

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
 Data File : VN072603.D
 Acq On : 24 May 2022 22:07
 Operator : JC\MD
 Sample : N2968-04
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-25

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\82N052422W.M
 Title : SW846 8260

Signal : TIC: VN072603.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.258	36	46	61	rBV	408901	774050	3.47%	0.536%
2	2.434	66	76	87	rVV	831021	1398734	6.27%	0.969%
3	3.122	183	193	213	rBV	957403	2243985	10.05%	1.555%
4	3.416	234	243	250	rBV	112942	264826	1.19%	0.184%
5	3.504	250	258	277	rVB3	541551	1653629	7.41%	1.146%
6	3.710	283	293	308	rBV	453807	1122219	5.03%	0.778%
7	3.887	310	323	331	rVV	279163	730589	3.27%	0.506%
8	3.987	331	340	361	rVB	579259	1582962	7.09%	1.097%
9	4.951	490	504	516	rBV	193645	670354	3.00%	0.465%
10	5.181	528	543	567	rVB2	373899	1755304	7.86%	1.216%
11	5.616	601	617	636	rBV	204475	733907	3.29%	0.509%
12	6.404	739	751	754	rVV2	85910	280589	1.26%	0.194%
13	6.463	755	761	773	rVV	137159	418586	1.88%	0.290%
14	6.598	773	784	792	rVV	101472	317763	1.42%	0.220%
15	6.698	792	801	813	rVV5	115463	562041	2.52%	0.389%
16	6.898	826	835	852	rVB	123172	363708	1.63%	0.252%
17	7.145	864	877	886	rBV	635487	1901653	8.52%	1.318%
18	7.840	976	995	1005	rBV	186587	468294	2.10%	0.325%
19	8.016	1015	1025	1029	rBV	121192	275701	1.23%	0.191%
20	8.087	1029	1037	1048	rVB2	681952	1765671	7.91%	1.224%
21	8.457	1088	1100	1108	rBV	2469303	5779181	25.89%	4.005%
22	8.581	1116	1121	1128	rVB2	138538	292141	1.31%	0.202%
23	8.963	1176	1186	1199	rBV	387898	886779	3.97%	0.614%
24	9.451	1256	1269	1277	rBV2	130248	364534	1.63%	0.253%
25	9.969	1348	1357	1363	rBV	117906	227760	1.02%	0.158%
26	10.439	1429	1437	1441	rBV	569195	1049382	4.70%	0.727%
27	10.504	1441	1448	1462	rVV	9206839	16652693	74.59%	11.539%
28	10.639	1464	1471	1477	rVB	338223	588343	2.64%	0.408%
29	10.710	1477	1483	1489	rBV	320831	520727	2.33%	0.361%
30	11.739	1650	1658	1667	rBV	630416	1111018	4.98%	0.770%
31	11.839	1667	1675	1685	rVV	9388137	15490422	69.39%	10.734%
32	11.951	1685	1694	1706	rVB	11698252	22324218	100.00%	15.470%
33	12.275	1737	1749	1761	rBV	7017487	11392824	51.03%	7.895%
34	12.574	1793	1800	1808	rVB	377456	594828	2.66%	0.412%
35	12.727	1819	1826	1834	rBV	522183	885448	3.97%	0.614%
36	12.916	1851	1858	1863	rBV	832344	1308371	5.86%	0.907%

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37	12.980	1863	1869	1872	rVV	1767682	3159228	14.15%	2.189%
38	13.010	1872	1874	1878	rVV	1288577	1702726	7.63%	1.180%
39	13.051	1878	1881	1892	rVB	1085839	1653433	7.41%	1.146%
40	13.216	1901	1909	1917	rBV	2106165	3373853	15.11%	2.338%
41	13.363	1926	1934	1947	rBV	7127504	10877172	48.72%	7.537%
42	13.698	1980	1991	2001	rBV2	2138418	4374221	19.59%	3.031%
43	13.869	2008	2020	2037	rBV	2921361	5848587	26.20%	4.053%
44	14.057	2046	2052	2058	rVV2	281595	512245	2.29%	0.355%
45	14.121	2058	2063	2066	rVV	341660	558063	2.50%	0.387%
46	14.151	2066	2068	2073	rVV	265197	381835	1.71%	0.265%
47	14.210	2073	2078	2084	rVV	648571	989527	4.43%	0.686%
48	14.274	2084	2089	2092	rVV	179073	286558	1.28%	0.199%
49	14.321	2092	2097	2106	rVB2	679025	1122616	5.03%	0.778%
50	14.451	2113	2119	2126	rBV2	160293	257815	1.15%	0.179%
51	14.533	2126	2133	2136	rBV	399777	629311	2.82%	0.436%
52	14.574	2136	2140	2145	rVB	477556	720402	3.23%	0.499%
53	14.804	2174	2179	2184	rBV	599629	900886	4.04%	0.624%
54	14.927	2190	2200	2206	rBV2	1019513	2139035	9.58%	1.482%
55	15.074	2218	2225	2233	rBV2	250369	456780	2.05%	0.317%
56	15.186	2233	2244	2248	rBV2	141651	356597	1.60%	0.247%
57	15.304	2256	2264	2272	rVB3	142407	348493	1.56%	0.241%
58	15.498	2289	2297	2306	rBV	2263086	4230668	18.95%	2.932%
59	15.598	2308	2314	2321	rVV	166198	322929	1.45%	0.224%
60	16.610	2479	2486	2502	rVB	148889	354261	1.59%	0.245%

