

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020421\
 Data File : VN065726.D
 Acq On : 4 Feb 2021 18:47
 Operator : JC/MD
 Sample : M1314-04 100X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 40966

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\82N012521W.M
 Title : SW846 8260

Signal : TIC: VN065726.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.779	614	634	669	rBV	1296619	3306085	100.00%	25.590%
2	6.020	1315	1331	1350	rBV4	17399	55370	1.67%	0.429%
3	7.550	1789	1807	1817	rBV	114738	288034	8.71%	2.229%
4	7.624	1818	1830	1851	rVB2	230465	545129	16.49%	4.219%
5	7.987	1926	1943	1967	rBV2	146225	344188	10.41%	2.664%
6	8.547	2101	2117	2144	rBV	348790	731461	22.12%	5.662%
7	10.058	2571	2587	2597	rBV	568290	1032794	31.24%	7.994%
8	10.122	2597	2607	2637	rVB	879173	1600357	48.41%	12.387%
9	11.376	2983	2997	3019	rBV	472547	831823	25.16%	6.438%
10	11.479	3019	3029	3044	rVB	78059	132614	4.01%	1.026%
11	11.589	3049	3063	3082	rBV	300123	578804	17.51%	4.480%
12	11.917	3145	3165	3180	rBV	151276	256393	7.76%	1.985%
13	12.373	3294	3307	3331	rVB	335009	572811	17.33%	4.434%
14	12.624	3375	3385	3393	rBV	51775	88127	2.67%	0.682%
15	12.701	3401	3409	3419	rVB2	43616	69593	2.10%	0.539%
16	12.862	3448	3459	3470	rBV	31627	53037	1.60%	0.411%
