

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
 Data File : VN073375.D
 Acq On : 07 Jul 2022 16:46
 Operator : JC\MD
 Sample : N3620-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 BP-TB-20220706

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\82N062822W.M
 Title : SW846 8260

Signal : TIC: VN073375.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.005	17	20	25	rVB2	5328	7494	7.17%	1.027%
2	2.193	48	52	54	rBV	3464	4605	4.40%	0.631%
3	2.228	54	58	63	rVB	23880	32817	31.38%	4.499%
4	2.369	75	82	90	rBV	70087	104567	100.00%	14.337%
5	2.552	108	113	122	rBV	12372	23190	22.18%	3.179%
6	2.640	125	128	131	rBV3	1228	1706	1.63%	0.234%
7	2.681	131	135	136	rBV	1348	1593	1.52%	0.218%
8	2.699	136	138	142	rBV5	1682	2262	2.16%	0.310%
9	3.081	197	203	204	rBV4	1943	2923	2.80%	0.401%
10	3.169	215	218	220	rBV	1268	1481	1.42%	0.203%
11	3.646	293	299	301	rVV	1772	3367	3.22%	0.462%
12	3.693	305	307	313	rVB4	1488	2791	2.67%	0.383%
13	4.240	391	400	409	rBV2	9263	26629	25.47%	3.651%
14	4.516	439	447	449	rBV3	2055	4227	4.04%	0.580%
15	5.293	569	579	589	rBV3	5034	16131	15.43%	2.212%
16	5.828	663	670	671	rBV2	791	1453	1.39%	0.199%
17	5.887	678	680	688	rVB4	2591	4987	4.77%	0.684%
18	7.010	859	871	877	rBV5	4559	15744	15.06%	2.159%
19	7.263	909	914	915	rBV3	2257	3161	3.02%	0.433%
20	7.287	917	918	923	rVB	2673	2222	2.12%	0.305%
21	7.728	990	993	995	rBV2	1246	1551	1.48%	0.213%
22	7.951	1025	1031	1037	rBV2	4842	10957	10.48%	1.502%
23	8.016	1037	1042	1050	rVV3	8332	16380	15.66%	2.246%
24	8.369	1096	1102	1109	rVB4	6081	12540	11.99%	1.719%
25	8.792	1171	1174	1175	rBV3	1261	1385	1.32%	0.190%
26	8.816	1175	1178	1180	rVB	1263	1519	1.45%	0.208%
27	8.904	1185	1193	1199	rVV2	11497	22701	21.71%	3.112%
28	9.469	1282	1289	1297	rVB3	4072	8713	8.33%	1.195%
29	9.722	1331	1332	1338	rVB4	3234	4017	3.84%	0.551%
30	10.269	1420	1425	1433	rVB3	5404	9168	8.77%	1.257%
31	10.381	1437	1444	1450	rBV	13965	25912	24.78%	3.553%
32	10.445	1450	1455	1462	rVV2	9000	17199	16.45%	2.358%
33	10.563	1471	1475	1479	rVV2	2171	3781	3.62%	0.518%
34	11.028	1553	1554	1558	rVB2	2095	1635	1.56%	0.224%
35	11.122	1565	1570	1576	rBV4	4275	7504	7.18%	1.029%
36	11.598	1649	1651	1655	rBV4	1032	1506	1.44%	0.206%

