

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010422\
 Data File : VN070473.D
 Acq On : 4 Jan 2022 19:14
 Operator : JC/MD
 Sample : N1012-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31212

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070473.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.685	610	632	673	rBV	1466881	4037250	9.18%	3.339%
2	4.285	831	856	892	rBV	437096	1308138	2.98%	1.082%
3	4.578	937	965	1001	rBV	589122	1949872	4.43%	1.613%
4	7.332	1965	1992	2073	rBV2	15826336	43969281	100.00%	36.366%
5	8.021	2228	2249	2260	rBV	735152	1755173	3.99%	1.452%
6	8.083	2261	2272	2297	rVB	1167036	2641462	6.01%	2.185%
7	8.437	2381	2404	2434	rBV	956555	2278757	5.18%	1.885%
8	8.965	2571	2601	2619	rBV	1823986	3745117	8.52%	3.097%
9	9.051	2619	2633	2663	rVB	493259	1065787	2.42%	0.881%
10	10.440	3127	3151	3164	rBV	3011519	5582653	12.70%	4.617%
11	10.502	3164	3174	3203	rVB	922273	1730432	3.94%	1.431%
12	11.741	3618	3636	3659	rBV	2288340	4167820	9.48%	3.447%
13	11.843	3660	3674	3694	rVB	656766	1144281	2.60%	0.946%
14	11.948	3695	3713	3737	rBV	2466044	4768137	10.84%	3.944%
15	12.280	3813	3837	3860	rBV4	1969534	3894907	8.86%	3.221%
16	12.728	3990	4004	4028	rVB	2120600	3712216	8.44%	3.070%
17	12.919	4059	4075	4085	rBV	326460	553091	1.26%	0.457%
18	12.980	4085	4098	4106	rBV	1361859	2298327	5.23%	1.901%
19	13.053	4117	4125	4140	rVB2	872082	1568700	3.57%	1.297%
20	13.219	4170	4187	4202	rBV	837290	1533524	3.49%	1.268%
