

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
 Data File : VN071808.D
 Acq On : 02 Apr 2022 19:22
 Operator : JC\MD
 Sample : N2200-17
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DUP033022

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\82N033022W.M
 Title : SW846 8260

Signal : TIC: VN071808.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	34	41	60	rBV	1069938	4062568	92.50%	12.371%
2	2.434	74	76	88	rVB2	156305	323241	7.36%	0.984%
3	2.787	132	136	139	rBV	29966	63354	1.44%	0.193%
4	3.128	188	194	204	rVB2	124052	320459	7.30%	0.976%
5	3.510	250	259	273	rVB4	37310	120970	2.75%	0.368%
6	3.716	286	294	305	rVB2	22245	53973	1.23%	0.164%
7	3.993	332	341	352	rVB	76258	201928	4.60%	0.615%
8	4.575	422	440	452	rBV3	21609	100738	2.29%	0.307%
9	5.187	531	544	554	rVB4	26578	124497	2.83%	0.379%
10	5.363	563	574	589	rVB2	78028	275648	6.28%	0.839%
11	5.616	601	617	637	rBV	660337	2348605	53.47%	7.152%
12	6.487	755	765	778	rVB5	33833	117151	2.67%	0.357%
13	7.145	866	877	887	rBV2	48529	143810	3.27%	0.438%
14	8.022	1014	1026	1031	rBV	420956	1029669	23.44%	3.135%
15	8.081	1031	1036	1046	rVB	789938	1805125	41.10%	5.497%
16	8.457	1087	1100	1108	rBV3	1643028	4391972	100.00%	13.374%
17	8.528	1108	1112	1120	rVB2	65685	144999	3.30%	0.442%
18	8.963	1175	1186	1199	rBV	1217031	2483290	56.54%	7.562%
19	10.439	1427	1437	1444	rBV	1943445	3526230	80.29%	10.738%
20	10.504	1444	1448	1460	rVB	200213	365372	8.32%	1.113%
21	11.739	1650	1658	1669	rBV	1817010	3253115	74.07%	9.906%
22	11.839	1669	1675	1686	rVV	337830	596291	13.58%	1.816%
23	11.951	1686	1694	1705	rVB	463847	910729	20.74%	2.773%
24	12.275	1743	1749	1758	rVB	85347	148819	3.39%	0.453%
25	12.727	1819	1826	1841	rBV	1348238	2311336	52.63%	7.038%
26	12.916	1853	1858	1864	rBV	33840	59623	1.36%	0.182%
27	12.980	1864	1869	1872	rVV	66253	114298	2.60%	0.348%
