

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
 Data File : VN073686.D
 Acq On : 02 Aug 2022 14:47
 Operator : JC\MD
 Sample : N3971-12
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-19

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_N\methods\82N072822W.M
 Title : SW846 8260

Signal : TIC: VN073686.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	48	59	66	rBV	748668	1131329	17.01%	2.919%
2	2.310	66	72	78	rBV	39355	113382	1.70%	0.293%
3	2.399	80	87	98	rVV	1585265	2458347	36.96%	6.343%
4	2.699	136	138	152	rVB4	40909	96653	1.45%	0.249%
5	3.087	194	204	232	rVB	2978310	6652053	100.00%	17.164%
6	3.457	258	267	283	rVB2	287082	798444	12.00%	2.060%
7	3.657	293	301	312	rVB2	70255	165761	2.49%	0.428%
8	3.828	319	330	337	rBV3	33173	94382	1.42%	0.244%
9	3.928	337	347	362	rVB	341791	898704	13.51%	2.319%
10	4.222	382	397	406	rBV2	30686	114937	1.73%	0.297%
11	4.510	434	446	459	rBV2	52713	181027	2.72%	0.467%
12	4.881	496	509	518	rBV4	23152	81224	1.22%	0.210%
13	4.993	518	528	532	rVV3	36402	113143	1.70%	0.292%
14	5.104	534	547	572	rVB4	167318	848850	12.76%	2.190%
15	5.528	607	619	636	rBV3	49331	175137	2.63%	0.452%
16	6.387	745	765	777	rBV	73752	232804	3.50%	0.601%
17	6.522	777	788	797	rBV4	49582	158903	2.39%	0.410%
18	6.822	829	839	852	rVB2	60111	176619	2.66%	0.456%
19	7.063	870	880	889	rBV	228116	681011	10.24%	1.757%
20	7.134	890	892	903	rVB3	35136	83030	1.25%	0.214%
21	7.339	919	927	937	rBV	77696	189116	2.84%	0.488%
22	7.775	989	1001	1008	rVB2	32876	86240	1.30%	0.223%
23	7.951	1021	1031	1036	rBV	273453	658478	9.90%	1.699%
24	8.022	1036	1043	1054	rVB2	552539	1306128	19.63%	3.370%
25	8.392	1093	1106	1114	rBV2	998449	2620859	39.40%	6.763%
26	8.469	1114	1119	1124	rVB2	41142	89125	1.34%	0.230%
27	8.904	1183	1193	1207	rBV	687823	1398456	21.02%	3.608%
28	10.380	1437	1444	1450	rBV	971512	1768351	26.58%	4.563%
29	10.445	1450	1455	1461	rVV	269474	505585	7.60%	1.305%
30	11.233	1583	1589	1602	rVB	61658	119460	1.80%	0.308%
31	11.686	1658	1666	1676	rBV	954039	1696850	25.51%	4.378%
32	11.786	1676	1683	1693	rVV	1268174	2080563	31.28%	5.368%
33	11.892	1693	1701	1713	rVB	2388658	4524335	68.01%	11.674%
34	12.221	1749	1757	1766	rBV	427204	704826	10.60%	1.819%
35	12.521	1800	1808	1815	rVB	63910	111100	1.67%	0.287%
36	12.674	1826	1834	1845	rBV	844338	1423469	21.40%	3.673%

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37	12.863	1859	1866	1871	rBV	83809	137057	2.06%	0.354%
38	12.927	1871	1877	1880	rVV	172150	294747	4.43%	0.761%
39	12.957	1880	1882	1886	rVV	78690	106218	1.60%	0.274%
40	12.998	1886	1889	1898	rVB	68079	108560	1.63%	0.280%
41	13.163	1908	1917	1924	rBV	166879	269620	4.05%	0.696%
42	13.310	1933	1942	1948	rBV	417223	664488	9.99%	1.715%
43	13.616	1986	1994	2006	rBV2	1091859	2086782	31.37%	5.384%
44	13.710	2006	2010	2017	rVB	81528	131376	1.97%	0.339%
45	13.816	2022	2028	2039	rVB	146384	250994	3.77%	0.648%
46	15.439	2293	2304	2312	rBV	81458	167113	2.51%	0.431%

