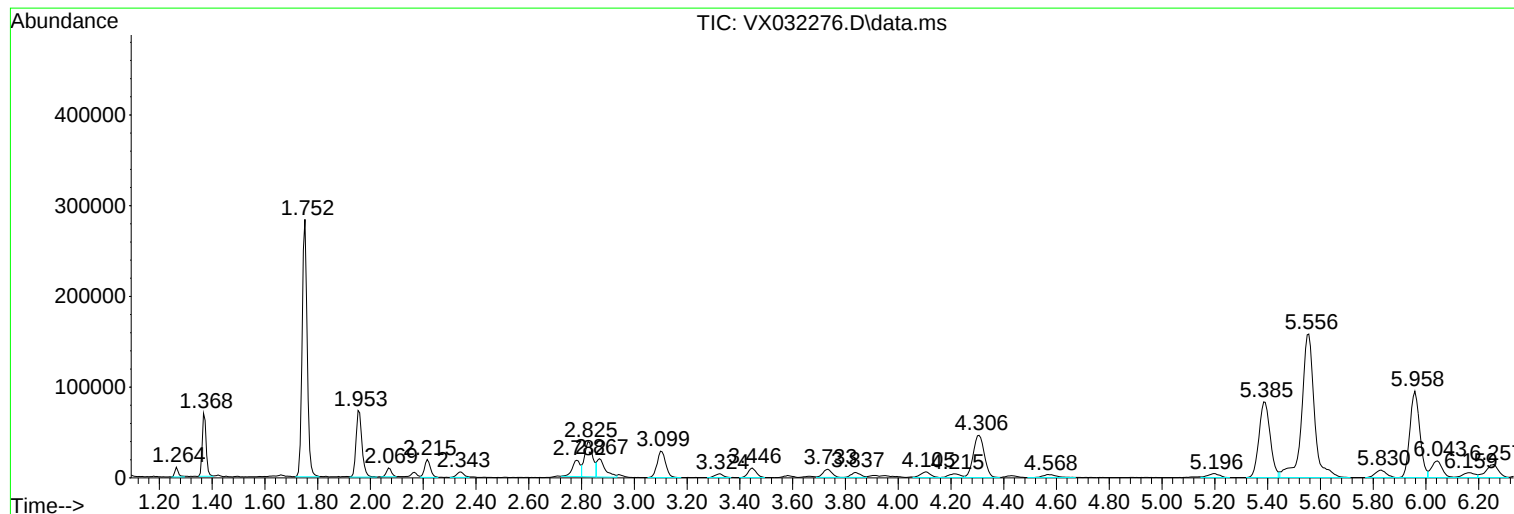
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

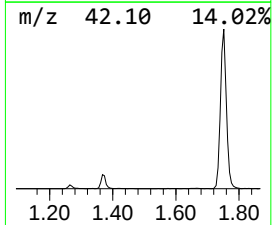
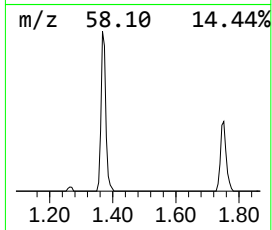
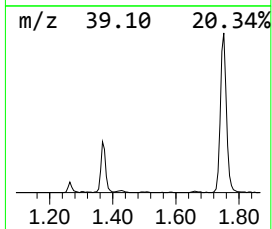
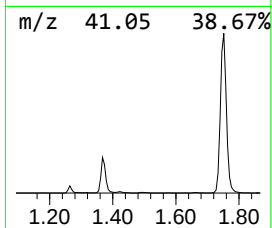
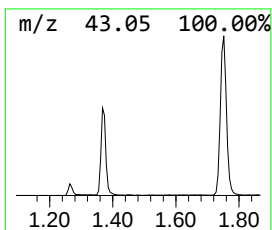
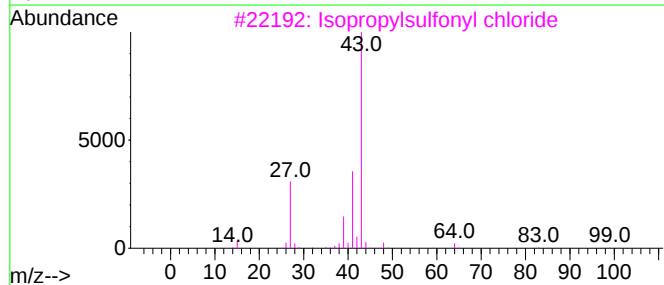
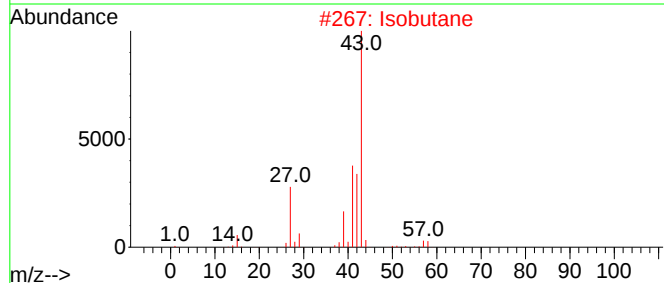
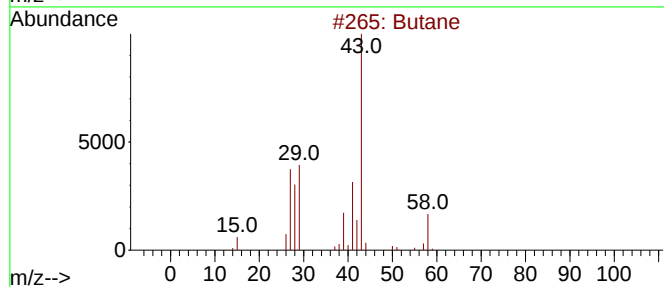
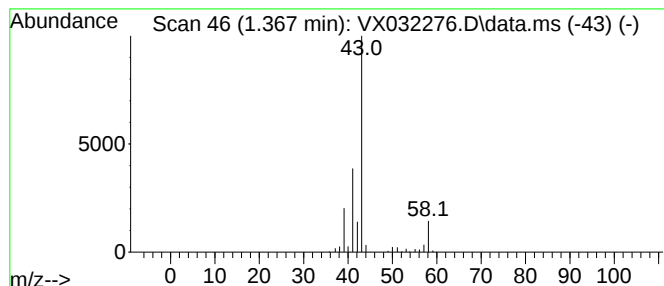
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Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.367	6.83 ug/l	71671	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane			58	C4H10	000106-97-8	80
2	Isobutane			58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride			142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-			89	C3H7NO2	000108-03-2	9
5	Acetone			58	C3H6O	000067-64-1	4



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MSVOA_X
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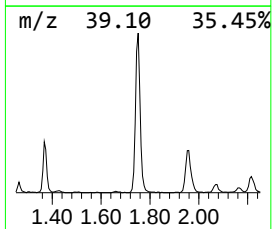
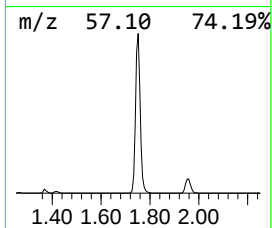
