

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074533.D
 Acq On : 17 Sep 2022 01:19
 Operator : JC\MD
 Sample : N4549-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-50

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: VN074533.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.198	47	53	62	rBV	236007	536038	25.63%	2.200%
2	2.404	84	88	92	rBV3	41227	64799	3.10%	0.266%
3	2.693	132	137	141	rBV4	61990	129959	6.21%	0.533%
4	3.081	196	203	215	rVB	582953	1372442	65.63%	5.633%
5	3.451	261	266	273	rVB3	18469	36866	1.76%	0.151%
6	4.187	379	391	406	rBV2	116081	428901	20.51%	1.760%
7	4.992	514	528	549	rBV5	252721	1039012	49.69%	4.265%
8	5.528	608	619	634	rVB3	42107	146676	7.01%	0.602%
9	6.798	824	835	836	rBV3	21666	41028	1.96%	0.168%
10	6.963	853	863	873	rBV3	118484	349785	16.73%	1.436%
11	7.063	873	880	888	rVV3	51335	139994	6.69%	0.575%
12	7.128	888	891	892	rVV2	24532	28127	1.35%	0.115%
13	7.139	892	893	900	rVV3	30558	46424	2.22%	0.191%
14	7.233	900	909	923	rVB3	35822	123634	5.91%	0.507%
15	7.769	991	1000	1012	rVB2	51550	150010	7.17%	0.616%
16	7.951	1019	1031	1037	rBV2	267401	699759	33.46%	2.872%
17	8.016	1037	1042	1050	rVV	436144	997595	47.71%	4.095%
18	8.104	1050	1057	1068	rVB2	214267	545292	26.08%	2.238%
19	8.286	1081	1088	1094	rBV5	15104	34145	1.63%	0.140%
20	8.369	1094	1102	1114	rVV3	345521	911849	43.61%	3.743%
21	8.486	1116	1122	1123	rVV4	20671	32867	1.57%	0.135%
22	8.545	1124	1132	1143	rVV	410329	1030471	49.28%	4.230%
23	8.639	1143	1148	1157	rVB	57295	119053	5.69%	0.489%
24	8.904	1184	1193	1205	rBV	704004	1490055	71.26%	6.116%
25	8.998	1205	1209	1215	rVB4	25346	48175	2.30%	0.198%
26	9.139	1225	1233	1237	rBV5	29411	66745	3.19%	0.274%
27	9.186	1237	1241	1247	rVB4	16691	30608	1.46%	0.126%
28	9.357	1262	1270	1282	rBV6	109025	325805	15.58%	1.337%
29	9.463	1282	1288	1294	rVB6	14215	33790	1.62%	0.139%
30	9.533	1294	1300	1305	rBV3	21419	49183	2.35%	0.202%
31	9.674	1313	1324	1330	rBV4	56946	133820	6.40%	0.549%
32	9.816	1342	1348	1358	rVB	197053	408712	19.54%	1.678%
33	9.951	1358	1371	1384	rBV2	265793	620901	29.69%	2.549%
34	10.139	1395	1403	1409	rVB4	52861	103925	4.97%	0.427%
35	10.204	1409	1414	1419	rBV2	21977	35275	1.69%	0.145%
36	10.263	1419	1424	1427	rVV5	24249	48116	2.30%	0.197%

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37	10.304	1427	1431	1437	rVV3	52152	93629	4.48%	0.384%
38	10.380	1437	1444	1458	rVV	1125474	2091145	100.00%	8.583%
39	10.580	1466	1478	1484	rBV3	162860	401887	19.22%	1.650%
40	10.657	1484	1491	1497	rVB2	152158	262075	12.53%	1.076%
41	10.716	1497	1501	1507	rVB5	32261	52116	2.49%	0.214%
42	10.798	1507	1515	1525	rVB4	175680	384850	18.40%	1.580%
43	10.880	1525	1529	1534	rBV7	17392	36646	1.75%	0.150%
44	11.068	1555	1561	1566	rVV3	39097	71714	3.43%	0.294%
45	11.198	1579	1583	1588	rVB4	35004	57324	2.74%	0.235%
46	11.251	1588	1592	1597	rBV4	15897	29385	1.41%	0.121%
47	11.345	1603	1608	1611	rBV5	15946	26461	1.27%	0.109%
48	11.386	1611	1615	1622	rVB3	35651	61411	2.94%	0.252%
49	11.604	1646	1652	1655	rBV8	16925	31016	1.48%	0.127%
50	11.686	1659	1666	1673	rBV	1114363	1952443	93.37%	8.014%
51	11.774	1678	1681	1686	rVB2	16324	30454	1.46%	0.125%
52	11.933	1701	1708	1712	rVB9	30231	57373	2.74%	0.235%
53	12.198	1748	1753	1759	rVV8	12109	28573	1.37%	0.117%
54	12.392	1779	1786	1790	rBV7	14653	24325	1.16%	0.100%
55	12.521	1801	1808	1814	rBV	128355	225456	10.78%	0.925%
56	12.674	1827	1834	1843	rVB	923375	1527954	73.07%	6.272%
57	12.862	1858	1866	1871	rVB	74948	134821	6.45%	0.553%
58	12.945	1877	1880	1886	rBV8	10172	22132	1.06%	0.091%
59	13.168	1911	1918	1922	rVB4	22117	38410	1.84%	0.158%
60	13.262	1931	1934	1946	rVB4	15030	38117	1.82%	0.156%
61	13.421	1955	1961	1970	rVB2	98090	174393	8.34%	0.716%
62	13.615	1984	1994	2008	rVV	1116243	1910188	91.35%	7.840%
63	13.709	2008	2010	2014	rVV3	14984	21247	1.02%	0.087%
64	13.780	2017	2022	2023	rVV4	27590	38088	1.82%	0.156%
65	13.821	2023	2029	2035	rVV	322792	579655	27.72%	2.379%
66	13.862	2035	2036	2040	rVV4	24855	23825	1.14%	0.098%
67	13.945	2044	2050	2057	rBV4	80544	135273	6.47%	0.555%
68	14.009	2057	2061	2068	rBV2	29903	49394	2.36%	0.203%
69	14.092	2068	2075	2082	rBV	138012	233998	11.19%	0.960%
70	14.274	2100	2106	2111	rVB	96913	164578	7.87%	0.676%
71	14.345	2111	2118	2124	rVV8	47978	104745	5.01%	0.430%
72	14.409	2124	2129	2133	rVV2	63583	93529	4.47%	0.384%
73	14.480	2134	2141	2148	rVB5	33933	71516	3.42%	0.294%
74	14.598	2156	2161	2166	rVB3	44591	65641	3.14%	0.269%
75	14.709	2174	2180	2184	rVB	50403	84316	4.03%	0.346%
76	14.762	2184	2189	2196	rVB3	61518	108405	5.18%	0.445%

