

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032622\
 Data File : VN071580.D
 Acq On : 26 Mar 2022 18:14
 Operator : JC\MD
 Sample : N2131-04
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-4

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\82N032522W.M
 Title : SW846 8260

Signal : TIC: VN071580.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.134	181	195	226	rVB	3929994	9048536	9.85%	1.594%
2	3.510	250	259	277	rVB2	1087593	2803692	3.05%	0.494%
3	3.716	283	294	308	rBV	467796	1146645	1.25%	0.202%
4	3.993	333	341	359	rVB	487240	1331522	1.45%	0.235%
5	5.081	515	526	530	rVV	667060	2218825	2.42%	0.391%
6	5.151	530	538	576	rVB6	1598253	8647709	9.42%	1.523%
7	5.616	603	617	635	rBV	1431011	4952120	5.39%	0.872%
8	6.122	689	703	720	rBV	585954	1812000	1.97%	0.319%
9	6.469	755	762	774	rVB2	383513	1150938	1.25%	0.203%
10	7.045	849	860	867	rBV	381557	1124143	1.22%	0.198%
11	7.145	867	877	899	rVB	2887992	8657454	9.43%	1.525%
12	8.016	1016	1025	1029	rBV	495465	1191000	1.30%	0.210%
13	8.086	1029	1037	1045	rVV3	2109545	5914287	6.44%	1.042%
14	8.175	1045	1052	1063	rVB	1090675	2813703	3.06%	0.496%
15	8.292	1063	1072	1079	rBV	601119	1416389	1.54%	0.249%
16	8.457	1089	1100	1110	rBV2	3263544	8215818	8.95%	1.447%
17	8.575	1110	1120	1122	rBV4	839366	1942704	2.12%	0.342%
18	8.963	1175	1186	1199	rBV3	1760904	4149443	4.52%	0.731%
19	9.457	1254	1270	1276	rBV2	1085287	3336639	3.63%	0.588%
20	9.880	1336	1342	1350	rVB	504540	1023544	1.11%	0.180%
21	9.969	1350	1357	1360	rBV	564267	1037762	1.13%	0.183%
22	10.010	1360	1364	1371	rVB	865840	1701232	1.85%	0.300%
23	10.439	1429	1437	1441	rBV	2366734	4360196	4.75%	0.768%
24	10.504	1441	1448	1461	rVB	18668909	34189762	37.23%	6.021%
25	11.739	1651	1658	1666	rBV	2243418	3894009	4.24%	0.686%
26	11.839	1667	1675	1686	rVV2	37654271	65178760	70.97%	11.479%
27	11.957	1686	1695	1707	rVB2	47528397	88144077	95.97%	15.524%
28	12.274	1738	1749	1761	rBV	6069353	9964196	10.85%	1.755%
29	12.574	1790	1800	1808	rBV	3072102	4886588	5.32%	0.861%
30	12.727	1818	1826	1835	rBV	1775360	2936457	3.20%	0.517%
31	12.916	1850	1858	1864	rBV	8015237	12667385	13.79%	2.231%
32	13.010	1864	1874	1879	rVV	12513092	23115246	25.17%	4.071%
33	13.057	1879	1882	1901	rVB	2013670	2923011	3.18%	0.515%
34	13.216	1901	1909	1918	rBV	2575854	4227681	4.60%	0.745%
35	13.363	1924	1934	1948	rBV2	55147473	91845937	100.00%	16.176%
36	13.492	1948	1956	1962	rVB3	861419	2067070	2.25%	0.364%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	13.704	1981	1992	2000	rBV2	11941873	23002945	25.05%	4.051%
38	13.833	2008	2014	2016	rBV	3287619	4760444	5.18%	0.838%
39	13.874	2016	2021	2025	rVV	11377317	19632084	21.38%	3.458%
40	13.915	2025	2028	2037	rVV3	3087253	5614613	6.11%	0.989%
41	13.998	2037	2042	2047	rVV	619953	959022	1.04%	0.169%
42	14.057	2047	2052	2058	rVV2	1364184	2442928	2.66%	0.430%
43	14.127	2058	2064	2067	rVV	4649352	8160136	8.88%	1.437%
44	14.157	2067	2069	2074	rVV	3692066	4746526	5.17%	0.836%
45	14.215	2074	2079	2084	rVV	7494269	11609399	12.64%	2.045%
46	14.274	2084	2089	2092	rVV	920249	1465870	1.60%	0.258%
47	14.321	2092	2097	2105	rVB2	3376558	5851933	6.37%	1.031%
48	14.457	2114	2120	2125	rBV	1208472	1869586	2.04%	0.329%
49	14.533	2125	2133	2137	rBV	3671268	6393110	6.96%	1.126%
50	14.574	2137	2140	2145	rVB	4992900	6984701	7.60%	1.230%
51	14.804	2174	2179	2184	rBV	3143056	4958480	5.40%	0.873%
52	14.927	2191	2200	2206	rBV3	5369523	11588138	12.62%	2.041%
53	14.986	2206	2210	2217	rVB2	448831	926263	1.01%	0.163%
54	15.080	2219	2226	2234	rBV2	650436	1201627	1.31%	0.212%
55	15.192	2234	2245	2257	rVV3	902864	2849114	3.10%	0.502%
56	15.304	2257	2264	2274	rVB3	670762	1578055	1.72%	0.278%
57	15.504	2290	2298	2306	rVB	6044145	11314616	12.32%	1.993%
58	16.609	2478	2486	2503	rVB	1740726	3849407	4.19%	0.678%