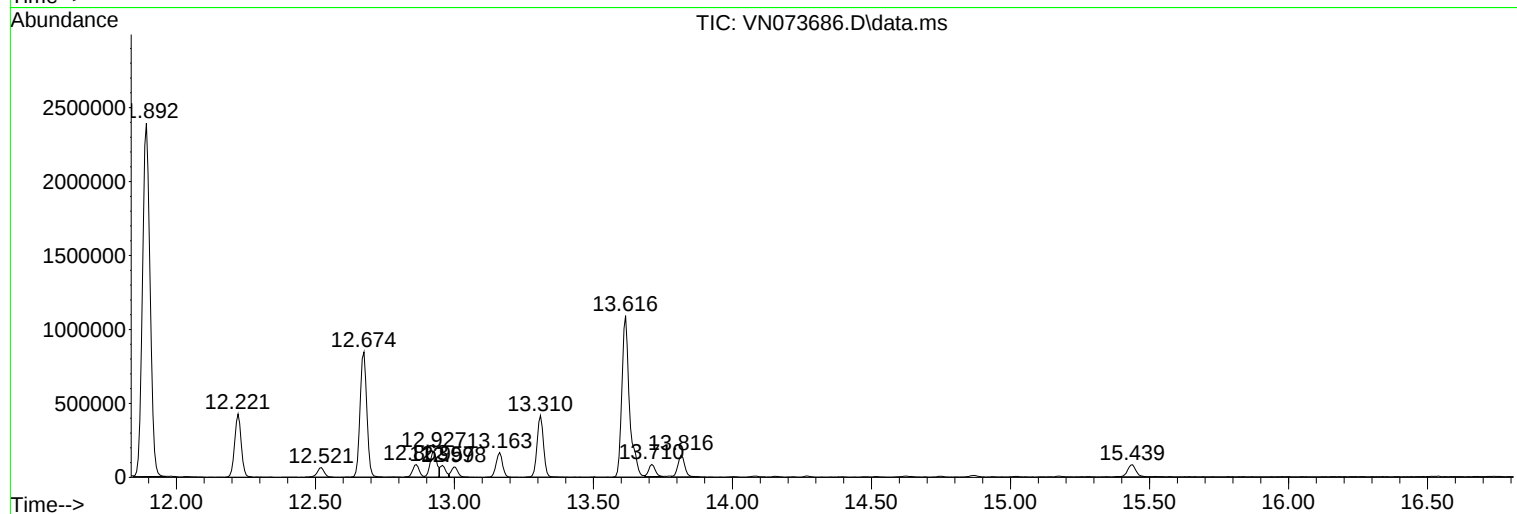
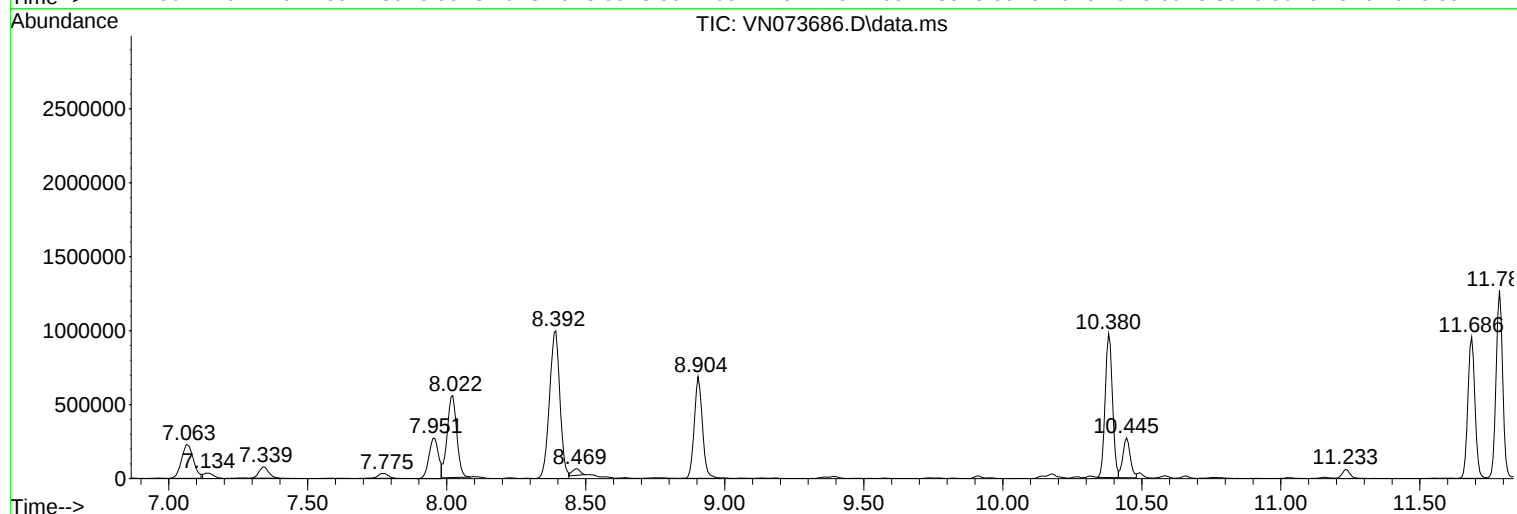
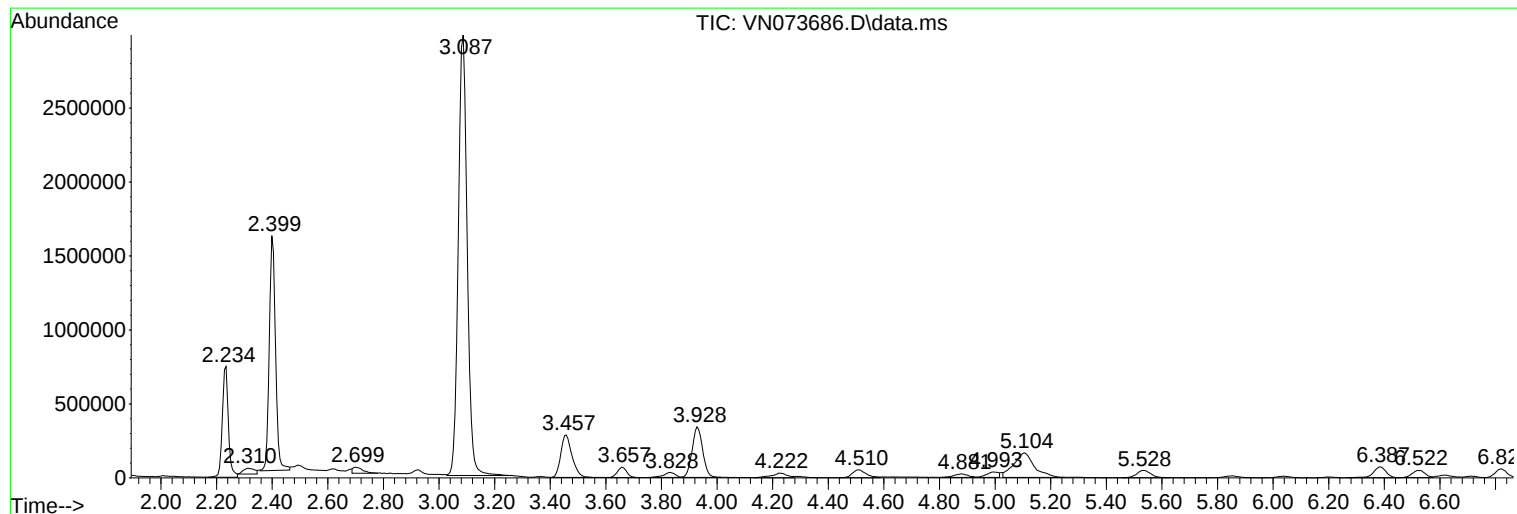
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



