

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032621\
 Data File : VN066356.D
 Acq On : 26 Mar 2021 17:56
 Operator : JC/MD
 Sample : M1777-04
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 245

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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

Signal : TIC: VN066356.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.269	205	216	231	rVB	156103	237241	1.52%	0.449%
2	3.213	545	568	628	rBV	6432528	15609079	100.00%	29.568%
3	3.738	746	764	791	rVB	320650	798223	5.11%	1.512%
4	6.750	1867	1887	1906	rBV2	57028	163495	1.05%	0.310%
5	7.507	2148	2169	2183	rBV2	328389	814030	5.22%	1.542%
6	7.584	2184	2198	2222	rVB2	547932	1292631	8.28%	2.449%
7	7.949	2313	2334	2358	rBV	415706	984459	6.31%	1.865%
8	8.512	2525	2544	2566	rBV	793624	1635560	10.48%	3.098%
9	10.028	3089	3109	3123	rBV	1382767	2595726	16.63%	4.917%
10	10.092	3123	3133	3163	rVB	298393	555962	3.56%	1.053%
11	11.350	3584	3602	3626	rBV	1080848	1881691	12.06%	3.564%
12	11.562	3664	3681	3708	rBV	293397	561852	3.60%	1.064%
13	11.892	3789	3804	3828	rVB	269599	451795	2.89%	0.856%
14	12.345	3958	3973	4001	rBV	851156	1451309	9.30%	2.749%
15	12.600	4055	4068	4076	rBV	266834	452954	2.90%	0.858%
16	12.677	4088	4097	4112	rVB2	239633	384618	2.46%	0.729%
17	12.836	4144	4156	4173	rBV	191170	326767	2.09%	0.619%
18	12.983	4197	4211	4227	rBV	971807	1582022	10.14%	2.997%
19	13.289	4311	4325	4331	rBV	811474	1411369	9.04%	2.674%
20	13.487	4380	4399	4407	rBV	516515	947430	6.07%	1.795%
21	13.528	4408	4414	4435	rVB3	326334	580642	3.72%	1.100%
22	13.619	4437	4448	4460	rBV	254717	379643	2.43%	0.719%
23	13.683	4464	4472	4483	rVB	127301	194650	1.25%	0.369%
24	13.745	4485	4495	4500	rVV	246450	366656	2.35%	0.695%
25	13.774	4502	4506	4517	rVV	290490	388447	2.49%	0.736%
26	13.833	4517	4528	4539	rVV	403789	618767	3.96%	1.172%
27	13.938	4556	4567	4579	rVB2	358353	574797	3.68%	1.089%
28	14.069	4606	4616	4625	rBV2	183127	327271	2.10%	0.620%
29	14.153	4638	4647	4653	rBV	286997	428335	2.74%	0.811%
30	14.190	4654	4661	4672	rVB	586868	869508	5.57%	1.647%
31	14.238	4672	4679	4687	rBV3	141077	181259	1.16%	0.343%
32	14.418	4737	4746	4756	rBV	480983	729009	4.67%	1.381%
33	14.466	4757	4764	4774	rVB	533306	722762	4.63%	1.369%
34	14.533	4775	4789	4802	rBV3	1303331	2624156	16.81%	4.971%
35	14.587	4804	4809	4824	rVB5	193566	314566	2.02%	0.596%
36	14.684	4833	4845	4864	rVB	866979	1399504	8.97%	2.651%

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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

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37	14.794	4878	4886	4892	rBV5	215189	310361	1.99%	0.588%
38	14.898	4915	4925	4938	rVB3	377649	724483	4.64%	1.372%
39	15.126	5002	5010	5019	rVB	261334	360481	2.31%	0.683%
40	15.188	5023	5033	5044	rBV5	219188	511077	3.27%	0.968%
41	15.266	5054	5062	5078	rVB	507360	795866	5.10%	1.508%
42	15.349	5083	5093	5109	rVB2	320158	632964	4.06%	1.199%
43	15.542	5157	5165	5184	rVB	864667	1544688	9.90%	2.926%
44	15.834	5262	5274	5289	rBV	630121	1217187	7.80%	2.306%
45	16.081	5357	5366	5381	rVV2	352098	651084	4.17%	1.233%
46	16.153	5385	5393	5418	rVB	368383	678764	4.35%	1.286%
47	16.269	5425	5436	5449	rBV6	247907	524686	3.36%	0.994%