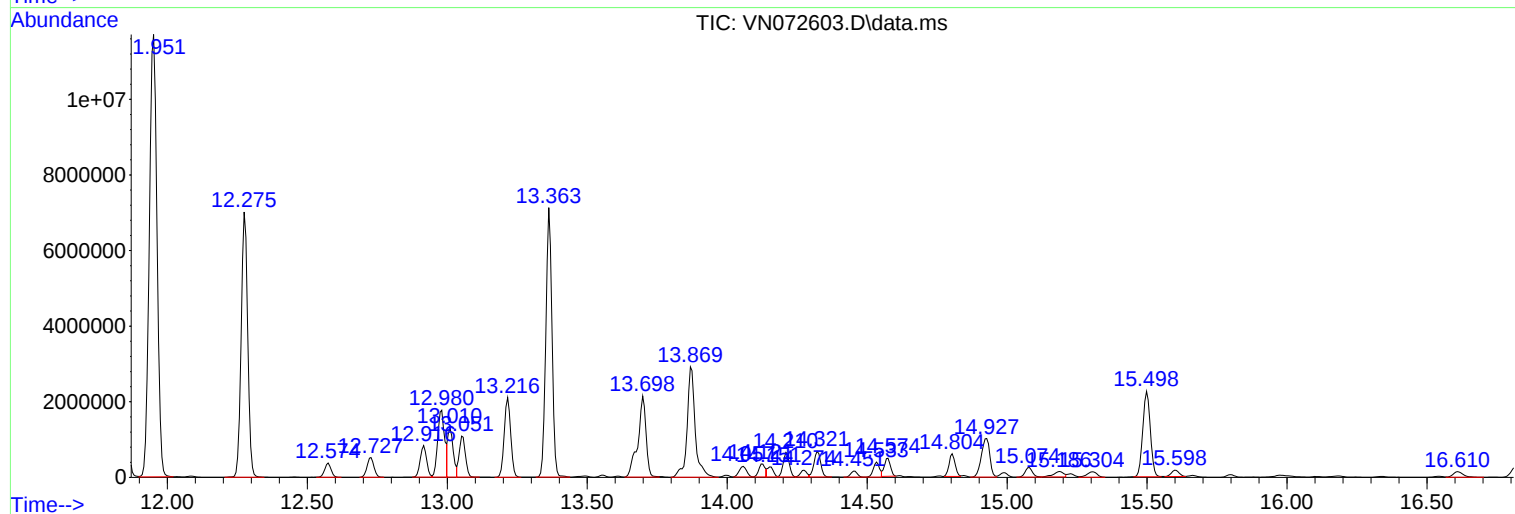
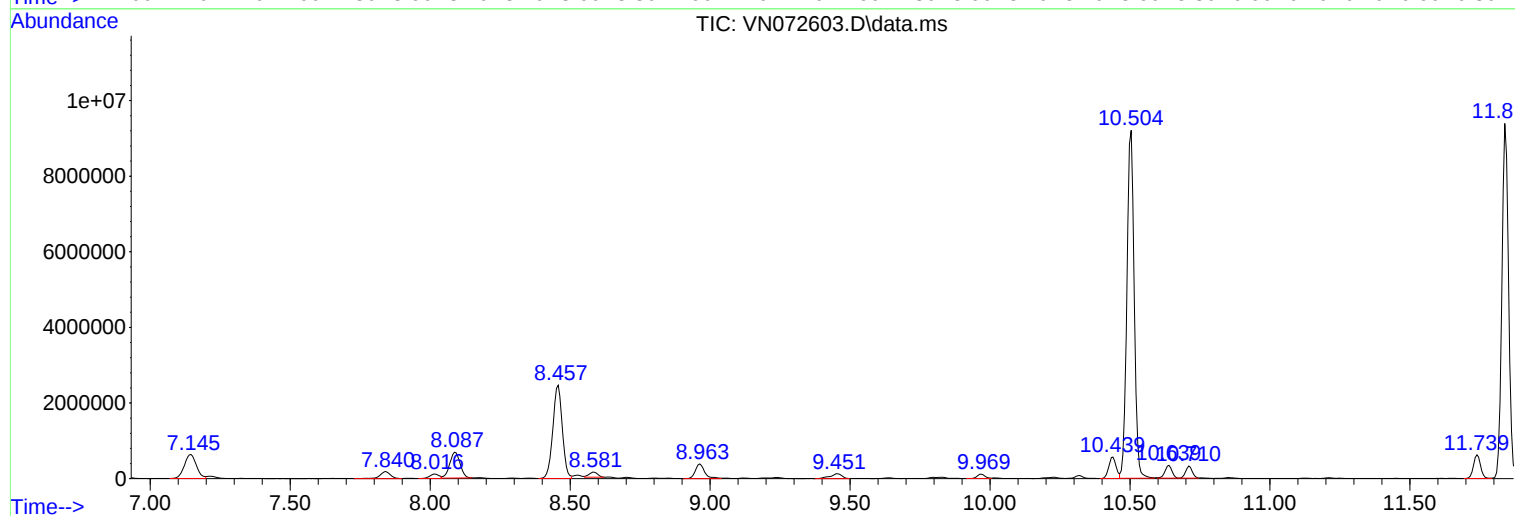
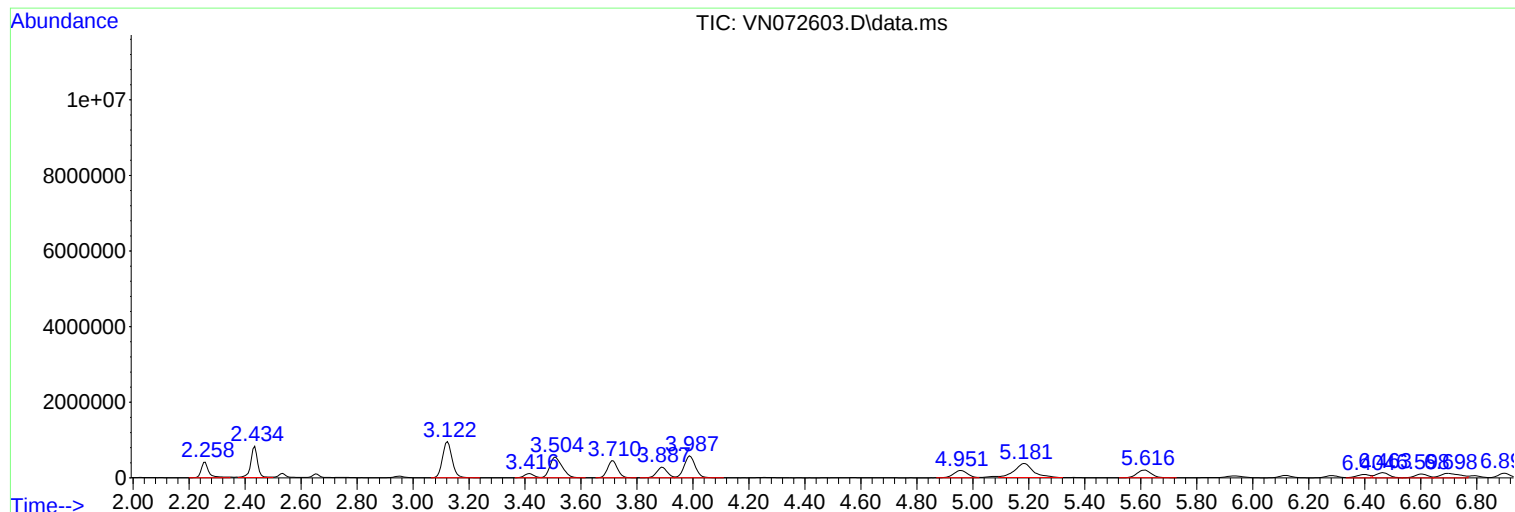
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