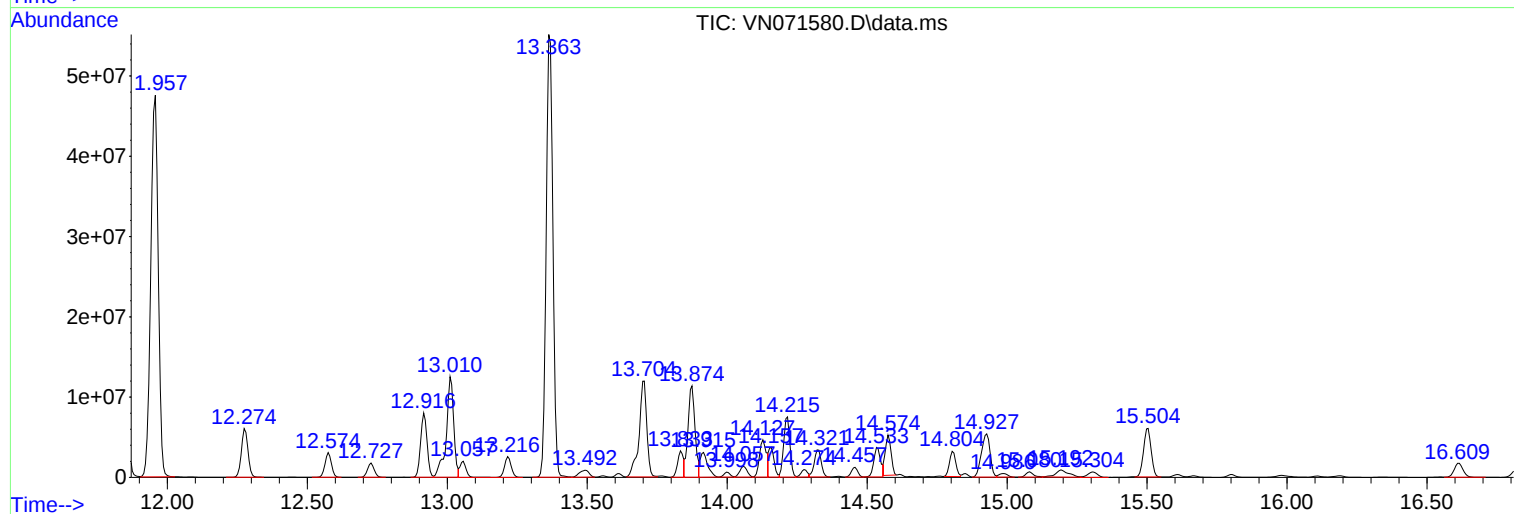
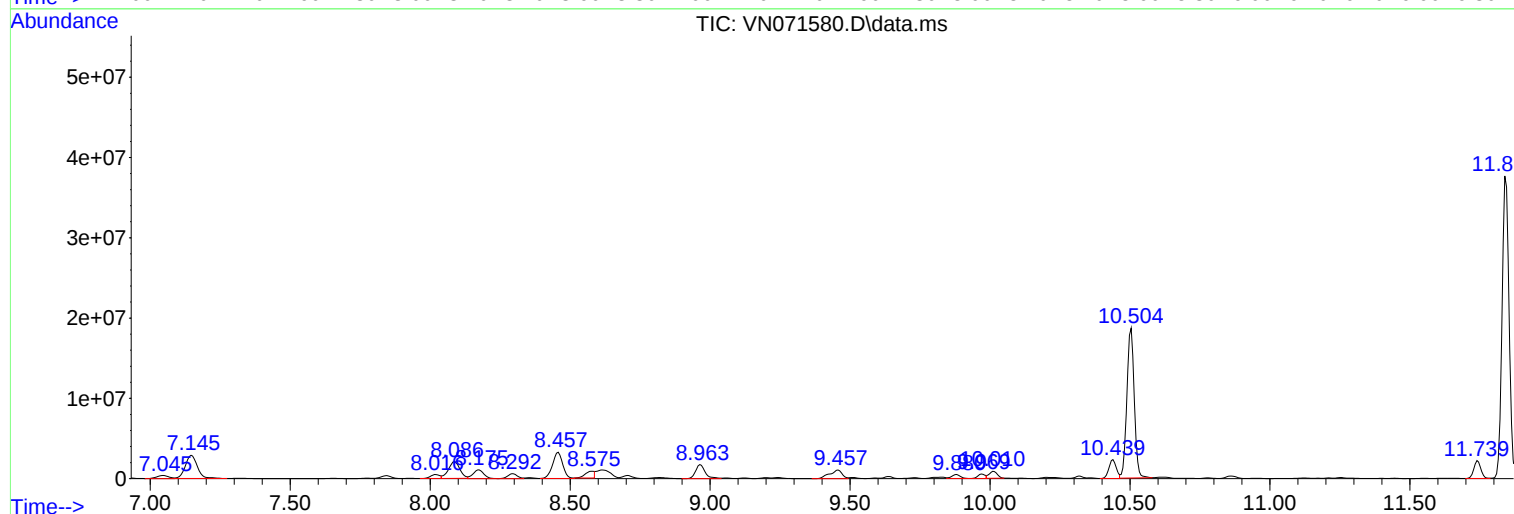
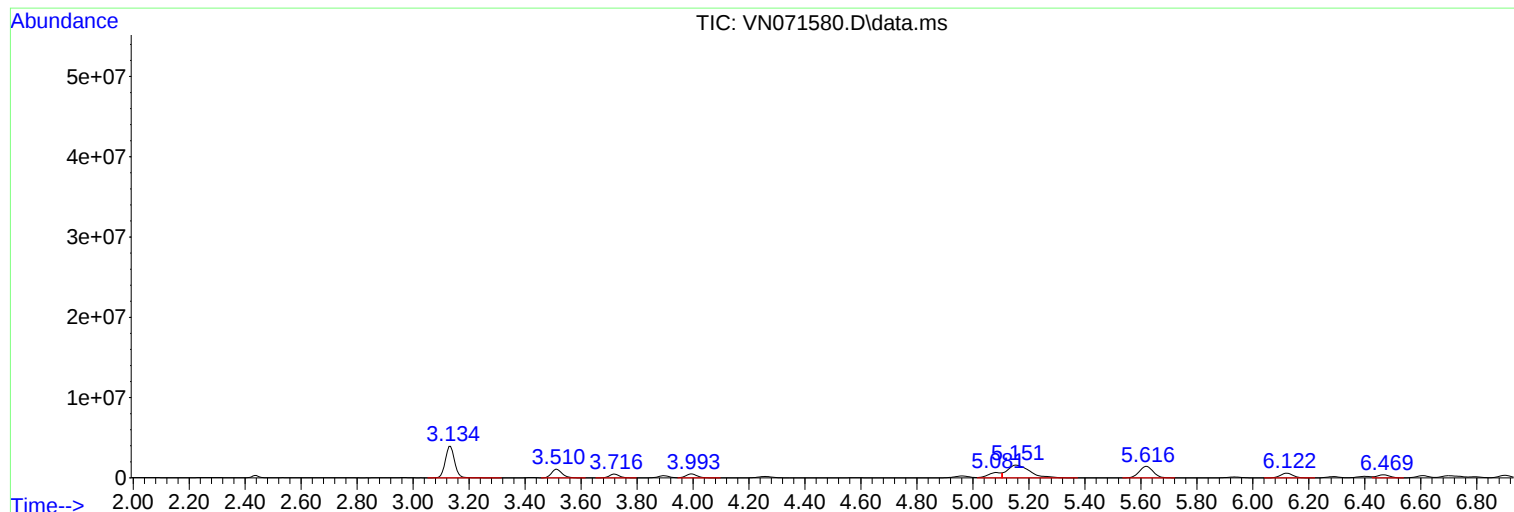
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Instrument :
MSVOA_N
ClientSampleId :
MW-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032522W.M
Quant Title : SW846 8260

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



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Data File : VN071580.D
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-4