21	13.366	4226	4242	4270	rBV2	3222651	8628025	19.62%	7.136%
22	13.672	4343	4356	4363	rBV	1619275	2913699	6.63%	2.410%
23	13.871	4407	4430	4439	rBV3	1052127	2160418	4.91%	1.787%
24	13.991	4464	4475	4488	rBV4	581696	925143	2.10%	0.765%
25	14.128	4516	4526	4531	rBV	323996	501113	1.14%	0.414%
26	14.211	4548	4557	4569	rVB	460175	690380	1.57%	0.571%
27	14.324	4588	4599	4611	rVB3	544312	903276	2.05%	0.747%
28	14.576	4687	4693	4702	rVB	450217	600720	1.37%	0.497%
29	14.807	4769	4779	4785	rBV	510951	797942	1.81%	0.660%
30	14.844	4786	4793	4805	rVB2	682760	1048626	2.38%	0.867%
31	14.927	4807	4824	4857	rBV4	1249598	3217003	7.32%	2.661%
32	15.080	4870	4881	4898	rVB	969555	1701362	3.87%	1.407%
33	15.697	5103	5111	5132	rVB	682559	1213047	2.76%	1.003%
34	16.014	5222	5229	5252	rVB2	587532	1125789	2.56%	0.931%
35	16.673	5466	5475	5490	rVB	421243	777587	1.77%	0.643%

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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\82N122721W.M
Title : SW846 8260

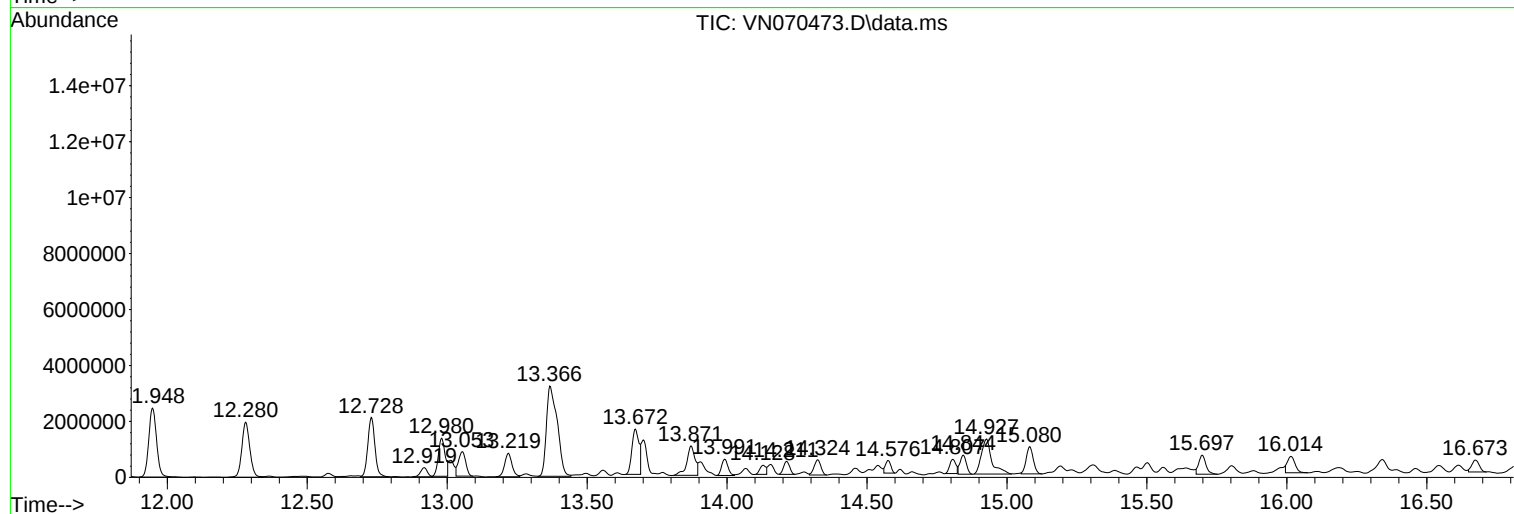
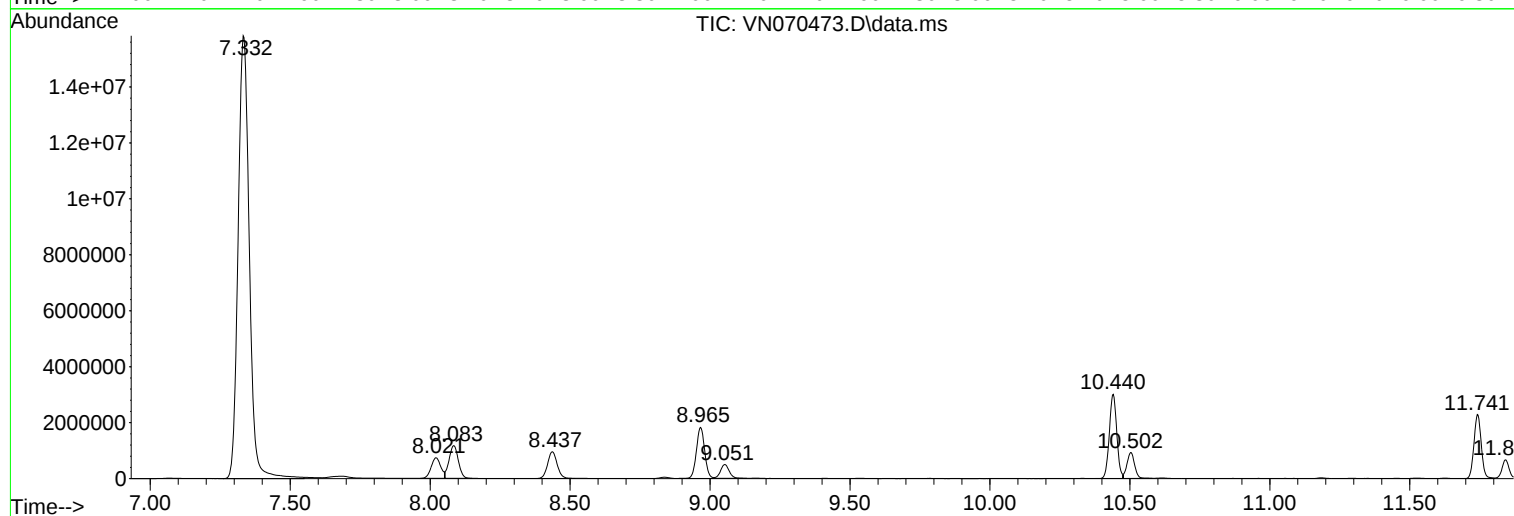
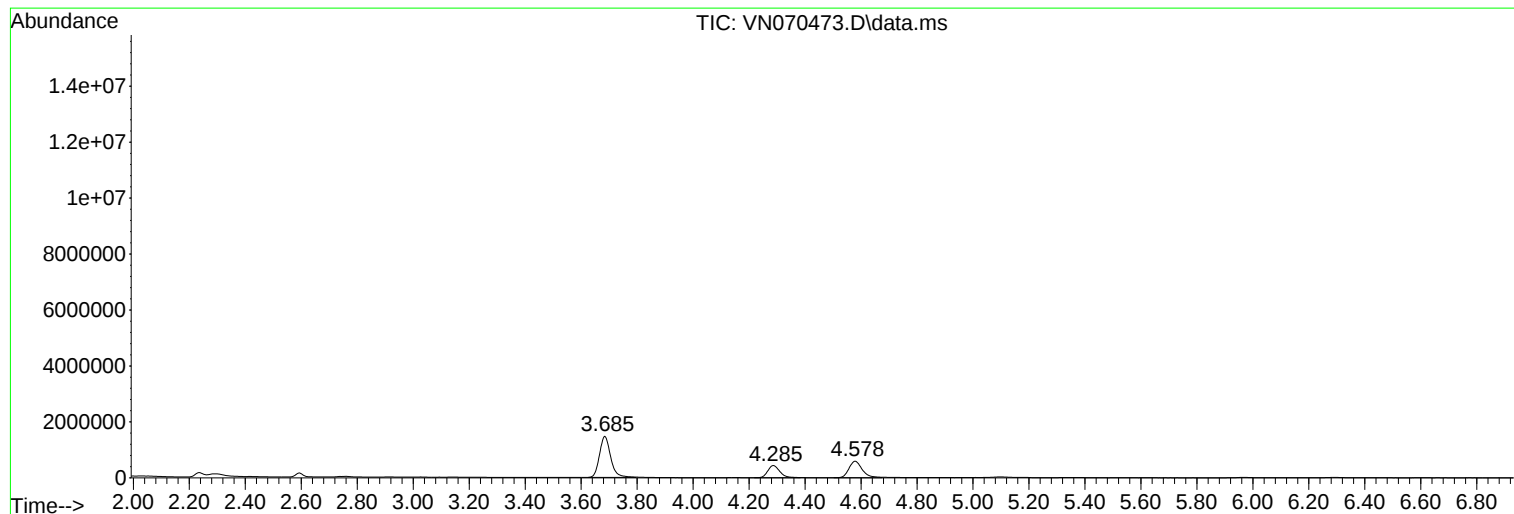
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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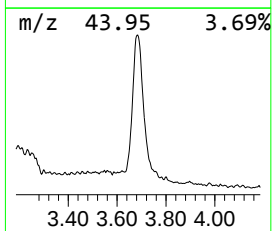
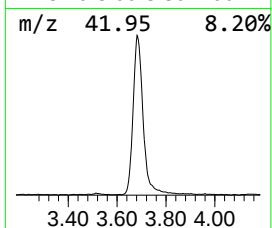
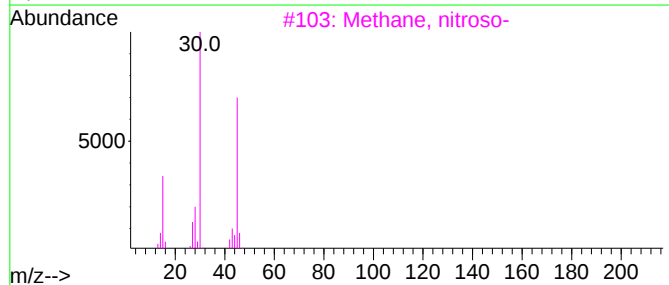
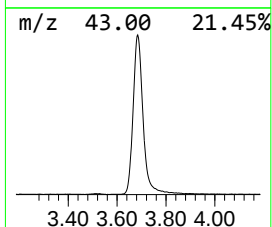
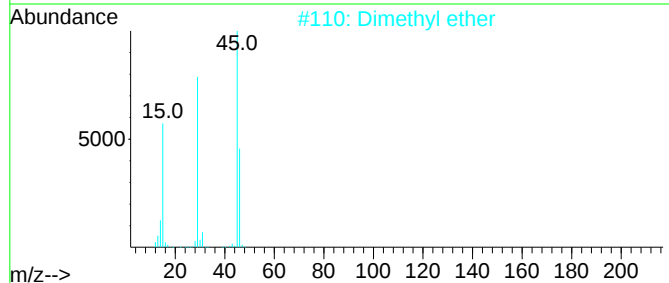
