

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
 Data File : VN073683.D
 Acq On : 02 Aug 2022 13:33
 Operator : JC\MD
 Sample : N3971-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-9R

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: VN073683.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	48	58	75	rBV	6339168	9572632	15.89%	3.759%
2	2.404	77	88	99	rVV	12703617	21912437	36.38%	8.603%
3	2.498	99	104	117	rVV	2236220	3675799	6.10%	1.443%
4	2.622	118	125	133	rVB	1353095	2244715	3.73%	0.881%
5	2.922	167	176	187	rBV	754325	1550756	2.57%	0.609%
6	3.081	193	203	242	rVB	11329953	25180054	41.80%	9.886%
7	3.363	242	251	259	rVV	510166	1162253	1.93%	0.456%
8	3.463	259	268	290	rVV3	1726837	6067080	10.07%	2.382%
9	3.657	291	301	318	rVV	2767271	6591925	10.94%	2.588%
10	3.834	319	331	338	rVV	1529509	3958092	6.57%	1.554%
11	3.928	338	347	381	rVB	3751918	10067100	16.71%	3.953%
12	4.881	491	509	520	rBV2	376198	1321124	2.19%	0.519%
13	5.104	533	547	572	rVB4	648001	3329848	5.53%	1.307%
14	6.381	757	764	777	rVB	320411	960310	1.59%	0.377%
15	6.522	777	788	796	rBV	202882	642750	1.07%	0.252%
16	6.822	829	839	854	rVB	265771	788839	1.31%	0.310%
17	7.069	868	881	889	rBV	752386	2256044	3.75%	0.886%
18	7.951	1020	1031	1036	rBV	281408	687036	1.14%	0.270%
19	8.016	1036	1042	1053	rVB2	737514	1801330	2.99%	0.707%
20	8.386	1094	1105	1112	rBV3	780979	2106062	3.50%	0.827%
21	8.469	1112	1119	1125	rBV	592072	1264335	2.10%	0.496%
22	8.904	1182	1193	1206	rBV	743854	1631808	2.71%	0.641%
23	10.380	1436	1444	1449	rBV	1049448	1913453	3.18%	0.751%
24	10.445	1449	1455	1472	rVB	4989886	9299865	15.44%	3.651%
25	11.686	1658	1666	1675	rBV	1040557	1844464	3.06%	0.724%
26	11.786	1675	1683	1693	rVV	14910131	24320633	40.38%	9.549%
27	11.892	1693	1701	1721	rVB	32593354	60236232	100.00%	23.651%
28	12.221	1746	1757	1773	rBV	7900917	12774713	21.21%	5.016%
29	12.521	1795	1808	1817	rBV	583533	965674	1.60%	0.379%
30	12.674	1827	1834	1846	rVB	967148	1616991	2.68%	0.635%
31	12.863	1858	1866	1871	rBV	1030470	1582061	2.63%	0.621%
32	12.921	1871	1876	1879	rVV	1910801	3069223	5.10%	1.205%
33	12.957	1879	1882	1886	rVV	1562207	2391270	3.97%	0.939%
34	12.998	1886	1889	1897	rVB	1356943	2064924	3.43%	0.811%
35	13.162	1908	1917	1925	rBV	1709179	2784531	4.62%	1.093%
36	13.310	1932	1942	1956	rBV	6739011	10566075	17.54%	4.149%

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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

37	13.615	1987	1994	1996	rBV	1297793	2232114	3.71%	0.876%
38	13.645	1996	1999	2007	rVB	2283817	3378351	5.61%	1.326%
39	13.815	2016	2028	2044	rVB	1533481	2877306	4.78%	1.130%
40	15.433	2295	2303	2315	rBV	1092513	2002608	3.32%	0.786%

