

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
 Data File : VN067293.D
 Acq On : 11 Jun 2021 17:07
 Operator : JC/MD
 Sample : M2659-01
 Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31454

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\82N061021W.M
 Title : SW846 8260

Signal : TIC: VN067293.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.022	3	12	38	rVB	343066	609820	1.55%	0.358%
2	8.019	2225	2248	2258	rBV	298727	711814	1.81%	0.418%
3	8.080	2259	2271	2297	rVB	540497	1243228	3.16%	0.730%
4	8.434	2381	2403	2428	rBV2	365428	843354	2.14%	0.495%
5	8.963	2583	2600	2634	rBV	800816	1704039	4.32%	1.000%
6	10.440	3136	3151	3169	rBV	1258113	2414061	6.13%	1.417%
7	11.747	3624	3638	3660	rBV	1157361	2121451	5.38%	1.245%
8	11.953	3704	3715	3754	rVB6	173283	564195	1.43%	0.331%
9	12.734	3995	4006	4021	rVB2	1138638	1928004	4.89%	1.132%
10	12.986	4088	4100	4117	rBV2	906561	2536995	6.44%	1.489%
11	13.061	4118	4128	4146	rVB	1322493	2565637	6.51%	1.506%
12	13.372	4233	4244	4256	rBV	2742177	4745077	12.04%	2.786%
13	13.914	4439	4446	4464	rVB3	2319022	4694641	11.91%	2.756%
14	13.999	4468	4478	4500	rBV6	4940199	10201666	25.89%	5.989%
15	14.217	4552	4559	4570	rVB5	2776233	3900155	9.90%	2.290%
16	14.327	4590	4600	4609	rBV5	3923364	6506158	16.51%	3.819%
17	14.383	4611	4621	4637	rBV5	7805285	16302475	41.37%	9.570%
18	14.541	4662	4680	4690	rBV2	18618595	39404801	100.00%	23.132%
19	14.648	4705	4720	4737	rBV4	8212612	26032716	66.06%	15.282%
20	14.852	4789	4796	4809	rVB3	13702445	21188764	53.77%	12.439%
21	14.919	4813	4821	4835	rBV3	9442115	20127350	51.08%	11.816%

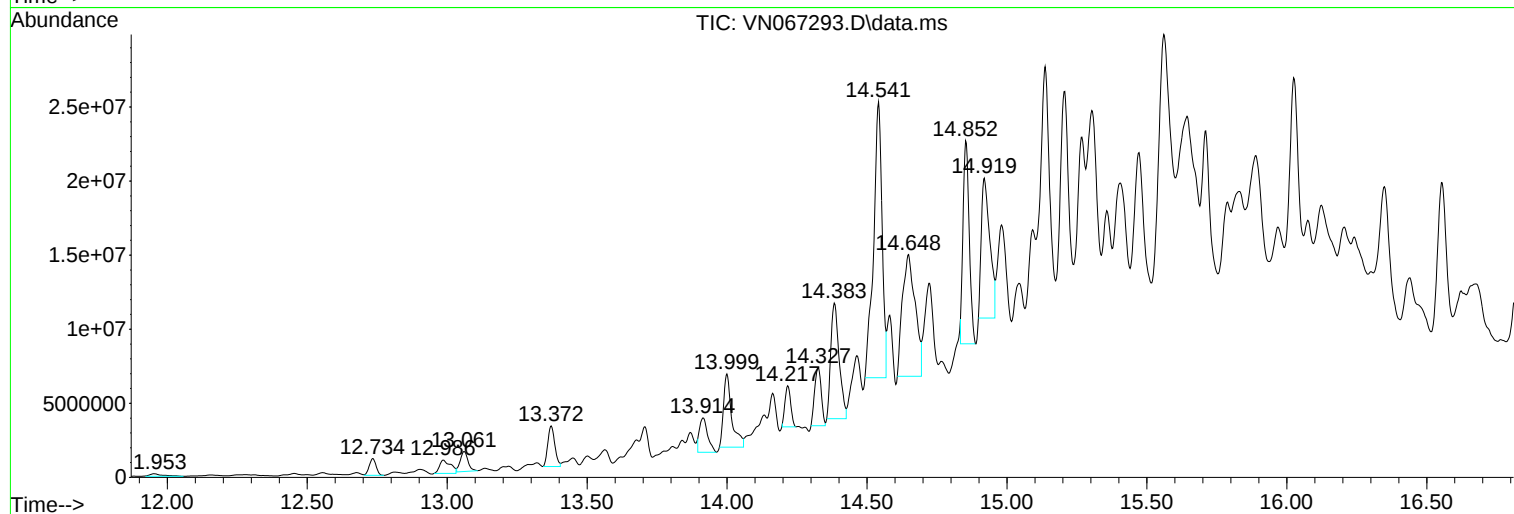
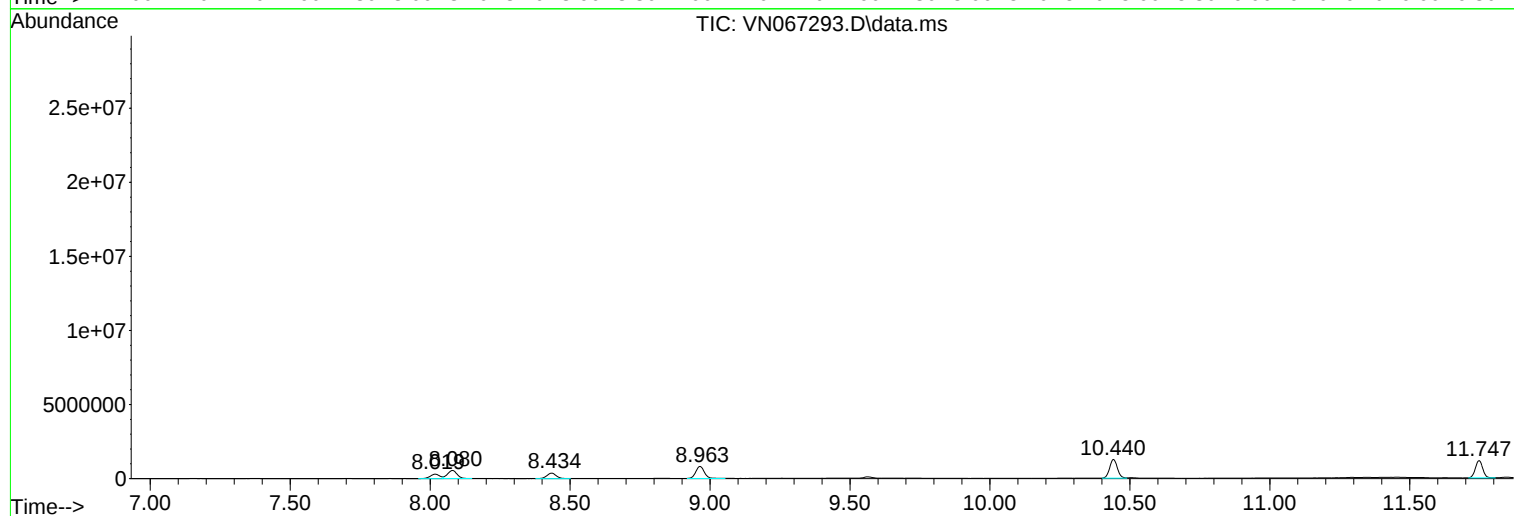
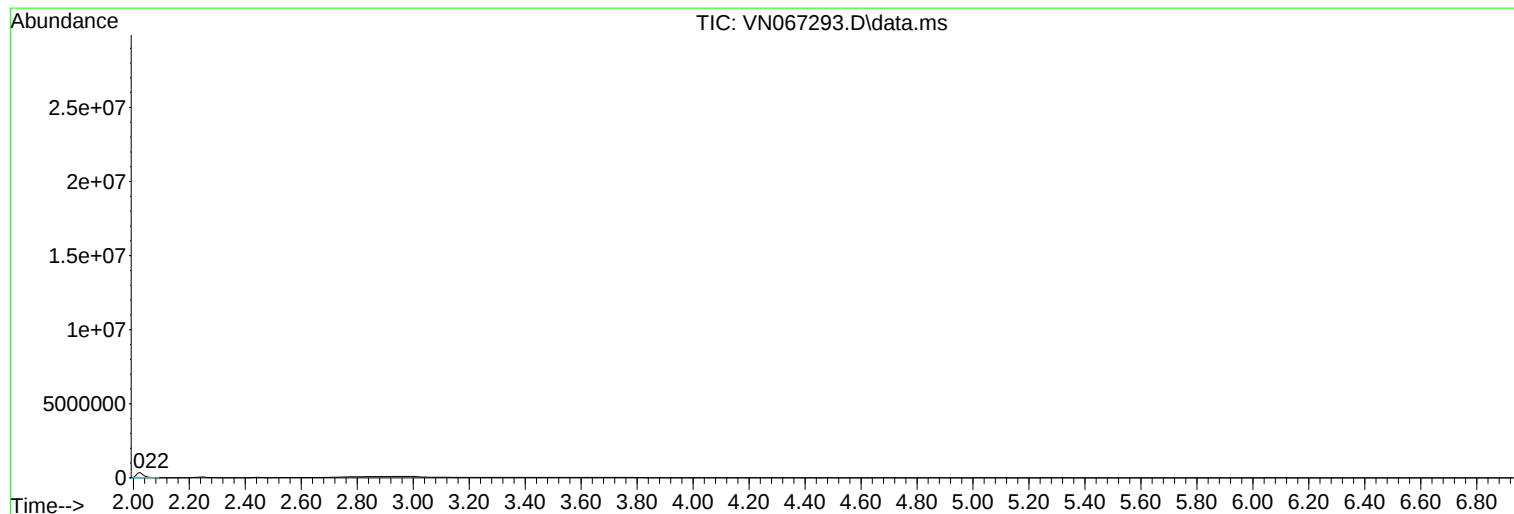
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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



