

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074535.D
 Acq On : 17 Sep 2022 02:07
 Operator : JC\MD
 Sample : N4549-07
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-51

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\82N091522W.M
 Title : SW846 8260

Signal : TIC: VN074535.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	47	53	61	rBV	239667	513170	25.02%	3.294%
2	2.410	84	89	92	rBV3	32011	63635	3.10%	0.408%
3	2.681	132	135	137	rBV	63600	73757	3.60%	0.473%
4	3.081	199	203	214	rVB5	80161	217255	10.59%	1.394%
5	3.157	214	216	227	rVB6	34488	99519	4.85%	0.639%
6	3.934	340	348	353	rBV4	19390	47176	2.30%	0.303%
7	4.992	517	528	538	rBV3	43269	157570	7.68%	1.011%
8	5.098	538	546	547	rBV2	34803	60954	2.97%	0.391%
9	5.528	606	619	631	rBV2	70920	264247	12.88%	1.696%
10	7.063	871	880	885	rBV5	32586	82787	4.04%	0.531%
11	7.145	887	894	901	rVV3	46123	116130	5.66%	0.745%
12	7.228	901	908	922	rVB2	27684	87286	4.26%	0.560%
13	7.722	981	992	994	rBV6	8014	22887	1.12%	0.147%
14	7.769	994	1000	1007	rVB4	35371	79773	3.89%	0.512%
