

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
 Data File : VN066380.D
 Acq On : 29 Mar 2021 16:34
 Operator : JC/MD
 Sample : M1835-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 ASR7

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: VN066380.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	145	168	187	rBV	4232347	7552619	4.14%	0.945%
2	2.751	377	396	420	rBV	6019809	11910549	6.53%	1.490%
3	3.087	502	521	554	rVB4	2225498	6333412	3.47%	0.792%
4	3.256	566	584	609	rVB	1810727	3756367	2.06%	0.470%
5	3.406	622	640	654	rBV	953904	2105675	1.15%	0.263%
6	3.492	655	672	699	rVB	3810961	8762350	4.80%	1.096%
7	4.328	959	984	1003	rBV	1146735	3341993	1.83%	0.418%
8	4.943	1173	1213	1310	rBV	43022273	182438494	100.00%	22.818%
9	6.525	1778	1803	1824	rBV3	1166827	3665442	2.01%	0.458%
10	7.576	2180	2195	2213	rVB7	1094645	3067833	1.68%	0.384%
11	7.965	2313	2340	2366	rBV	45271722	118600599	65.01%	14.833%
12	8.161	2402	2413	2461	rVB	2804036	7509729	4.12%	0.939%
13	8.512	2522	2544	2570	rBV3	1243592	2994984	1.64%	0.375%
14	10.030	3094	3110	3120	rBV2	1913764	4176864	2.29%	0.522%
15	10.092	3120	3133	3164	rVB	20674733	41387145	22.69%	5.176%
16	11.347	3584	3601	3624	rBV2	1352944	2754990	1.51%	0.345%
17	11.454	3624	3641	3663	rVV	37371239	65492426	35.90%	8.191%
18	11.567	3664	3683	3722	rVB	68506771	143133532	78.46%	17.902%
19	11.892	3787	3804	3830	rVB	13418634	22756869	12.47%	2.846%
20	12.192	3902	3916	3930	rBV	1667138	2661240	1.46%	0.333%
21	12.345	3958	3973	4001	rBV	1056987	1865490	1.02%	0.233%
22	12.535	4029	4044	4055	rBV	3346888	5299767	2.90%	0.663%
23	12.600	4055	4068	4075	rVV	8442801	14137884	7.75%	1.768%
24	12.632	4076	4080	4088	rVV	6111751	7938215	4.35%	0.993%
25	12.677	4088	4097	4120	rVB	8395173	13153497	7.21%	1.645%
26	12.836	4140	4156	4185	rBV	5279209	8661050	4.75%	1.083%
27	12.983	4195	4211	4242	rBV	24452300	40891208	22.41%	5.114%
28	13.316	4312	4335	4373	rVB	10433996	18796306	10.30%	2.351%
29	13.485	4375	4398	4409	rBV	10643546	18856205	10.34%	2.358%
30	13.670	4455	4467	4483	rVB2	886909	1885172	1.03%	0.236%
31	13.831	4516	4527	4540	rVB	1663811	2494620	1.37%	0.312%
32	13.935	4556	4566	4582	rVB2	1266846	2022929	1.11%	0.253%
33	14.190	4654	4661	4673	rVB	1694684	2513177	1.38%	0.314%
34	14.533	4773	4789	4804	rBV3	2433384	4598535	2.52%	0.575%
35	15.070	4973	4989	5013	rBV	6633518	12029334	6.59%	1.505%

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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