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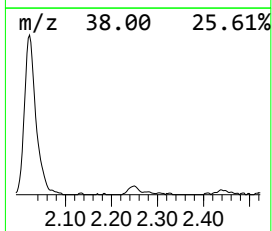
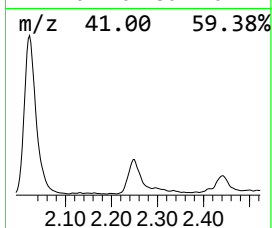
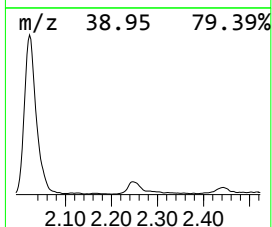
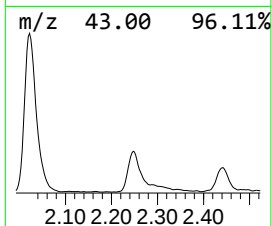
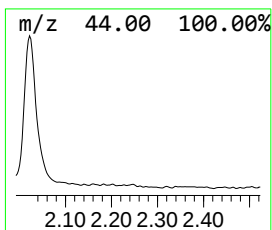
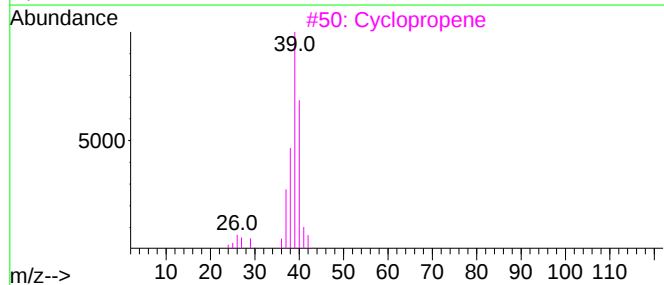
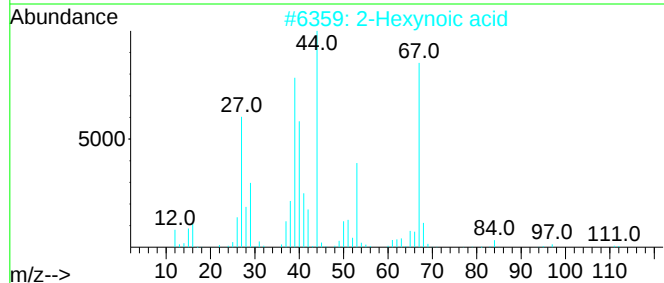
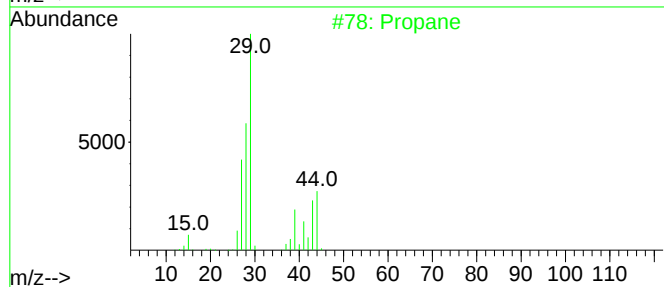
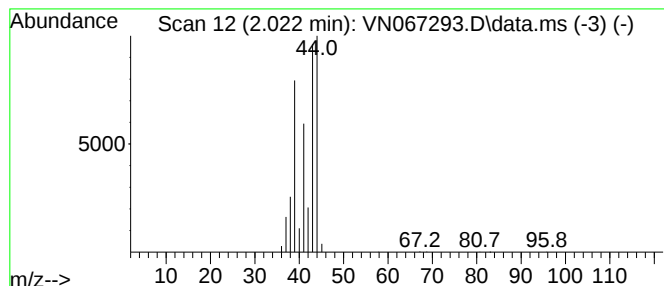
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.022	24.53 ug/l	609820	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	83
2			2-Hexynoic acid	112	C6H8O2	000764-33-0	43
3			Cyclopropene	40	C3H4	002781-85-3	38
4			Propene	42	C3H6	000115-07-1	9
5			2-Butynal	68	C4H4O	001119-19-3	9