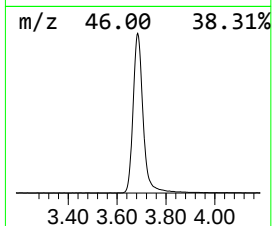
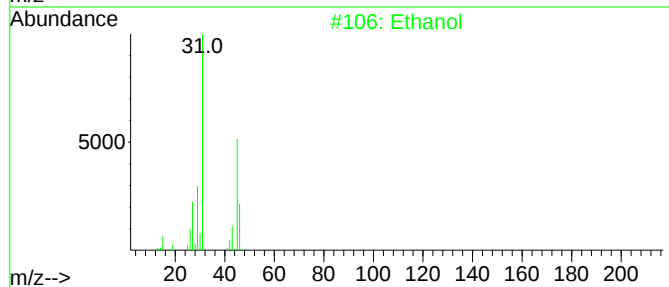
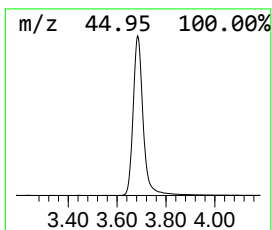
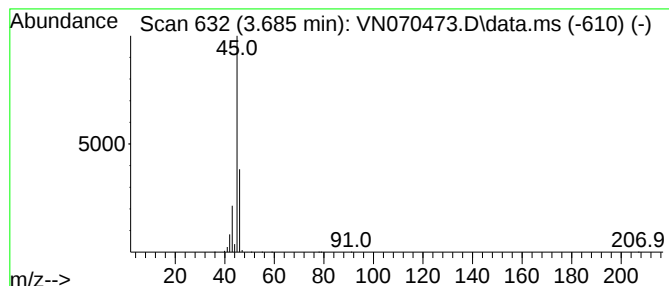
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.685	76.42 ug/l	4037250	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	64
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Formic acid			46	CH2O2	000064-18-6	4
5	L-Lactic acid			90	C3H6O3	000079-33-4	2



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Instrument :
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ClientSampleId :
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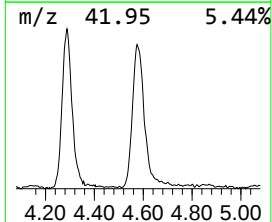
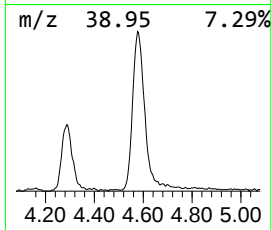
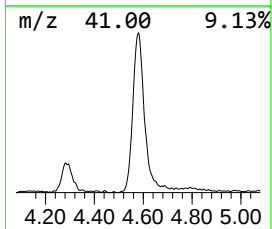
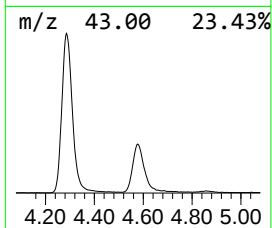
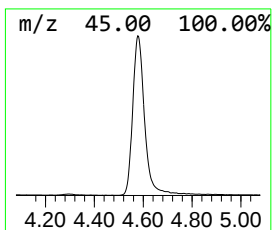
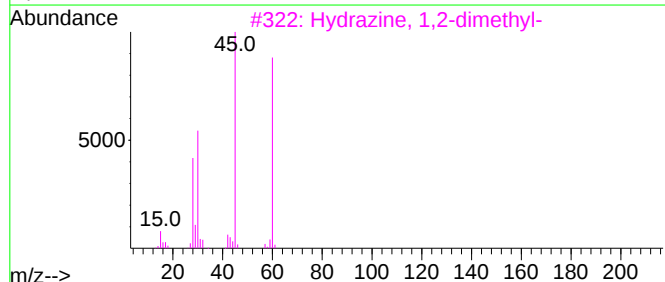
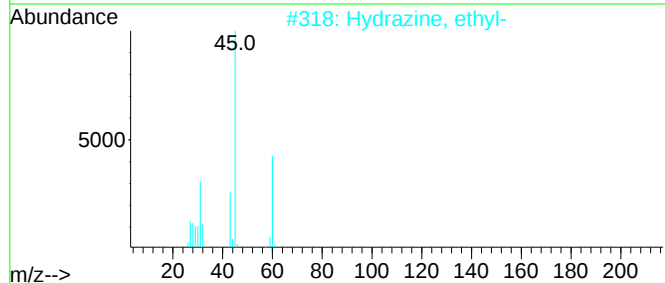
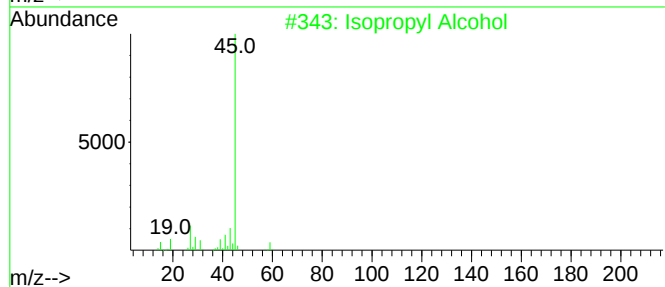
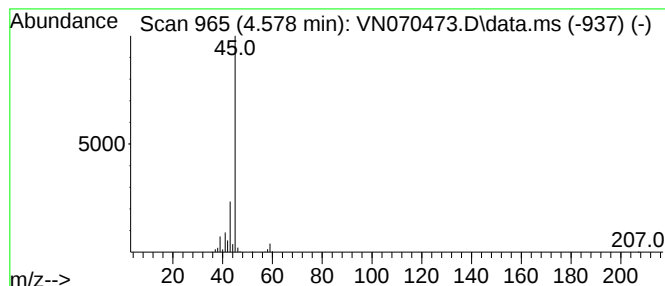
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.578	36.91 ug/l	1949870	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4
5			Formamide	45	CH3NO	000075-12-7	4



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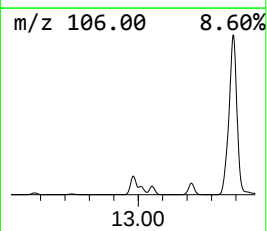
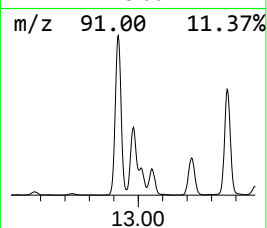
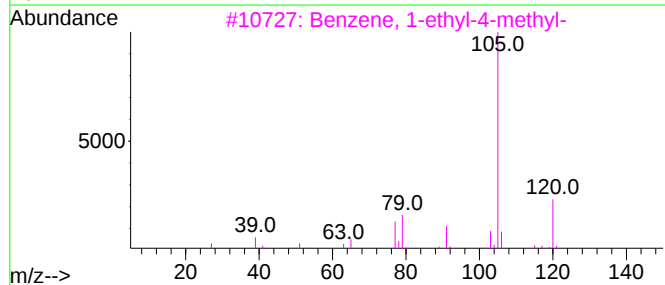
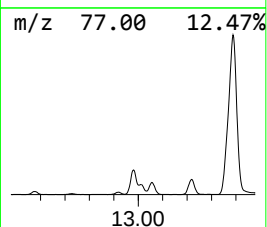
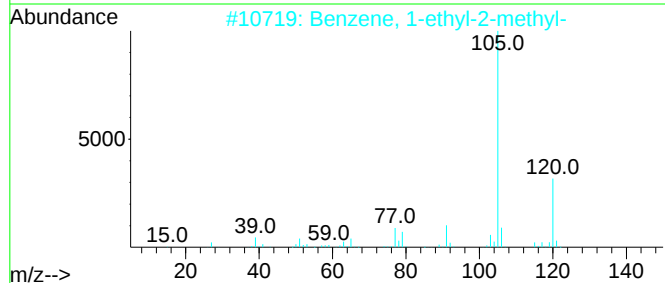
