

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
 Data File : VN065629.D
 Acq On : 27 Jan 2021 14:59
 Operator : JC/MD
 Sample : M1190-08
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41709

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: VN065629.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.550	1789	1807	1817	rBV2	133324	333158	3.91%	0.767%
2	7.624	1818	1830	1850	rVB	280602	679476	7.97%	1.565%
3	8.000	1925	1947	1973	rBV3	646932	1632521	19.15%	3.759%
4	8.550	2101	2118	2139	rBV	406407	855186	10.03%	1.969%
5	10.058	2568	2587	2595	rBV	646010	1178469	13.82%	2.714%
6	10.122	2595	2607	2636	rVB	4635435	8526969	100.00%	19.635%
7	11.376	2981	2997	3015	rBV	552529	969378	11.37%	2.232%
8	11.479	3017	3029	3047	rVV	575215	979951	11.49%	2.257%
9	11.588	3047	3063	3097	rVB	3322382	6259698	73.41%	14.414%
10	11.916	3146	3165	3191	rBV	2251053	3830482	44.92%	8.820%
11	12.373	3294	3307	3323	rBV	402539	689794	8.09%	1.588%
12	12.624	3374	3385	3392	rBV	968687	1592886	18.68%	3.668%
13	12.704	3402	3410	3432	rVB	506486	815267	9.56%	1.877%
14	12.862	3446	3459	3472	rBV	496293	807399	9.47%	1.859%
15	13.010	3491	3505	3530	rBV	1781728	2876829	33.74%	6.624%