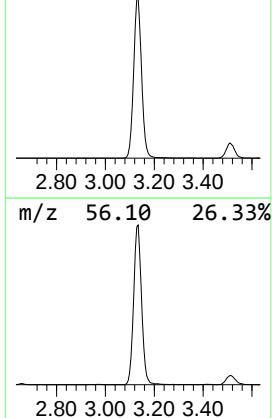
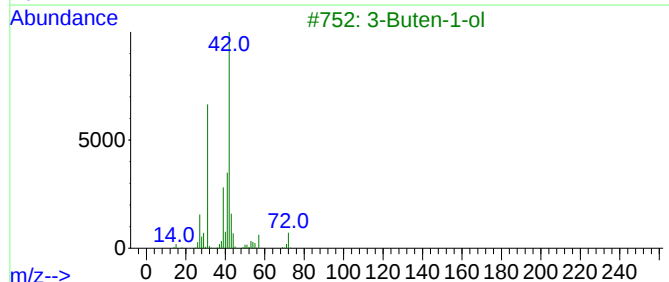
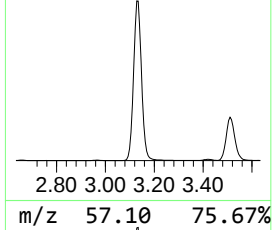
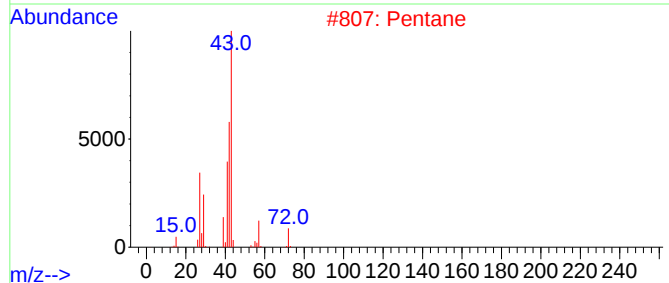
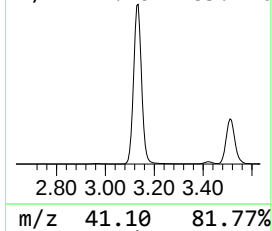
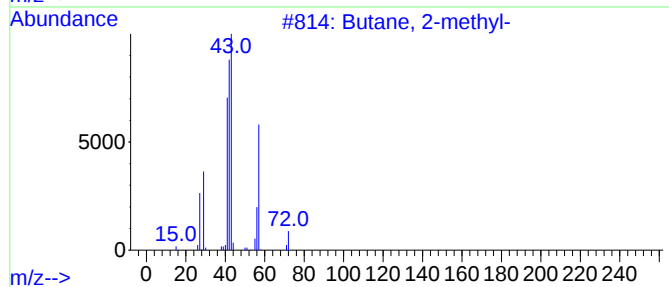
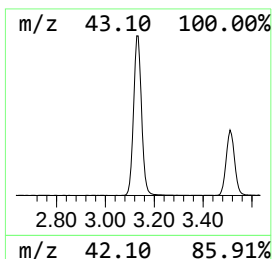
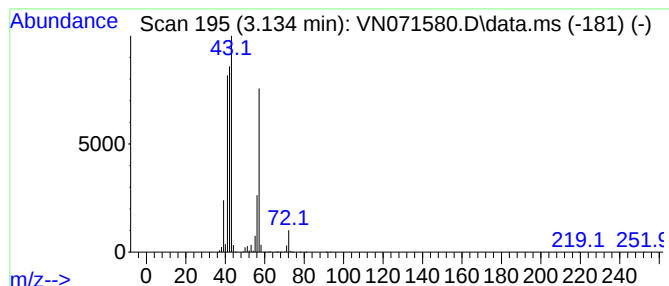
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032522W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	76.50 ug/l	9048540	Pentafluorobenzene	8.081

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	45
3			3-Buten-1-ol	72	C4H8O	000627-27-0	43
4			Butane, 2-nitro-	103	C4H9NO2	000600-24-8	10
5			Azetidine	57	C3H7N	000503-29-7	9



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-4

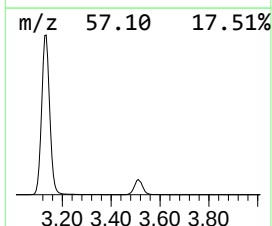
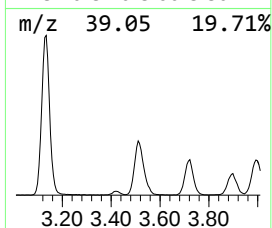
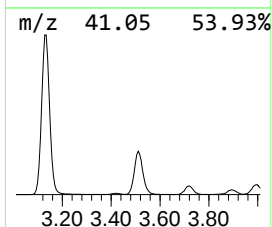
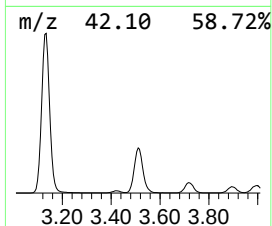
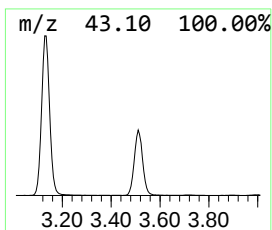
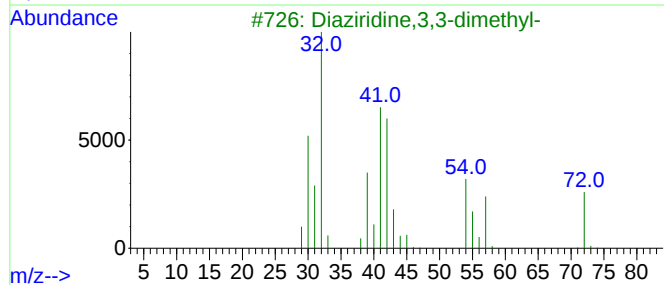
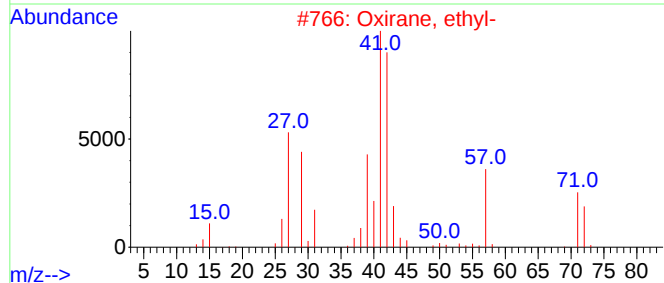
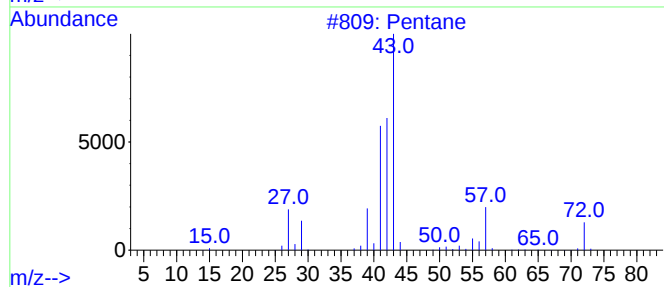
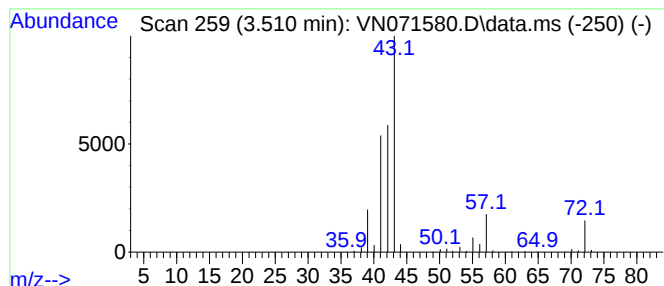
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032522W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.510	23.70 ug/l	2803690	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	43
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	10
5			Tetrahydrofuran	72	C4H8O	000109-99-9	9



