

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010622\
 Data File : VX026379.D
 Acq On : 06 Jan 2022 17:26
 Operator : JC/MD
 Sample : N1020-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-3

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\82X123021W.M
 Title : SW846 8260

Signal : TIC: VX026379.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	26	30	41	rVB	65604	61870	1.64%	0.263%
2	1.374	41	47	53	rBV	258633	267907	7.09%	1.137%
3	1.752	104	109	120	rVB	315894	445110	11.78%	1.889%
4	1.965	138	144	156	rVB2	178917	372623	9.86%	1.582%
5	2.075	157	162	169	rVV	74517	104582	2.77%	0.444%
6	2.172	173	178	181	rVV	51896	79473	2.10%	0.337%
7	2.221	181	186	200	rVB	350310	537346	14.23%	2.281%
8	2.752	261	273	282	rBV	119503	271923	7.20%	1.154%
9	2.873	287	293	308	rVB2	173504	413175	10.94%	1.754%
10	3.105	323	331	342	rVB	23195	52278	1.38%	0.222%
11	3.325	358	367	378	rVB2	24251	53130	1.41%	0.226%
12	3.739	427	435	443	rVB	65743	154467	4.09%	0.656%
13	3.843	443	452	458	rVV	43634	111113	2.94%	0.472%
14	3.910	458	463	472	rVV	32889	94083	2.49%	0.399%
15	4.001	472	478	486	rVB	17799	46973	1.24%	0.199%
16	4.105	486	495	508	rVB2	43751	115652	3.06%	0.491%
17	4.312	517	529	540	rBV	124312	355275	9.41%	1.508%
18	4.434	540	549	561	rVB2	21759	60960	1.61%	0.259%
19	5.202	662	675	690	rVB	74441	221932	5.88%	0.942%
20	5.391	694	706	714	rBV	95566	280017	7.41%	1.189%
21	5.477	714	720	726	rVV2	46465	141020	3.73%	0.599%
22	5.556	726	733	760	rVB	165833	498280	13.19%	2.115%
23	5.958	789	799	805	rBV	108612	284152	7.52%	1.206%
24	6.044	805	813	827	rVV	686156	1799118	47.63%	7.636%
25	6.202	827	839	858	rVB	51938	174103	4.61%	0.739%
26	6.763	922	931	942	rBV	253451	640241	16.95%	2.718%
27	7.171	990	998	1007	rVB2	19093	43068	1.14%	0.183%
28	7.385	1022	1033	1045	rBV5	15886	45589	1.21%	0.194%
29	8.147	1146	1158	1163	rBV	42377	75081	1.99%	0.319%
30	8.507	1210	1217	1224	rBV	39569	65390	1.73%	0.278%
31	8.653	1234	1241	1247	rBV	495438	793620	21.01%	3.369%
32	8.720	1247	1252	1263	rVB	431951	651561	17.25%	2.766%
33	9.049	1297	1306	1315	rVB	25374	40331	1.07%	0.171%
34	10.055	1461	1471	1483	rBV	512793	688570	18.23%	2.923%
35	10.195	1488	1494	1504	rVV	2134152	2763641	73.16%	11.730%
36	10.305	1505	1512	1525	rVB	2772764	3777317	100.00%	16.033%

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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

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37	10.640	1562	1567	1578	rVB	1045282	1353538	35.83%	5.745%
38	10.963	1613	1620	1626	rVB	55296	67801	1.79%	0.288%
39	11.079	1634	1639	1652	rVB	389805	513364	13.59%	2.179%
40	11.305	1668	1676	1682	rBV	76122	93045	2.46%	0.395%
41	11.378	1683	1688	1690	rBV	237932	309081	8.18%	1.312%
42	11.451	1696	1700	1711	rVB	194436	230767	6.11%	0.980%
43	11.616	1721	1727	1735	rBV	378083	477721	12.65%	2.028%
44	11.750	1744	1749	1756	rBV	992918	1236260	32.73%	5.247%
45	12.024	1789	1794	1799	rVB	490515	614073	16.26%	2.606%
46	12.091	1799	1805	1810	rBV	491268	624117	16.52%	2.649%
47	12.244	1822	1830	1838	rBV	558756	693549	18.36%	2.944%
48	12.414	1852	1858	1863	rBV	54979	69814	1.85%	0.296%
49	12.616	1886	1891	1894	rBV	38535	45313	1.20%	0.192%
50	12.701	1900	1905	1914	rVB2	51592	70630	1.87%	0.300%
51	13.292	1997	2002	2007	rVB2	80190	100149	2.65%	0.425%
52	13.774	2076	2081	2090	rBV	374900	479363	12.69%	2.035%