Sum of corrected areas: 52789826

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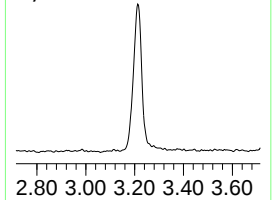
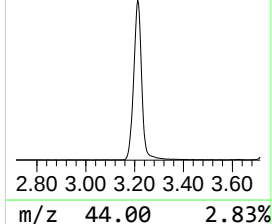
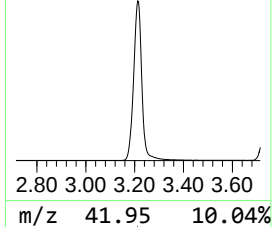
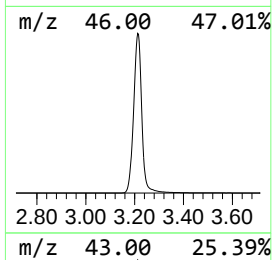
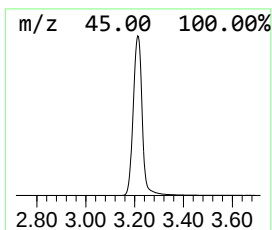
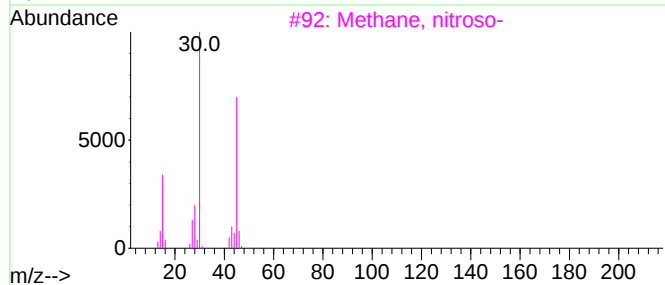
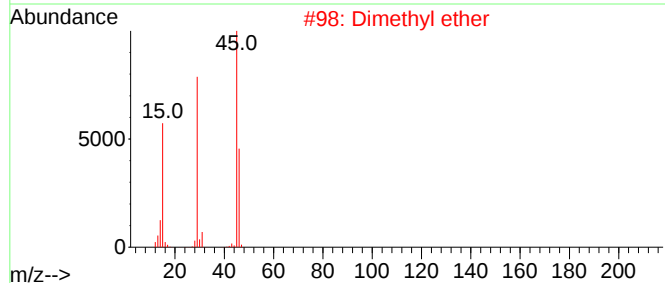
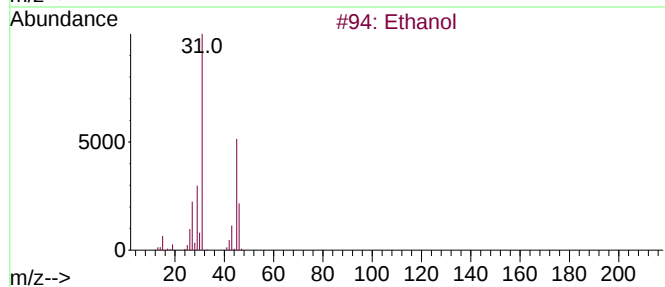
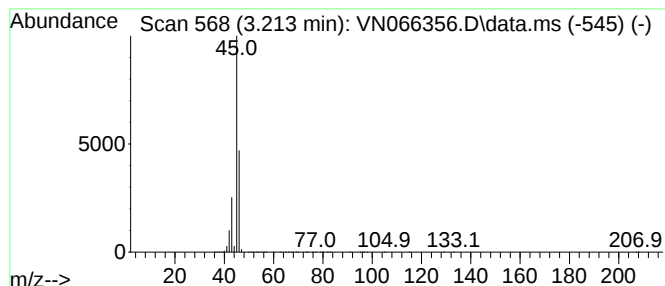
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.213	603.77 ug/l	15609100	Pentafluorobenzene	7.584

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	Oxalic acid			90	C2H2O4	000144-62-7	4



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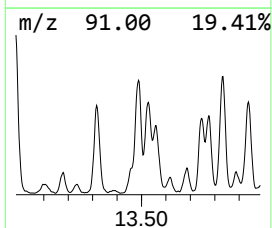
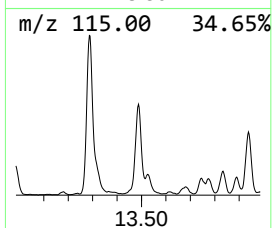
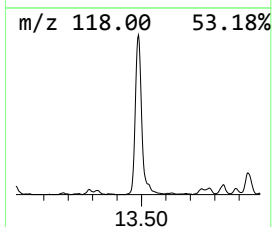
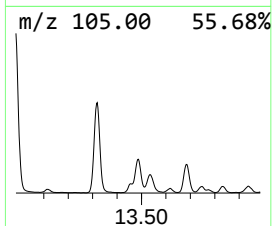
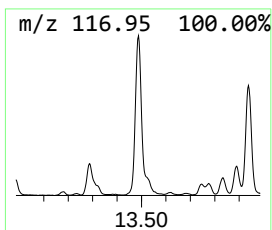
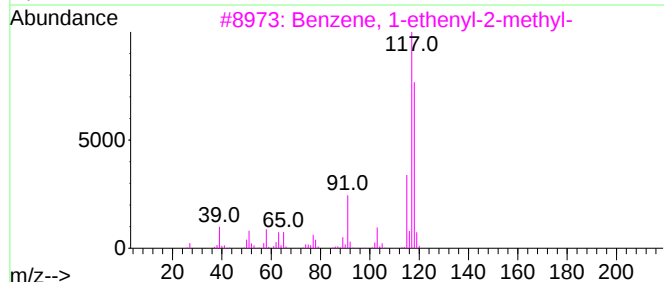
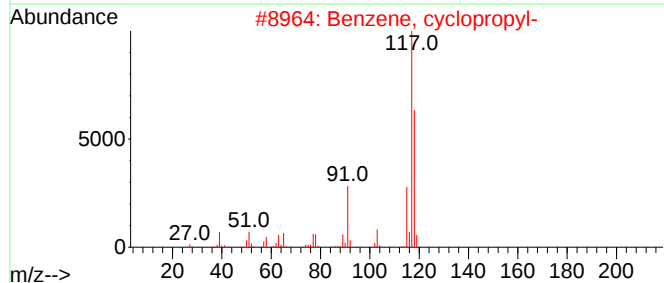
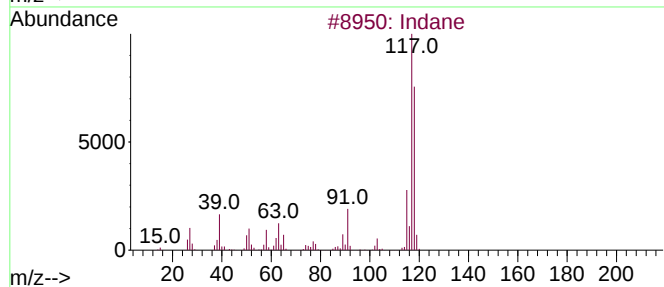
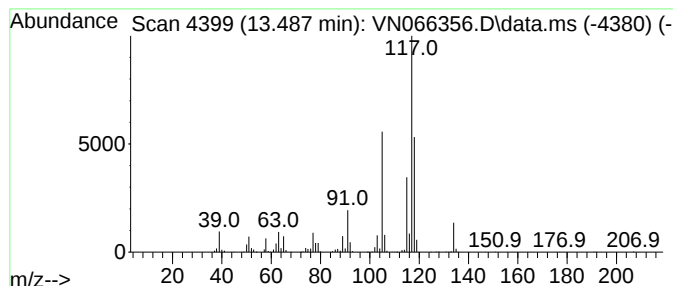
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