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

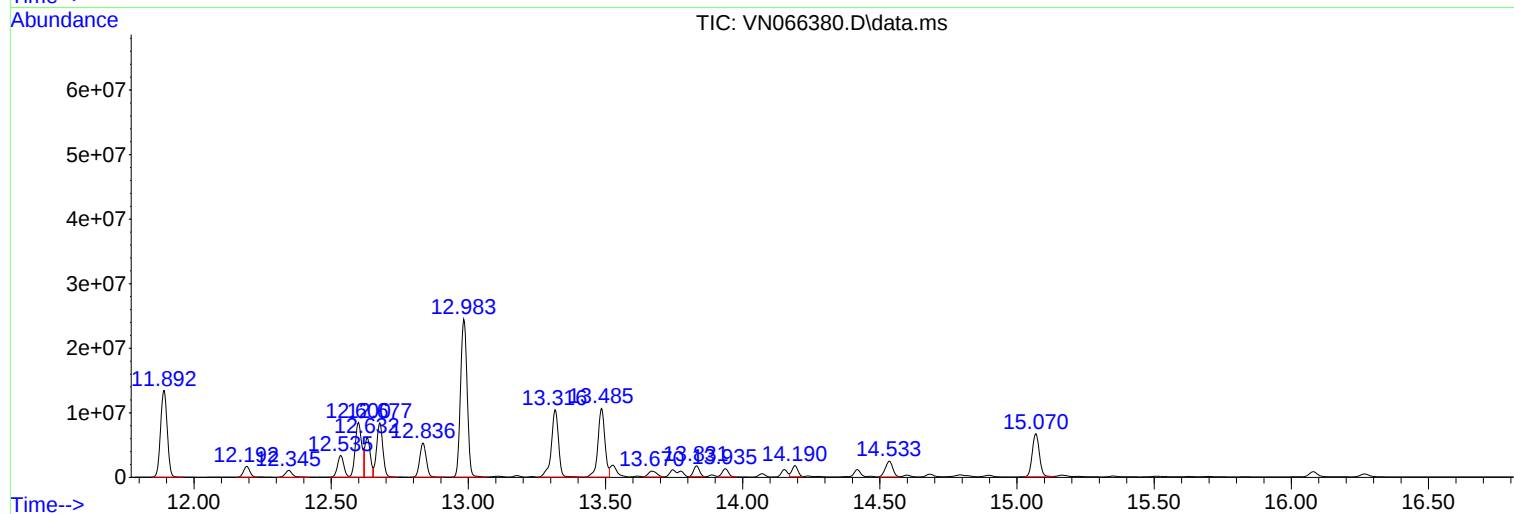
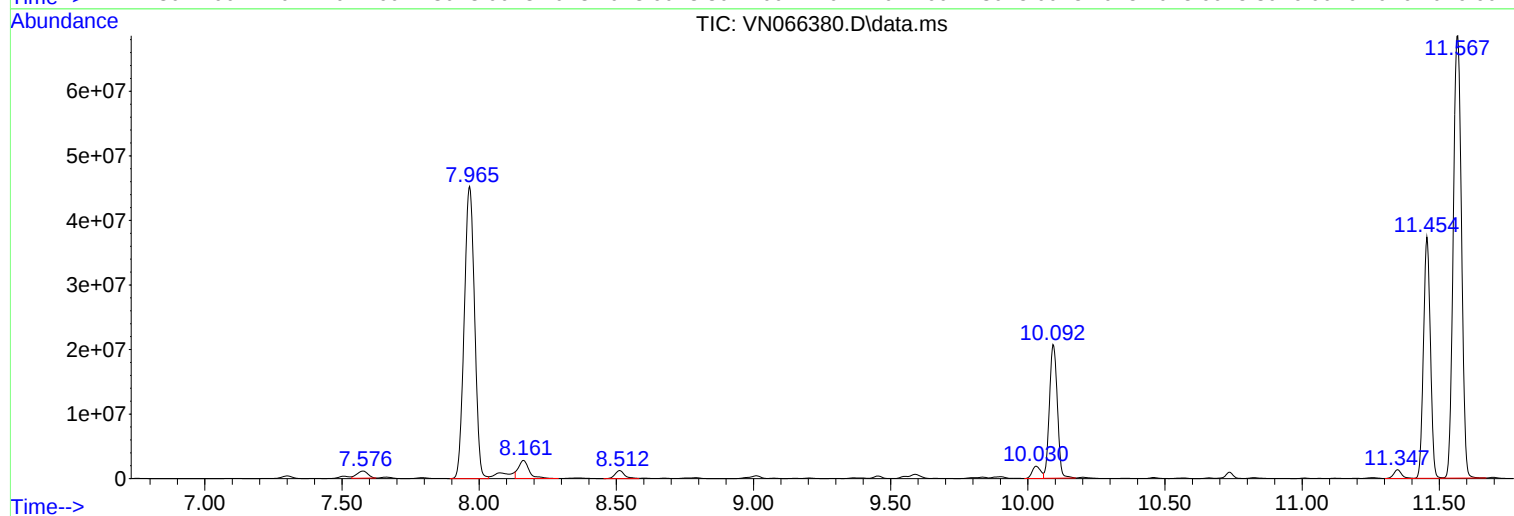
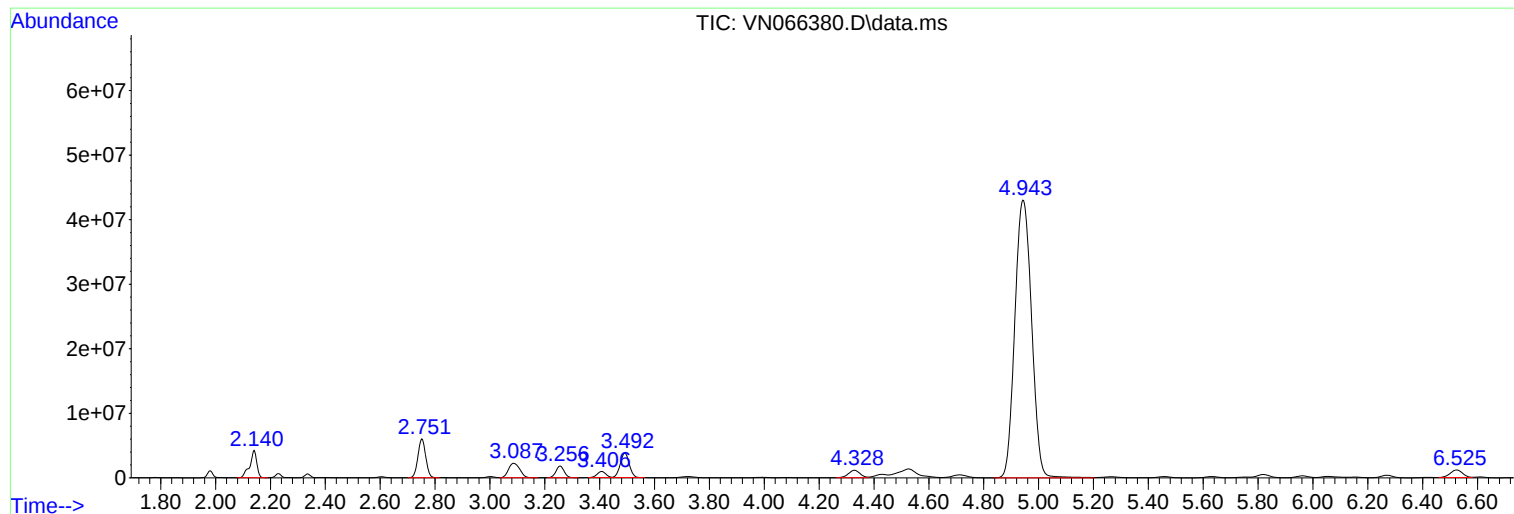
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

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



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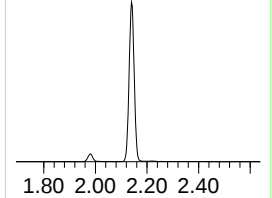
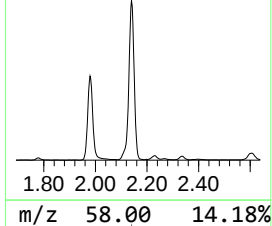
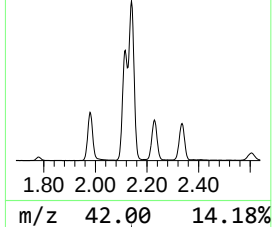
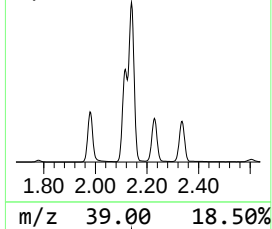
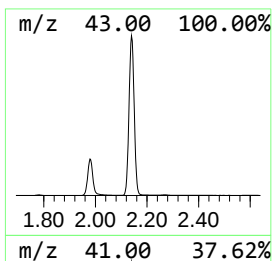
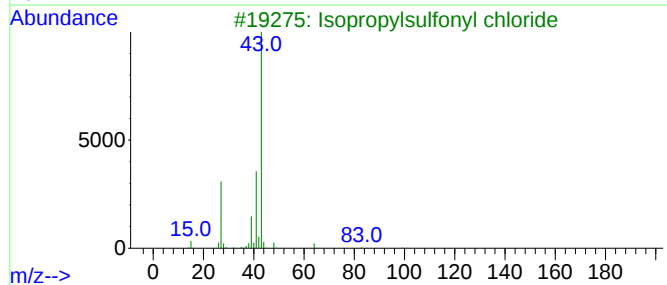
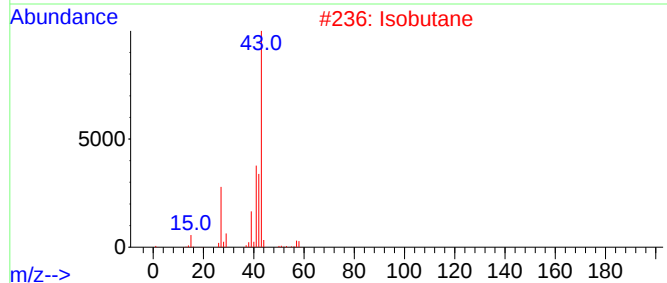
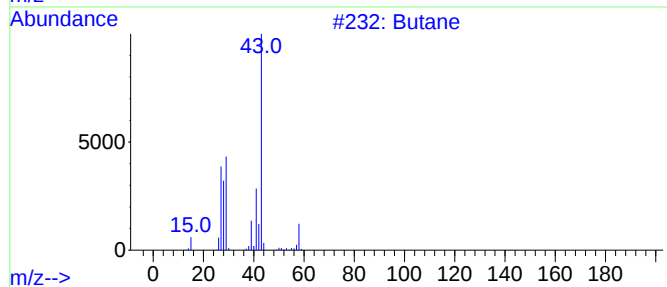
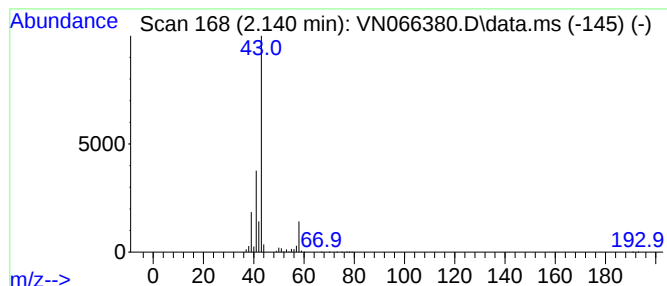
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	123.09 ug/l	7552620	Pentafluorobenzene	7.584