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



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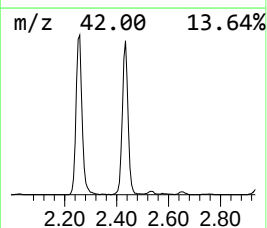
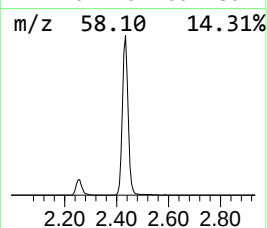
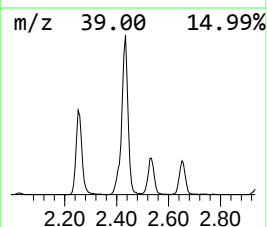
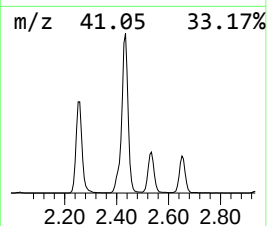
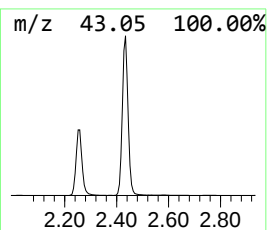
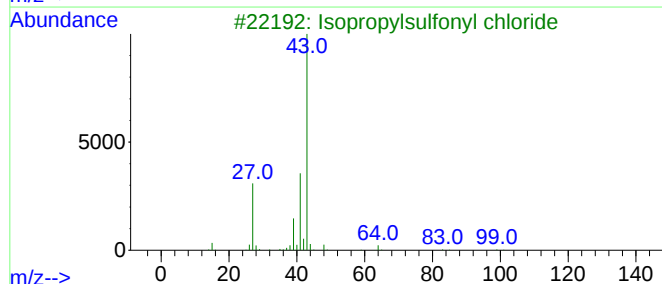
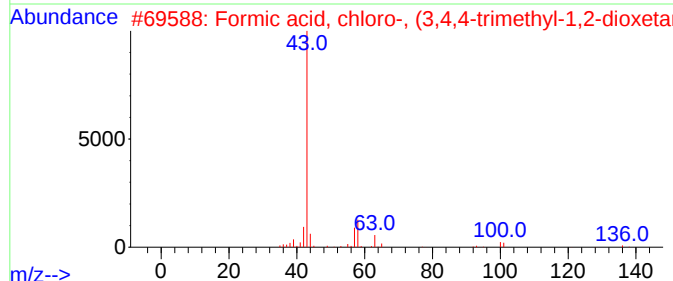
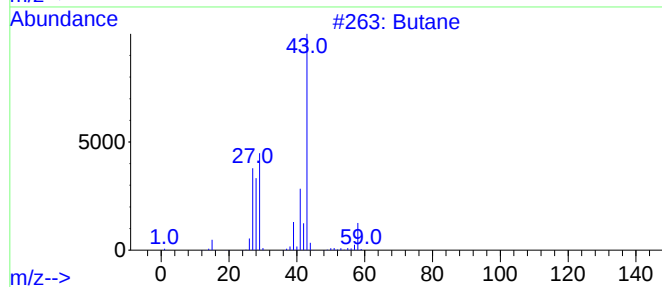
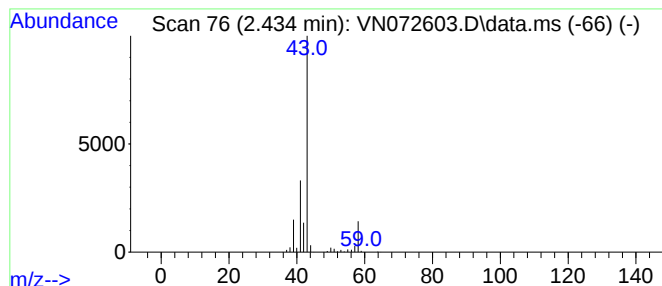
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.434	39.61 ug/l	1398730	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	9
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Allyl acetate	100	C5H8O2	000591-87-7	9
5			Isobutane	58	C4H10	000075-28-5	9