17	13.010	3492	3505	3516	rBV	98674	161667	4.89%	1.251%
18	13.312	3587	3599	3619	rBV2	394243	734903	22.23%	5.688%
19	13.515	3645	3662	3669	rBV	47829	87700	2.65%	0.679%
20	13.553	3669	3674	3691	rVB4	24072	47761	1.44%	0.370%
21	13.643	3691	3702	3711	rBV2	39243	61043	1.85%	0.472%
22	13.859	3761	3769	3777	rVB2	25116	36614	1.11%	0.283%
23	13.965	3793	3802	3811	rVB2	34736	53310	1.61%	0.413%
24	14.215	3875	3880	3889	rVB	25109	37948	1.15%	0.294%
25	14.444	3944	3951	3959	rBV2	26697	40554	1.23%	0.314%
26	14.492	3959	3966	3975	rVB	49237	72282	2.19%	0.559%
27	14.563	3975	3988	3997	rBV3	71774	146797	4.44%	1.136%
28	14.611	3998	4003	4016	rVB5	19868	33190	1.00%	0.257%
29	14.711	4024	4034	4043	rVB2	53886	87757	2.65%	0.679%
30	14.817	4051	4067	4074	rBV5	21623	51689	1.56%	0.400%
31	14.926	4090	4101	4110	rVB5	24028	47738	1.44%	0.370%
32	15.096	4140	4154	4164	rBV3	48559	107427	3.25%	0.832%
33	15.222	4182	4193	4208	rVV7	18383	58632	1.77%	0.454%
34	15.296	4209	4216	4230	rVB	45038	69225	2.09%	0.536%
35	15.383	4232	4243	4255	rBV3	19868	42616	1.29%	0.330%
36	15.576	4296	4303	4320	rVB3	47664	85321	2.58%	0.660%

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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 >