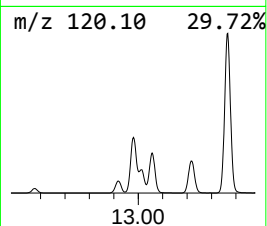
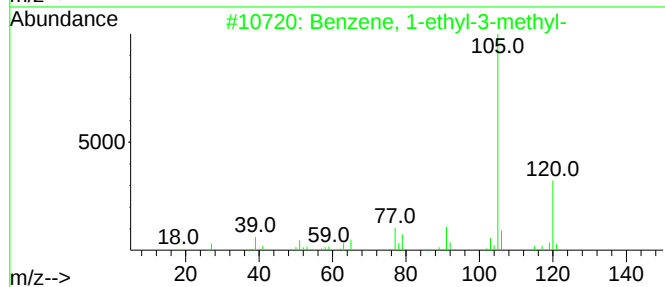
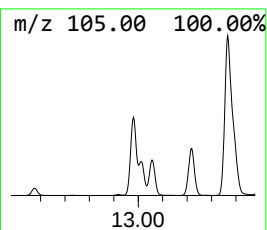
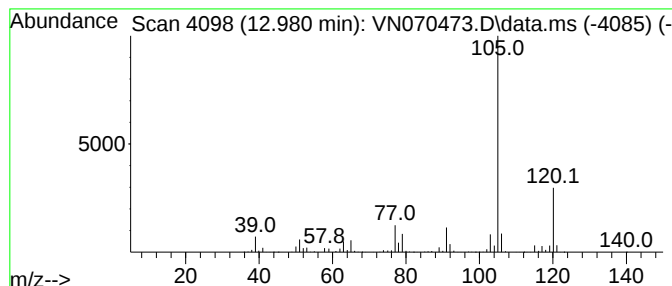
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	39.44 ug/l	2298330	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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Instrument :
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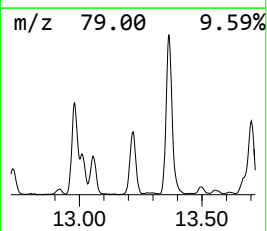
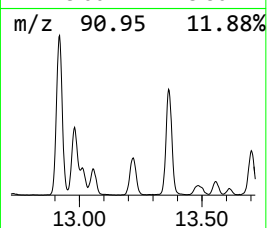
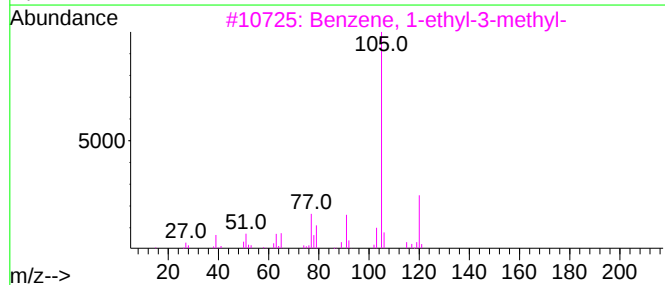
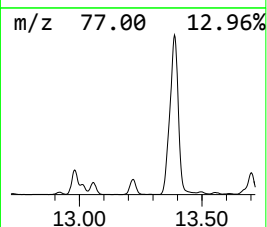
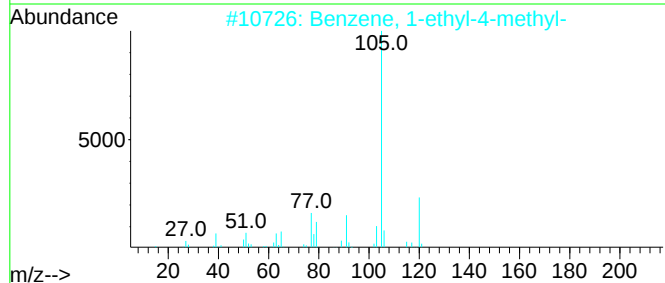
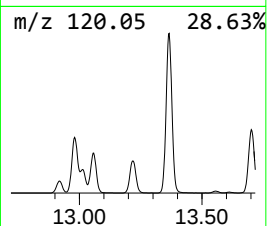
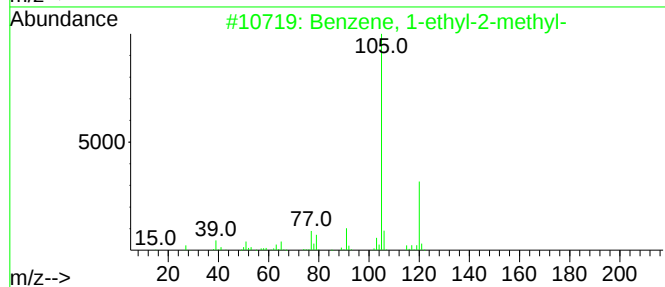
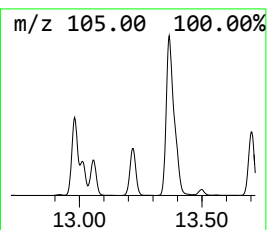
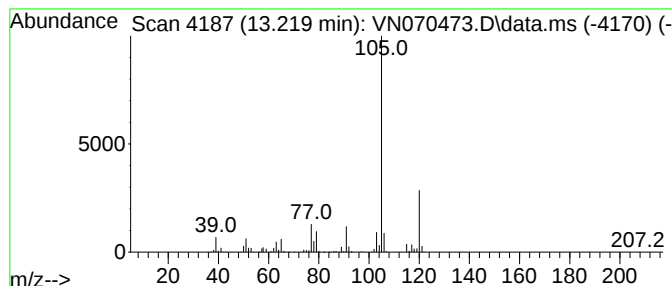
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	26.32 ug/l	1533520	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	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



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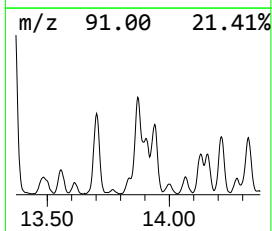
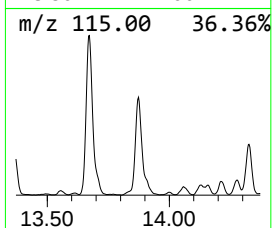
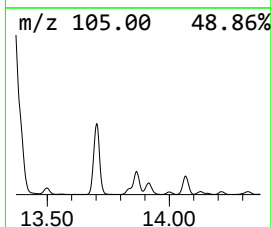
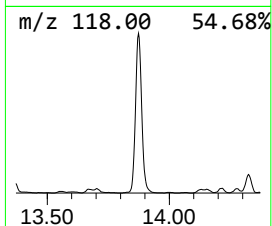
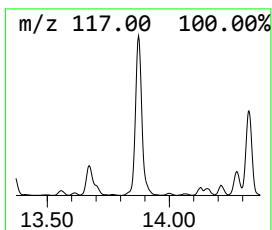
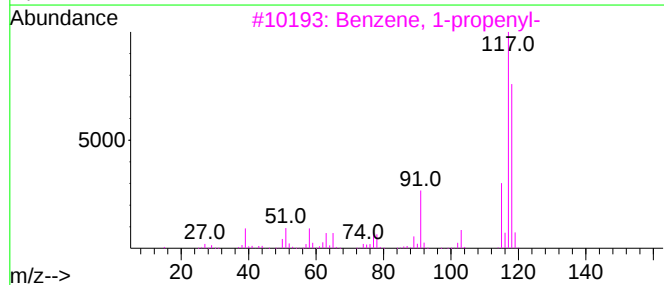
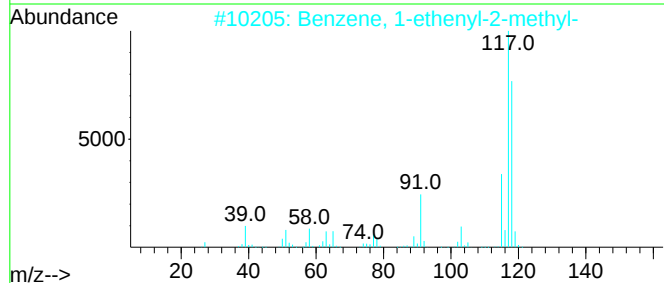
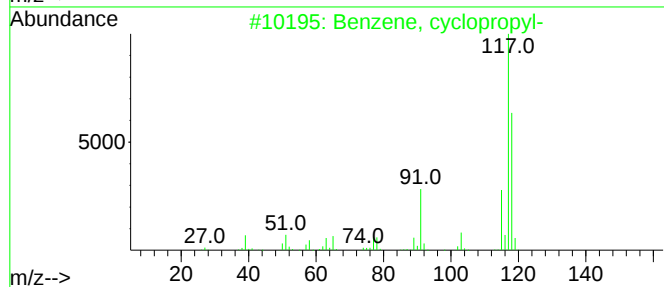
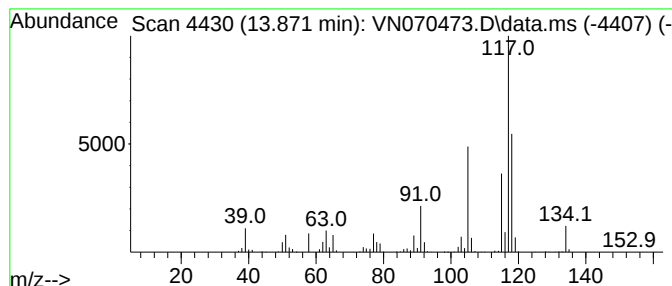