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

Peak Number 2 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.487	33.56 ug/l	947430	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	93
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	92
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
5			Deltacyclene	118	C9H10	007785-10-6	70



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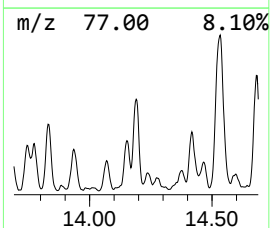
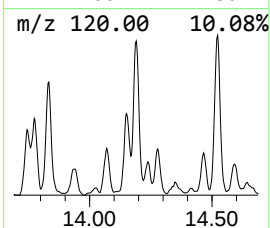
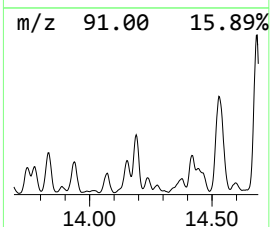
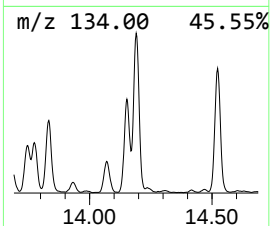
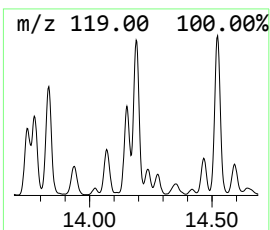
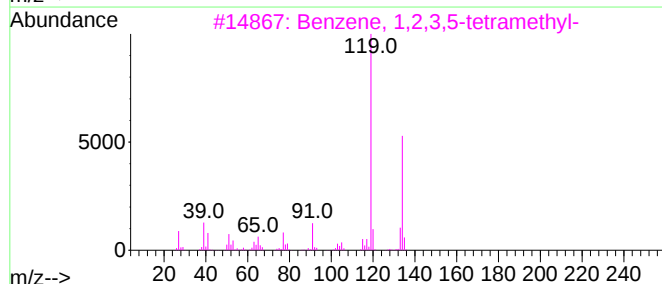
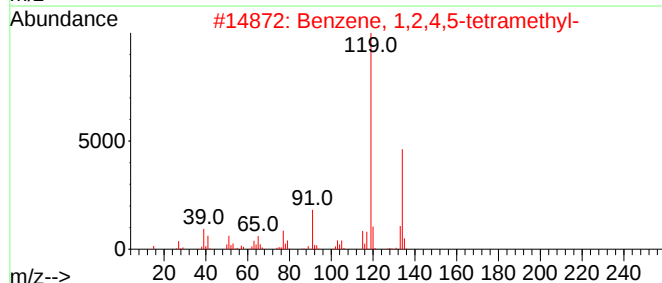
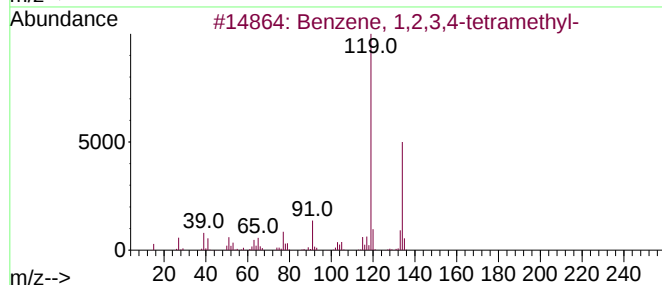
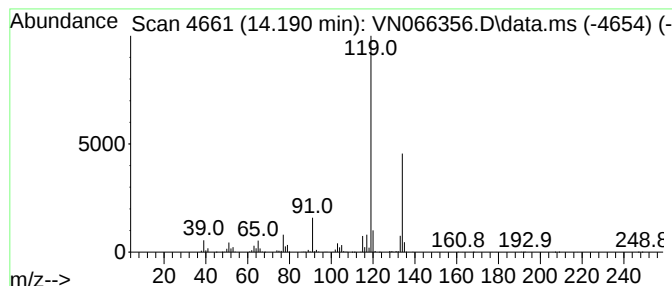
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.190	30.80 ug/l	869508	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91