28	13.010	1872	1874	1878	rVV	57978	80967	1.84%	0.247%
29	13.057	1878	1882	1890	rVB	51198	82533	1.88%	0.251%
30	13.216	1904	1909	1915	rVB	46728	73592	1.68%	0.224%
31	13.363	1927	1934	1944	rVB	138671	229400	5.22%	0.699%
32	13.669	1979	1986	1998	rBV	1457751	2592002	59.02%	7.893%
33	13.874	2016	2021	2032	rVB3	72458	145724	3.32%	0.444%
34	14.927	2192	2200	2206	rBV4	30133	61987	1.41%	0.189%
35	15.504	2290	2298	2305	rBV2	88899	175579	4.00%	0.535%

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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\82N033022W.M
Title : SW846 8260

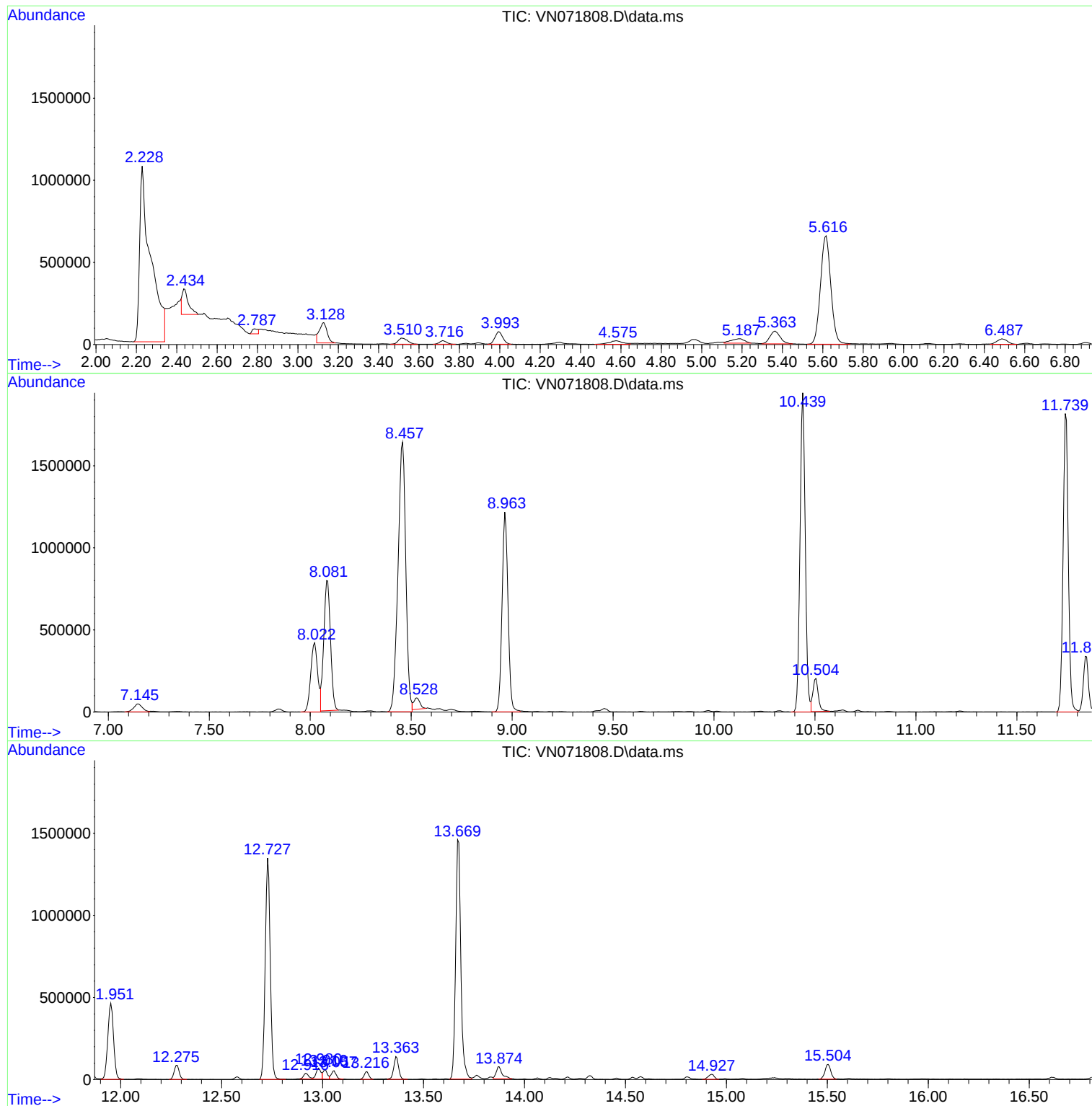
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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



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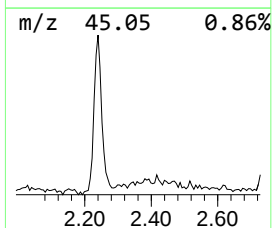
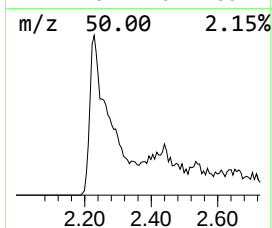
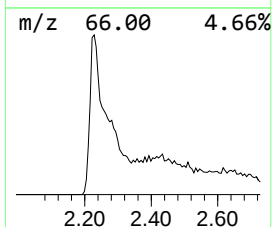