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, cyclopropyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	37.07 ug/l	2160420	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	94
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	93
4			Indane	118	C9H10	000496-11-7	93
5			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010422\
Data File : VN070473.D
Acq On : 4 Jan 2022 19:14
Operator : JC/MD
Sample : N1012-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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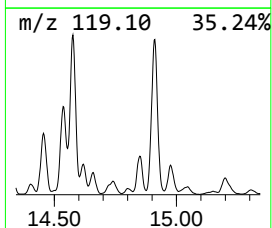
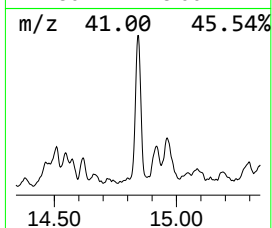
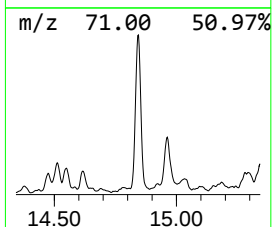
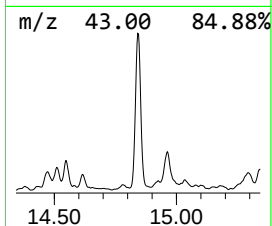
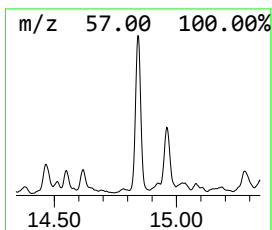
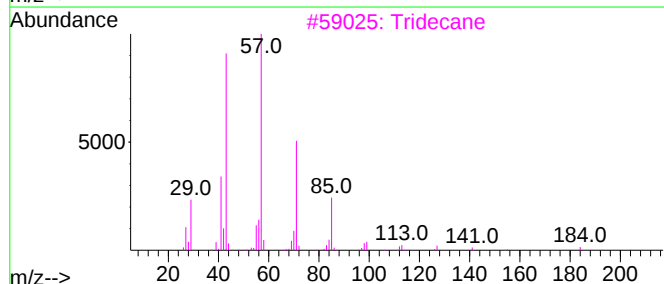
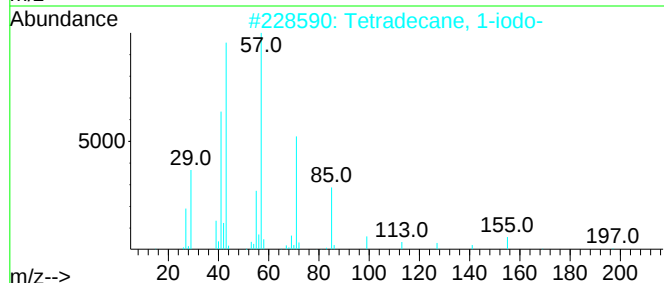
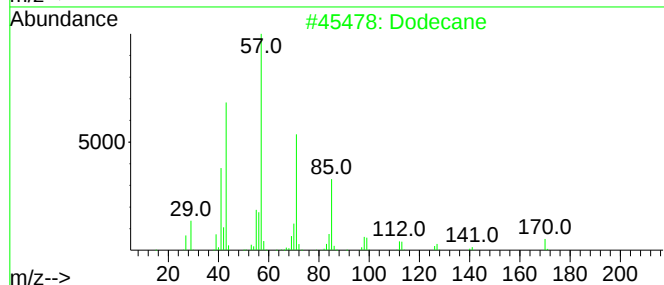
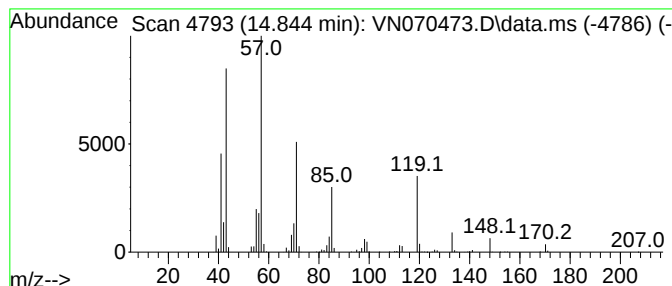
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Quant Title : SW846 8260

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

Peak Number 6 Dodecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.844	17.99 ug/l	1048630	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	86
2			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	53
3			Tridecane	184	C13H28	000629-50-5	52
4			Tetradecane	198	C14H30	000629-59-4	52
5			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010422\
Data File : VN070473.D
Acq On : 4 Jan 2022 19:14
Operator : JC/MD