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37	11.680	1661	1665	1672	rVB2	14620	24791	23.71%	3.399%
38	11.780	1678	1682	1685	rBV2	2652	3525	3.37%	0.483%
39	11.886	1694	1700	1708	rVB4	6680	13178	12.60%	1.807%
40	12.216	1750	1756	1762	rVB3	5044	9413	9.00%	1.291%
41	12.286	1765	1768	1770	rVB	1716	1651	1.58%	0.226%
42	12.310	1770	1772	1774	rBV2	1510	1424	1.36%	0.195%
43	12.398	1780	1787	1794	rBV5	5723	11144	10.66%	1.528%
44	12.516	1804	1807	1810	rVB3	2003	3069	2.93%	0.421%
45	12.675	1829	1834	1841	rVB3	13256	22691	21.70%	3.111%
46	12.869	1862	1867	1870	rBV3	913	1496	1.43%	0.205%
47	12.916	1872	1875	1877	rBV2	1920	1719	1.64%	0.236%
48	12.986	1884	1887	1888	rBV3	2765	2919	2.79%	0.400%
49	13.086	1900	1904	1906	rBV5	1853	2657	2.54%	0.364%
50	13.222	1925	1927	1929	rBV3	2546	2428	2.32%	0.333%
51	13.298	1937	1940	1941	rBV3	2528	2676	2.56%	0.367%
52	13.392	1953	1956	1958	rBV4	1832	2194	2.10%	0.301%
53	13.410	1958	1959	1962	rBV3	2277	2258	2.16%	0.310%
54	13.457	1964	1967	1968	rBV3	4045	3146	3.01%	0.431%
55	13.504	1973	1975	1978	rVV4	4664	5373	5.14%	0.737%
56	13.610	1986	1993	2000	rVV4	19245	40352	38.59%	5.532%
57	13.669	2002	2003	2006	rBV3	2695	2106	2.01%	0.289%
58	13.704	2006	2009	2011	rVV4	3016	3012	2.88%	0.413%
59	13.804	2024	2026	2028	rVV3	2882	2731	2.61%	0.374%
60	13.833	2028	2031	2033	rVB4	2488	3196	3.06%	0.438%
61	13.927	2044	2047	2049	rBV4	1931	1998	1.91%	0.274%
62	14.069	2065	2071	2073	rBV6	2870	4507	4.31%	0.618%
63	14.092	2073	2075	2076	rBV2	3023	2878	2.75%	0.395%
64	14.210	2092	2095	2096	rBV3	1495	1864	1.78%	0.256%
65	14.286	2106	2108	2111	rVB3	2069	1850	1.77%	0.254%
66	14.316	2111	2113	2114	rBV2	2618	1582	1.51%	0.217%
67	14.392	2123	2126	2127	rBV2	3824	2960	2.83%	0.406%
68	14.445	2131	2135	2140	rVB7	5131	10867	10.39%	1.490%
69	14.521	2147	2148	2150	rBV2	3053	2785	2.66%	0.382%
70	14.563	2154	2155	2158	rVB3	3572	2259	2.16%	0.310%
71	14.751	2185	2187	2188	rBV2	2566	1636	1.56%	0.224%
72	14.892	2209	2211	2217	rVB6	5841	9096	8.70%	1.247%
73	14.951	2217	2221	2222	rBV4	1873	2078	1.99%	0.285%
74	15.080	2241	2243	2246	rVB4	2975	2690	2.57%	0.369%
75	15.145	2252	2254	2255	rBV2	3390	2056	1.97%	0.282%
76	15.210	2259	2265	2267	rBV6	6316	10404	9.95%	1.426%

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77	15.316	2281	2283	2286	rVB4	2036	1997	1.91%	0.274%
78	15.357	2288	2290	2291	rBV2	2072	1719	1.64%	0.236%
79	15.533	2318	2320	2324	rBV4	2180	2581	2.47%	0.354%
80	15.568	2324	2326	2329	rBV4	3580	5365	5.13%	0.736%
81	15.727	2351	2353	2354	rBV2	3669	2325	2.22%	0.319%
82	15.751	2355	2357	2358	rVV2	2787	1692	1.62%	0.232%
83	15.886	2378	2380	2381	rBV2	2549	1860	1.78%	0.255%
84	15.904	2381	2383	2385	rVB3	3464	2303	2.20%	0.316%
85	15.927	2385	2387	2392	rVB6	2846	4645	4.44%	0.637%
86	15.968	2392	2394	2396	rBV3	2157	1751	1.67%	0.240%
87	16.033	2403	2405	2406	rBV2	2253	1838	1.76%	0.252%
88	16.098	2410	2416	2418	rBV7	4571	8474	8.10%	1.162%
89	16.198	2431	2433	2434	rBV2	2312	1828	1.75%	0.251%
90	16.268	2441	2445	2447	rBV5	4366	6555	6.27%	0.899%
91	16.345	2456	2458	2459	rVB2	3641	2148	2.05%	0.294%
92	16.368	2459	2462	2464	rBV4	3664	4545	4.35%	0.623%
93	16.392	2464	2466	2468	rVV3	6337	5095	4.87%	0.699%
94	16.421	2468	2471	2476	rVB7	4240	7317	7.00%	1.003%
95	16.510	2484	2486	2488	rBV3	3013	2623	2.51%	0.360%
96	16.527	2488	2489	2491	rVB2	4632	2589	2.48%	0.355%
97	16.580	2496	2498	2501	rVV4	3734	4924	4.71%	0.675%
98	16.621	2503	2505	2514	rVB10	5685	9496	9.08%	1.302%
99	16.692	2516	2517	2519	rVB2	3463	2219	2.12%	0.304%
100	16.721	2519	2522	2523	rBV3	2921	3008	2.88%	0.412%