15	7.951	1019	1031	1036	rBV2	281382	684022	33.35%	4.390%
16	8.016	1036	1042	1052	rVB	463667	1042513	50.83%	6.691%
17	8.375	1093	1103	1115	rBV4	426624	1205241	58.76%	7.735%
18	8.528	1121	1129	1133	rBV6	21179	56461	2.75%	0.362%
19	8.904	1184	1193	1205	rBV	736471	1562561	76.18%	10.029%
20	8.992	1205	1208	1215	rVB7	16679	30947	1.51%	0.199%
21	9.133	1226	1232	1235	rBV5	24771	46869	2.29%	0.301%
22	9.175	1236	1239	1247	rVB4	20184	42617	2.08%	0.274%
23	9.357	1263	1270	1275	rBV5	20583	46844	2.28%	0.301%
24	9.757	1329	1338	1339	rBV6	14624	29305	1.43%	0.188%
25	9.910	1356	1364	1368	rBV4	35672	64762	3.16%	0.416%
26	9.957	1368	1372	1383	rVB4	22344	55541	2.71%	0.356%
27	10.151	1397	1405	1412	rBV9	12873	37321	1.82%	0.240%
28	10.257	1418	1423	1435	rVB3	55057	119578	5.83%	0.767%
29	10.380	1435	1444	1453	rBV	1139973	2051119	100.00%	13.164%
30	10.580	1473	1478	1484	rVB7	20931	42738	2.08%	0.274%
31	10.804	1512	1516	1525	rVB7	13046	26886	1.31%	0.173%
32	11.069	1557	1561	1565	rBV4	20942	32333	1.58%	0.208%
33	11.127	1566	1571	1573	rVV4	11515	21400	1.04%	0.137%
34	11.145	1573	1574	1580	rVB4	16390	21488	1.05%	0.138%