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Title : SW846 8260

77	14.939	2212	2219	2226	rBV4	32812	60756	2.91%	0.249%
78	15.127	2247	2251	2256	rVV6	17179	32185	1.54%	0.132%
79	15.221	2260	2267	2278	rVB6	36143	117923	5.64%	0.484%
80	15.492	2308	2313	2319	rBV4	20388	41165	1.97%	0.169%
81	15.580	2320	2328	2333	rVB8	27937	57998	2.77%	0.238%
82	16.039	2399	2406	2412	rBV4	30030	65905	3.15%	0.271%
83	16.474	2476	2480	2485	rVB4	13985	23487	1.12%	0.096%
84	16.733	2515	2524	2525	rBV6	17342	25546	1.22%	0.105%

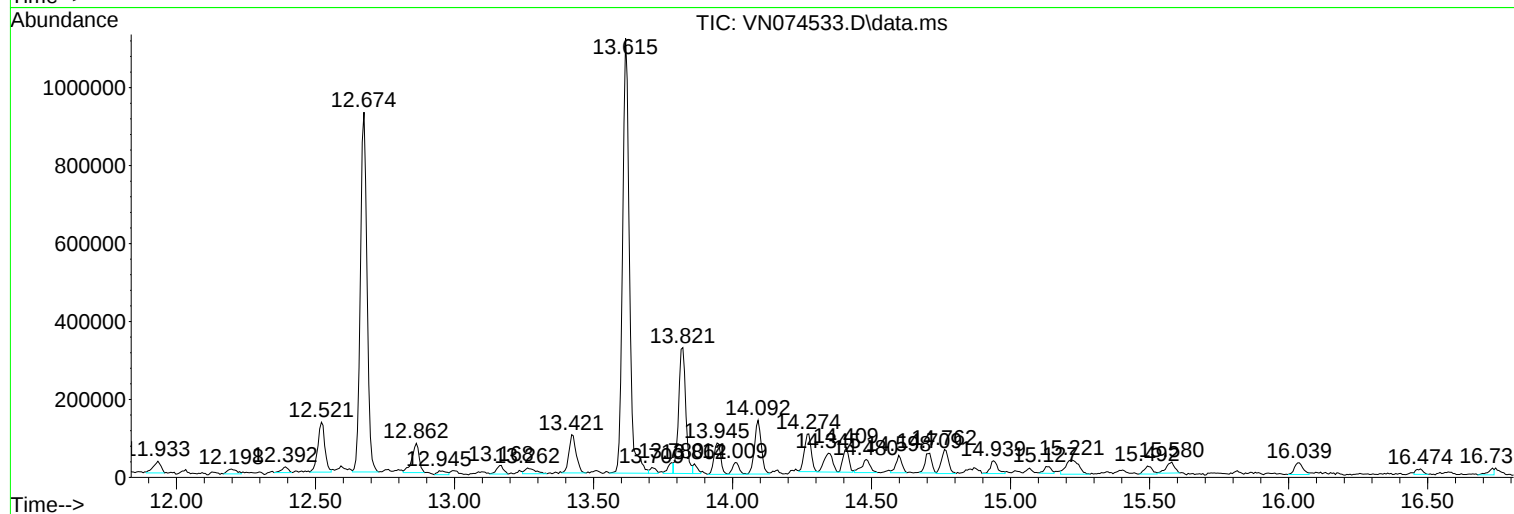
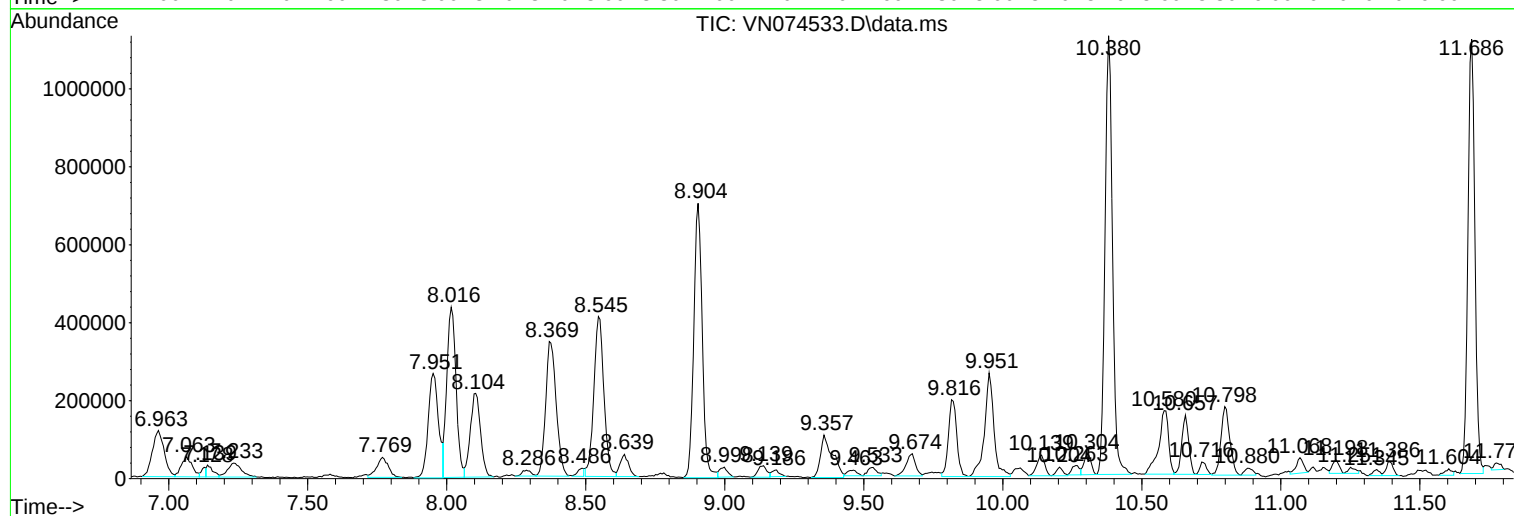
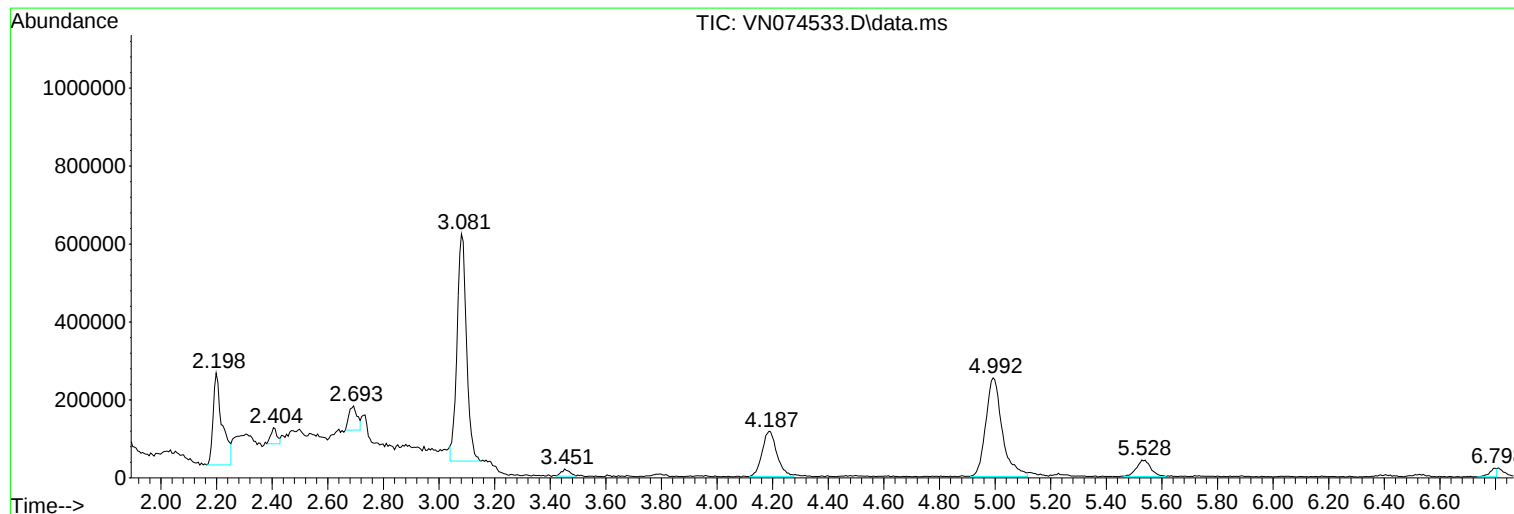
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



