

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
 Data File : VN071100.D
 Acq On : 28 Feb 2022 17:32
 Operator : JC\MD
 Sample : N1689-03 10X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-39

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\82N021522W.M
 Title : SW846 8260

Signal : TIC: VN071100.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.440	69	77	87	rVB	105400	202508	1.11%	0.210%
2	3.128	186	194	207	rVB	136240	332040	1.82%	0.344%
3	3.999	332	342	354	rVB2	89064	249558	1.36%	0.259%
4	5.622	602	618	631	rBV3	61947	231252	1.26%	0.240%
5	7.145	868	877	886	rBV3	108550	286635	1.57%	0.297%
6	8.016	1015	1025	1030	rBV2	488810	1152018	6.30%	1.194%
7	8.081	1030	1036	1046	rVB	1024264	2360516	12.91%	2.446%
8	8.451	1086	1099	1112	rBV2	2011322	5545030	30.32%	5.746%
9	8.963	1175	1186	1200	rBV	1440349	3020071	16.52%	3.130%
10	9.457	1256	1270	1282	rBV2	69235	203776	1.11%	0.211%
11	10.433	1428	1436	1442	rBV	2125337	3993078	21.84%	4.138%
12	10.498	1442	1447	1462	rVV	4781397	8854821	48.42%	9.176%
13	11.739	1650	1658	1667	rBV	1916424	3384529	18.51%	3.507%
14	11.839	1667	1675	1685	rVV	4918841	8292449	45.35%	8.594%
15	11.945	1685	1693	1712	rVB	9372759	18285857	100.00%	18.950%
16	12.275	1737	1749	1764	rBV	7725287	12913068	70.62%	13.382%
17	12.575	1793	1800	1807	rVB	206273	330945	1.81%	0.343%
18	12.727	1815	1826	1837	rBV	1557581	2686484	14.69%	2.784%
19	12.916	1852	1858	1863	rBV	504293	803601	4.39%	0.833%
20	12.980	1863	1869	1872	rVV	1268866	2288924	12.52%	2.372%
21	13.010	1872	1874	1878	rVV	929421	1296332	7.09%	1.343%
22	13.057	1878	1882	1895	rVB	815886	1330138	7.27%	1.378%
23	13.216	1901	1909	1919	rBV	1180843	1913901	10.47%	1.983%
24	13.363	1926	1934	1947	rVB	3944604	6332410	34.63%	6.562%
25	13.669	1980	1986	1989	rBV	1594146	2833250	15.49%	2.936%
26	13.698	1989	1991	2000	rVB	1325823	1864849	10.20%	1.933%
27	13.869	2008	2020	2037	rBV3	1022017	2287536	12.51%	2.371%
28	14.057	2046	2052	2058	rBV2	124149	230953	1.26%	0.239%
29	14.127	2058	2064	2066	rVV	133759	216795	1.19%	0.225%
30	14.210	2073	2078	2084	rVB	197756	309373	1.69%	0.321%
31	14.321	2092	2097	2107	rVB2	189886	323712	1.77%	0.335%
32	14.533	2125	2133	2136	rBV	119810	195139	1.07%	0.202%
33	14.574	2136	2140	2145	rVB	176301	268464	1.47%	0.278%
34	14.921	2191	2199	2206	rBV3	299450	681882	3.73%	0.707%
35	15.498	2290	2297	2305	rBV	515730	993563	5.43%	1.030%

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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\82N021522W.M
Title : SW846 8260