Sum of corrected areas: 729374

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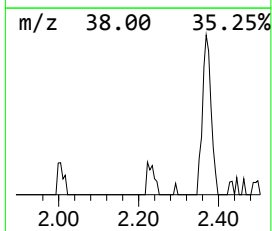
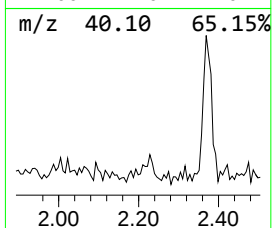
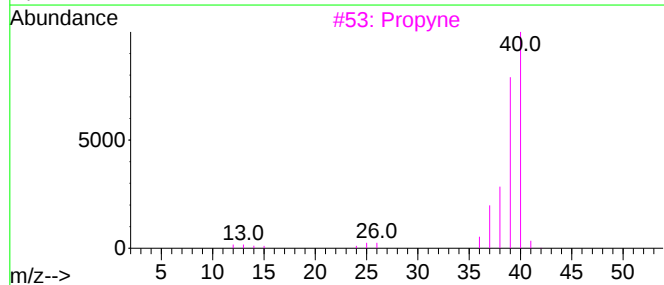
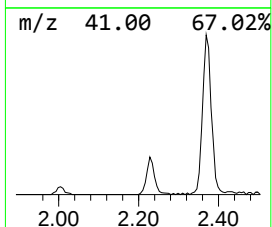
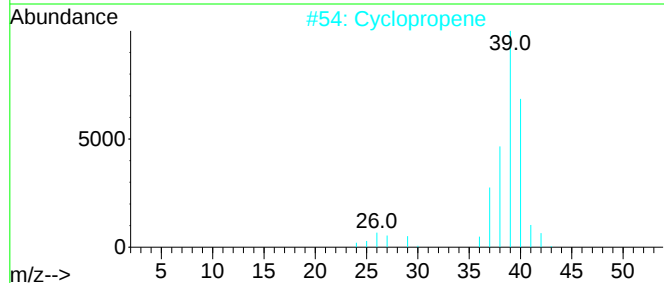
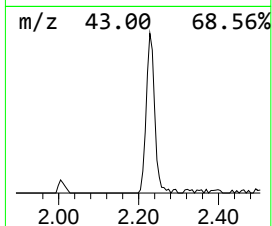
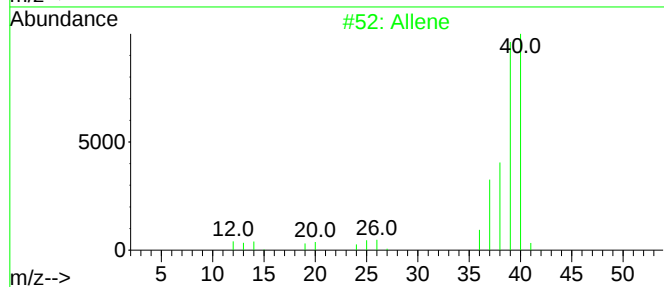
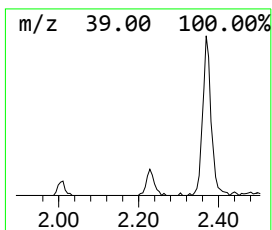
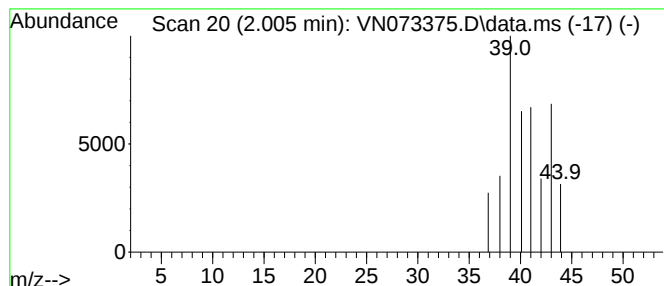
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Allene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.005	22.88 ug/l	7494	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allene			40	C3H4	000463-49-0	78
2	Cyclopropene			40	C3H4	002781-85-3	78
3	Propyne			40	C3H4	000074-99-7	9
4	Propene			42	C3H6	000115-07-1	4
5	Pyrimidine-2,4(1H,3H)-dione, 5-a...			156	C4H4N4O3	1000270-67-7	2