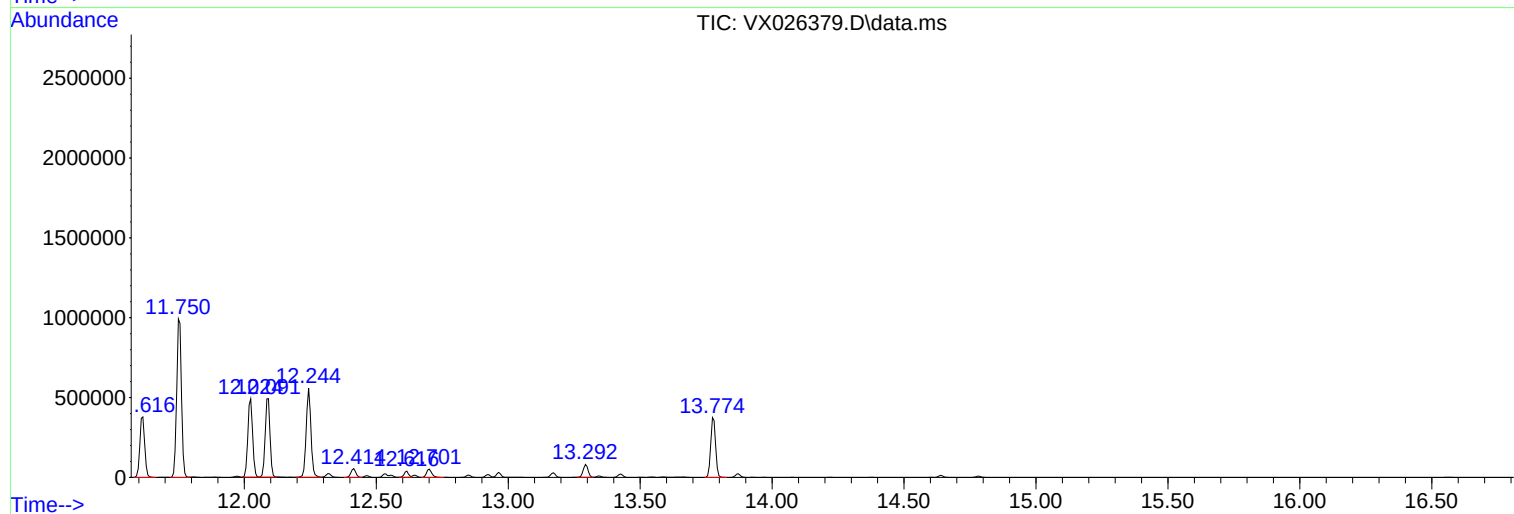
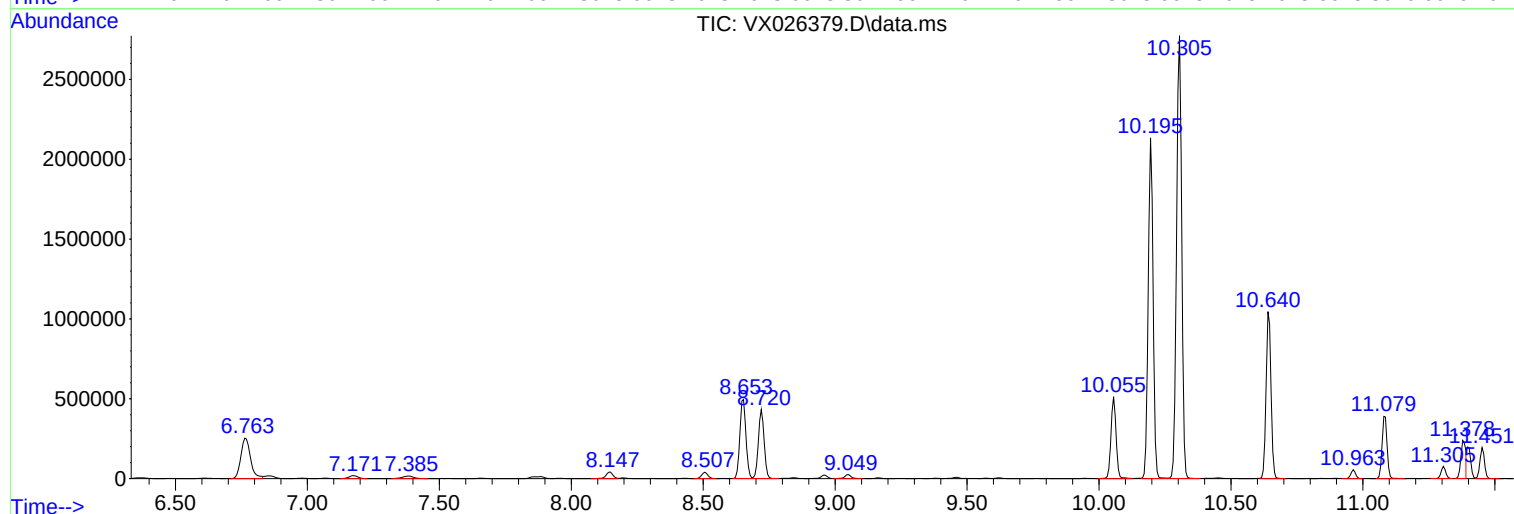
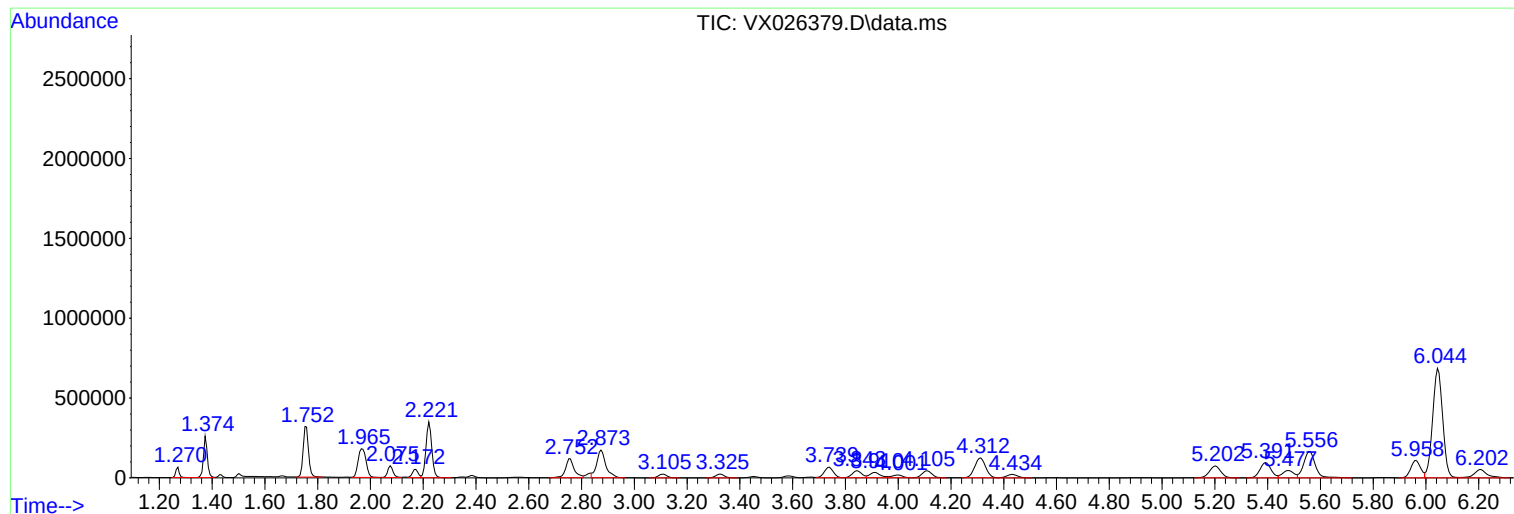
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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