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Acq On : 26 Mar 2022 18:14
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Sample : N2131-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-4

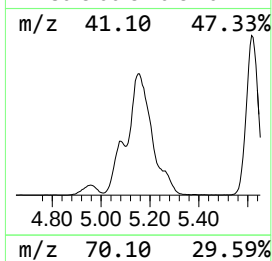
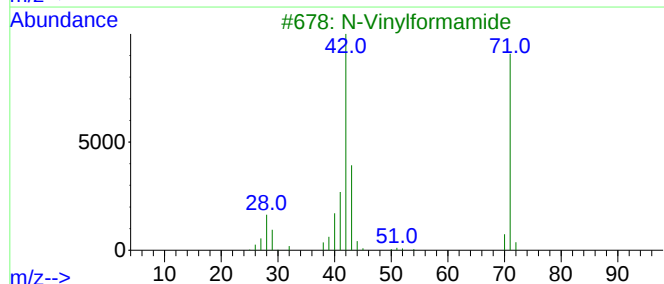
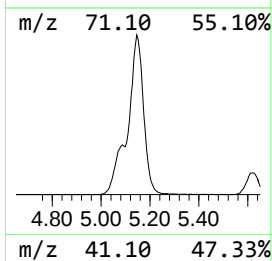
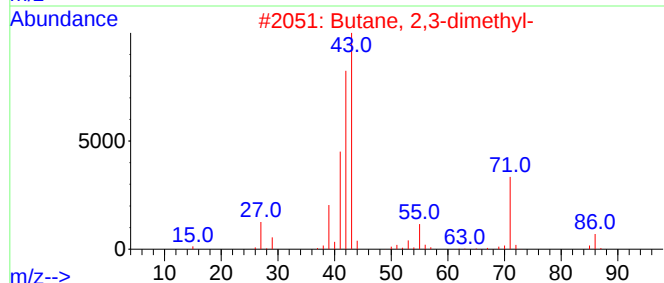
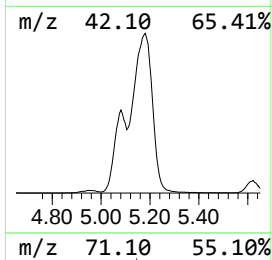
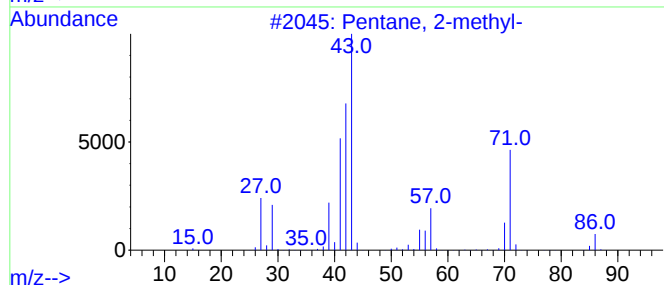
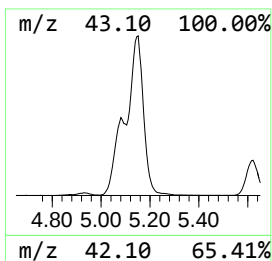
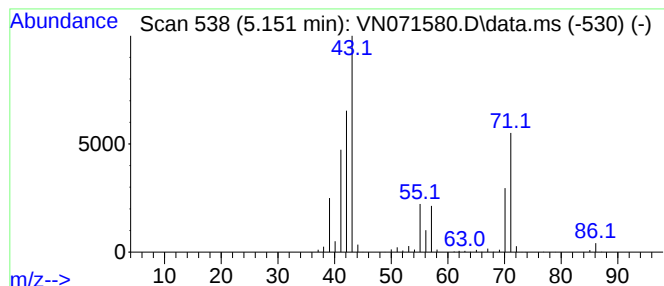
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032522W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	73.11 ug/l	8647710	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	47
3			N-Vinylformamide	71	C3H5NO	013162-05-5	47
4			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	43
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	40



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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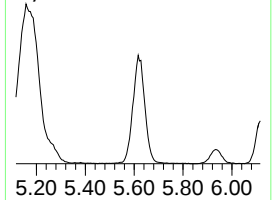
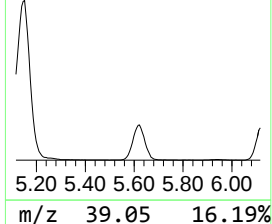
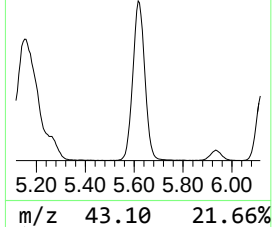
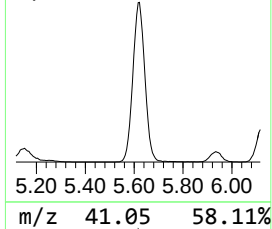
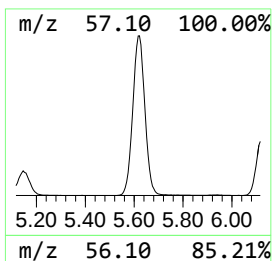
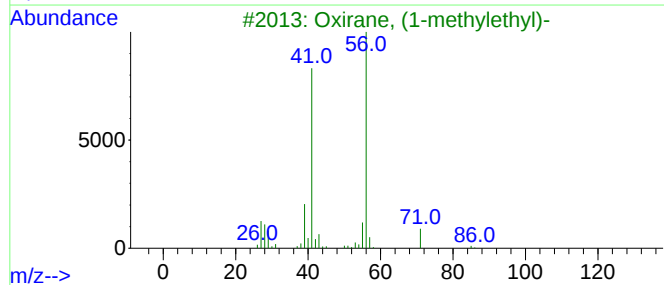
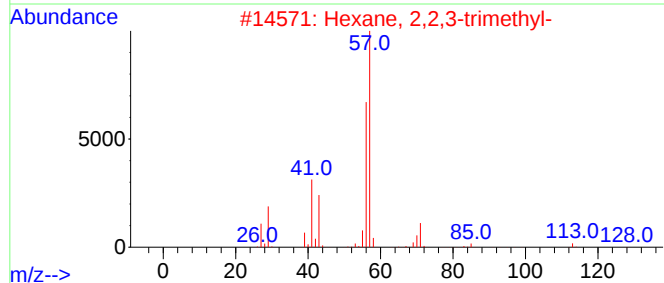
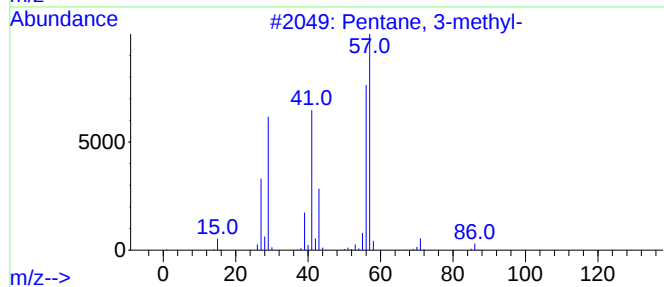
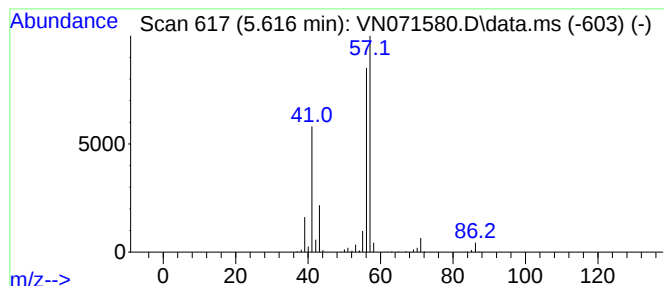
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032522W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.616	41.87 ug/l	4952120	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	83
3			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	64
4			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
5			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	43



