

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
 Data File : VN081796.D
 Acq On : 18 Apr 2024 18:42
 Operator : JC\MD
 Sample : P2121-04
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 4826

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\82N041524W.M
 Title : SW846 8260

Signal : TIC: VN081796.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.077	16	21	27	rBV	35720	57422	1.47%	0.249%
2	2.812	138	146	152	rBV2	33413	66276	1.69%	0.287%
3	4.430	410	421	434	rBV	29243	87462	2.23%	0.379%
4	6.677	792	803	811	rBV4	15681	54847	1.40%	0.238%
5	7.230	886	897	906	rBV4	30793	88445	2.26%	0.383%
6	8.165	1046	1056	1061	rBV	208182	489927	12.51%	2.122%
7	8.224	1061	1066	1079	rVB	382482	820893	20.96%	3.555%
8	8.582	1111	1127	1135	rBV	212037	518588	13.24%	2.246%
9	9.100	1205	1215	1227	rBV	528627	1082953	27.65%	4.690%
10	9.271	1237	1244	1254	rBV	39729	95980	2.45%	0.416%
11	9.647	1302	1308	1314	rBV9	14308	39411	1.01%	0.171%
12	10.565	1458	1464	1478	rVB	855790	1600378	40.86%	6.931%
13	11.865	1679	1685	1697	rVB	779939	1484577	37.90%	6.430%
14	12.141	1707	1732	1733	rBV3	674577	2825503	72.13%	12.237%
15	12.847	1846	1852	1860	rVB	625349	1150417	29.37%	4.982%
16	13.059	1880	1888	1899	rBV4	256757	942268	24.05%	4.081%
17	13.223	1906	1916	1917	rBV5	282413	834426	21.30%	3.614%
18	13.259	1918	1922	1928	rVB	913493	1532811	39.13%	6.639%
19	13.335	1929	1935	1955	rVB	1800900	3917159	100.00%	16.965%
20	13.506	1958	1964	1970	rBV	330099	598506	15.28%	2.592%
21	13.612	1976	1982	1987	rBV10	110796	295217	7.54%	1.279%