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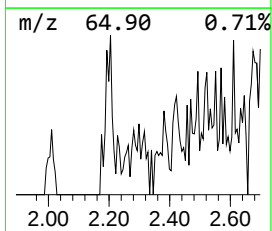
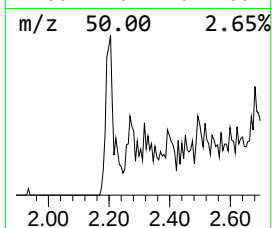
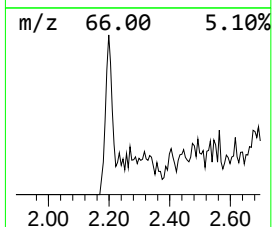
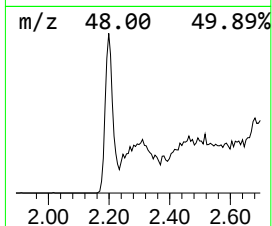
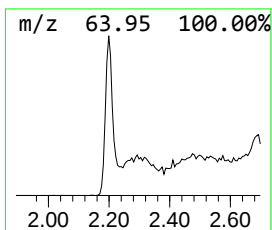
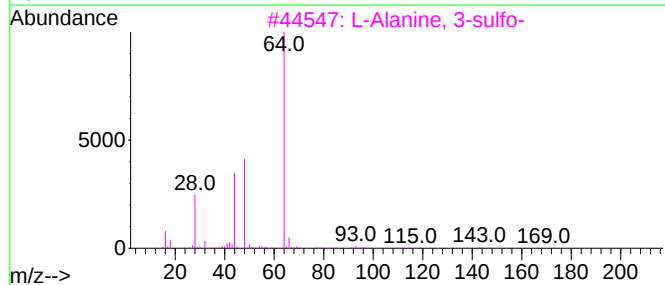
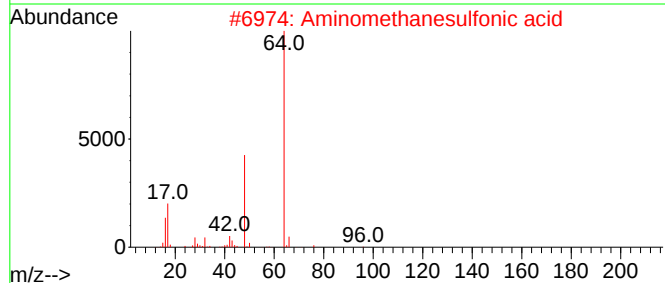
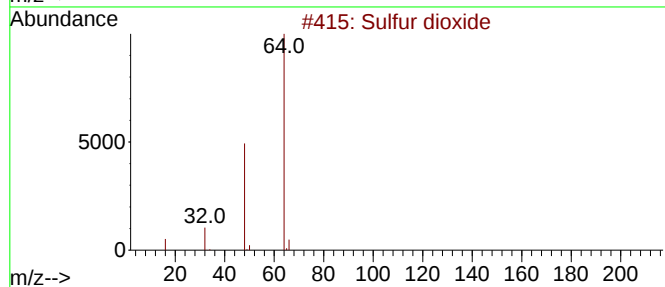
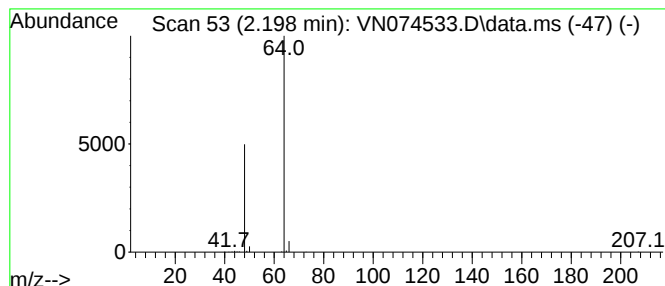
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.198	26.87 ug/l	536038	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			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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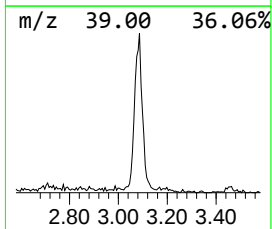
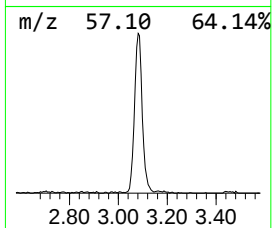
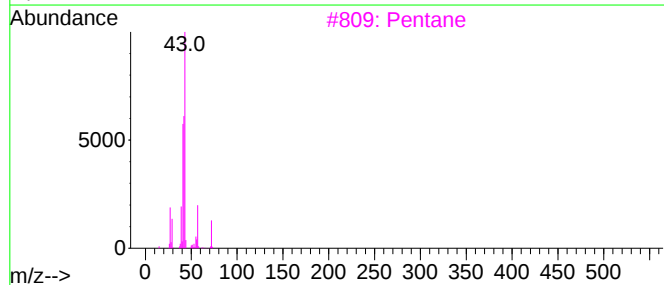
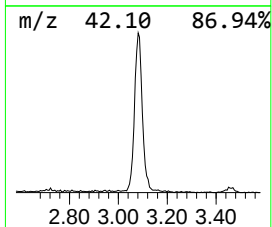
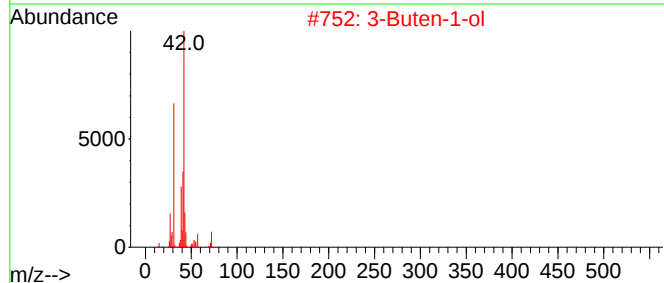
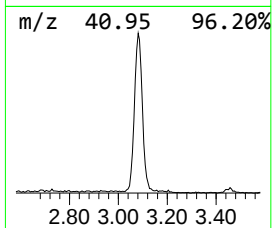
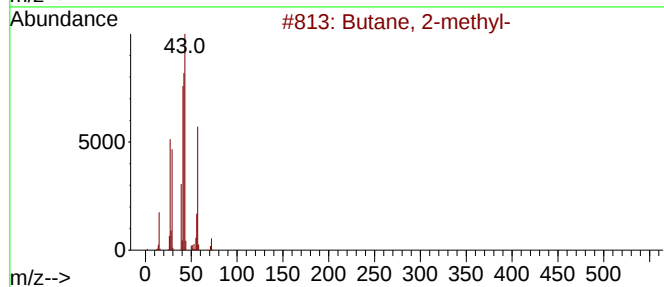
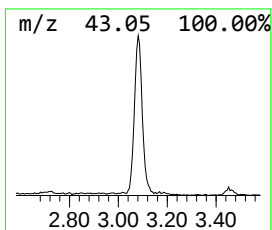
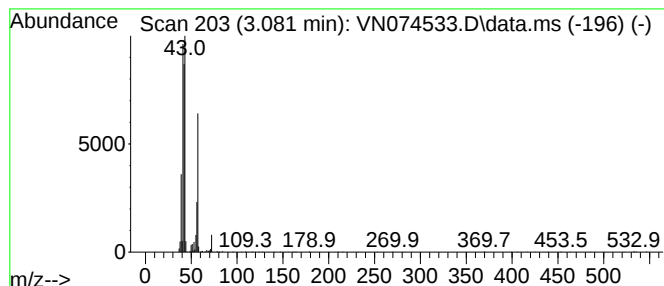
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	68.79 ug/l	1372440	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
5			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12