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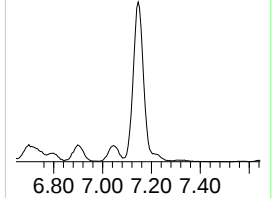
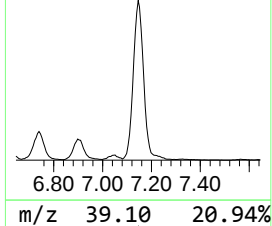
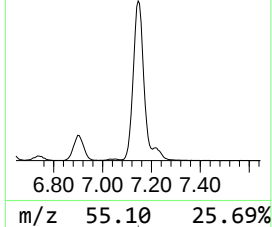
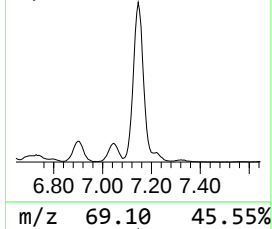
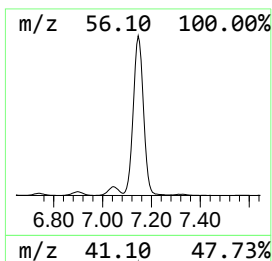
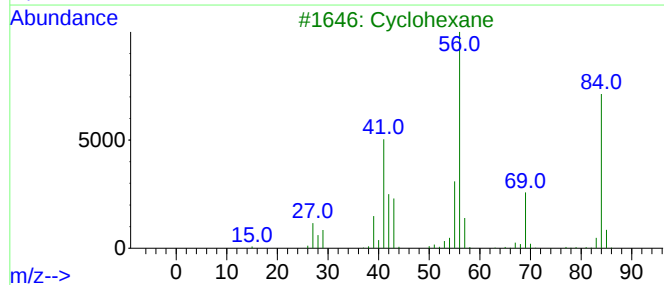
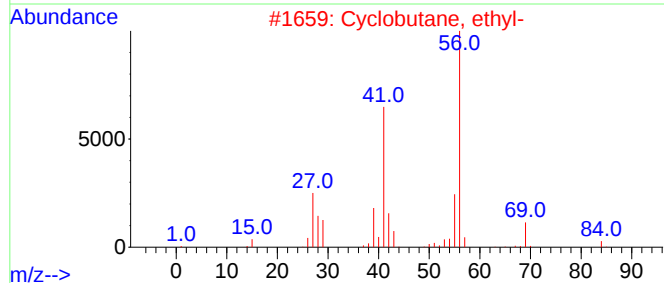
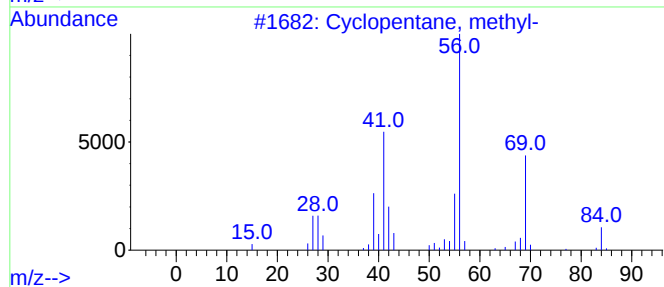
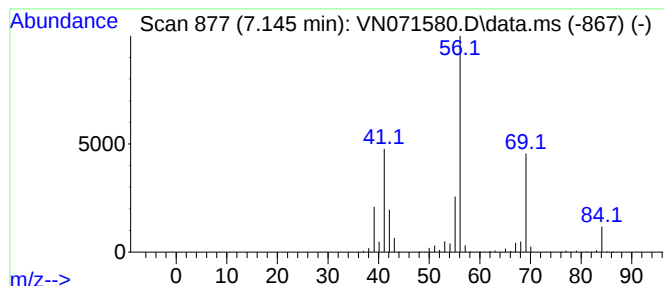
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	73.19 ug/l	8657450	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3			Cyclohexane	84	C6H12	000110-82-7	64
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032622\
Data File : VN071580.D
Acq On : 26 Mar 2022 18:14
Operator : JC\MD
Sample : N2131-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-4

