

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
 Data File : VN066379.D
 Acq On : 29 Mar 2021 16:11
 Operator : JC/MD
 Sample : M1835-01
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 LMW01

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\82N032521W.M
 Title : SW846 8260

Signal : TIC: VN066379.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.979	96	108	130	rBV	649664	921778	1.29%	0.256%
2	2.140	147	168	188	rBV	3023359	4464776	6.24%	1.238%
3	2.752	377	396	419	rBV	4811243	9534365	13.33%	2.644%
4	3.082	502	519	551	rVB3	1414790	3678717	5.14%	1.020%
5	3.256	567	584	606	rVB	637222	1330721	1.86%	0.369%
6	3.492	654	672	707	rVB	2985934	6904312	9.65%	1.915%
7	4.329	964	984	1000	rBV3	256584	733923	1.03%	0.204%
8	4.428	1002	1021	1032	rBV2	394016	1231222	1.72%	0.341%
9	4.712	1099	1127	1177	rVB	3945273	13409983	18.75%	3.719%
10	4.937	1187	1211	1248	rVB5	360717	1317629	1.84%	0.365%
11	5.820	1523	1540	1566	rVB	403363	1233476	1.72%	0.342%
12	5.959	1570	1592	1612	rBV3	241478	758914	1.06%	0.210%
13	6.268	1685	1707	1742	rVB3	297865	906683	1.27%	0.251%
14	6.525	1777	1803	1824	rBV2	1327476	4112562	5.75%	1.141%
15	7.298	2075	2091	2116	rVB2	512466	1335653	1.87%	0.370%
16	7.507	2141	2169	2177	rBV2	329389	811512	1.13%	0.225%
17	7.574	2179	2194	2214	rVV4	1171653	3413465	4.77%	0.947%
18	7.960	2313	2338	2364	rBV	9860818	24156321	33.77%	6.700%
19	8.081	2366	2383	2395	rBV5	424803	1287691	1.80%	0.357%
20	8.510	2518	2543	2571	rBV3	1153887	2836468	3.97%	0.787%
21	9.009	2695	2729	2745	rBV4	391802	1189670	1.66%	0.330%
22	9.550	2914	2931	2938	rBV	470273	905777	1.27%	0.251%
23	10.028	3093	3109	3119	rBV	1541341	2924870	4.09%	0.811%
24	10.092	3119	3133	3166	rVB	12937961	25128057	35.13%	6.970%
25	11.350	3585	3602	3622	rBV	1211496	2230725	3.12%	0.619%
26	11.455	3624	3641	3662	rVV	16509022	28704737	40.13%	7.962%
27	11.565	3663	3682	3713	rVV	35034207	71537137	100.00%	19.842%
28	11.889	3786	3803	3834	rBV	15812198	26763107	37.41%	7.423%
29	12.192	3902	3916	3929	rBV	1167329	1853984	2.59%	0.514%
30	12.345	3957	3973	4005	rBV	947791	1707998	2.39%	0.474%
31	12.535	4029	4044	4055	rBV	1995231	3167577	4.43%	0.879%
32	12.600	4055	4068	4073	rVV	3182980	4987091	6.97%	1.383%
33	12.632	4073	4080	4089	rVV	4783421	7545981	10.55%	2.093%
34	12.678	4089	4097	4121	rVB	3505508	5420165	7.58%	1.503%
35	12.833	4140	4155	4179	rBV	3959792	6425412	8.98%	1.782%
36	12.983	4195	4211	4242	rBV	20001438	32879729	45.96%	9.120%

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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

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37	13.316	4312	4335	4356	rBV	8220632	14795294	20.68%	4.104%
38	13.485	4375	4398	4409	rBV	8020899	13817090	19.31%	3.832%
39	13.678	4456	4470	4483	rVB2	470373	948843	1.33%	0.263%
40	13.745	4484	4495	4501	rBV	787176	1212028	1.69%	0.336%
41	13.831	4516	4527	4539	rBV	1305503	1982833	2.77%	0.550%
42	13.935	4556	4566	4583	rVB2	1279681	2099137	2.93%	0.582%
43	14.153	4634	4647	4653	rBV	846344	1317227	1.84%	0.365%
44	14.190	4653	4661	4673	rVB	1136245	1753762	2.45%	0.486%
45	14.418	4734	4746	4759	rBV	945762	1518211	2.12%	0.421%
46	14.534	4773	4789	4804	rBV3	2082129	3902567	5.46%	1.082%
47	15.067	4974	4988	5016	rBV	4109059	7321768	10.23%	2.031%
48	16.078	5352	5365	5394	rVB	635302	1334298	1.87%	0.370%
49	16.266	5421	5435	5459	rVB	356260	787231	1.10%	0.218%