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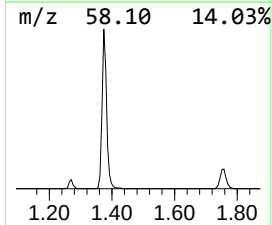
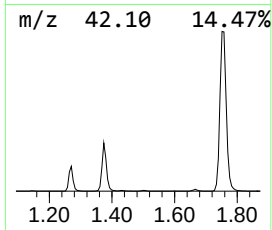
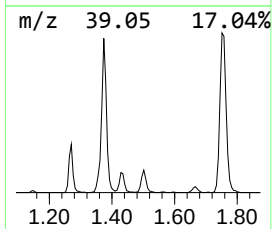
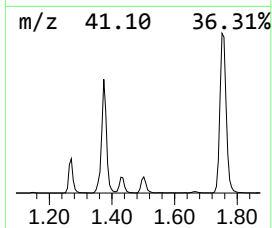
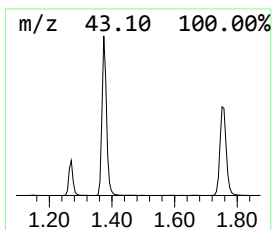
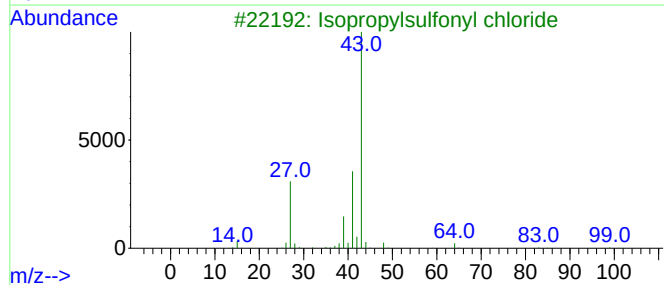
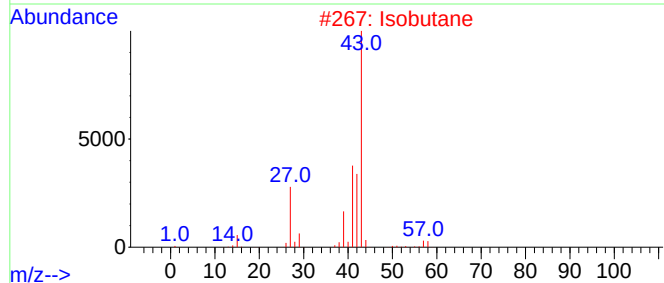
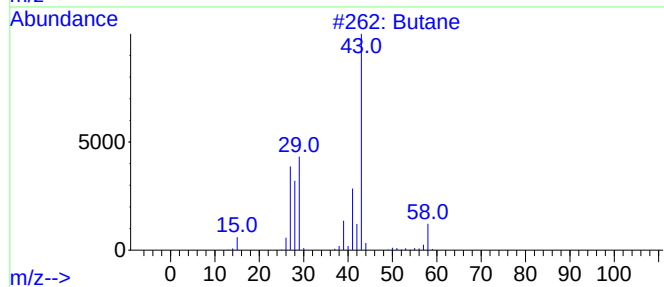
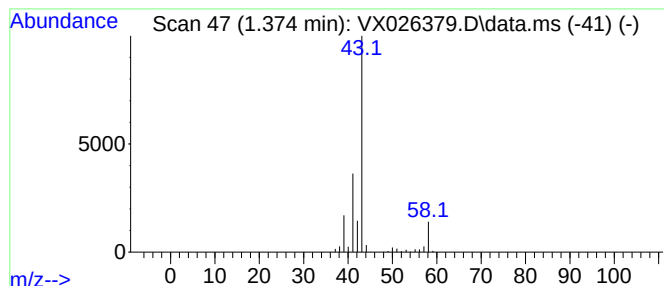
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	26.88 ug/l	267907	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
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			Diazene, dimethyl-	58	C2H6N2	000503-28-6	5



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-3

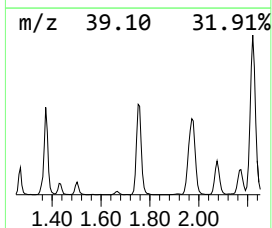
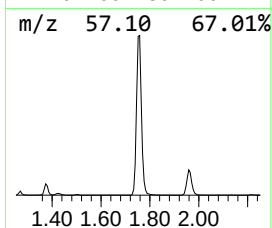
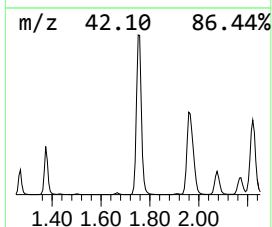
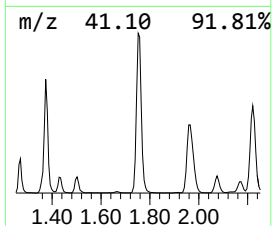
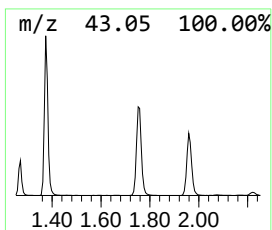
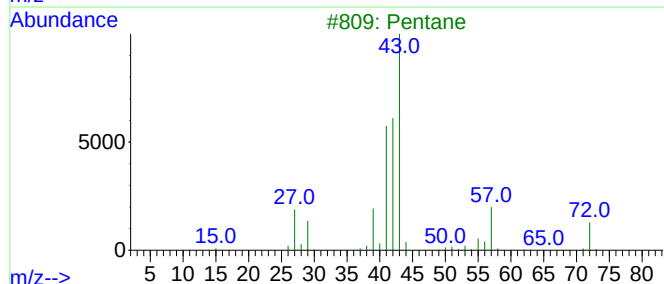
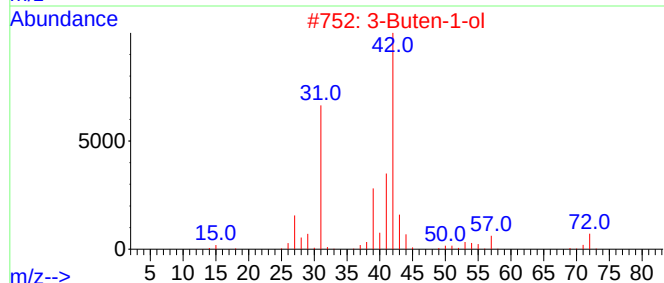
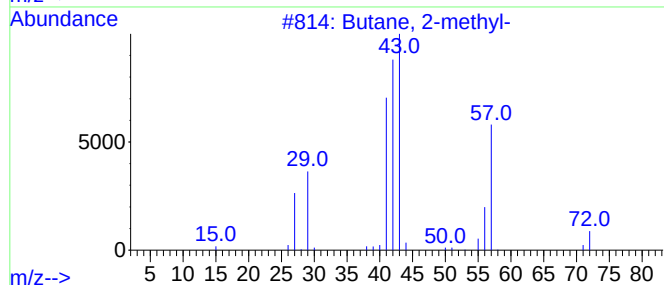
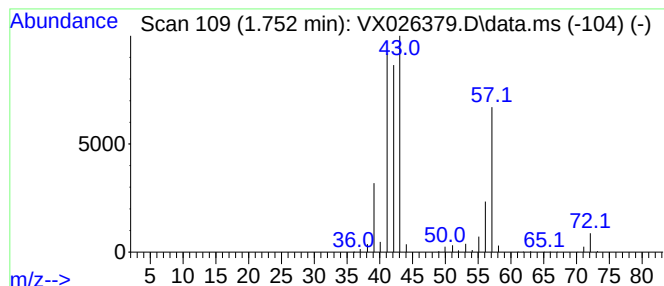
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	44.66 ug/l	445110	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	25
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	14