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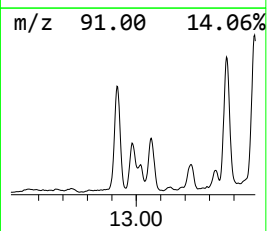
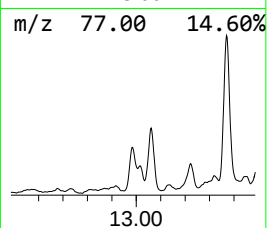
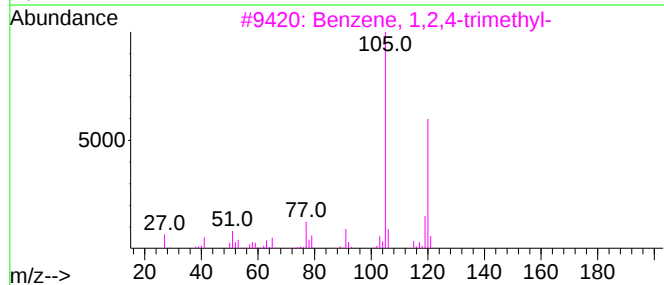
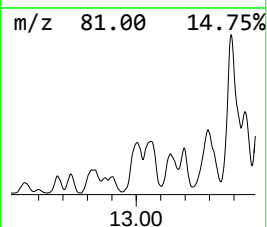
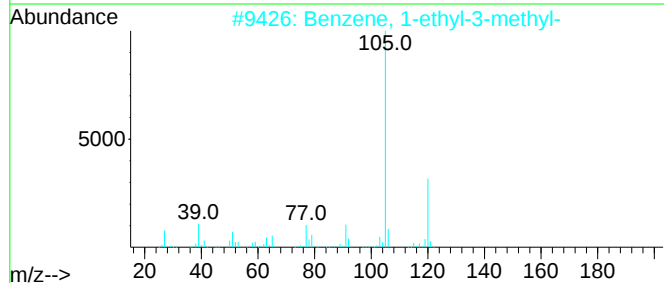
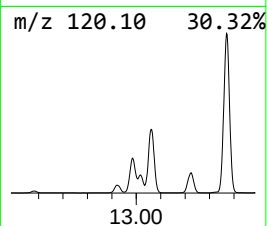
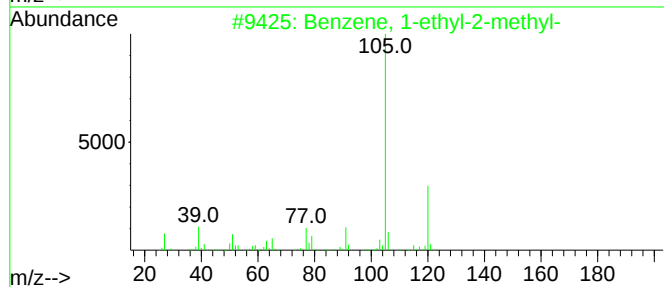
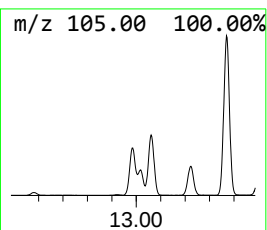
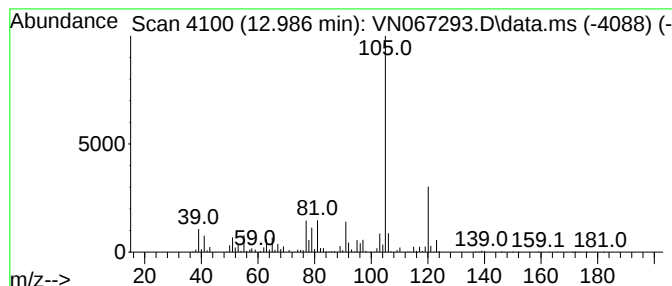
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	27.02 ug/l	2537000	1,4-Dichlorobenzene-d4	13.675

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-3-methyl-	120	C9H12	000620-14-4	89
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	76
4			Mesitylene	120	C9H12	000108-67-8	76
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	70