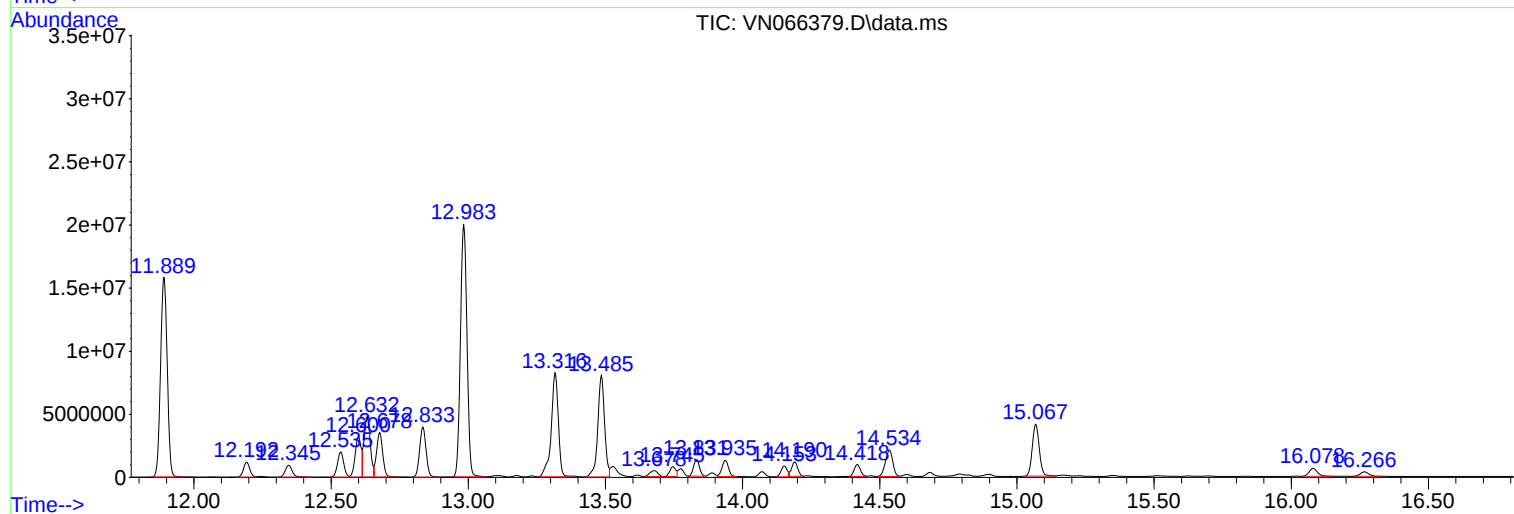
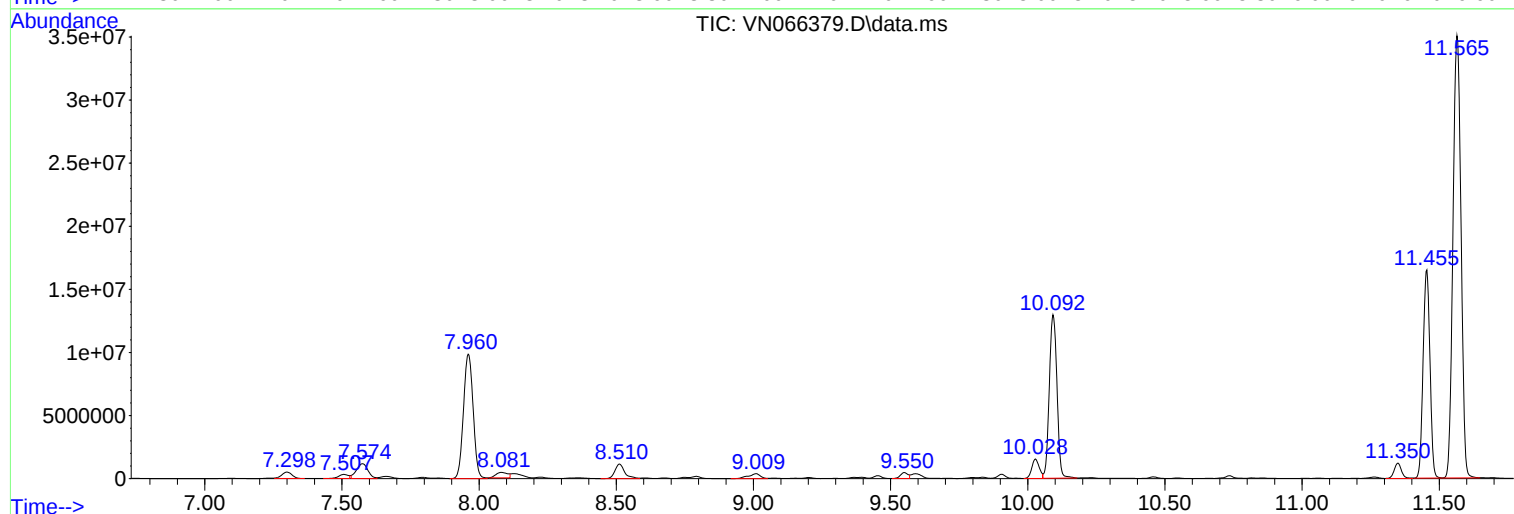
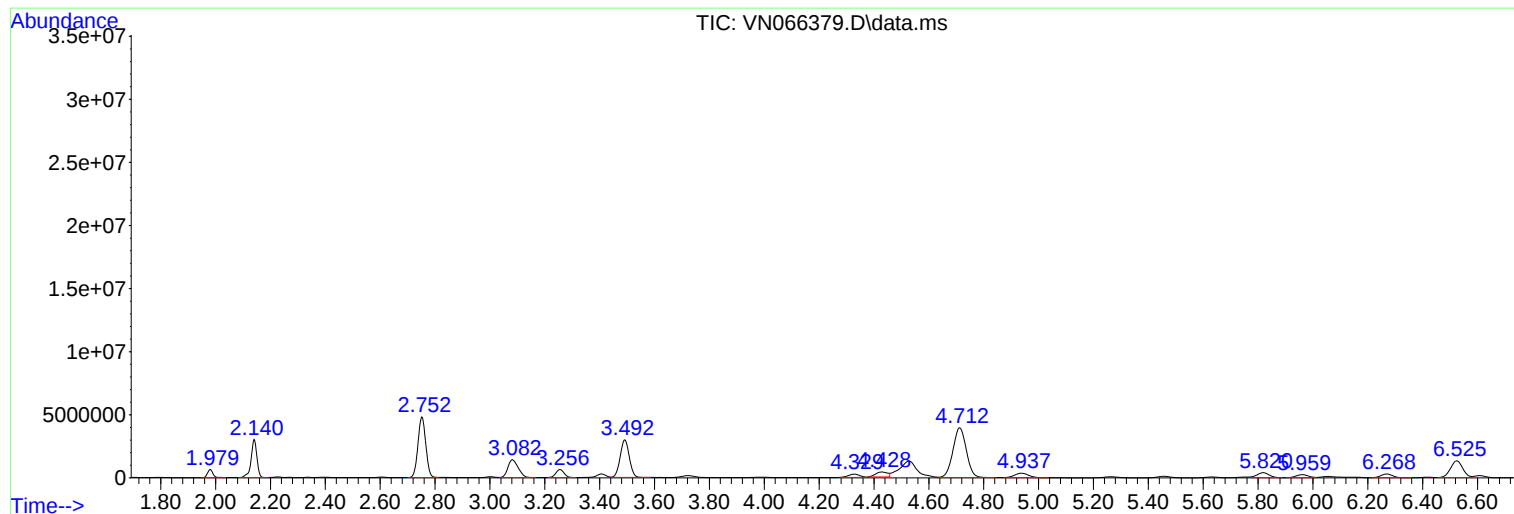
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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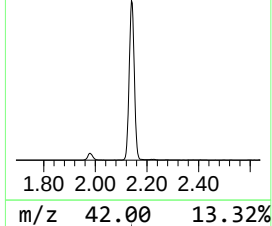
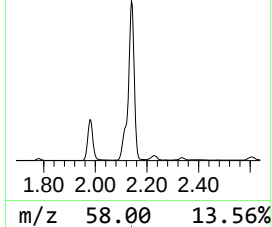
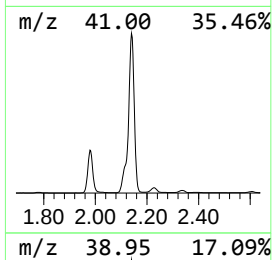
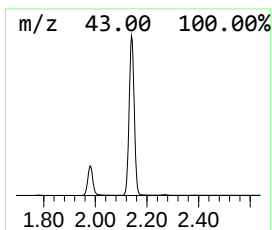
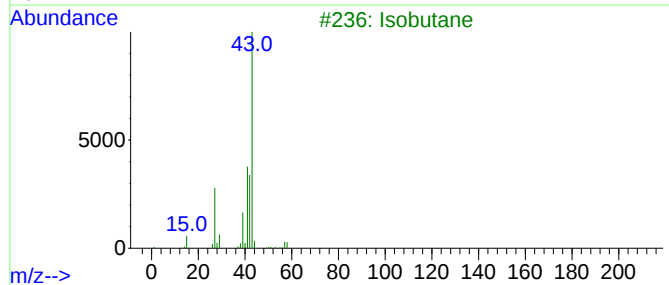
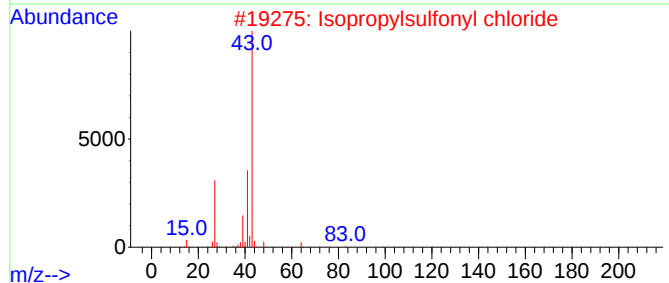
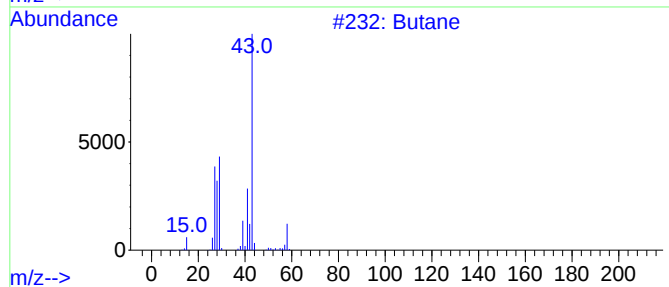
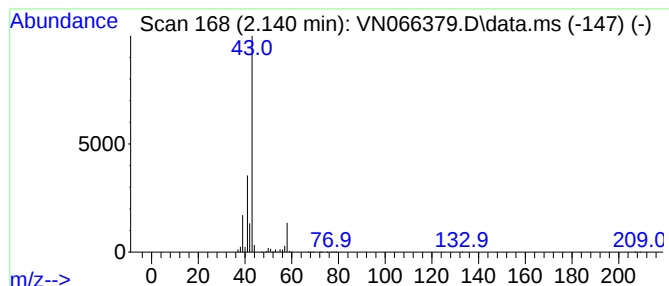
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	65.40 ug/l	4464780	Pentafluorobenzene	7.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3			Isobutane	58	C4H10	000075-28-5	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Diazene, dimethyl-	58	C2H6N2	000503-28-6	4