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Instrument :
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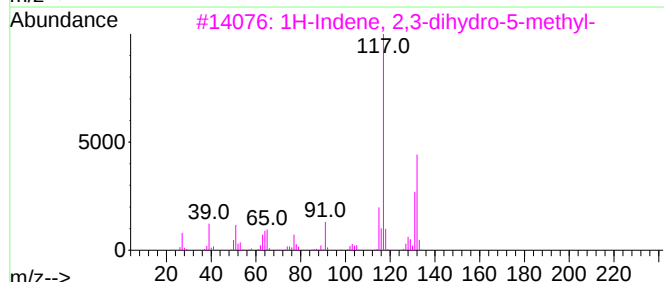
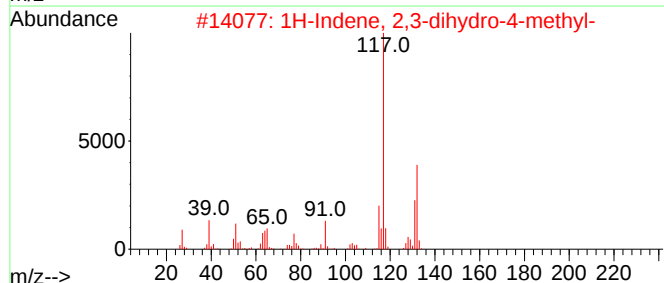
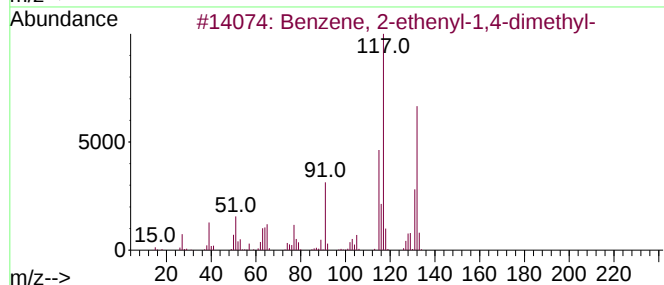
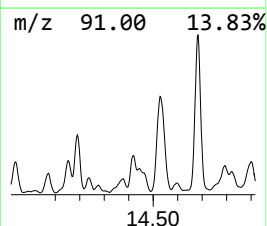
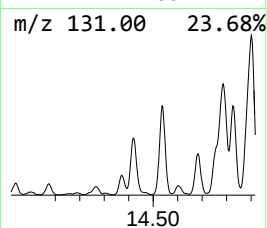
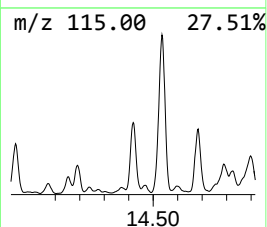
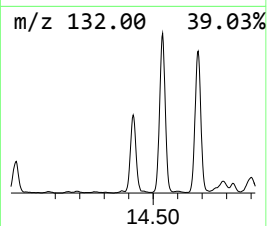
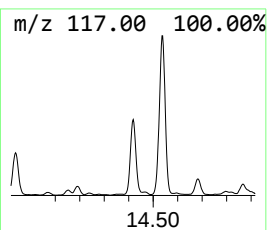
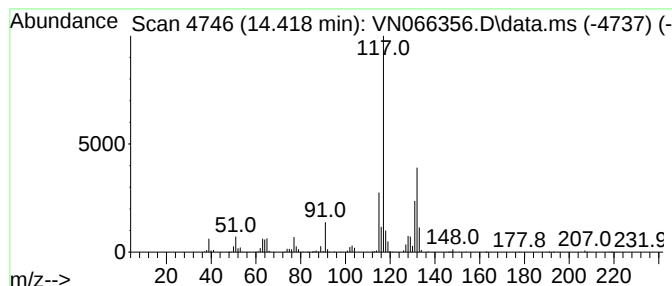
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.418	25.83 ug/l	729009	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
2			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	86
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	80



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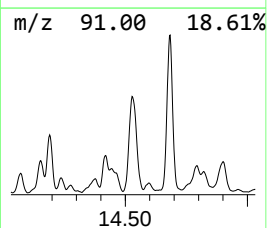
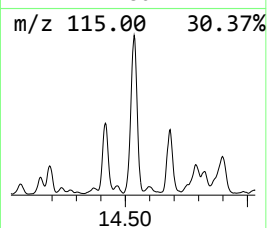
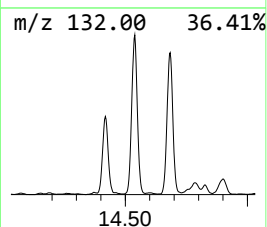
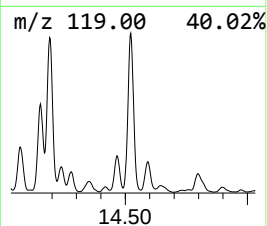
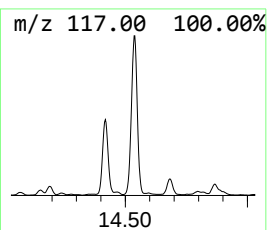
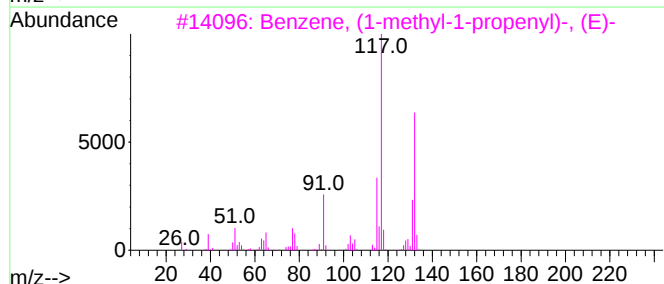
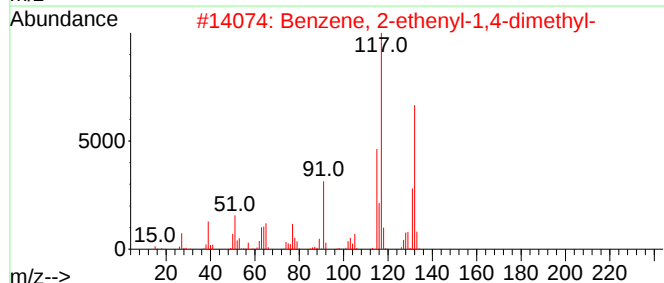
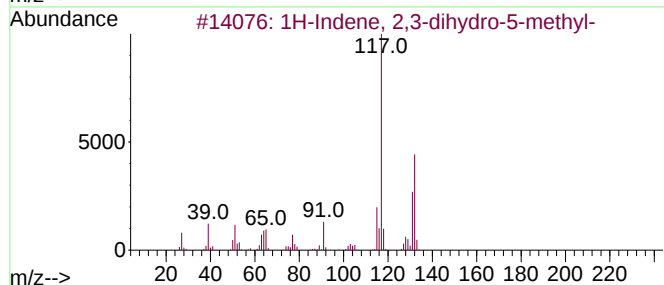
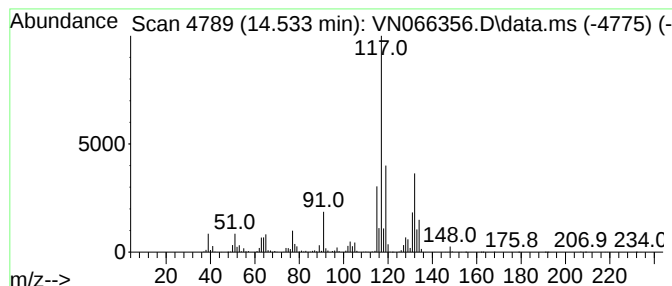
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