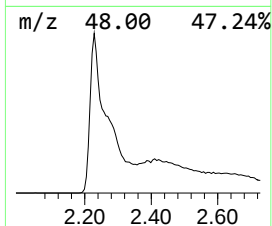
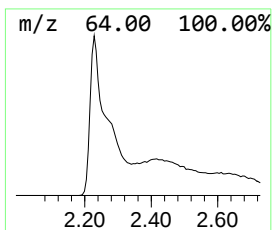
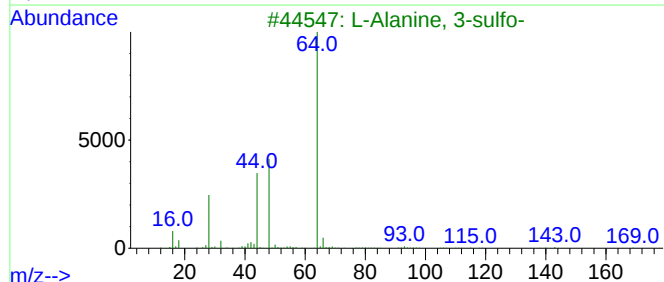
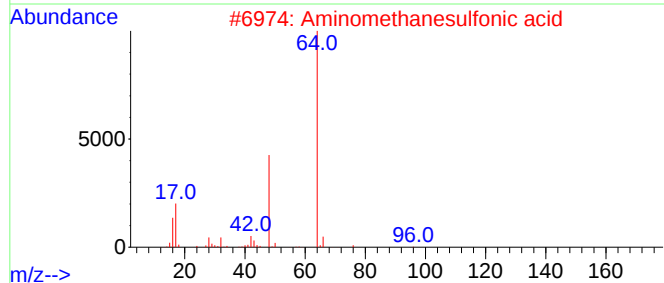
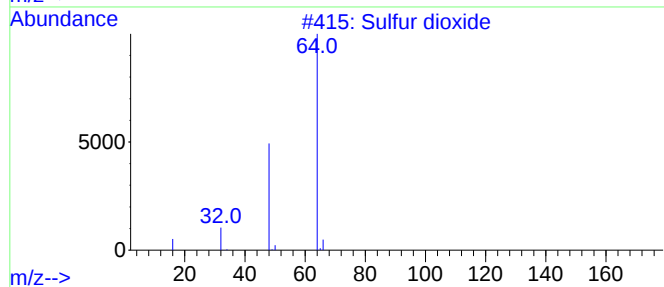
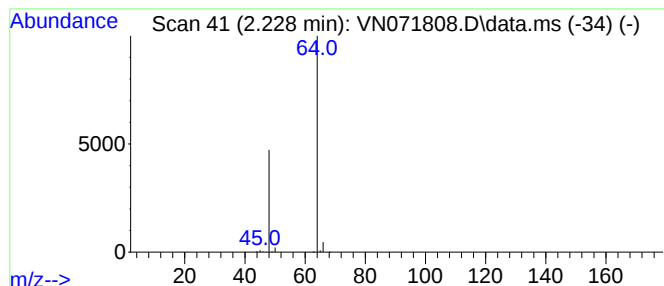
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	112.53 ug/l	4062570	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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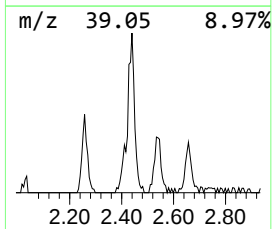
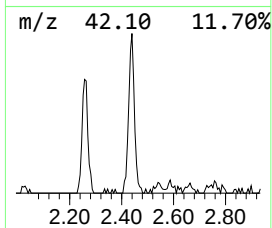
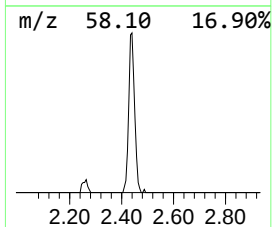
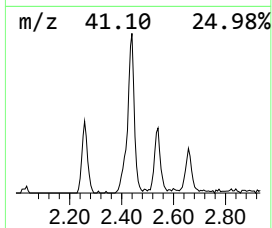
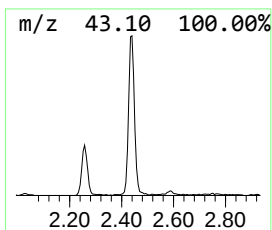
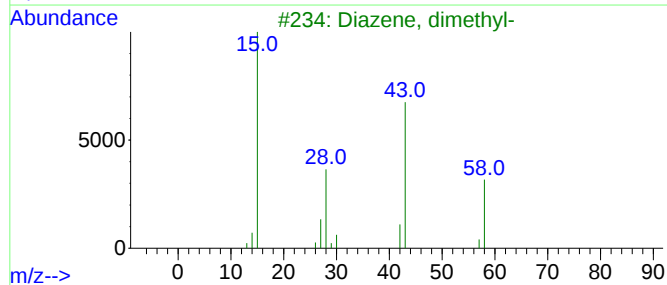
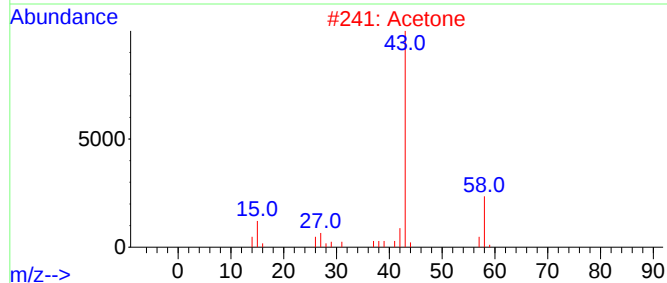
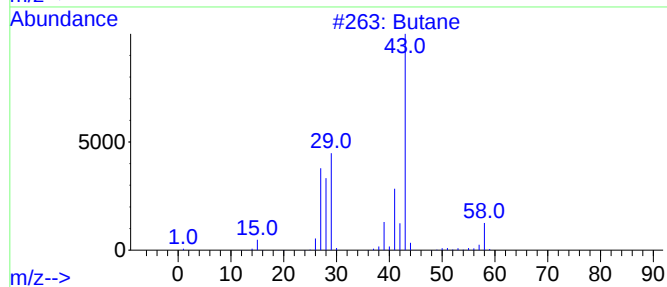
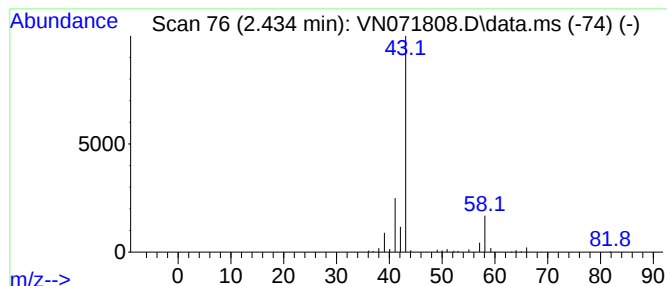
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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.