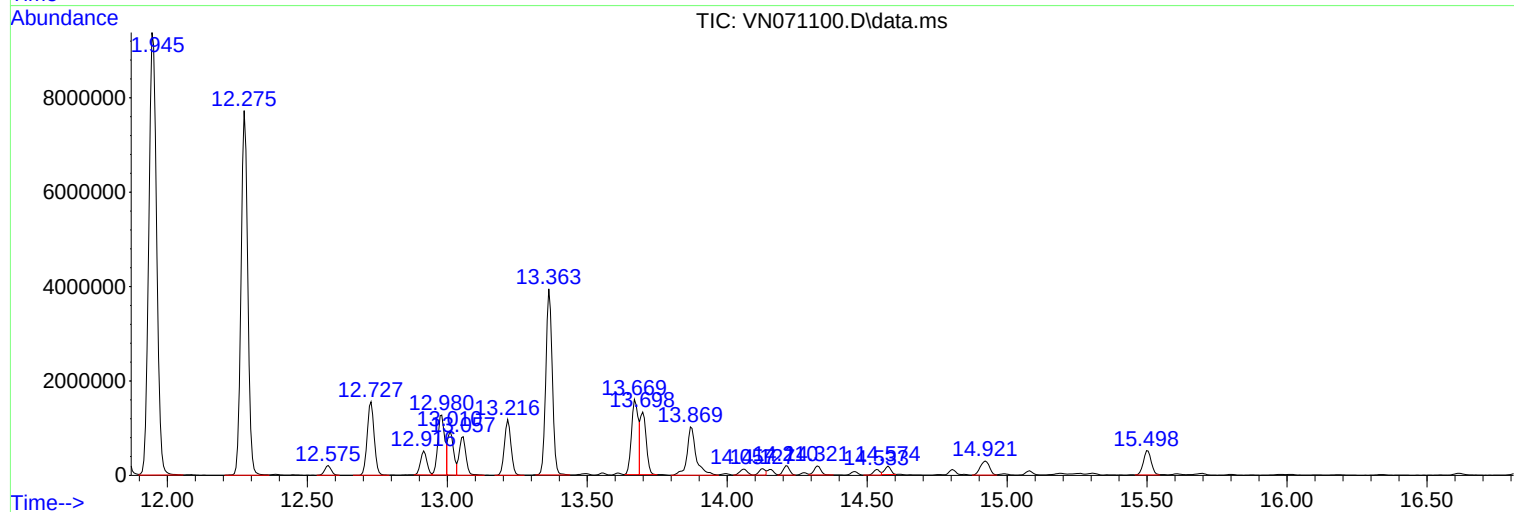
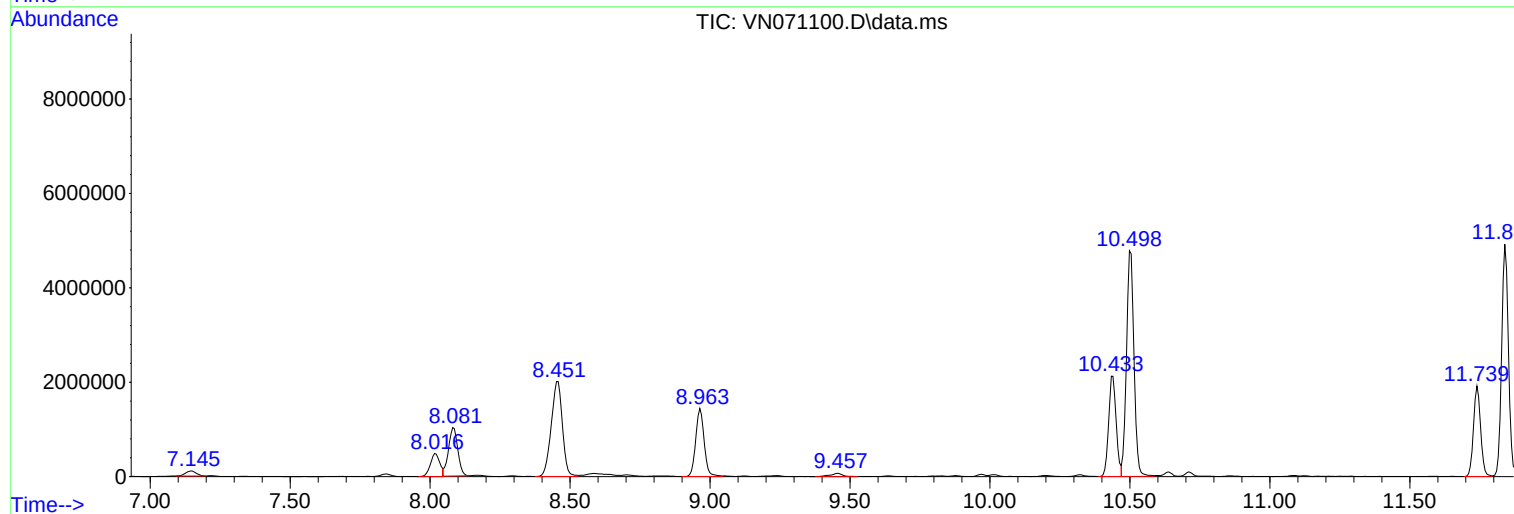
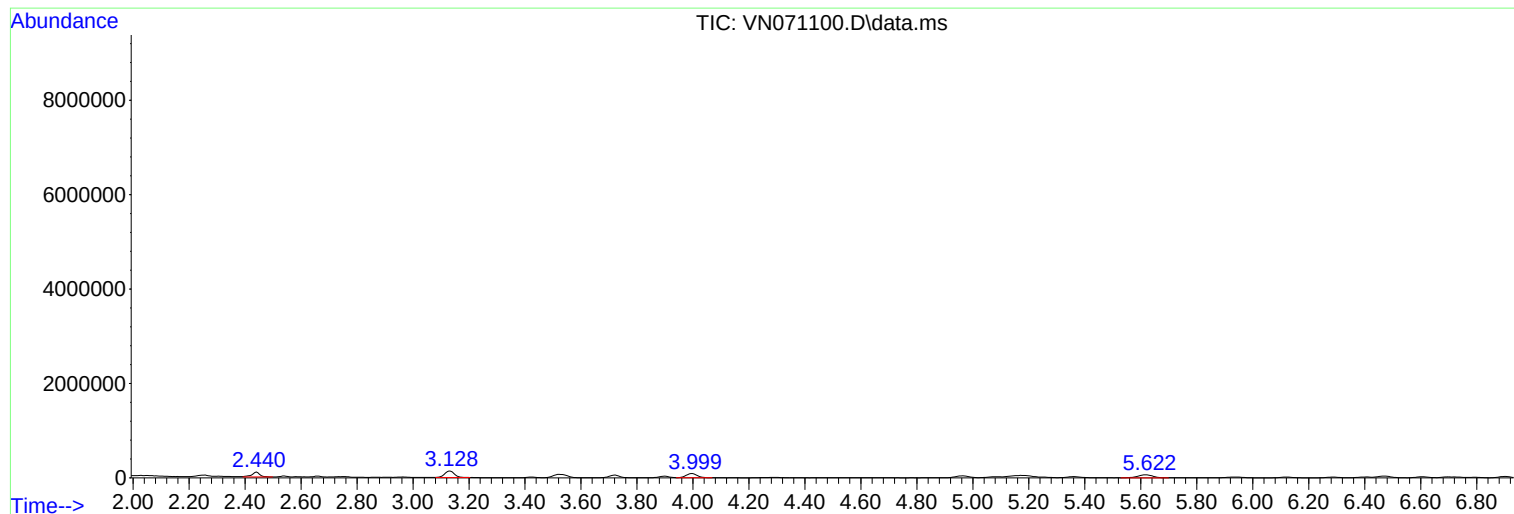
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