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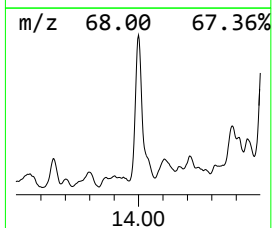
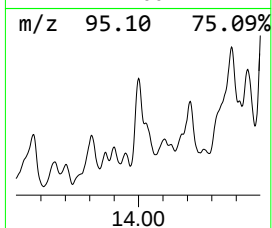
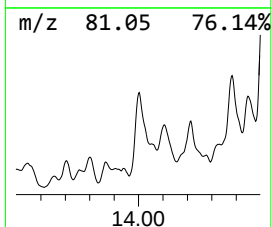
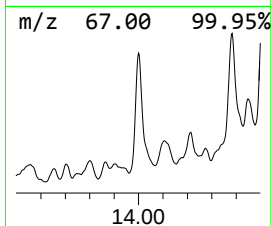
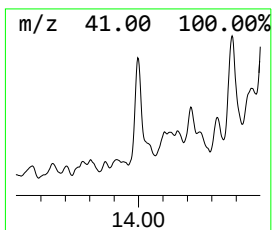
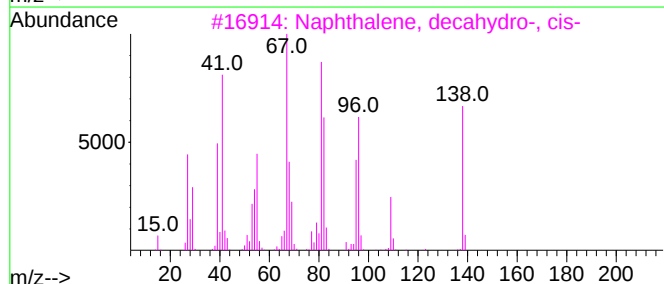
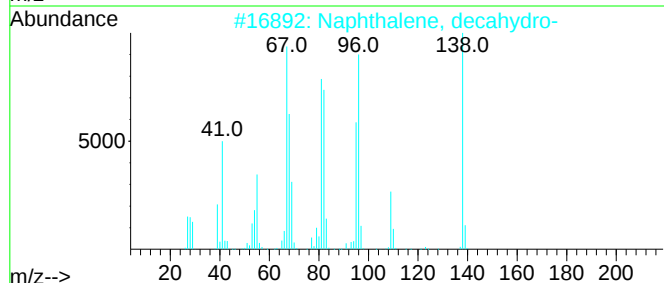
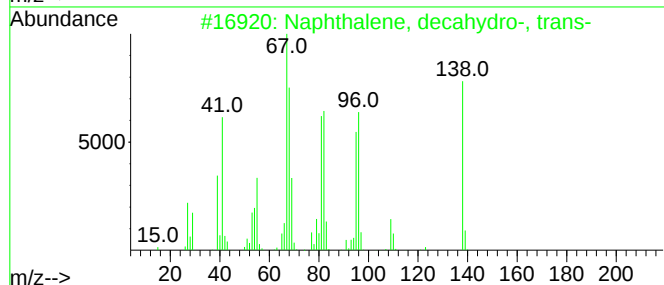
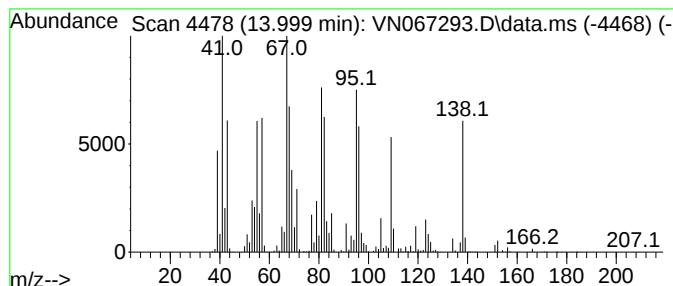
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, decahydro-, tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.999	108.65 ug/l	10201700	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	95
2			Naphthalene, decahydro-	138	C10H18	000091-17-8	94
3			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	93
4			Cyclohexane, 1-methyl-3-(1-methy...	138	C10H18	024399-15-3	90
5			Cyclohexene, 3-methyl-6-(1-methy...	138	C10H18	005256-65-5	70



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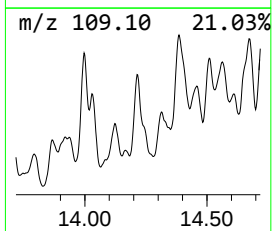
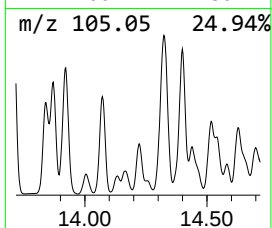
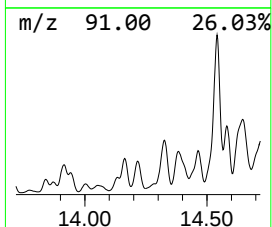
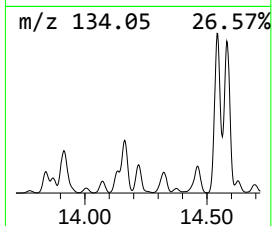
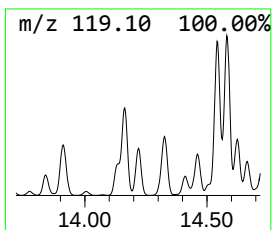
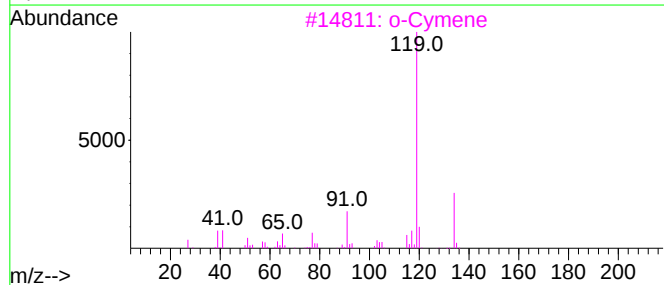
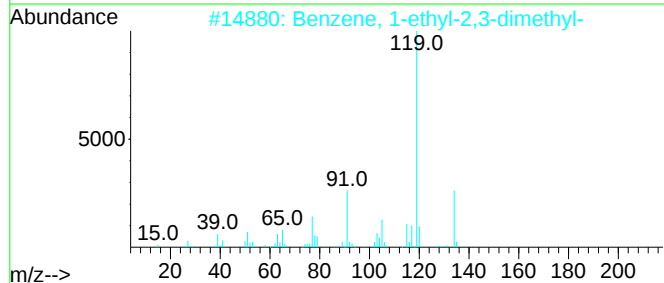
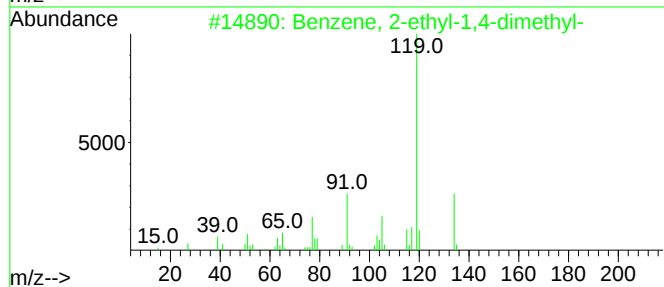
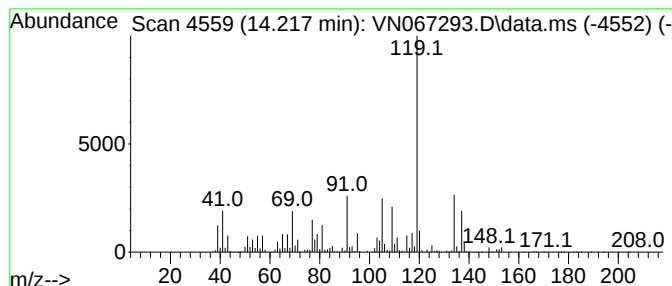
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	41.54 ug/l	3900160	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	92
2			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
3			o-Cymene	134	C10H14	000527-84-4	91
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	90
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	64