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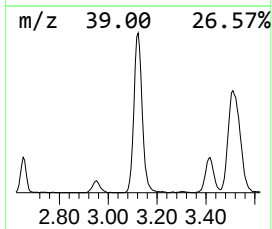
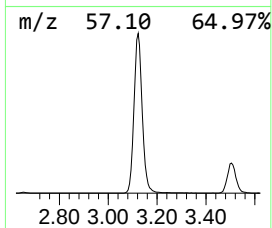
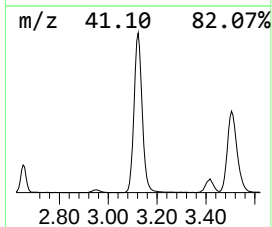
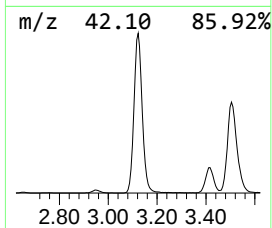
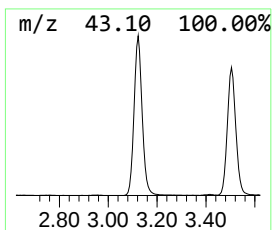
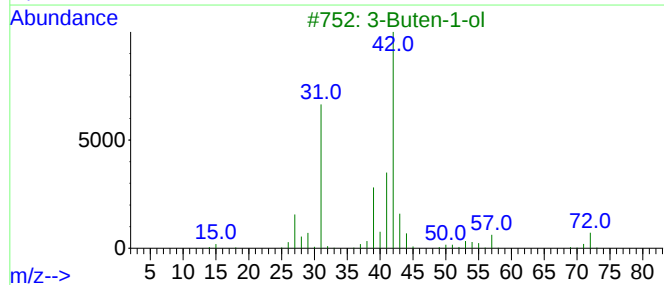
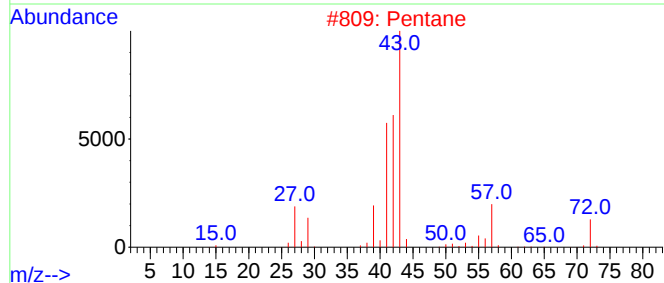
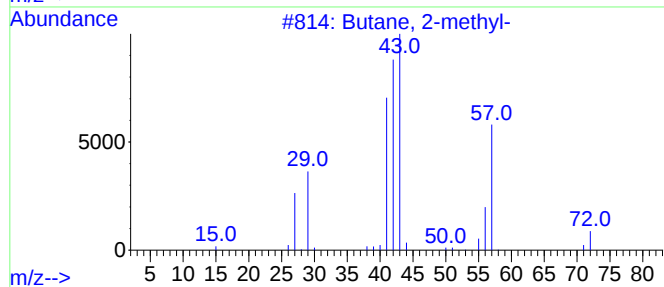
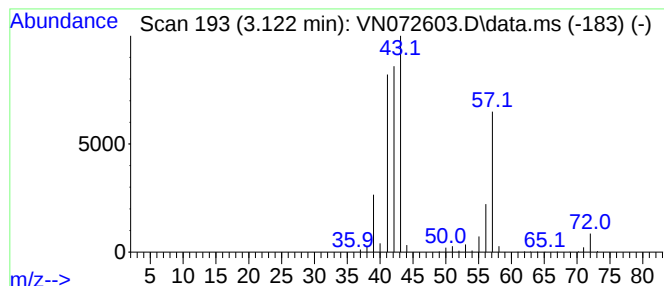
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.122	63.54 ug/l	2243990	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	36
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			1-Butene	56	C4H8	000106-98-9	10
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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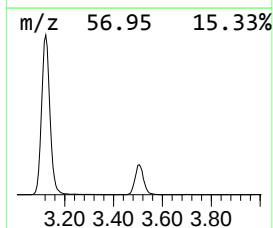
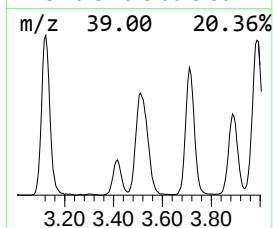
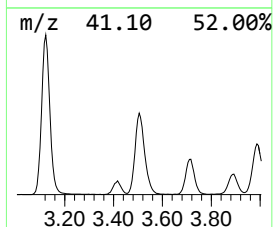
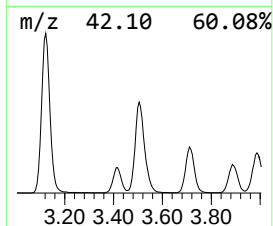
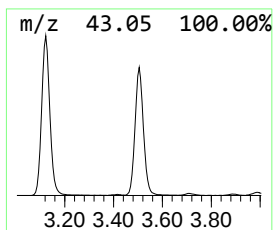
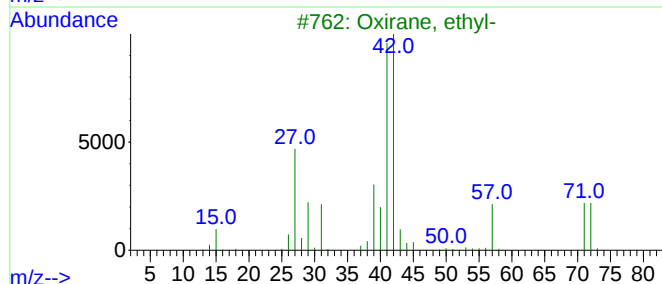
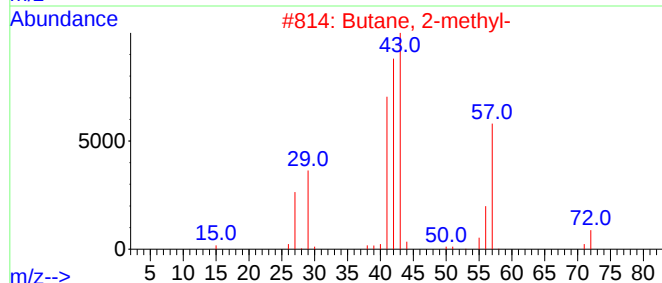
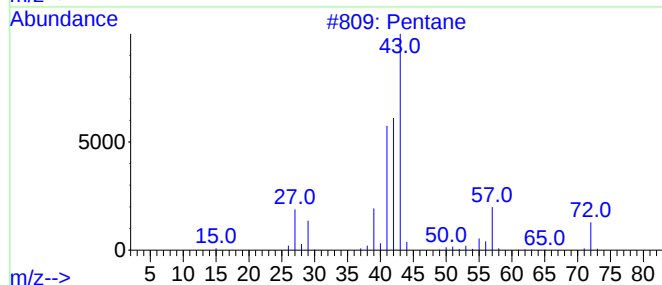
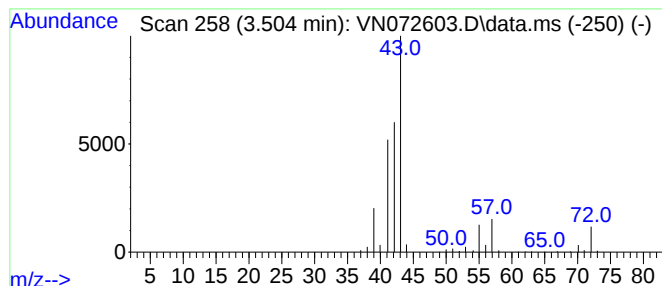
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.504	46.83 ug/l	1653630	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Butane, 2-methyl-	72	C5H12	000078-78-4	64
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	40
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5			Cyclobutane, methyl-	70	C5H10	000598-61-8	9



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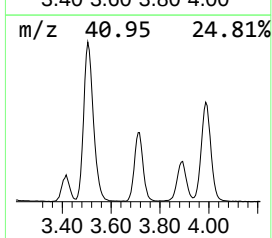
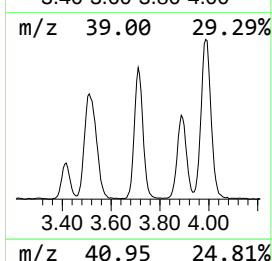
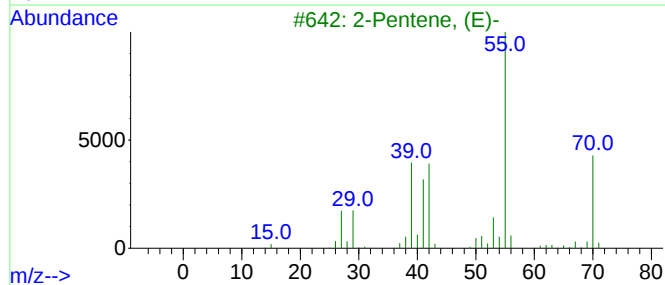
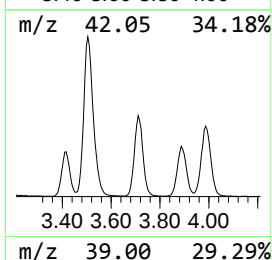
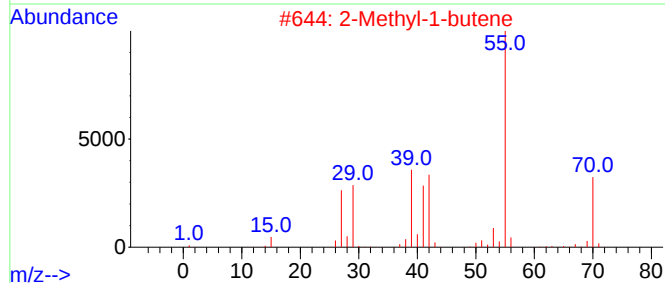
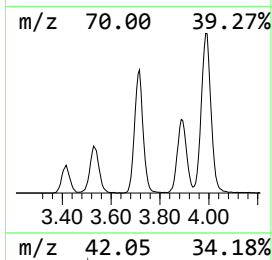
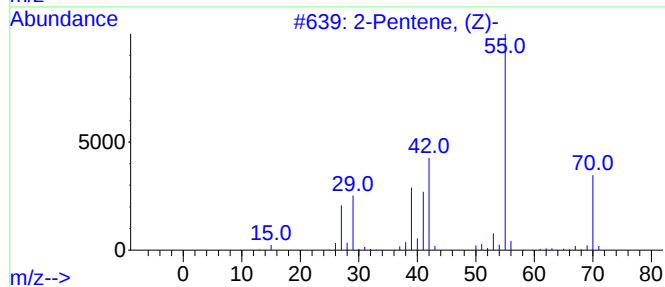
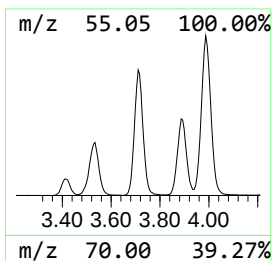
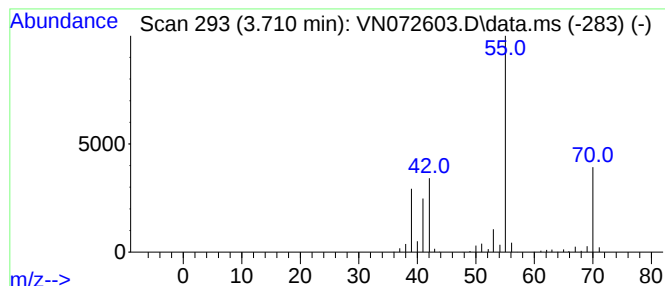
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Quant Title : SW846 8260