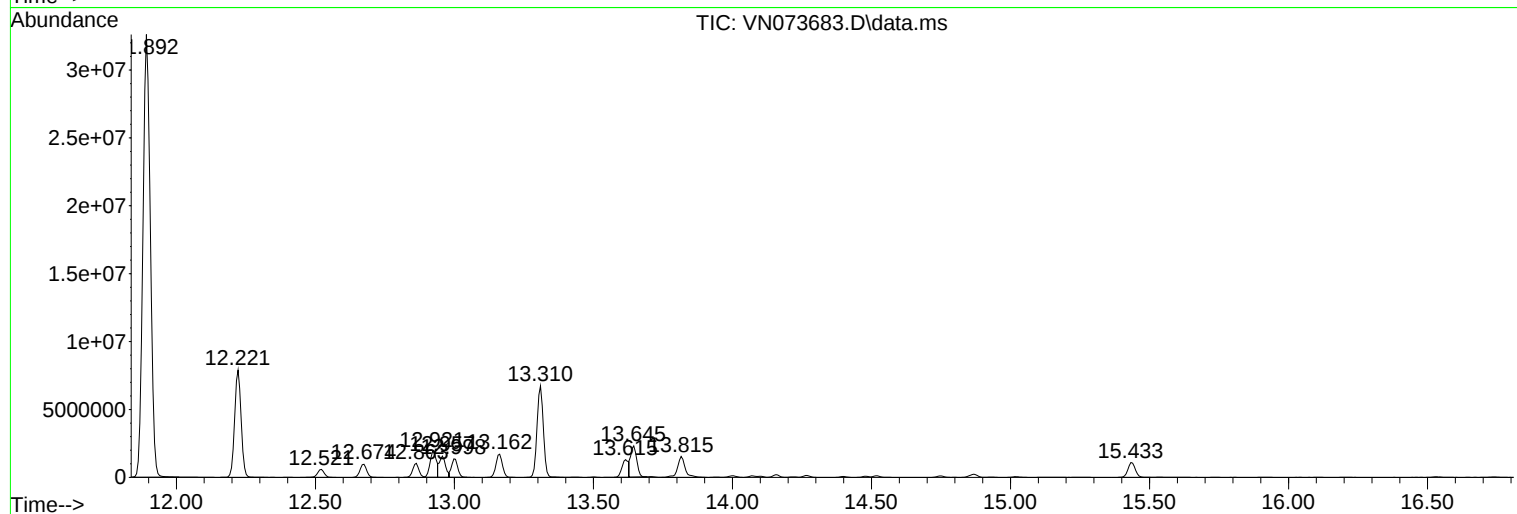
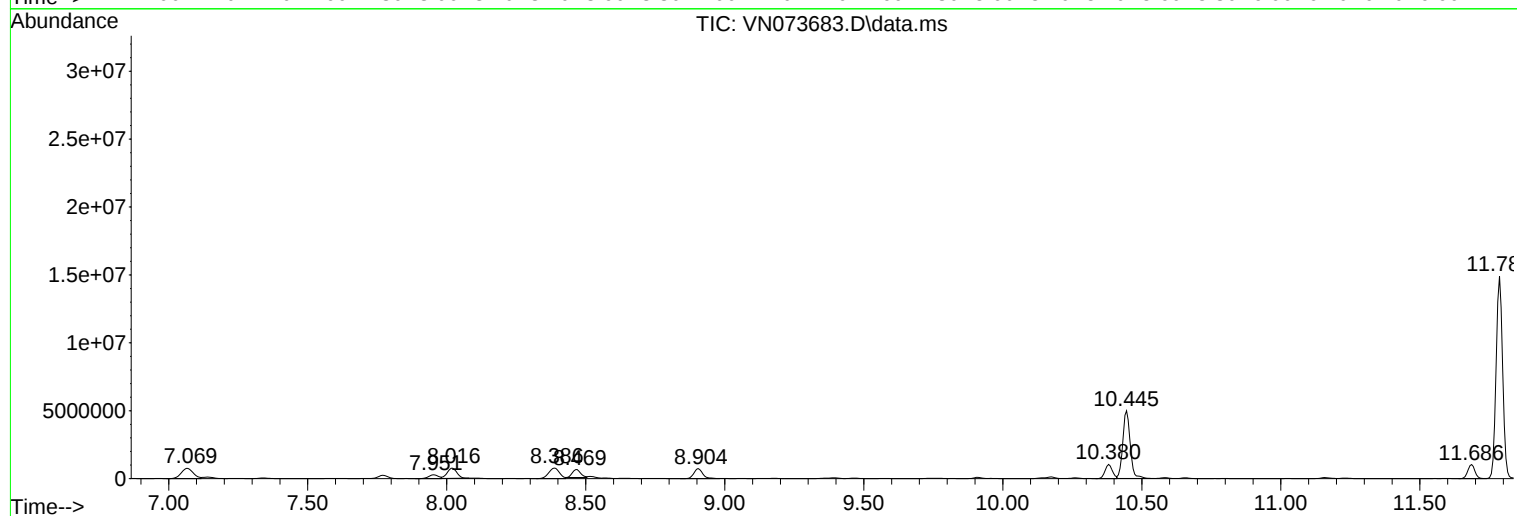
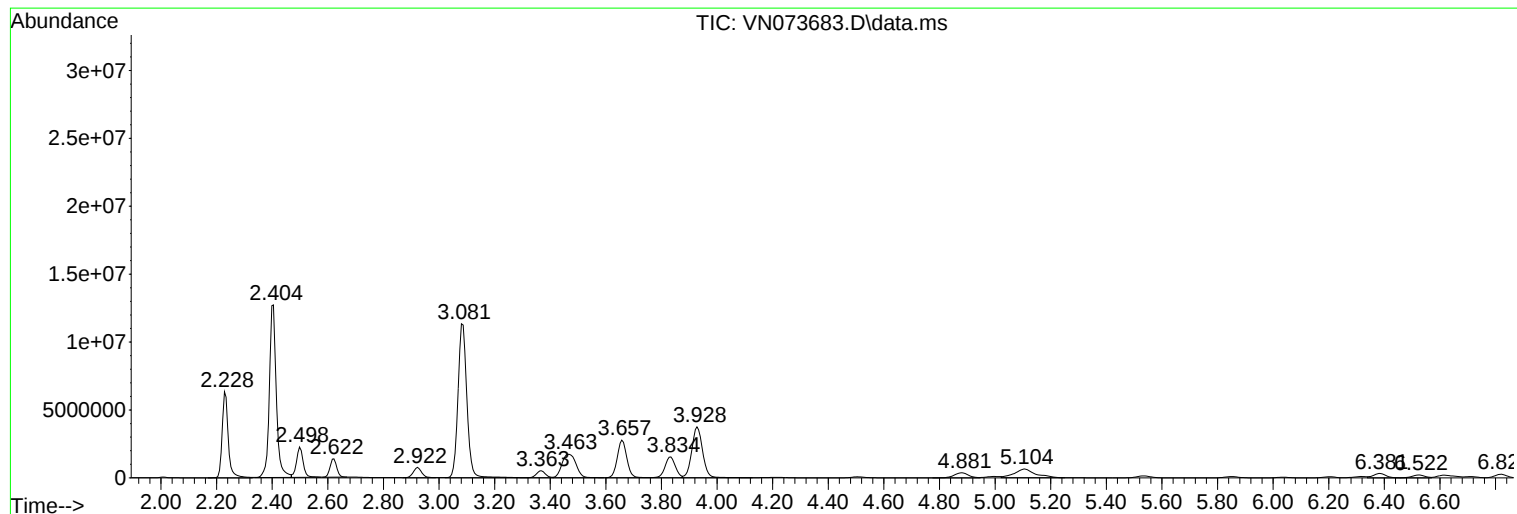
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