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

Peak Number 5 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	92.96 ug/l	2624160	1,4-Dichlorobenzene-d4	13.286

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	92
2		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	76
4		Benzene, 2-butenyl-	132	C10H12	001560-06-1	76
5		3-Phenylbut-1-ene	132	C10H12	000934-10-1	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032621\
Data File : VN066356.D
Acq On : 26 Mar 2021 17:56
Operator : JC/MD
Sample : M1777-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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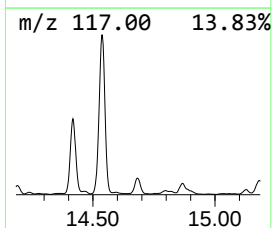
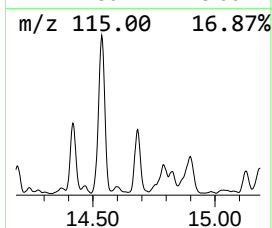
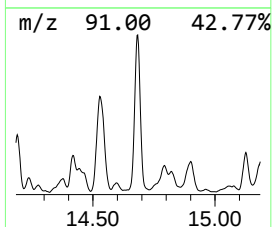
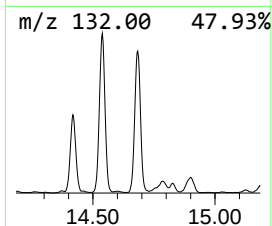
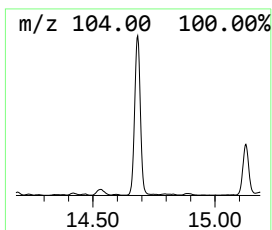
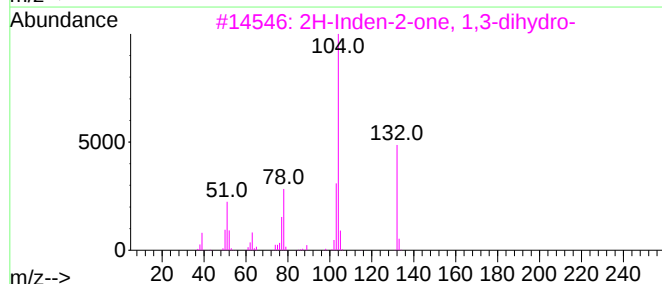
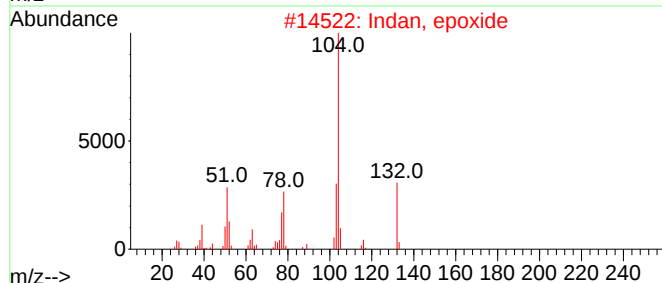
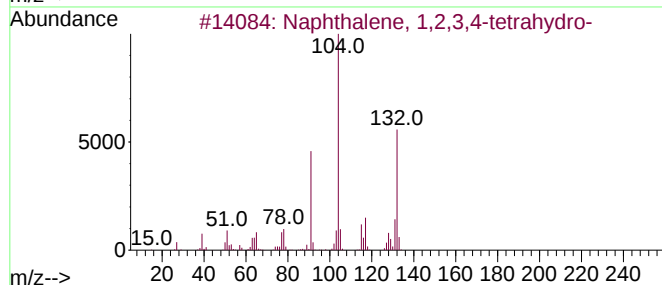
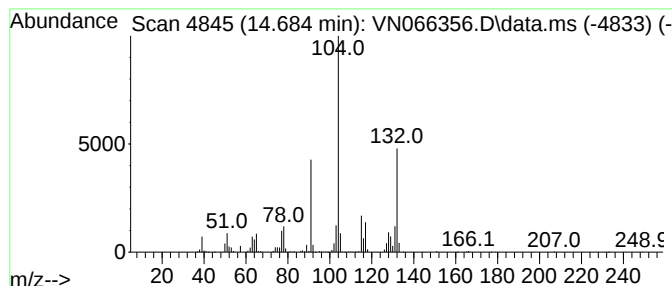
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.684	49.58 ug/l	1399500	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2			Indan, epoxide	132	C9H8O	000768-22-9	58
3			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	53
4			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	46
5			Isoquinoline, 1,2,3,4-tetrahydro-	133	C9H11N	000091-21-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032621\
Data File : VN066356.D