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Isobutane	58	C4H10	000075-28-5	9
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Diazene, dimethyl-	58	C2H6N2	000503-28-6	4



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ALS Vial : 18 Sample Multiplier: 1

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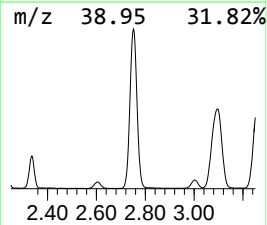
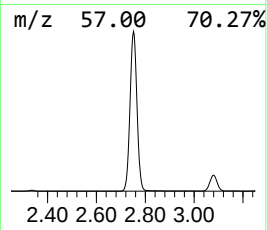
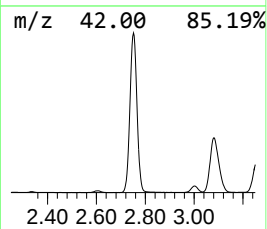
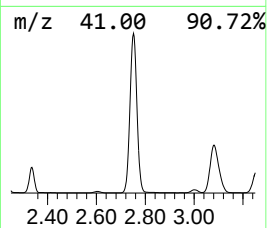
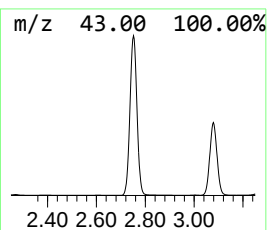
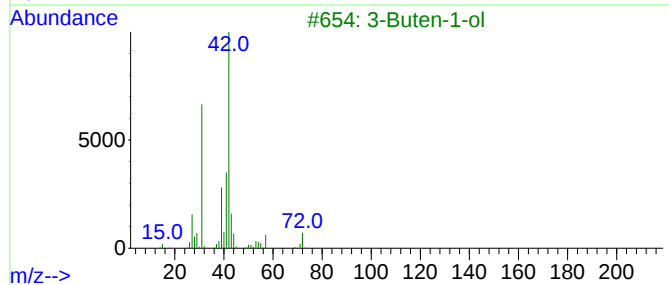
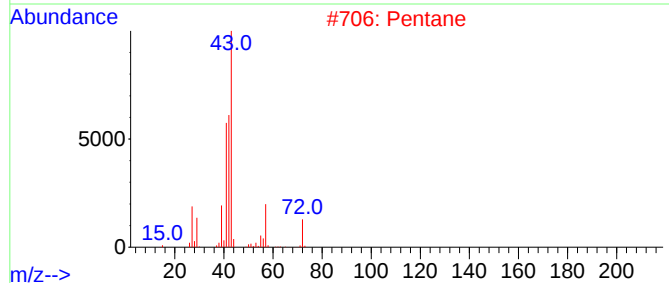
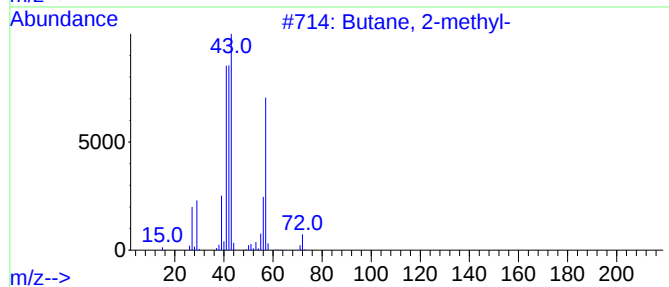
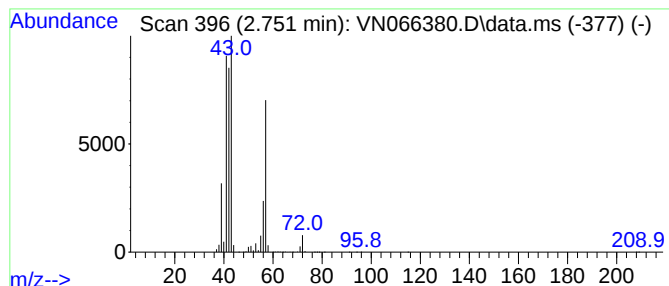
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.751	194.12 ug/l	11910500	Pentafluorobenzene	7.584

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	94
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	9
5	1-Propene, 2-methyl-			56	C4H8	000115-11-7	9