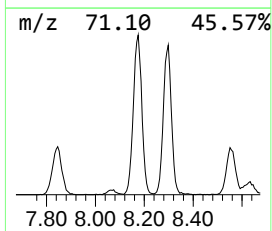
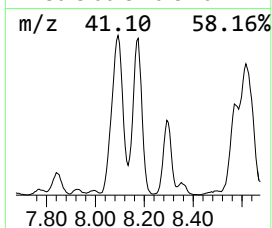
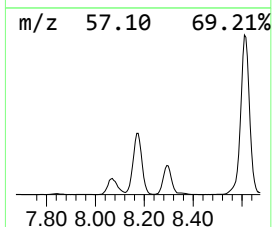
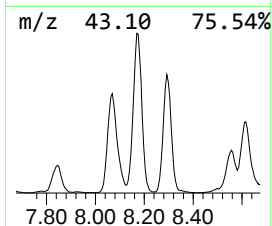
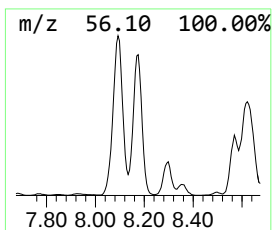
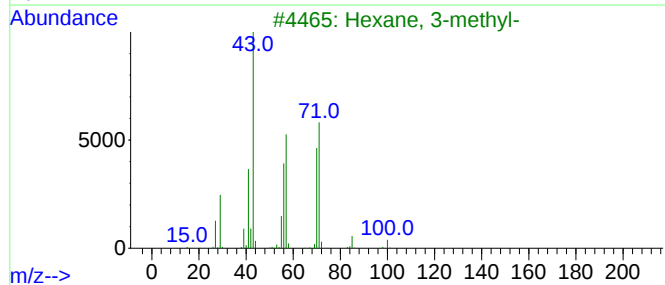
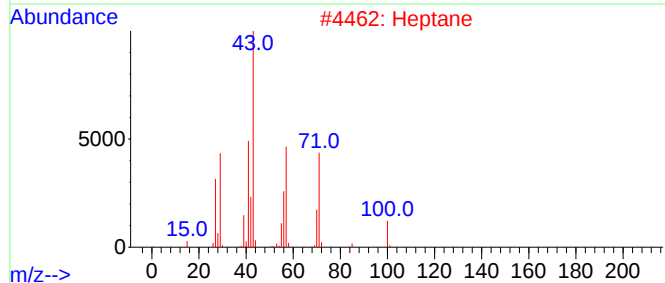
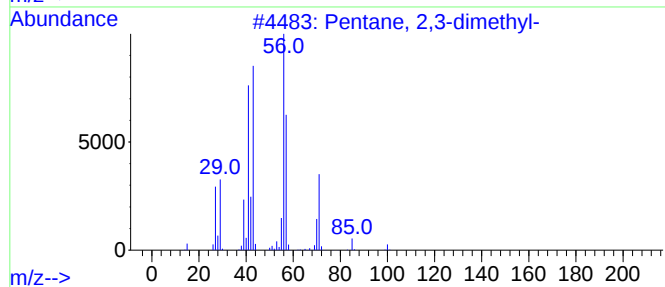
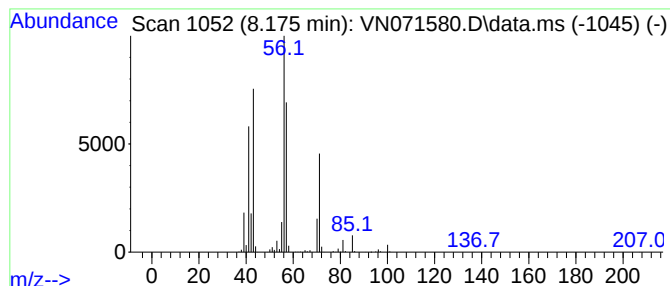
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.175	23.79 ug/l	2813700	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Heptane	100	C7H16	000142-82-5	47
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	43
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
5			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032622\
Data File : VN071580.D
Acq On : 26 Mar 2022 18:14
Operator : JC\MD
Sample : N2131-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-4

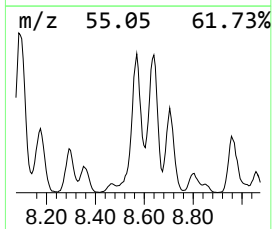
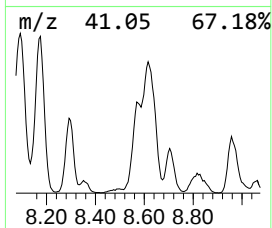
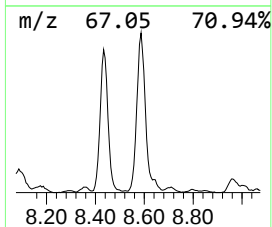
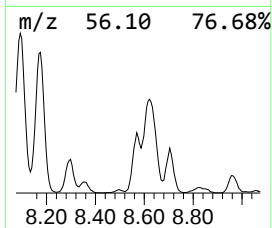
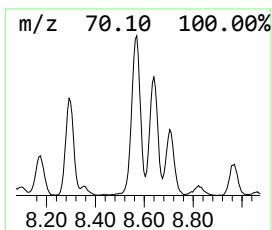
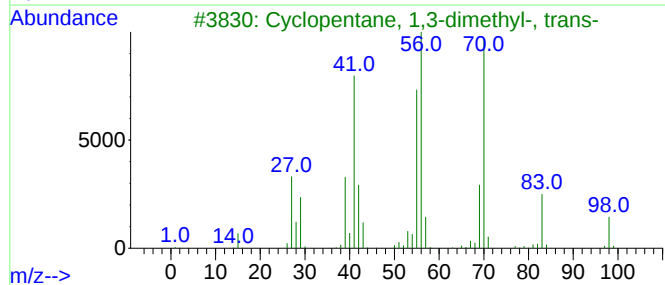
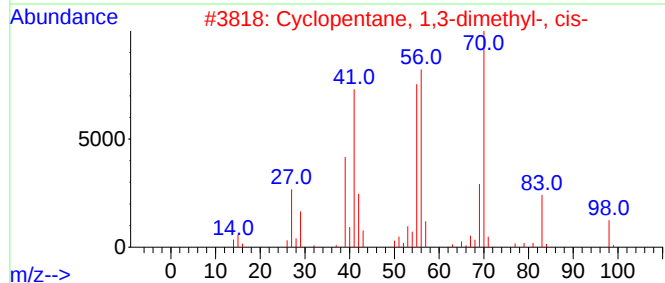
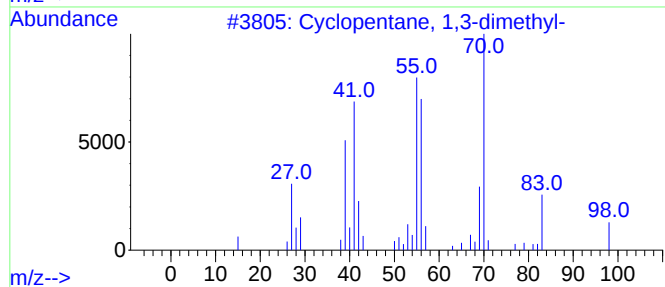
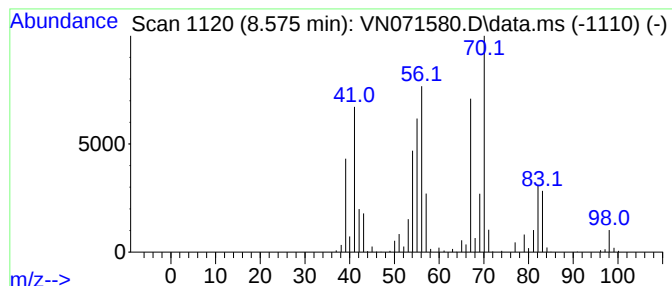
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, 1,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.575	23.41 ug/l	1942700	1,4-Difluorobenzene	8.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	70
2			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	70
3			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	53
4			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	38
5			Cyclohexene	82	C6H10	000110-83-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032622\
Data File : VN071580.D
Acq On : 26 Mar 2022 18:14
Operator : JC\MD
Sample : N2131-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-4