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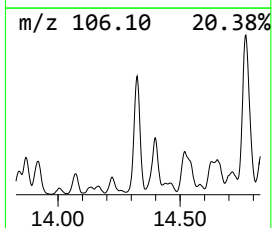
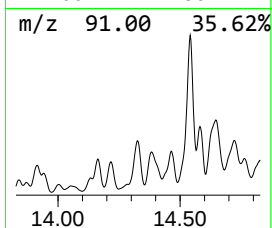
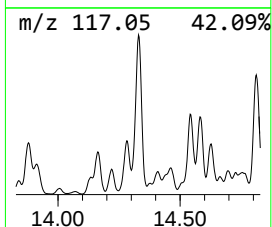
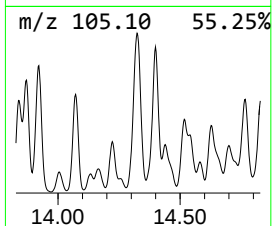
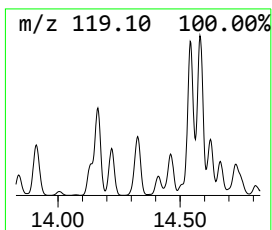
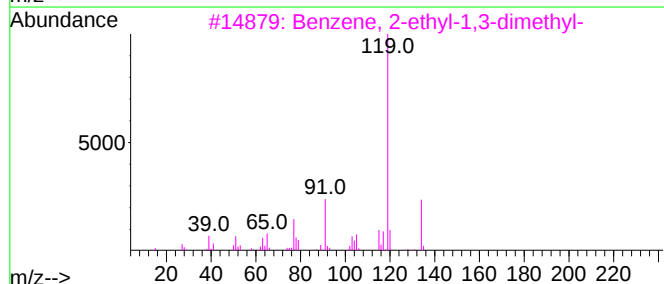
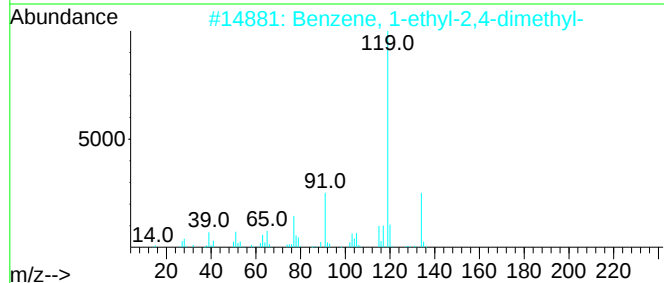
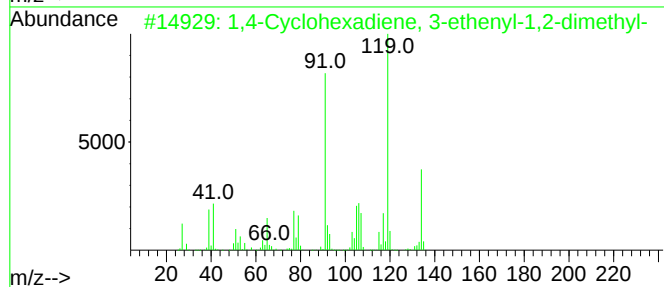
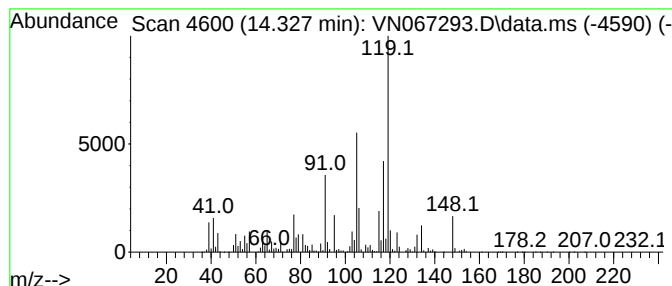
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TIC Integration Parameters: LSCINT.P

Peak Number 5 1,4-Cyclohexadiene, 3-ethen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	69.29 ug/l	6506160	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Cyclohexadiene, 3-ethenyl-1,...	134	C10H14	062338-57-2	52
2			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	49
3			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	46
4			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	46
5			1-Methyl-1-silabenzocyclobutene	134	C8H10Si	160841-06-5	46



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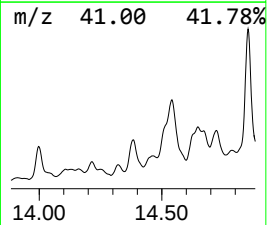
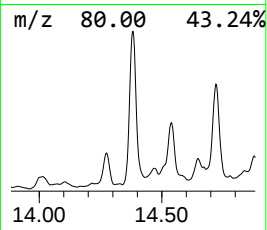
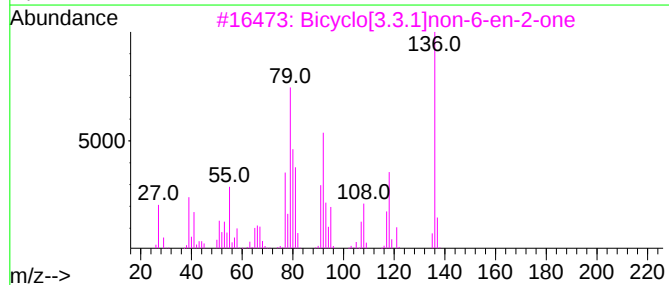
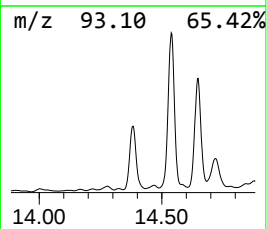
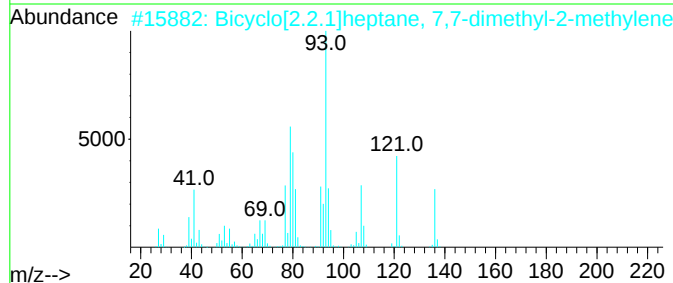
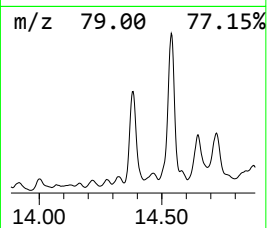
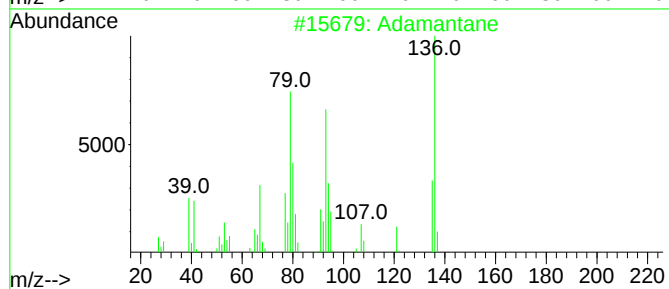
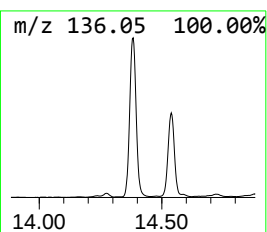
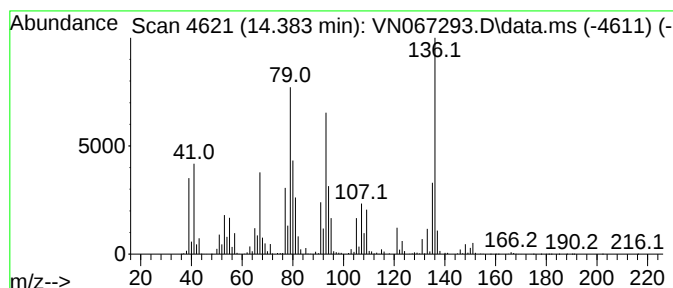
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Quant Title : SW846 8260