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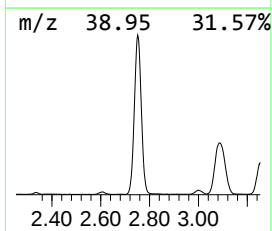
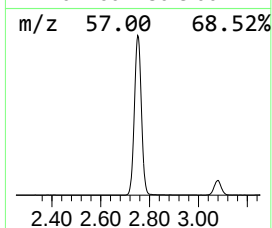
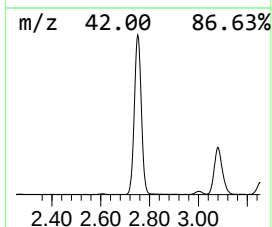
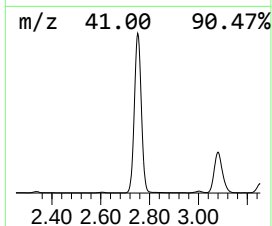
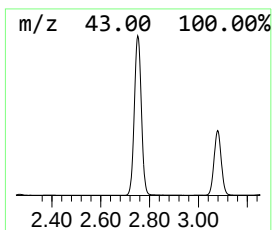
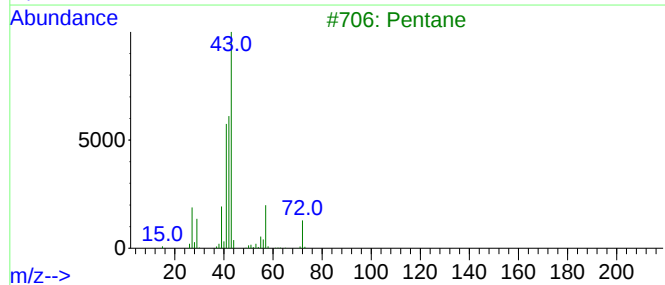
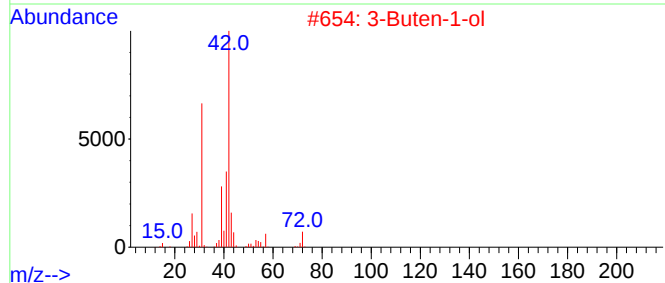
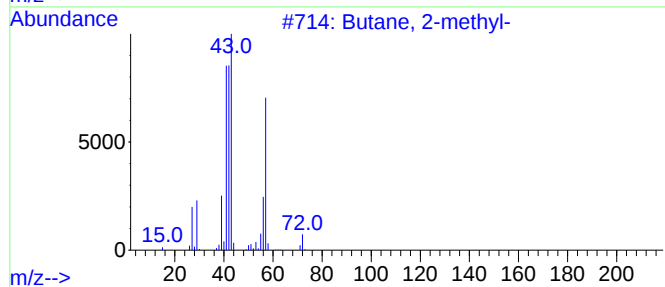
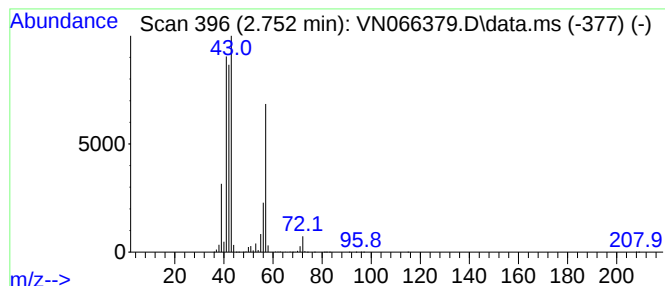
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.752	139.66 ug/l	9534370	Pentafluorobenzene	7.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
5			Azetidine	57	C3H7N	000503-29-7	9