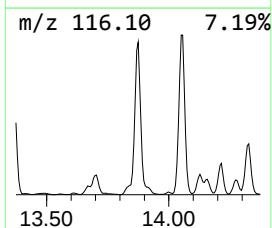
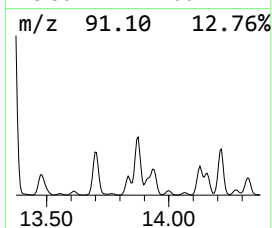
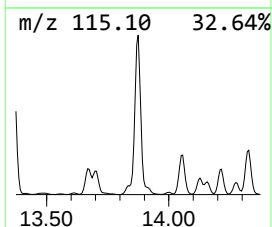
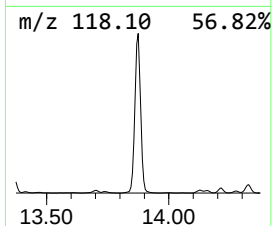
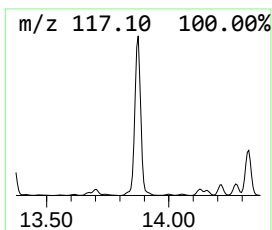
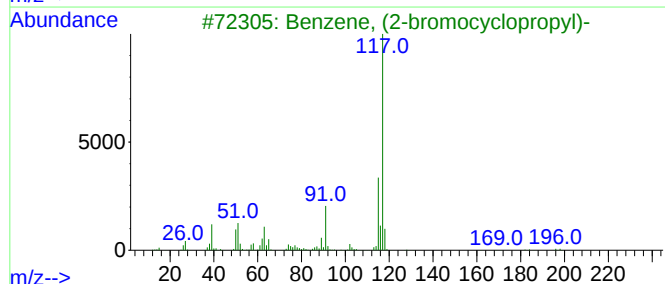
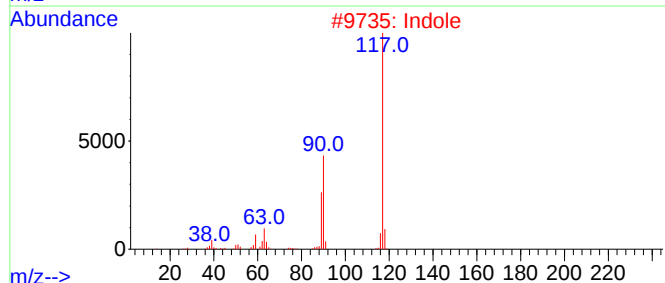
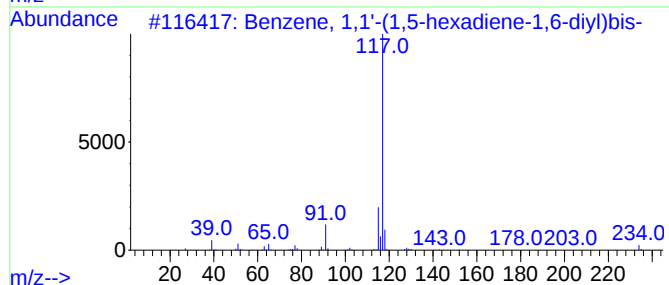
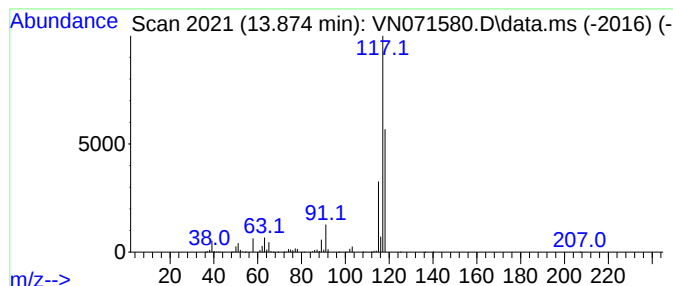
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	42.67 ug/l	19632100	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
2			Indole	117	C8H7N	000120-72-9	46
3			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
4			Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	42
5			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032622\
Data File : VN071580.D
Acq On : 26 Mar 2022 18:14
Operator : JC\MD
Sample : N2131-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

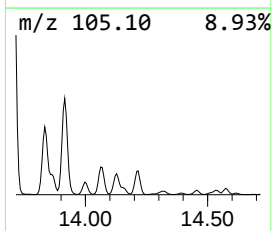
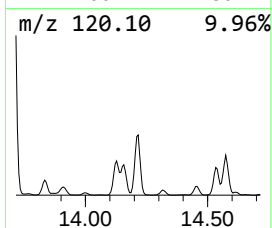
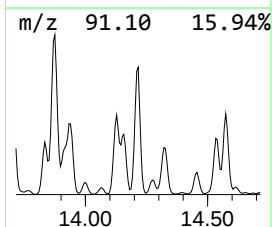
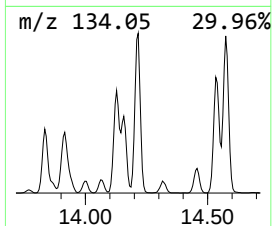
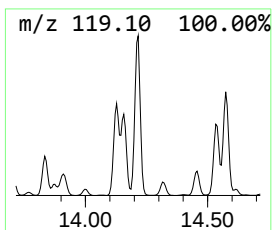
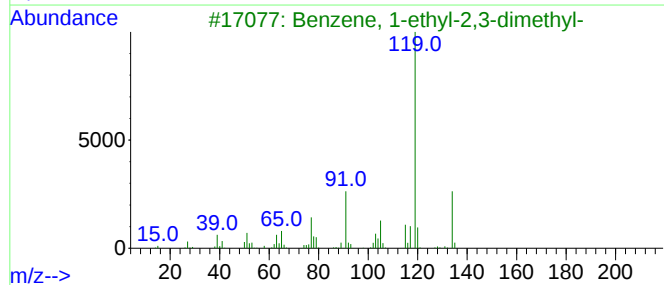
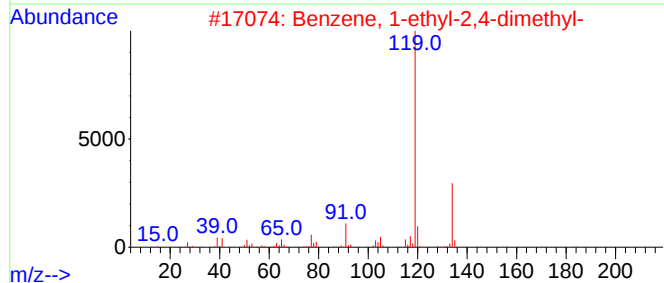
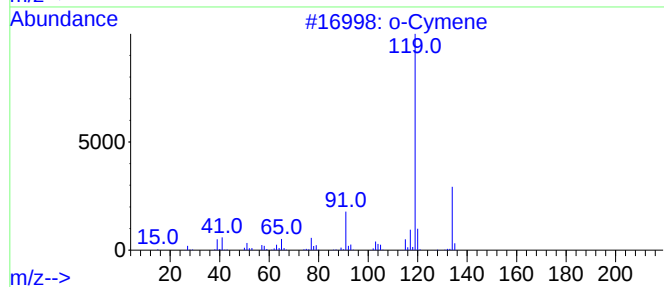
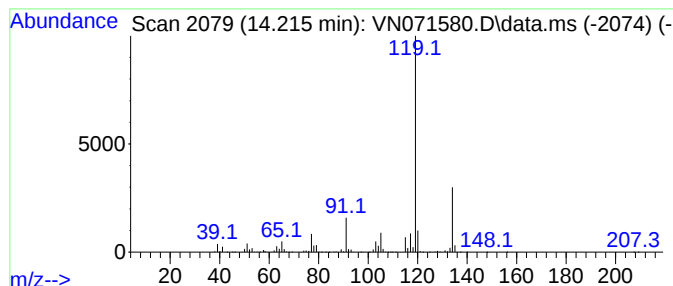
Instrument :
MSVOA_N
ClientSampleId :
MW-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032522W.M
Quant Title : SW846 8260