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37	15.727	4341	4350	4370	rVB5	16529	39057	1.18%	0.302%
38	15.868	4382	4394	4407	rBV5	34152	72014	2.18%	0.557%
39	16.119	4462	4472	4483	rVV	51424	99266	3.00%	0.768%
40	16.190	4485	4494	4506	rVB	28618	51983	1.57%	0.402%
41	16.305	4517	4530	4543	rBV2	45305	106503	3.22%	0.824%

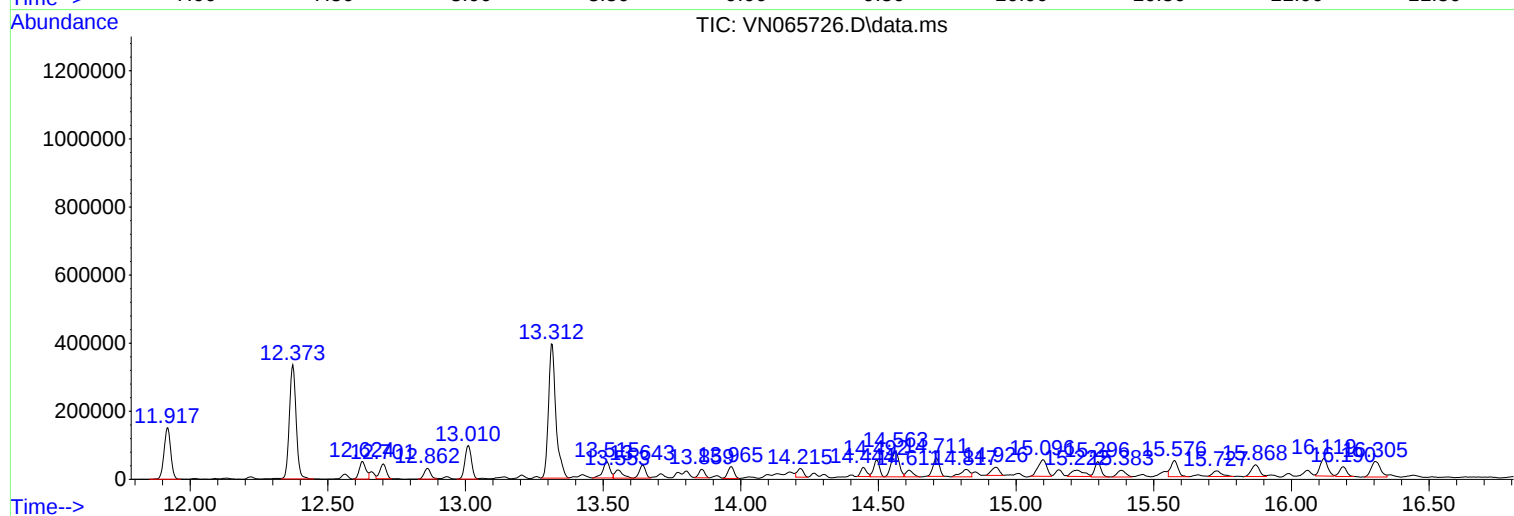
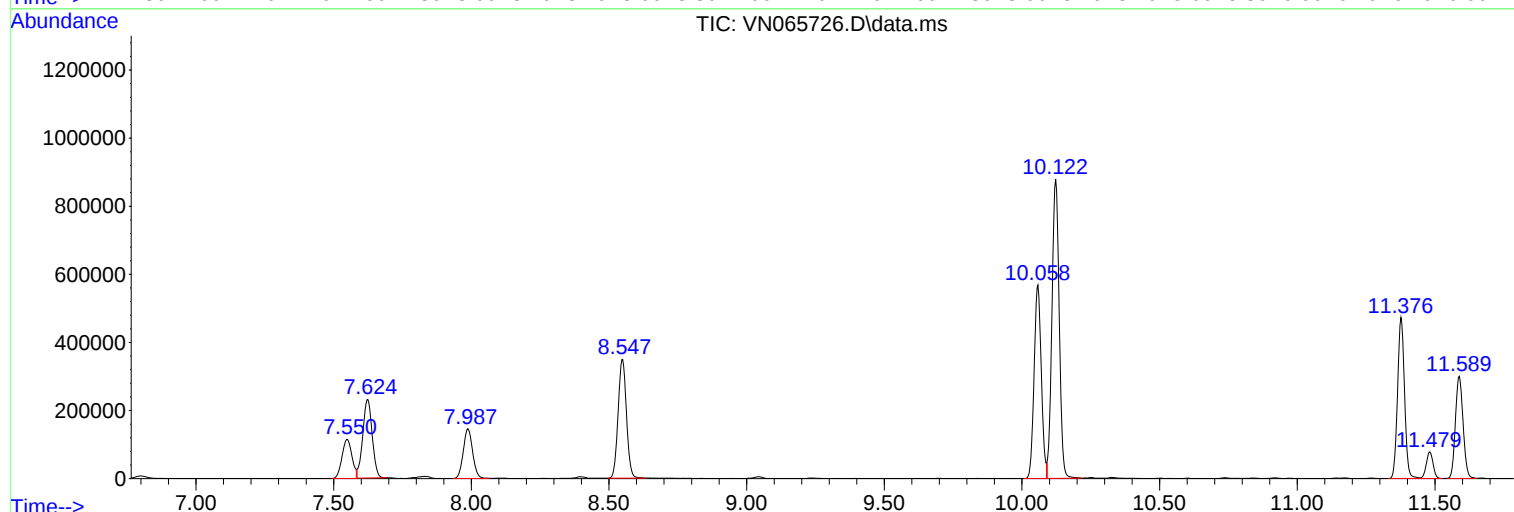
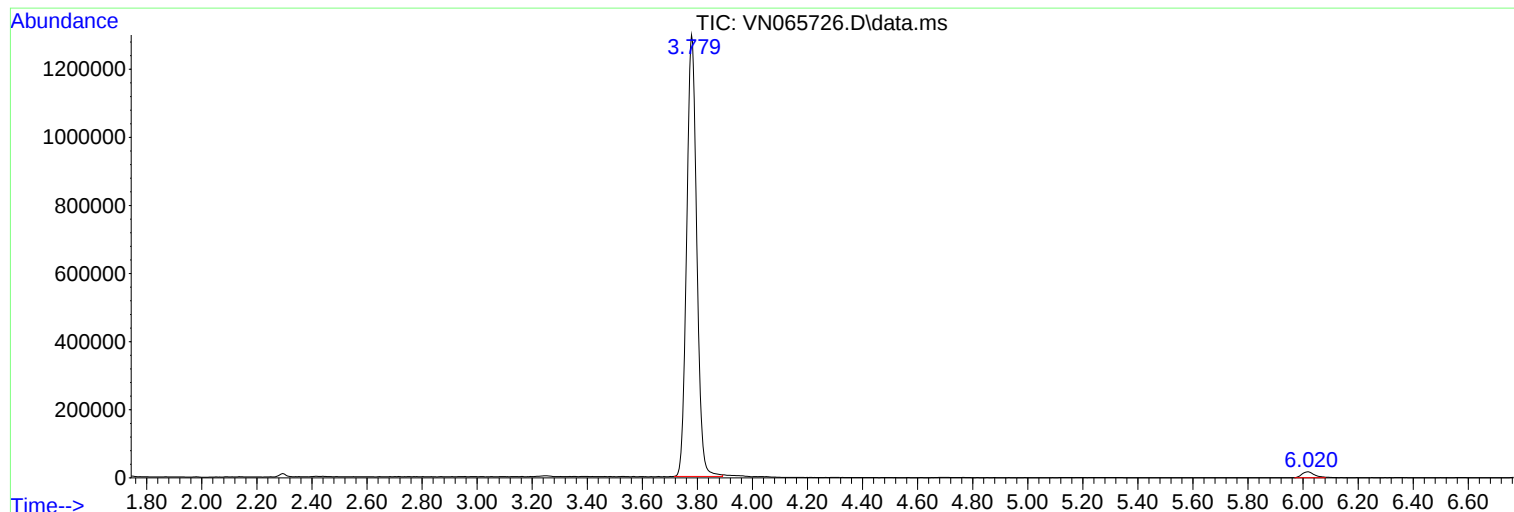
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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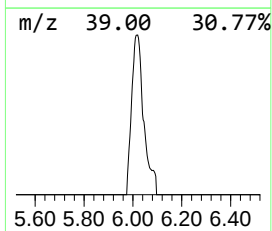
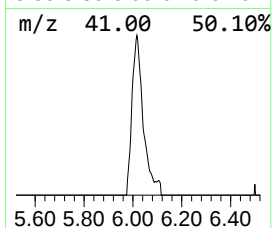
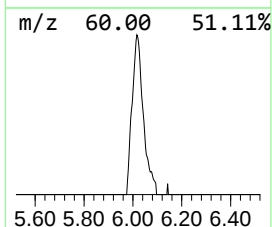
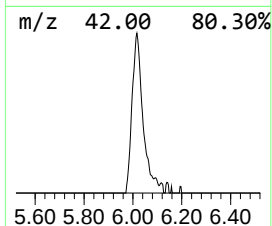
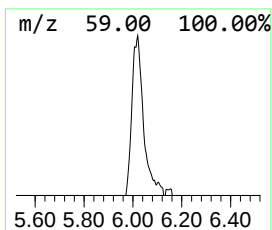
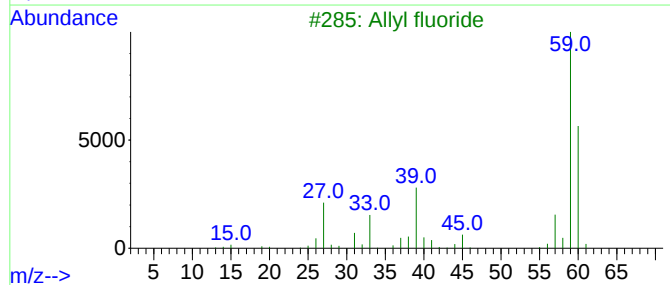
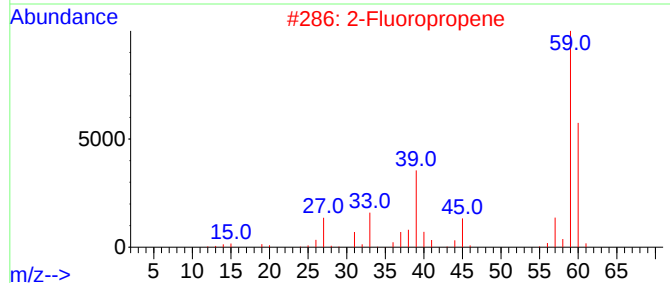
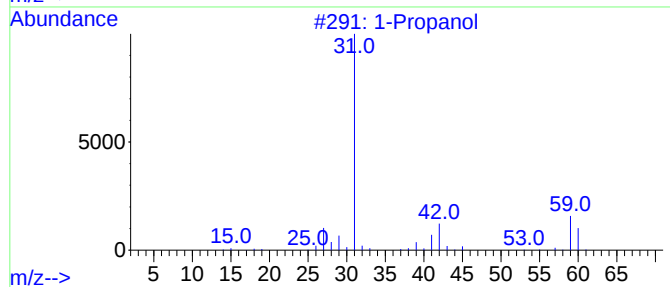
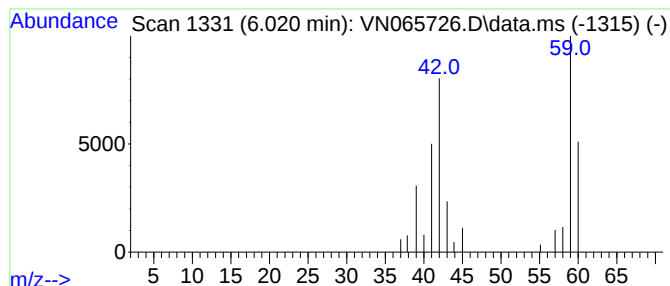
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Propanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.020	5.08 ug/l	55370	Pentafluorobenzene	7.624

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	78
2		2-Fluoropropene	60	C3H5F	001184-60-7	49
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		Acetaldoxime	59	C2H5NO	000107-29-9	7
5		3-Pentanol	88	C5H12O	000584-02-1	4