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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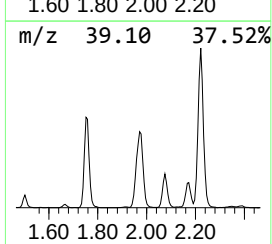
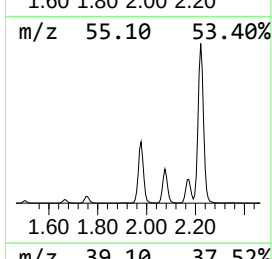
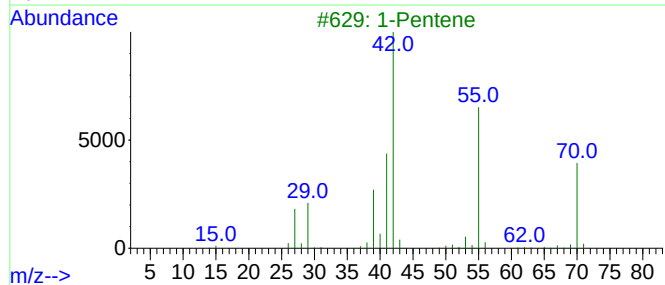
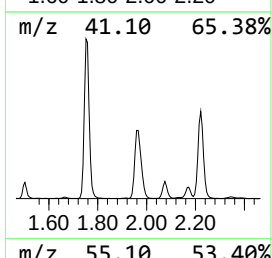
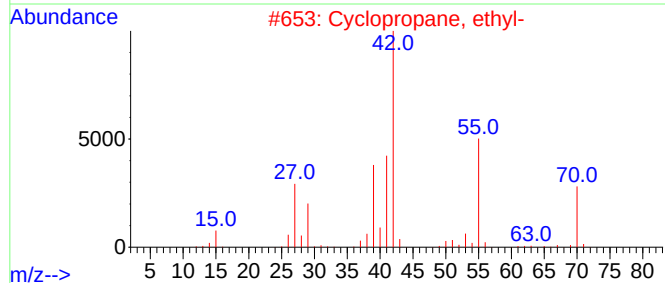
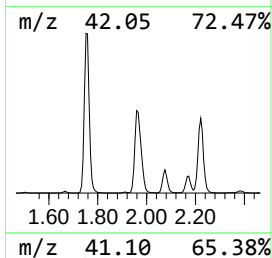
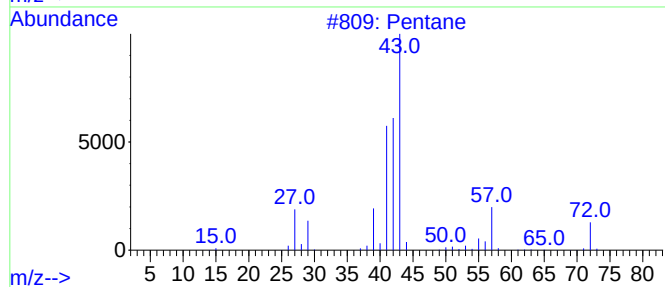
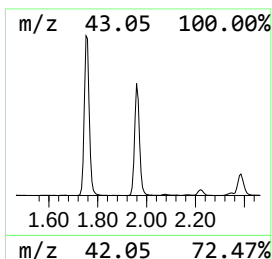
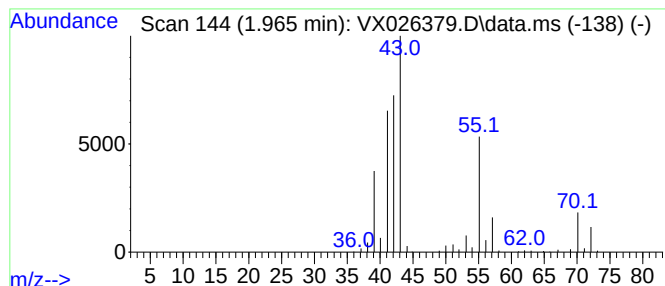
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.965	37.39 ug/l	372623	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	59
2	Cyclopropane, ethyl-			70	C5H10	001191-96-4	49
3	1-Pentene			70	C5H10	000109-67-1	47
4	Cyclobutane, methyl-			70	C5H10	000598-61-8	47
5	Butane, 2-methyl-			72	C5H12	000078-78-4	38



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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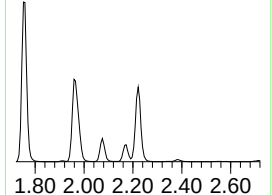
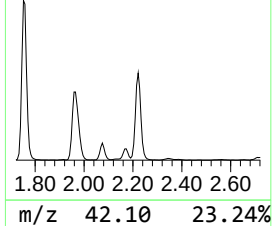
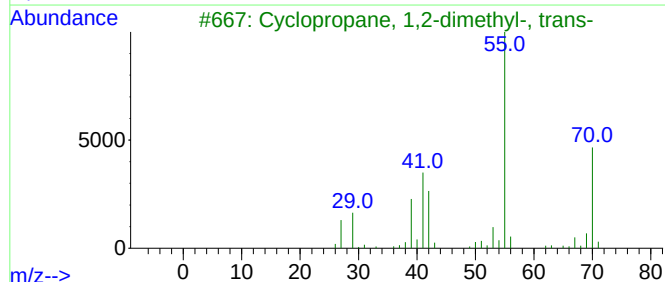
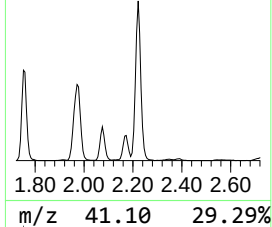
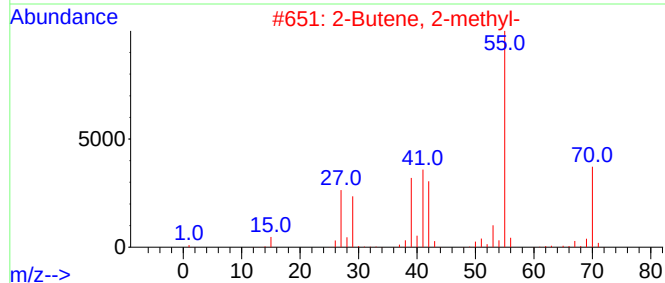
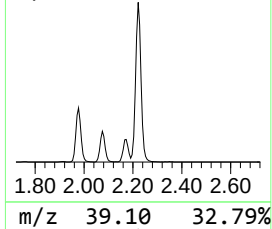
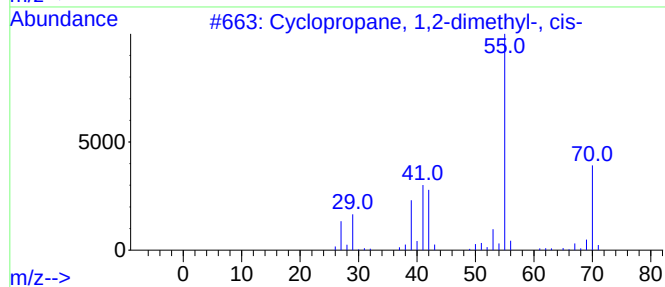
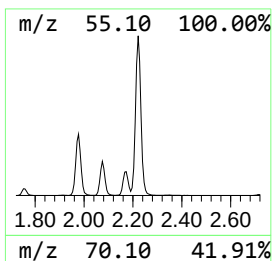
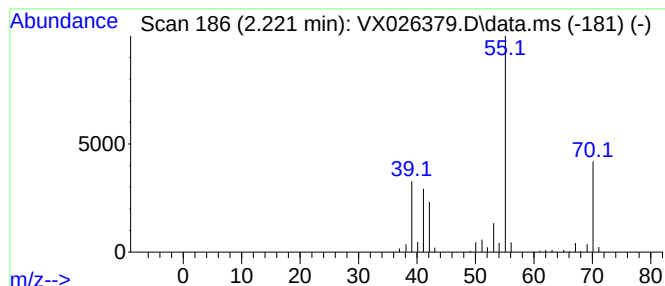
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopropane, 1,2-dimethyl-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.221	53.92 ug/l	537346	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
3			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
4			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
5			2-Methyl-1-butene	70	C5H10	000563-46-2	78