Acq On : 26 Mar 2021 17:56
Operator : JC/MD
Sample : M1777-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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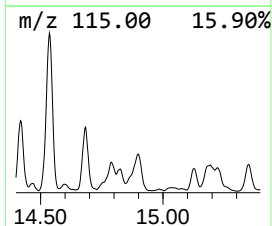
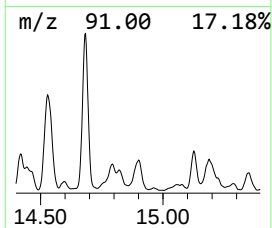
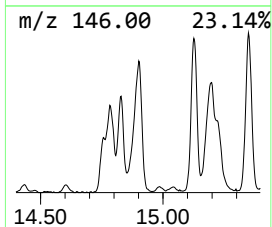
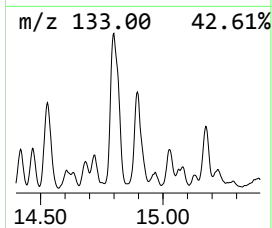
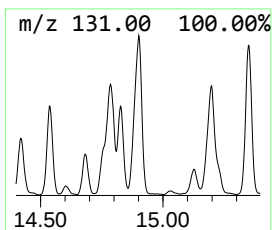
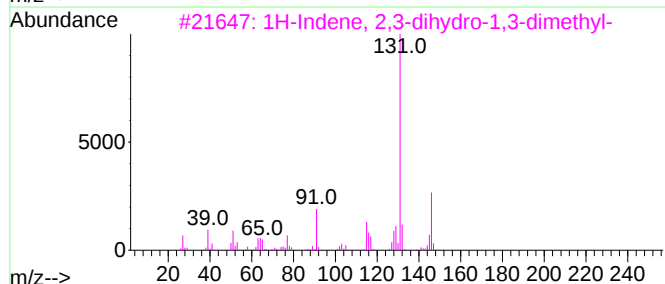
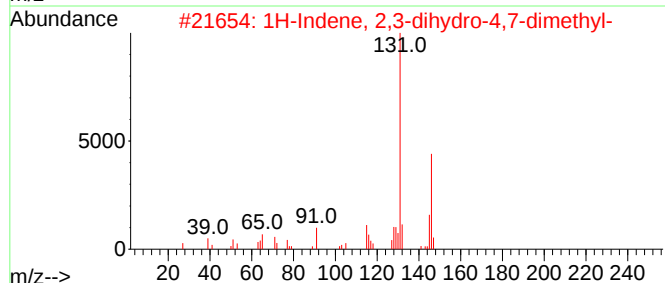
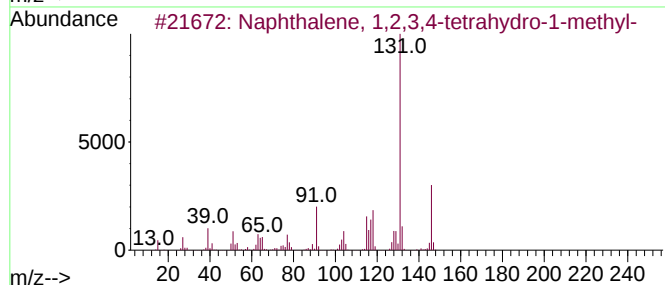
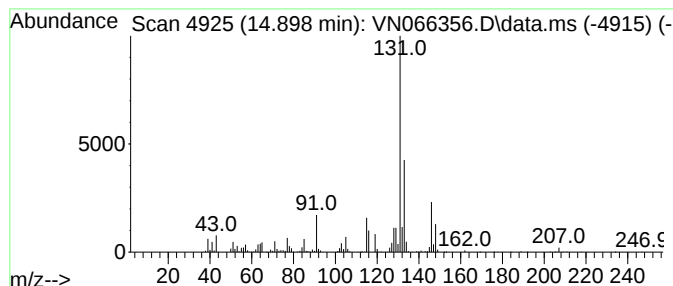
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	25.67 ug/l	724483	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	86
2			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	70
3			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	70
4			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	70
5			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032621\
Data File : VN066356.D
Acq On : 26 Mar 2021 17:56
Operator : JC/MD
Sample : M1777-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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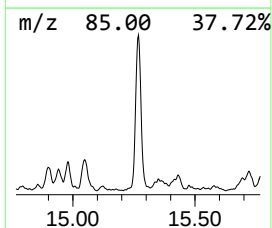
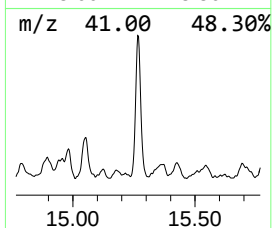
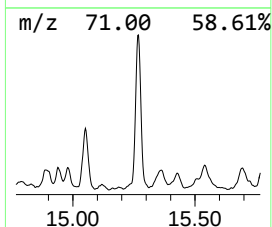
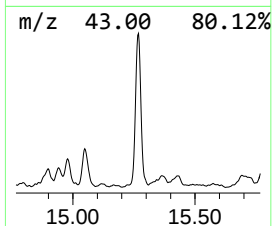
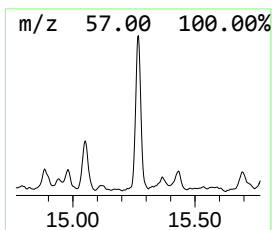
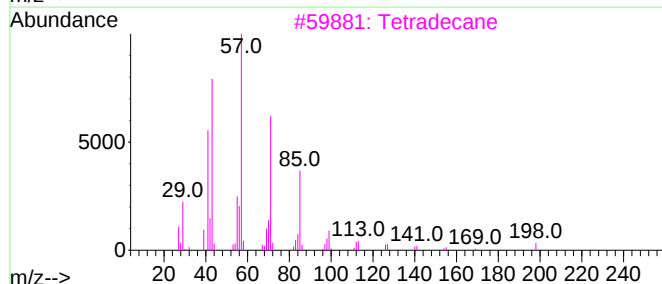
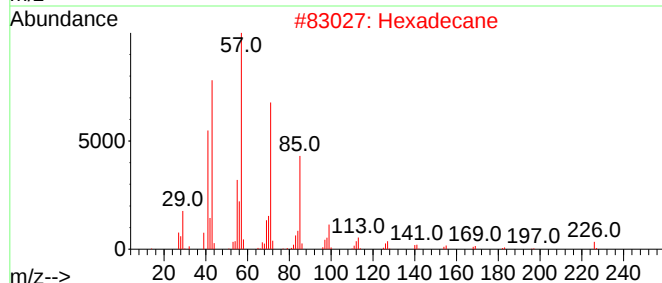
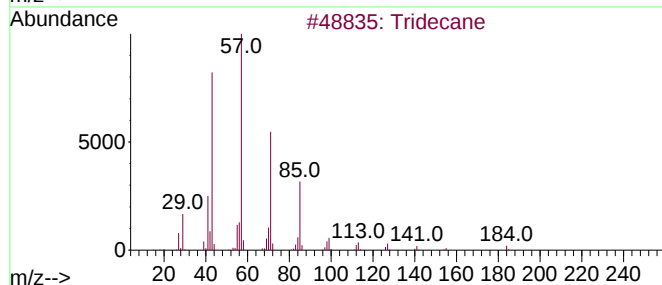