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

Peak Number 6 Adamantane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.383	173.63 ug/l	16302500	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane	136	C10H16	000281-23-2	98
2			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	81
3			Bicyclo[3.3.1]non-6-en-2-one	136	C9H12O	022482-58-2	70
4			Bicyclo[3.3.1]non-2-en-9-one	136	C9H12O	004844-11-5	64
5			Cyclohexene, 5-methyl-3-(1-methy...	136	C10H16	056816-08-1	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067293.D
Acq On : 11 Jun 2021 17:07
Operator : JC/MD
Sample : M2659-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31454

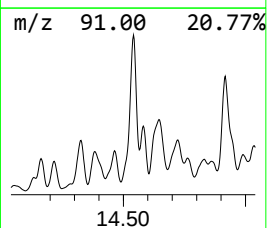
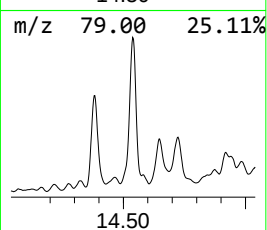
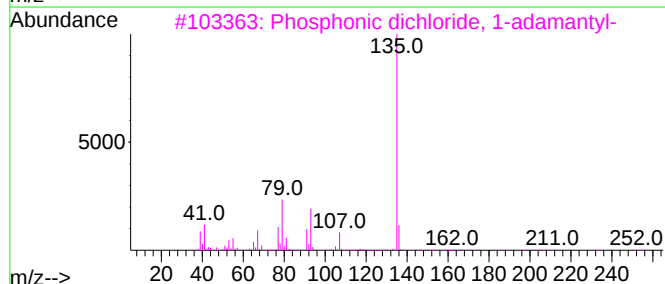
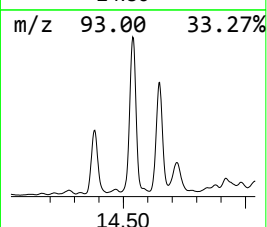
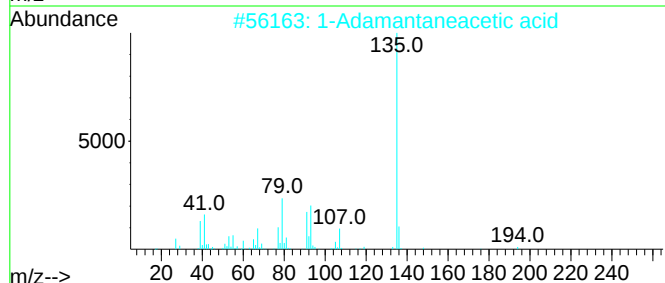
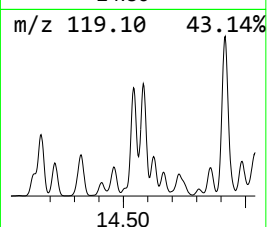
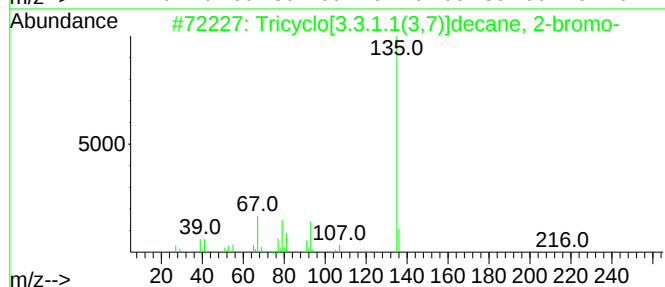
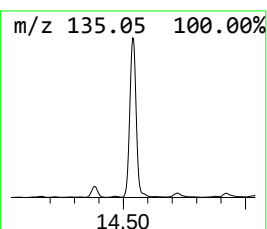
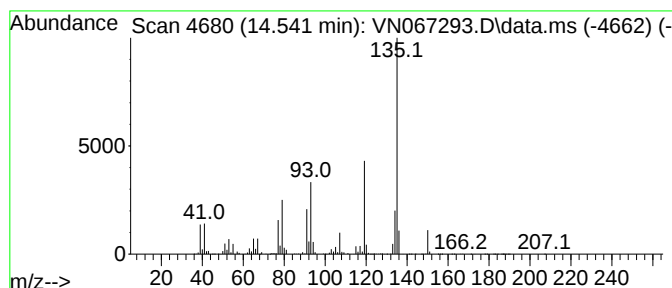
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.541 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.541	419.68 ug/l	39404800	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[3.3.1.1(3,7)]decane, 2-...	214	C10H15Br	007314-85-4	47
2			1-Adamantaneacetic acid	194	C12H18O2	004942-47-6	47
3			Phosphonic dichloride, 1-adamantyl-	252	C10H15Cl2OP	1000294-15-7	47
4			Tricyclo[3.3.1.1(3,7)]decane, 1-...	181	C10H15NO2	007575-82-8	47
5			1-Bromoadamantane	214	C10H15Br	000768-90-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067293.D
Acq On : 11 Jun 2021 17:07
Operator : JC/MD
Sample : M2659-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31454