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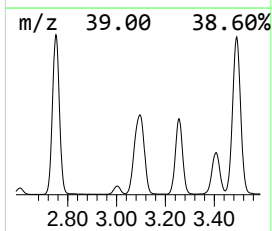
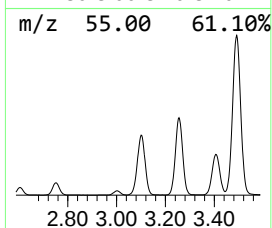
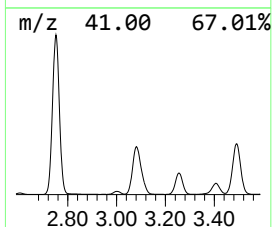
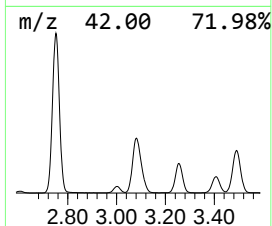
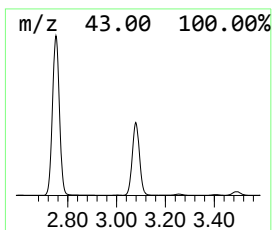
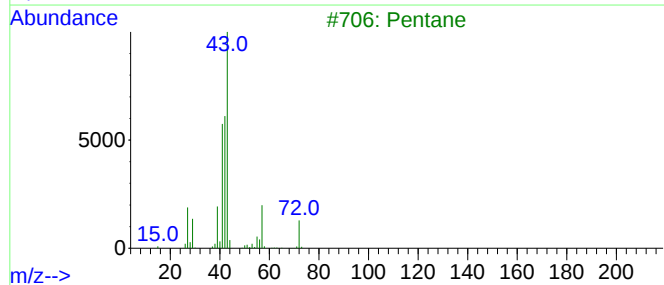
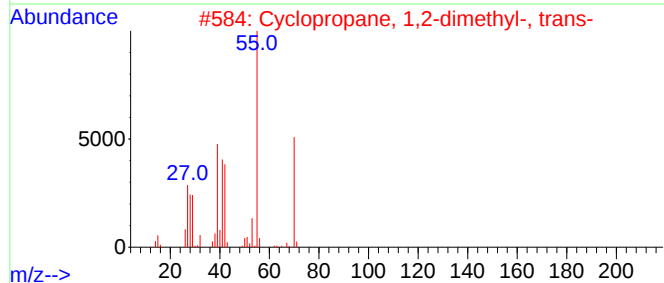
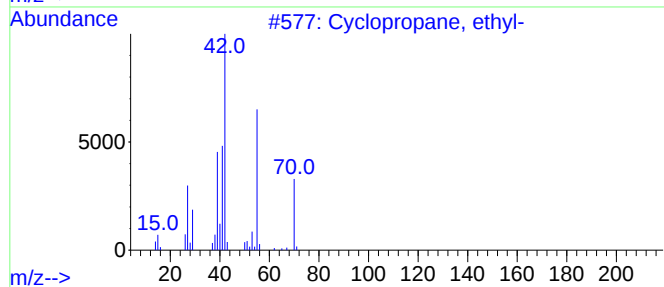
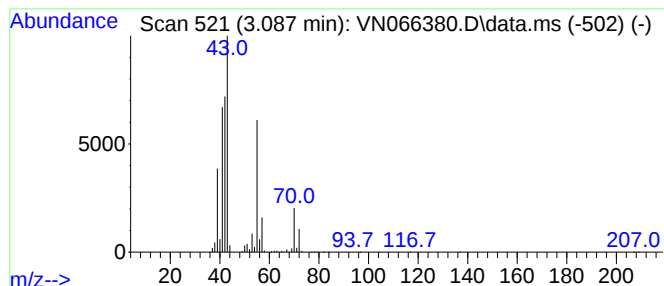
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Quant Title : SW846 8260

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

Peak Number 3 Cyclopropane, ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	103.22 ug/l	6333410	Pentafluorobenzene	7.584

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, ethyl-	70	C5H10	001191-96-4	58
2			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	49
3			Pentane	72	C5H12	000109-66-0	46
4			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	38
5			1-Pentene	70	C5H10	000109-67-1	38



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ALS Vial : 18 Sample Multiplier: 1

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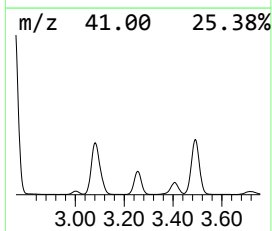
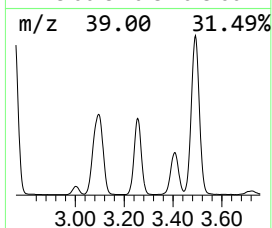
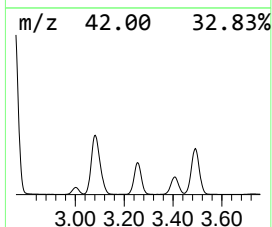
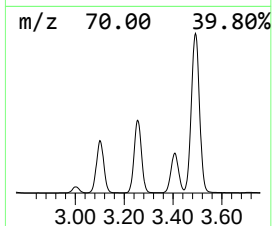
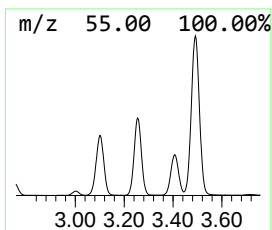
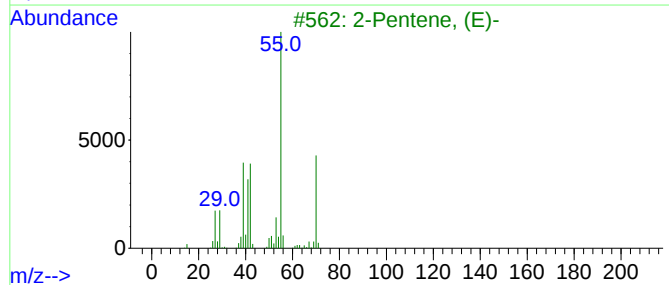
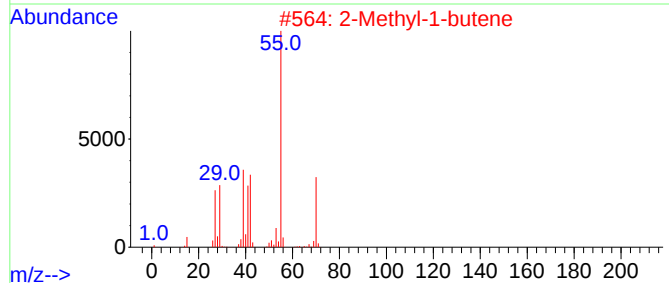
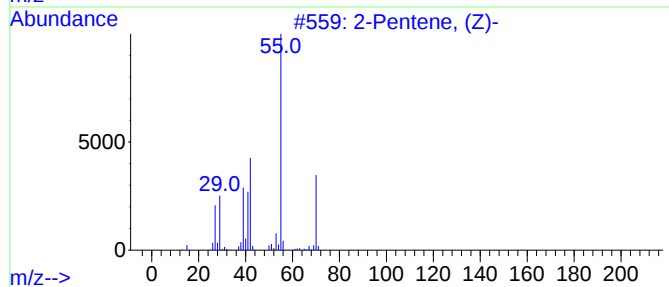
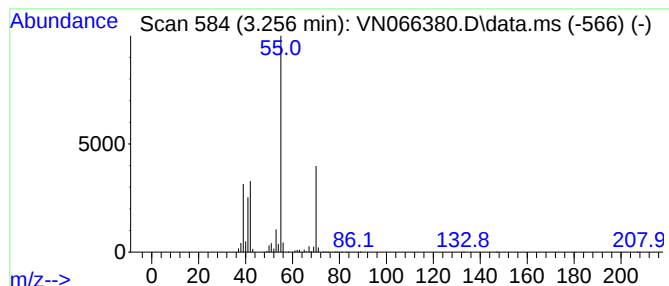
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentene, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.256	61.22 ug/l	3756370	Pentafluorobenzene	7.584