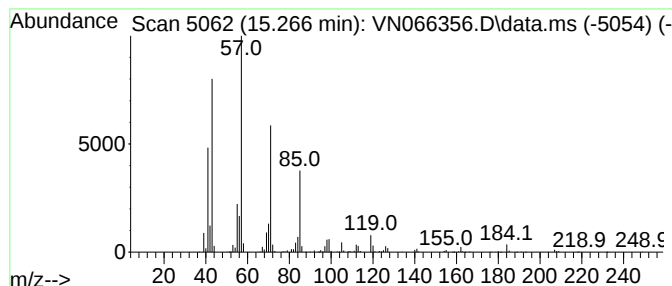
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.266	28.19 ug/l	795866	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	93
2			Hexadecane	226	C16H34	000544-76-3	87
3			Tetradecane	198	C14H30	000629-59-4	86
4			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80
5			Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032621\
Data File : VN066356.D
Acq On : 26 Mar 2021 17:56
Operator : JC/MD
Sample : M1777-04
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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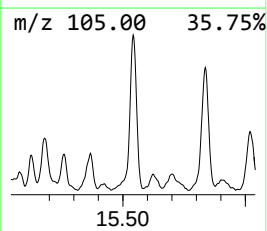
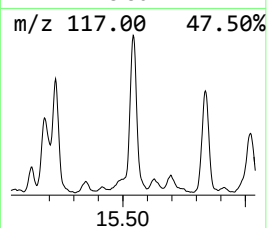
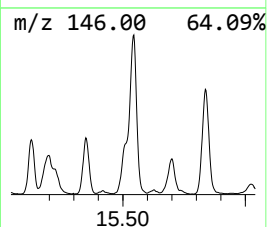
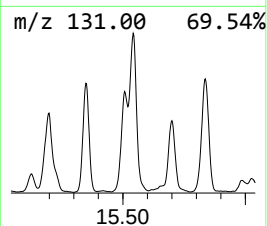
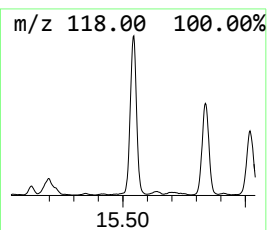
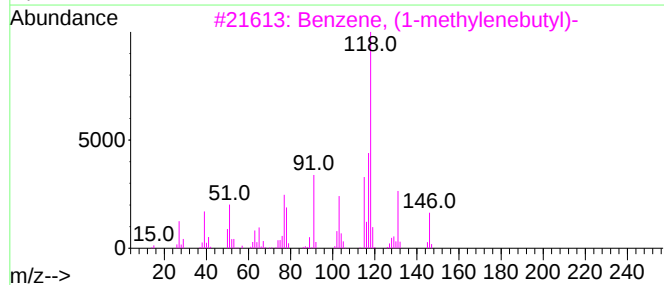
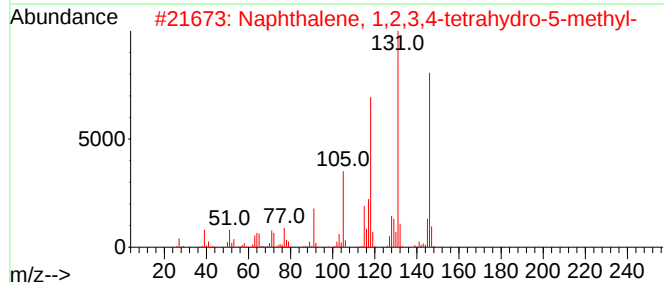
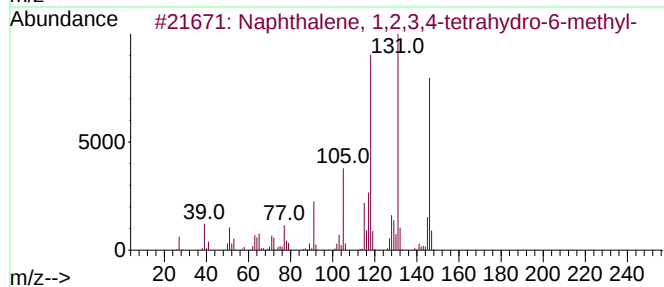
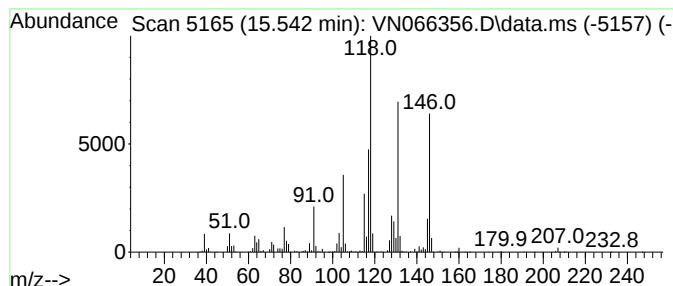
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.542	54.72 ug/l	1544690	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	92
3			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	83
4			Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	74
5			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032621\
Data File : VN066356.D
Acq On : 26 Mar 2021 17:56
Operator : JC/MD
Sample : M1777-04
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ALS Vial : 17 Sample Multiplier: 1