35	11.686	1658	1666	1673	rBV	1143811	1974137	96.25%	12.670%
36	11.739	1673	1675	1680	rVV6	29094	43080	2.10%	0.276%

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37	11.792	1680	1684	1692	rVB7	11662	21065	1.03%	0.135%
38	11.898	1695	1702	1713	rVB4	26209	65396	3.19%	0.420%
39	12.033	1718	1725	1729	rBV6	21509	36737	1.79%	0.236%
40	12.216	1752	1756	1762	rBV3	12263	23529	1.15%	0.151%
41	12.392	1780	1786	1790	rBV5	13805	24289	1.18%	0.156%
42	12.463	1793	1798	1802	rVV5	12735	25686	1.25%	0.165%
43	12.521	1802	1808	1815	rVB	104622	183323	8.94%	1.177%
44	12.674	1826	1834	1843	rBV	911838	1539986	75.08%	9.884%
45	12.863	1861	1866	1875	rVV	78797	130779	6.38%	0.839%
46	12.939	1875	1879	1886	rVV8	10931	22158	1.08%	0.142%
47	13.168	1910	1918	1923	rBV3	19203	32901	1.60%	0.211%
48	13.298	1936	1940	1947	rVB6	15108	26832	1.31%	0.172%
49	13.421	1954	1961	1971	rVB3	37305	84383	4.11%	0.542%
50	13.615	1986	1994	2006	rBV	1123017	1856499	90.51%	11.915%
51	13.715	2006	2011	2018	rVB4	14636	23235	1.13%	0.149%
52	13.786	2018	2023	2025	rBV4	14498	20582	1.00%	0.132%