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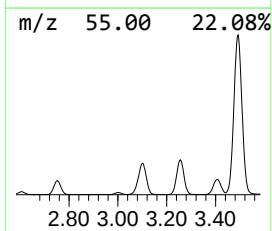
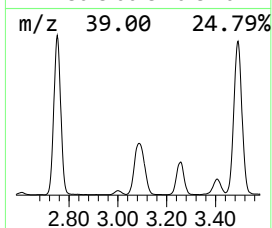
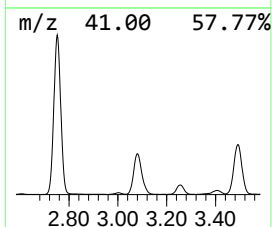
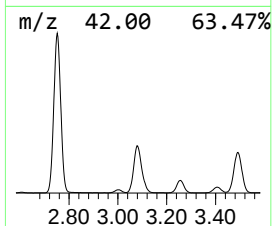
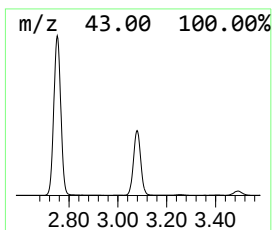
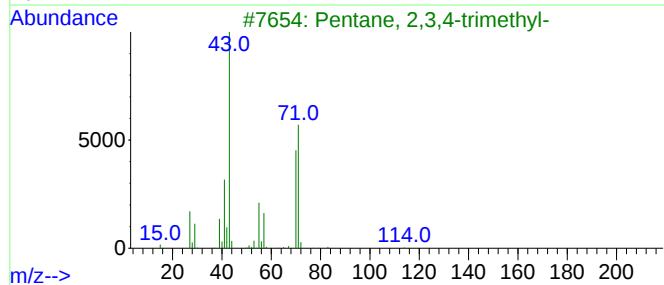
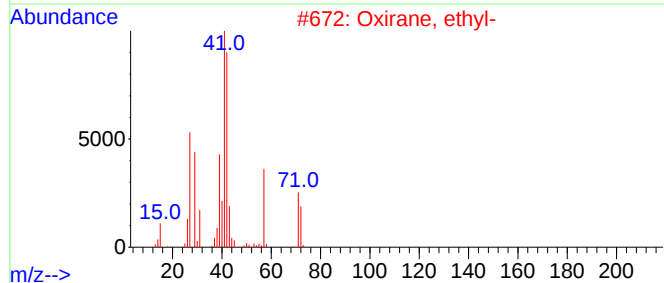
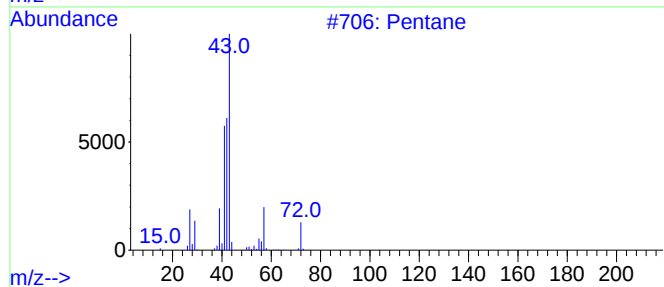
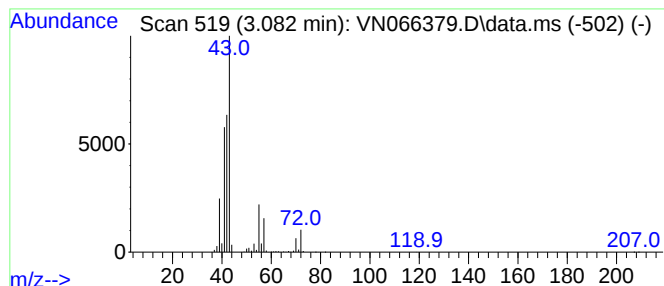
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.082	53.89 ug/l	3678720	Pentafluorobenzene	7.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	86
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	43
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	28
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	17
5			Butane, 2-methyl-	72	C5H12	000078-78-4	12



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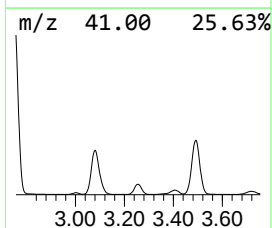
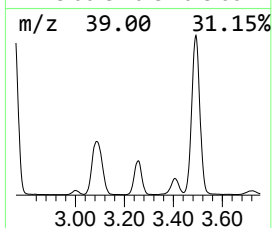
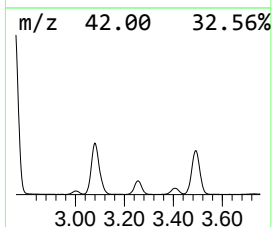
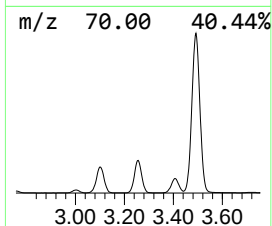
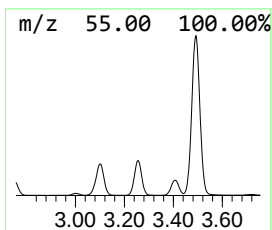
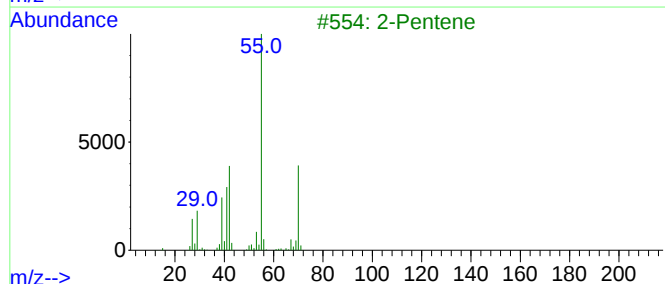
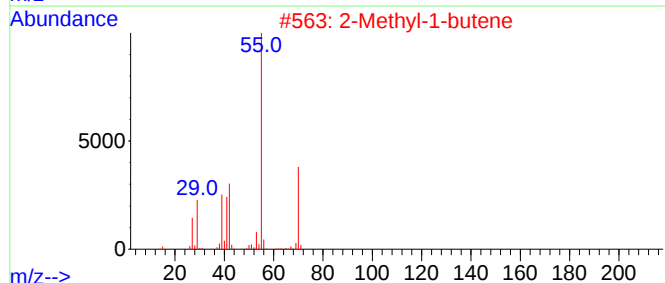
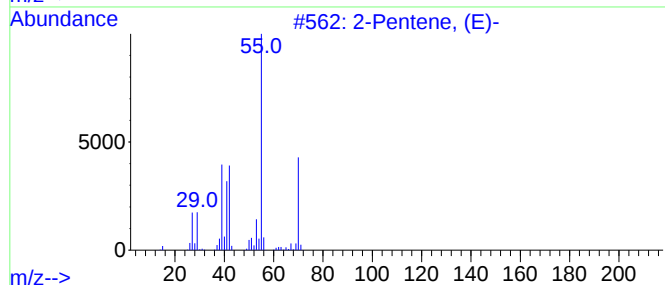
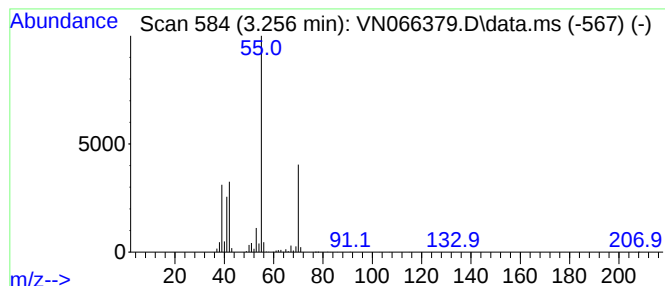
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.256	19.49 ug/l	1330720	Pentafluorobenzene	7.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentene, (E)-	70	C5H10	000646-04-8	94
2			2-Methyl-1-butene	70	C5H10	000563-46-2	91
3			2-Pentene	70	C5H10	000109-68-2	91
4			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
5			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87