22	13.688	1991	1995	2006	rVB7	356390	863283	22.04%	3.739%
23	13.794	2007	2013	2018	rBV	786804	1403684	35.83%	6.079%
24	14.017	2044	2051	2061	rVB5	252477	807230	20.61%	3.496%
25	14.694	2161	2166	2175	rVB7	99776	278833	7.12%	1.208%
26	15.223	2247	2256	2267	rVB4	188667	593658	15.16%	2.571%
27	15.394	2280	2285	2292	rBV5	139186	343384	8.77%	1.487%
28	16.500	2465	2473	2478	rBV5	67946	216033	5.52%	0.936%

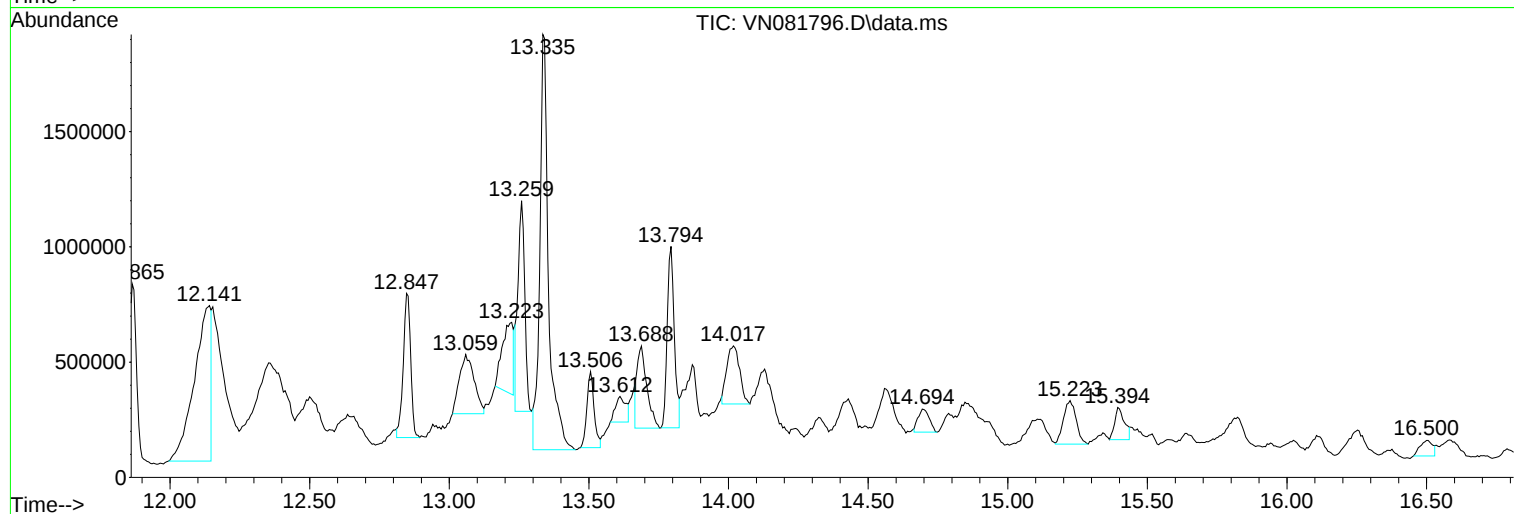
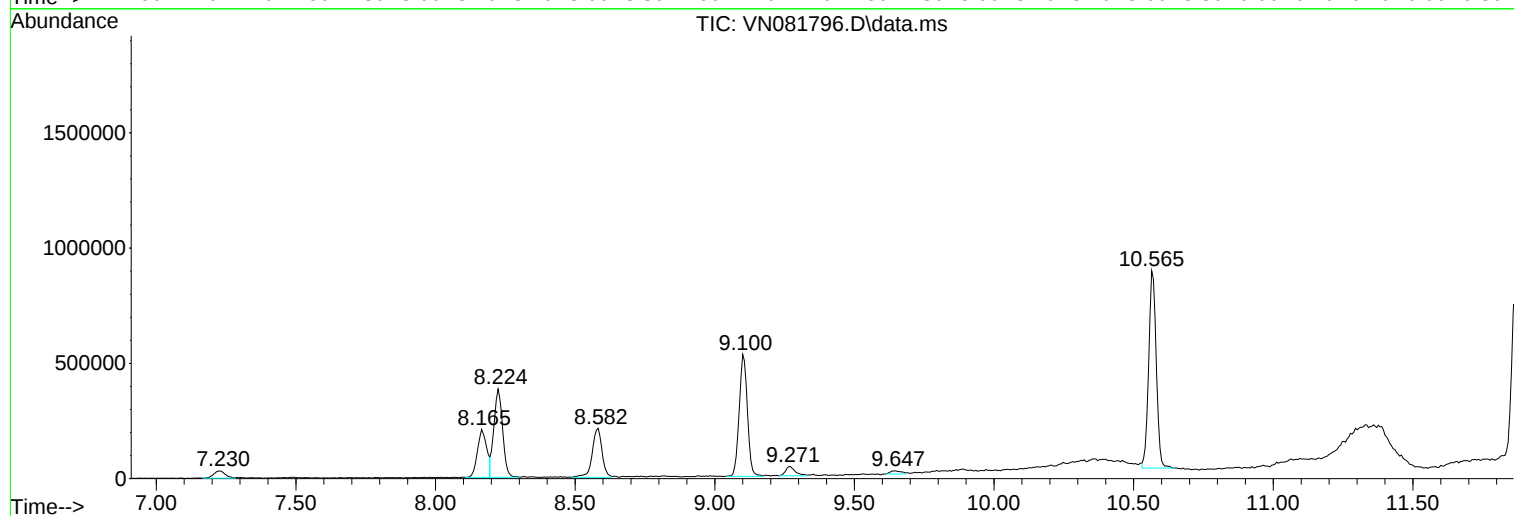
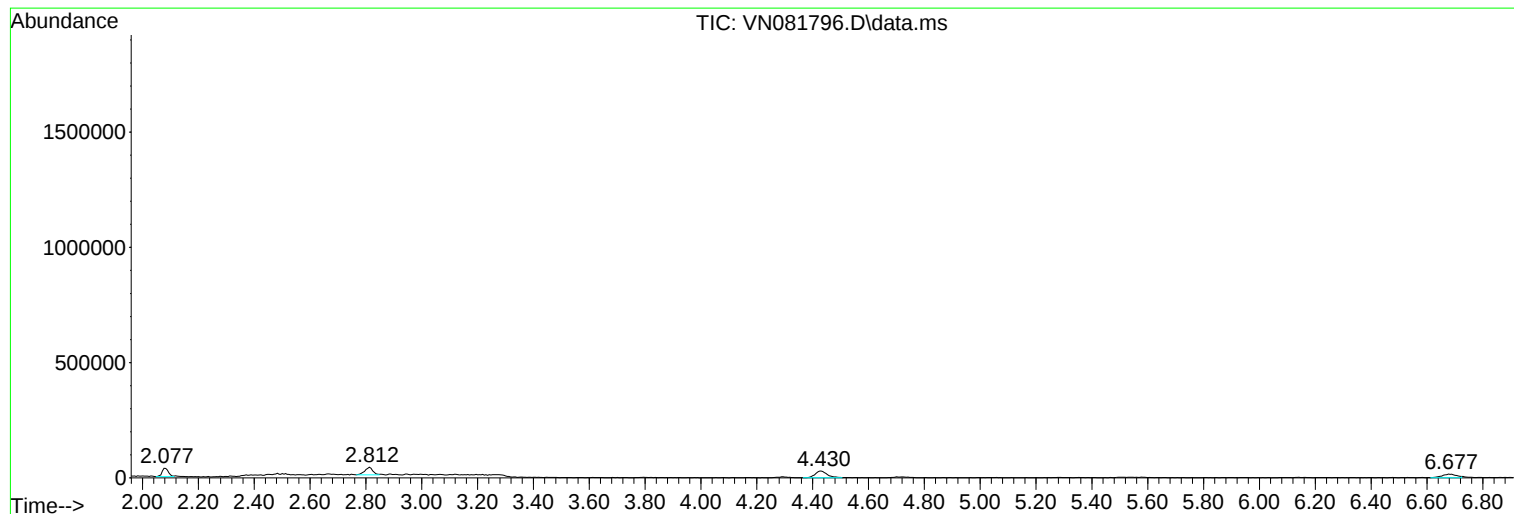
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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



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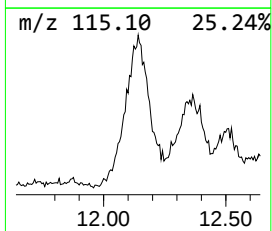
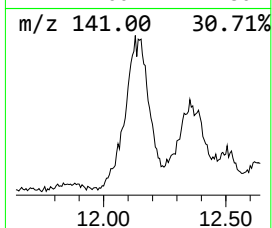
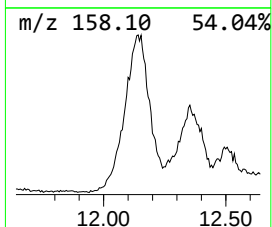
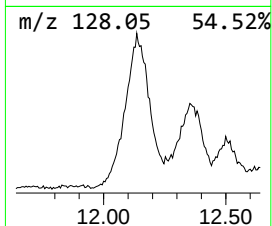
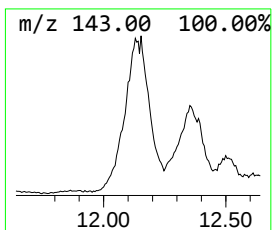
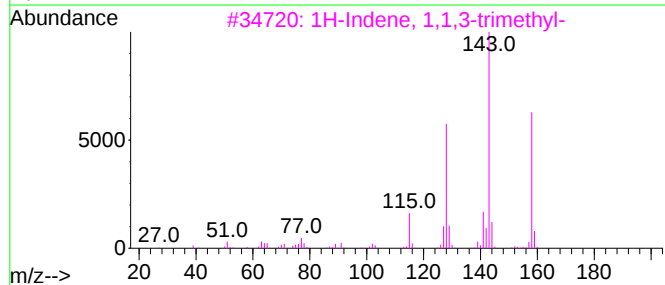
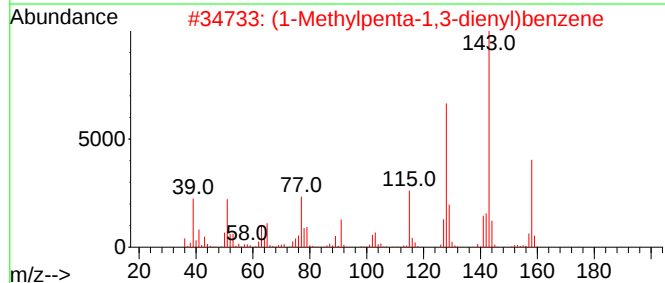
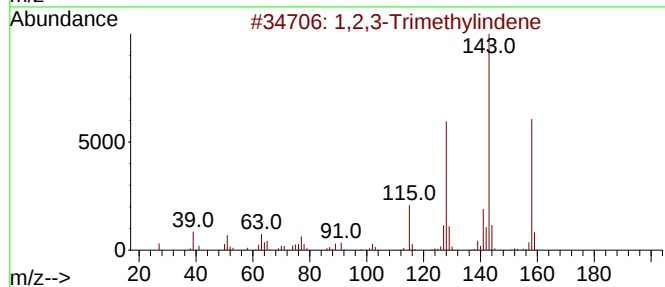
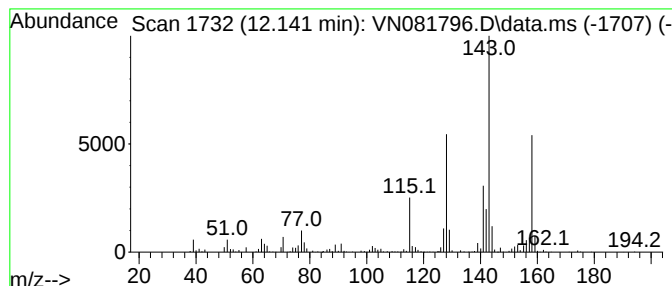
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1,2,3-Trimethylindene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.141	95.16 ug/l	2825500	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,3-Trimethylindene	158	C12H14	004773-83-5	94
2			(1-Methylpenta-1,3-dienyl)benzene	158	C12H14	116669-49-9	90
3			1H-Indene, 1,1,3-trimethyl-	158	C12H14	002177-45-9	87
4			Benzene, 1,3,5-trimethyl-2-(1,2-...	158	C12H14	029555-07-5	80
5			(1-Methylpenta-2,4-dienyl)benzene	158	C12H14	1000210-01-1	74