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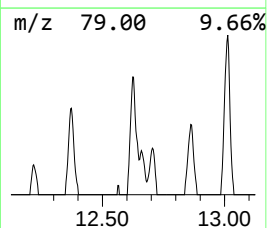
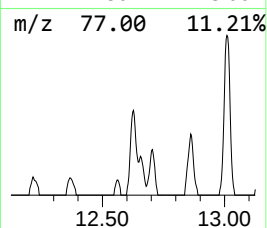
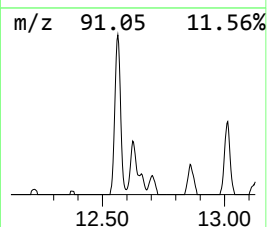
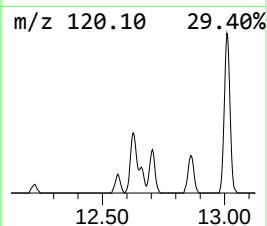
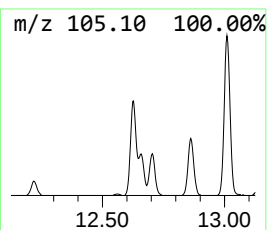
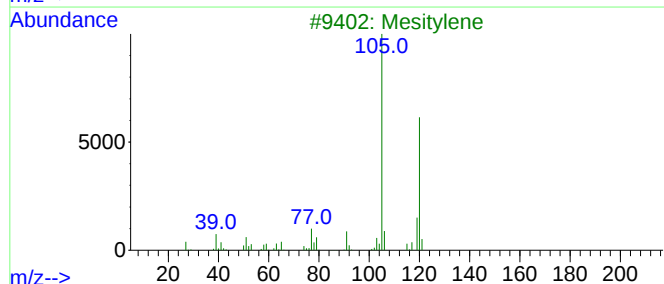
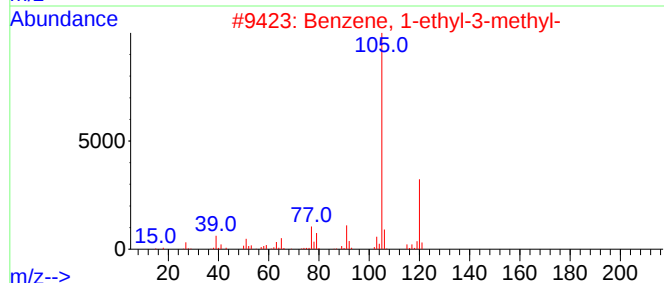
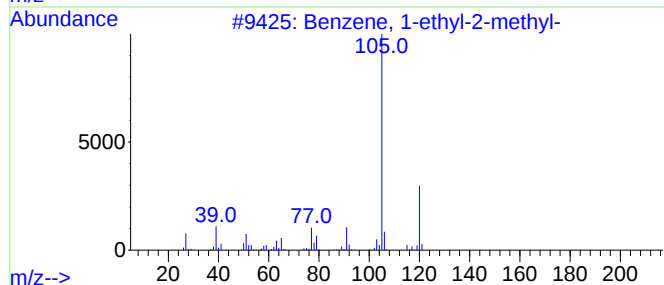
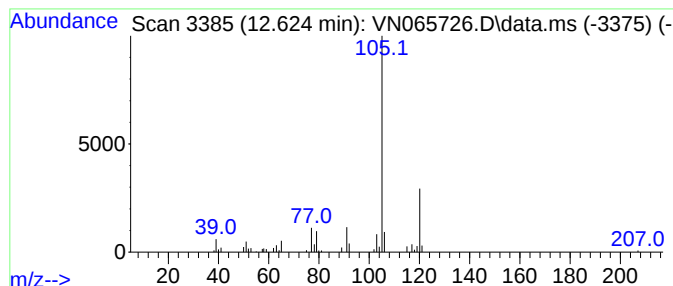
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.624	6.00 ug/l	88127	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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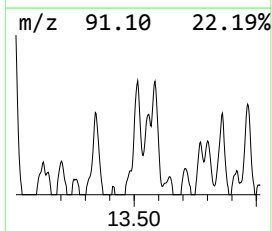
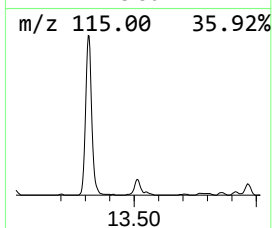
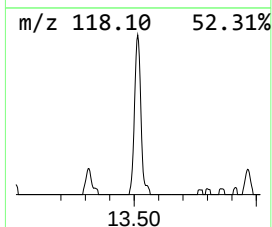
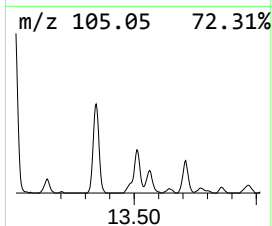
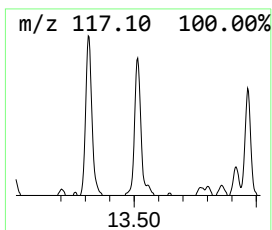
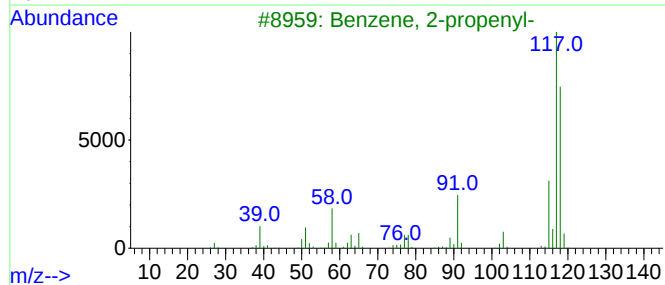
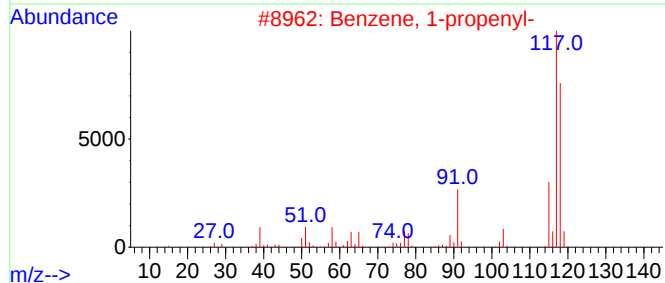
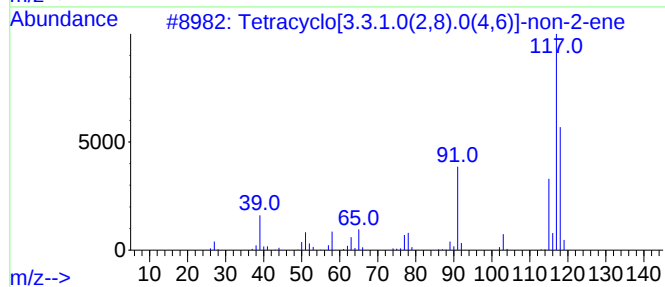
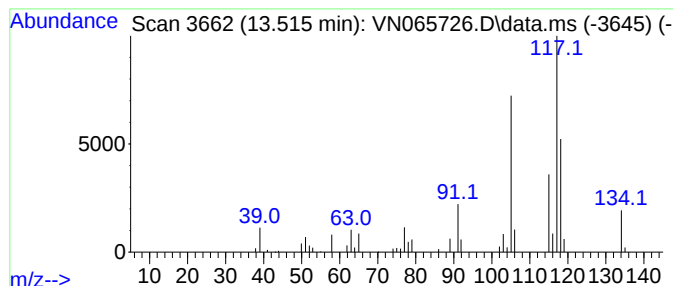
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tetracyclo[3.3.1.0(2,8).0(4... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.515	5.97 ug/l	87700	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	70
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4			Indane	118	C9H10	000496-11-7	64