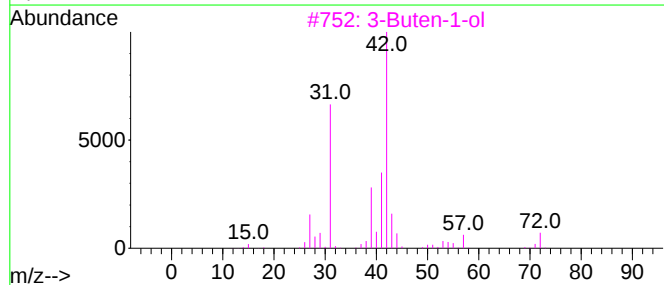
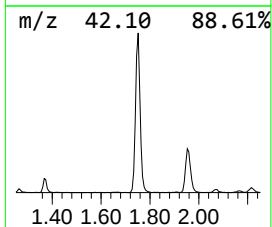
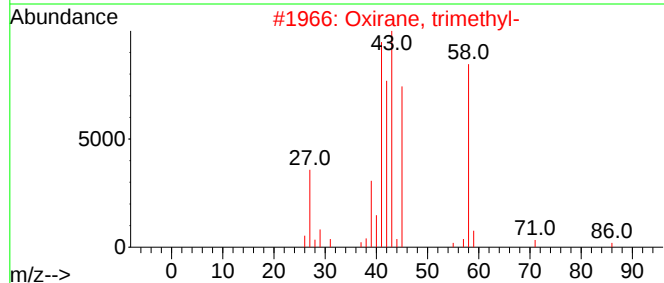
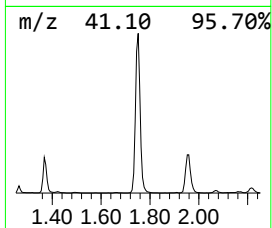
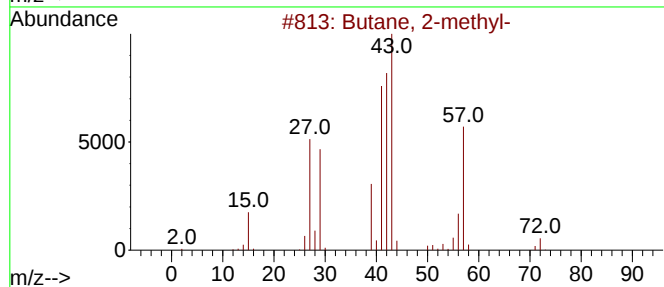
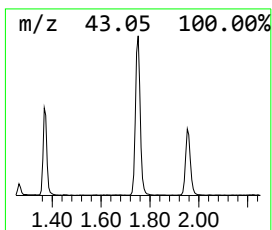
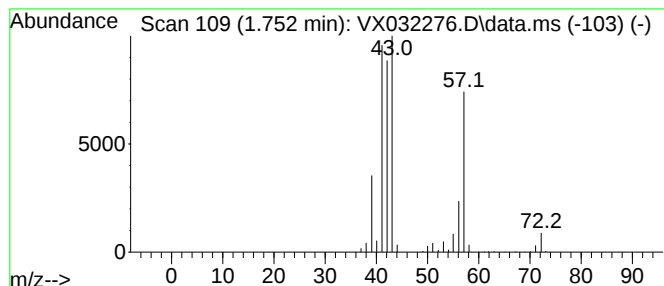
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	35.78 ug/l	375224	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Oxirane, trimethyl-	86	C5H10O	005076-19-7	40
3			3-Buten-1-ol	72	C4H8O	000627-27-0	37
4			Pentane	72	C5H12	000109-66-0	33
5			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28



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ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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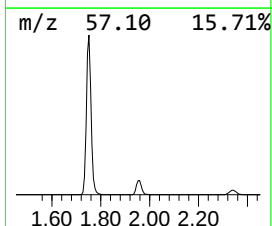
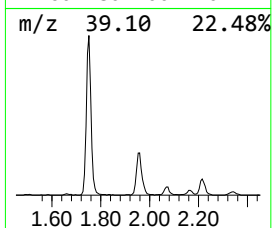
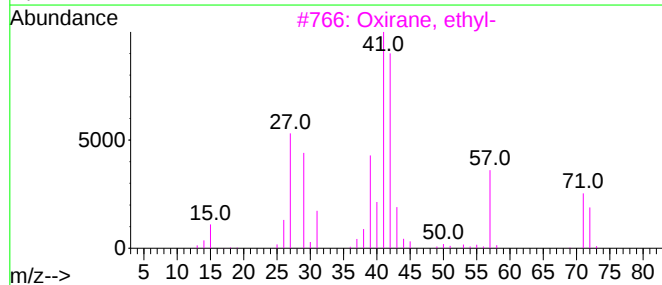
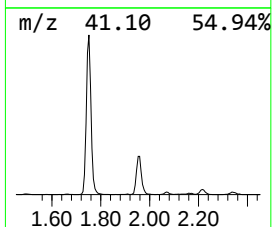
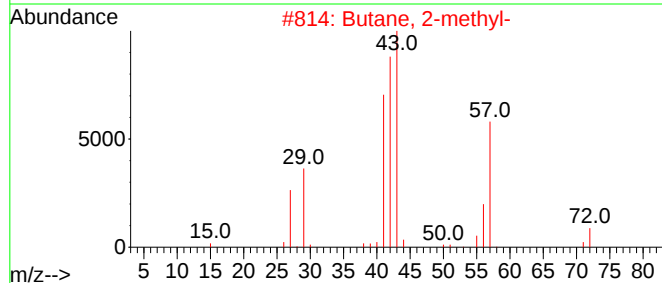
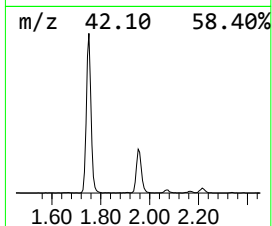
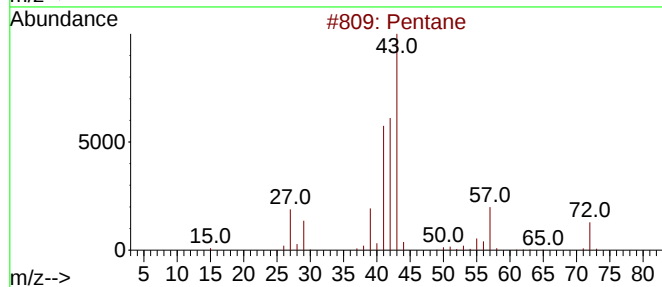