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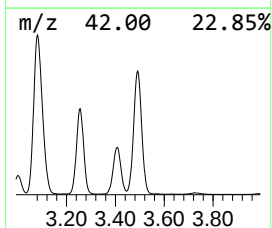
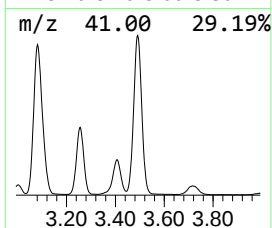
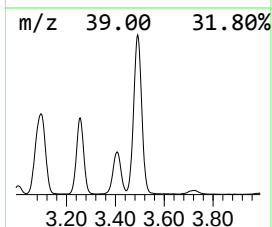
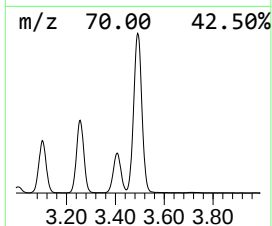
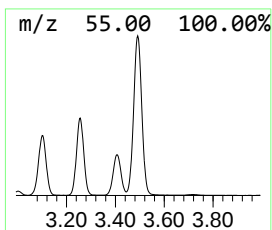
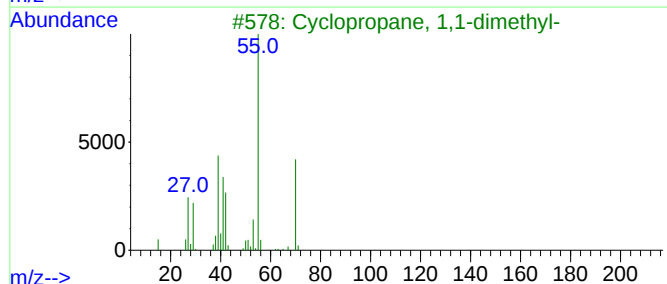
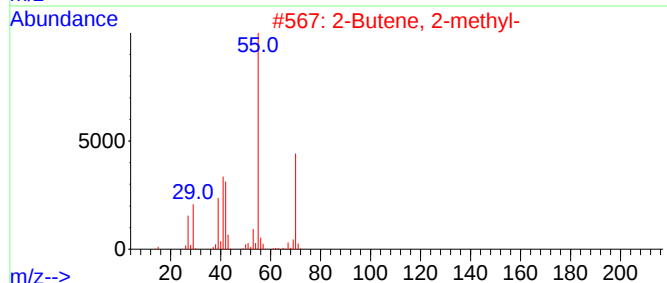
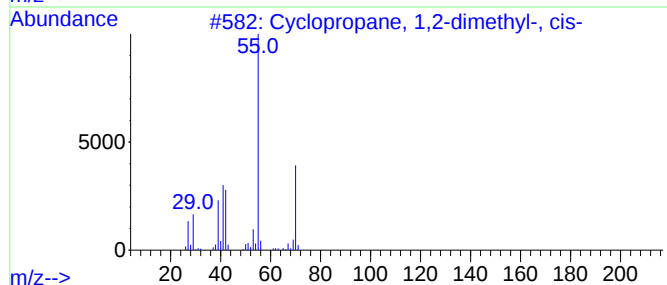
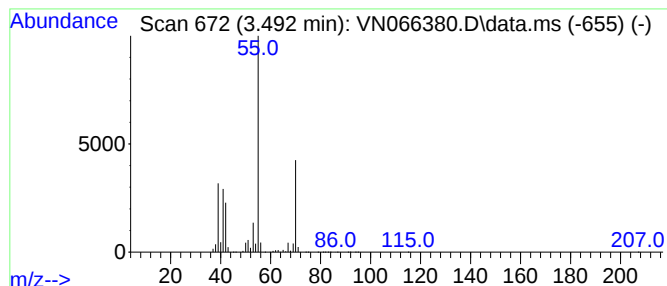
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.492	142.81 ug/l	8762350	Pentafluorobenzene	7.584

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	80
5			2-Pentene	70	C5H10	000109-68-2	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066380.D
Acq On : 29 Mar 2021 16:34
Operator : JC/MD
Sample : M1835-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR7