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64



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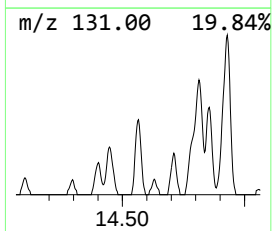
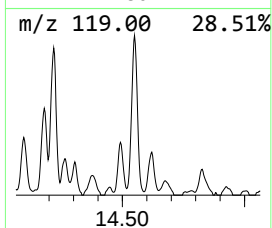
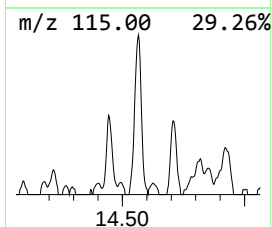
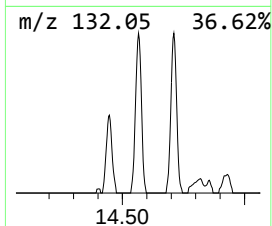
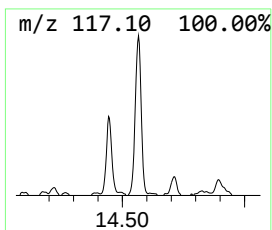
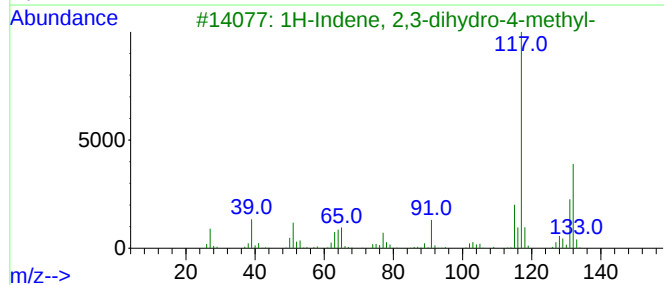
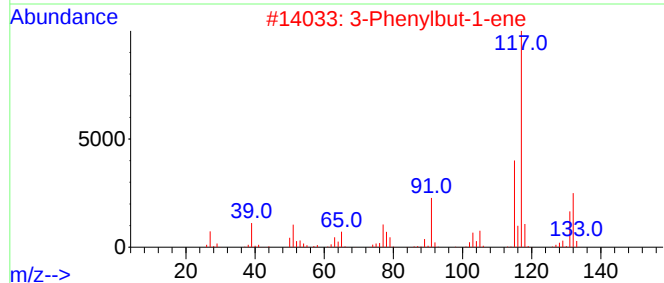
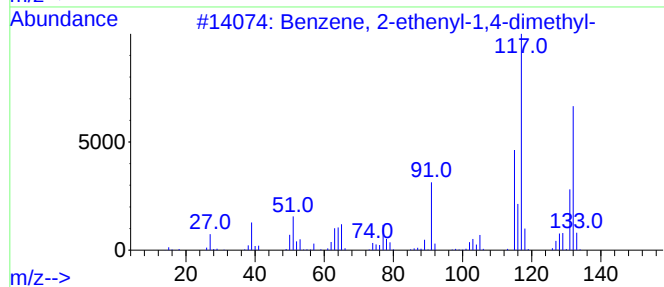
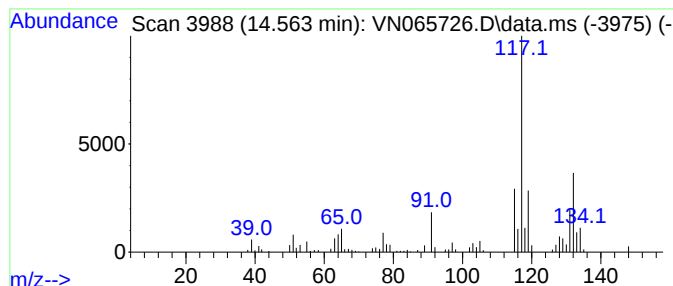
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Peak Number 4 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.563	9.99 ug/l	146797	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
3			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	76
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	76
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	72



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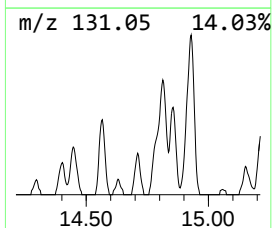
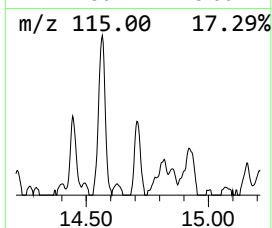
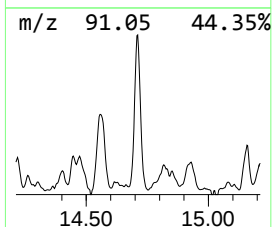
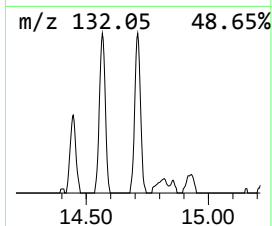
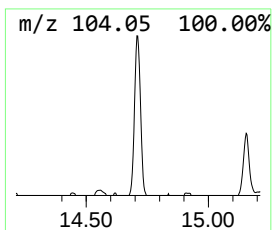
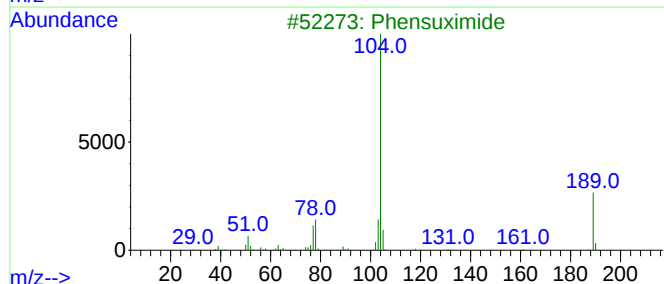
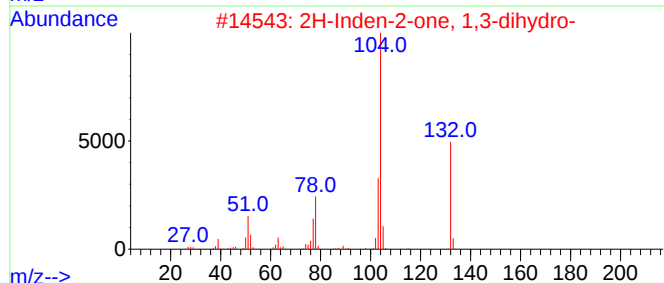
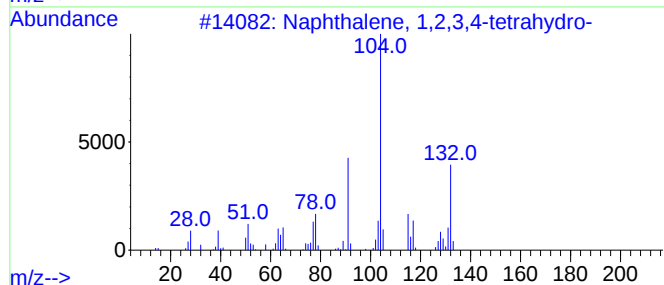