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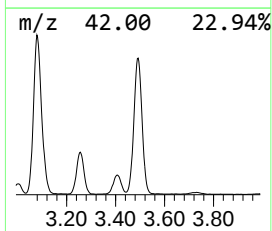
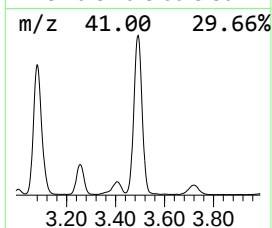
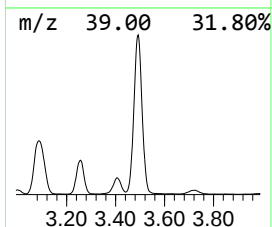
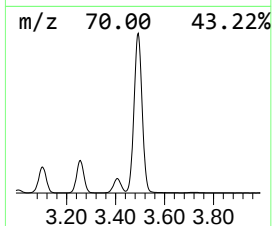
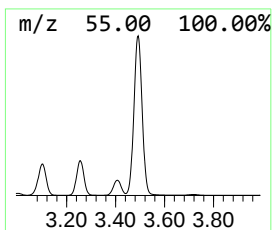
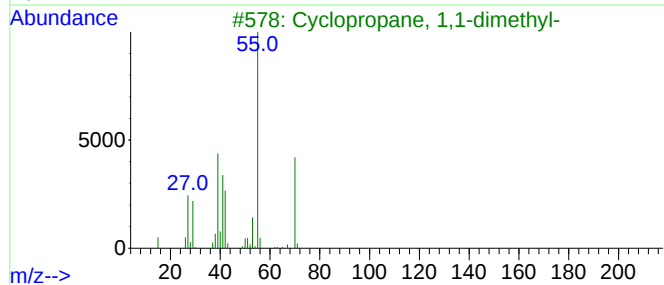
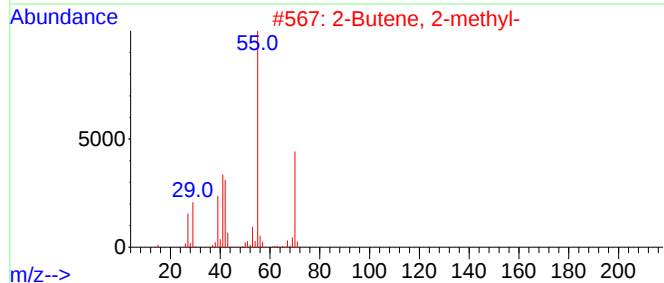
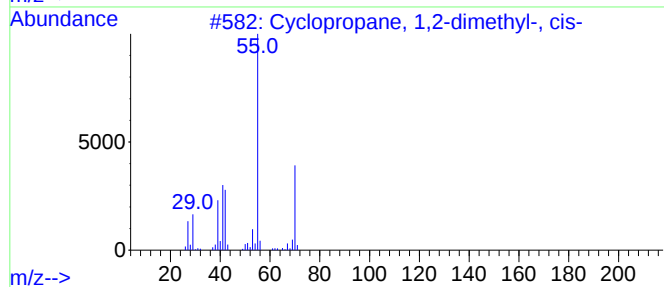
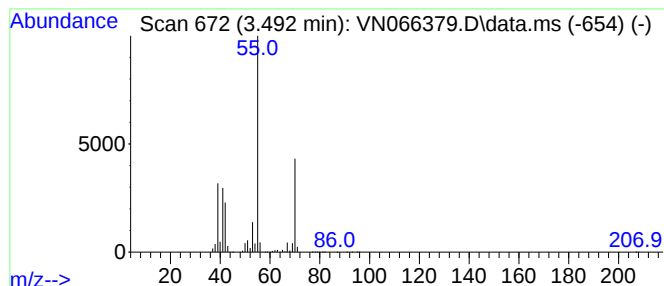
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.492	101.13 ug/l	6904310	Pentafluorobenzene	7.585

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	87
3			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
4			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	76
5			2-Methyl-1-butene	70	C5H10	000563-46-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066379.D
Acq On : 29 Mar 2021 16:11
Operator : JC/MD
Sample : M1835-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
LMW01