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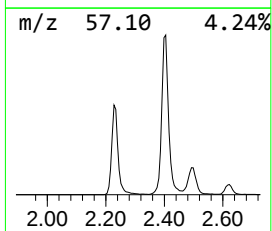
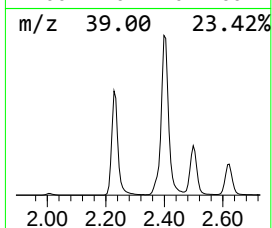
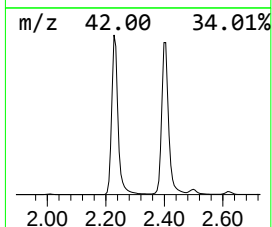
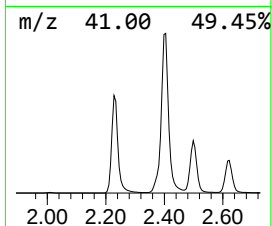
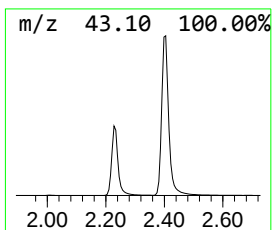
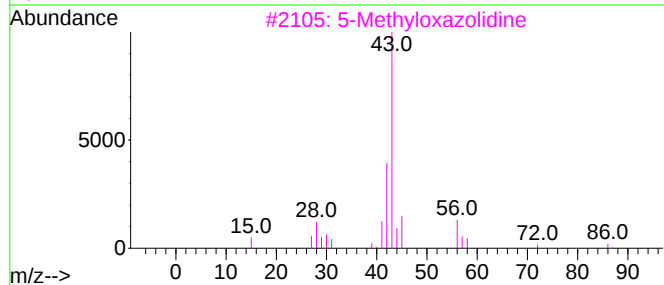
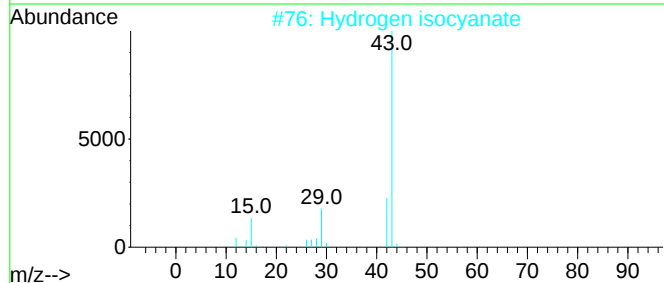
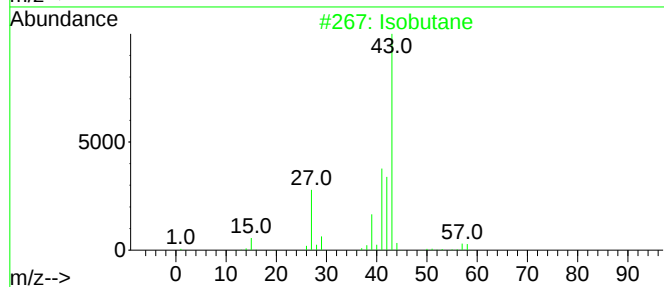
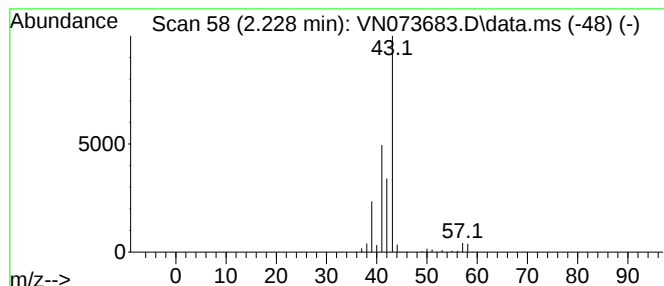
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	265.71 ug/l	9572630	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	80
2			Hydrogen isocyanate	43	CHNO	000075-13-8	4
3			5-Methyloxazolidine	87	C4H9NO	058328-22-6	4
4			Cyclobutylamine	71	C4H9N	002516-34-9	4
5			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

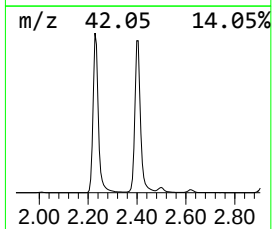
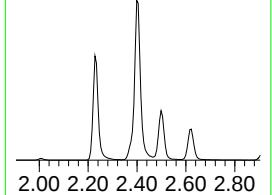
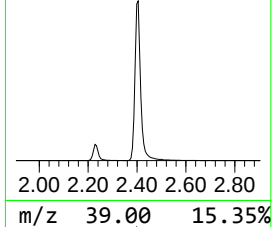
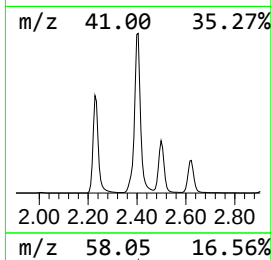
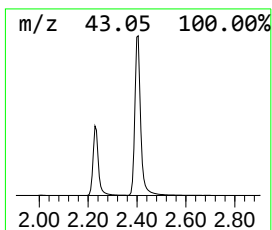
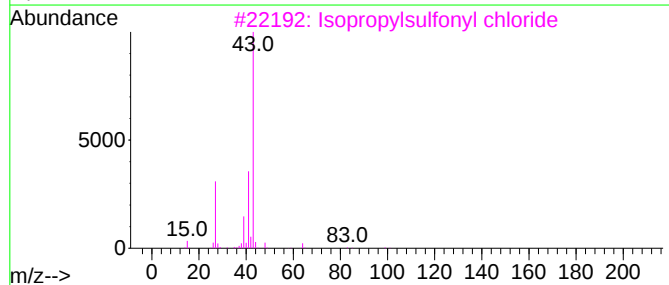
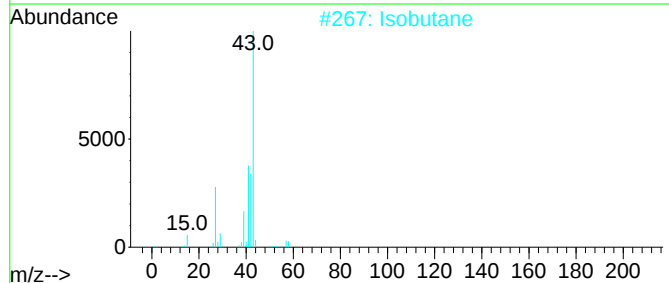
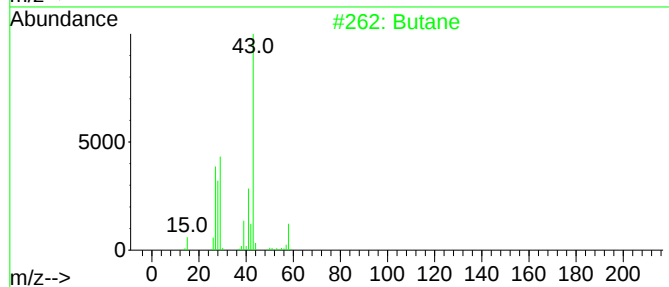
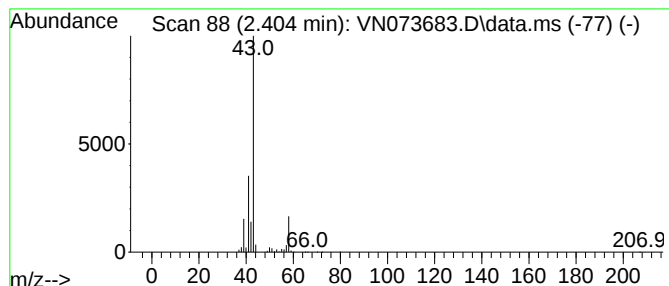
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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.
2.404	608.23 ug/l	21912400	Pentafluorobenzene	8.016