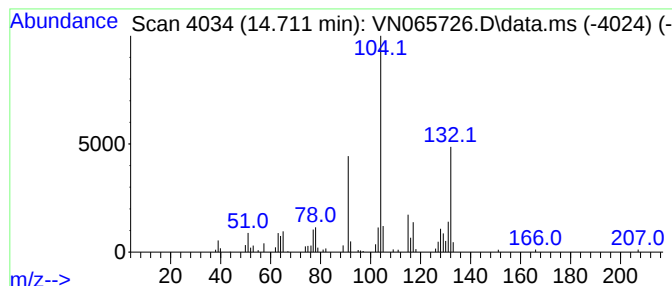
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.711	5.97 ug/l	87757	1,4-Dichlorobenzene-d4	13.315

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	53
3			Phensuximide	189	C11H11NO2	000086-34-0	38
4			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	38
5			2-Furanone, 4-phenyltetrahydro	162	C10H10O2	1000197-38-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020421\
Data File : VN065726.D
Acq On : 4 Feb 2021 18:47
Operator : JC/MD
Sample : M1314-04 100X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
40966

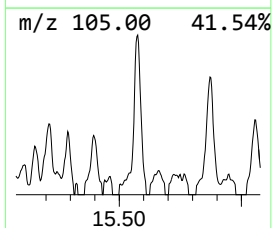
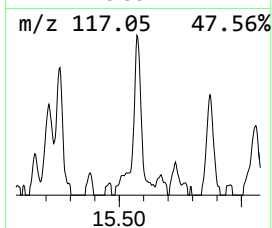
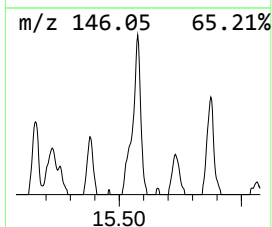
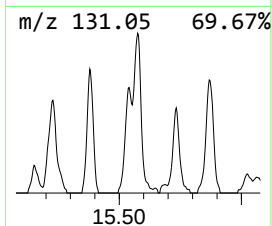
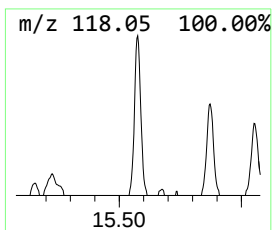
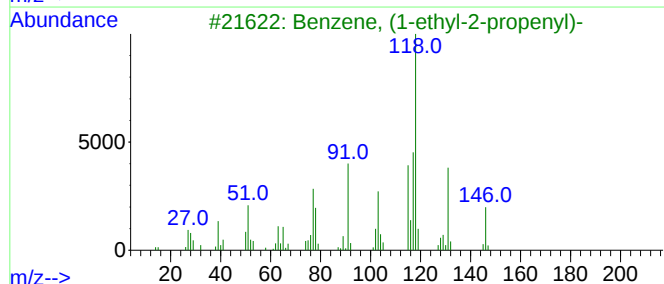
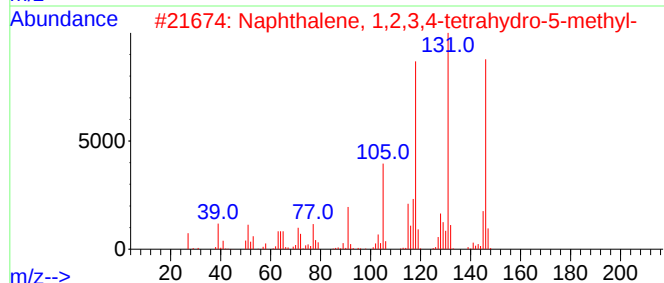
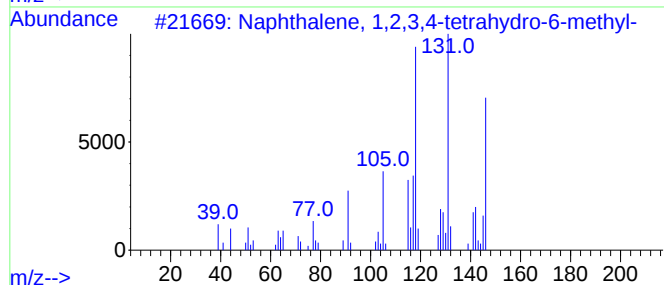
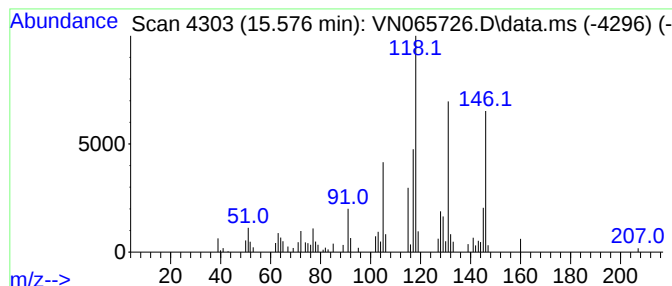
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.576	5.80 ug/l	85321	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	91
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	87
3			Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	87
4			2(1H)-Quinazolinone	146	C8H6N2O	007471-58-1	46