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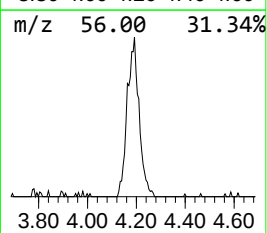
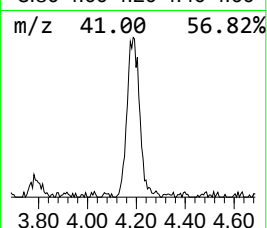
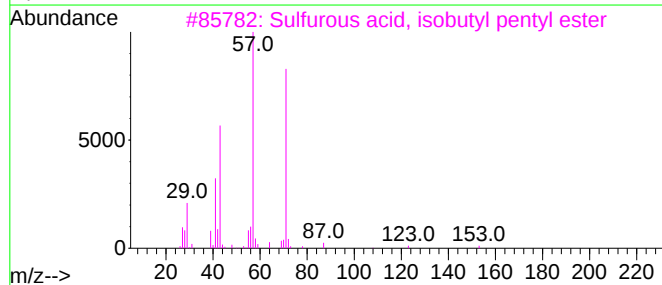
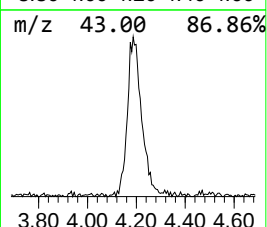
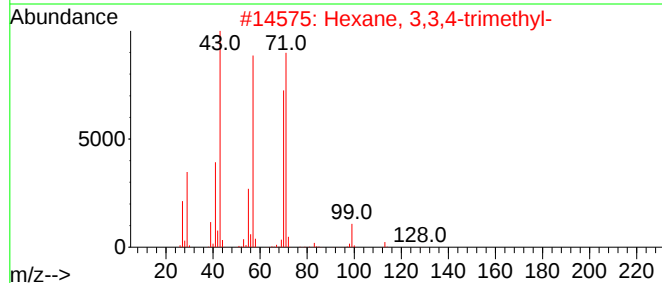
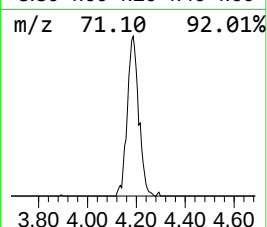
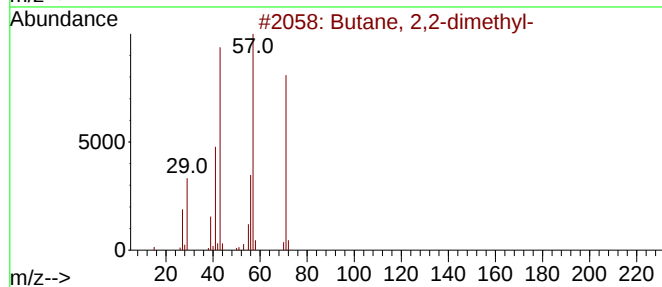
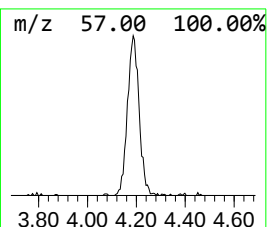
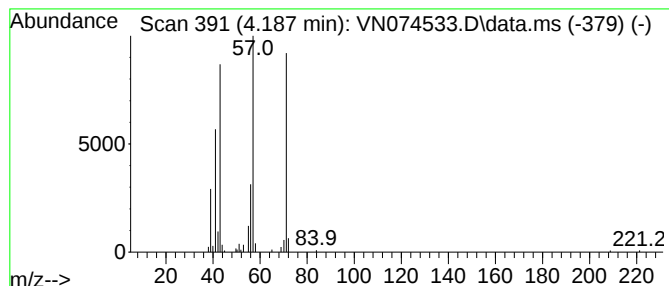
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.187	21.50 ug/l	428901	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	83
2			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	72
3			Sulfurous acid, isobutyl pentyl ...	208	C9H20O3S	1000309-13-8	72
4			Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	72
5			4-Heptanone, 3-methyl-	128	C8H16O	015726-15-5	56