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	7



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

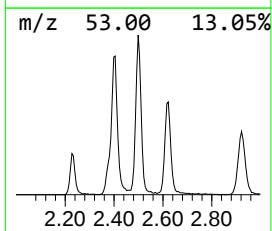
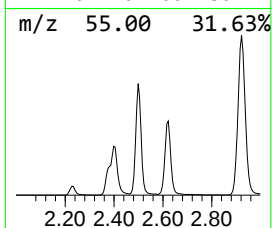
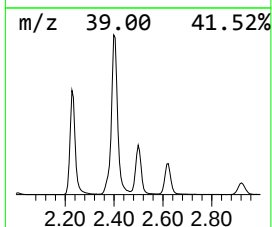
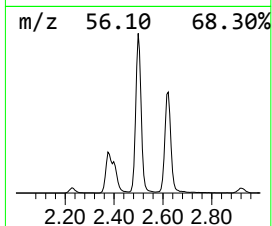
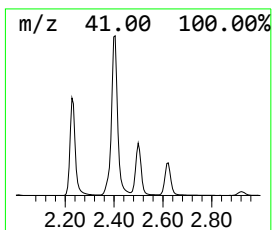
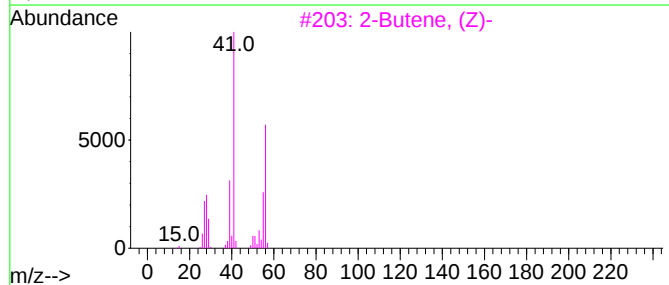
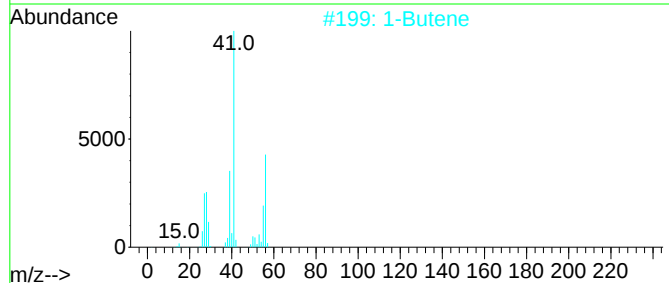
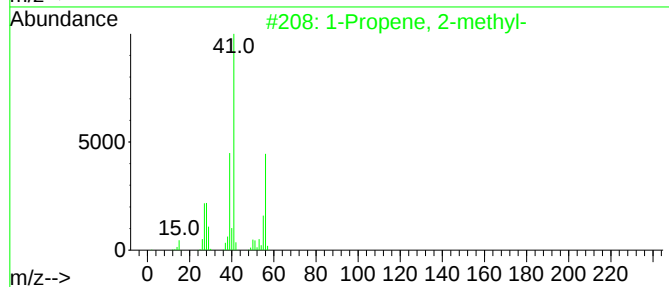
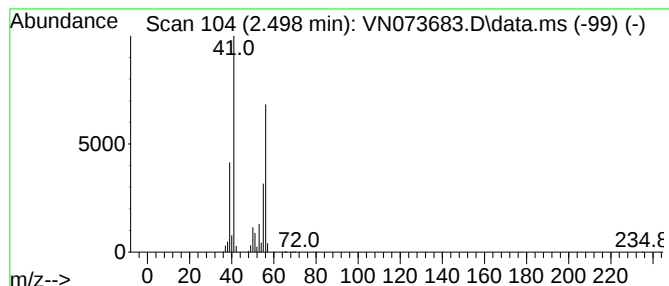
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Propene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.498	102.03 ug/l	3675800	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-			56	C4H8	000115-11-7	87
2	1-Butene			56	C4H8	000106-98-9	87
3	2-Butene, (Z)-			56	C4H8	000590-18-1	80
4	2-Butene			56	C4H8	000107-01-7	74
5	2-Butene, (E)-			56	C4H8	000624-64-6	72



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

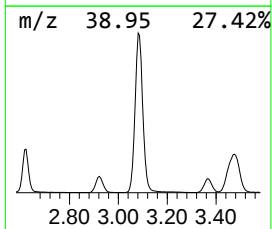
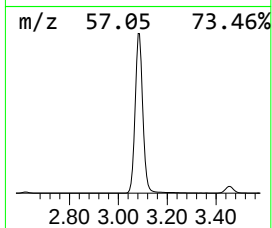
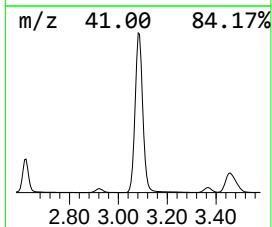
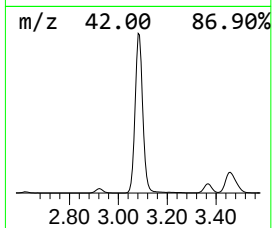
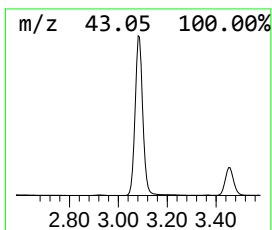
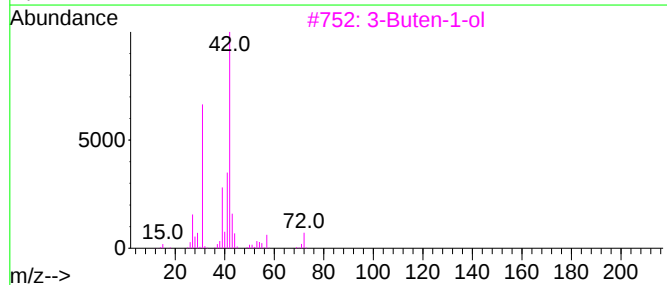
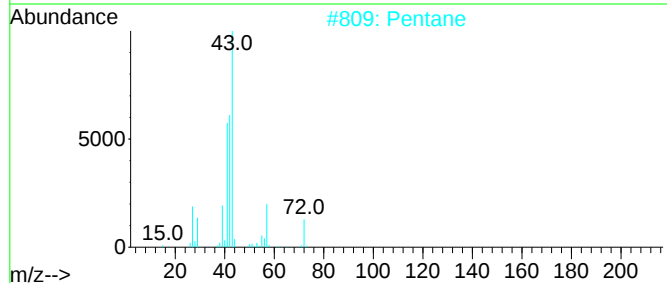
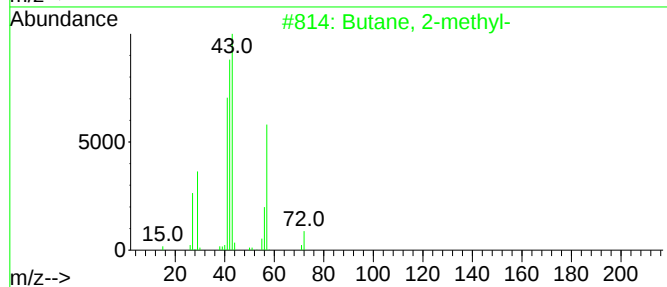
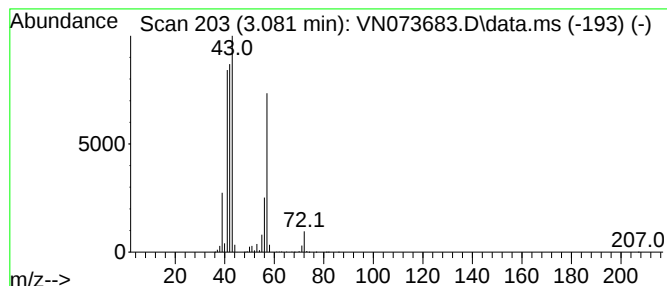
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Quant Title : SW846 8260