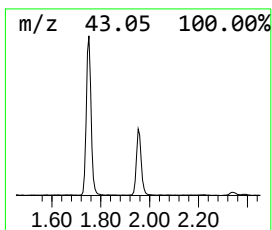
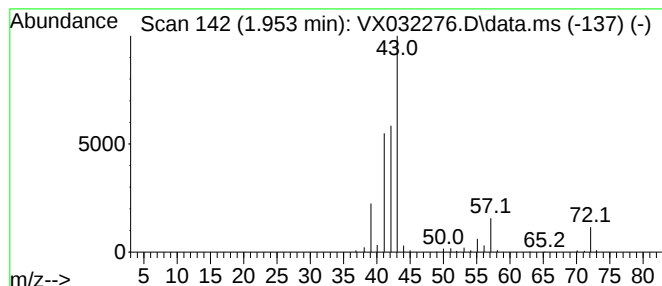
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	10.71 ug/l	112296	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Butane, 2-methyl-	72	C5H12	000078-78-4	53
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
4			2-Butanone	72	C4H8O	000078-93-3	9
5			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9



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ClientSampleId :
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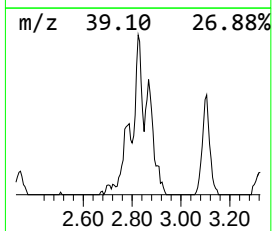
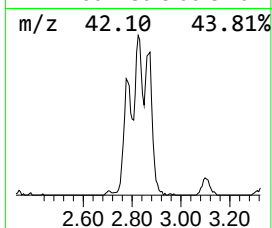
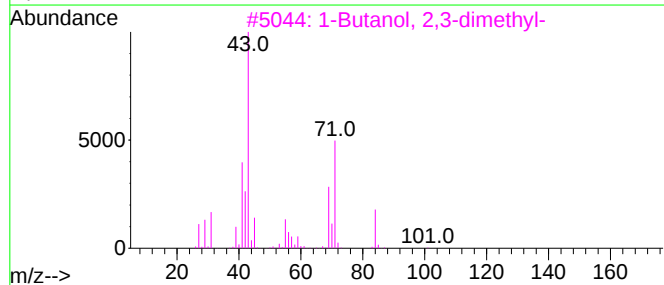
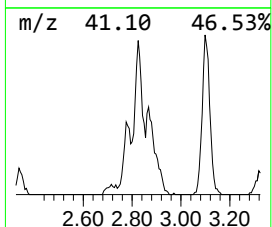
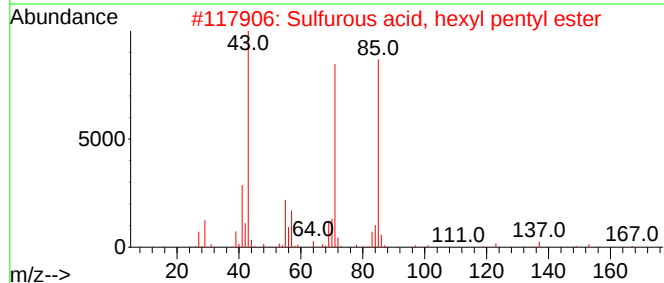
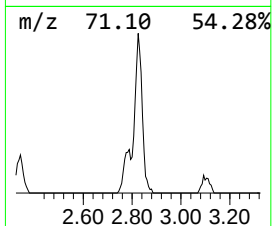
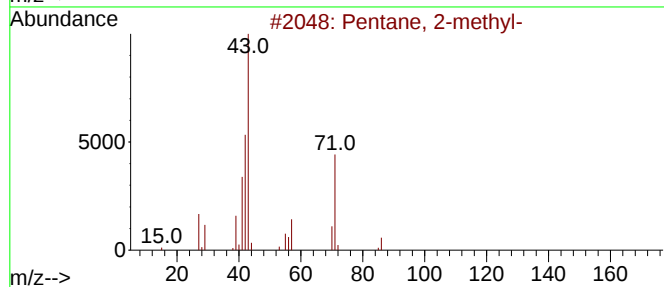
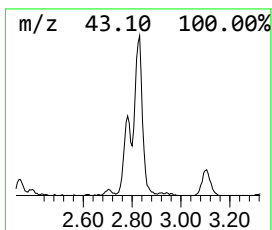
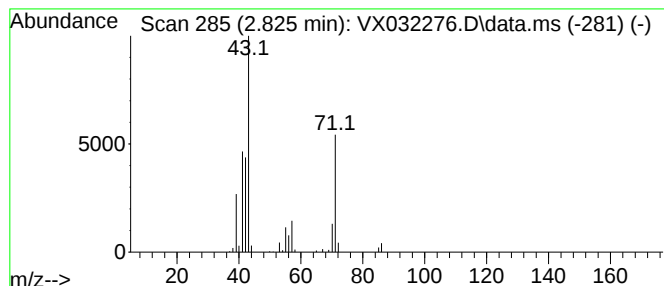
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	8.10 ug/l	84936	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	47
3			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