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MW-50

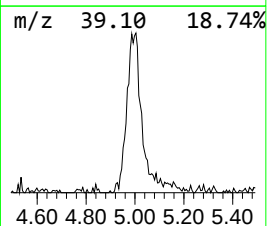
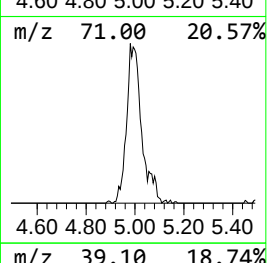
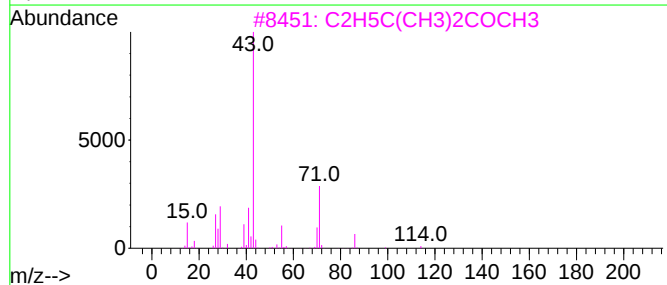
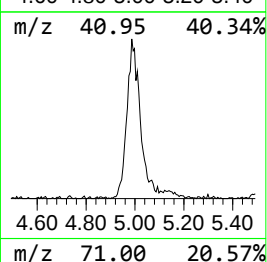
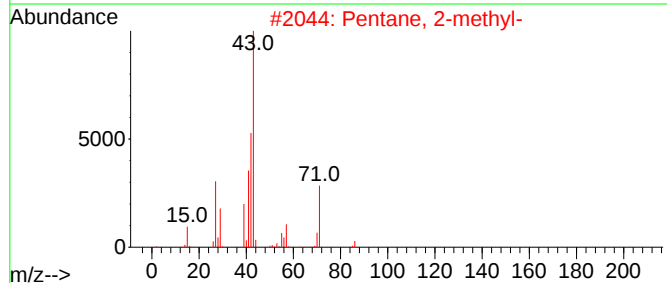
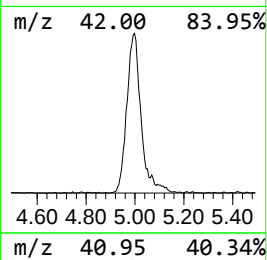
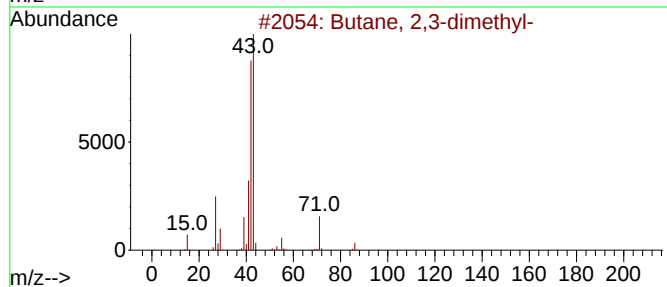
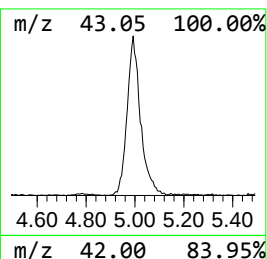
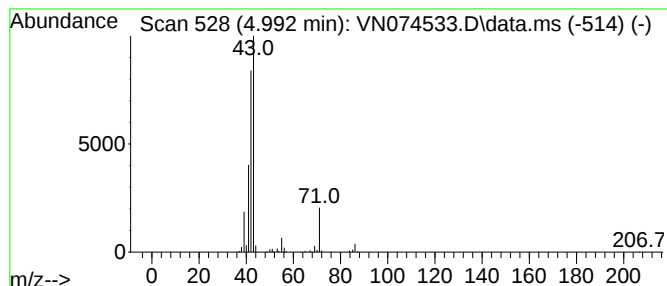
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Quant Title : SW846 8260

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

Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.992	52.08 ug/l	1039010	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	47
3			C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	9
4			Butanoic acid, 4-hydroxy-	104	C4H8O3	000591-81-1	9
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074533.D
Acq On : 17 Sep 2022 01:19
Operator : JC\MD
Sample : N4549-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-50

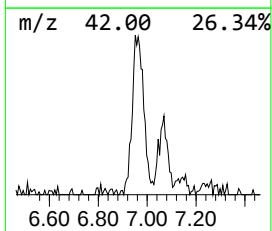
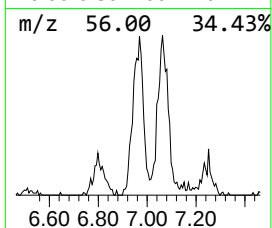
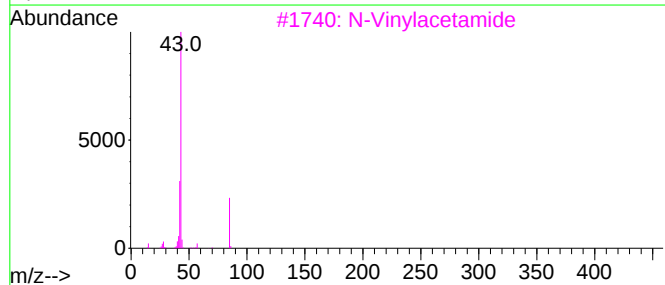
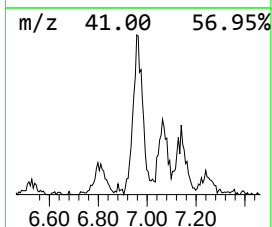
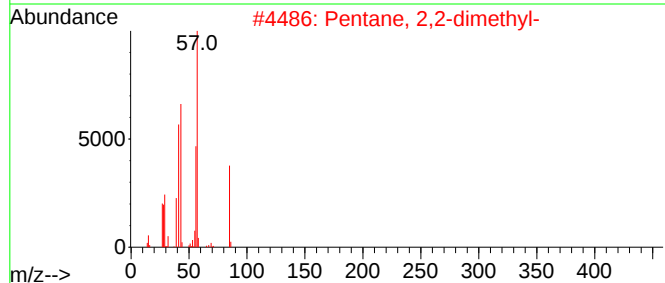
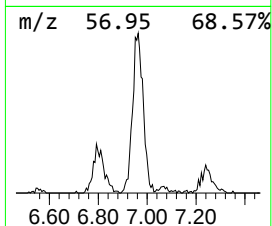
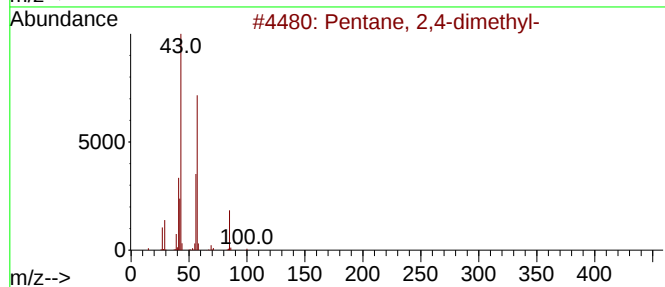
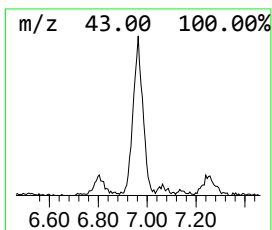
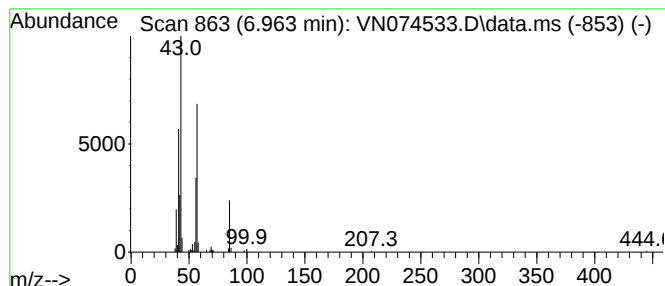
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.963	17.53 ug/l	349785	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50
3			N-Vinylacetamide	85	C4H7NO	005202-78-8	47
4			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	45
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074533.D
Acq On : 17 Sep 2022 01:19
Operator : JC\MD
Sample : N4549-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-50