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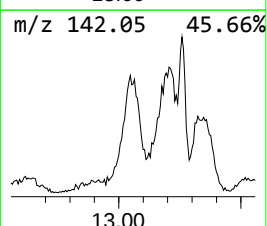
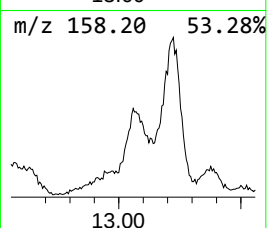
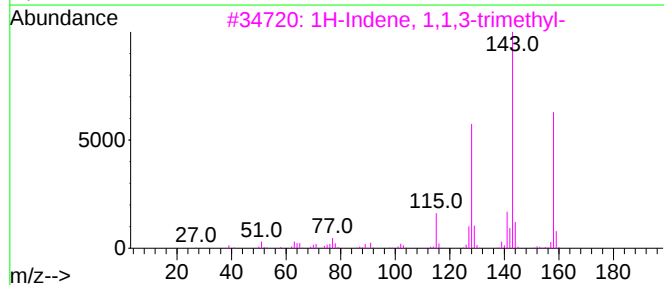
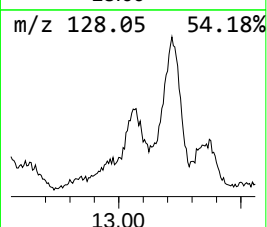
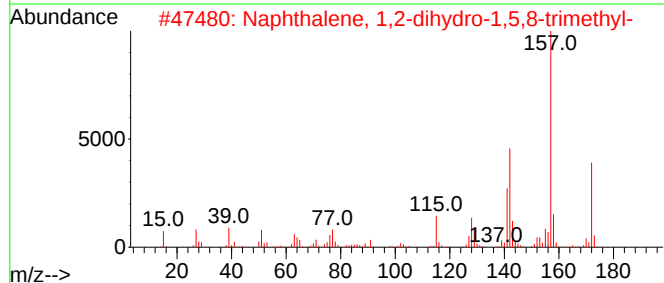
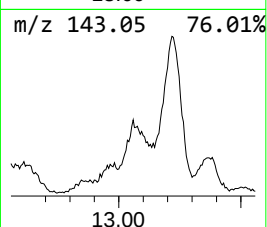
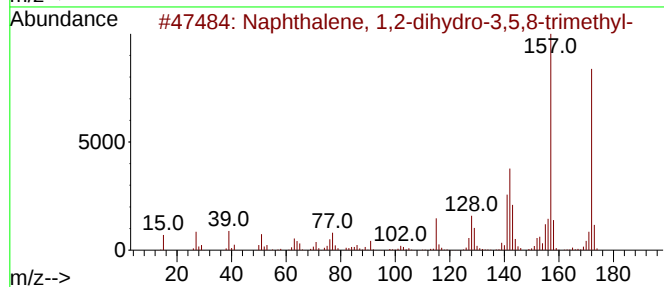
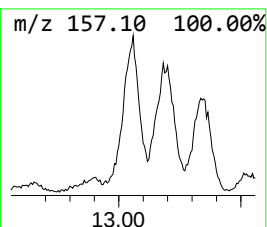
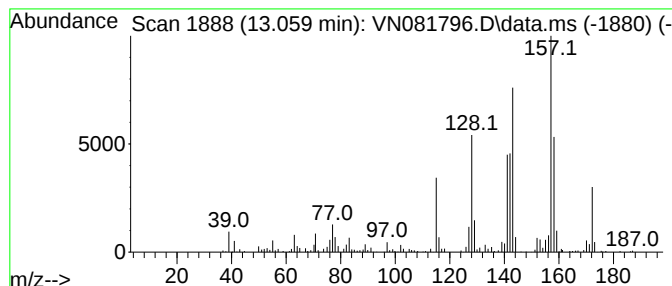
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
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Peak Number 2 Naphthalene, 1,2-dihydro-3,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.059	33.56 ug/l	942268	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2-dihydro-3,5,8-t...	172	C13H16	030316-18-8	52
2			Naphthalene, 1,2-dihydro-1,5,8-t...	172	C13H16	004506-36-9	50
3			1H-Indene, 1,1,3-trimethyl-	158	C12H14	002177-45-9	50
4			Benzene, 1,4-bis(1-methylethenyl)-	158	C12H14	001605-18-1	50
5			1,2,3-Trimethylindene	158	C12H14	004773-83-5	50



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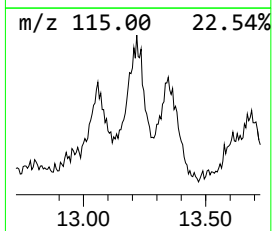
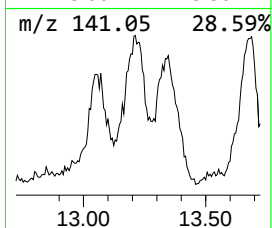
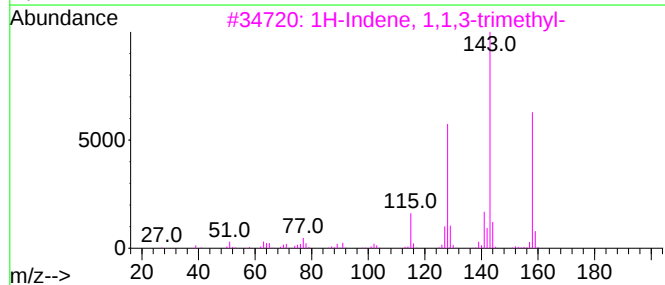
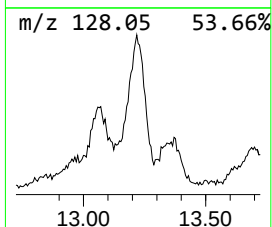
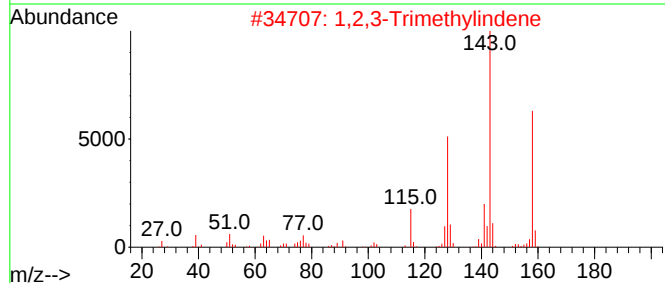
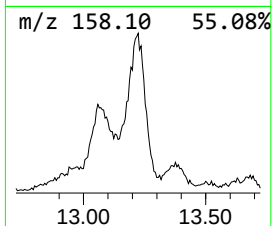
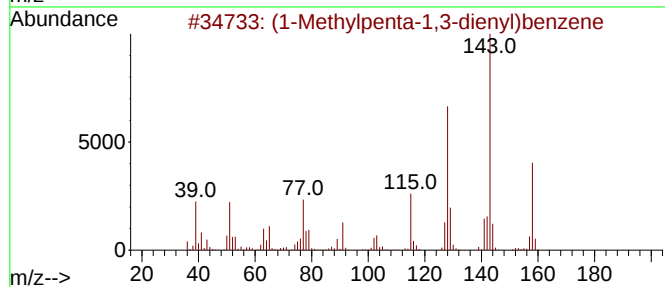
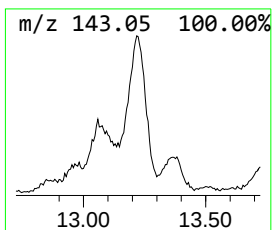
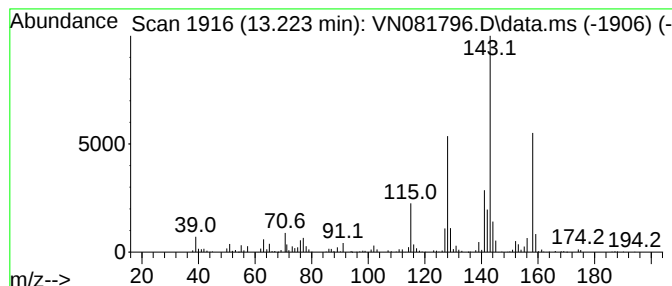
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (1-Methylpenta-1,3-dienyl)b... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.223	29.72 ug/l	834426	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1-Methylpenta-1,3-dienyl)benzene	158	C12H14	116669-49-9	90