16	13.203	3555	3565	3575	rBV	65556	104451	1.22%	0.241%
17	13.315	3589	3600	3603	rBV	500072	756424	8.87%	1.742%
18	13.344	3604	3609	3624	rVB	732912	1115260	13.08%	2.568%
19	13.511	3643	3661	3669	rVV	659716	1223864	14.35%	2.818%
20	13.553	3669	3674	3692	rVB2	271886	467623	5.48%	1.077%
21	13.707	3711	3722	3732	rVB	115721	188820	2.21%	0.435%
22	13.772	3732	3742	3747	rBV	192201	307938	3.61%	0.709%
23	13.801	3748	3751	3760	rVV	182316	230491	2.70%	0.531%
24	13.858	3760	3769	3779	rVV	279136	423819	4.97%	0.976%
25	13.916	3779	3787	3793	rVV	60843	94659	1.11%	0.218%
26	13.965	3793	3802	3812	rVB	264810	433990	5.09%	0.999%
27	14.096	3833	3843	3852	rBV	111445	175070	2.05%	0.403%
28	14.180	3859	3869	3874	rBV	185024	284072	3.33%	0.654%
29	14.219	3874	3881	3889	rVV	313318	470075	5.51%	1.082%
30	14.402	3924	3938	3943	rBV3	45351	86814	1.02%	0.200%
31	14.444	3943	3951	3960	rVV	266990	427262	5.01%	0.984%
32	14.492	3961	3966	3974	rVB	78728	109077	1.28%	0.251%
33	14.563	3974	3988	3999	rBV3	559979	1161061	13.62%	2.674%
34	14.711	4023	4034	4049	rBV	280824	448723	5.26%	1.033%
35	14.820	4049	4068	4074	rBV4	140400	330566	3.88%	0.761%
36	14.926	4090	4101	4118	rVB3	150445	322788	3.79%	0.743%