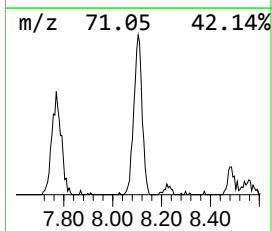
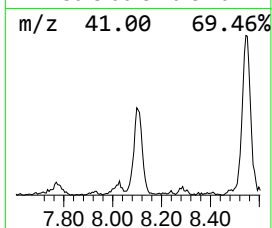
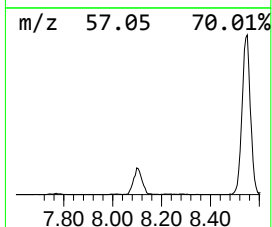
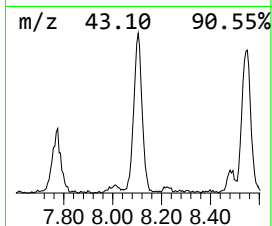
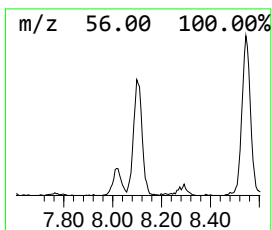
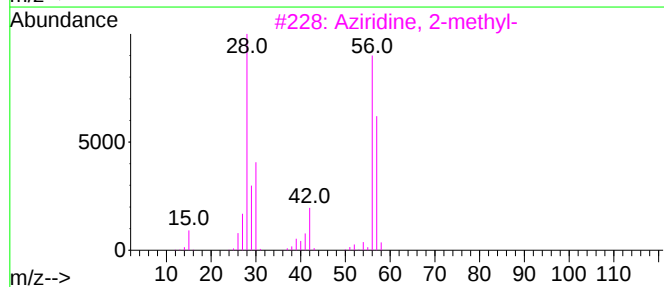
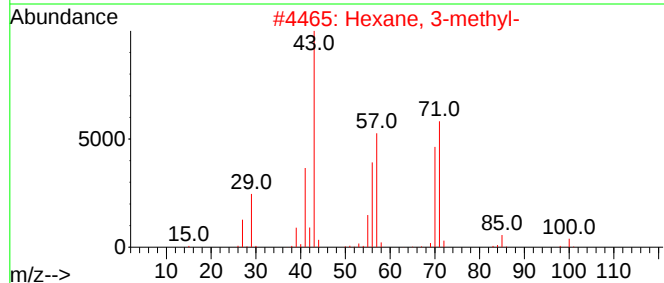
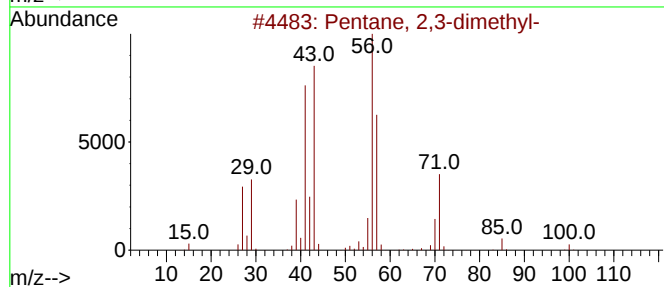
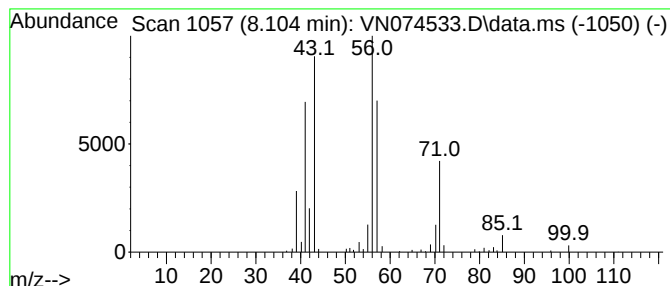
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	27.33 ug/l	545292	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	95
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	43
3			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43
4			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	40
5			Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074533.D
Acq On : 17 Sep 2022 01:19
Operator : JC\MD
Sample : N4549-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-50