Sample : N1012-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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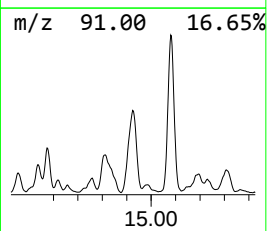
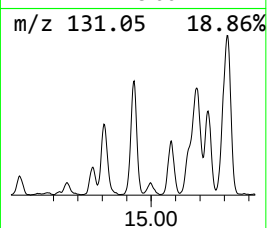
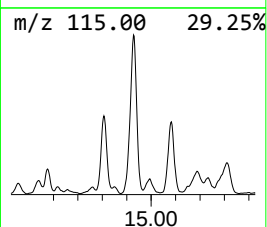
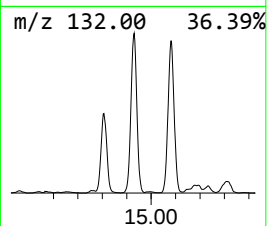
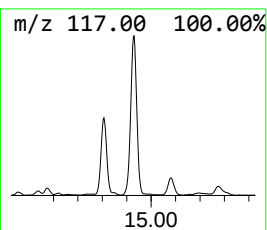
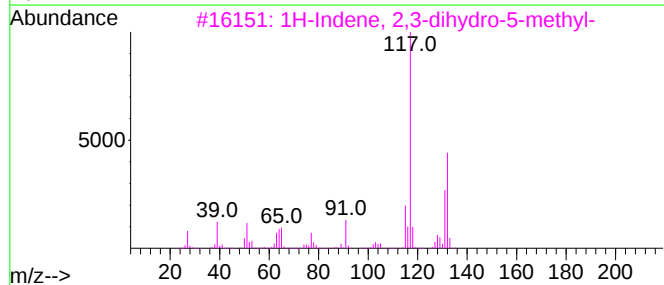
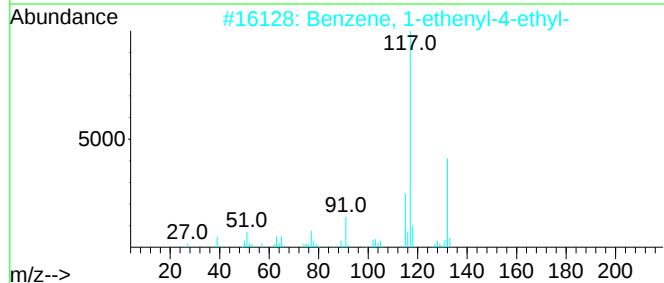
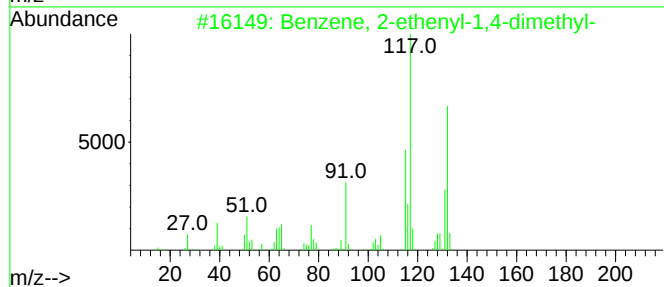
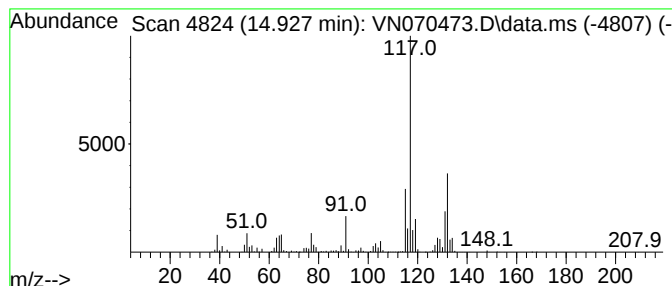
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	55.20 ug/l	3217000	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010422\
Data File : VN070473.D
Acq On : 4 Jan 2022 19:14
Operator : JC/MD
Sample : N1012-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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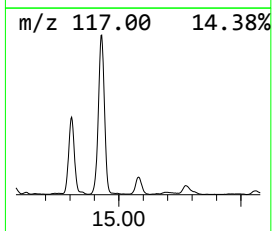
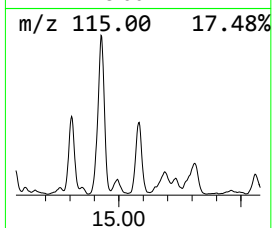
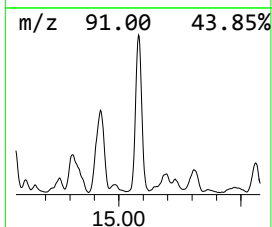
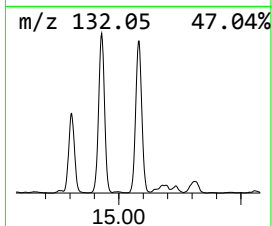
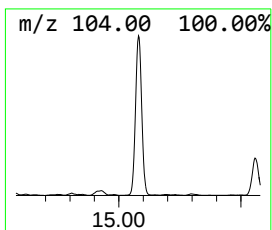
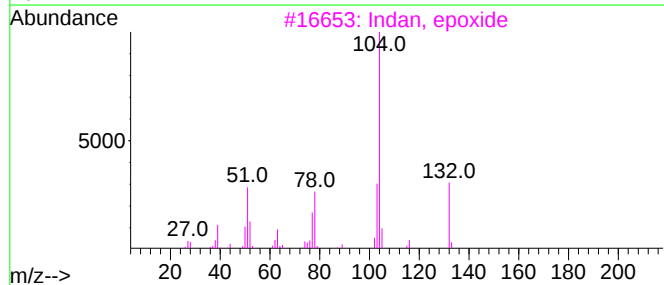
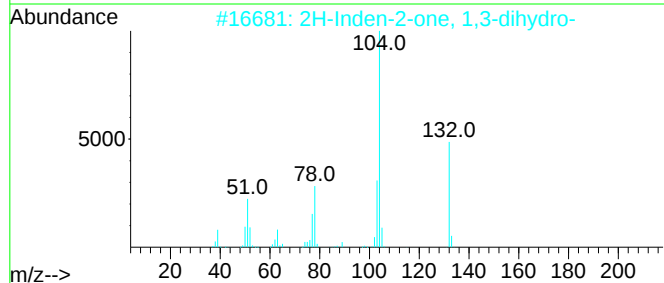
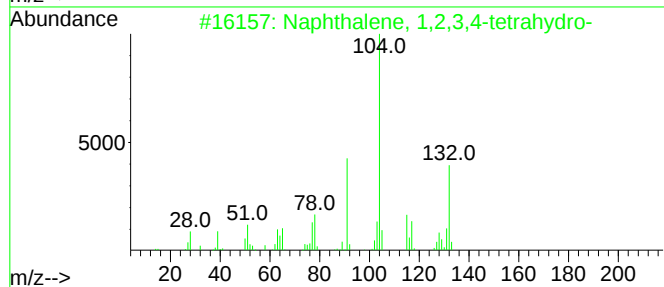
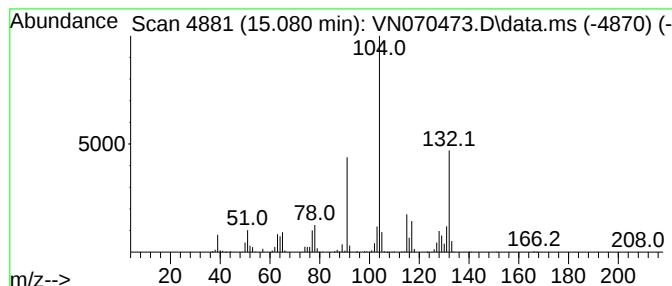
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetrahydro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	29.20 ug/l	1701360	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	58
3			Indan, epoxide	132	C9H8O	000768-22-9	52
4			Benzene, 3-cyclohexen-1-yl-	158	C12H14	004994-16-5	47