53	13.945	2045	2050	2056	rVB6	17032	26445	1.29%	0.170%
54	14.162	2081	2087	2092	rBV4	24526	36561	1.78%	0.235%
55	14.268	2100	2105	2113	rVB3	54669	94810	4.62%	0.609%
56	14.480	2132	2141	2148	rBV3	41739	80756	3.94%	0.518%
57	14.874	2200	2208	2213	rBV6	15766	35645	1.74%	0.229%
58	14.933	2214	2218	2224	rVB4	16852	29400	1.43%	0.189%
59	15.245	2265	2271	2276	rVB10	16564	35900	1.75%	0.230%

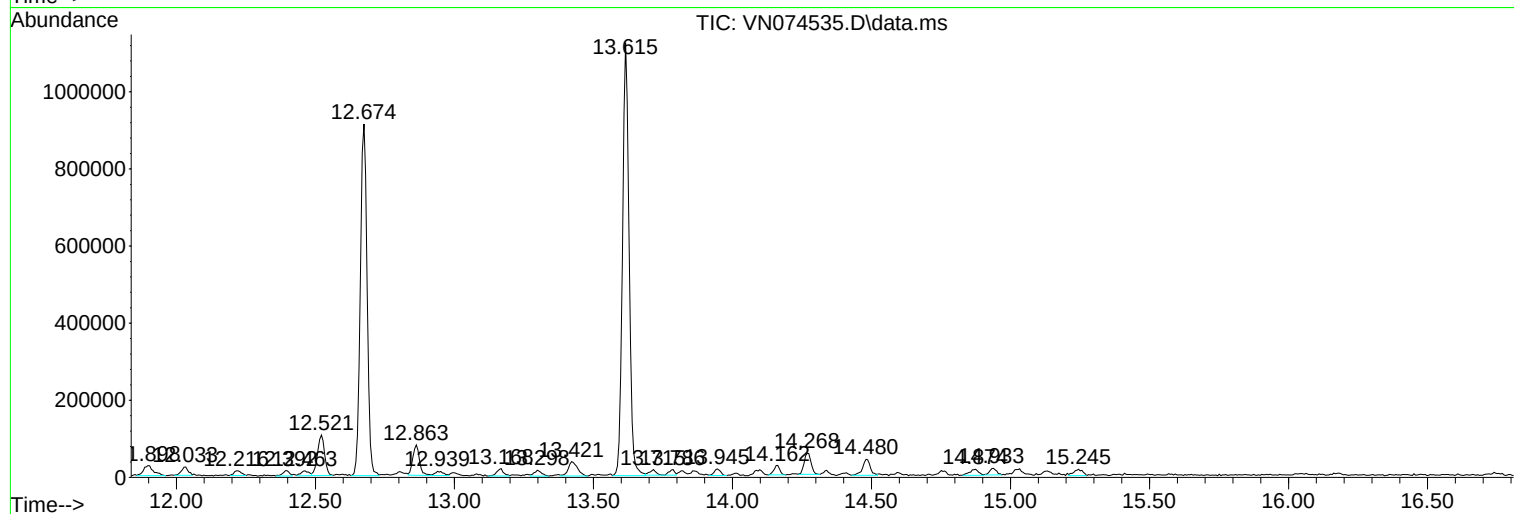
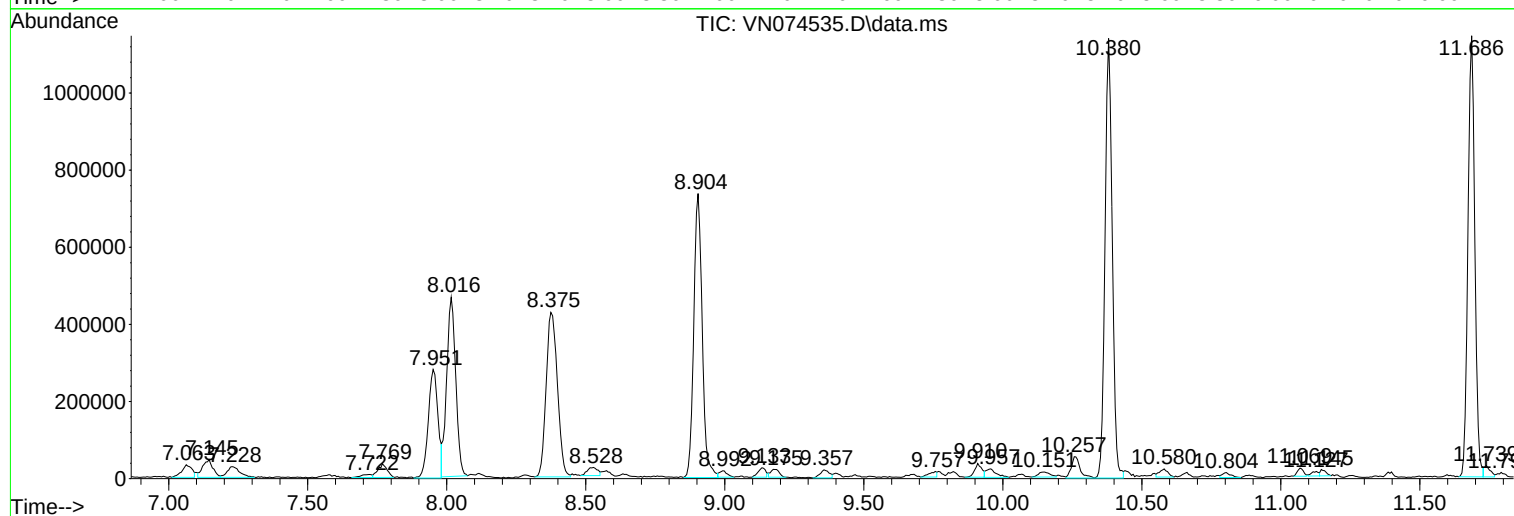
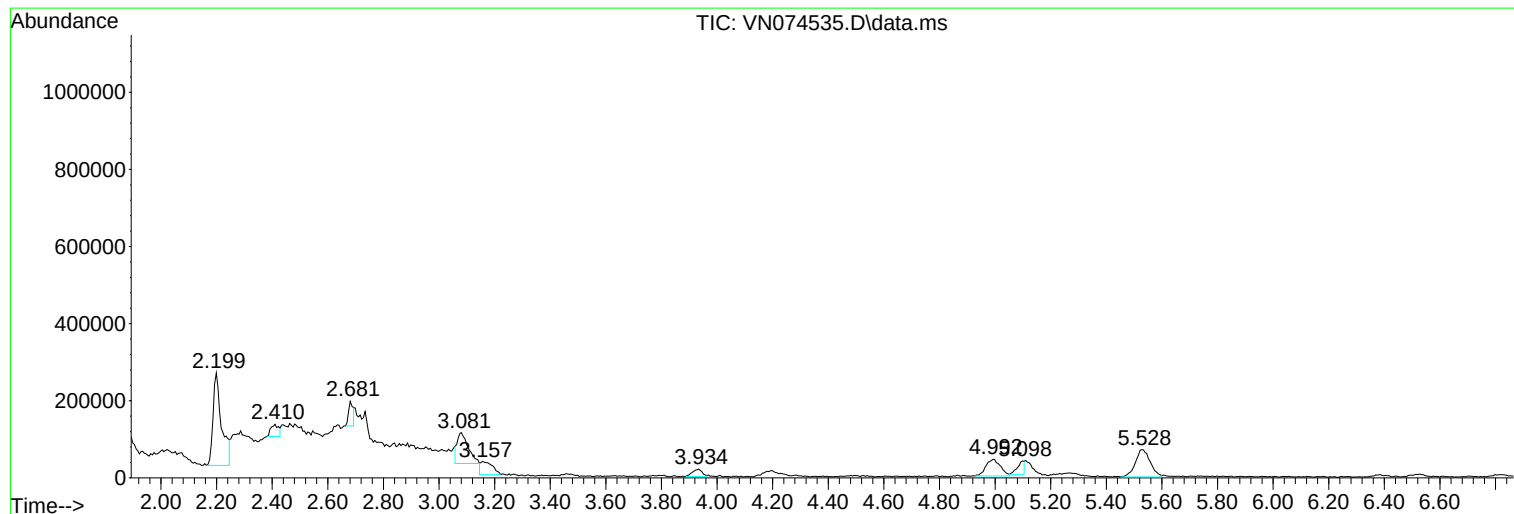
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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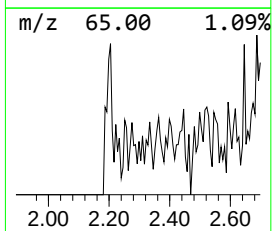
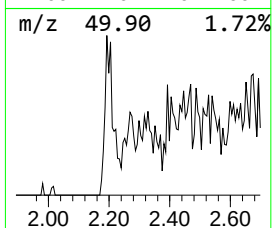
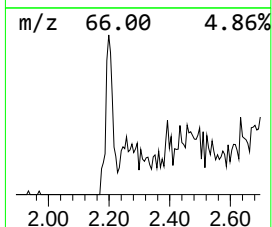
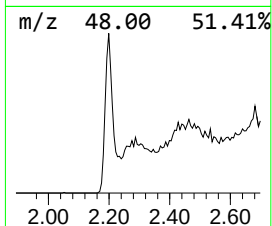
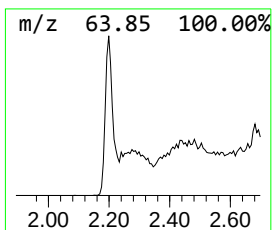
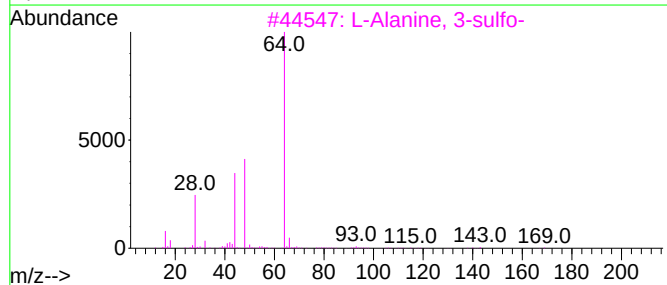
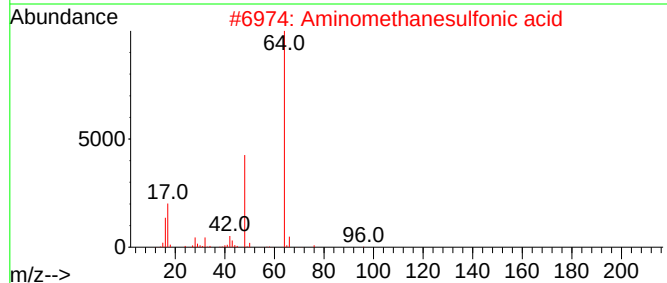
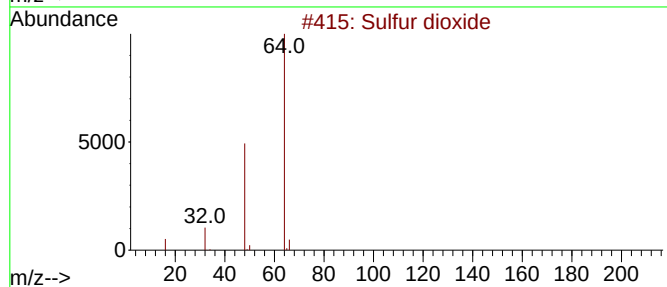
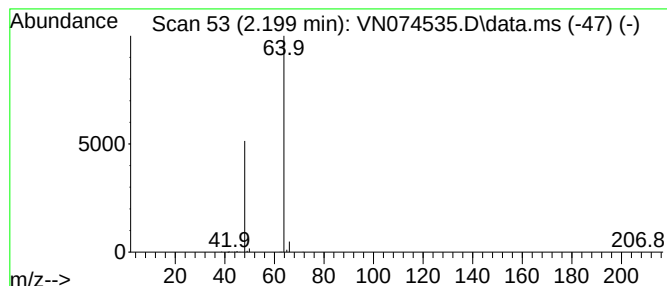
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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.