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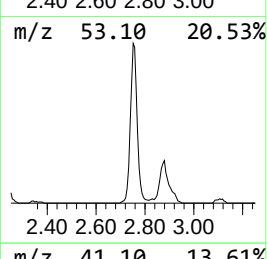
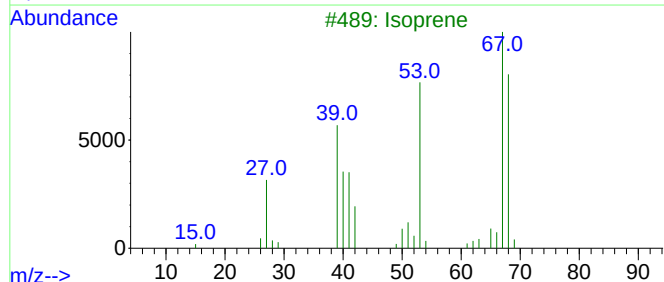
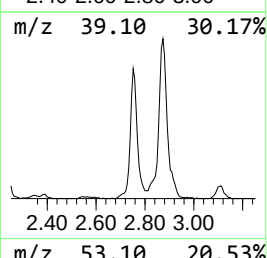
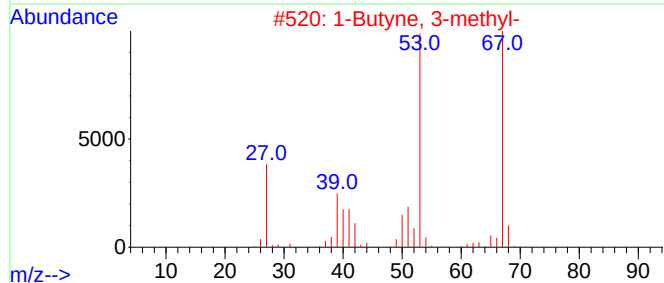
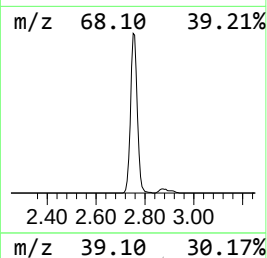
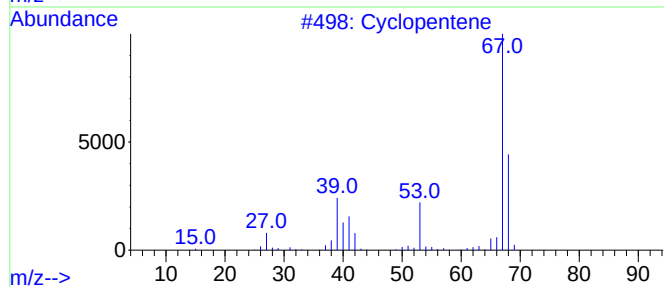
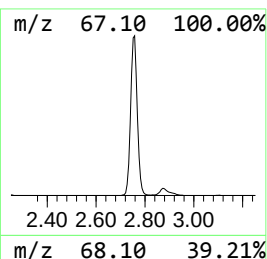
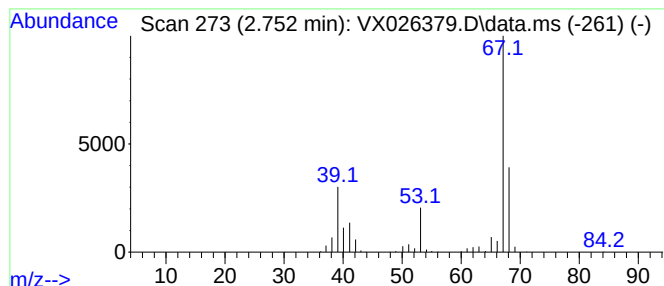
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.752	27.29 ug/l	271923	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene	68	C5H8	000142-29-0	91
2			1-Butyne, 3-methyl-	68	C5H8	000598-23-2	64
3			Isoprene	68	C5H8	000078-79-5	59
4			1,4-Pentadiene	68	C5H8	000591-93-5	58
5			1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010622\
Data File : VX026379.D
Acq On : 06 Jan 2022 17:26
Operator : JC/MD
Sample : N1020-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