5			Benzene, cyclobutyl-	132	C10H12	004392-30-7	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010422\
Data File : VN070473.D
Acq On : 4 Jan 2022 19:14
Operator : JC/MD
Sample : N1012-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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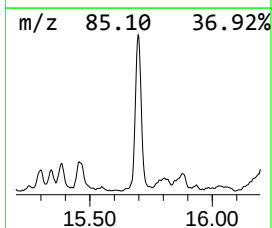
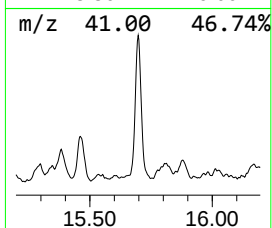
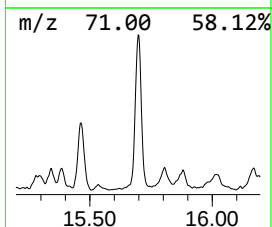
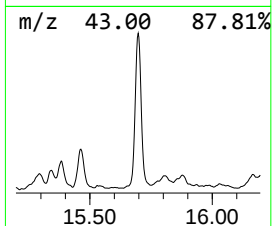
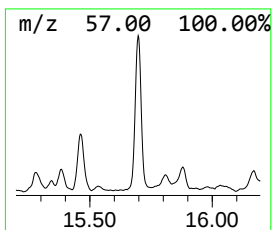
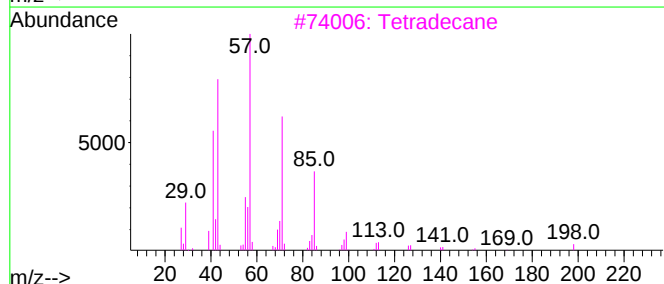
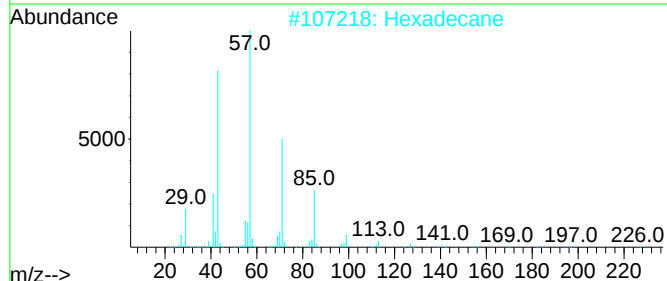
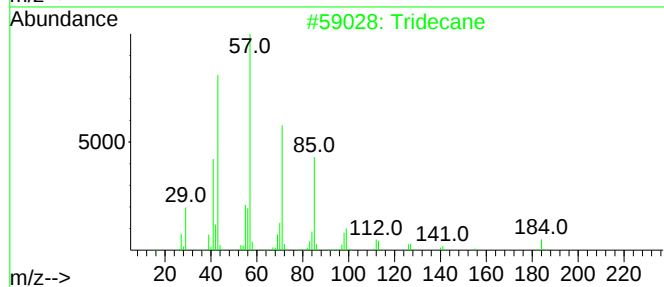
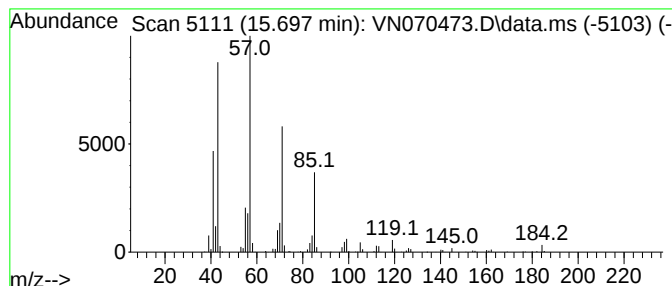
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Quant Title : SW846 8260

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

Peak Number 9 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.697	20.82 ug/l	1213050	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	93
2			Hexadecane	226	C16H34	000544-76-3	86
3			Tetradecane	198	C14H30	000629-59-4	86
4			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010422\
Data File : VN070473.D
Acq On : 4 Jan 2022 19:14
Operator : JC/MD
Sample : N1012-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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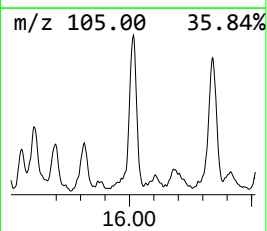
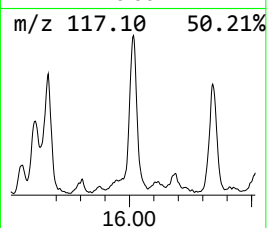
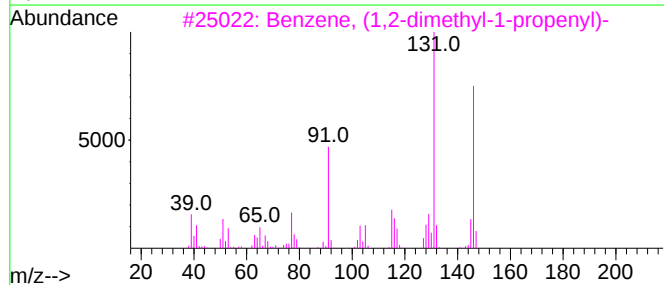
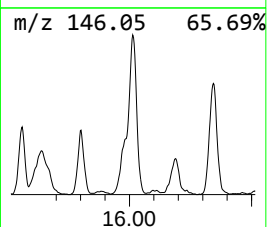