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

Peak Number 4 2-Pentene, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.710	31.78 ug/l	112220	Pentafluorobenzene	8.081

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentene, (Z)-	70	C5H10	000627-20-3	91
2		2-Methyl-1-butene	70	C5H10	000563-46-2	91
3		2-Pentene, (E)-	70	C5H10	000646-04-8	90
4		2-Pentene	70	C5H10	000109-68-2	90
5		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87



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MW-25

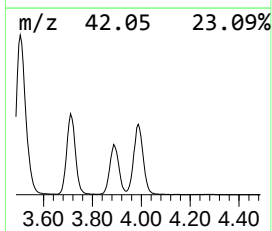
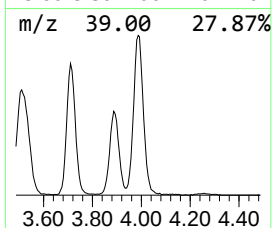
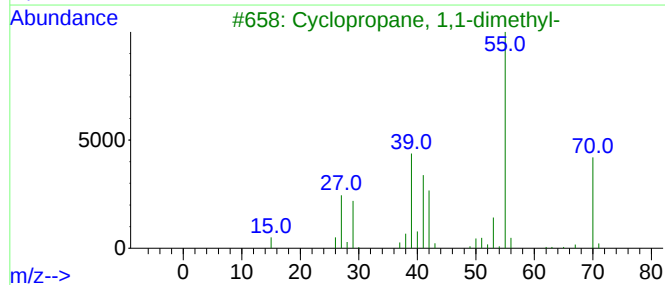
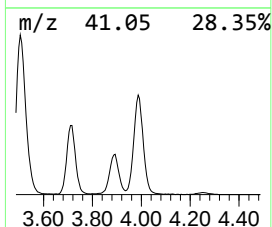
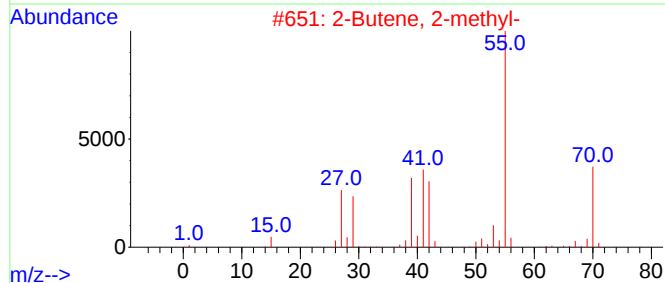
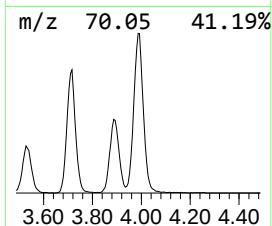
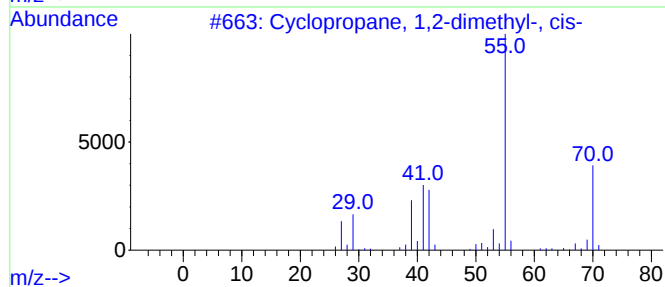
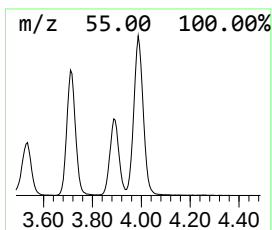
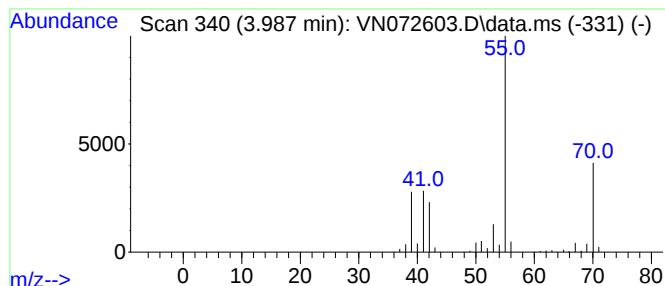
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.987	44.83 ug/l	1582960	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
3			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
4			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80
5			2-Pentene, (E)-	70	C5H10	000646-04-8	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072603.D
Acq On : 24 May 2022 22:07
Operator : JC\MD
Sample : N2968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-25