2			1,2,3-Trimethylindene	158	C12H14	004773-83-5	90
3			1H-Indene, 1,1,3-trimethyl-	158	C12H14	002177-45-9	87
4			Benzene, 1,4-bis(1-methylethenyl)-	158	C12H14	001605-18-1	72
5			Benzene, 1,3,5-trimethyl-2-(1,2-...	158	C12H14	029555-07-5	72



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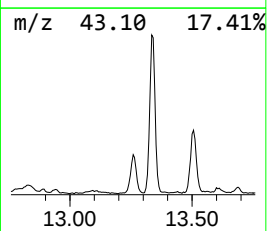
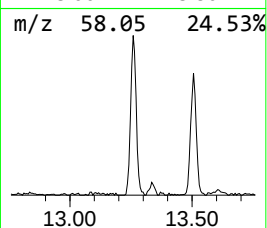
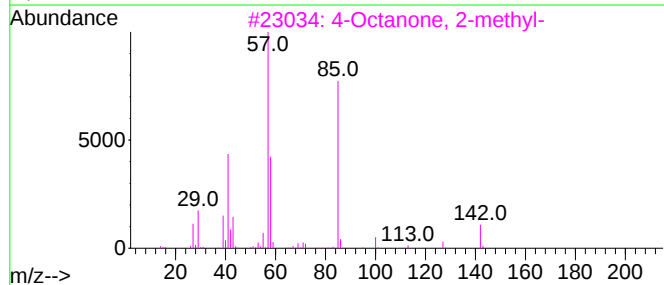
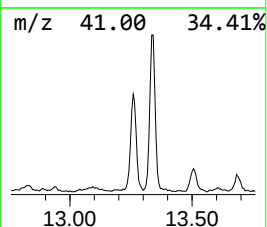
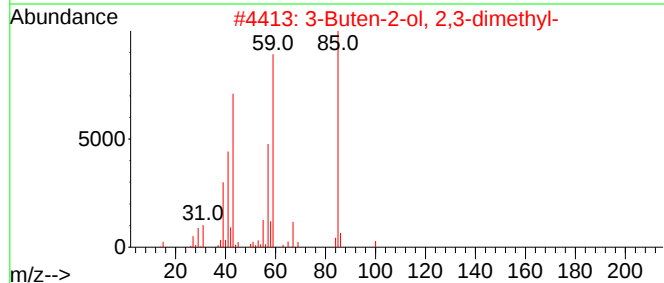
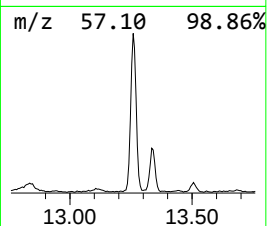
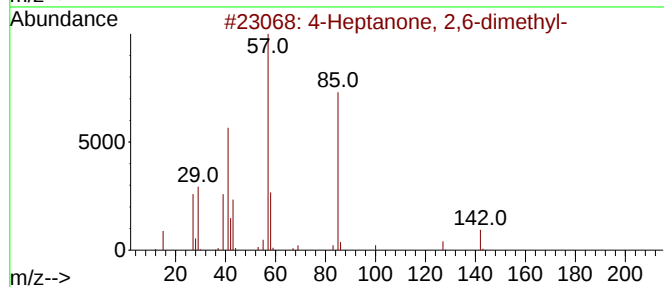
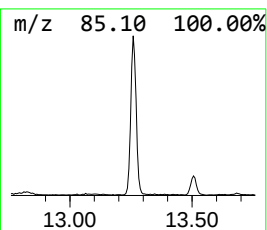
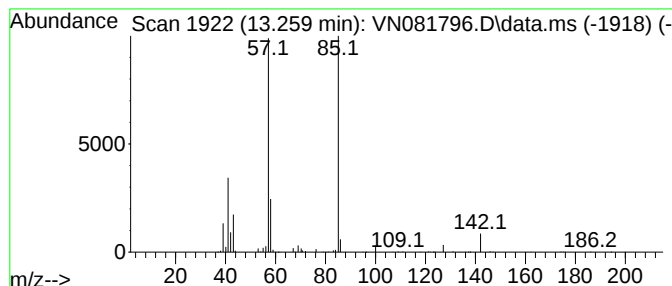
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Peak Number 4 4-Heptanone, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	54.60 ug/l	1532810	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	80
2		3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	59
3		4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	47
4		3,5-Heptanedione, 4-acetyl-2,2,6...	226	C13H22O3	1000161-42-4	45
5		2-Methylbutanoic anhydride	186	C10H18O3	001468-39-9	42



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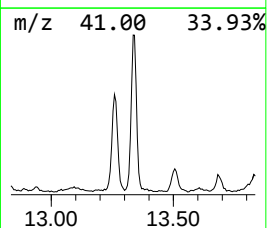
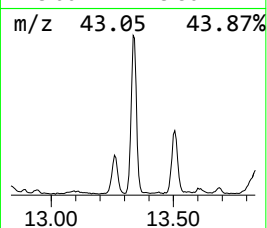
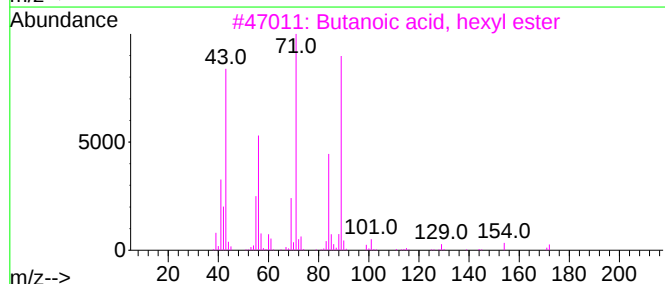
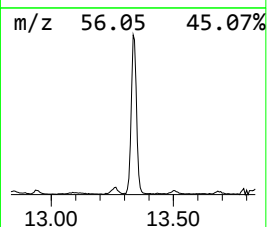
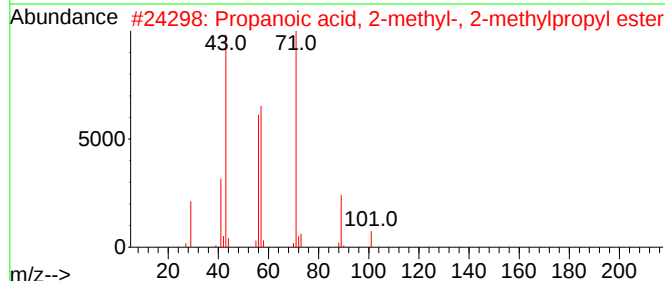
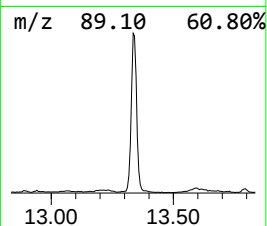