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

Peak Number 4 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	698.93 ug/l	25180100	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			Pentane	72	C5H12	000109-66-0	43
3			3-Buten-1-ol	72	C4H8O	000627-27-0	25
4			Butane, 2-nitro-	103	C4H9NO2	000600-24-8	10
5			1-Butene	56	C4H8	000106-98-9	10



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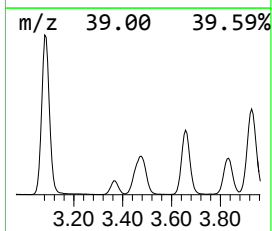
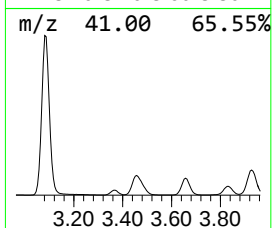
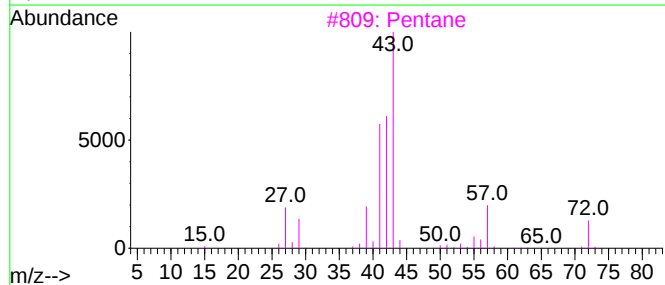
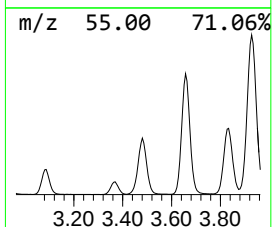
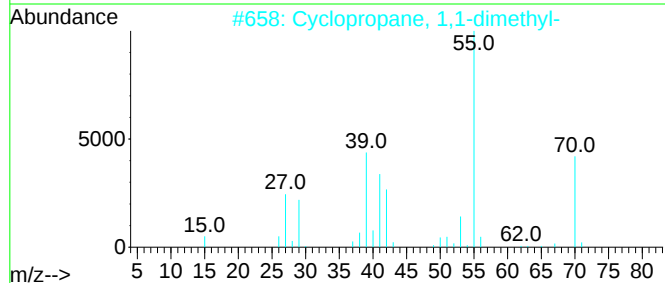
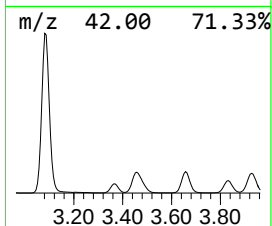
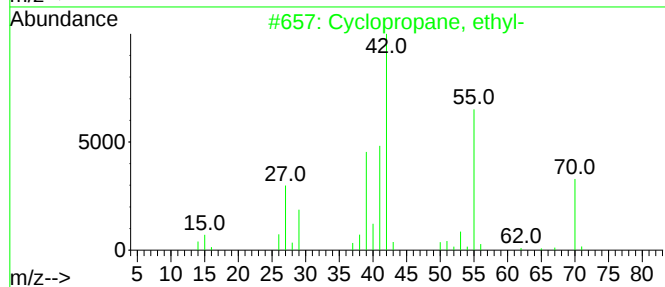
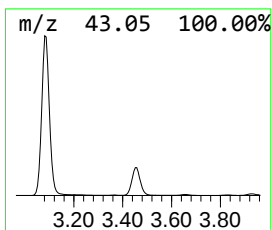
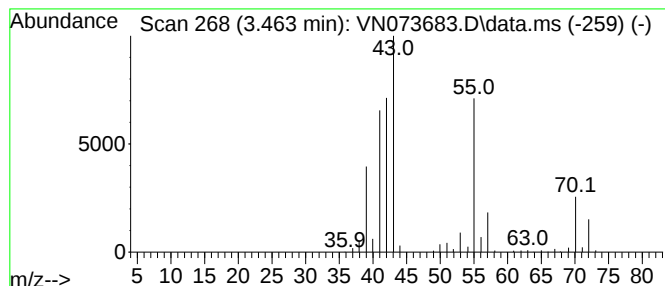
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclopropane, ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.463	168.41 ug/l	6067080	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, ethyl-	70	C5H10	001191-96-4	58
2			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	46
3			Pentane	72	C5H12	000109-66-0	46
4			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	43
5			1-Pentene	70	C5H10	000109-67-1	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073683.D
Acq On : 02 Aug 2022 13:33
Operator : JC\MD
Sample : N3971-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