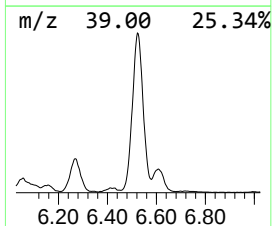
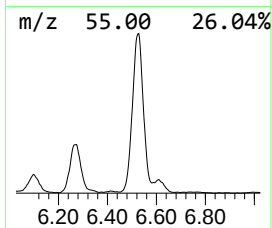
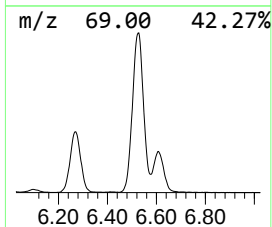
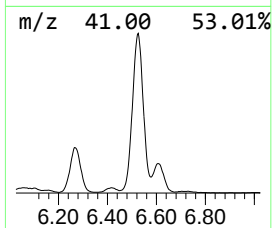
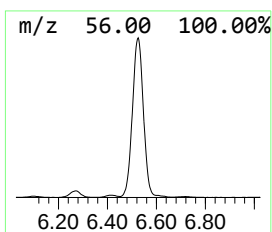
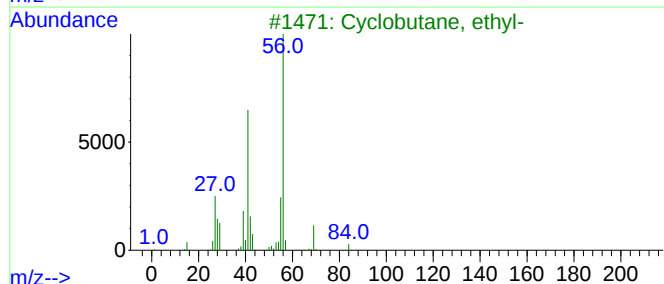
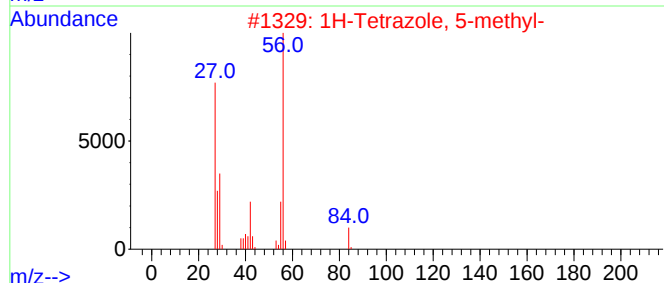
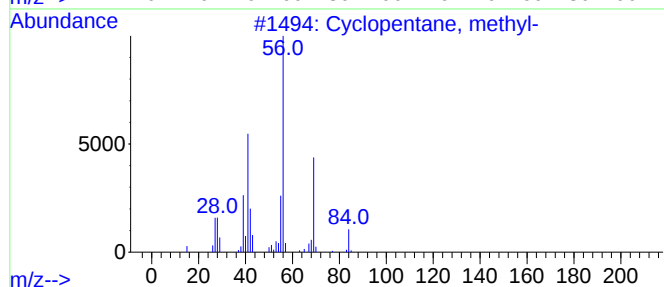
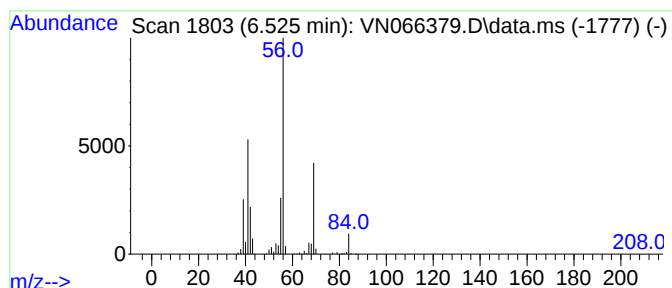
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.525	60.24 ug/l	4112560	Pentafluorobenzene	7.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			Cyclobutane	56	C4H8	000287-23-0	50
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066379.D
Acq On : 29 Mar 2021 16:11
Operator : JC/MD
Sample : M1835-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
LMW01

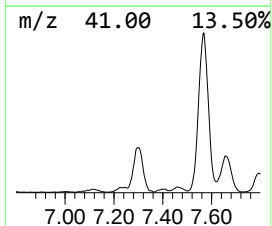
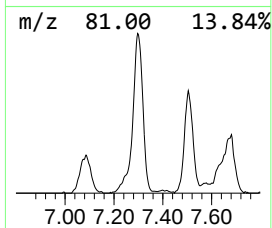
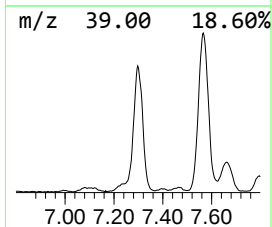
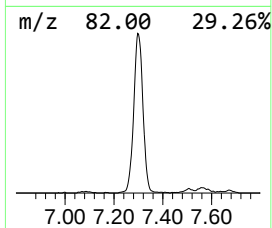
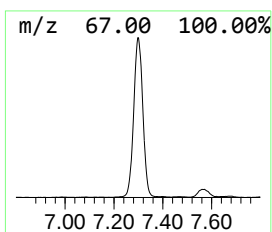
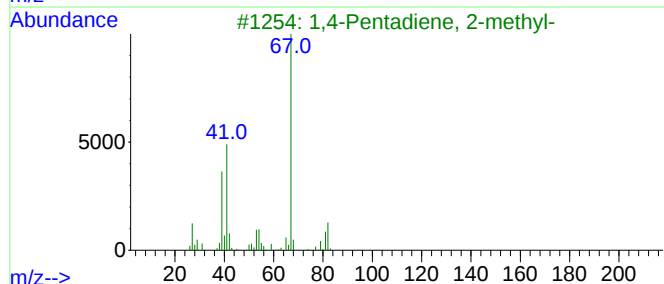
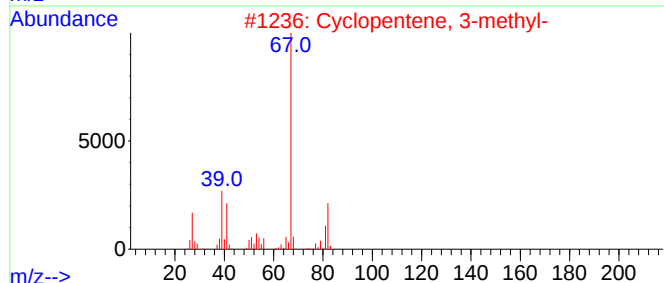
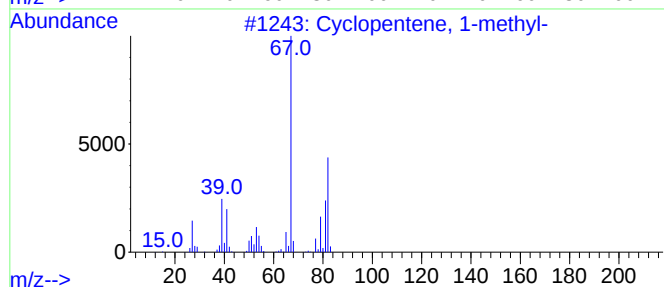
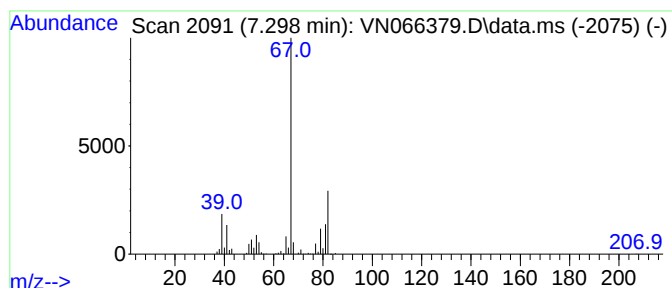
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclopentene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.298	19.56 ug/l	1335650	Pentafluorobenzene	7.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	90
2			Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	86
3			1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	83
4			Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	83
5			1,4-Pentadiene, 3-methyl-	82	C6H10	001115-08-8	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066379.D
Acq On : 29 Mar 2021 16:11
Operator : JC/MD
Sample : M1835-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
LMW01