4			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	38



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Operator : JC/MD
Sample : N5185-19 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

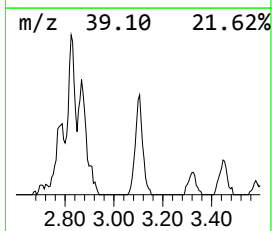
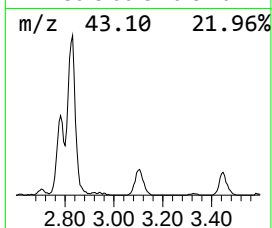
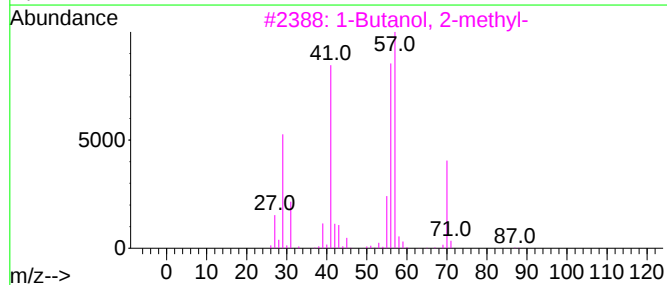
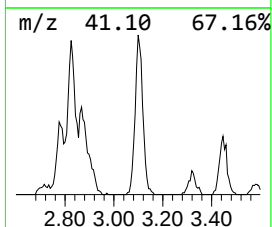
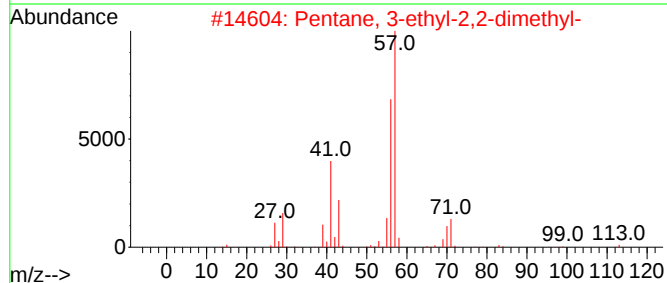
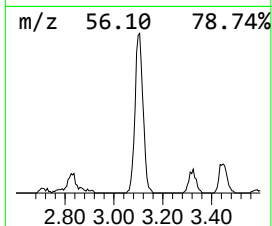
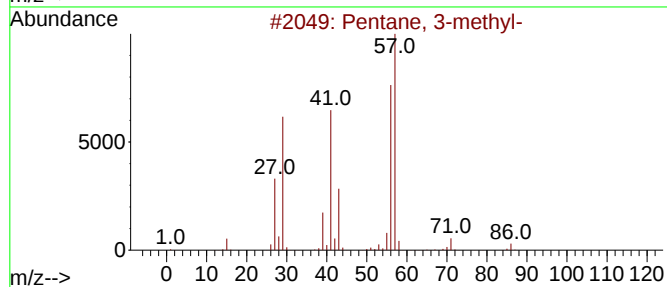
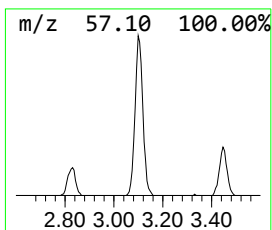
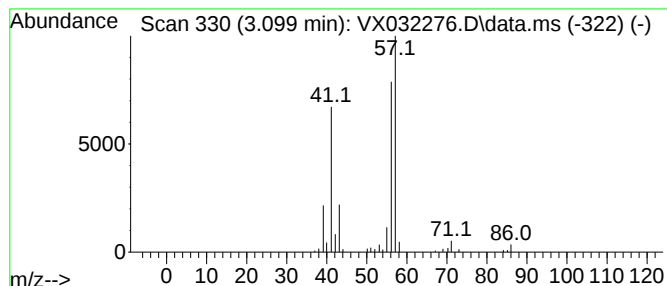
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.099	6.30 ug/l	66116	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
3			1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	64
4			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	53
5			Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
Data File : VX032276.D
Acq On : 20 Oct 2022 20:20
Operator : JC/MD
Sample : N5185-19 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

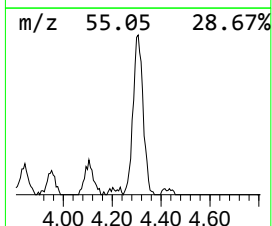