2.199	24.61 ug/l	513170	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	3
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3



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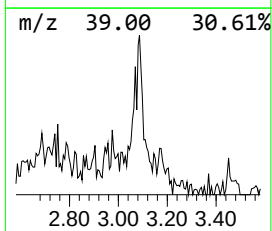
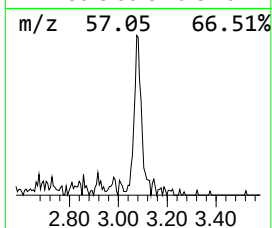
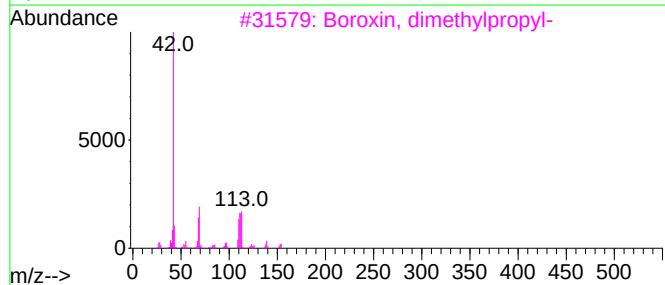
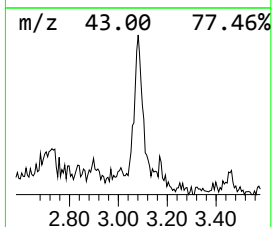
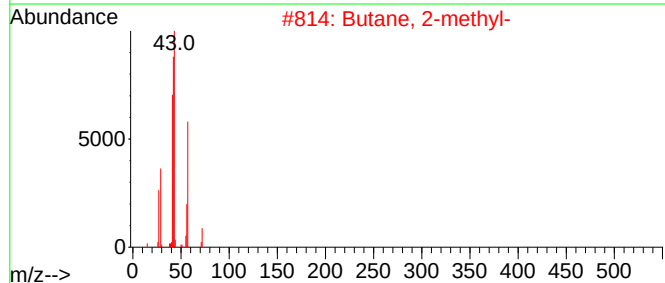
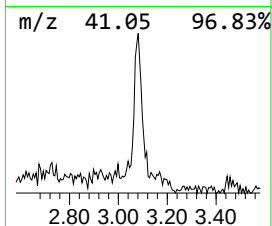
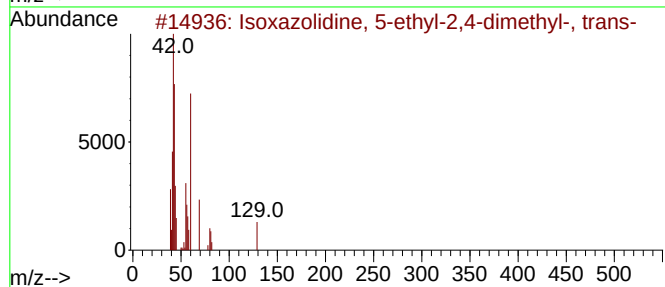
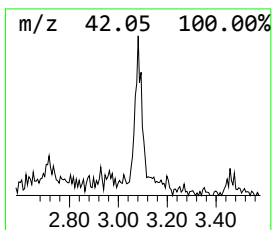
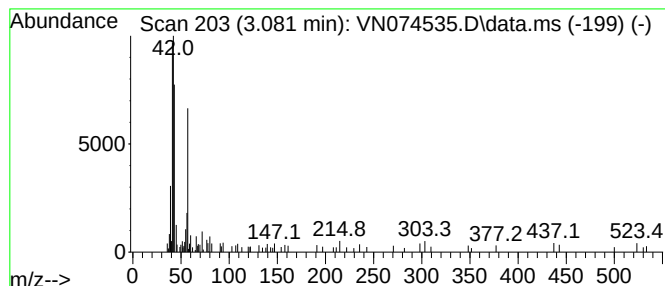
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 2 Isoxazolidine, 5-ethyl-2,4-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	10.42 ug/l	217255	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isoxazolidine, 5-ethyl-2,4-dimet...	129	C7H15NO	056728-14-4	53
2		Butane, 2-methyl-	72	C5H12	000078-78-4	53
3		Boroxin, dimethylpropyl-	154	C5H13B3O3	1000162-61-0	42
4		3-Buten-1-ol	72	C4H8O	000627-27-0	42