2.434	8.95 ug/l	323241	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	59
2			Acetone	58	C3H6O	000067-64-1	7
3			Diazene, dimethyl-	58	C2H6N2	000503-28-6	4
4			2-(2-Aminoethanesulfonyl)propane	151	C5H13NO2S	320337-16-4	4
5			Oxirane, trimethyl-	86	C5H10O	005076-19-7	4



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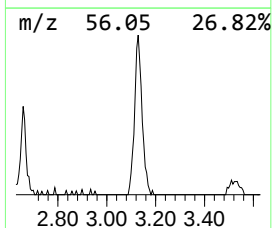
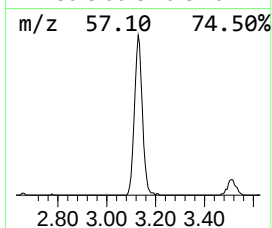
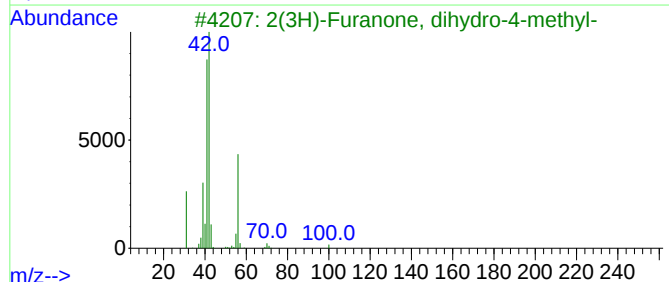
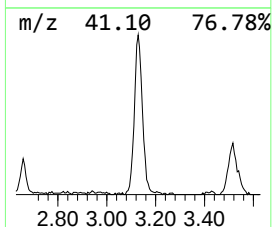
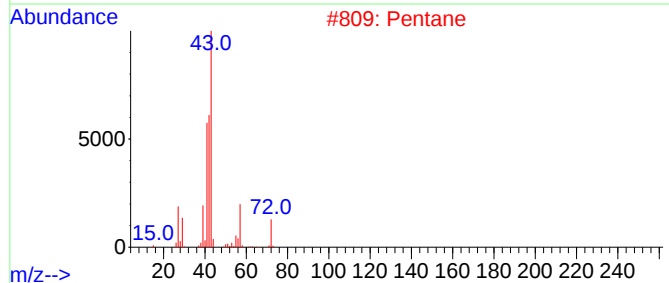
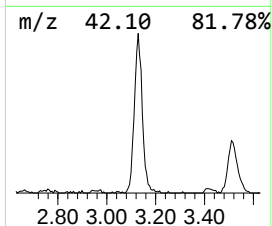
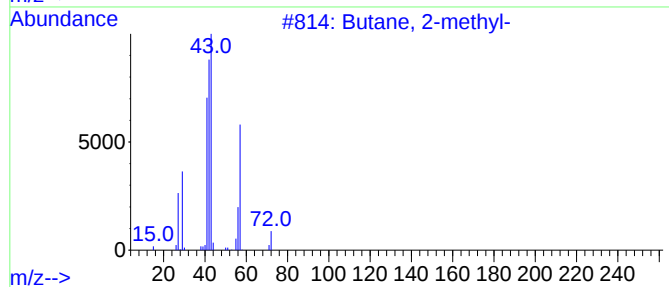
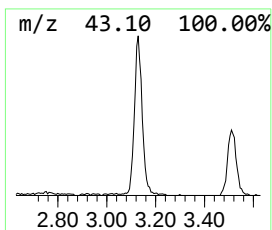
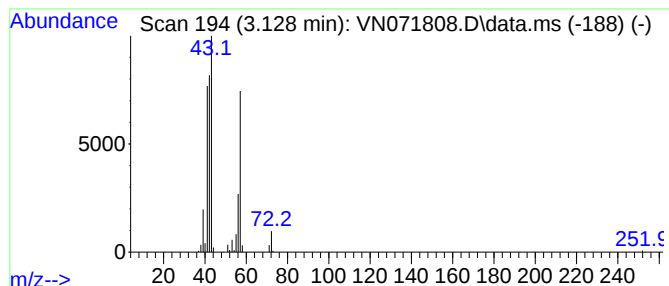
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	8.88 ug/l	320459	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	38
3			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	36
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5			Acetic acid, butoxyhydroxy-, but...	204	C10H20O4	068575-73-5	12