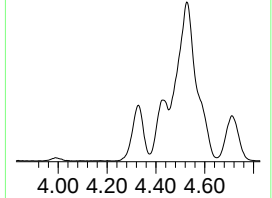
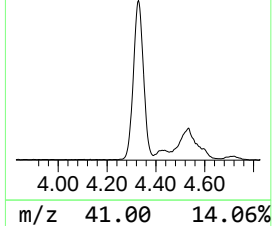
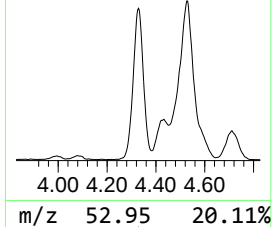
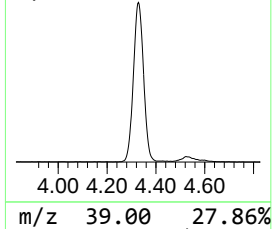
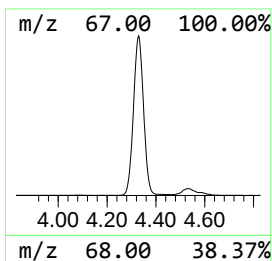
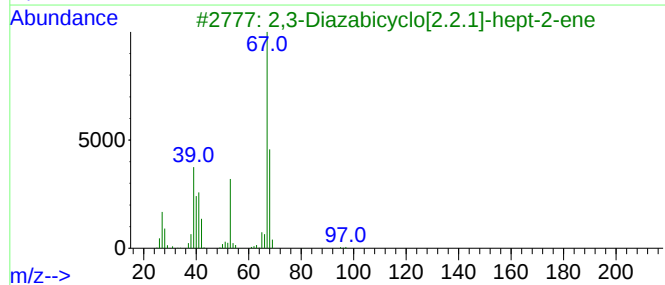
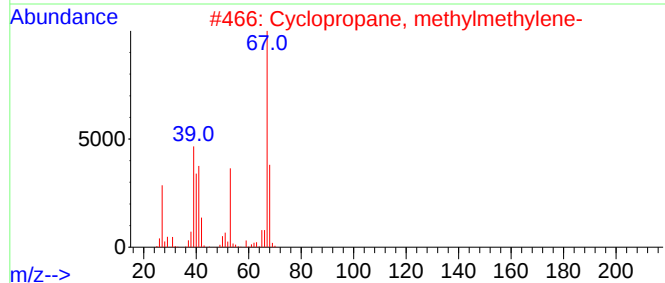
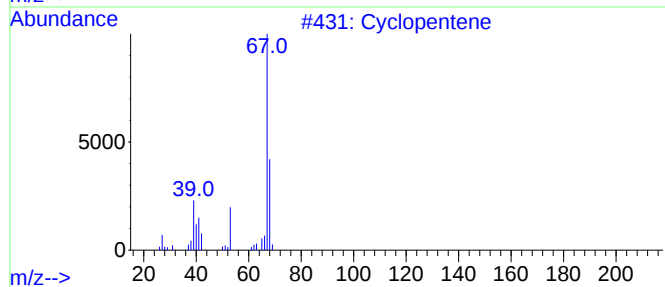
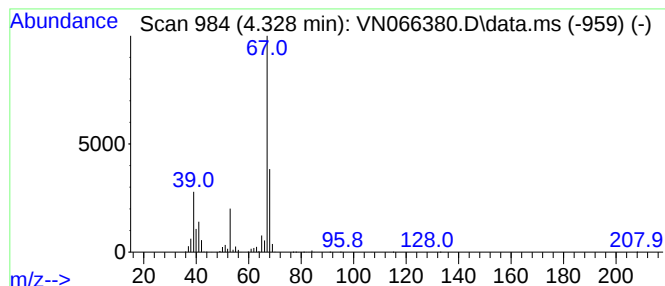
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.328	54.47 ug/l	3341990	Pentafluorobenzene	7.584

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene	68	C5H8	000142-29-0	91
2			Cyclopropane, methylmethylene-	68	C5H8	018631-84-0	91
3			2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	83
4			1-Butyne, 3-methyl-	68	C5H8	000598-23-2	59
5			1,4-Pentadiene	68	C5H8	000591-93-5	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066380.D
Acq On : 29 Mar 2021 16:34
Operator : JC/MD
Sample : M1835-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR7

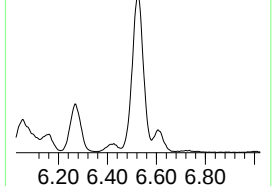
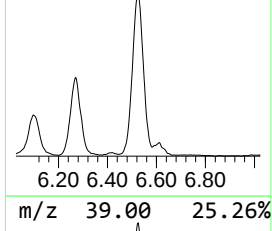
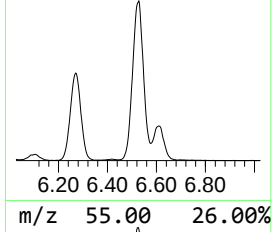
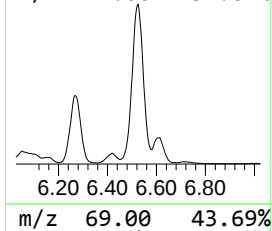
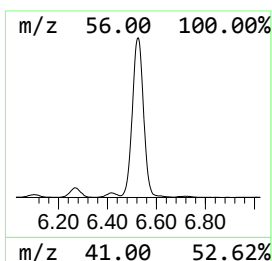
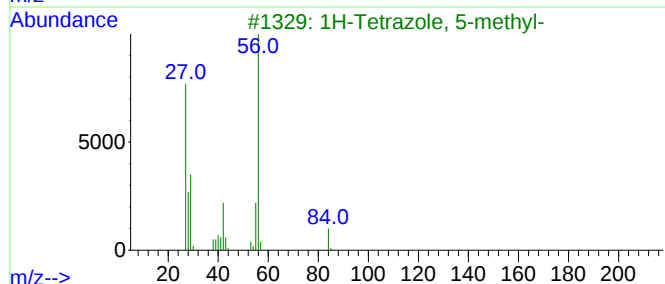
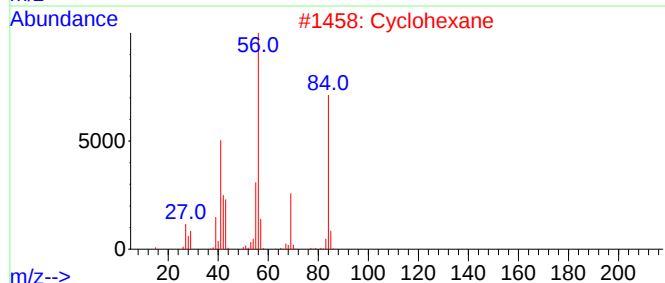
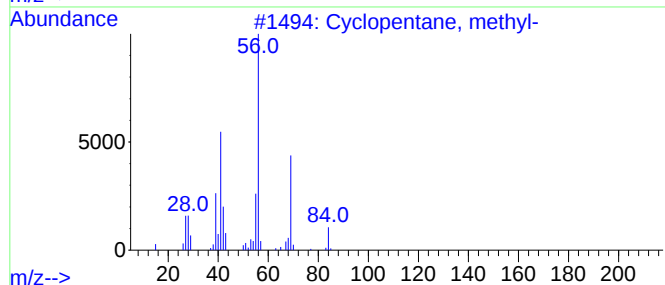
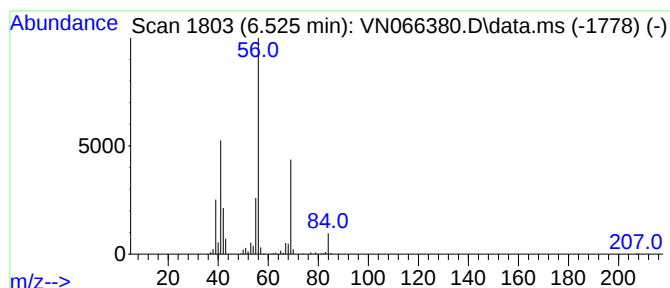
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.525	59.74 ug/l	3665440	Pentafluorobenzene	7.584