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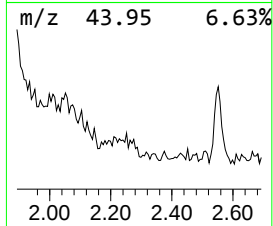
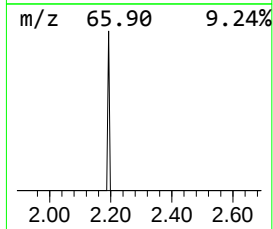
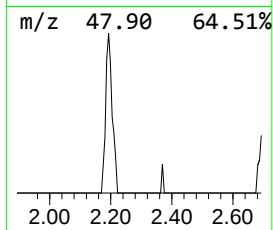
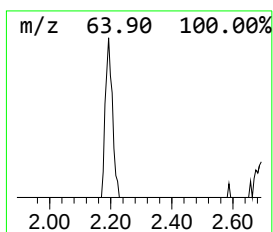
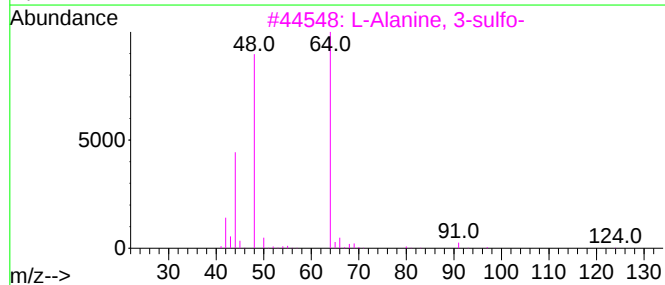
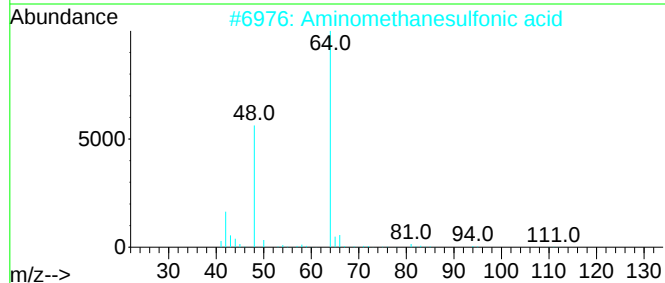
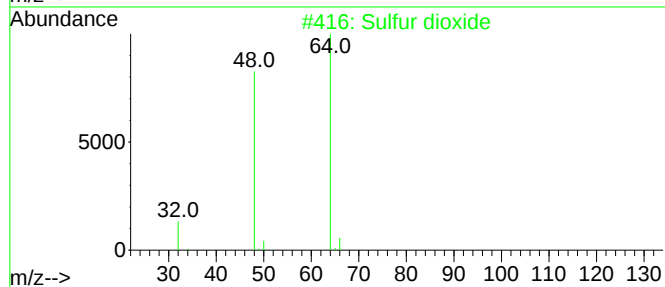
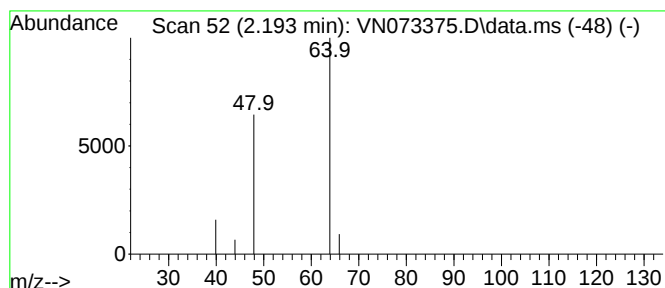
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 2 Sulfur dioxide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	14.06 ug/l	4605	Pentafluorobenzene	8.022

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



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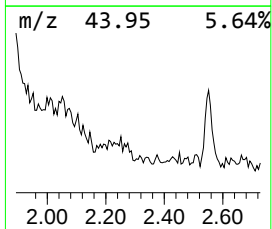
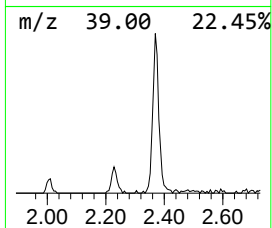
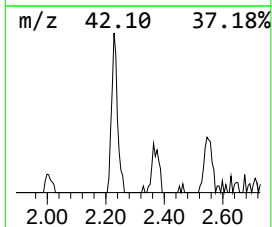
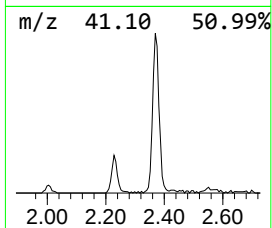
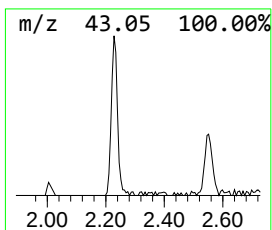
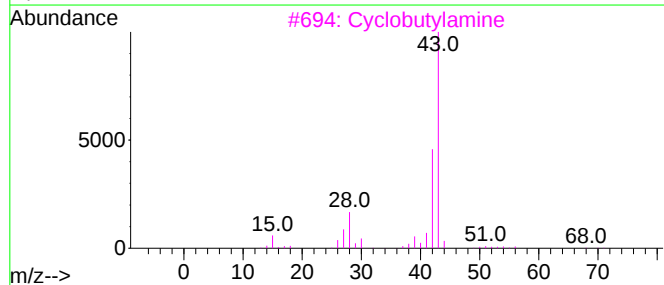
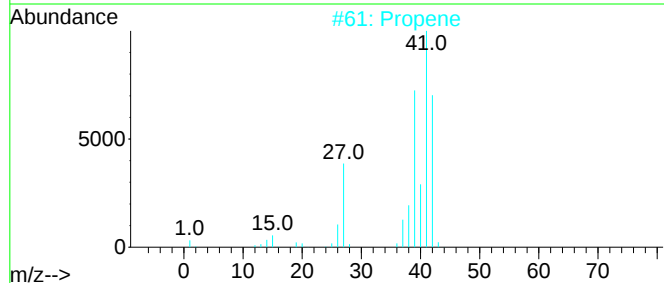
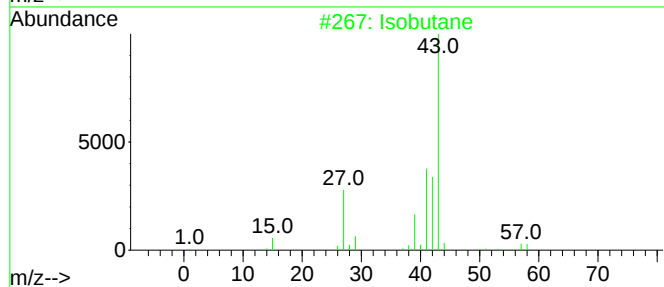
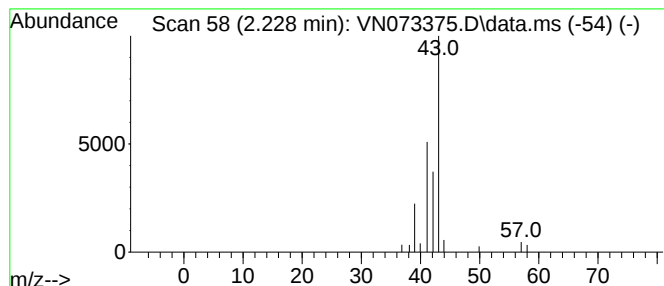
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 3 Isobutane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	100.17 ug/l	32817	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	83
2	Propene	42	C3H6	000115-07-1	4
3	Cyclobutylamine	71	C4H9N	002516-34-9	4
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	4
5	Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4