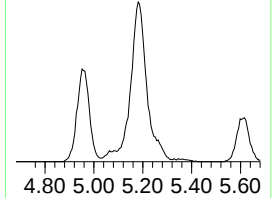
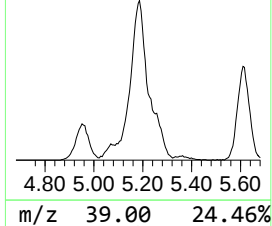
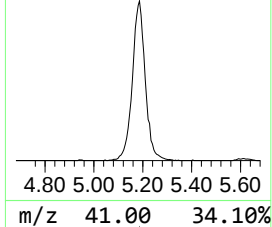
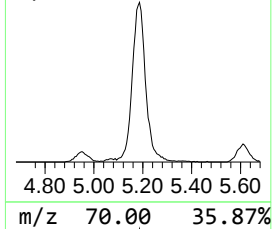
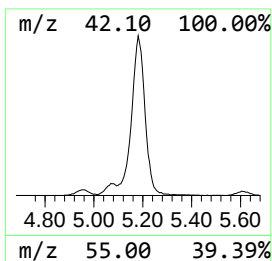
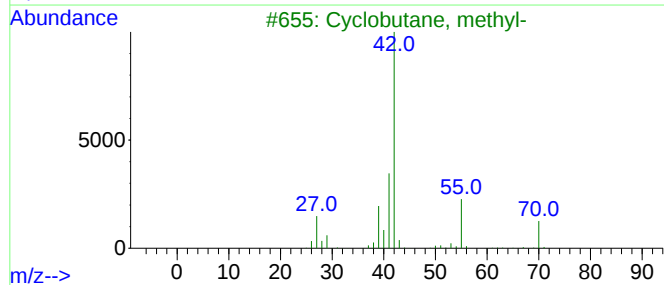
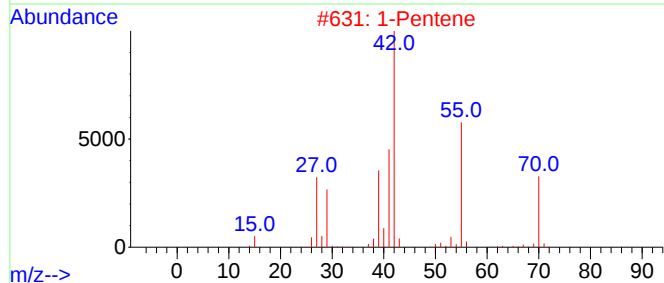
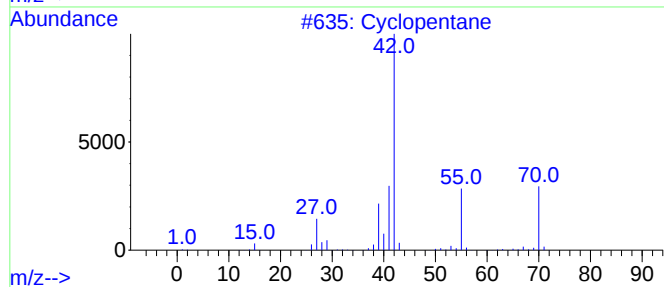
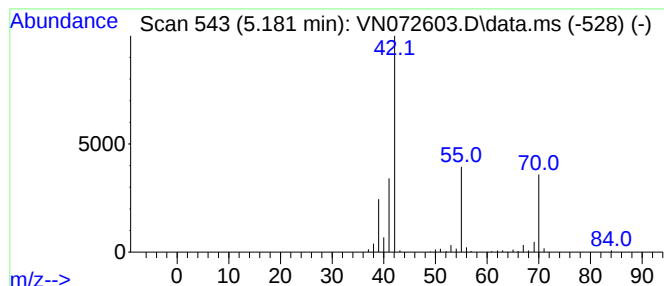
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	49.71 ug/l	1755300	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	86
2			1-Pentene	70	C5H10	000109-67-1	78
3			Cyclobutane, methyl-	70	C5H10	000598-61-8	72
4			Methyl propargyl ether	70	C4H6O	000627-41-8	9
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072603.D
Acq On : 24 May 2022 22:07
Operator : JC\MD
Sample : N2968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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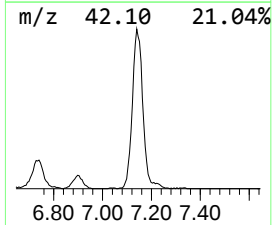
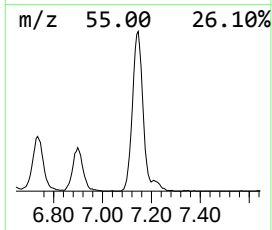
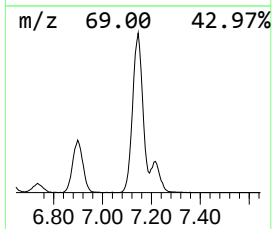
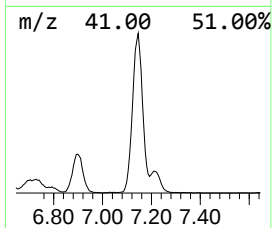
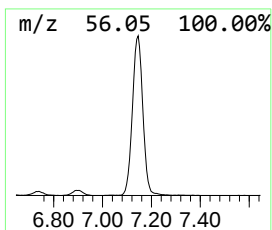
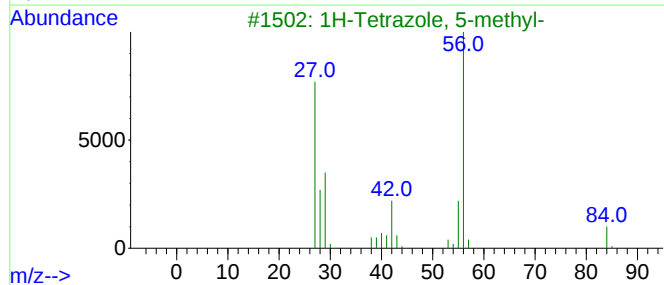
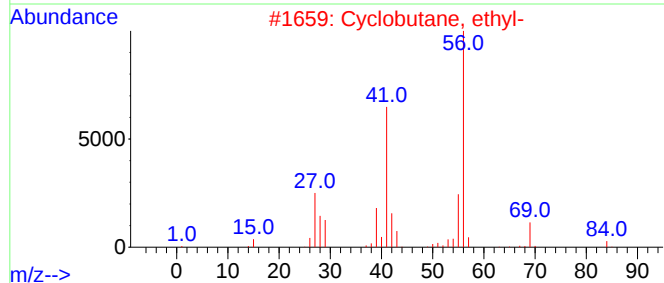
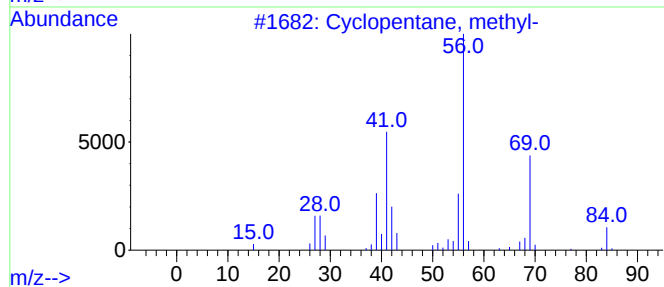
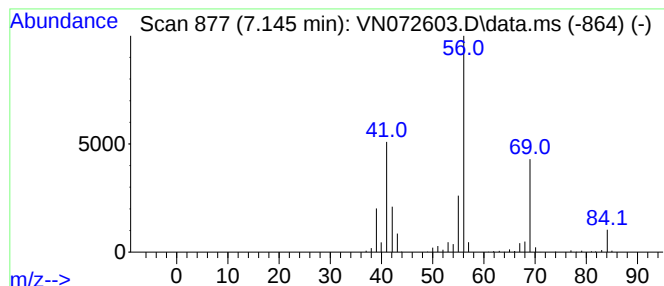
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	53.85 ug/l	1901650	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	80
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
4			Cyclopropane, propyl-	84	C6H12	002415-72-7	78
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072603.D
Acq On : 24 May 2022 22:07
Operator : JC\MD
Sample : N2968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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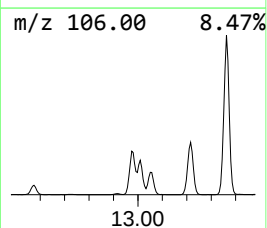
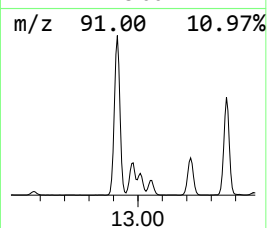
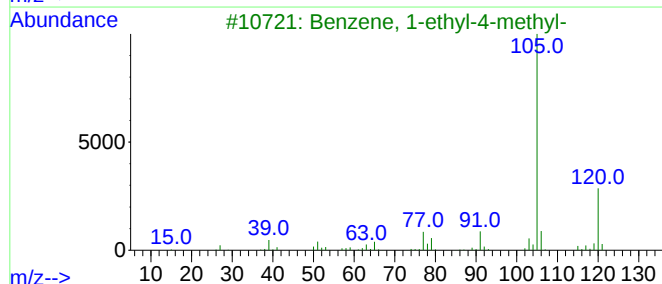
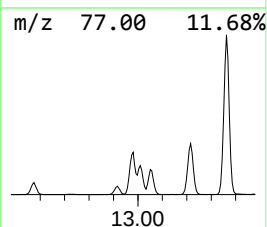
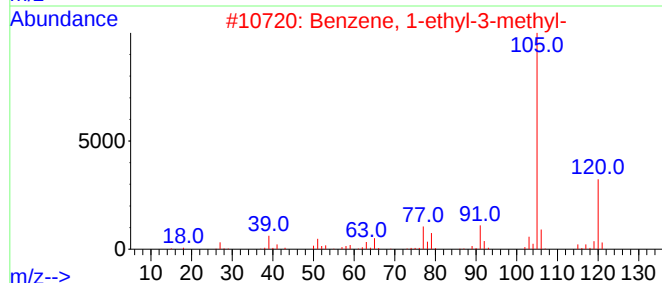
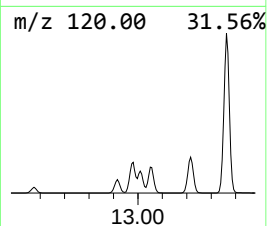
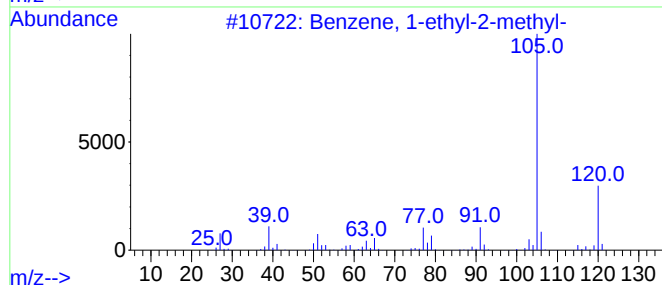
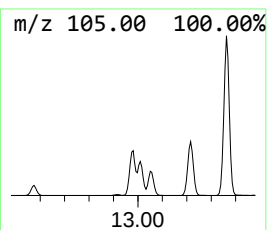
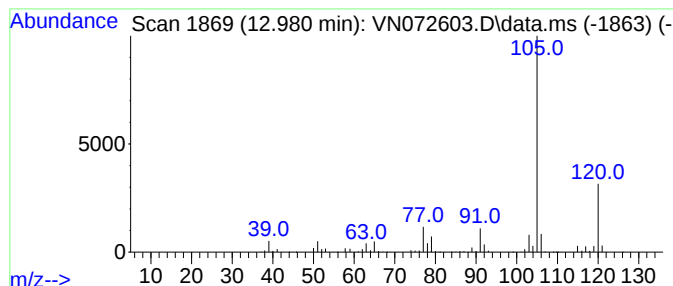
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	36.11 ug/l	3159230	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072603.D
Acq On : 24 May 2022 22:07
Operator : JC\MD
Sample : N2968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-25