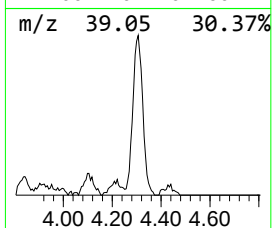
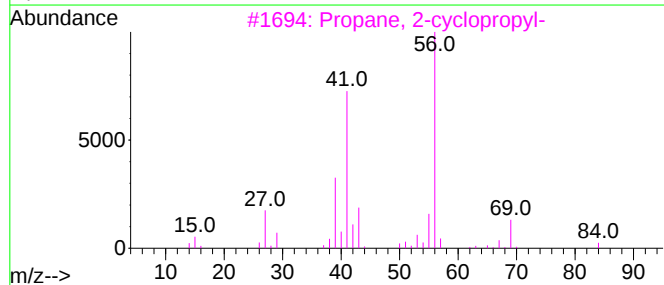
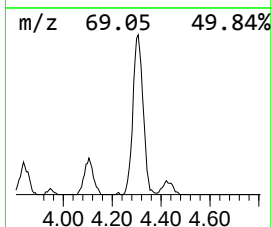
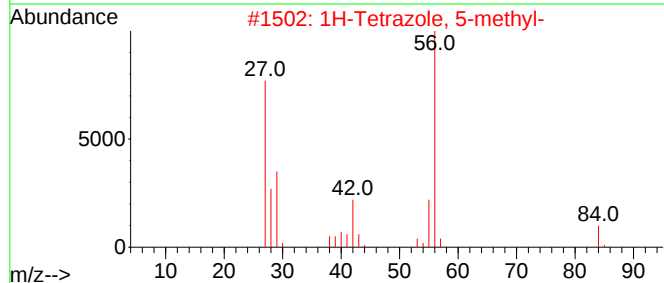
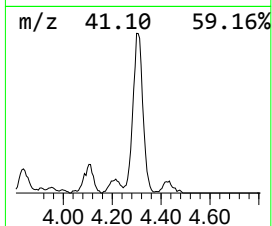
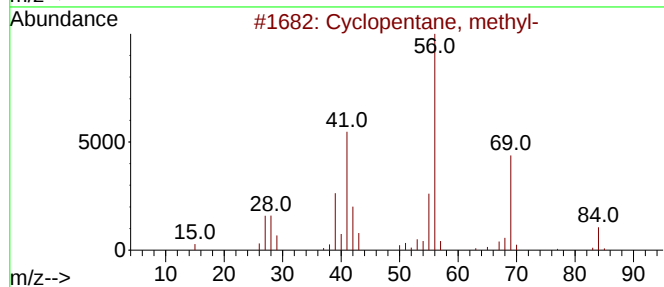
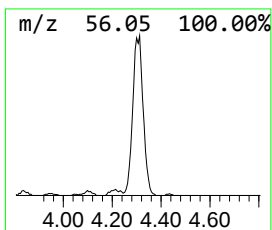
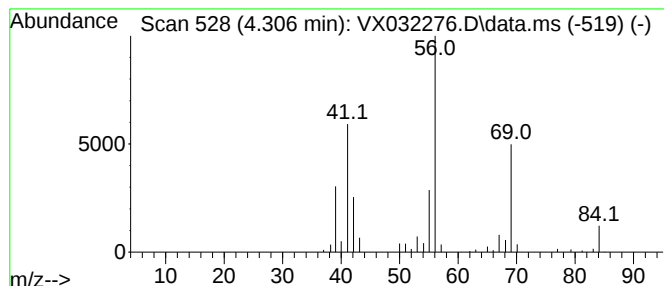
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	12.89 ug/l	135212	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
3			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	59
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
Data File : VX032276.D
Acq On : 20 Oct 2022 20:20
Operator : JC/MD
Sample : N5185-19 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

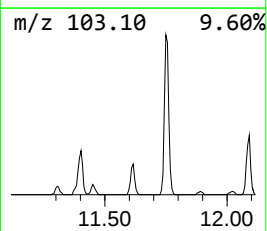
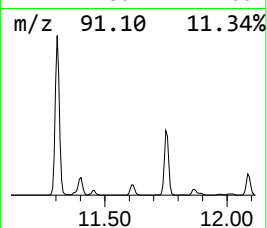
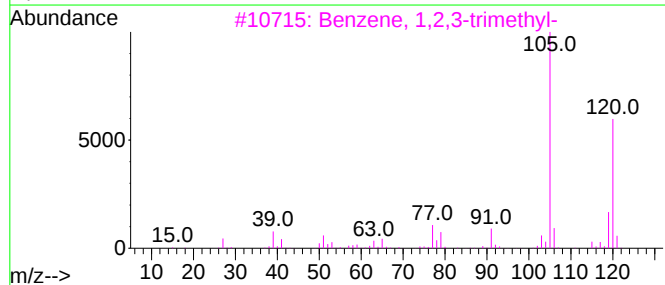
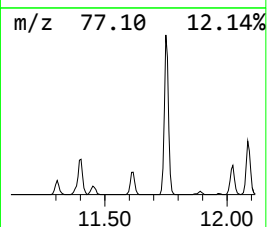
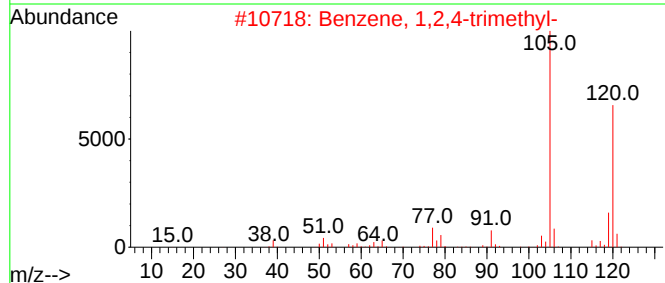
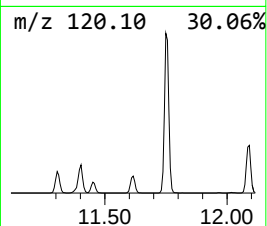
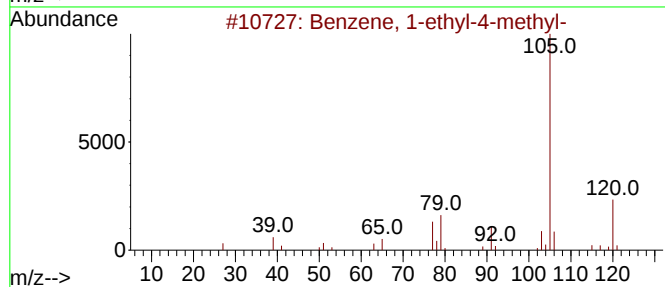
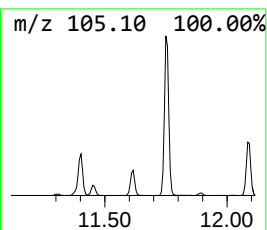
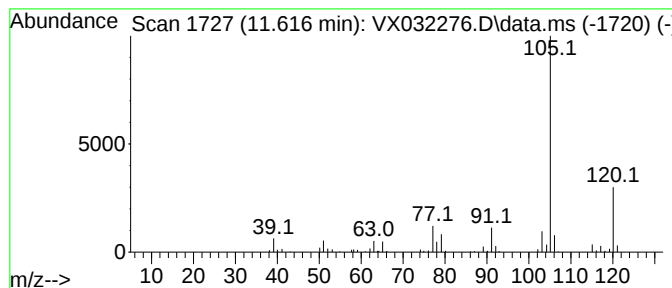