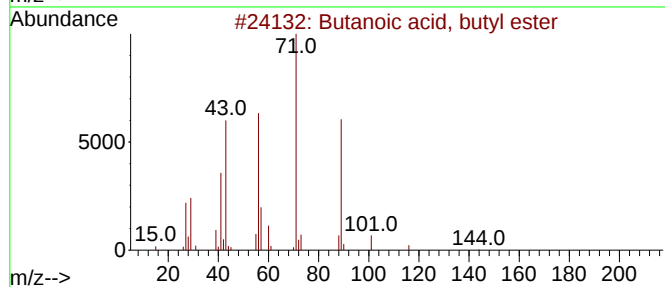
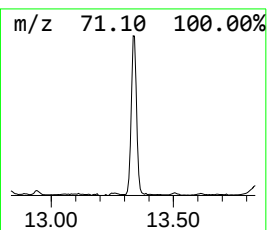
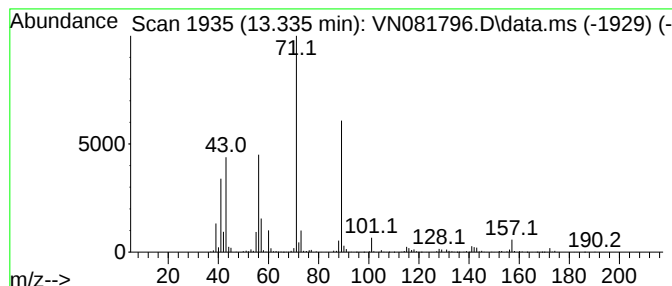
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Peak Number 5 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	139.53 ug/l	3917160	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	95
2			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59
5			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	59



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ClientSampleId :
4826

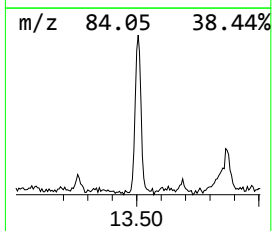
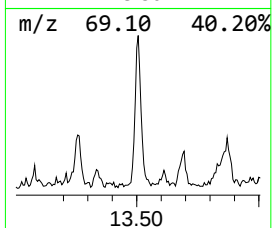
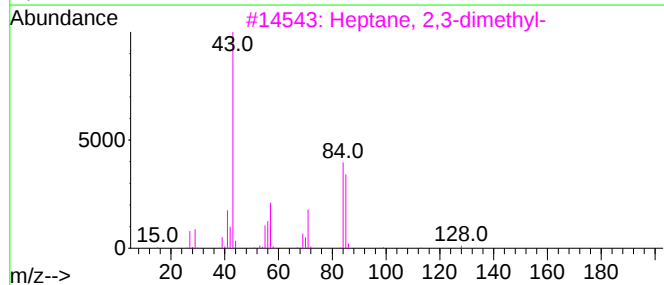
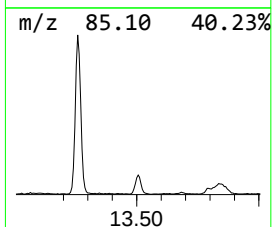
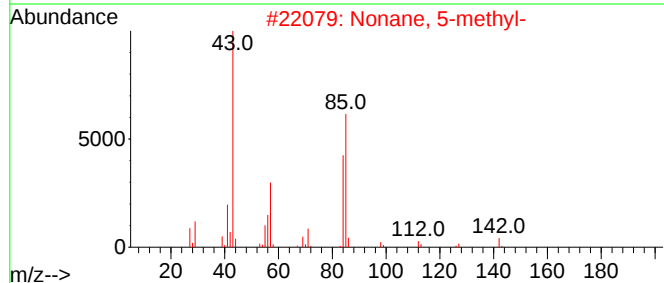
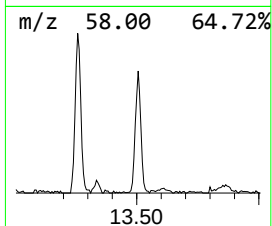
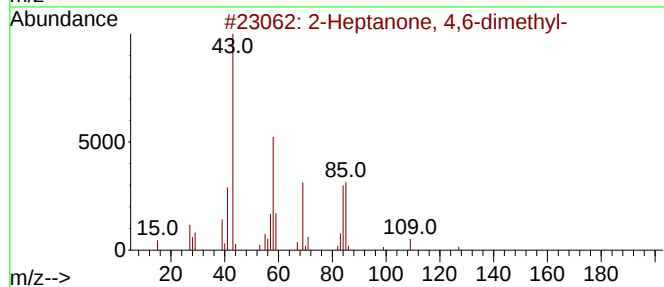
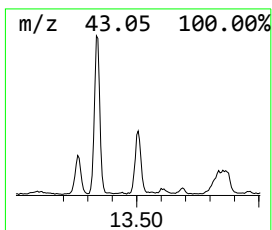
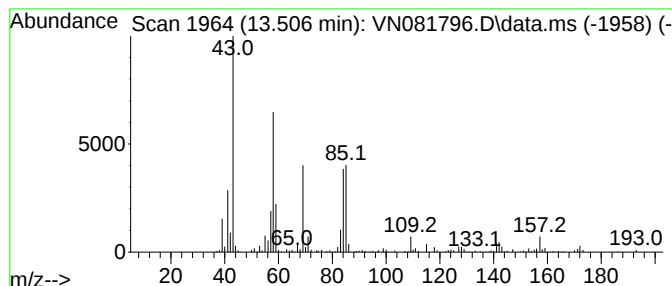
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Quant Title : SW846 8260

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

Peak Number 6 2-Heptanone, 4,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.506	21.32 ug/l	598506	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	80
2		Nonane, 5-methyl-	142	C10H22	015869-85-9	43
3		Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	35
4		Hexane, 3-ethyl-	114	C8H18	000619-99-8	35
5		2-Heptanone, 4-methyl-	128	C8H16O	006137-06-0	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081796.D
Acq On : 18 Apr 2024 18:42
Operator : JC\MD