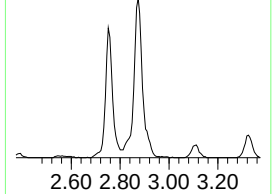
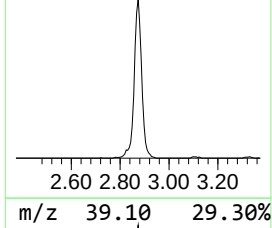
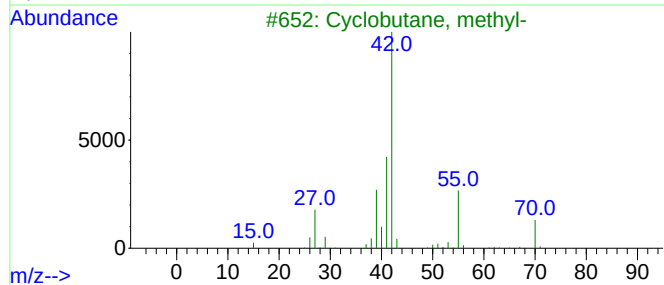
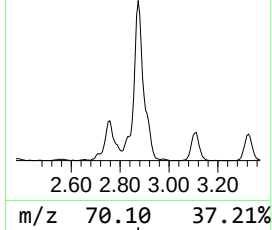
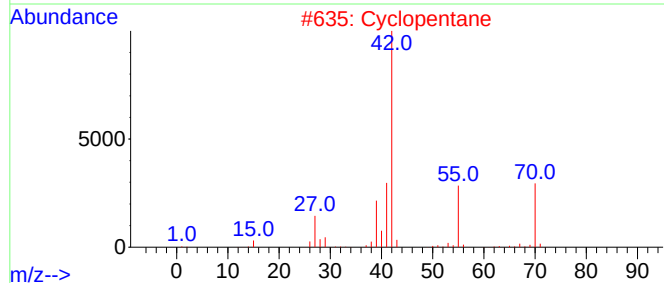
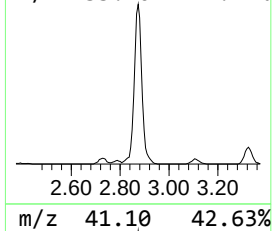
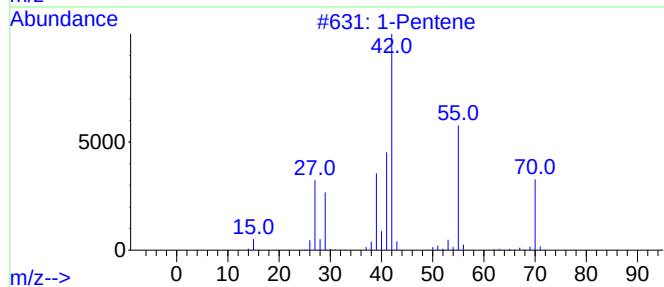
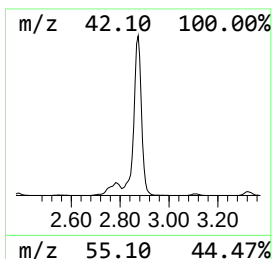
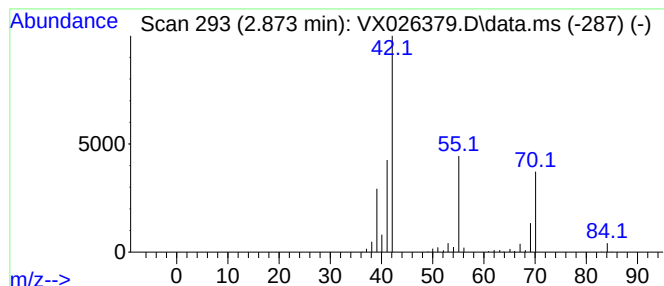
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 6 1-Pentene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.873	41.46 ug/l	413175	Pentafluorobenzene	5.556	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	80
2	Cyclopentane	70	C5H10	000287-92-3	72
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	59
5	2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VOX010622\
Data File : VX026379.D
Acq On : 06 Jan 2022 17:26
Operator : JC/MD
Sample : N1020-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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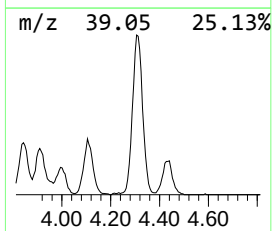
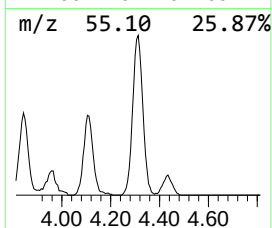
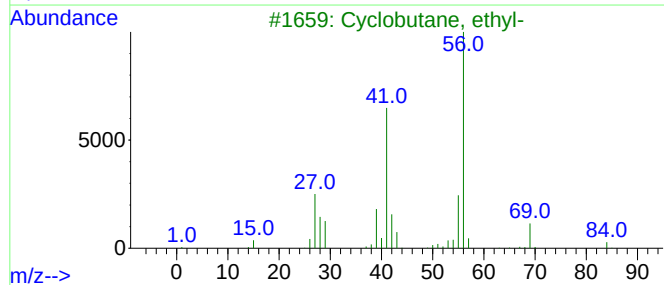
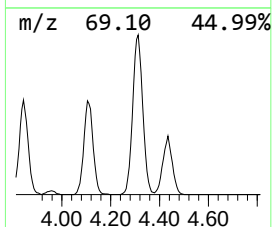
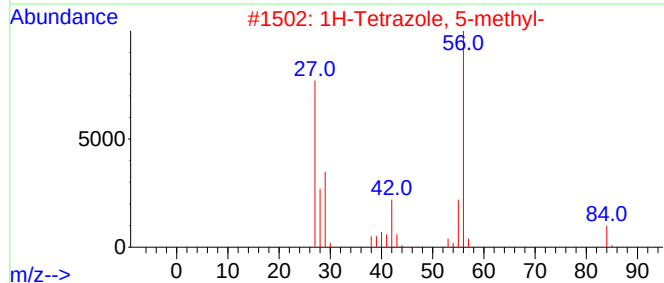
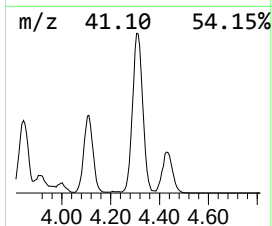
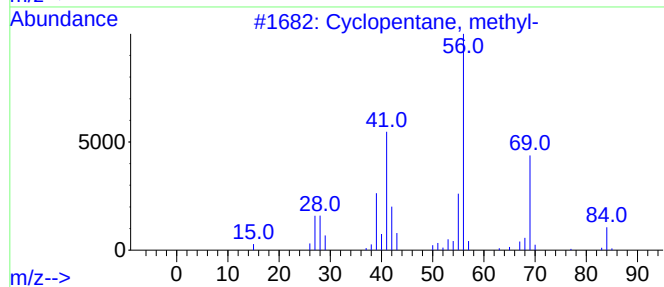
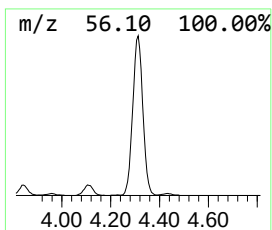
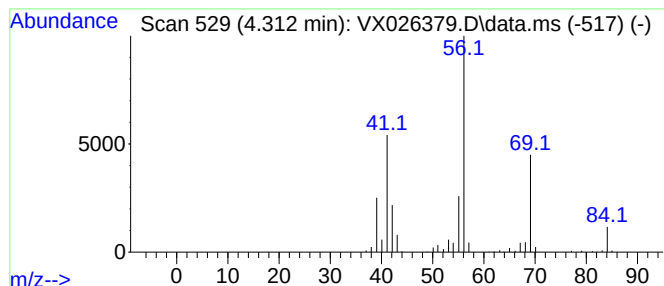
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	35.65 ug/l	355275	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	80
4			Cyclohexane	84	C6H12	000110-82-7	50
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010622\
Data File : VX026379.D
Acq On : 06 Jan 2022 17:26
Operator : JC/MD
Sample : N1020-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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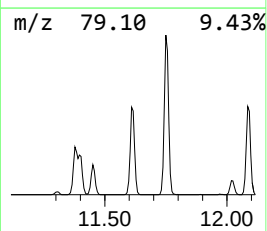
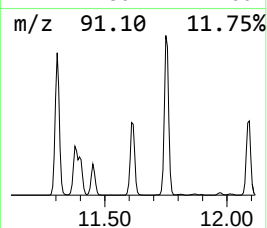
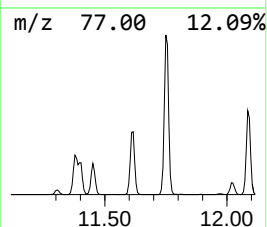
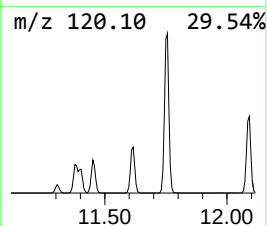
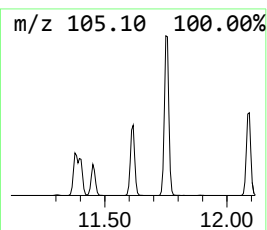
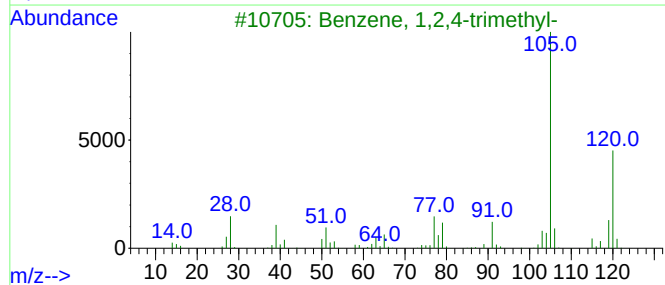
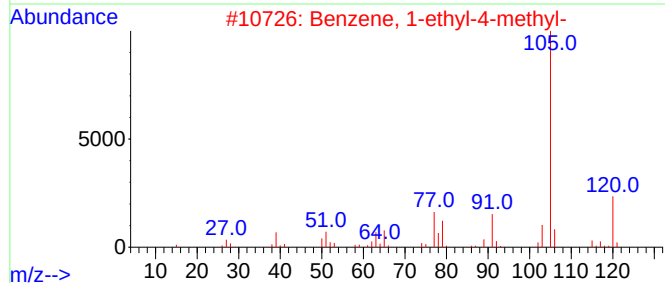
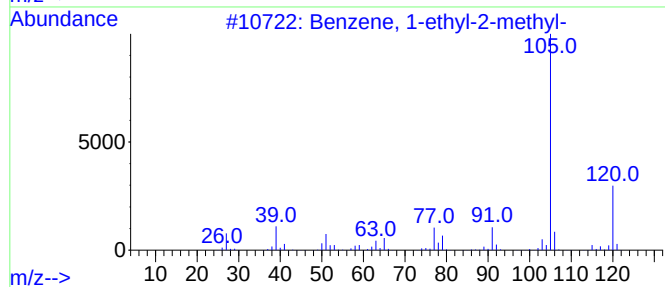
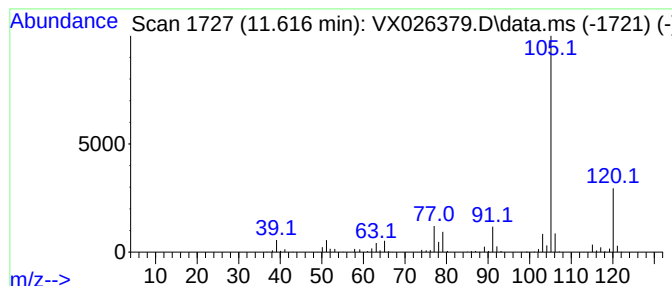
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	38.90 ug/l	477721	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VOX010622\
Data File : VX026379.D
Acq On : 06 Jan 2022 17:26
Operator : JC/MD
Sample : N1020-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