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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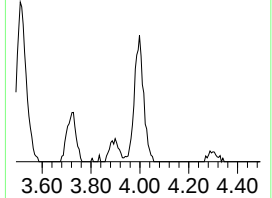
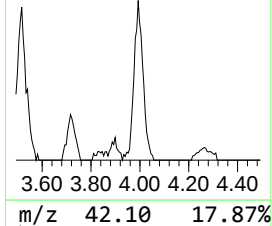
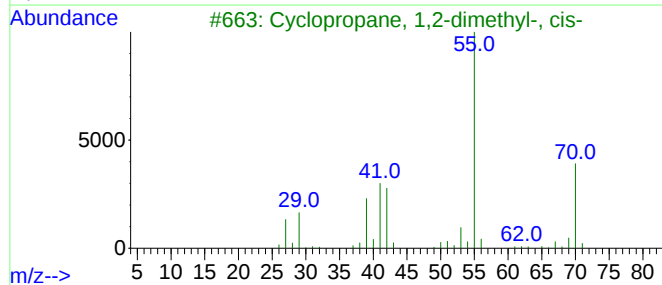
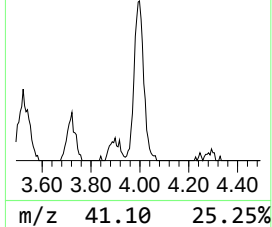
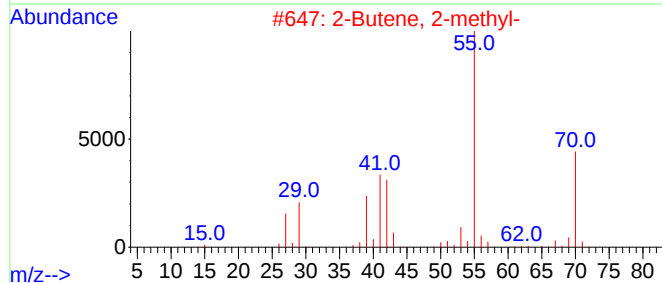
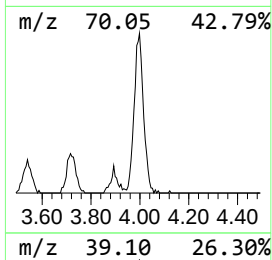
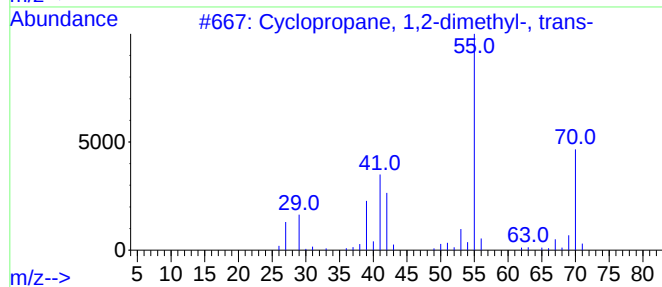
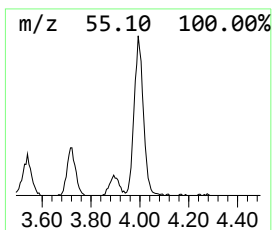
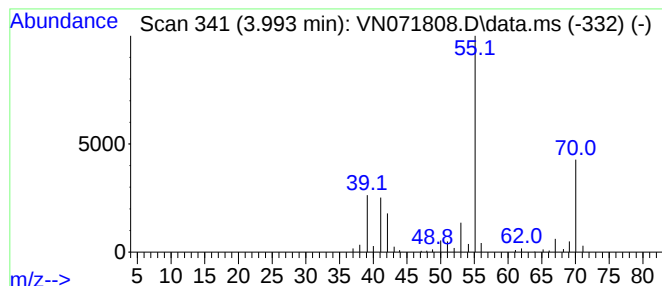
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.993	5.59 ug/l	201928	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	91
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
3			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	86
4			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
5			1-Butene, 3-methyl-	70	C5H10	000563-45-1	72



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.228	112.5	ug/l	4062570	1	8.081	1805130	50.0
Butane	2.434	8.9	ug/l	323241	1	8.081	1805130	50.0
Butane, 2-methyl-	3.128	8.9	ug/l	320459	1	8.081	1805130	50.0
Cyclopropane, 1...	3.993	5.6	ug/l	201928	1	8.081	1805130	50.0