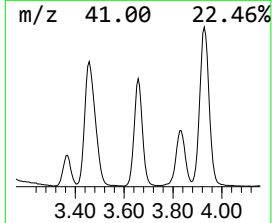
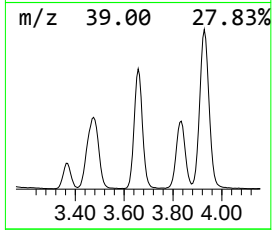
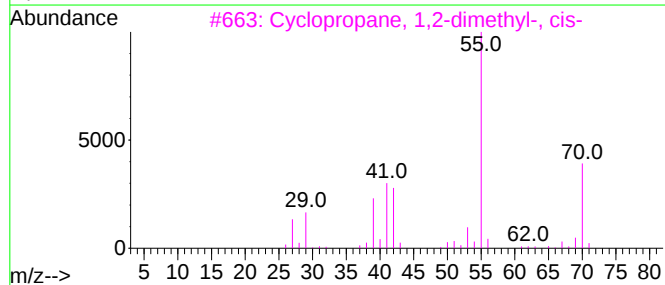
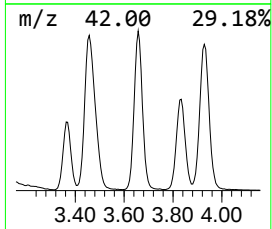
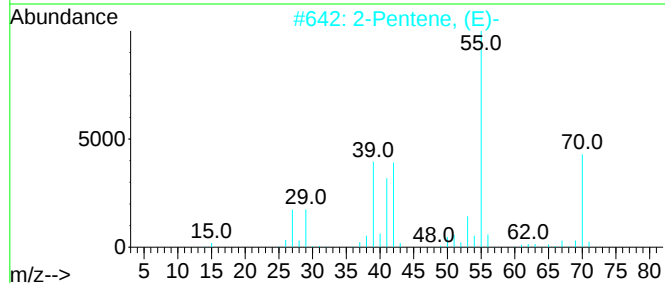
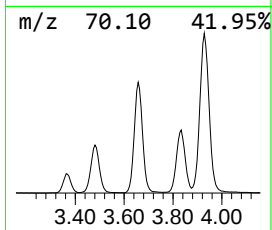
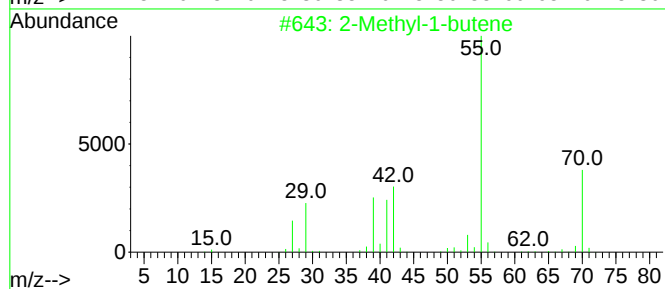
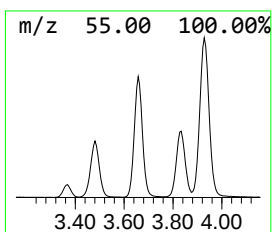
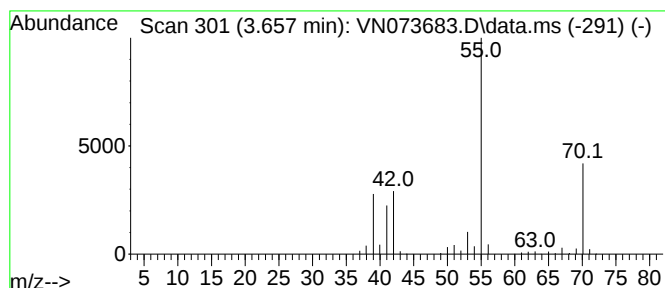
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Quant Title : SW846 8260

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

Peak Number 6 2-Methyl-1-butene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.657	182.97 ug/l	6591930	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-1-butene	70	C5H10	000563-46-2	91	
2	2-Pentene, (E)-	70	C5H10	000646-04-8	91	
3	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90	
4	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87	
5	2-Butene, 2-methyl-	70	C5H10	000513-35-9	87	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073683.D
Acq On : 02 Aug 2022 13:33
Operator : JC\MD
Sample : N3971-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