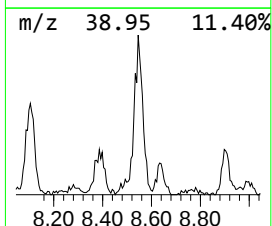
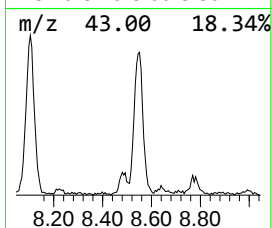
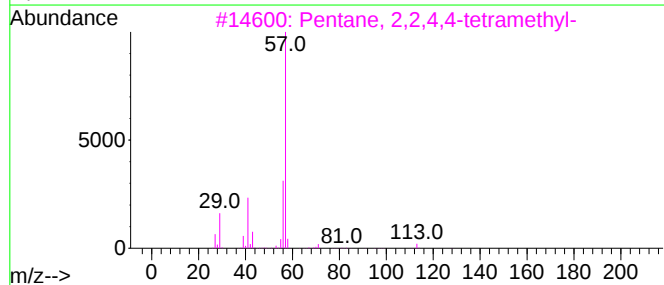
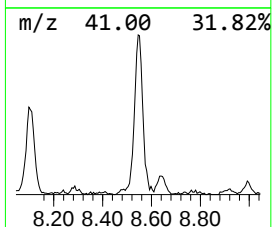
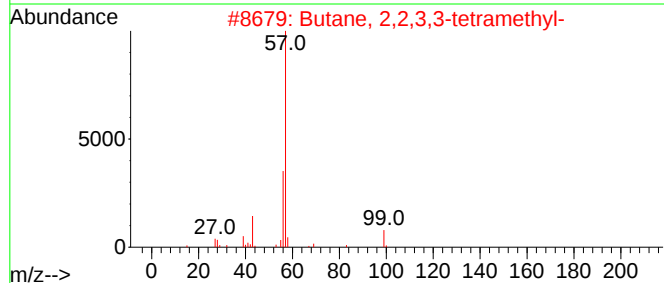
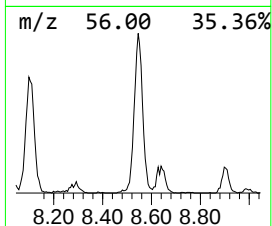
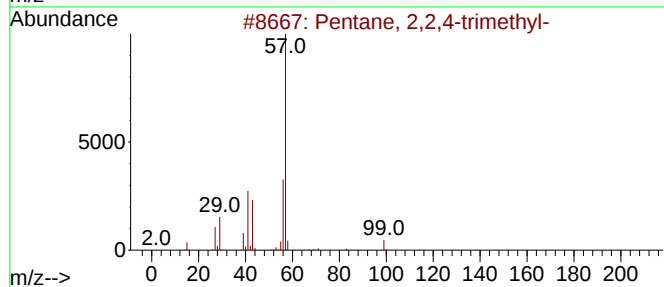
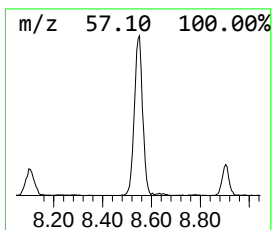
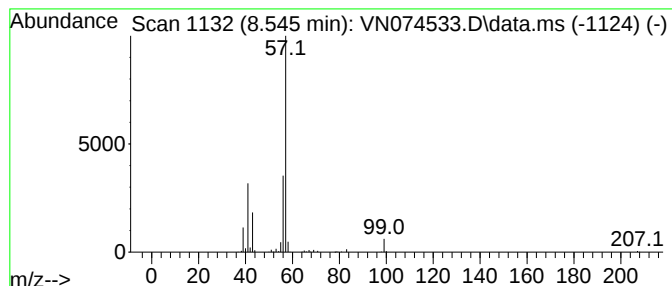
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,2,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	34.58 ug/l	1030470	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
4			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	59
5			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074533.D
Acq On : 17 Sep 2022 01:19
Operator : JC\MD
Sample : N4549-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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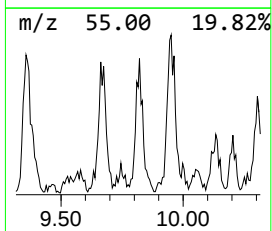
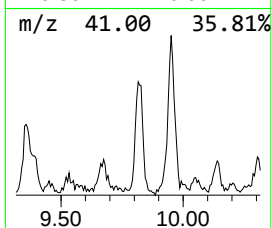
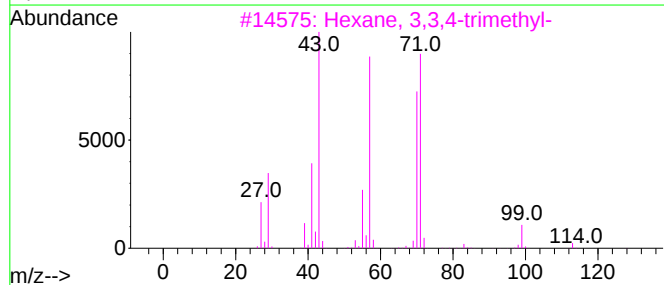
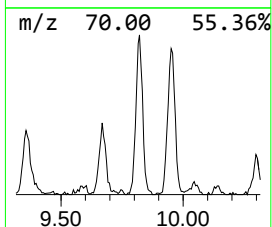
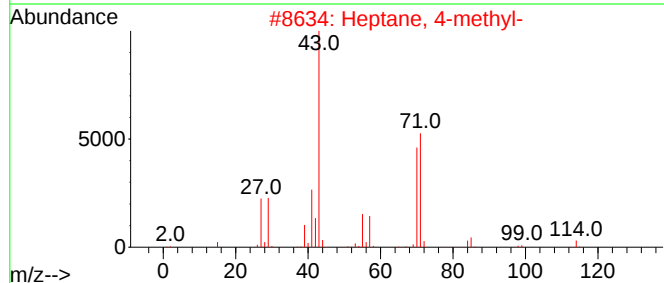
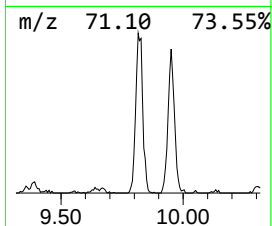
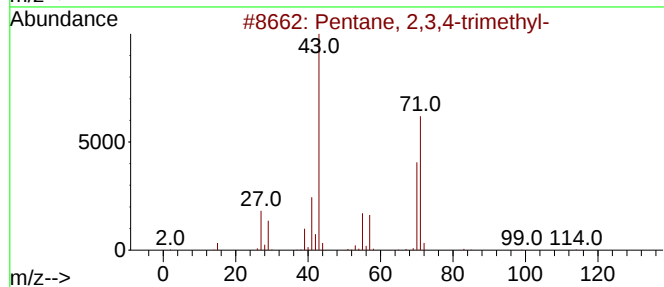
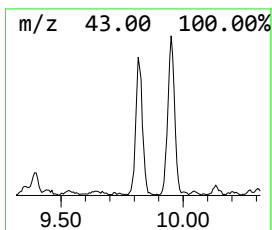
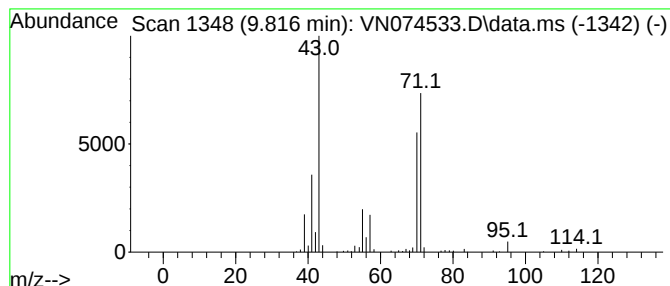
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Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3,4-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	13.71 ug/l	408712	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	78
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	72
3			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	72
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	72
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074533.D
Acq On : 17 Sep 2022 01:19
Operator : JC\MD
Sample : N4549-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-50

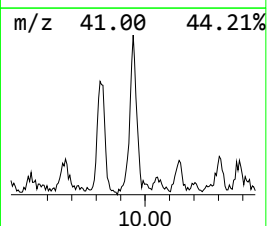
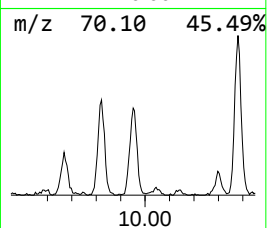
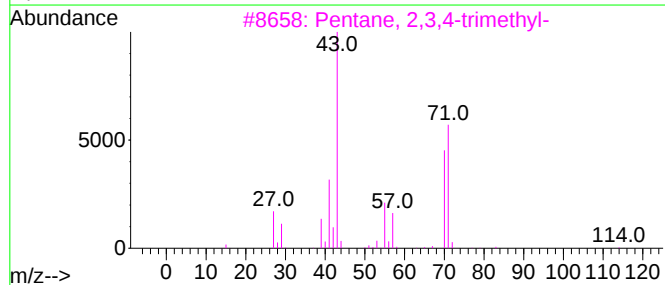
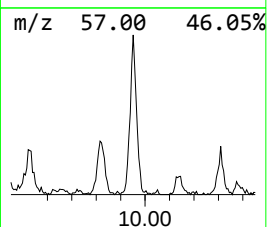
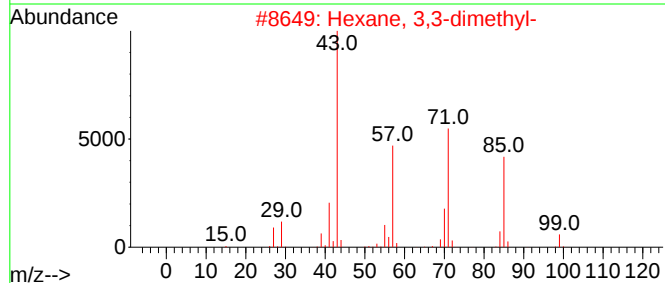
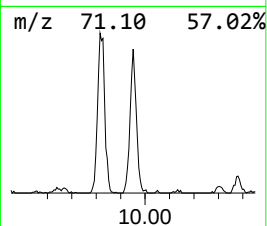
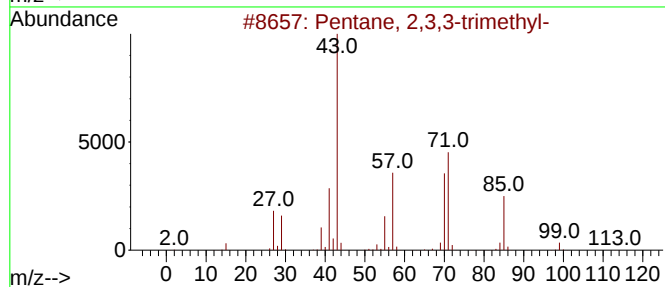
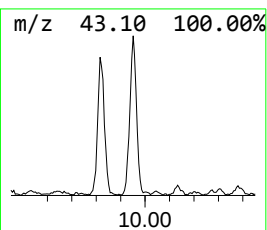
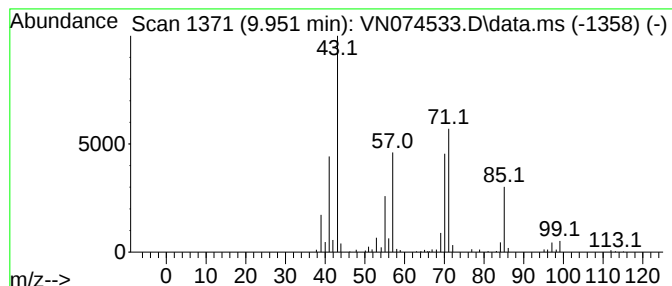
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Quant Title : SW846 8260