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	5.85 ug/l	69112	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
Data File : VX032276.D
Acq On : 20 Oct 2022 20:20
Operator : JC/MD
Sample : N5185-19 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

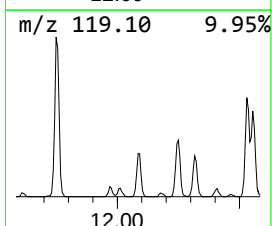
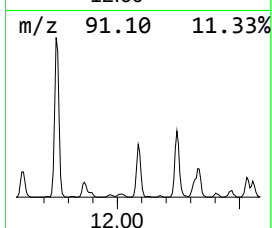
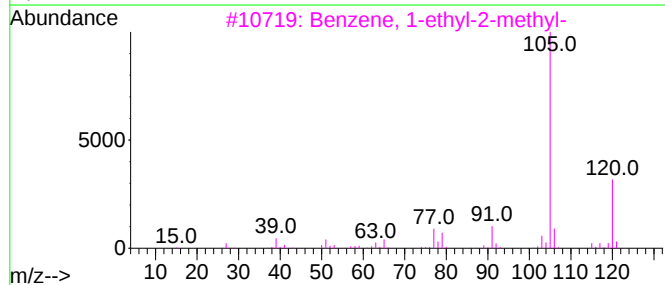
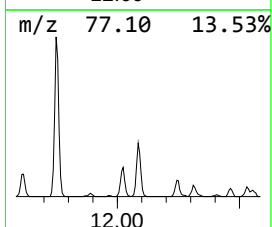
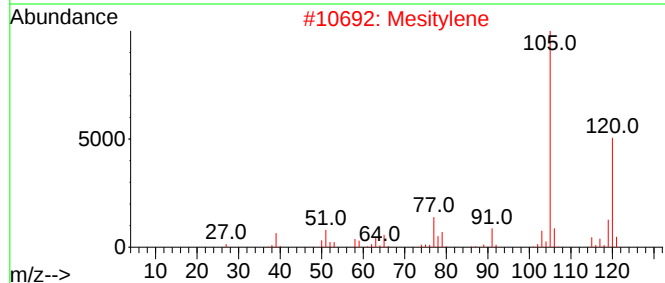
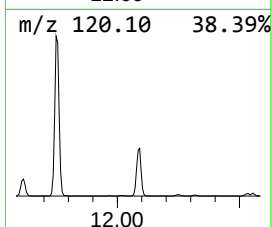
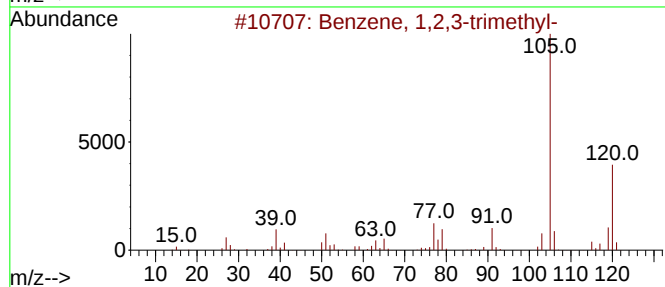
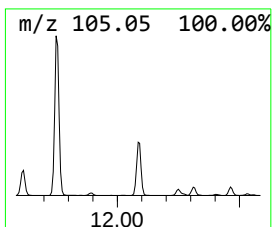
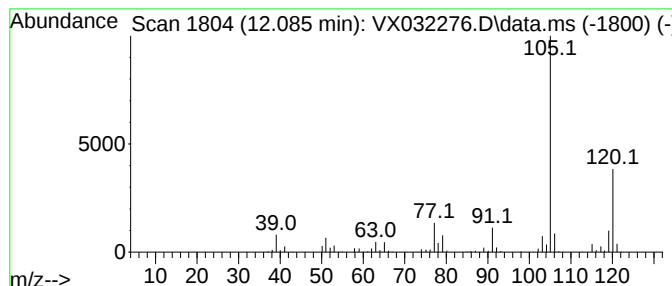
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	13.73 ug/l	162278	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Mesitylene	120	C9H12	000108-67-8	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
Data File : VX032276.D
Acq On : 20 Oct 2022 20:20
Operator : JC/MD
Sample : N5185-19 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

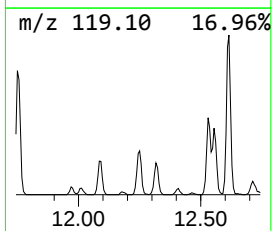
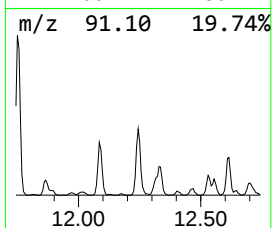