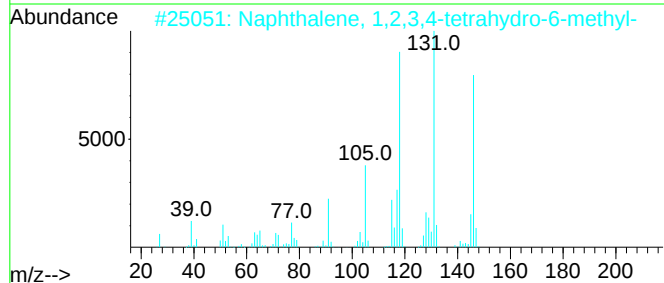
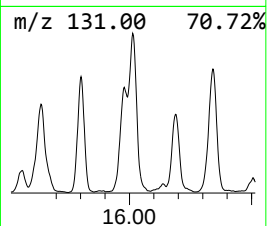
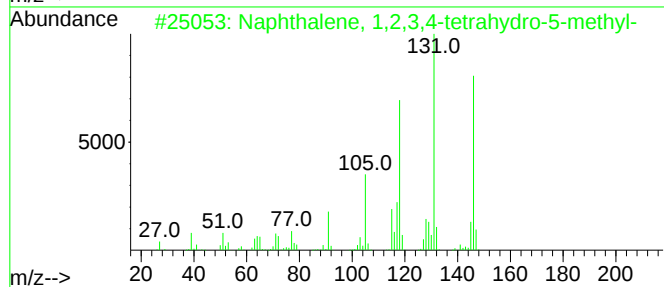
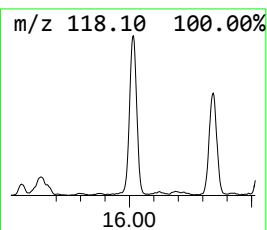
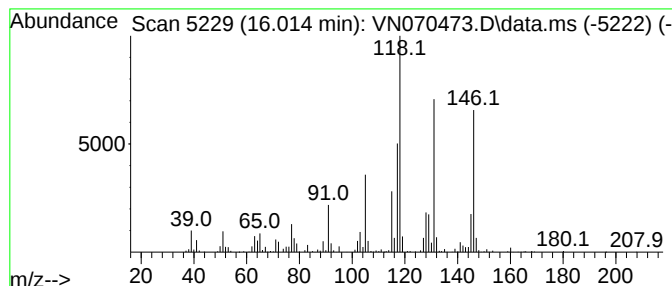
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.014	19.32 ug/l	1125790	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	91
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	64
3			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	46
4			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	45
5			7-Methylindan-1-one	146	C10H10O	039627-61-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010422\
Data File : VN070473.D
Acq On : 4 Jan 2022 19:14
Operator : JC/MD
Sample : N1012-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.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
Ethanol	3.685	76.4	ug/l	4037250	1	8.086	2641460	50.0
Isopropyl Alcohol	4.578	36.9	ug/l	1949870	1	8.086	2641460	50.0
Benzene, 1-ethy...	12.980	39.4	ug/l	2298330	4	13.672	2913700	50.0
Benzene, 1-ethy...	13.219	26.3	ug/l	1533520	4	13.672	2913700	50.0
Benzene, cyclop...	13.871	37.1	ug/l	2160420	4	13.672	2913700	50.0
Dodecane	14.844	18.0	ug/l	1048630	4	13.672	2913700	50.0
Benzene, 2-ethe...	14.927	55.2	ug/l	3217000	4	13.672	2913700	50.0
Naphthalene, 1,...	15.080	29.2	ug/l	1701360	4	13.672	2913700	50.0
Tridecane	15.697	20.8	ug/l	1213050	4	13.672	2913700	50.0
Naphthalene, 1,...	16.014	19.3	ug/l	1125790	4	13.672	2913700	50.0