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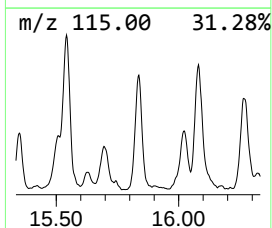
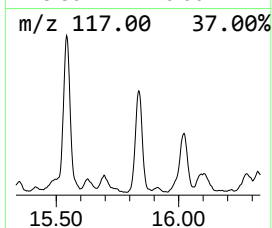
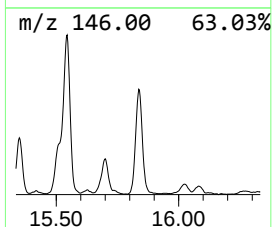
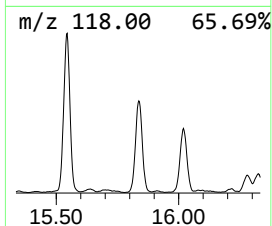
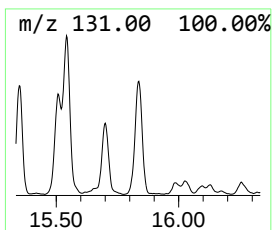
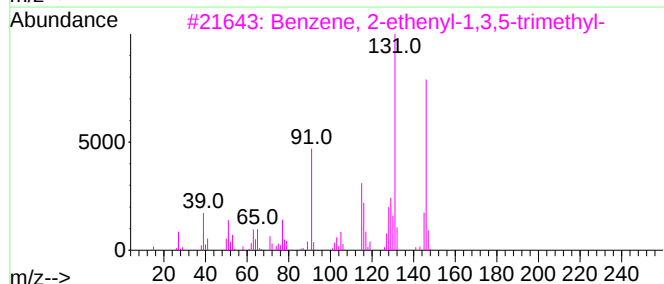
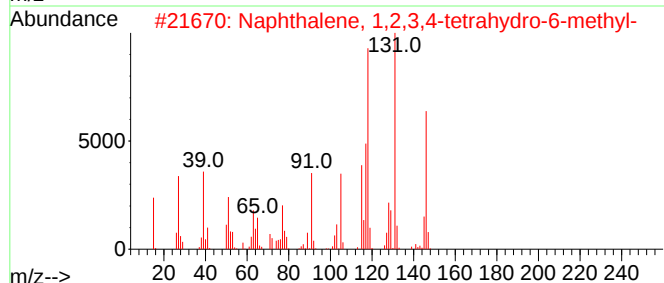
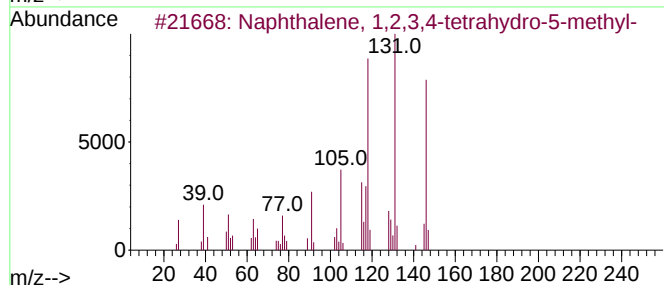
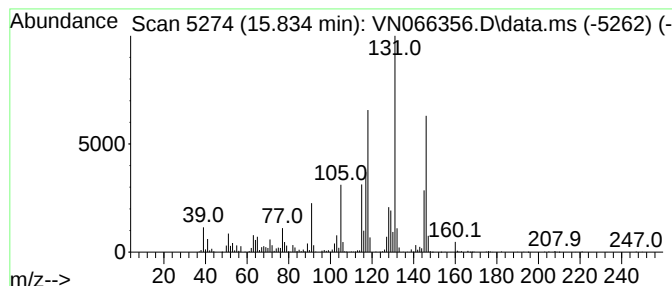
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.834	43.12 ug/l	1217190	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	94
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	83
4			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	81
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032621\
Data File : VN066356.D
Acq On : 26 Mar 2021 17:56
Operator : JC/MD
Sample : M1777-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Indane	13.487	33.6	ug/l	947430	4	13.286	1411370	50.0
Benzene, 1,2,3,...	14.190	30.8	ug/l	869508	4	13.286	1411370	50.0
Benzene, 2-ethe...	14.418	25.8	ug/l	729009	4	13.286	1411370	50.0
1H-Indene, 2,3-...	14.533	93.0	ug/l	2624160	4	13.286	1411370	50.0
Naphthalene, 1,...	14.684	49.6	ug/l	1399500	4	13.286	1411370	50.0
Naphthalene, 1,...	14.898	25.7	ug/l	724483	4	13.286	1411370	50.0
Tridecane	15.266	28.2	ug/l	795866	4	13.286	1411370	50.0
Naphthalene, 1,...	15.542	54.7	ug/l	1544690	4	13.286	1411370	50.0
Naphthalene, 1,...	15.834	43.1	ug/l	1217190	4	13.286	1411370	50.0