5			1H-Tetrazole, 5-phenyl-	146	C7H6N4	018039-42-4	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020421\
Data File : VN065726.D
Acq On : 4 Feb 2021 18:47
Operator : JC/MD
Sample : M1314-04 100X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
40966

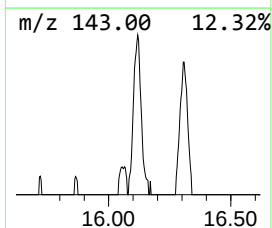
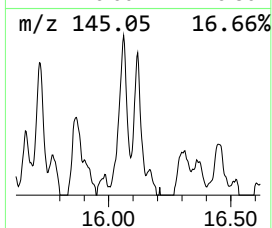
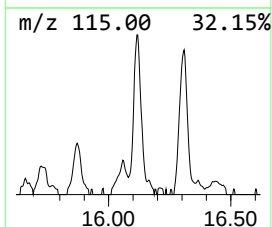
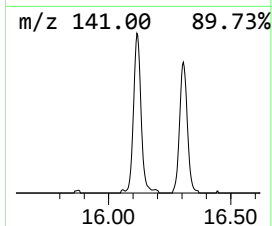
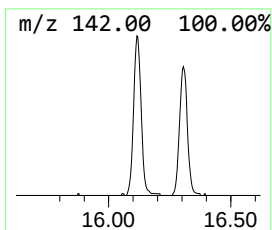
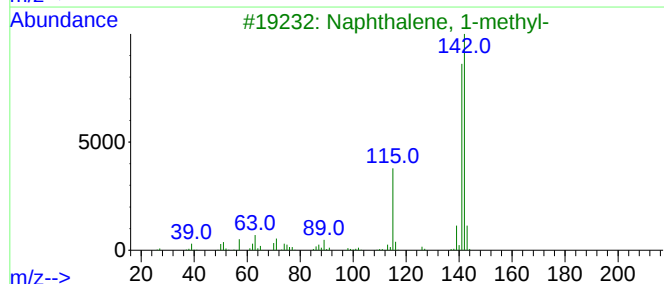
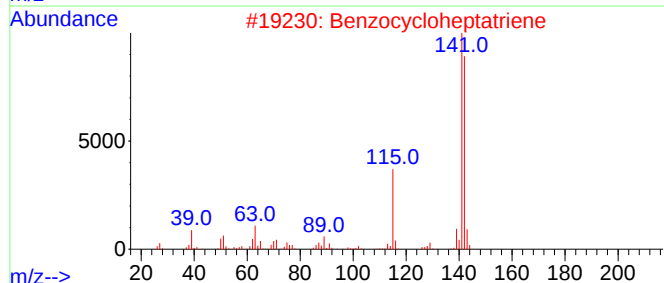
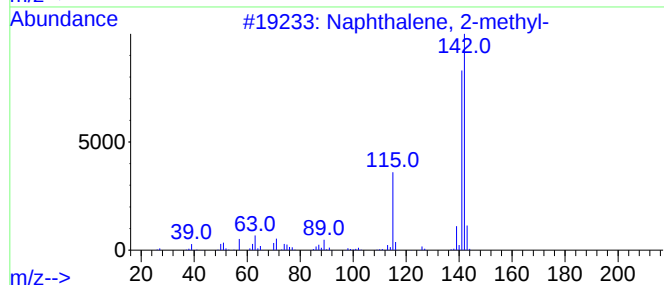
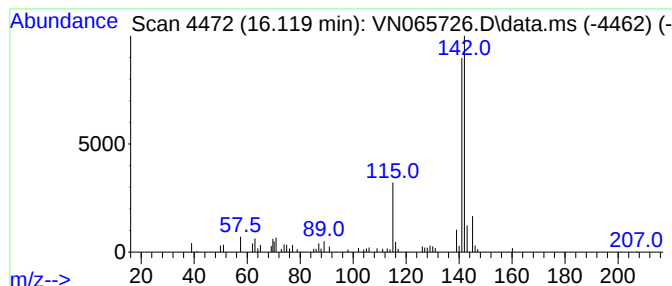
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.119	6.75 ug/l	99266	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Benzocycloheptatriene	142	C11H10	000264-09-5	93
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
4			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	87
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020421\
Data File : VN065726.D
Acq On : 4 Feb 2021 18:47
Operator : JC/MD
Sample : M1314-04 100X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
40966

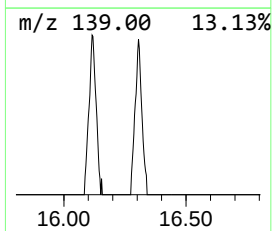
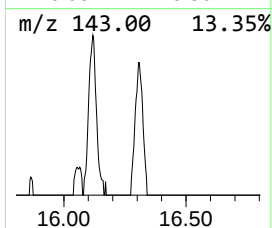
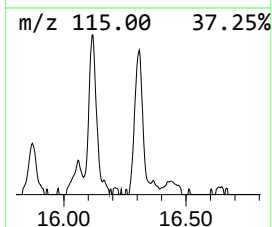
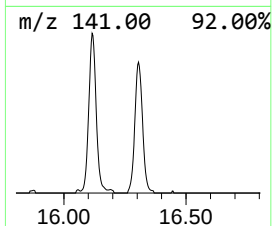