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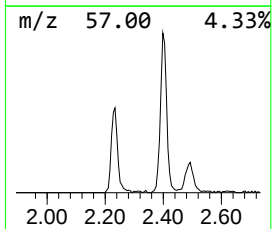
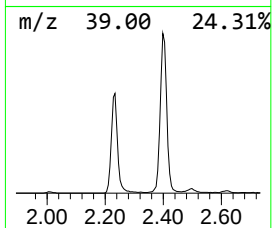
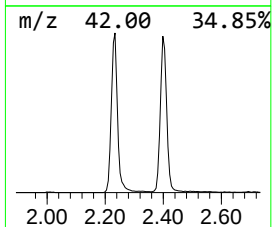
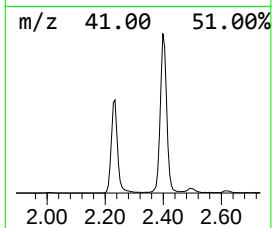
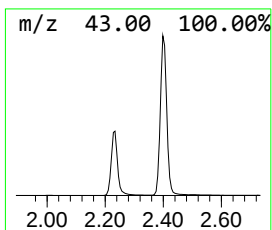
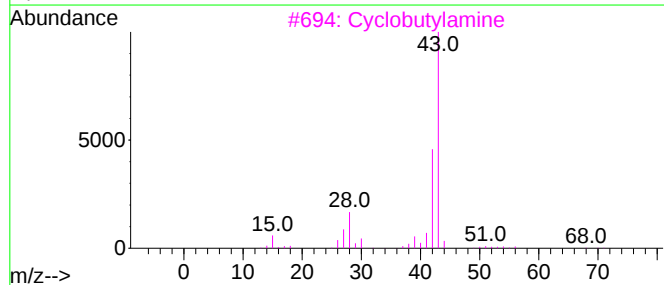
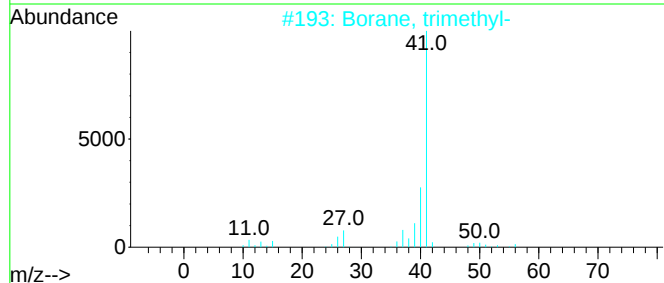
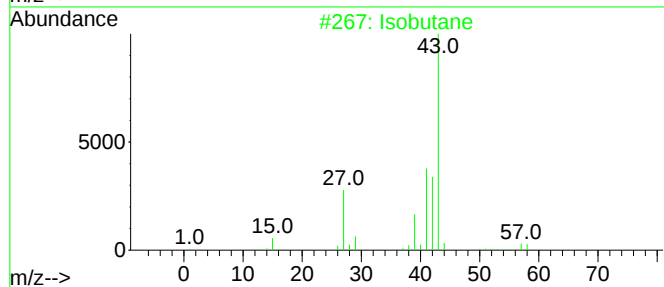
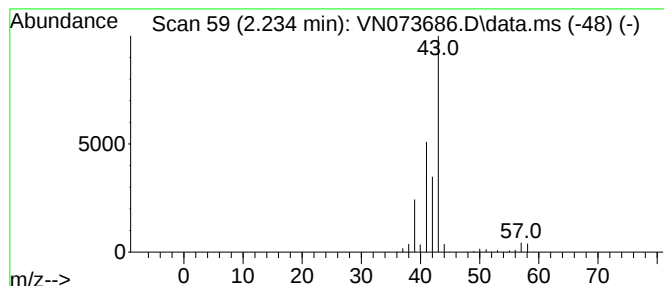
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Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	43.31 ug/l	1131330	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	80
2			Borane, trimethyl-	56	C3H9B	000593-90-8	5
3			Cyclobutylamine	71	C4H9N	002516-34-9	4
4			Propene	42	C3H6	000115-07-1	4
5			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4



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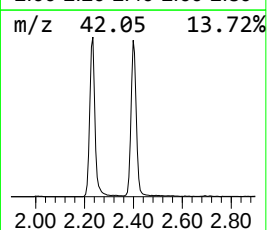
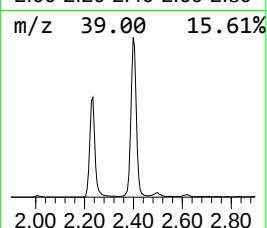
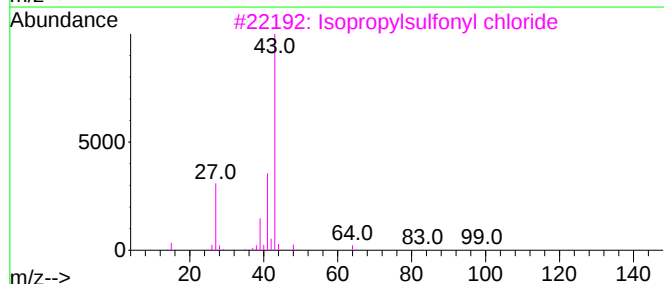
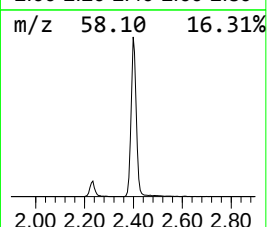
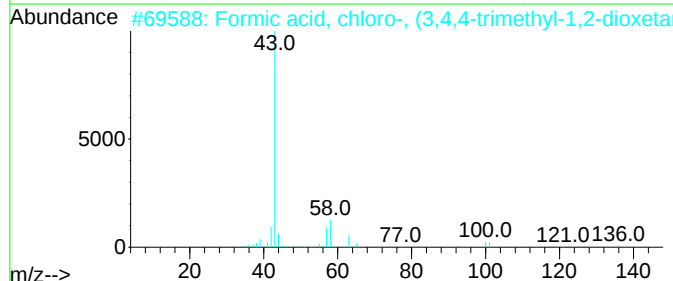
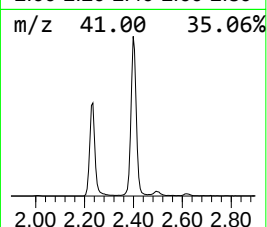
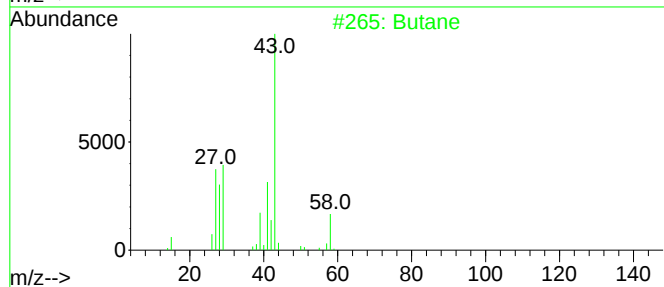
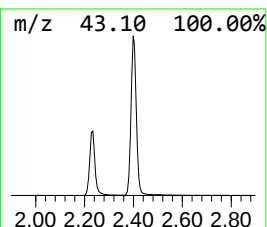
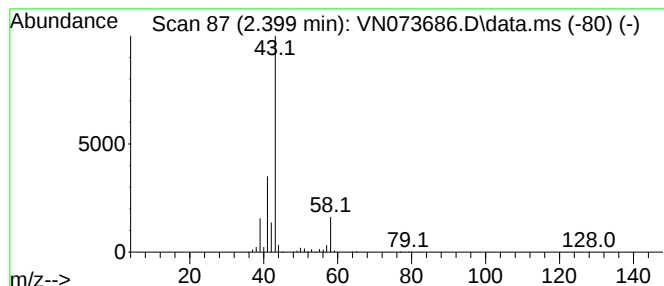
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	94.11 ug/l	2458350	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	39
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Isobutane	58	C4H10	000075-28-5	9
5			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9