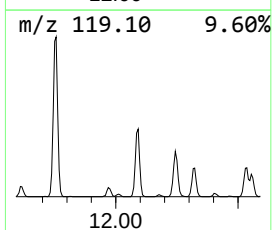
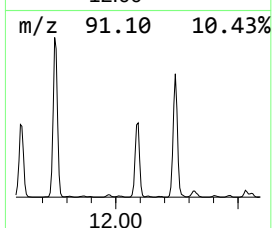
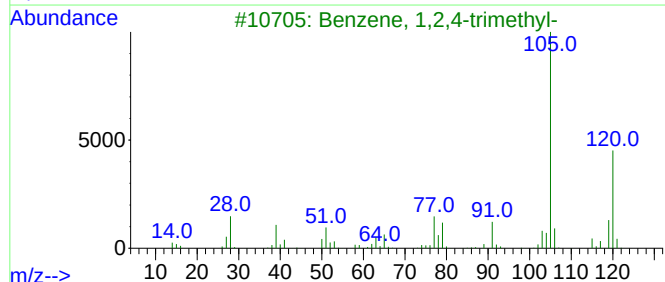
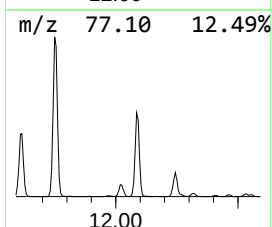
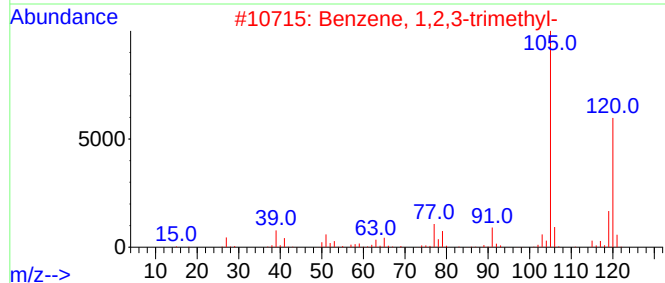
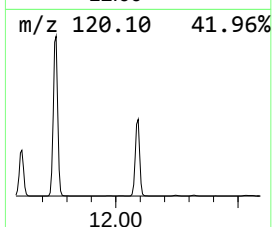
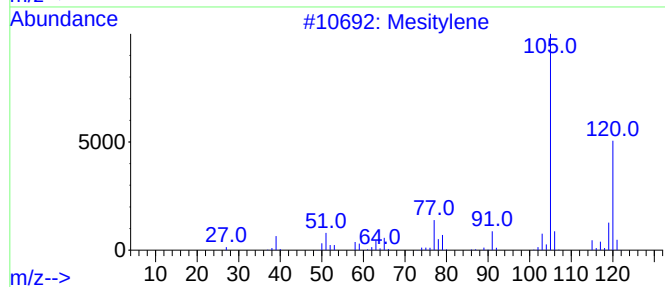
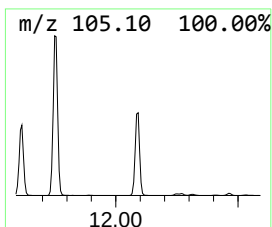
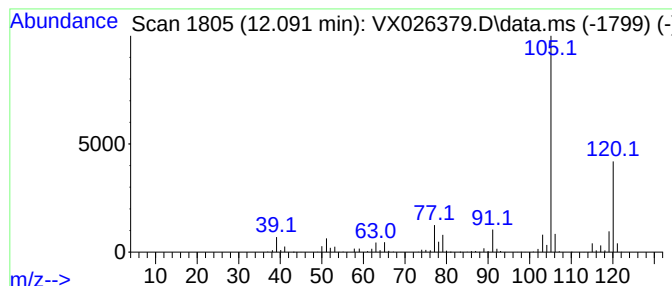
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	50.82 ug/l	624117	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010622\
Data File : VX026379.D
Acq On : 06 Jan 2022 17:26
Operator : JC/MD
Sample : N1020-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