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclohexane	84	C6H12	000110-82-7	83
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5			Cyclopropane, propyl-	84	C6H12	002415-72-7	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066380.D
Acq On : 29 Mar 2021 16:34
Operator : JC/MD
Sample : M1835-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR7

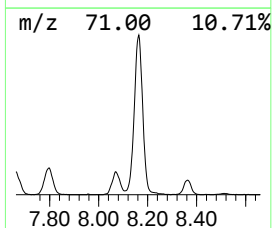
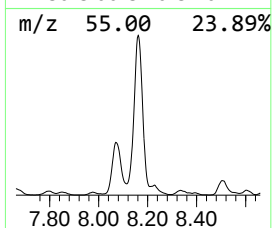
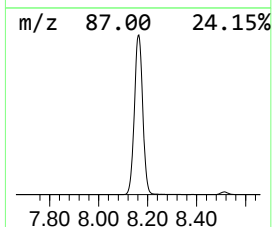
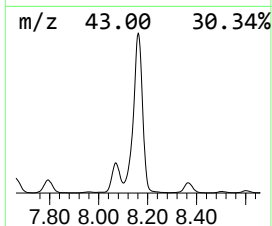
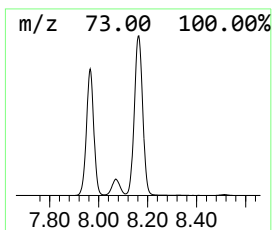
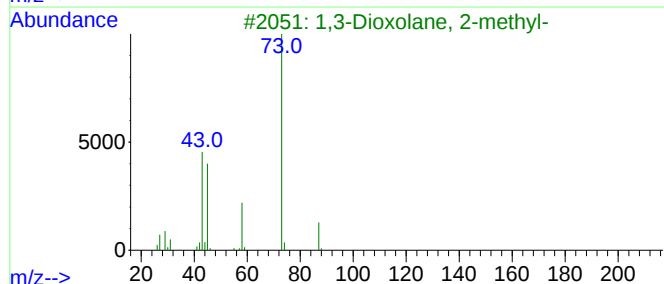
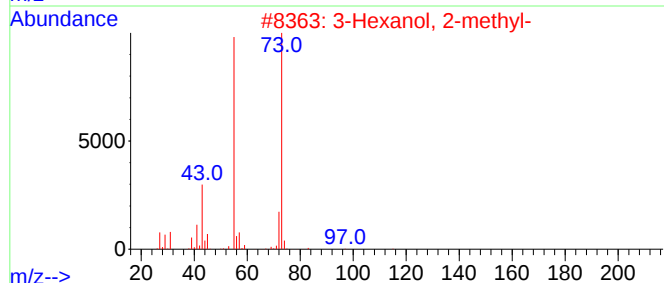
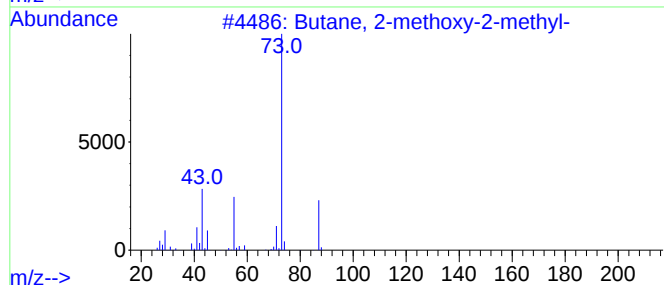
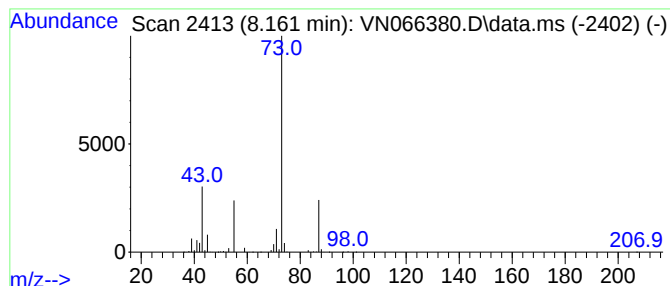
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Quant Title : SW846 8260

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

Peak Number 8 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.161	125.37 ug/l	7509730	1,4-Difluorobenzene	8.512

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066380.D
Acq On : 29 Mar 2021 16:34
Operator : JC/MD
Sample : M1835-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR7