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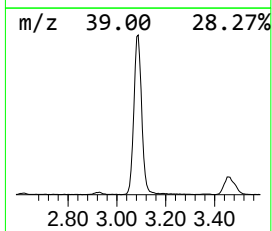
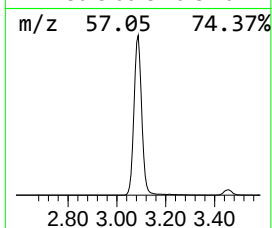
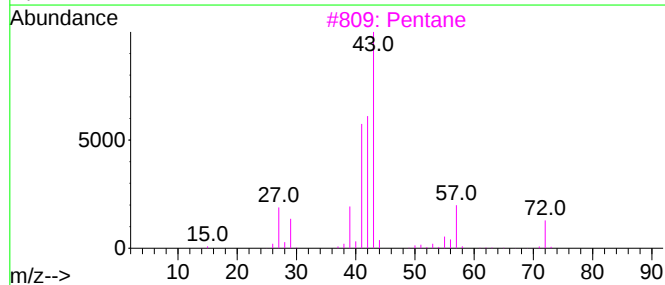
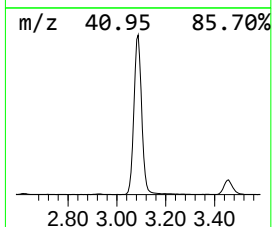
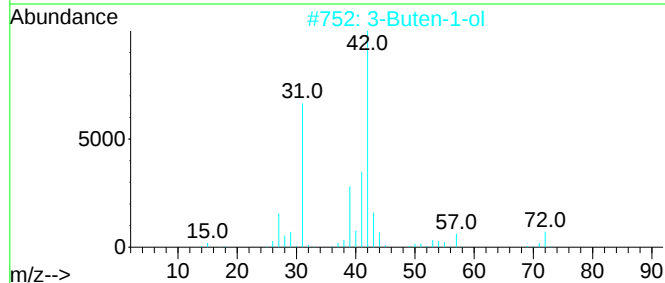
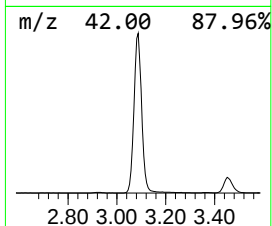
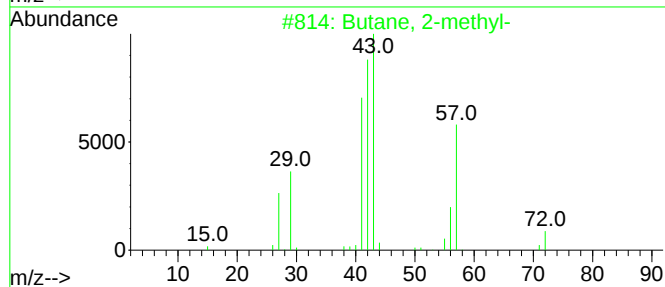
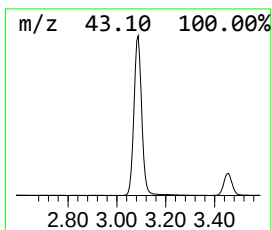
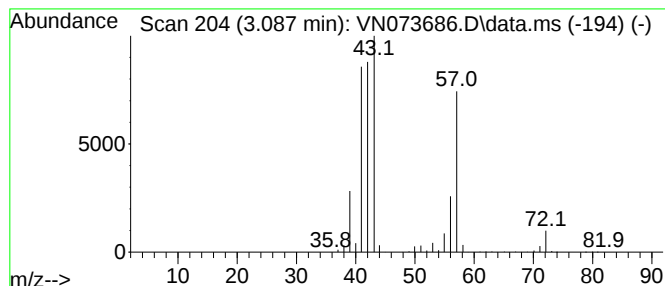
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Quant Title : SW846 8260

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

Peak Number 3 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	254.65 ug/l	6652050	Pentafluorobenzene	8.016

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	43
4			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	12
5			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10



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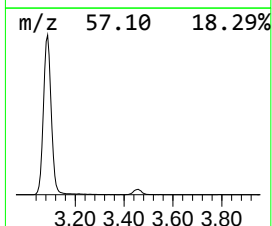
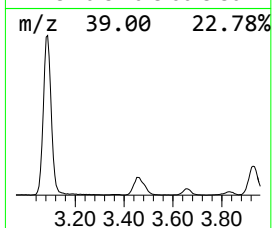
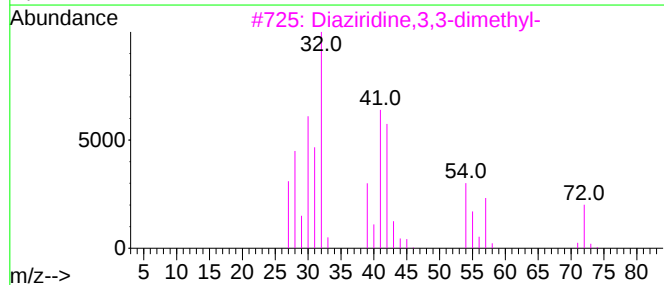
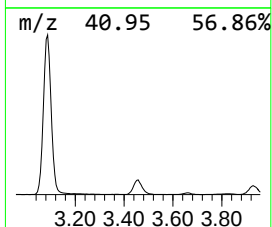
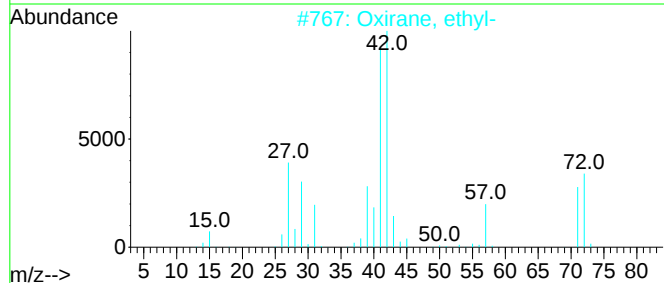
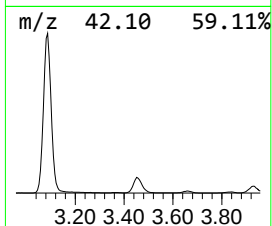
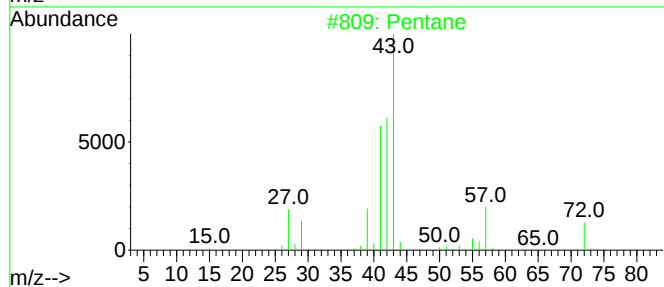
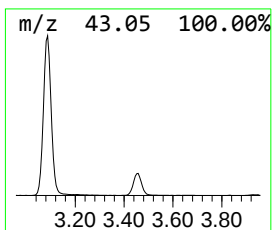
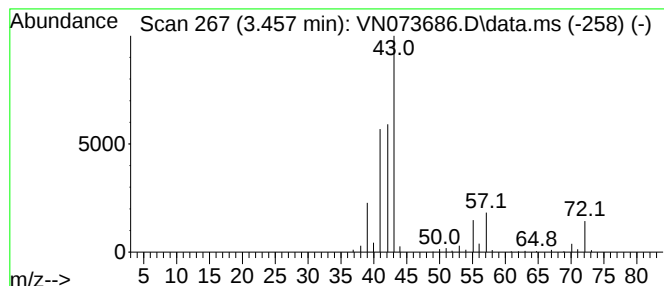
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Quant Title : SW846 8260