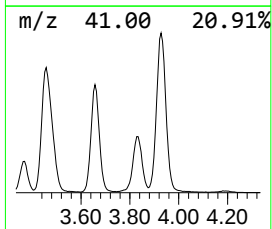
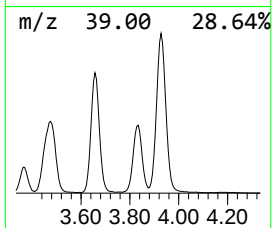
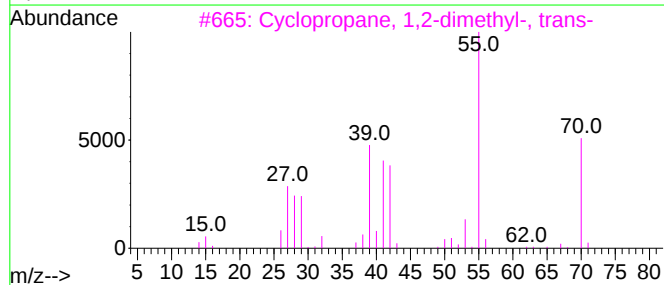
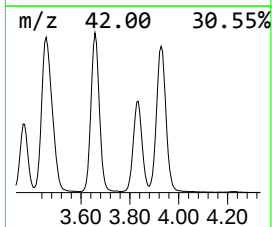
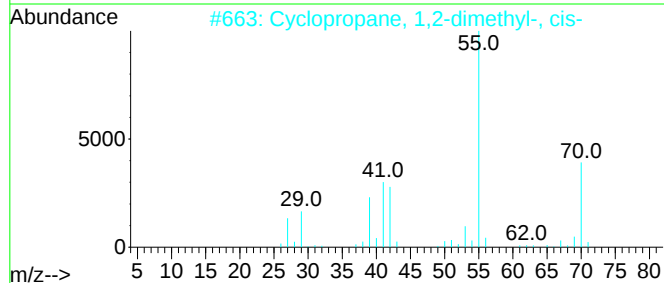
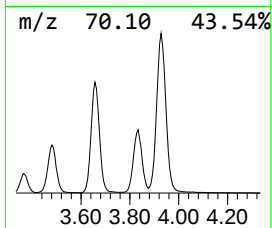
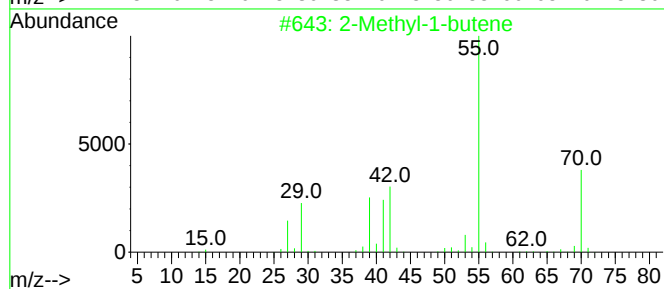
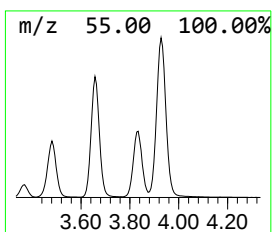
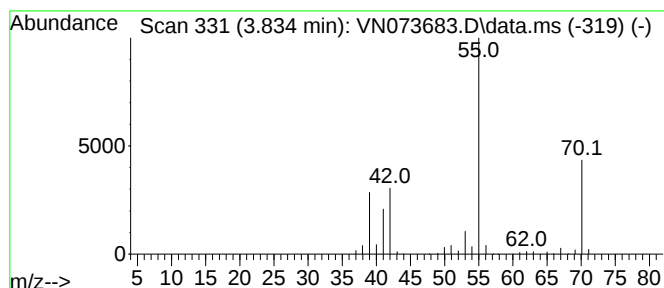
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopropane, 1,2-dimethyl-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.834	109.87 ug/l	3958090	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-1-butene		70	C5H10	000563-46-2	91
2	Cyclopropane, 1,2-dimethyl-, cis-		70	C5H10	000930-18-7	90
3	Cyclopropane, 1,2-dimethyl-, trans-		70	C5H10	002402-06-4	87
4	2-Butene, 2-methyl-		70	C5H10	000513-35-9	87
5	2-Pentene		70	C5H10	000109-68-2	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073683.D
Acq On : 02 Aug 2022 13:33
Operator : JC\MD
Sample : N3971-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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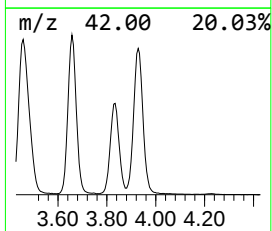
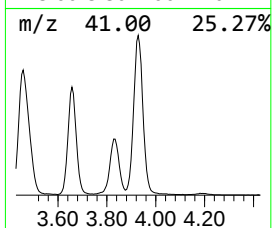
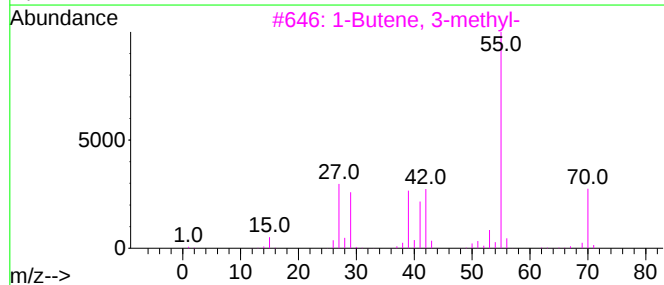
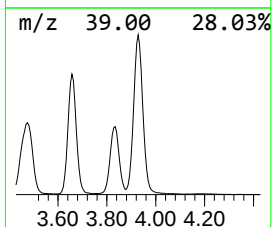
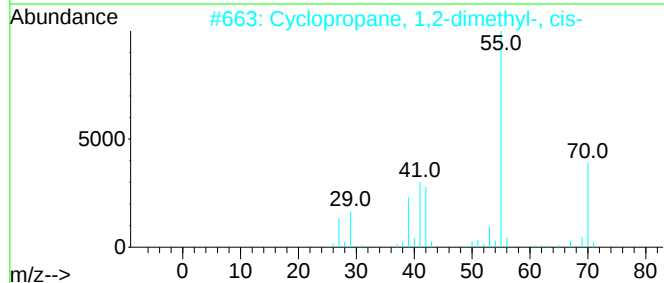
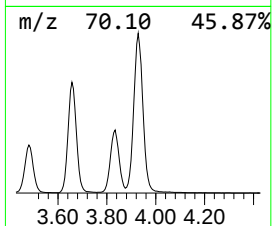
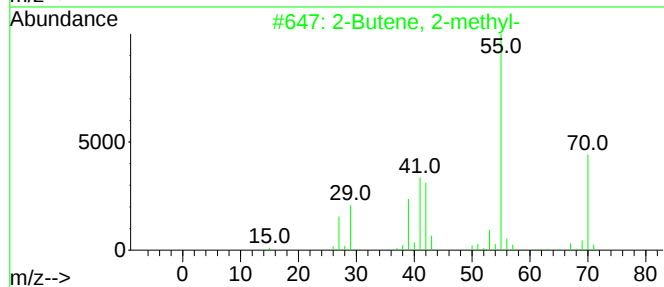
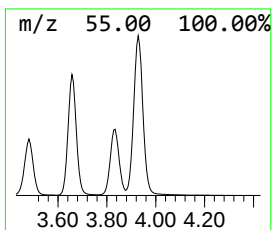
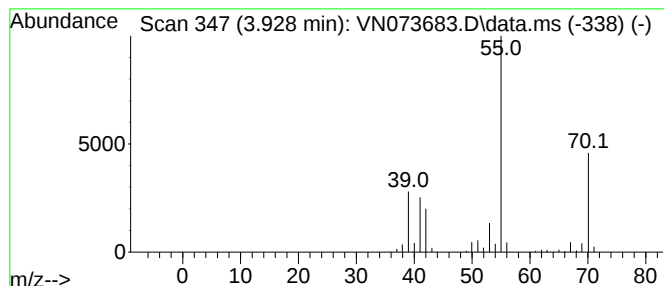
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.928	279.44 ug/l	10067100	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
2		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87
3		1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
4		Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83
5		Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073683.D
Acq On : 02 Aug 2022 13:33
Operator : JC\MD
Sample : N3971-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

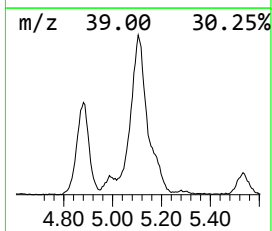
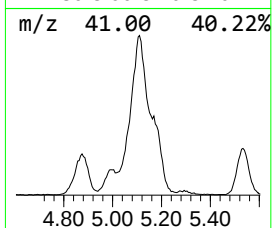
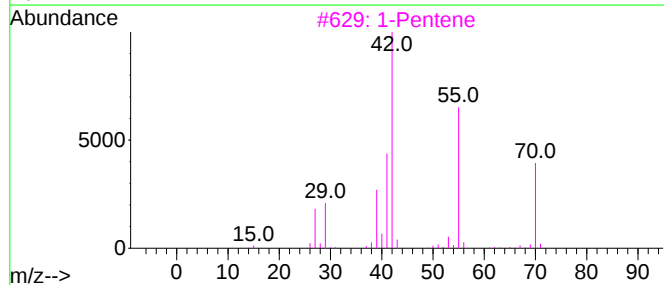
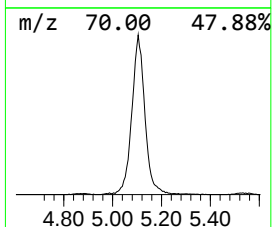
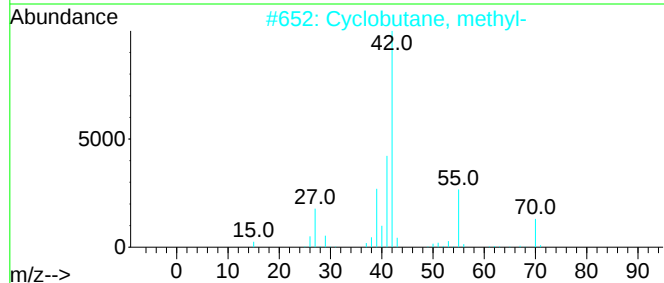
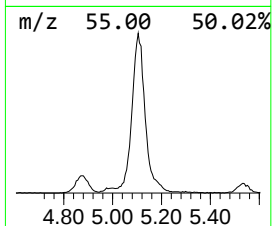
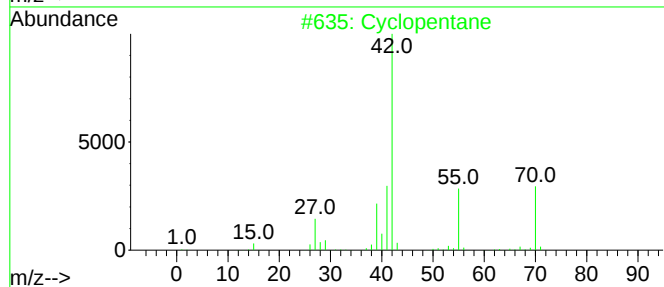
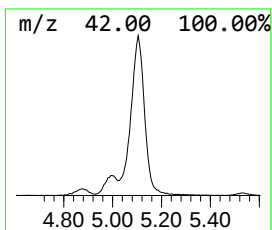
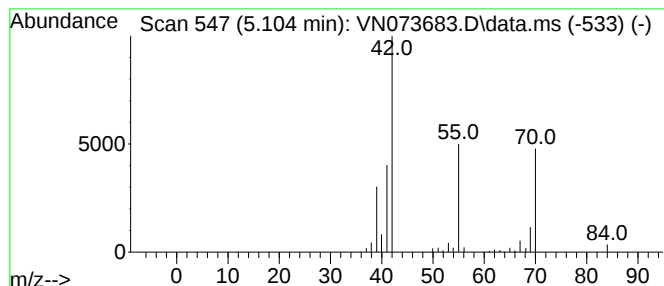
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Quant Title : SW846 8260