5		2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	36



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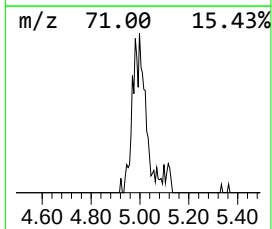
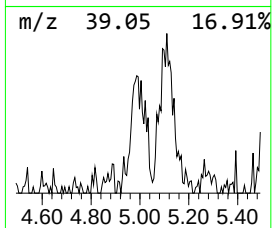
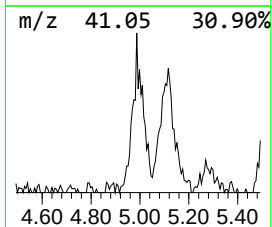
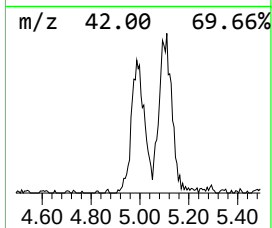
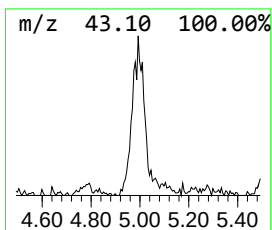
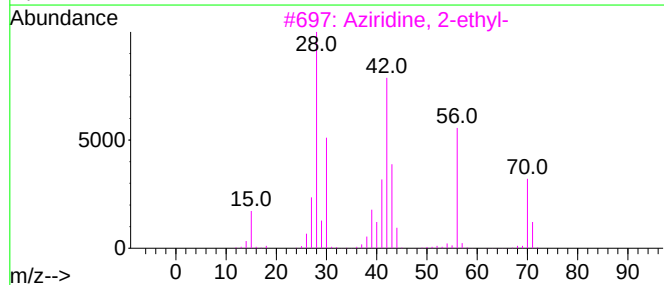
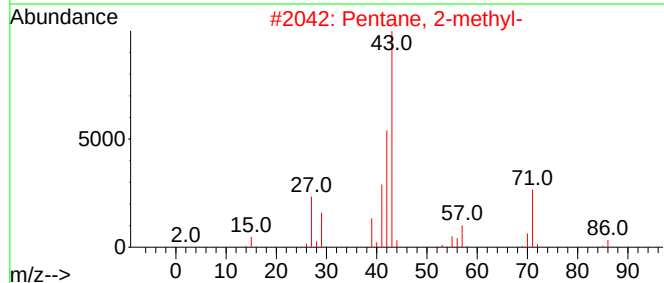
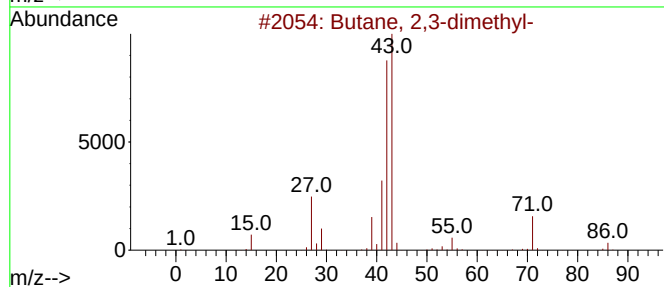
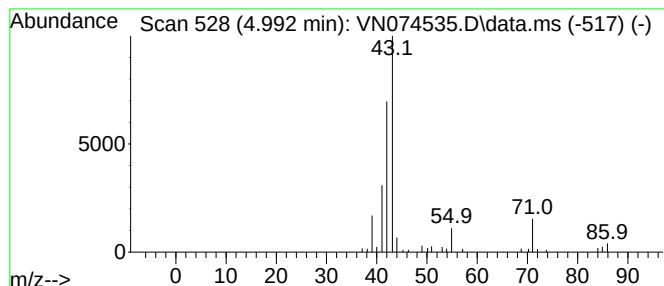
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Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.992	7.56 ug/l	157570	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	59
3			Aziridine, 2-ethyl-	71	C4H9N	002549-67-9	50
4			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9
5			1-Butanol	74	C4H10O	000071-36-3	9



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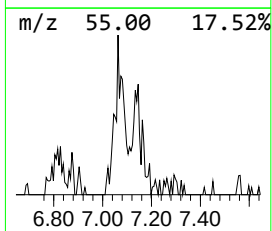
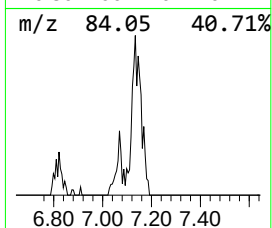
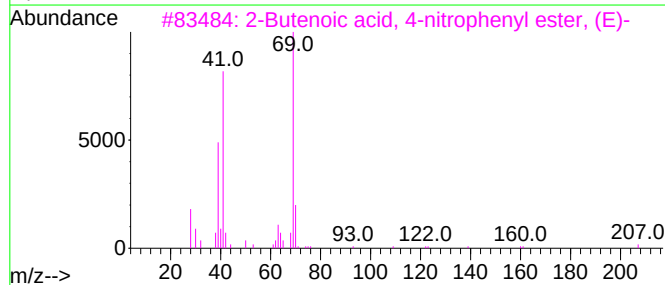
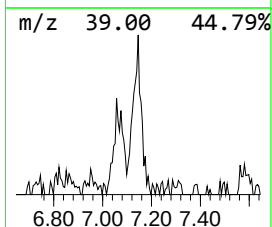