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

Peak Number 4 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.457	30.57 ug/l	798444	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	87
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	53
3			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	42
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	25
5			1-Pentene	70	C5H10	000109-67-1	17



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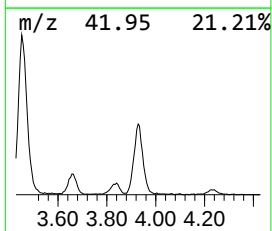
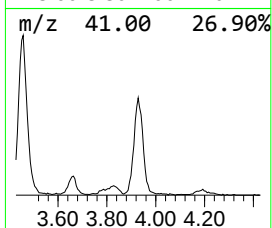
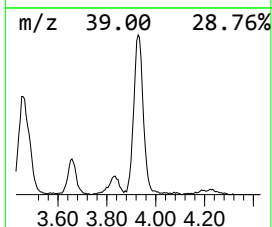
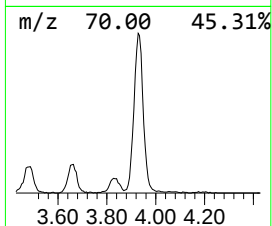
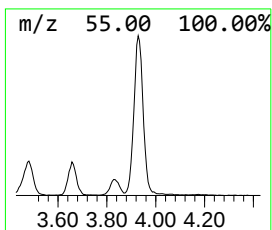
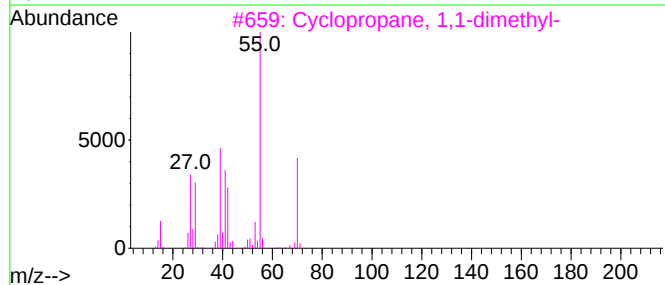
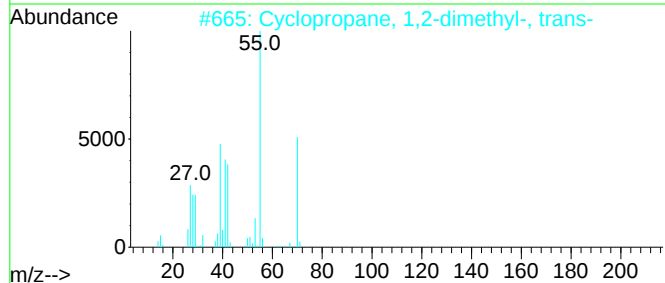
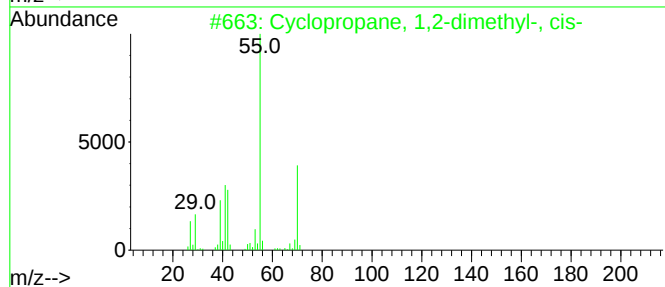
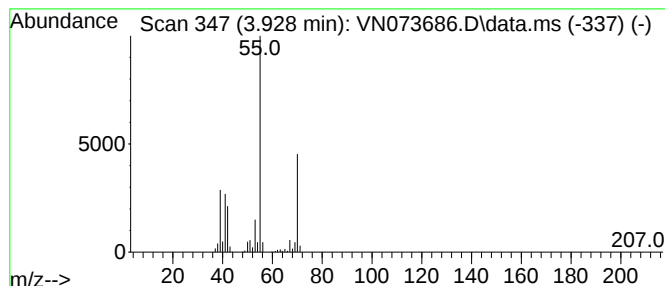
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.928	34.40 ug/l	898704	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2		Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83
3		Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
4		2-Butene, 2-methyl-	70	C5H10	000513-35-9	78
5		1-Butene, 3-methyl-	70	C5H10	000563-45-1	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073686.D
Acq On : 02 Aug 2022 14:47
Operator : JC\MD
Sample : N3971-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-19