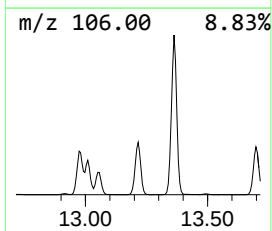
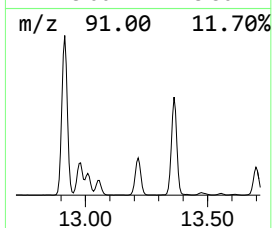
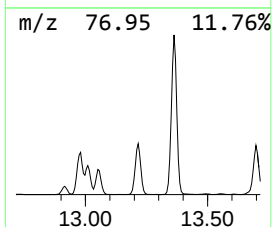
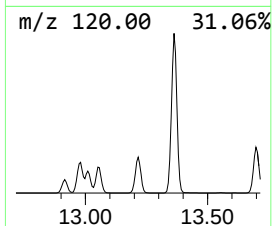
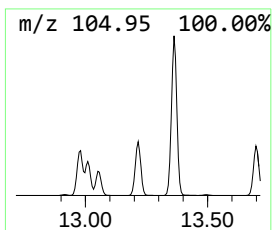
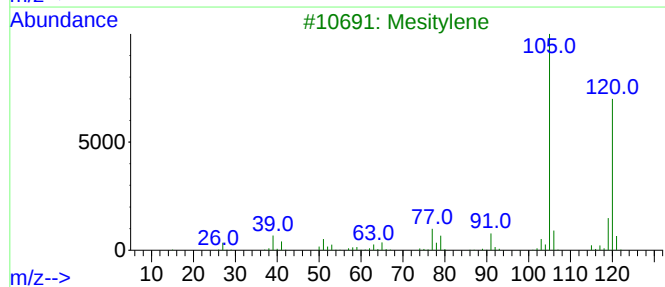
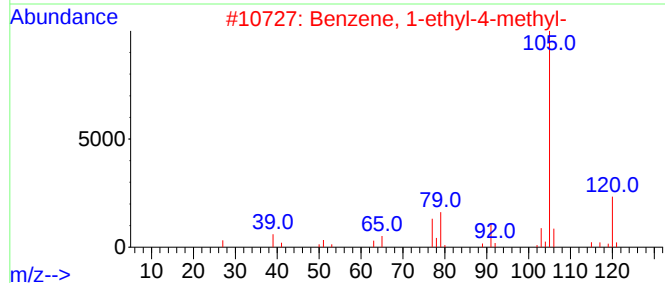
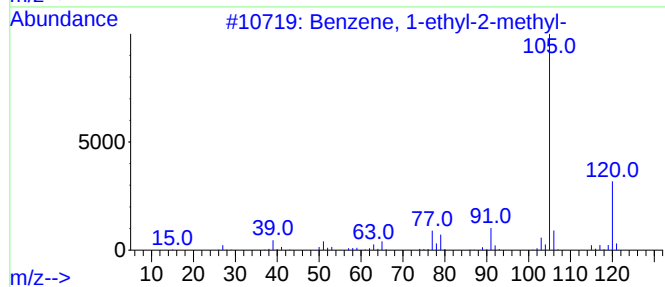
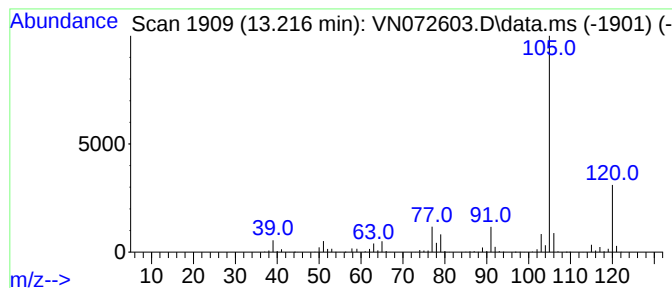
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	38.57 ug/l	3373850	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072603.D
Acq On : 24 May 2022 22:07
Operator : JC\MD
Sample : N2968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-25