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



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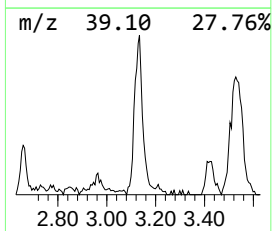
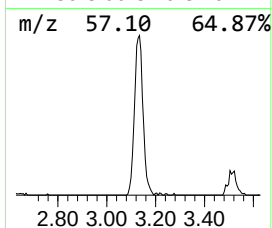
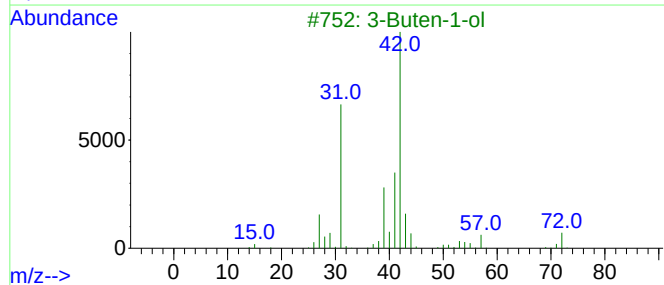
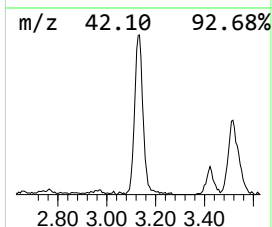
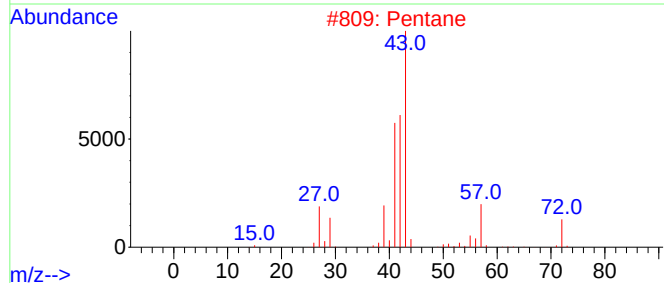
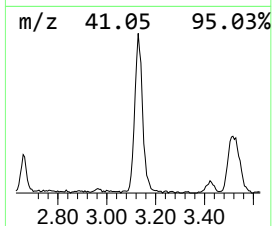
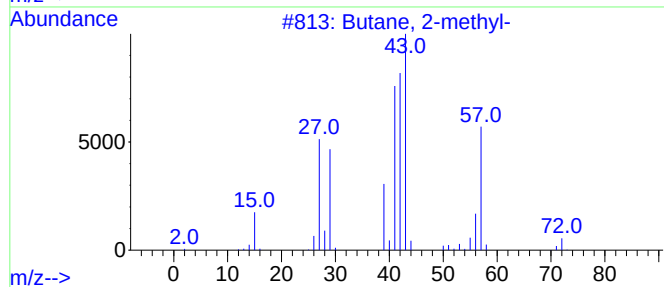
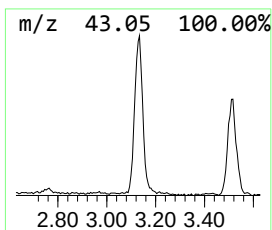
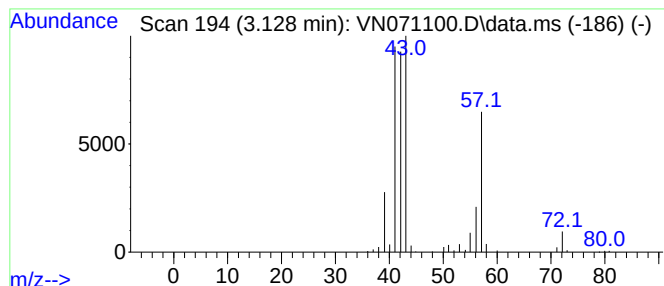
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	7.03 ug/l	332040	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	40
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	10
5			1-Butene	56	C4H8	000106-98-9	9



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Instrument :
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ClientSampleId :
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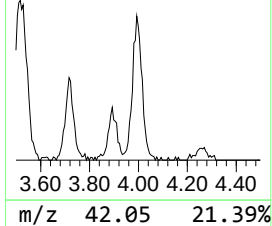
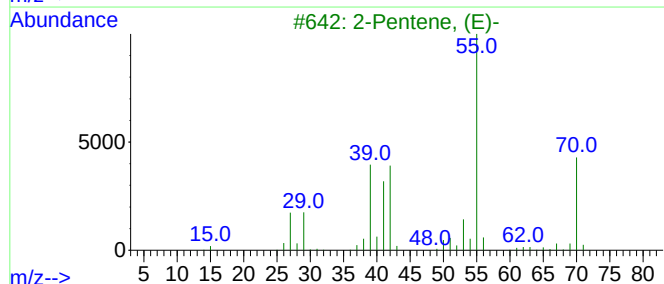
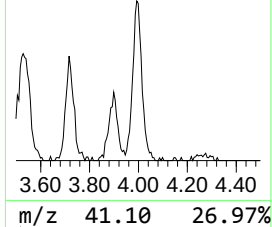
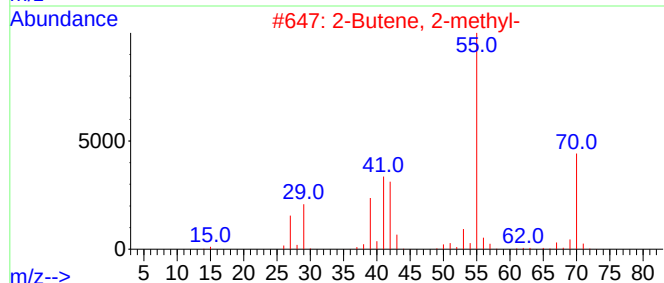
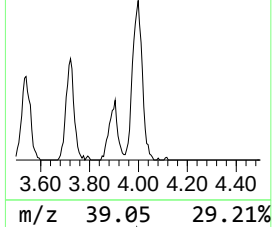
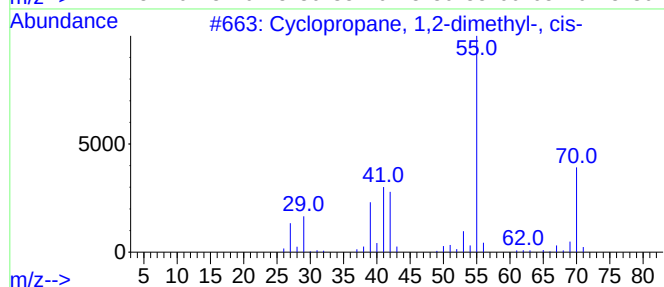
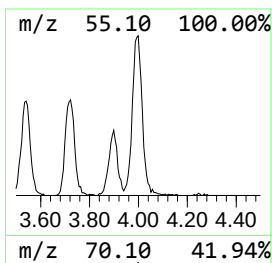
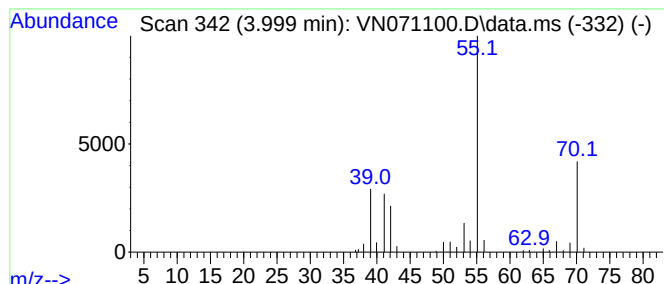
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopropane, 1,2-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.999	5.29 ug/l	249558	Pentafluorobenzene	8.081