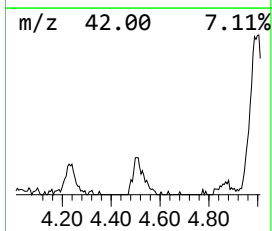
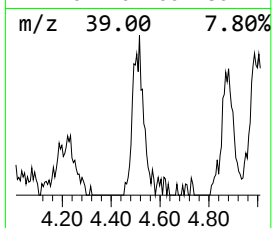
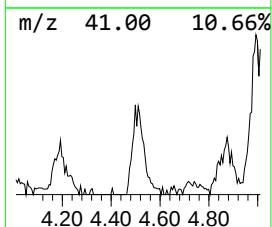
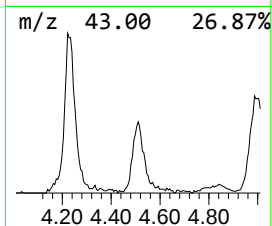
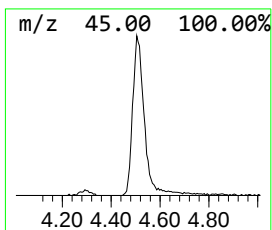
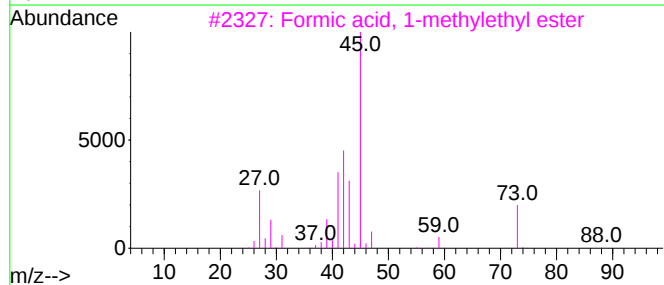
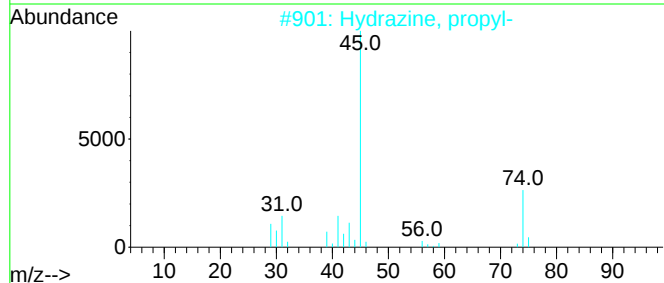
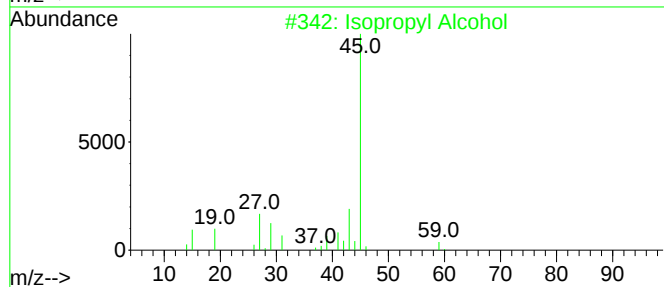
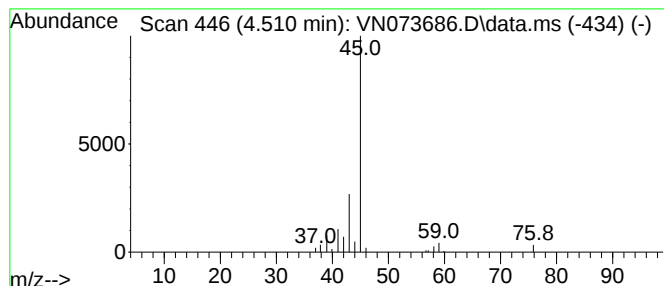
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Quant Title : SW846 8260

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

Peak Number 6 Isopropyl Alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	6.93 ug/l	181027	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	72
2			Hydrazine, propyl-	74	C3H10N2	005039-61-2	40
3			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
4			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
5			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073686.D
Acq On : 02 Aug 2022 14:47
Operator : JC\MD
Sample : N3971-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-19

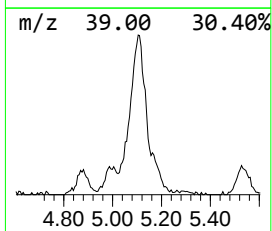
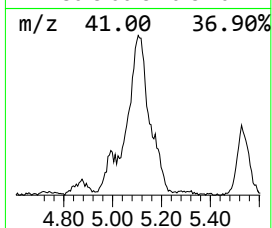
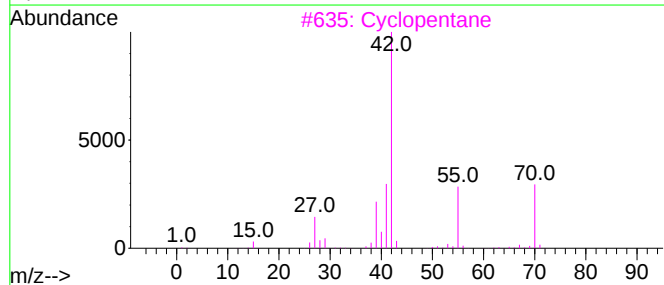
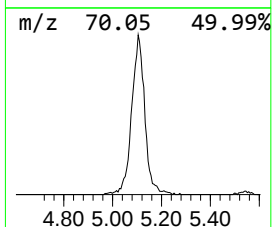
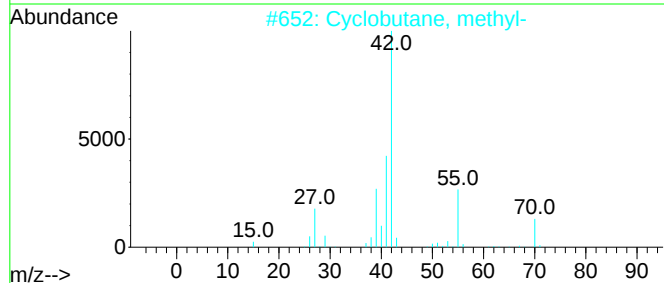
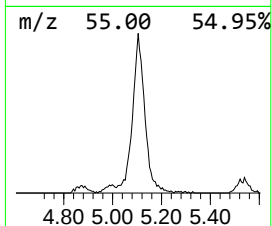
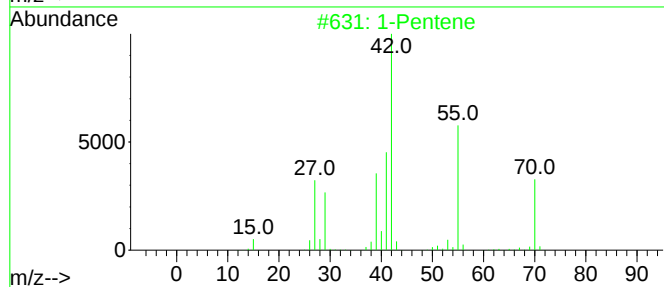
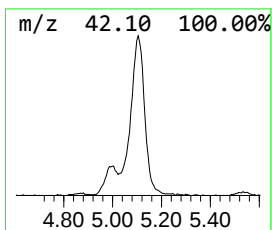
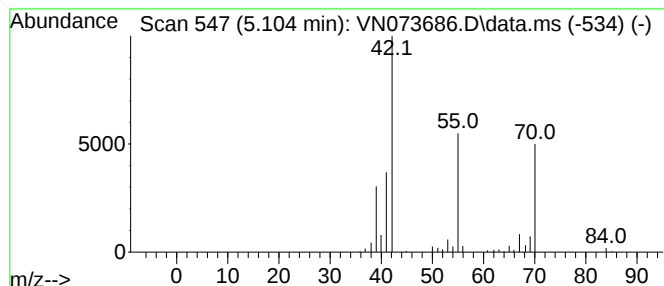
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Quant Title : SW846 8260