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BP-TB-20220706

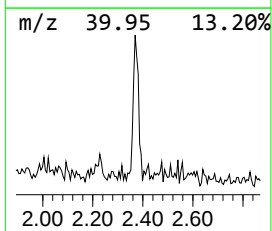
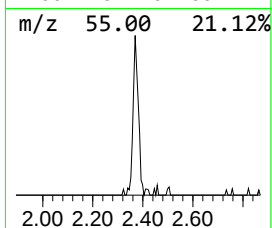
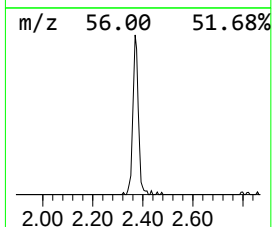
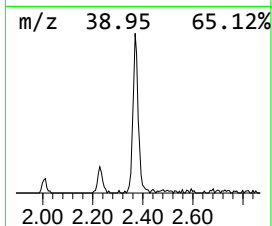
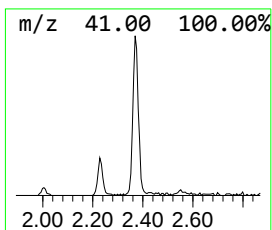
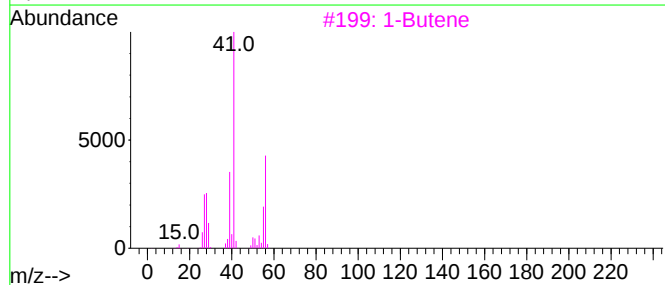
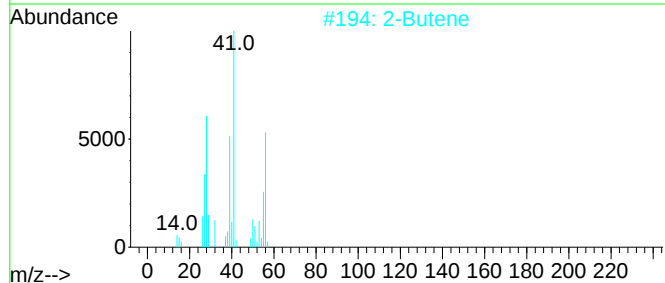
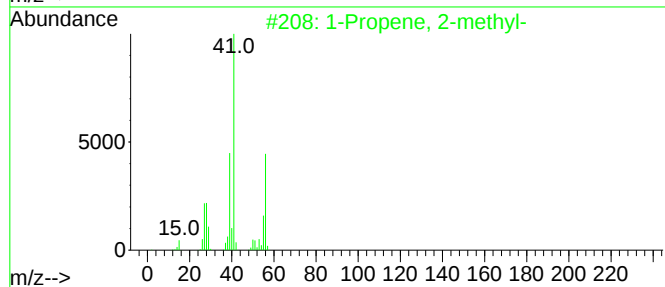
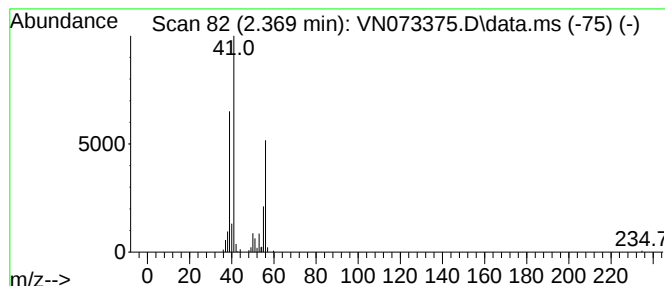
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.369	319.19 ug/l	104567	Pentafluorobenzene	8.022