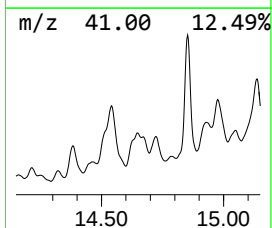
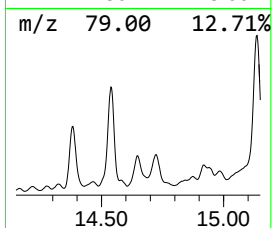
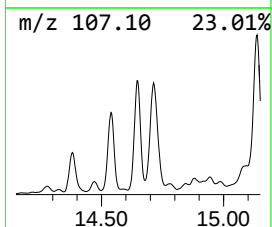
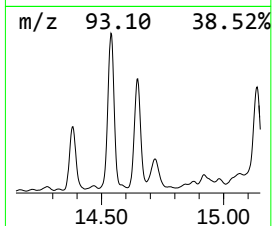
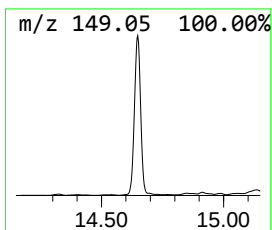
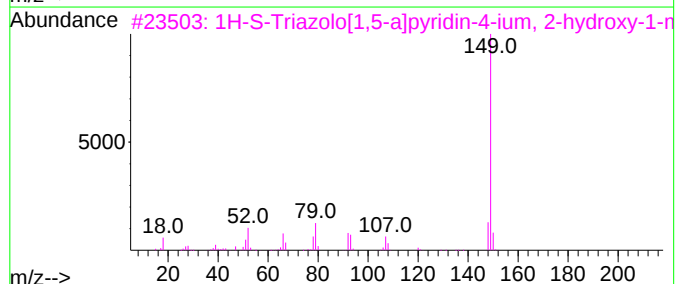
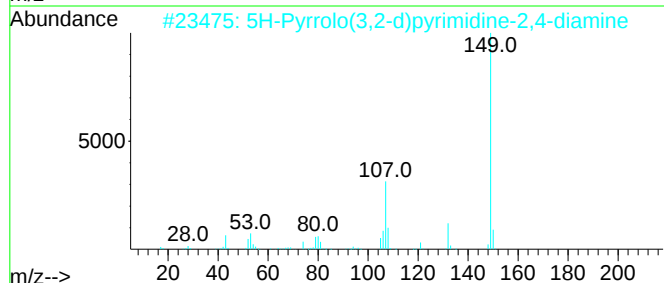
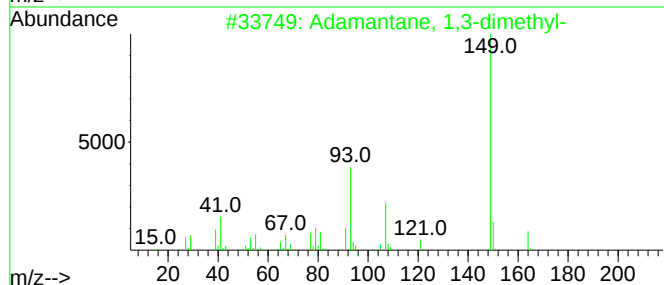
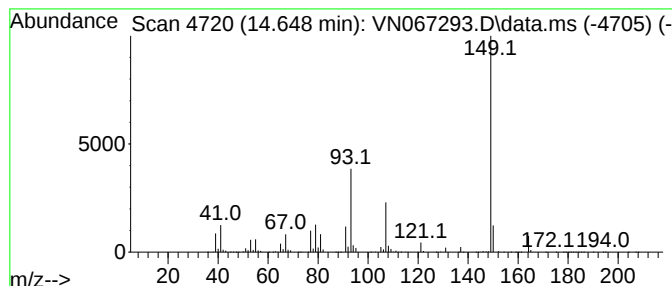
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Quant Title : SW846 8260

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

Peak Number 8 Adamantane, 1,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.649	277.26 ug/l	26032700	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	96
2			5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	47
3			1H-S-Triazolo[1,5-a]pyridin-4-iu...	149	C7H7N3O	013980-64-8	43
4			Cyclohexane, 1,1,4,4-tetramethyl...	164	C12H20	1000154-20-4	38
5			2,4,7-Trioxabicyclo[4.4.0]9-dece...	468	C30H44O4	1000160-93-8	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067293.D
Acq On : 11 Jun 2021 17:07
Operator : JC/MD
Sample : M2659-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31454

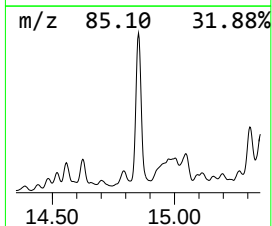
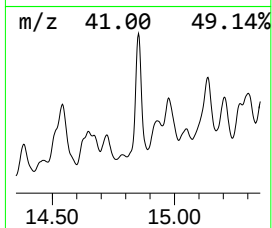
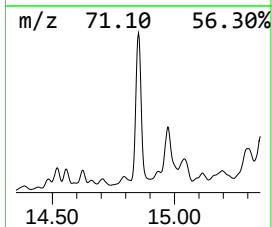
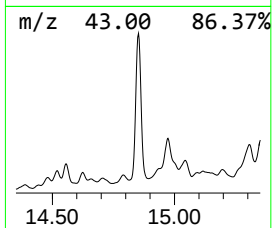
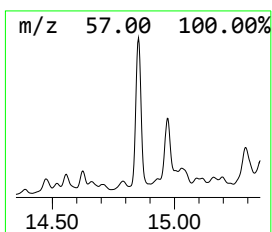
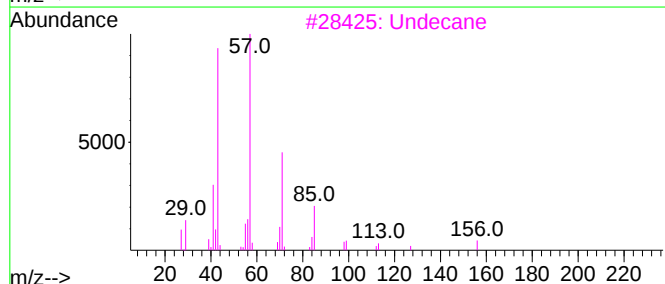
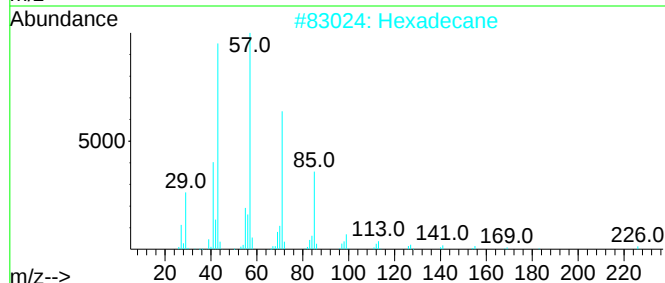
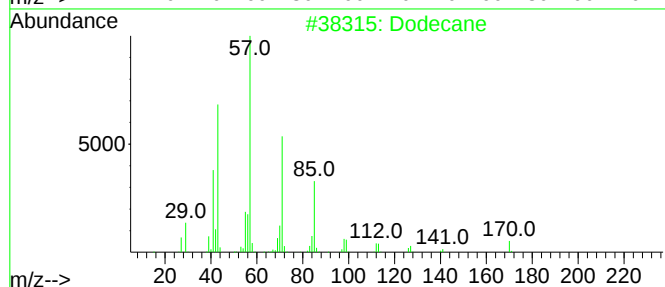
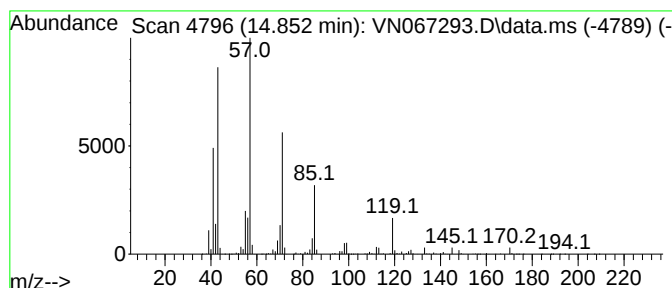
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Quant Title : SW846 8260