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

Peak Number 7 1-Pentene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	32.49 ug/l	848850	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene		70	C5H10	000109-67-1	86
2	Cyclobutane, methyl-		70	C5H10	000598-61-8	80
3	Cyclopentane		70	C5H10	000287-92-3	78
4	1-Pentanol		88	C5H12O	000071-41-0	56
5	Cyclopropane, ethyl-		70	C5H10	001191-96-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073686.D
Acq On : 02 Aug 2022 14:47
Operator : JC\MD
Sample : N3971-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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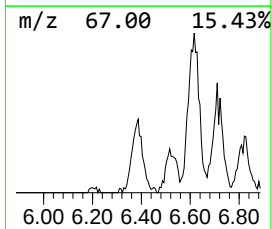
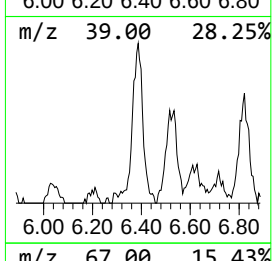
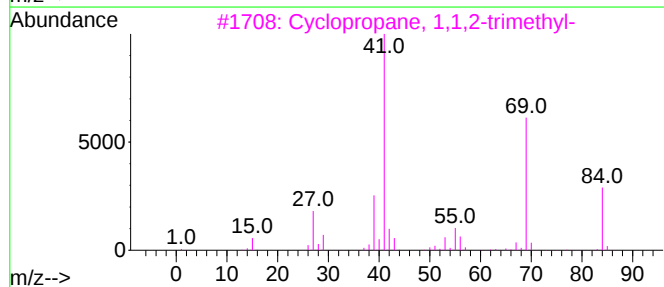
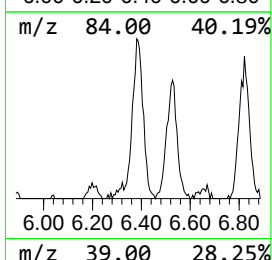
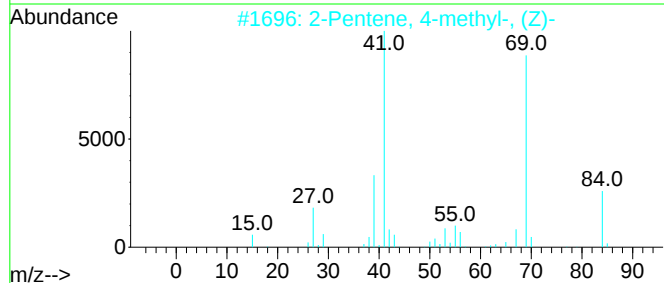
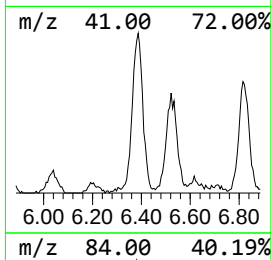
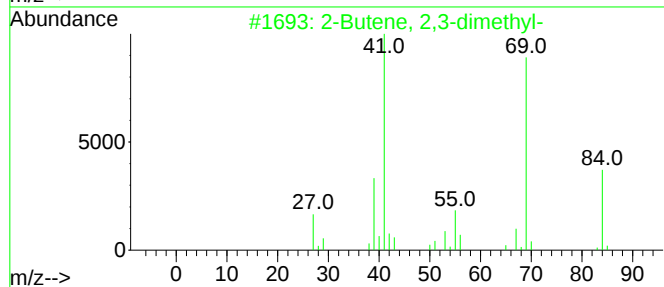
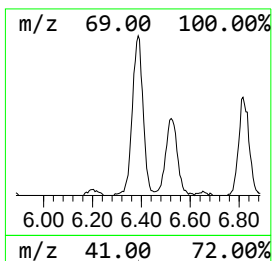
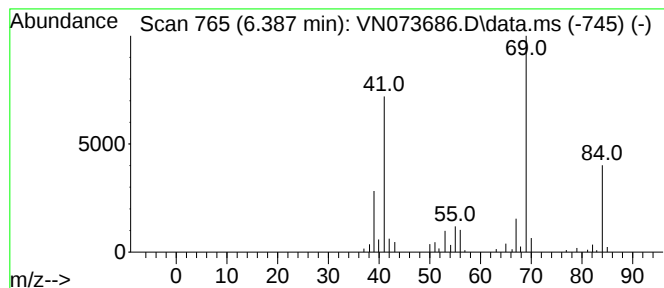
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Quant Title : SW846 8260

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

Peak Number 8 2-Butene, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.387	8.91 ug/l	232804	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2,3-dimethyl-			84	C6H12	000563-79-1	91
2	2-Pentene, 4-methyl-, (Z)-			84	C6H12	000691-38-3	90
3	Cyclopropane, 1,1,2-trimethyl-			84	C6H12	004127-45-1	87
4	2-Pentene, 4-methyl-			84	C6H12	004461-48-7	87
5	2-Pentene, 2-methyl-			84	C6H12	000625-27-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073686.D
Acq On : 02 Aug 2022 14:47
Operator : JC\MD
Sample : N3971-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-19

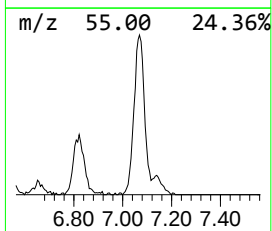
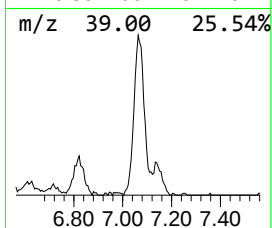
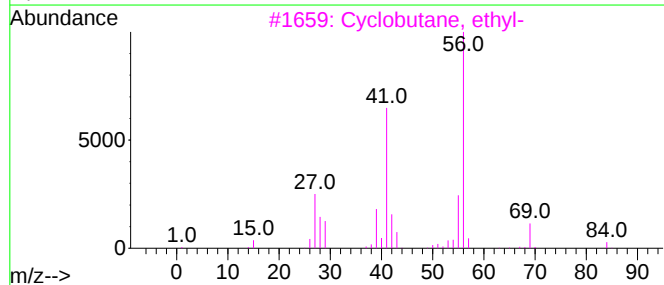
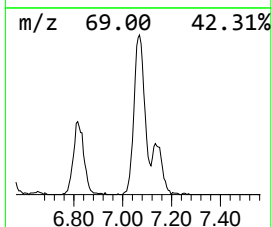
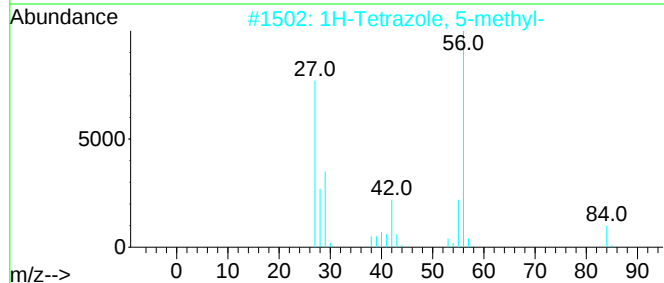
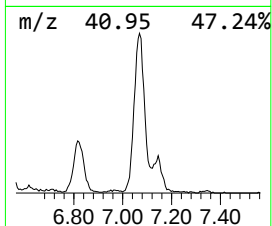
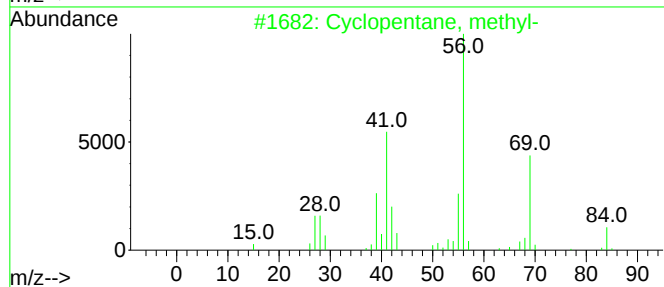
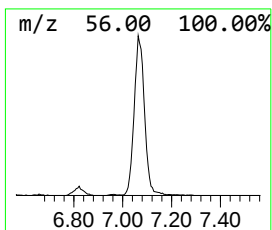
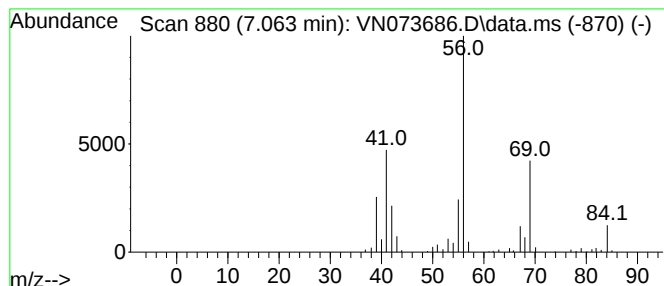
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Quant Title : SW846 8260