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propene, 2-methyl-	56	C4H8	000115-11-7	91
2		2-Butene	56	C4H8	000107-01-7	90
3		1-Butene	56	C4H8	000106-98-9	52
4		2-Butene, (Z)-	56	C4H8	000590-18-1	52
5		2-Butene, (E)-	56	C4H8	000624-64-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
Data File : VN073375.D
Acq On : 07 Jul 2022 16:46
Operator : JC\MD
Sample : N3620-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BP-TB-20220706

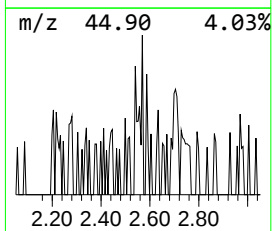
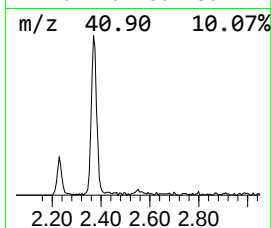
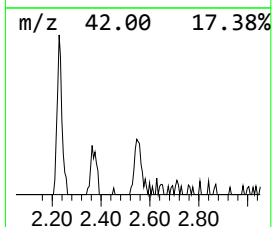
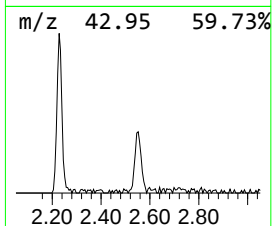
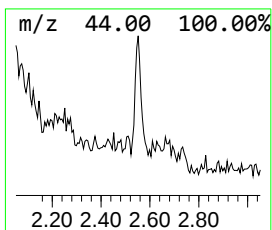
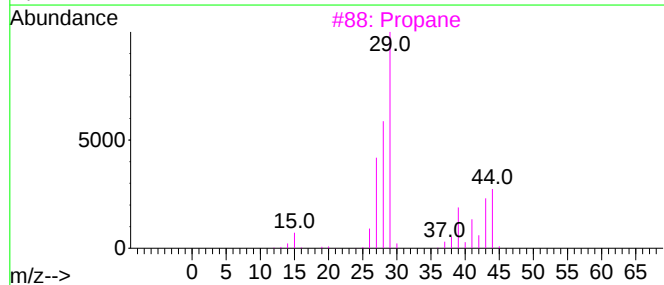
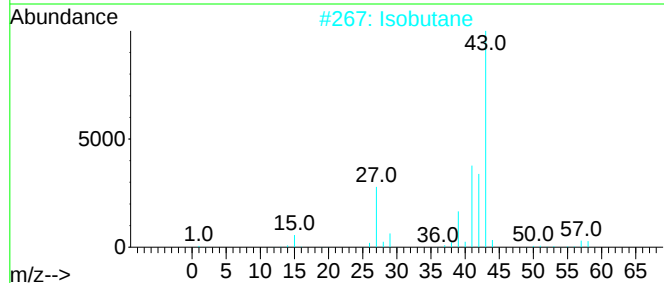
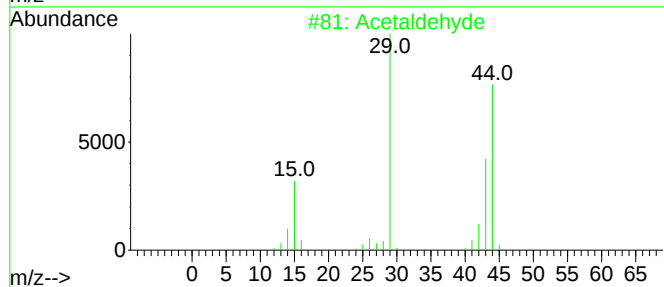
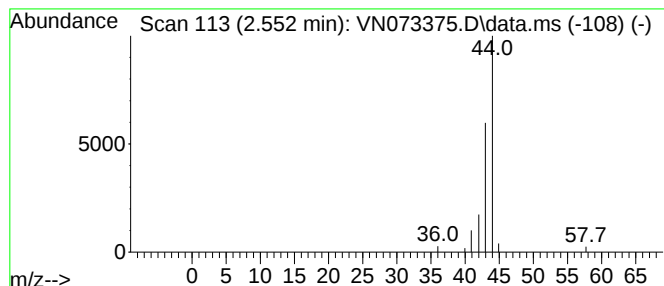
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Quant Title : SW846 8260