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87
2		2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
3		2-Pentene, (E)-	70	C5H10	000646-04-8	78
4		1-Butene, 3-methyl-	70	C5H10	000563-45-1	78
5		Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	74



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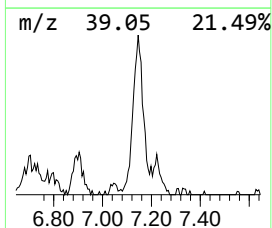
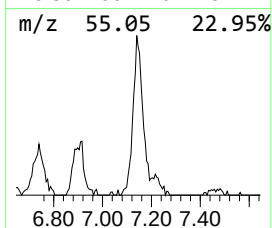
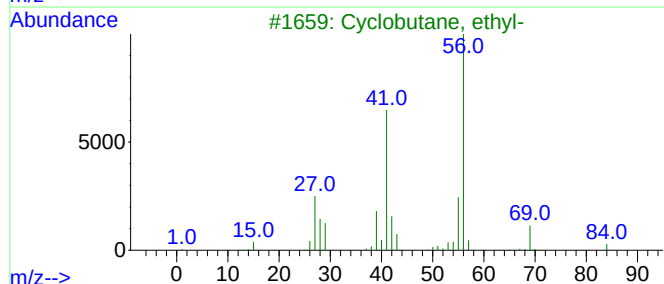
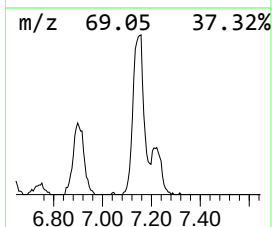
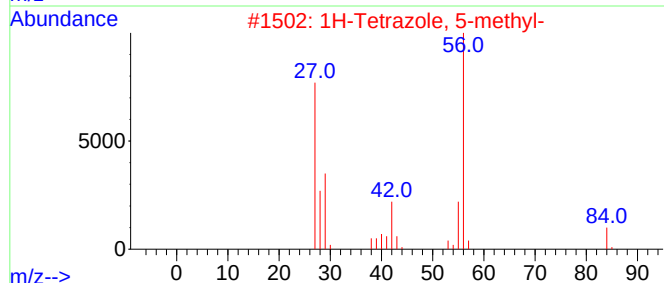
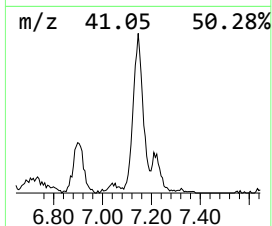
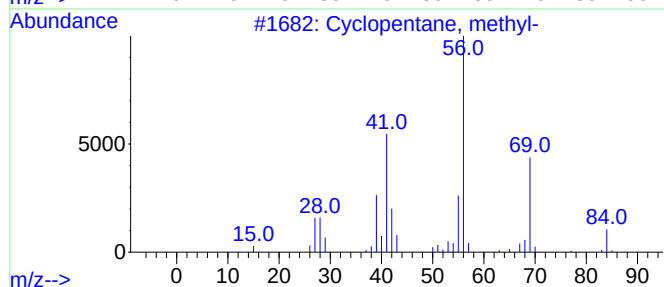
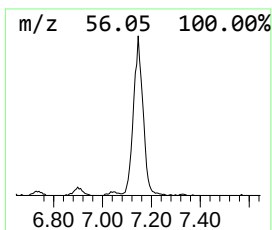
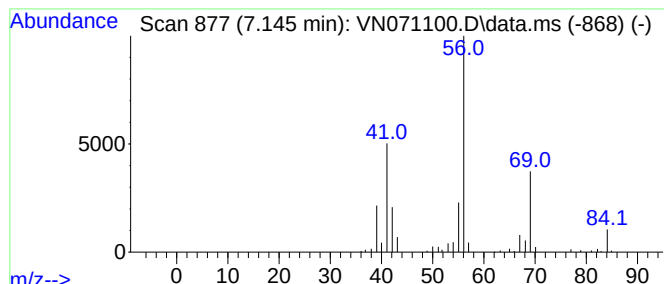
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Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	6.07 ug/l	286635	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	78
4			Cyclohexane	84	C6H12	000110-82-7	64
5			Aziridine, 1-(2-buten-2-yl)-	97	C6H11N	1000158-95-2	56