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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	15.100	4136	4155	4164	rBV	110938	236157	2.77%	0.544%
38	15.154	4164	4172	4180	rBV	79676	116249	1.36%	0.268%
39	15.219	4180	4192	4200	rBV5	67913	174146	2.04%	0.401%
40	15.379	4230	4242	4256	rBV	102831	199197	2.34%	0.459%
41	15.543	4278	4293	4294	rBV5	78902	131722	1.54%	0.303%
42	15.572	4295	4302	4318	rVV	215272	406721	4.77%	0.937%
43	15.730	4340	4351	4375	rVB3	68883	173739	2.04%	0.400%
44	15.871	4381	4395	4424	rVB3	145088	315796	3.70%	0.727%
45	16.058	4439	4453	4462	rBV4	71953	153922	1.81%	0.354%
46	16.119	4463	4472	4488	rVB	88136	169601	1.99%	0.391%
47	16.305	4517	4530	4542	rBV5	63640	160122	1.88%	0.369%

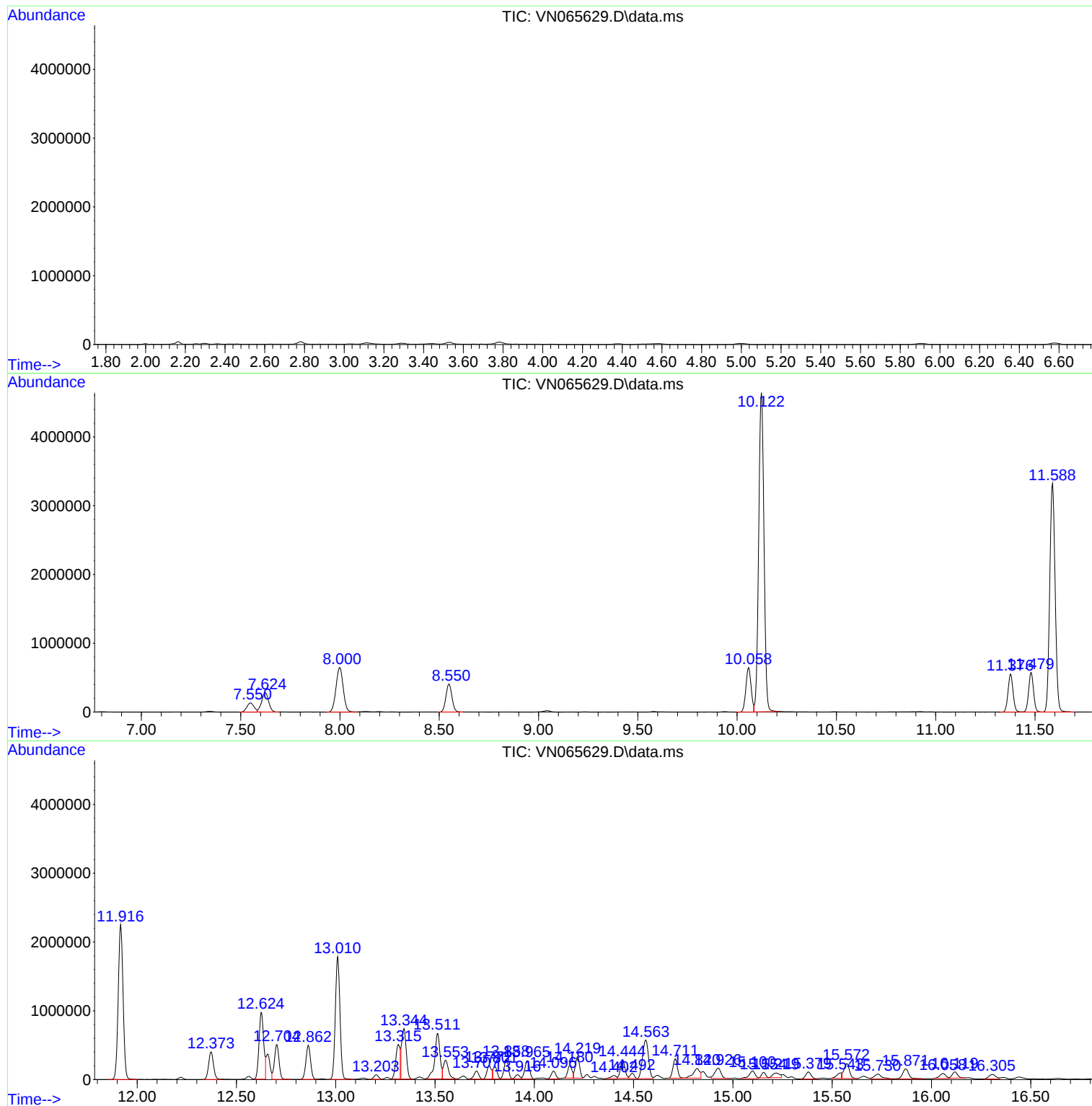
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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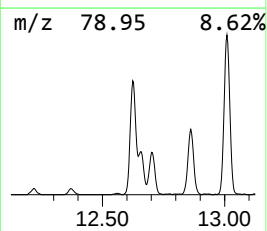
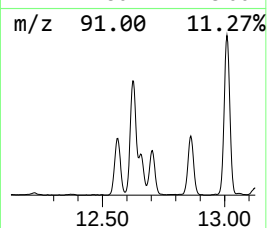
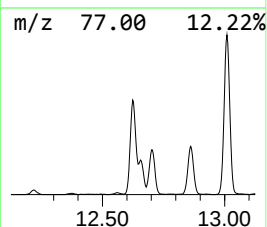
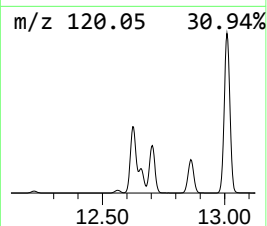
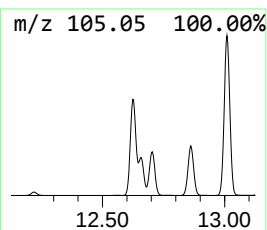
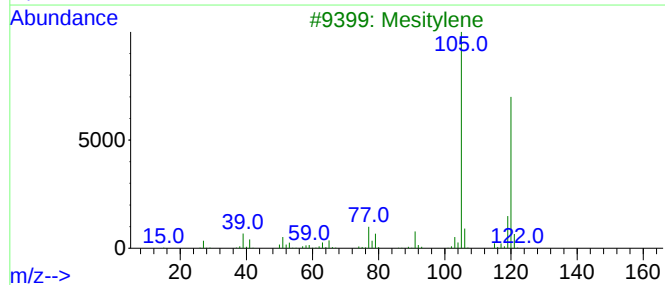
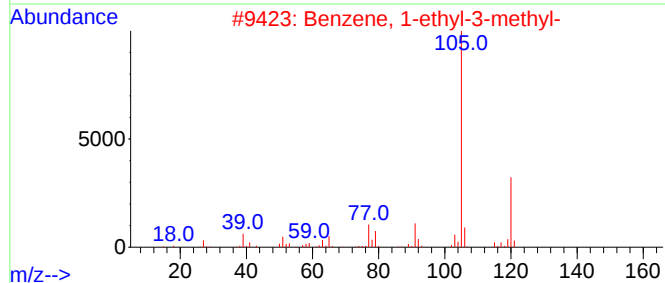