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

Peak Number 5 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.552	70.79 ug/l	23190	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Isobutane	58	C4H10	000075-28-5	5
3			Propane	44	C3H8	000074-98-6	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			1-Propanol, 2-amino-, (+/-)-	75	C3H9NO	006168-72-5	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
Data File : VN073375.D
Acq On : 07 Jul 2022 16:46
Operator : JC\MD
Sample : N3620-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BP-TB-20220706

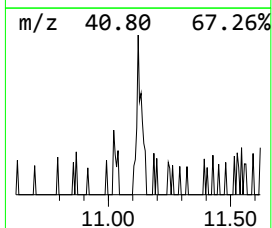
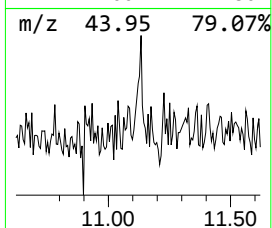
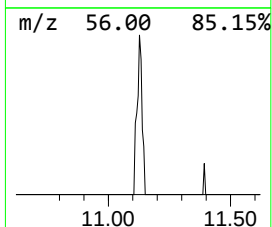
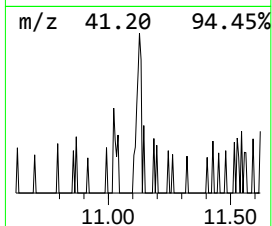
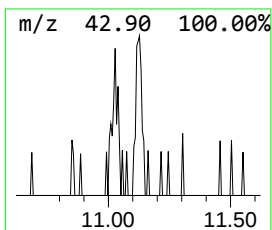
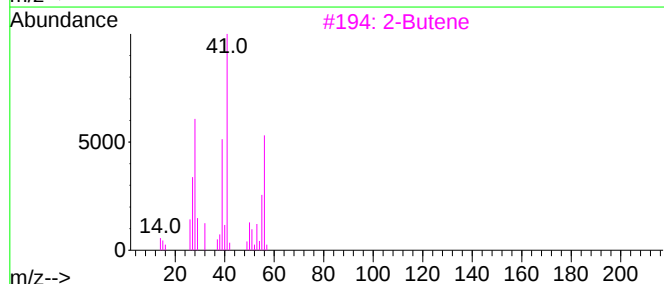
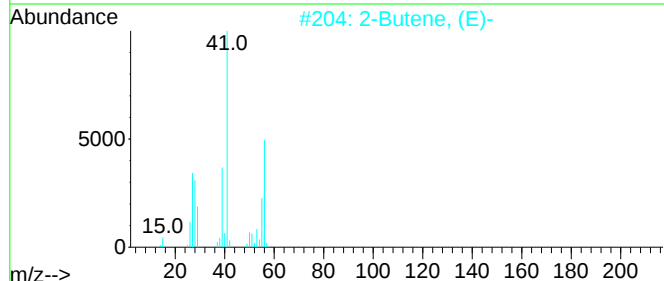
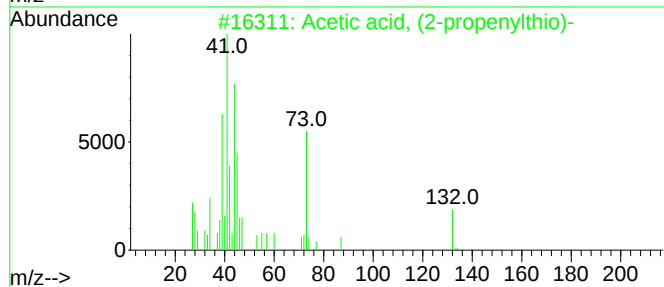
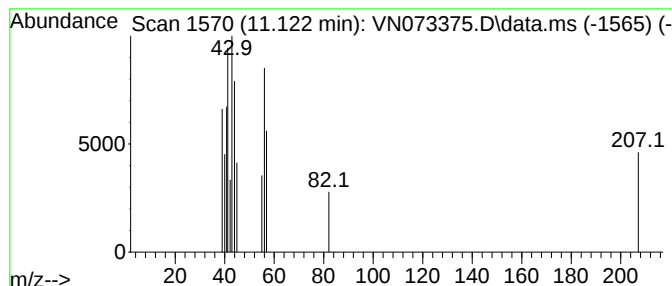
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Quant Title : SW846 8260

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

Peak Number 9 unknown11.112 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.122	15.13 ug/l	7504	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, (2-propenylthio)-	132	C5H8O2S	020600-63-9	25
2			2-Butene, (E)-	56	C4H8	000624-64-6	9
3			2-Butene	56	C4H8	000107-01-7	9
4			1-Butene	56	C4H8	000106-98-9	9
5			2-Butene, (Z)-	56	C4H8	000590-18-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
Data File : VN073375.D
Acq On : 07 Jul 2022 16:46
Operator : JC\MD
Sample : N3620-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BP-TB-20220706