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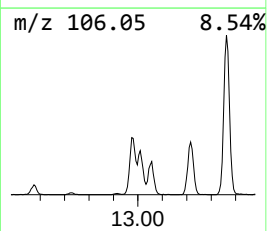
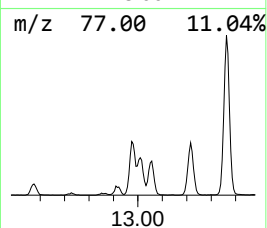
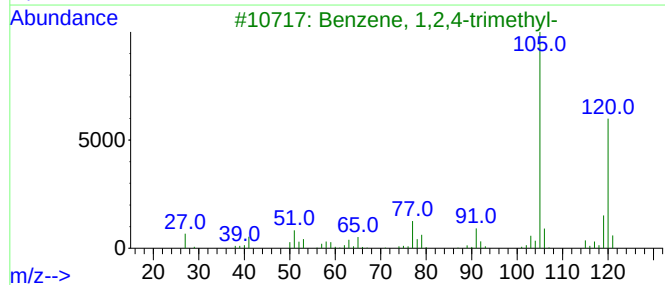
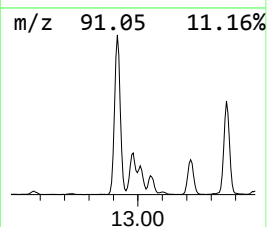
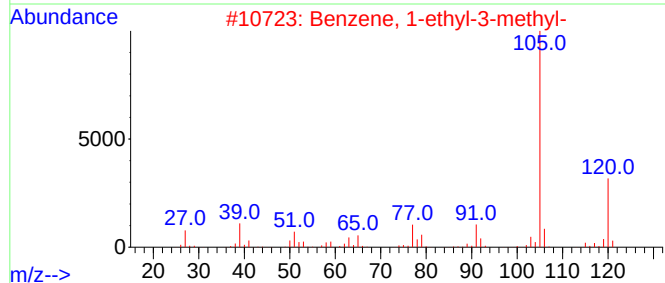
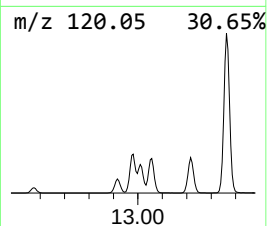
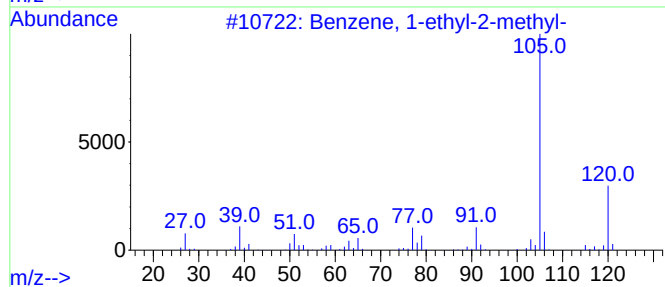
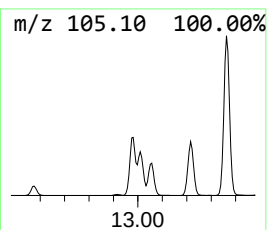
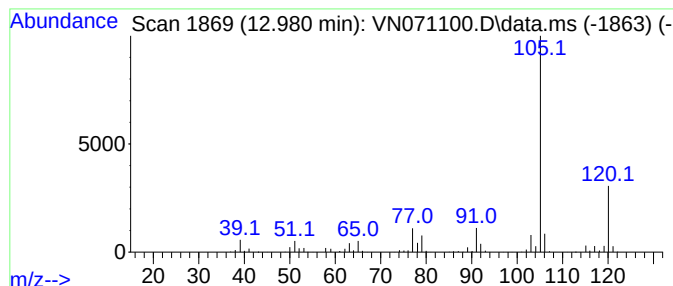
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	40.39 ug/l	2288920	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



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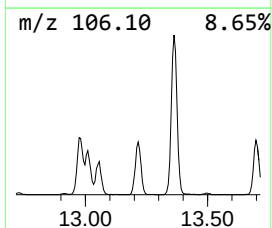
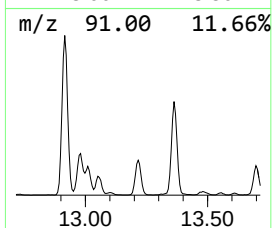
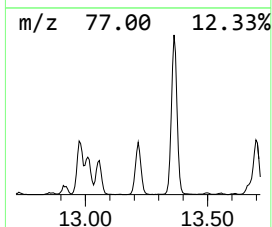
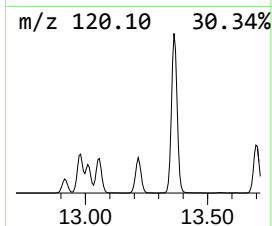
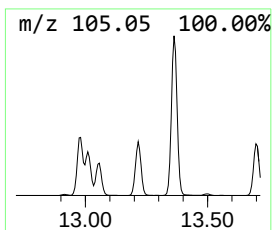
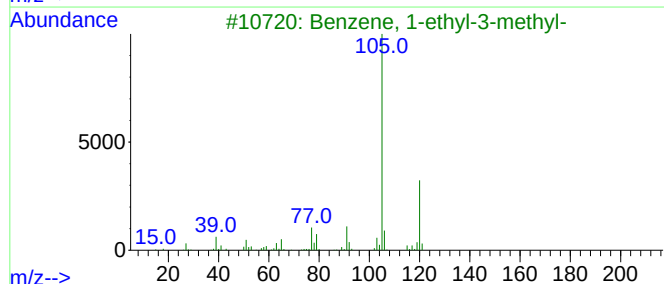
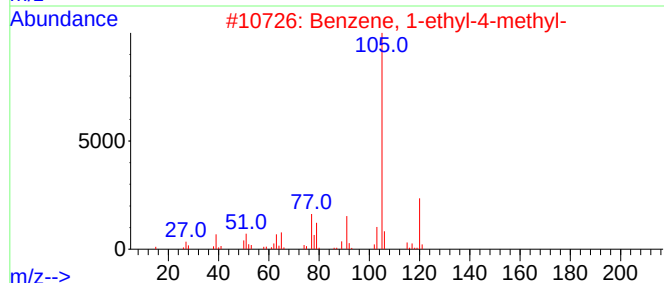
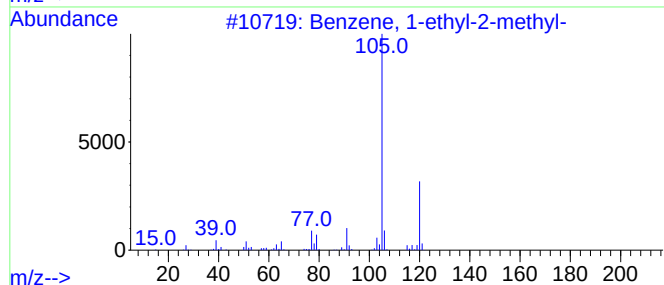
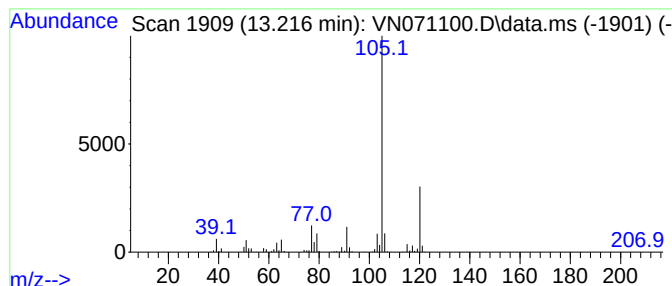
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	33.78 ug/l	1913900	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	93
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071100.D
Acq On : 28 Feb 2022 17:32
Operator : JC\MD
Sample : N1689-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-39