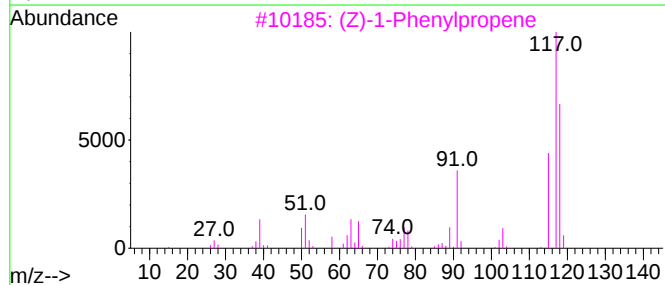
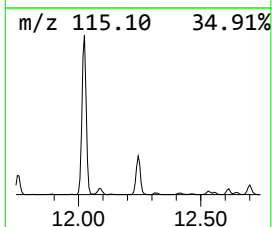
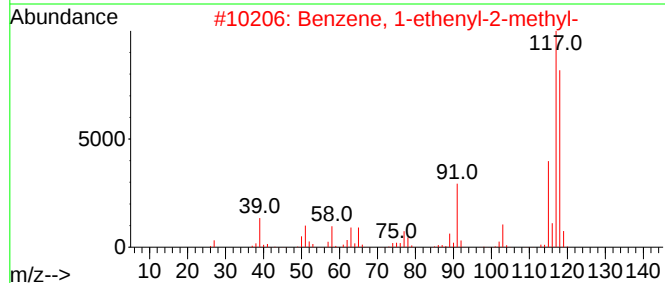
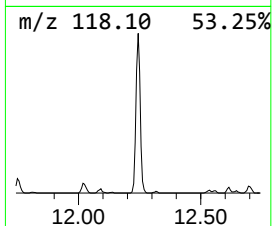
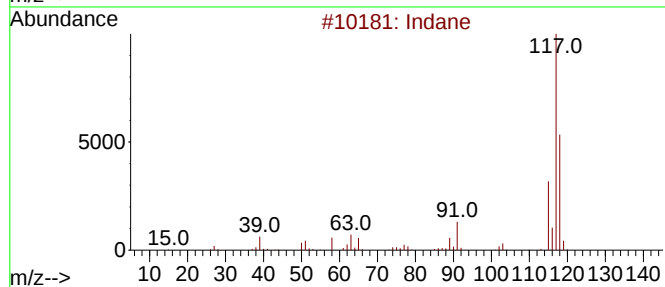
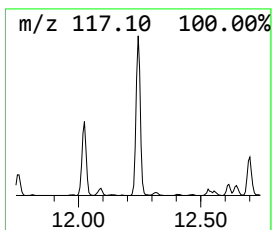
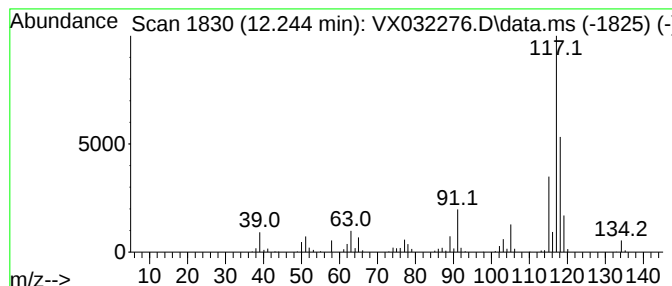
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Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	12.98 ug/l	153371	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
3			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	76
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
Data File : VX032276.D
Acq On : 20 Oct 2022 20:20
Operator : JC/MD
Sample : N5185-19 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

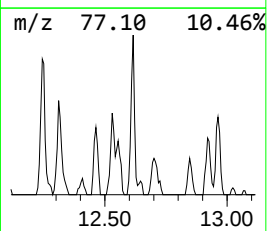
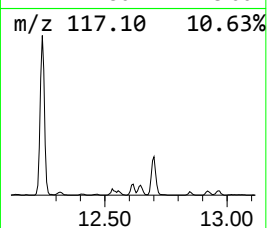
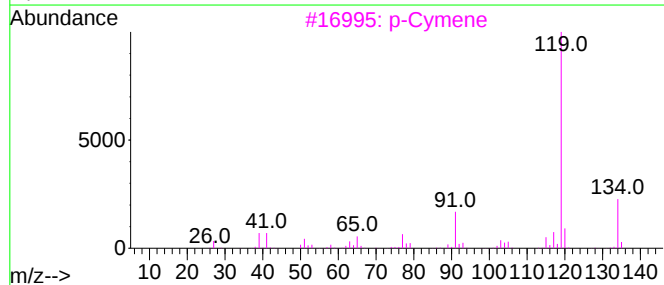
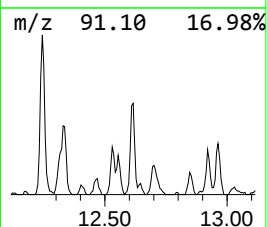
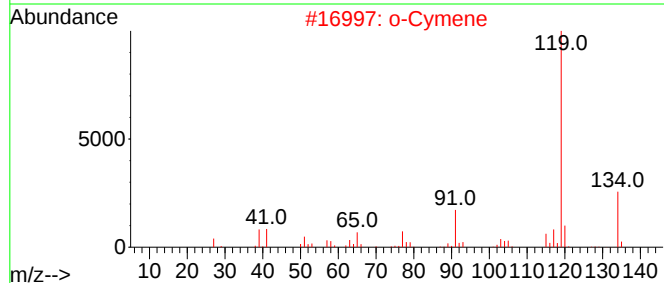
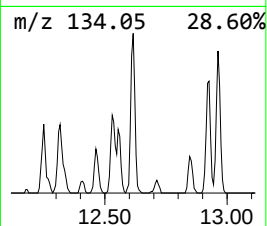
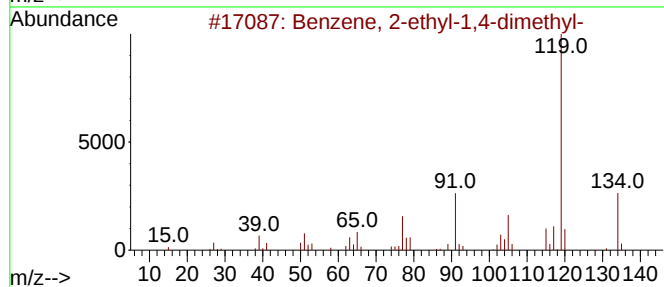
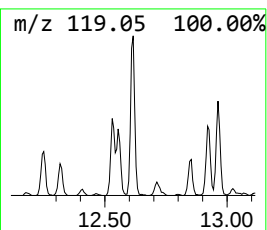