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

Peak Number 9 Pentane, 2,3,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.951	20.83 ug/l	620901	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	78
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074533.D
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Operator : JC\MD
Sample : N4549-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-50

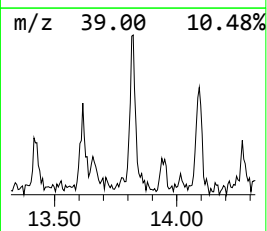
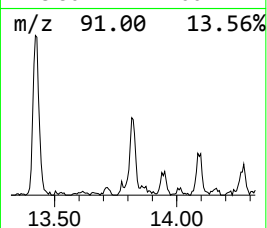
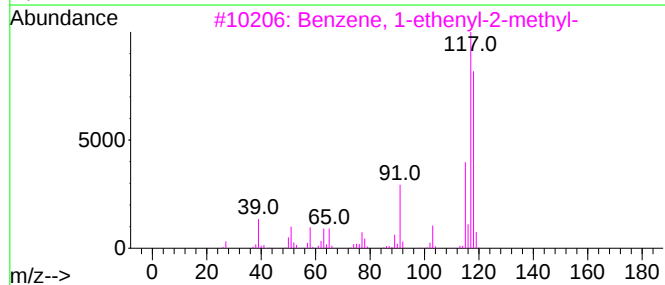
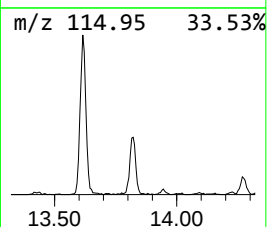
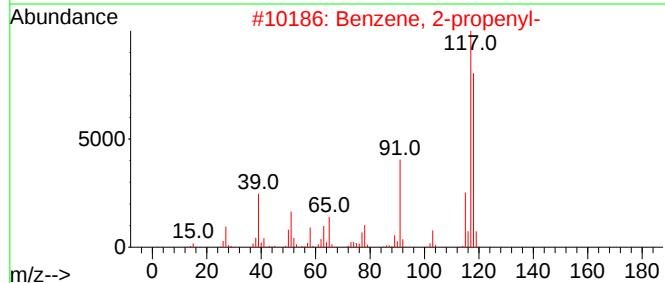
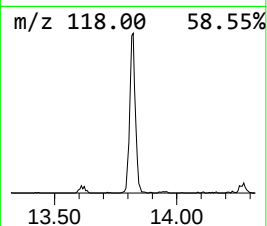
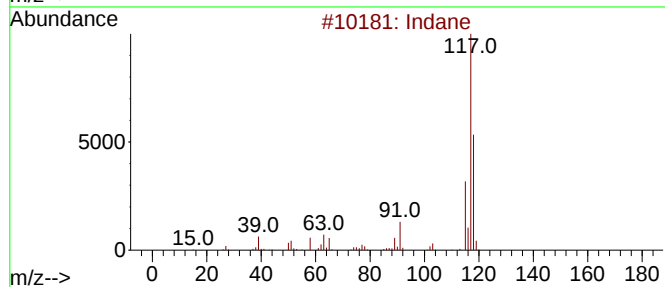
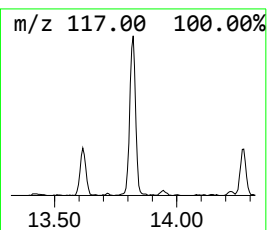
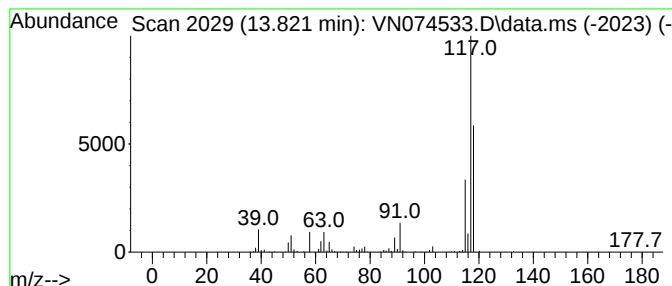
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	15.17 ug/l	579655	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	83
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	72
4			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	64
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074533.D
Acq On : 17 Sep 2022 01:19
Operator : JC\MD
Sample : N4549-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-50

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.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
Sulfur dioxide	2.198	26.9	ug/l	536038	1	8.016	997595	50.0
Butane, 2-methyl-	3.081	68.8	ug/l	1372440	1	8.016	997595	50.0
Butane, 2,2-dim...	4.187	21.5	ug/l	428901	1	8.016	997595	50.0
Butane, 2,3-dim...	4.992	52.1	ug/l	1039010	1	8.016	997595	50.0
Pentane, 2,4-di...	6.963	17.5	ug/l	349785	1	8.016	997595	50.0
Pentane, 2,3-di...	8.104	27.3	ug/l	545292	1	8.016	997595	50.0
Pentane, 2,2,4-...	8.545	34.6	ug/l	1030470	2	8.904	1490060	50.0
Pentane, 2,3,4-...	9.816	13.7	ug/l	408712	2	8.904	1490060	50.0
Pentane, 2,3,3-...	9.951	20.8	ug/l	620901	2	8.904	1490060	50.0
Indane	13.821	15.2	ug/l	579655	4	13.615	1910190	50.0