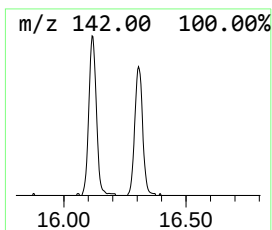
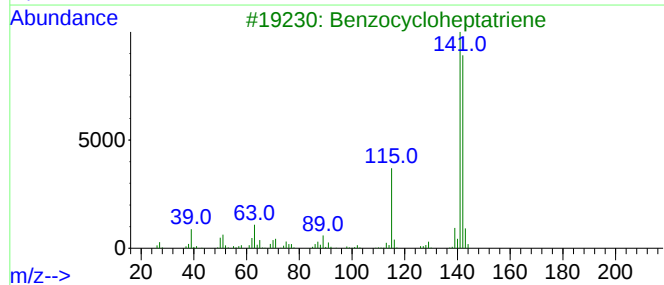
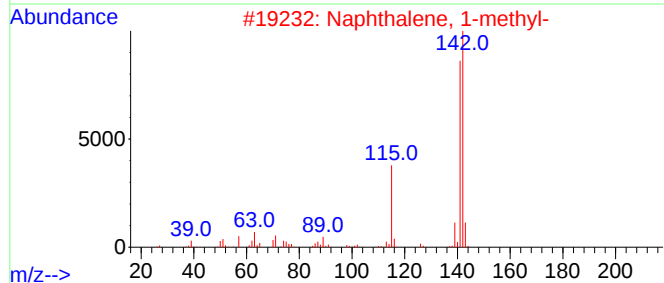
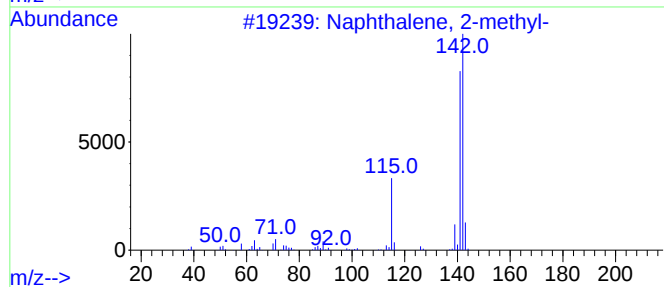
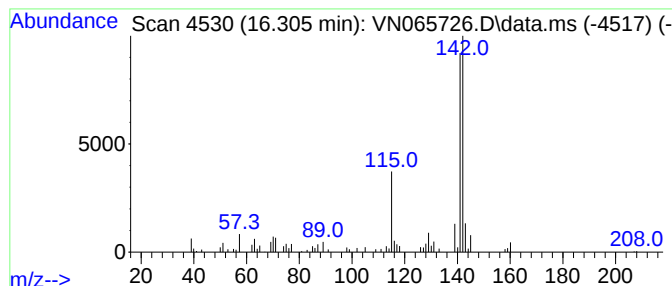
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.305	7.25 ug/l	106503	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3			Benzocycloheptatriene	142	C11H10	000264-09-5	90
4			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	87
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020421\
Data File : VN065726.D
Acq On : 4 Feb 2021 18:47
Operator : JC/MD
Sample : M1314-04 100X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
40966

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.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
1-Propanol	6.020	5.1	ug/l	55370	1	7.624	545129	50.0
Benzene, 1-ethy...	12.624	6.0	ug/l	88127	4	13.315	734903	50.0
Tetracyclo[3.3....	13.515	6.0	ug/l	87700	4	13.315	734903	50.0
Benzene, 2-ethe...	14.563	10.0	ug/l	146797	4	13.315	734903	50.0
Naphthalene, 1,...	14.711	6.0	ug/l	87757	4	13.315	734903	50.0
Naphthalene, 1,...	15.576	5.8	ug/l	85321	4	13.315	734903	50.0
Naphthalene, 2-...	16.119	6.8	ug/l	99266	4	13.315	734903	50.0
Naphthalene, 1-...	16.305	7.3	ug/l	106503	4	13.315	734903	50.0