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

Peak Number 9 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	26.07 ug/l	681011	Pentafluorobenzene	8.016

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	72
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4		Cyclohexane	84	C6H12	000110-82-7	56
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073686.D
Acq On : 02 Aug 2022 14:47
Operator : JC\MD
Sample : N3971-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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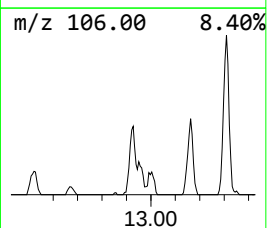
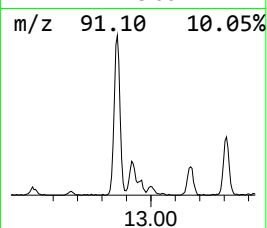
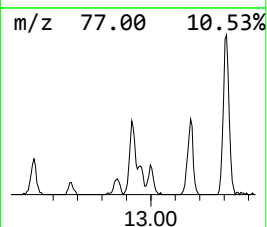
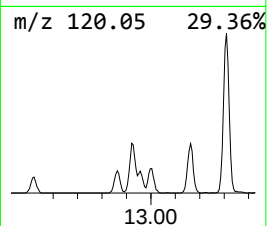
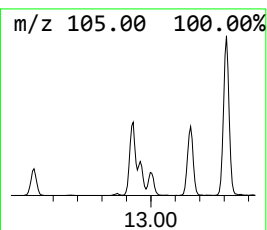
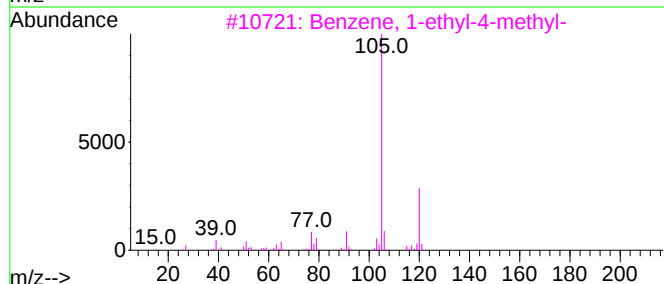
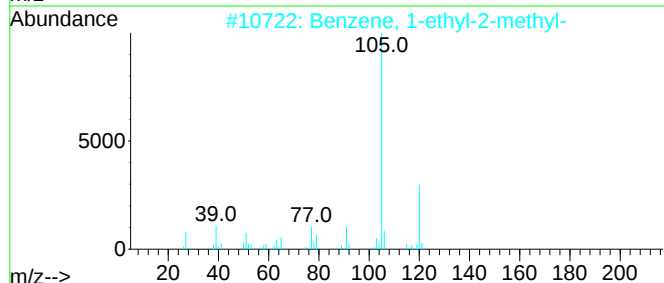
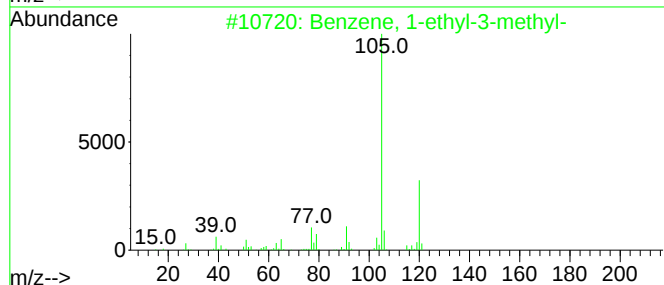
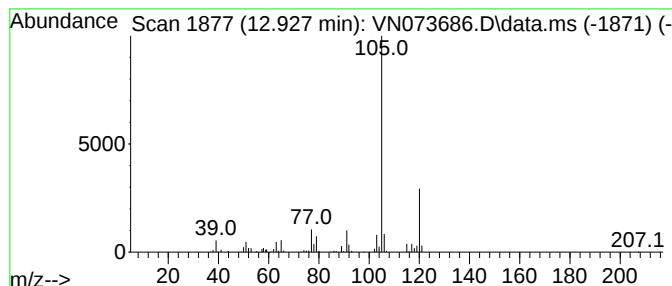
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.927	7.06 ug/l	294747	1,4-Dichlorobenzene-d4	13.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4		Mesitylene	120	C9H12	000108-67-8	91
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073686.D
Acq On : 02 Aug 2022 14:47
Operator : JC\MD
Sample : N3971-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-19

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.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	2.399	94.1	ug/l	2458350	1	8.016	1306130	50.0
Butane, 2-methyl-	3.087	254.7	ug/l	6652050	1	8.016	1306130	50.0
Pentane	3.457	30.6	ug/l	798444	1	8.016	1306130	50.0
Cyclopropane, 1...	3.928	34.4	ug/l	898704	1	8.016	1306130	50.0
Isopropyl Alcohol	4.510	6.9	ug/l	181027	1	8.016	1306130	50.0
1-Pentene	5.104	32.5	ug/l	848850	1	8.016	1306130	50.0
2-Butene, 2,3-d...	6.387	8.9	ug/l	232804	1	8.016	1306130	50.0
Cyclopentane, m...	7.063	26.1	ug/l	681011	1	8.016	1306130	50.0
Benzene, 1-ethy...	12.927	7.1	ug/l	294747	4	13.616	2086780	50.0