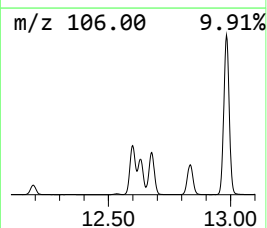
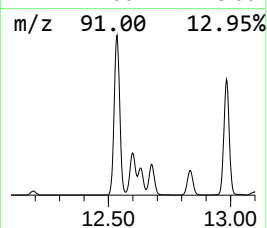
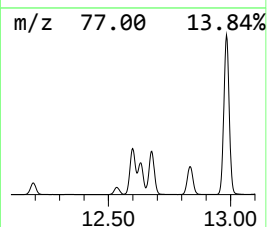
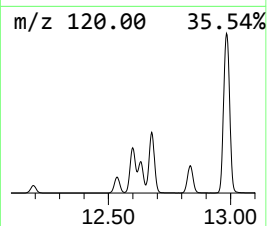
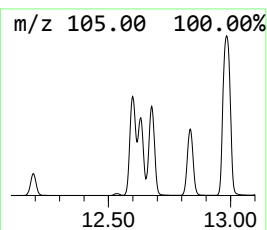
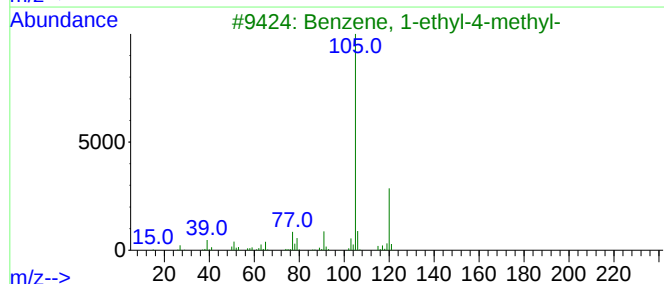
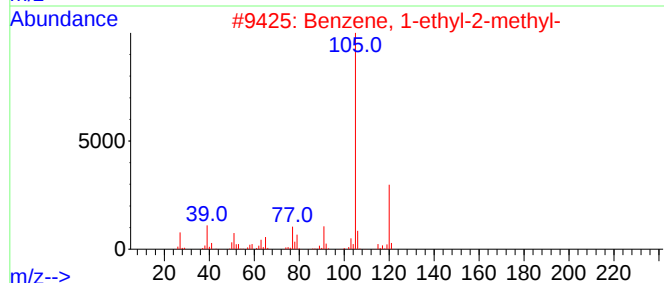
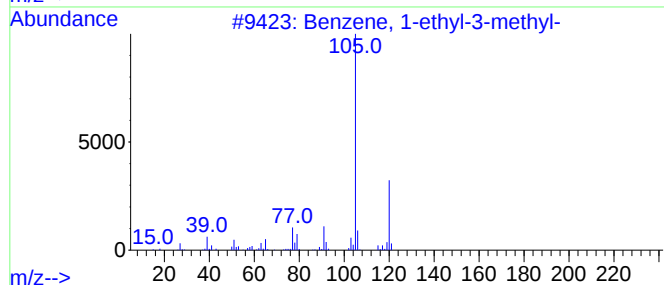
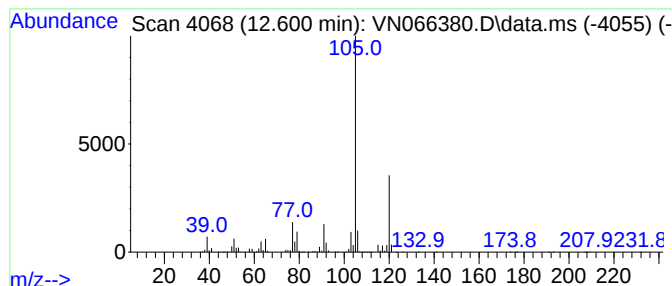
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.600	37.61 ug/l	14137900	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066380.D
Acq On : 29 Mar 2021 16:34
Operator : JC/MD
Sample : M1835-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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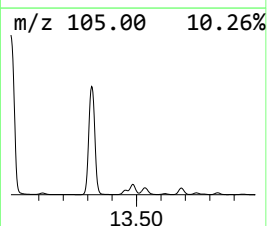
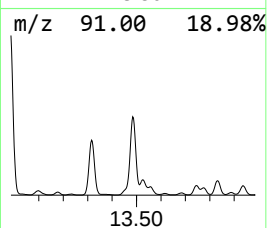
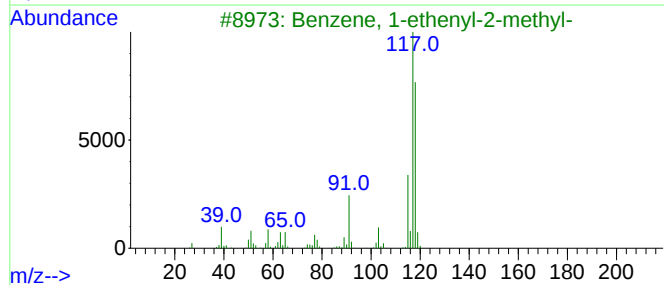
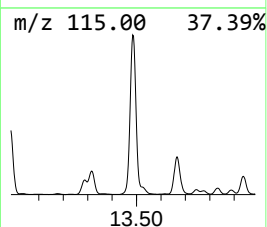
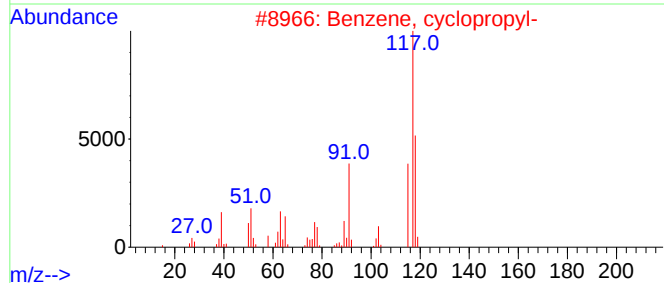
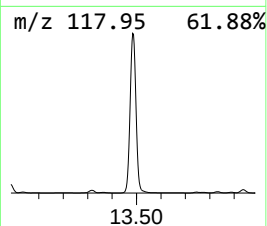
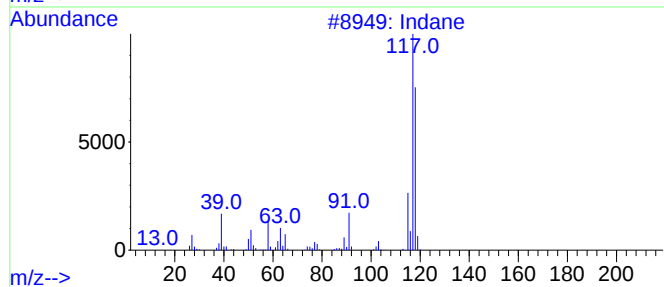
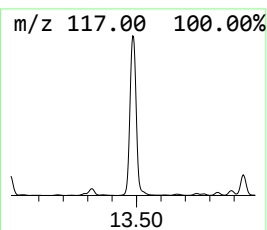
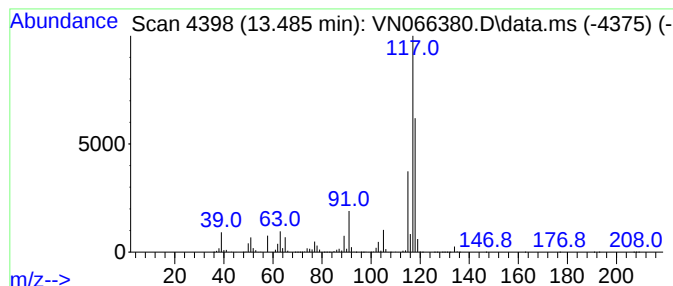
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.485	50.16 ug/l	18856200	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	90
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	89
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066380.D
Acq On : 29 Mar 2021 16:34
Operator : JC/MD
Sample : M1835-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR7

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-	2.751	194.1	ug/l	11910500	1	7.584	3067830	50.0
Cyclopropane, e...	3.087	103.2	ug/l	6333410	1	7.584	3067830	50.0
2-Pentene, (Z)-	3.256	61.2	ug/l	3756370	1	7.584	3067830	50.0
Cyclopropane, 1...	3.492	142.8	ug/l	8762350	1	7.584	3067830	50.0
Cyclopentene	4.328	54.5	ug/l	3341990	1	7.584	3067830	50.0
Cyclopentane, m...	6.525	59.7	ug/l	3665440	1	7.584	3067830	50.0
Butane, 2-metho...	8.161	125.4	ug/l	7509730	2	8.512	2994980	50.0
Benzene, 1-ethy...	12.600	37.6	ug/l	14137900	4	13.286	18796300	50.0
Indane	13.485	50.2	ug/l	18856200	4	13.286	18796300	50.0