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

Peak Number 9 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.216	25.23 ug/l	11609400	1,4-Dichlorobenzene-d4			13.668
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	o-Cymene		134	C10H14	000527-84-4	97
2	Benzene, 1-ethyl-2,4-dimethyl-		134	C10H14	000874-41-9	97
3	Benzene, 1-ethyl-2,3-dimethyl-		134	C10H14	000933-98-2	96
4	Benzene, 2-ethyl-1,3-dimethyl-		134	C10H14	002870-04-4	95
5	Benzene, 1-methyl-3-(1-methyleth...		134	C10H14	000535-77-3	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032622\
Data File : VN071580.D
Acq On : 26 Mar 2022 18:14
Operator : JC\MD
Sample : N2131-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-4

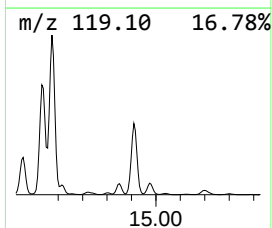
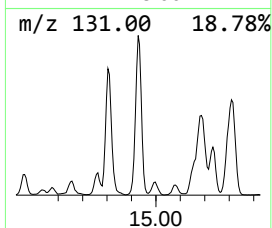
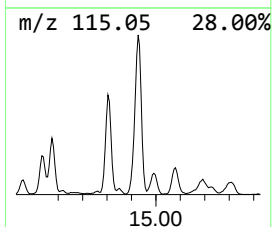
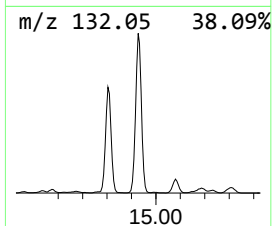
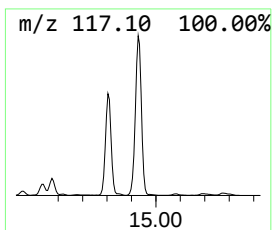
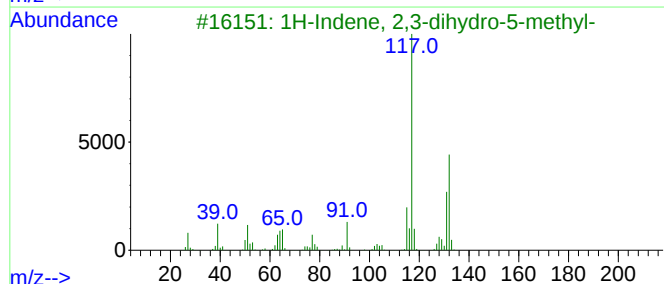
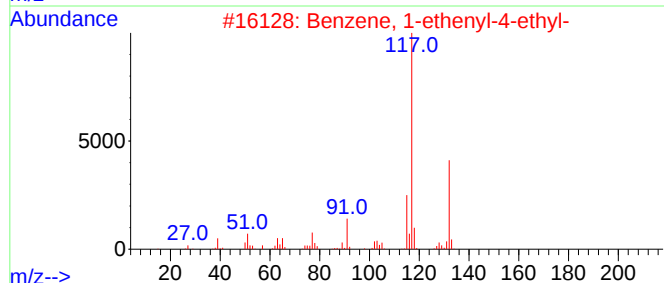
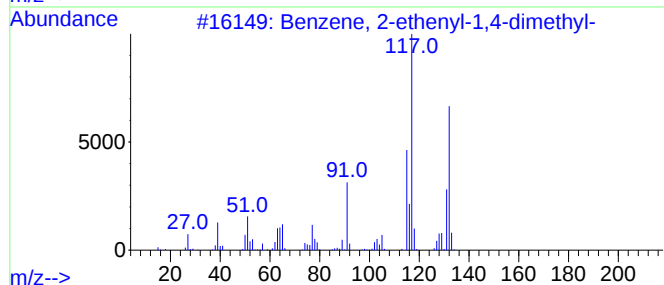
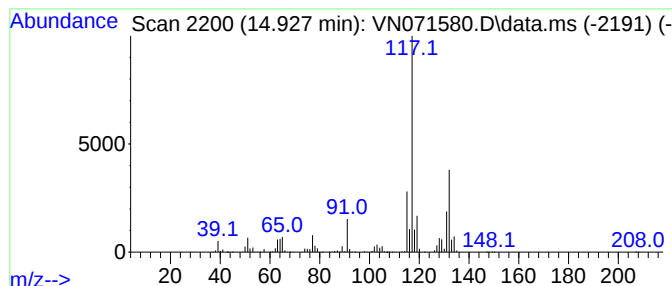
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	25.19 ug/l	11588100	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	91
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	90
5			Indan, 1-methyl-	132	C10H12	000767-58-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032622\
Data File : VN071580.D
Acq On : 26 Mar 2022 18:14
Operator : JC\MD
Sample : N2131-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032522W.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
Butane, 2-methyl-	3.134	76.5	ug/l	9048540	1	8.081	5914290	50.0
Pentane	3.510	23.7	ug/l	2803690	1	8.081	5914290	50.0
Pentane, 2-methyl-	5.151	73.1	ug/l	8647710	1	8.081	5914290	50.0
Pentane, 3-methyl-	5.616	41.9	ug/l	4952120	1	8.081	5914290	50.0
Cyclopentane, m...	7.145	73.2	ug/l	8657450	1	8.081	5914290	50.0
Pentane, 2,3-di...	8.175	23.8	ug/l	2813700	1	8.081	5914290	50.0
Cyclopentane, 1...	8.575	23.4	ug/l	1942700	2	8.963	4149440	50.0
Benzene, 1,1'-(...	13.874	42.7	ug/l	19632100	4	13.668	23002900	50.0
o-Cymene	14.216	25.2	ug/l	11609400	4	13.668	23002900	50.0
Benzene, 2-ethe...	14.927	25.2	ug/l	11588100	4	13.668	23002900	50.0