Sample : P2121-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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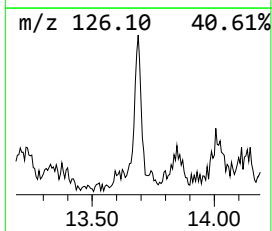
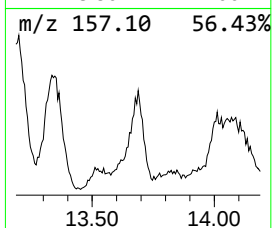
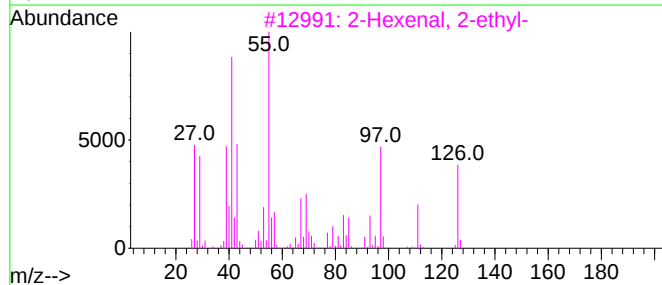
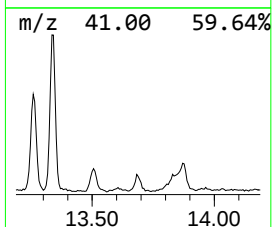
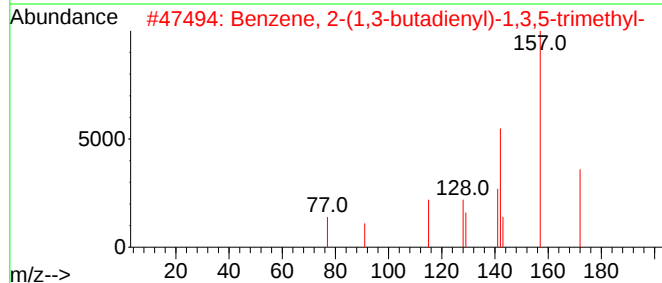
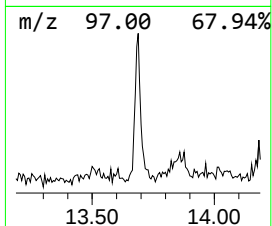
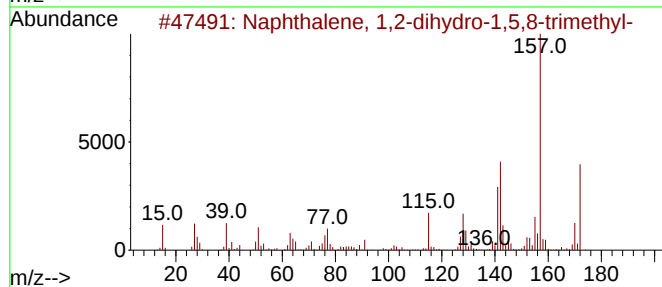
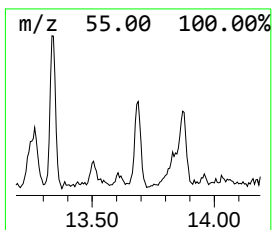
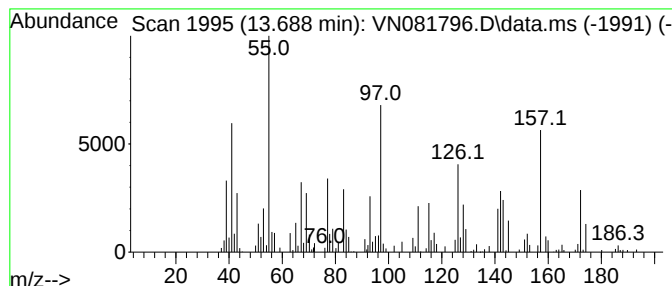
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.688 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	30.75 ug/l	863283	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2-dihydro-1,5,8-t...	172	C13H16	004506-36-9	46
2			Benzene, 2-(1,3-butadienyl)-1,3,...	172	C13H16	005732-00-3	41
3			2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	38
4			Naphthalene, 1,2-dihydro-1,1,6-t...	172	C13H16	030364-38-6	35
5			Naphthalene, 1,2-dihydro-1,4,6-t...	172	C13H16	055682-80-9	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081796.D
Acq On : 18 Apr 2024 18:42
Operator : JC\MD
Sample : P2121-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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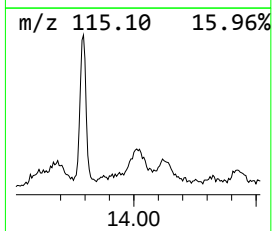
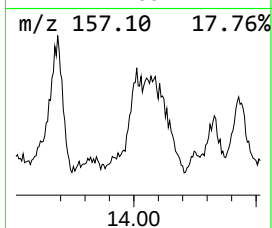
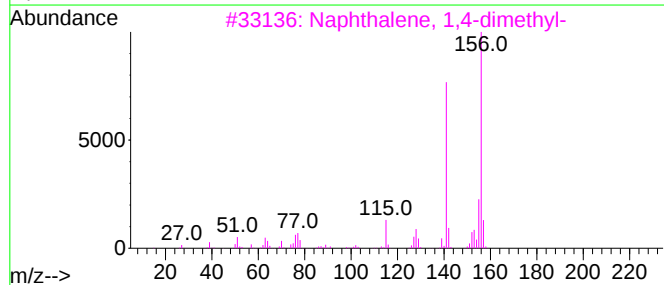
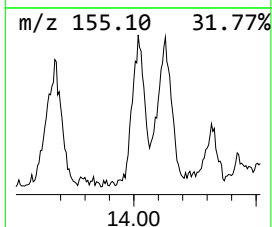
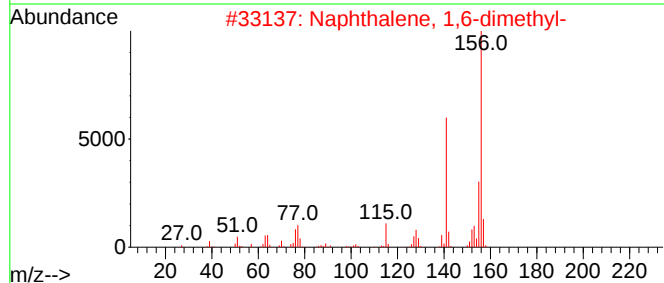
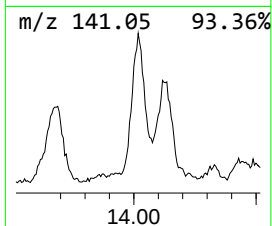
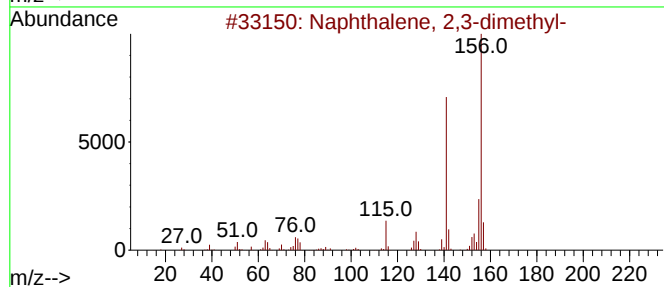
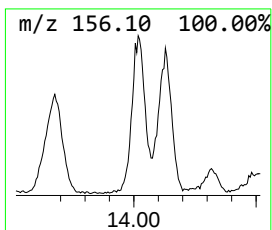
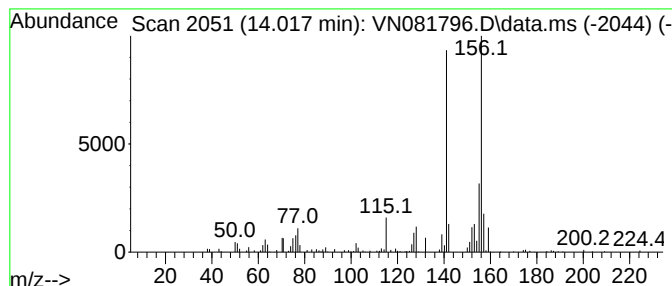