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

Peak Number 9 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.852	225.67 ug/l	21188800	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	95
2			Hexadecane	226	C16H34	000544-76-3	86
3			Undecane	156	C11H24	001120-21-4	72
4			Tridecane	184	C13H28	000629-50-5	72
5			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067293.D
Acq On : 11 Jun 2021 17:07
Operator : JC/MD
Sample : M2659-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31454

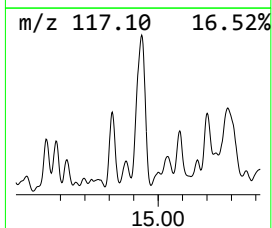
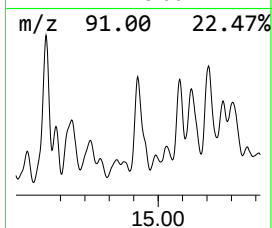
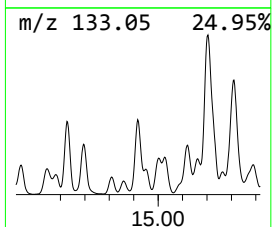
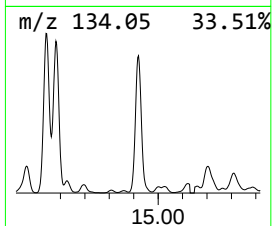
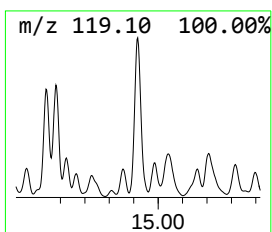
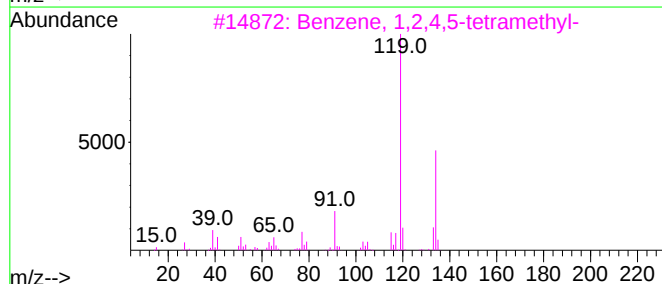
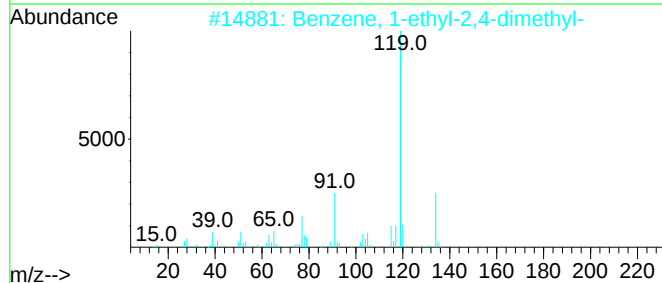
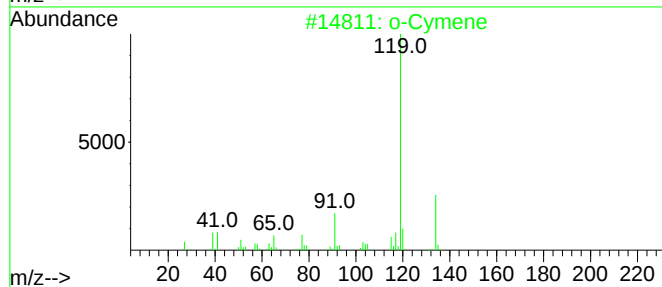
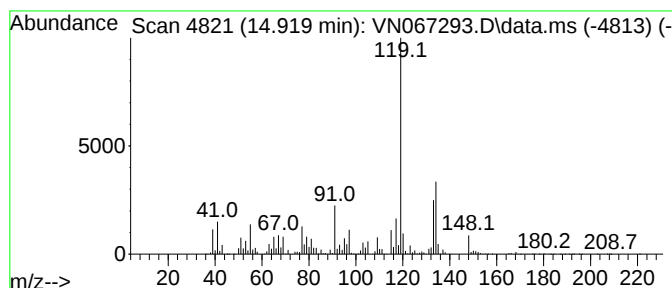
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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

Peak Number 10 o-Cymene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.919	214.37 ug/l	20127400	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	94
2			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	89
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	86
5			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067293.D
Acq On : 11 Jun 2021 17:07
Operator : JC/MD
Sample : M2659-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31454

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.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
Propane	2.022	24.5	ug/l	609820	1	8.080	1243230	50.0
Benzene, 1-ethy...	12.986	27.0	ug/l	2537000	4	13.675	4694640	50.0
Naphthalene, de...	13.999	108.7	ug/l	10201700	4	13.675	4694640	50.0
Benzene, 2-ethy...	14.217	41.5	ug/l	3900160	4	13.675	4694640	50.0
1,4-Cyclohexadi...	14.327	69.3	ug/l	6506160	4	13.675	4694640	50.0
Adamantane	14.383	173.6	ug/l	16302500	4	13.675	4694640	50.0
unknown14.541	14.541	419.7	ug/l	39404800	4	13.675	4694640	50.0
Adamantane, 1,3...	14.649	277.3	ug/l	26032700	4	13.675	4694640	50.0
Dodecane	14.852	225.7	ug/l	21188800	4	13.675	4694640	50.0
o-Cymene	14.919	214.4	ug/l	20127400	4	13.675	4694640	50.0