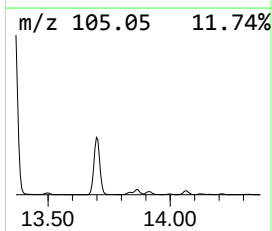
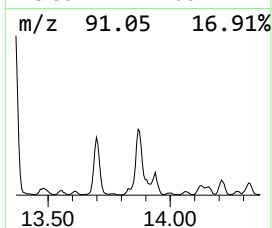
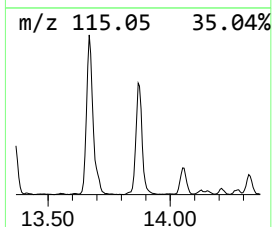
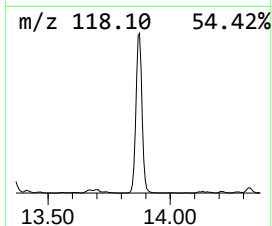
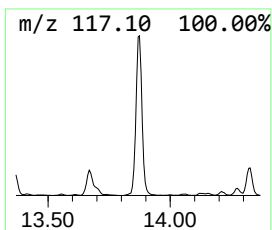
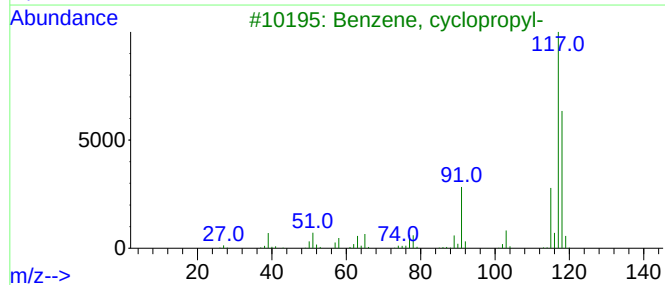
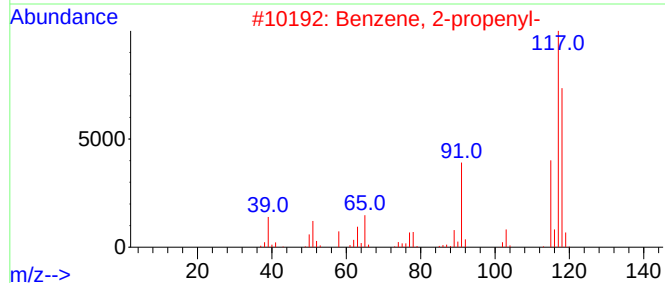
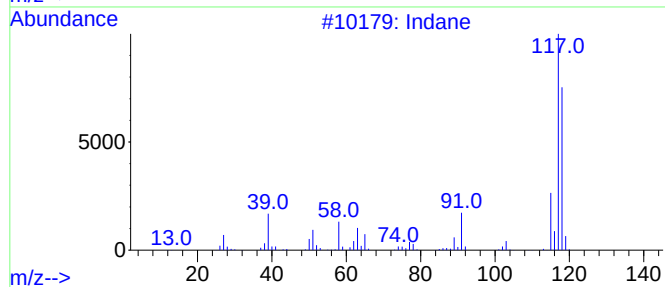
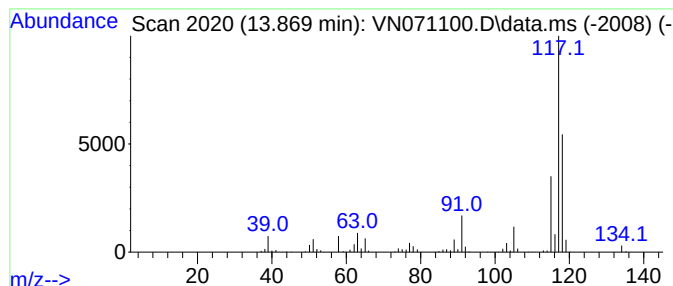
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Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.869	40.37 ug/l	2287540	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, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
5			Deltacyclene	118	C9H10	007785-10-6	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071100.D
Acq On : 28 Feb 2022 17:32
Operator : JC\MD
Sample : N1689-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-39