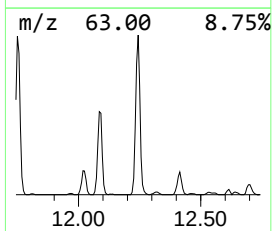
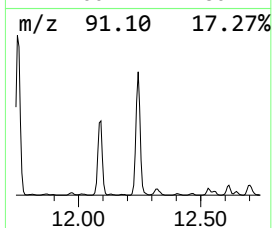
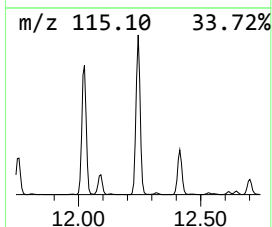
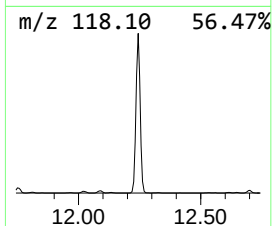
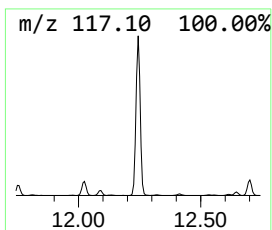
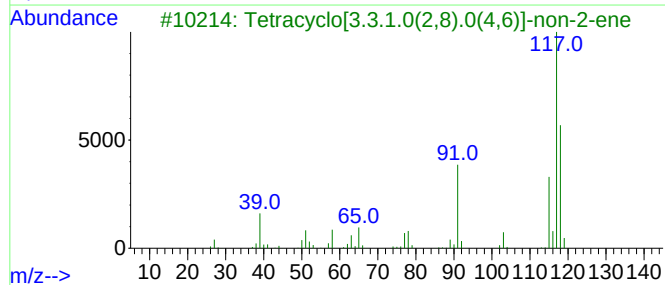
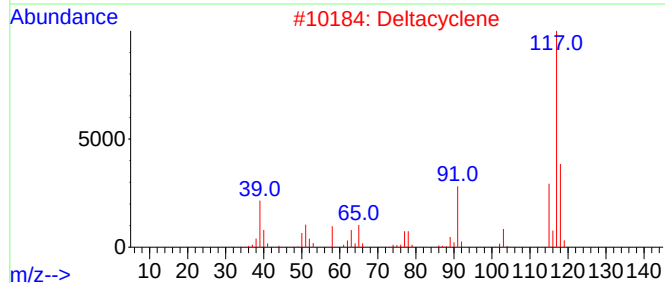
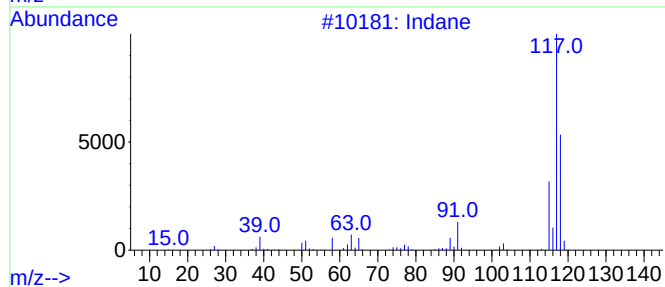
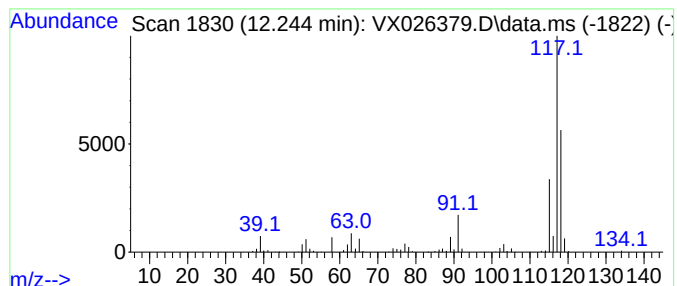
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	56.47 ug/l	693549	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Deltacyclene	118	C9H10	007785-10-6	74
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010622\
Data File : VX026379.D
Acq On : 06 Jan 2022 17:26
Operator : JC/MD
Sample : N1020-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.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	44.7	ug/l	445110	1	5.556	498280	50.0
Pentane	1.965	37.4	ug/l	372623	1	5.556	498280	50.0
Cyclopropane, 1...	2.221	53.9	ug/l	537346	1	5.556	498280	50.0
Cyclopentene	2.752	27.3	ug/l	271923	1	5.556	498280	50.0
1-Pentene	2.873	41.5	ug/l	413175	1	5.556	498280	50.0
Cyclopentane, m...	4.312	35.6	ug/l	355275	1	5.556	498280	50.0
Benzene, 1-ethy...	11.616	38.9	ug/l	477721	4	12.024	614073	50.0
Benzene, 1,2,3-...	12.091	50.8	ug/l	624117	4	12.024	614073	50.0
Indane	12.244	56.5	ug/l	693549	4	12.024	614073	50.0