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.017	28.75 ug/l	807230	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081796.D
Acq On : 18 Apr 2024 18:42
Operator : JC\MD
Sample : P2121-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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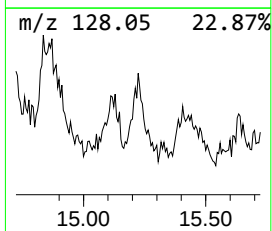
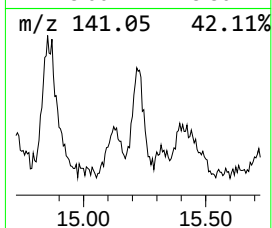
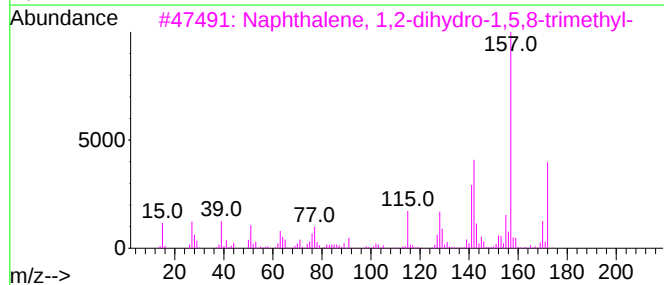
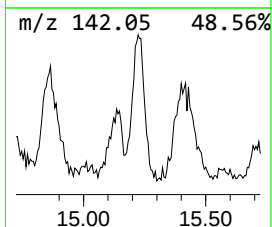
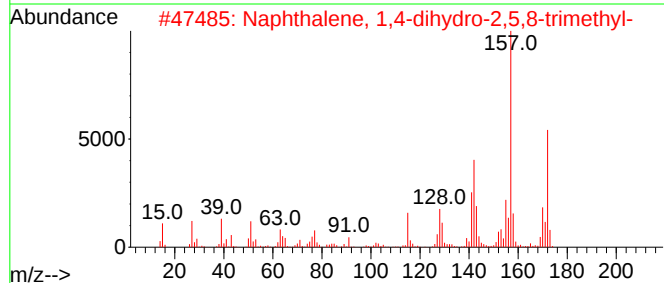
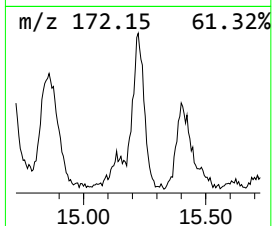
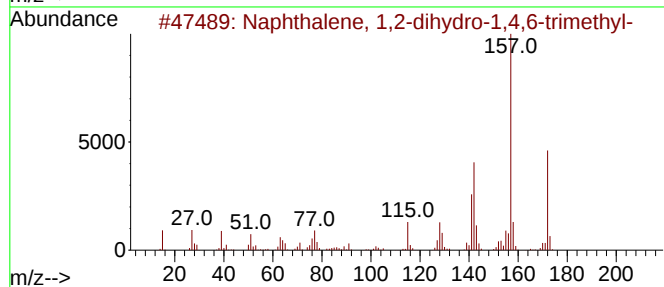
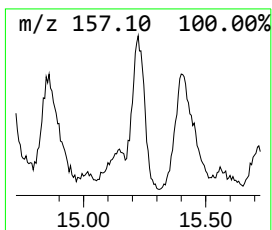
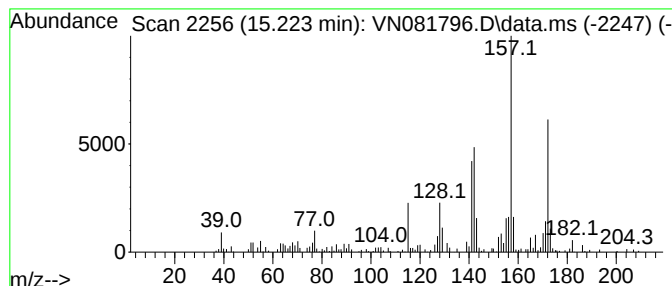
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2-dihydro-1,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.223	21.15 ug/l	593658	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2-dihydro-1,4,6-t...	172	C13H16	055682-80-9	93
2			Naphthalene, 1,4-dihydro-2,5,8-t...	172	C13H16	030316-19-9	93
3			Naphthalene, 1,2-dihydro-1,5,8-t...	172	C13H16	004506-36-9	91
4			Naphthalene, 1,2-dihydro-2,5,8-t...	172	C13H16	030316-23-5	90
5			Naphthalene, 1,2-dihydro-3,6,8-t...	172	C13H16	053156-06-2	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081796.D
Acq On : 18 Apr 2024 18:42
Operator : JC\MD
Sample : P2121-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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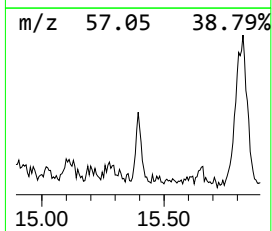
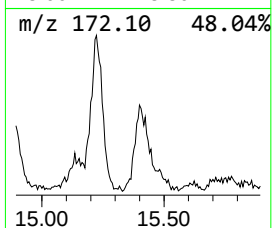
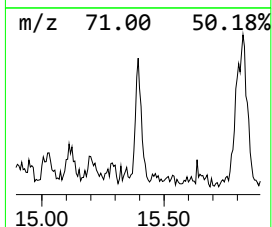
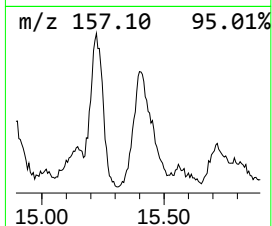
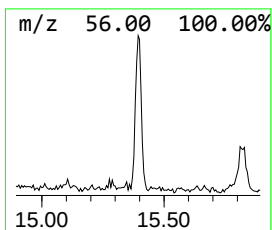