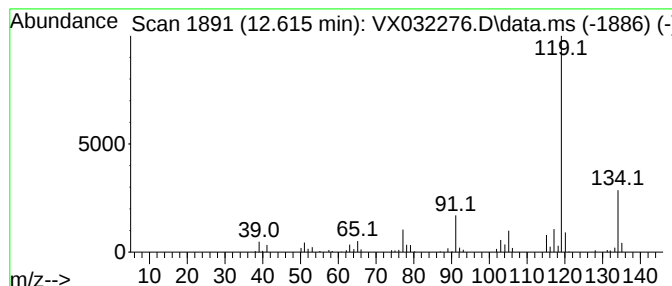
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	5.91 ug/l	69890	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			o-Cymene	134	C10H14	000527-84-4	95
3			p-Cymene	134	C10H14	000099-87-6	95
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
Data File : VX032276.D
Acq On : 20 Oct 2022 20:20
Operator : JC/MD
Sample : N5185-19 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.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
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Butane, 2-methyl-	1.752	35.8	ug/l	375224	1	5.556	524417	50.0
Pentane	1.953	10.7	ug/l	112296	1	5.556	524417	50.0
Pentane, 2-methyl-	2.825	8.1	ug/l	84936	1	5.556	524417	50.0
Pentane, 3-methyl-	3.099	6.3	ug/l	66116	1	5.556	524417	50.0
Cyclopentane, m...	4.306	12.9	ug/l	135212	1	5.556	524417	50.0
Benzene, 1-ethy...	11.616	5.8	ug/l	69112	4	12.024	590857	50.0
Benzene, 1,2,3-...	12.085	13.7	ug/l	162278	4	12.024	590857	50.0
Indane	12.244	13.0	ug/l	153371	4	12.024	590857	50.0
Benzene, 2-ethy...	12.616	5.9	ug/l	69890	4	12.024	590857	50.0