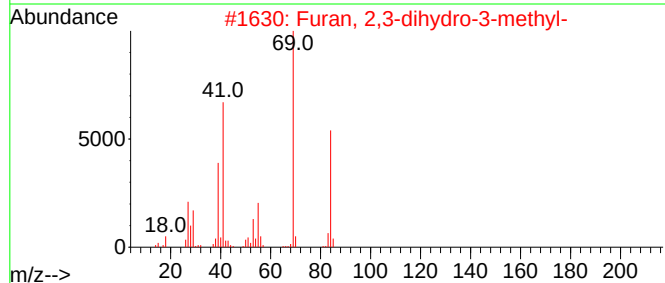
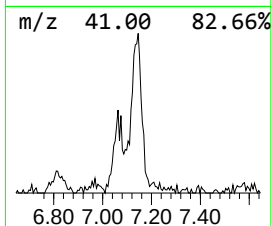
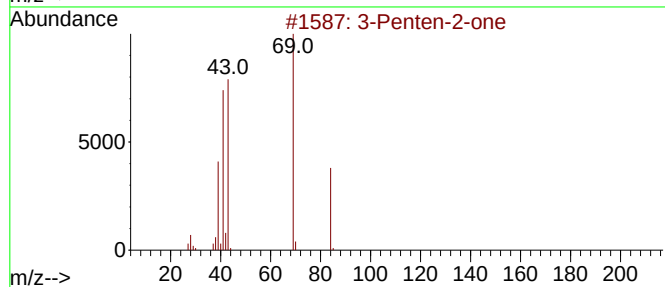
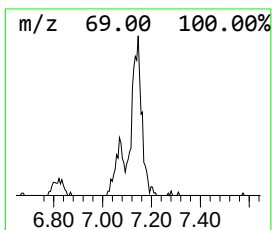
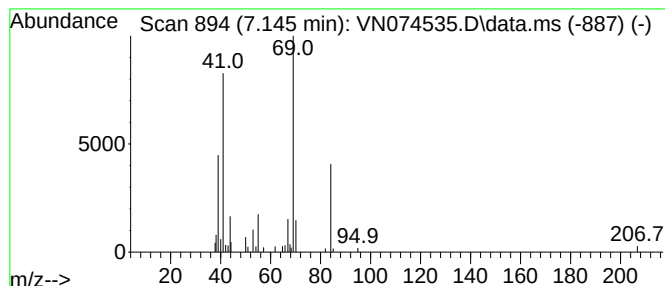
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 4 3-Penten-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	5.57 ug/l	116130	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one	84	C5H8O	000625-33-2	72
2			Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	64
3			2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	014617-88-0	52
4			2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	52
5			2-Pentene, 2-methyl-	84	C6H12	000625-27-4	50



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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	2.199	24.6	ug/l	513170	1	8.016	1042510	50.0
Isoxazolidine, ...	3.081	10.4	ug/l	217255	1	8.016	1042510	50.0
Butane, 2,3-dim...	4.992	7.6	ug/l	157570	1	8.016	1042510	50.0
3-Penten-2-one	7.145	5.6	ug/l	116130	1	8.016	1042510	50.0