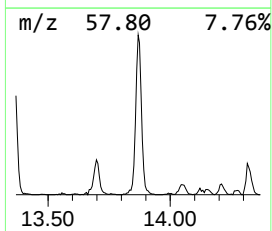
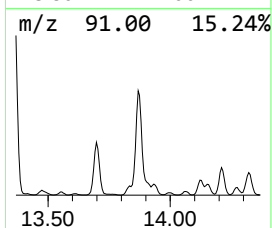
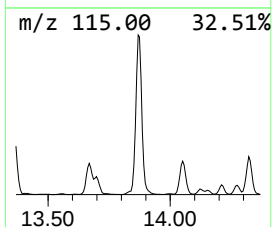
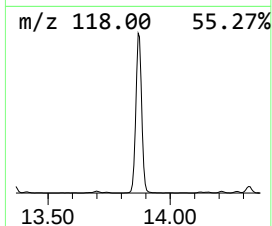
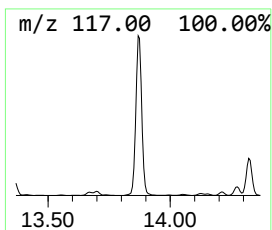
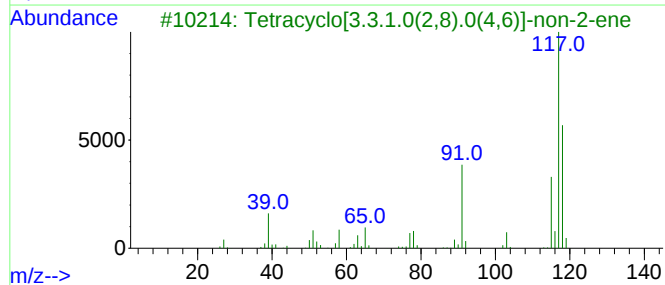
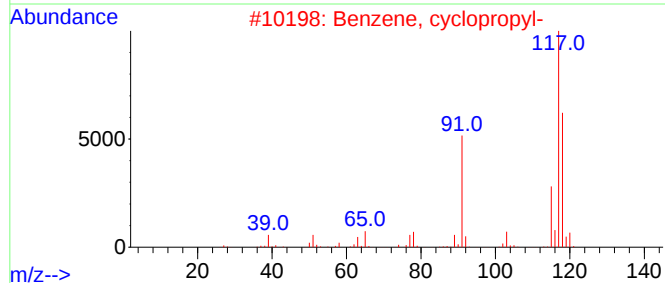
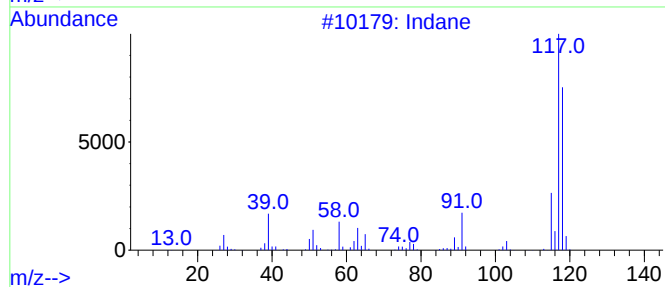
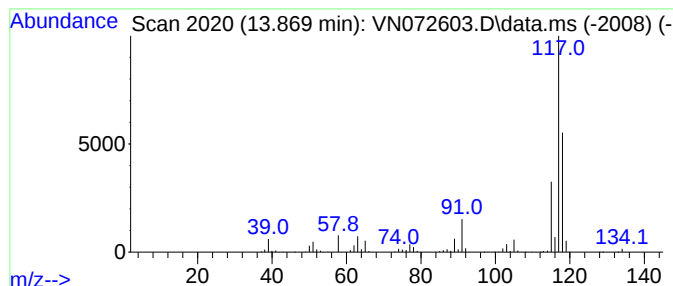
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	66.85 ug/l	5848590	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	90
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
4			Δtacyclene	118	C9H10	007785-10-6	72
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072603.D
Acq On : 24 May 2022 22:07
Operator : JC\MD
Sample : N2968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-25

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.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
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Butane, 2-methyl-	3.122	63.5	ug/l	2243990	1	8.081	1765670	50.0
Pentane	3.504	46.8	ug/l	1653630	1	8.081	1765670	50.0
2-Pentene, (Z)-	3.710	31.8	ug/l	1122220	1	8.081	1765670	50.0
Cyclopropane, 1...	3.987	44.8	ug/l	1582960	1	8.081	1765670	50.0
Cyclopentane	5.181	49.7	ug/l	1755300	1	8.081	1765670	50.0
Cyclopentane, m...	7.145	53.9	ug/l	1901650	1	8.081	1765670	50.0
Benzene, 1-ethy...	12.980	36.1	ug/l	3159230	4	13.669	4374220	50.0
Benzene, 1-ethy...	13.216	38.6	ug/l	3373850	4	13.669	4374220	50.0
Indane	13.868	66.8	ug/l	5848590	4	13.669	4374220	50.0