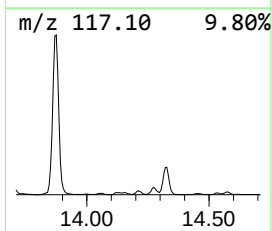
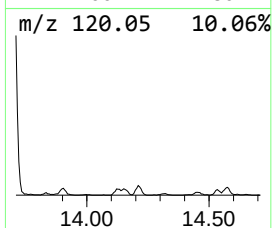
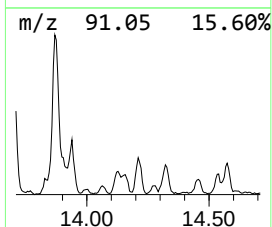
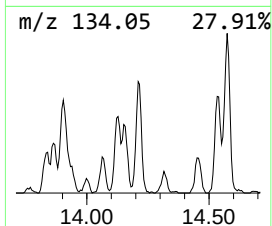
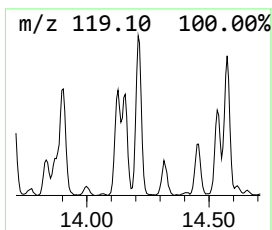
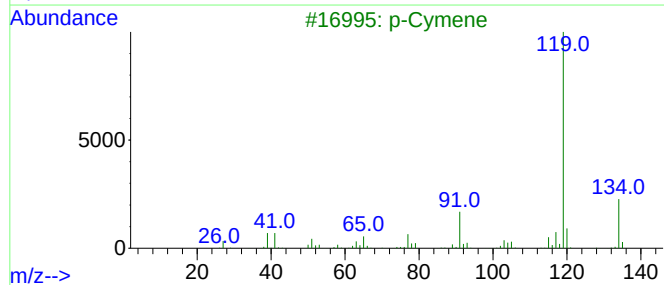
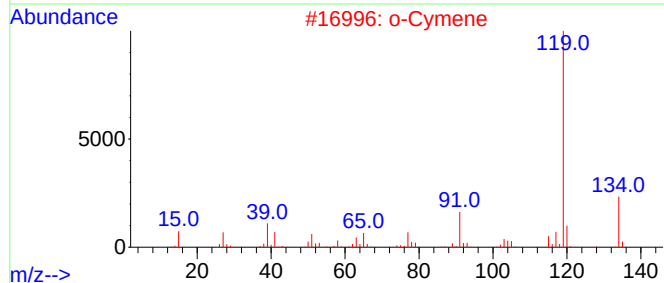
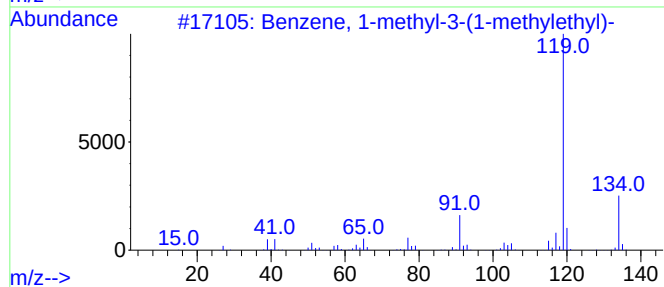
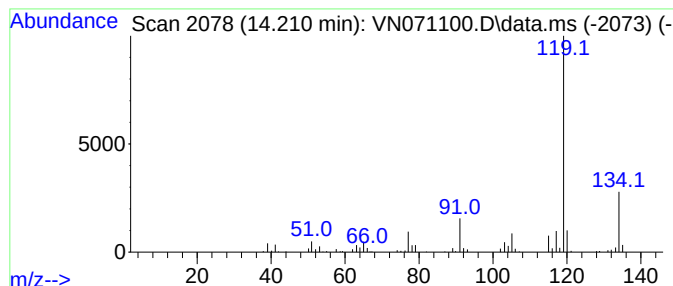
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-methyl-3-(1-meth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	5.46 ug/l	309373	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	97
2			o-Cymene	134	C10H14	000527-84-4	97
3			p-Cymene	134	C10H14	000099-87-6	97
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071100.D
Acq On : 28 Feb 2022 17:32
Operator : JC\MD
Sample : N1689-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-39

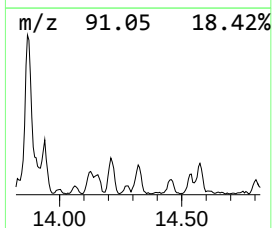
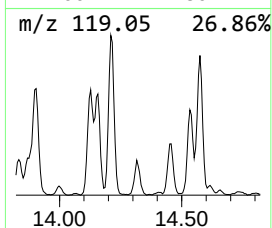
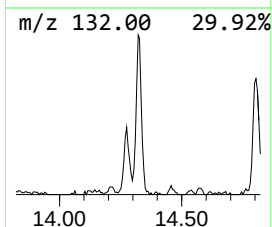
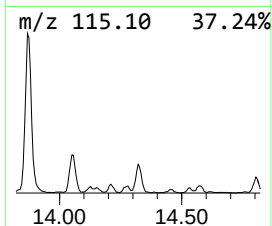
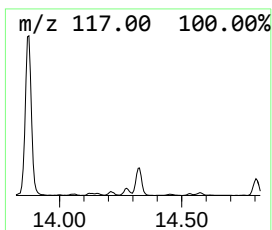
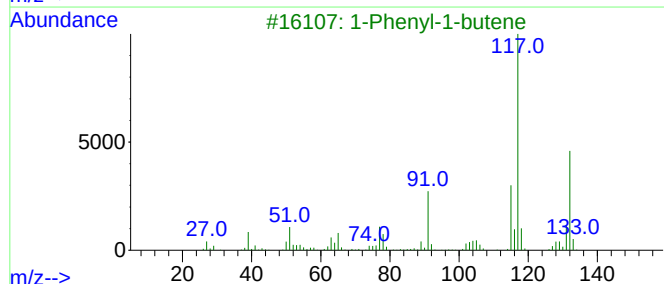
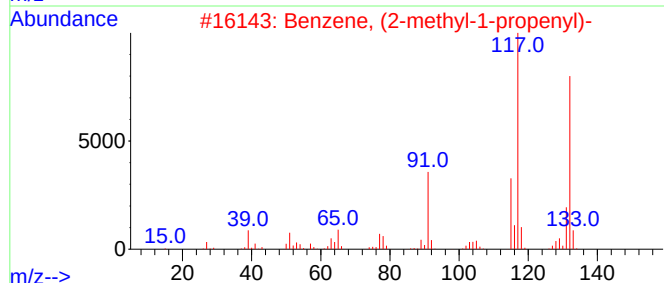
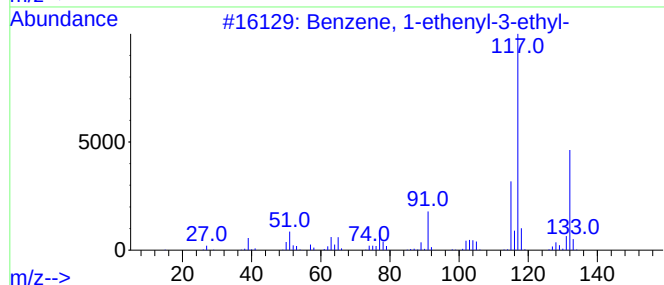
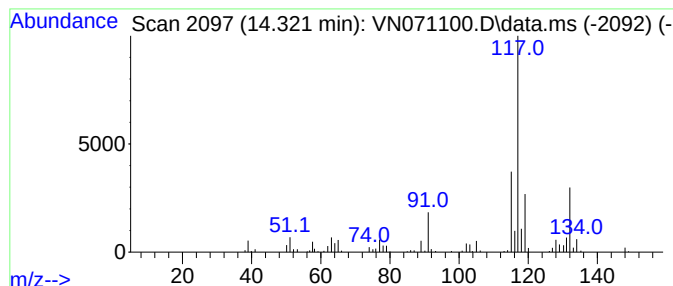
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.322	5.71 ug/l	323712	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	81
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	80
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	74
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	74
5			Indan, 1-methyl-	132	C10H12	000767-58-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071100.D
Acq On : 28 Feb 2022 17:32
Operator : JC\MD
Sample : N1689-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-39