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

Peak Number 9 Cyclopentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	92.43 ug/l	3329850	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane	70	C5H10	000287-92-3	86
2		Cyclobutane, methyl-	70	C5H10	000598-61-8	72
3		1-Pentene	70	C5H10	000109-67-1	72
4		2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	39
5		Methyl propargyl ether	70	C4H6O	000627-41-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073683.D
Acq On : 02 Aug 2022 13:33
Operator : JC\MD
Sample : N3971-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

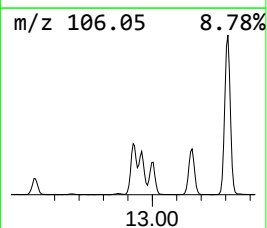
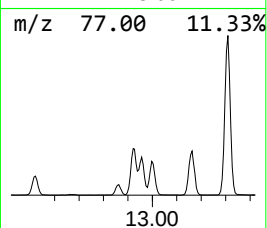
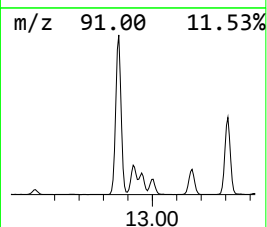
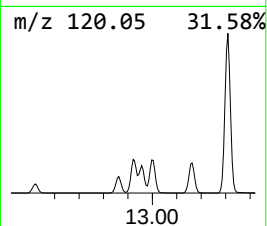
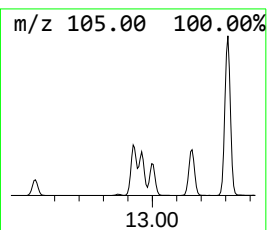
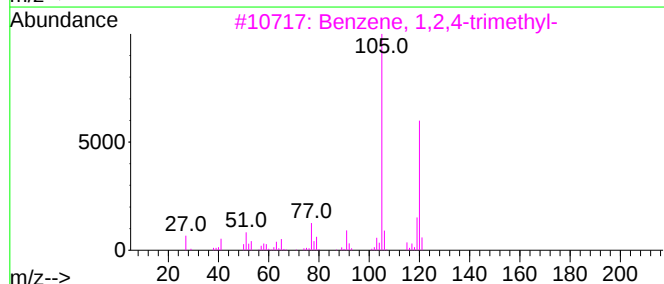
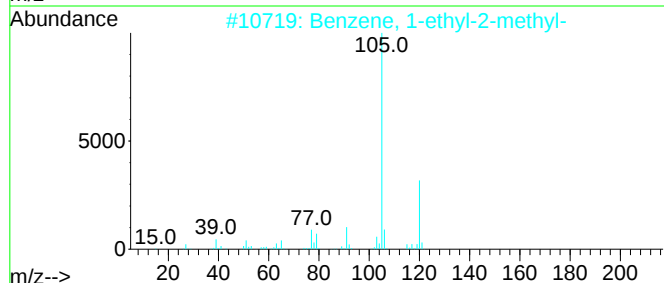
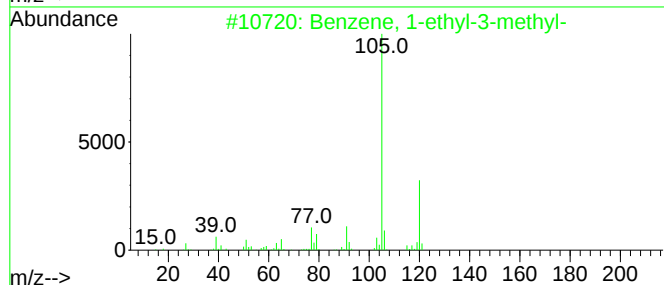
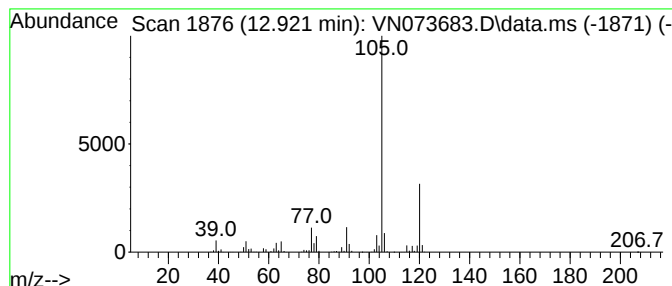
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.921	68.75 ug/l	3069220	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073683.D
Acq On : 02 Aug 2022 13:33
Operator : JC\MD
Sample : N3971-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

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	2.404	608.2	ug/l	21912400	1	8.016	1801330	50.0
1-Propene, 2-me...	2.498	102.0	ug/l	3675800	1	8.016	1801330	50.0
Butane, 2-methyl-	3.081	698.9	ug/l	25180100	1	8.016	1801330	50.0
Cyclopropane, e...	3.463	168.4	ug/l	6067080	1	8.016	1801330	50.0
2-Methyl-1-butene	3.657	183.0	ug/l	6591930	1	8.016	1801330	50.0
Cyclopropane, 1...	3.834	109.9	ug/l	3958090	1	8.016	1801330	50.0
2-Butene, 2-met...	3.928	279.4	ug/l	10067100	1	8.016	1801330	50.0
Cyclopentane	5.104	92.4	ug/l	3329850	1	8.016	1801330	50.0
Benzene, 1-ethy...	12.921	68.8	ug/l	3069220	4	13.615	2232110	50.0