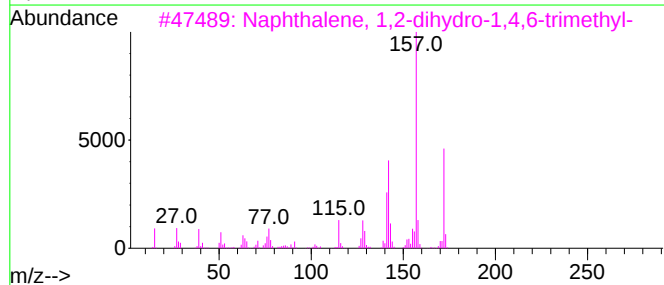
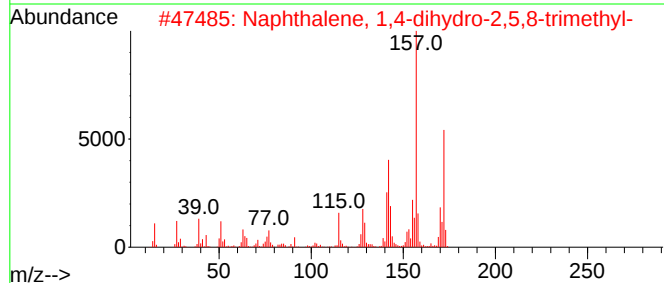
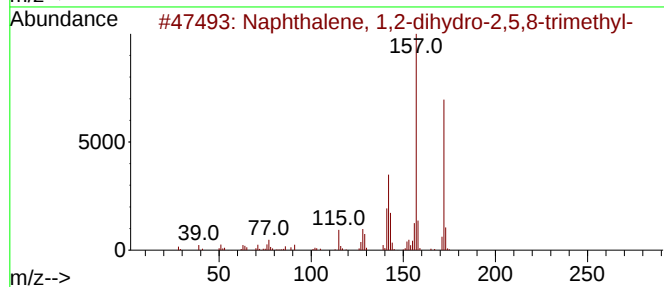
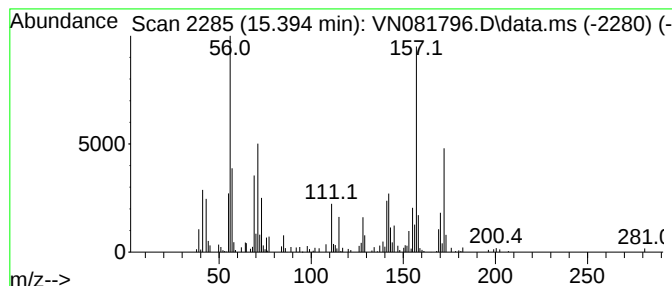
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2-dihydro-2,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.394	12.23 ug/l	343384	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2-dihydro-2,5,8-t...	172	C13H16	030316-23-5	86
2			Naphthalene, 1,4-dihydro-2,5,8-t...	172	C13H16	030316-19-9	70
3			Naphthalene, 1,2-dihydro-1,4,6-t...	172	C13H16	055682-80-9	64
4			Naphthalene, 1,2-dihydro-4,6,8-t...	172	C13H16	053156-12-0	58
5			Naphthalene, 1,2-dihydro-4,5,7-t...	172	C13H16	053156-11-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081796.D
Acq On : 18 Apr 2024 18:42
Operator : JC\MD
Sample : P2121-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.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
1,2,3-Trimethyl...	12.141	95.2	ug/l	2825500	3	11.865	1484580	50.0
Naphthalene, 1,...	13.059	33.6	ug/l	942268	4	13.794	1403680	50.0
(1-Methylpenta-...	13.223	29.7	ug/l	834426	4	13.794	1403680	50.0
4-Heptanone, 2,...	13.259	54.6	ug/l	1532810	4	13.794	1403680	50.0
Butanoic acid, ...	13.335	139.5	ug/l	3917160	4	13.794	1403680	50.0
2-Heptanone, 4,...	13.506	21.3	ug/l	598506	4	13.794	1403680	50.0
unknown13.688	13.688	30.8	ug/l	863283	4	13.794	1403680	50.0
Naphthalene, 2,...	14.017	28.8	ug/l	807230	4	13.794	1403680	50.0
Naphthalene, 1,...	15.223	21.1	ug/l	593658	4	13.794	1403680	50.0
Naphthalene, 1,...	15.394	12.2	ug/l	343384	4	13.794	1403680	50.0