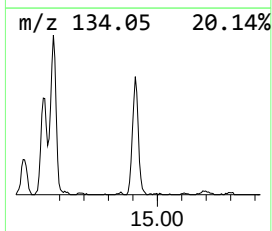
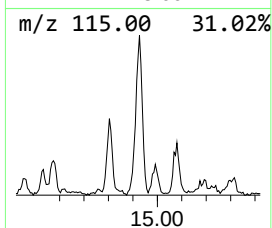
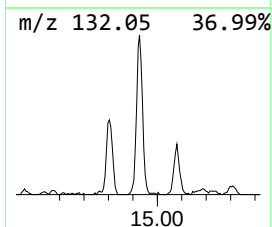
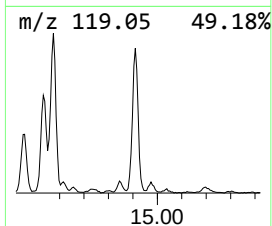
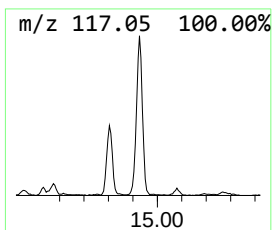
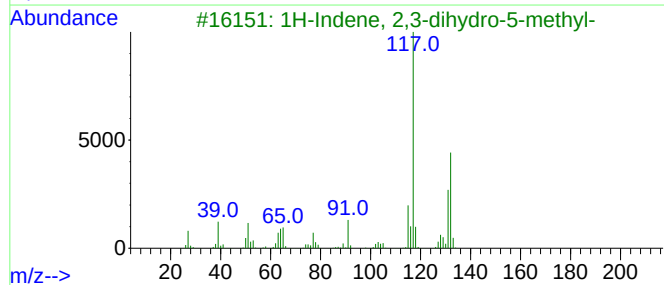
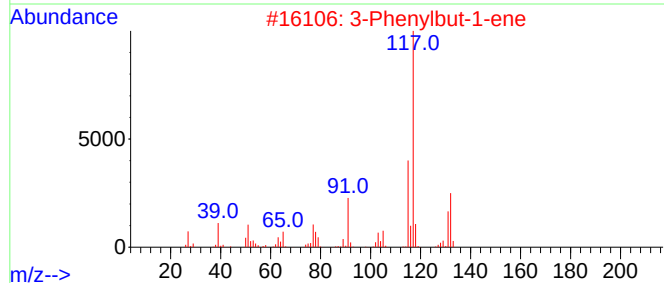
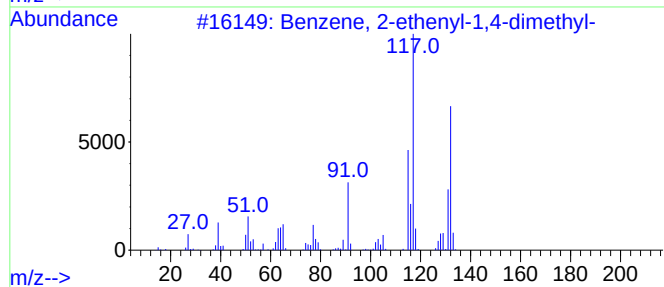
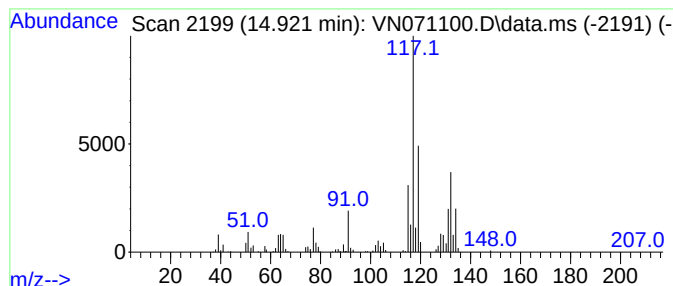
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	12.03 ug/l	681882	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	64
4			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	64
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071100.D
Acq On : 28 Feb 2022 17:32
Operator : JC\MD
Sample : N1689-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-39

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.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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Cyclopropane, 1...	3.999	5.3	ug/l	249558	1	8.081	2360520	50.0
Cyclopentane, m...	7.145	6.1	ug/l	286635	1	8.081	2360520	50.0
Benzene, 1-ethy...	12.980	40.4	ug/l	2288920	4	13.669	2833250	50.0
Benzene, 1-ethy...	13.216	33.8	ug/l	1913900	4	13.669	2833250	50.0
Indane	13.869	40.4	ug/l	2287540	4	13.669	2833250	50.0
Benzene, 1-meth...	14.210	5.5	ug/l	309373	4	13.669	2833250	50.0
Benzene, 1-ethe...	14.322	5.7	ug/l	323712	4	13.669	2833250	50.0
Benzene, 2-ethe...	14.921	12.0	ug/l	681882	4	13.669	2833250	50.0