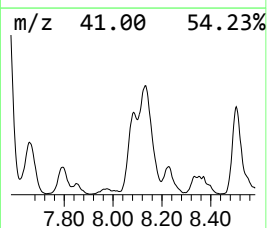
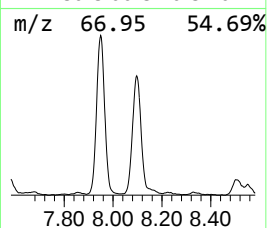
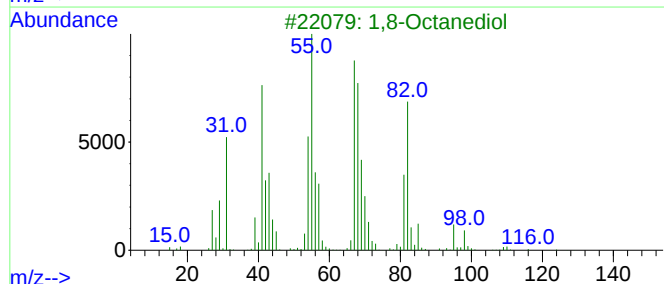
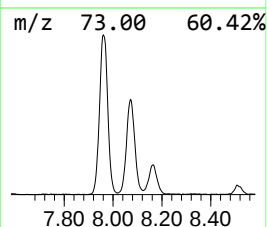
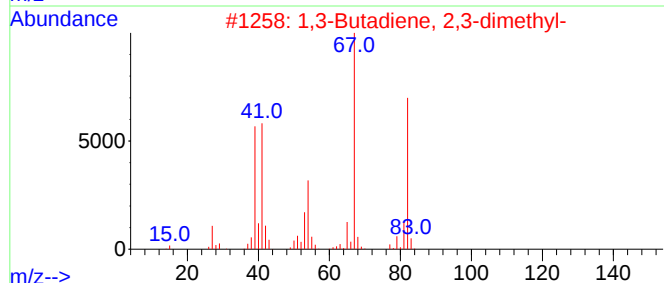
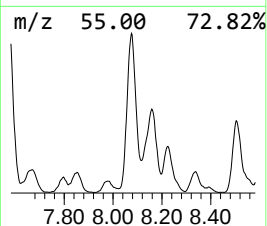
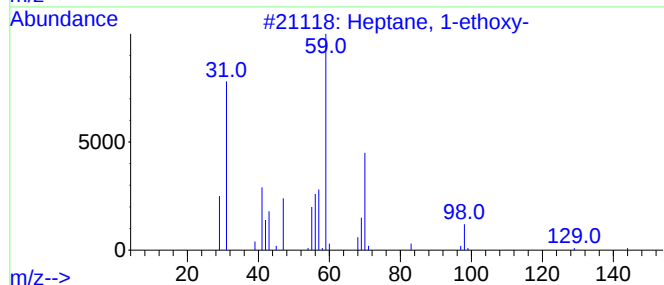
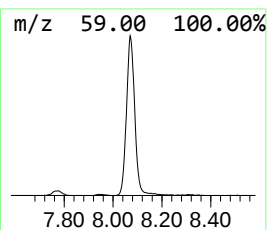
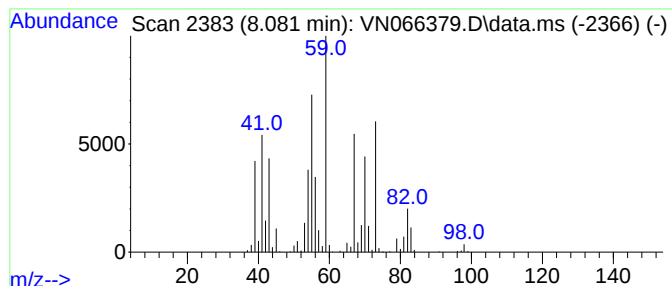
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown8.081 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	22.70 ug/l	1287690	1,4-Difluorobenzene	8.512

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 1-ethoxy-	144	C9H20O	001969-43-3	35
2			1,3-Butadiene, 2,3-dimethyl-	82	C6H10	000513-81-5	30
3			1,8-Octanediol	146	C8H18O2	000629-41-4	27
4			Ethylidenecyclobutane	82	C6H10	001528-21-8	25
5			Cyclohexene	82	C6H10	000110-83-8	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066379.D
Acq On : 29 Mar 2021 16:11
Operator : JC/MD
Sample : M1835-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
LMW01

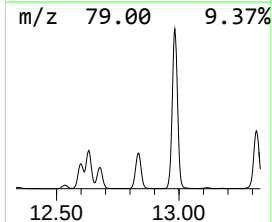
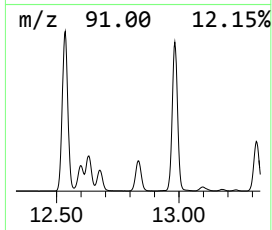
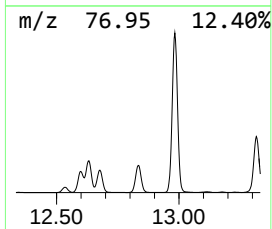
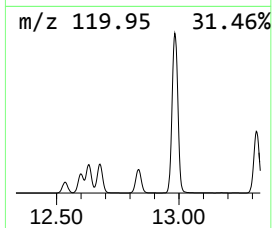
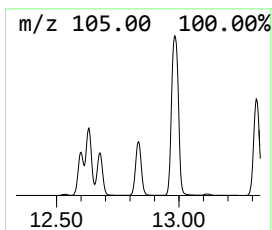
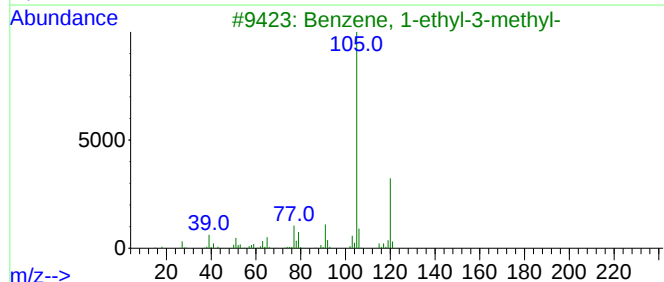
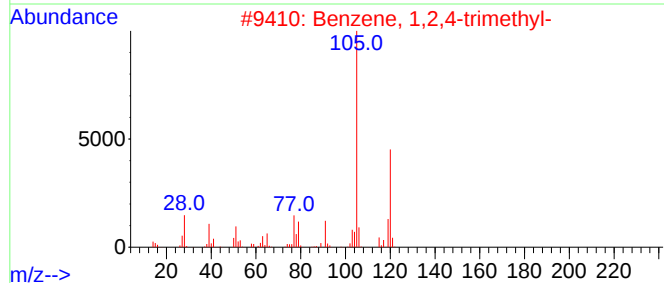
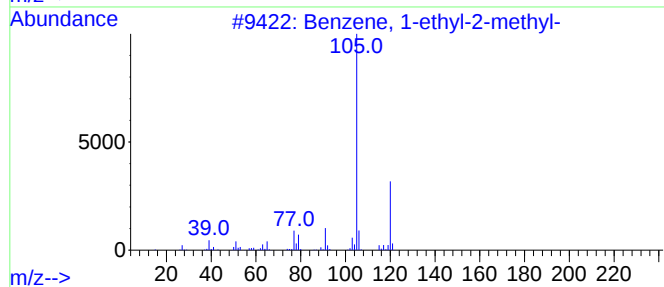
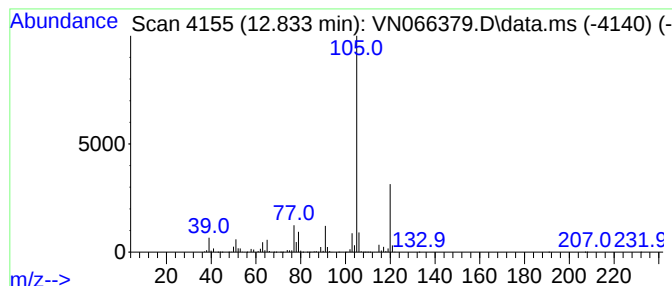
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.833	21.71 ug/l	6425410	1,4-Dichlorobenzene-d4	13.286