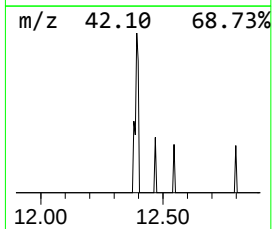
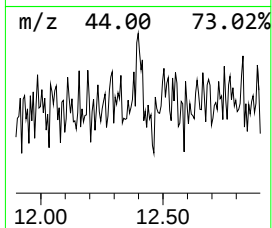
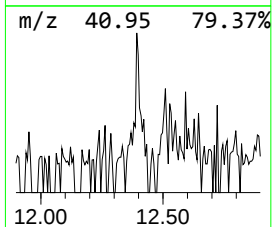
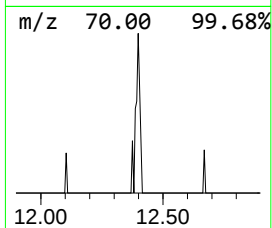
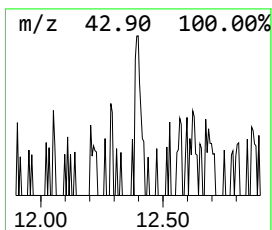
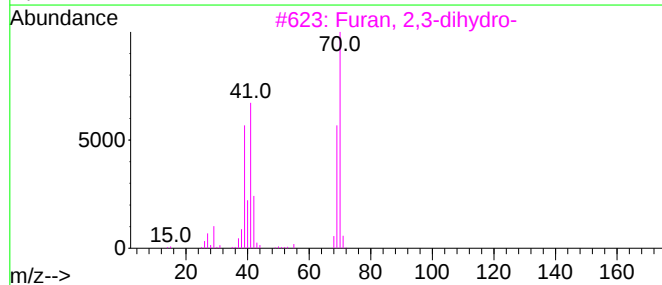
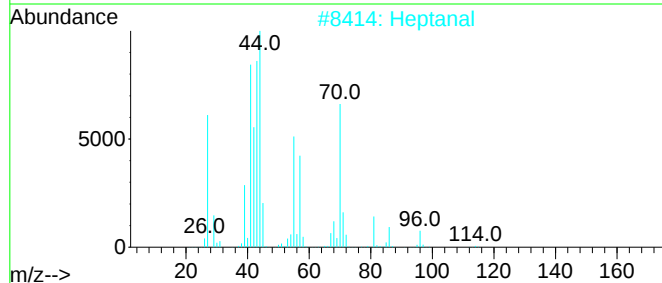
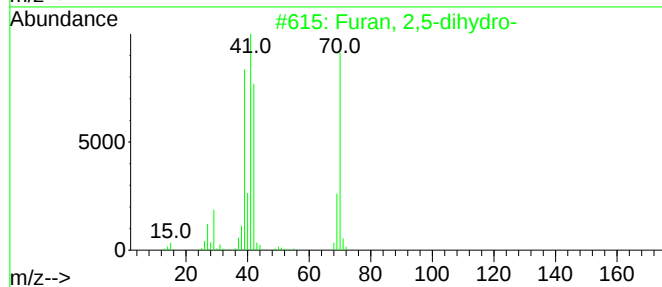
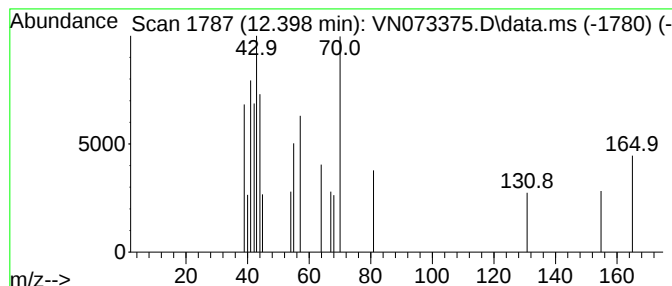
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Quant Title : SW846 8260

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

Peak Number 10 unknown12.398 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.398	22.48 ug/l	11144	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	11
2			Heptanal	114	C7H14O	000111-71-7	10
3			Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	10
4			Cycloheptane	98	C7H14	000291-64-5	10
5			2-Methyl-1-butene	70	C5H10	000563-46-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
Data File : VN073375.D
Acq On : 07 Jul 2022 16:46
Operator : JC\MD
Sample : N3620-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BP-TB-20220706

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.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
Allene	2.005	22.9	ug/l	7494	1	8.022	16380	50.0
Sulfur dioxide	2.193	14.1	ug/l	4605	1	8.022	16380	50.0
Isobutane	2.228	100.2	ug/l	32817	1	8.022	16380	50.0
1-Propene, 2-me...	2.369	319.2	ug/l	104567	1	8.022	16380	50.0
Acetaldehyde	2.552	70.8	ug/l	23190	1	8.022	16380	50.0
unknown11.112	11.122	15.1	ug/l	7504	3	11.686	24791	50.0
unknown12.398	12.398	22.5	ug/l	11144	3	11.686	24791	50.0