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066379.D
Acq On : 29 Mar 2021 16:11
Operator : JC/MD
Sample : M1835-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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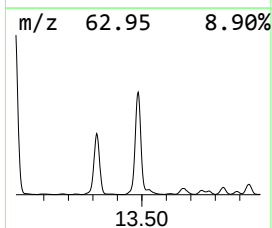
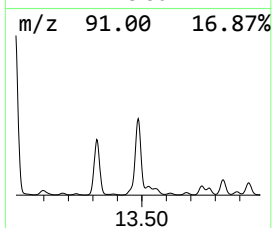
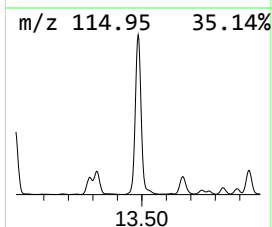
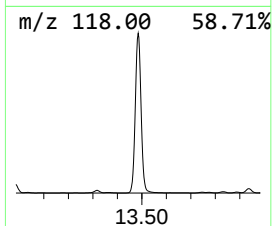
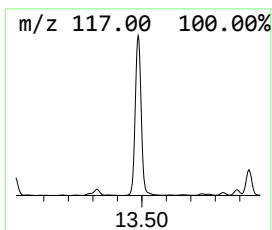
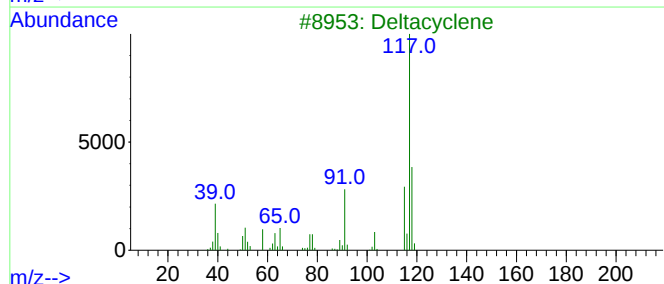
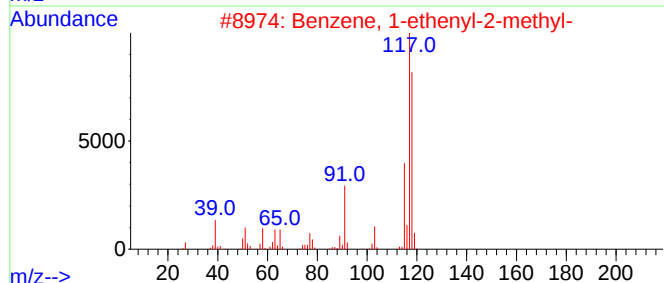
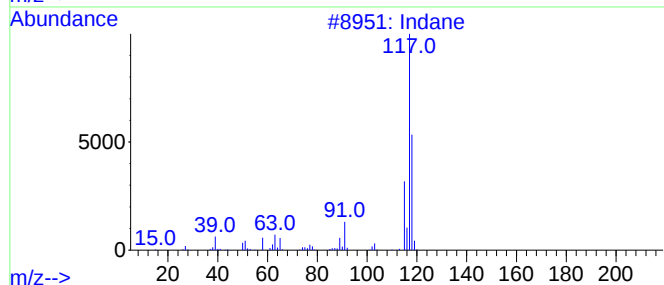
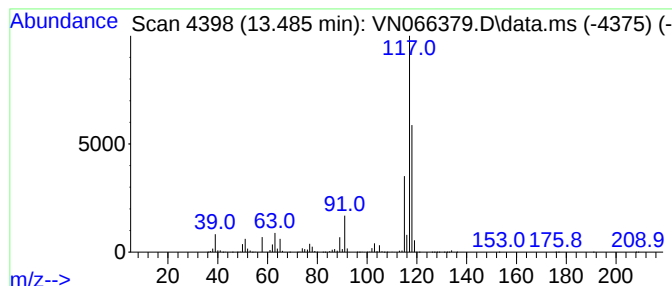
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.485	46.69 ug/l	13817100	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
3			Deltacyclene	118	C9H10	007785-10-6	74
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066379.D
Acq On : 29 Mar 2021 16:11
Operator : JC/MD
Sample : M1835-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
LMW01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.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-	2.752	139.7	ug/l	9534370	1	7.585	3413470	50.0
Pentane	3.082	53.9	ug/l	3678720	1	7.585	3413470	50.0
2-Pentene, (E)-	3.256	19.5	ug/l	1330720	1	7.585	3413470	50.0
Cyclopropane, 1...	3.492	101.1	ug/l	6904310	1	7.585	3413470	50.0
Cyclopentane, m...	6.525	60.2	ug/l	4112560	1	7.585	3413470	50.0
Cyclopentene, 1...	7.298	19.6	ug/l	1335650	1	7.585	3413470	50.0
unknown8.081	8.081	22.7	ug/l	1287690	2	8.512	2836470	50.0
Benzene, 1-ethy...	12.833	21.7	ug/l	6425410	4	13.286	14795300	50.0
Indane	13.485	46.7	ug/l	13817100	4	13.286	14795300	50.0