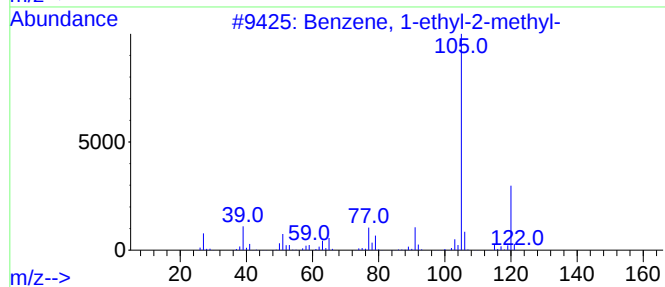
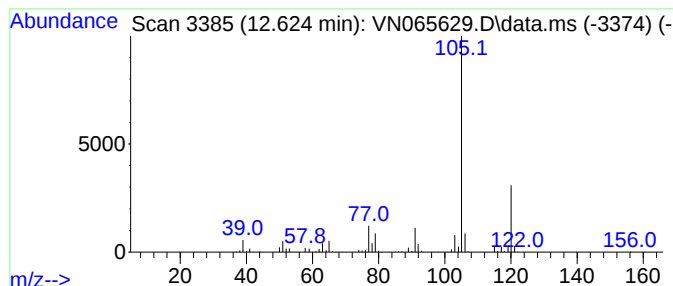
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.624	105.29 ug/l	1592890	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	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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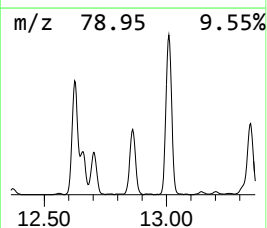
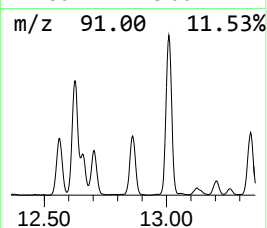
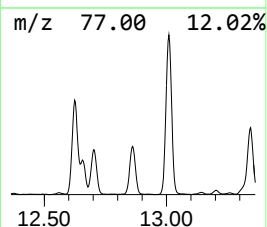
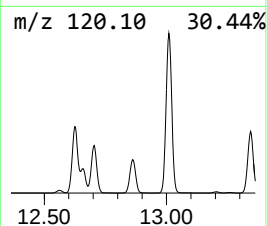
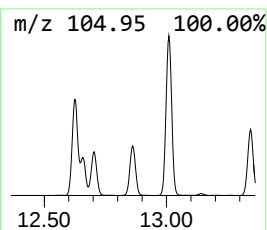
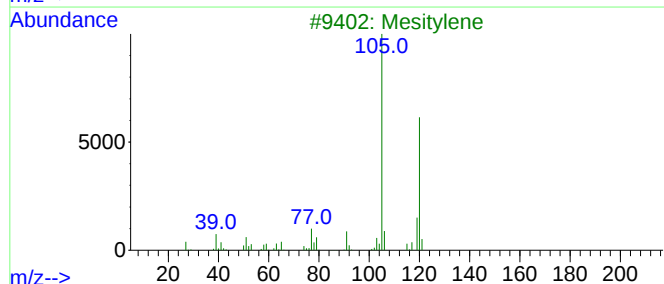
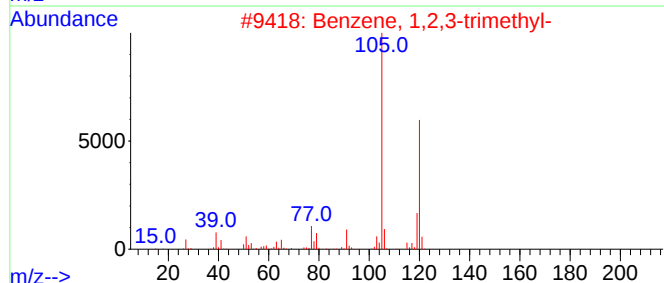
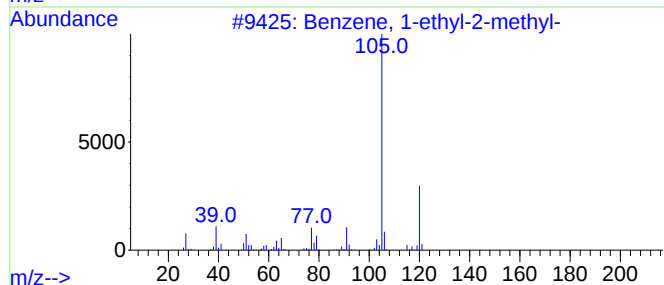
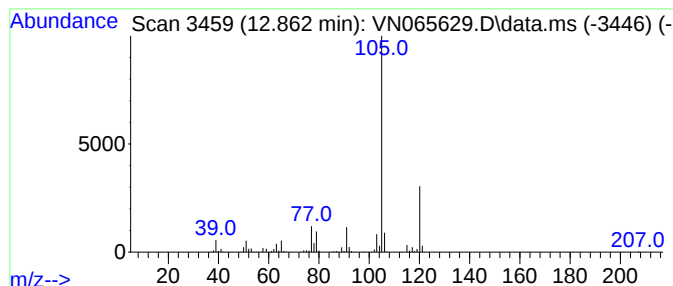
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.862	53.37 ug/l	807399	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	94
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

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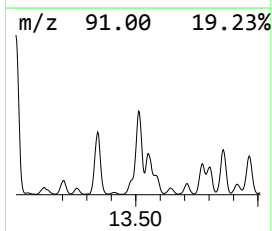
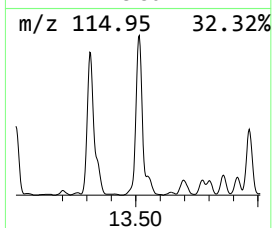
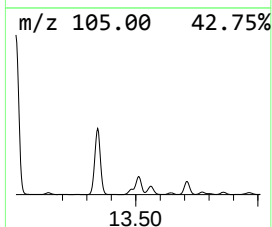
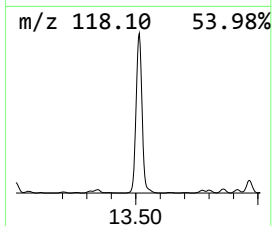
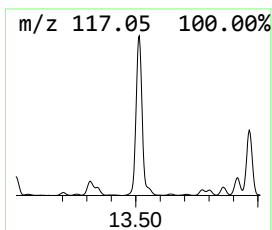
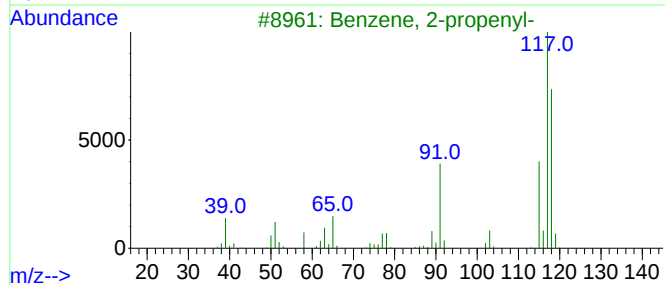
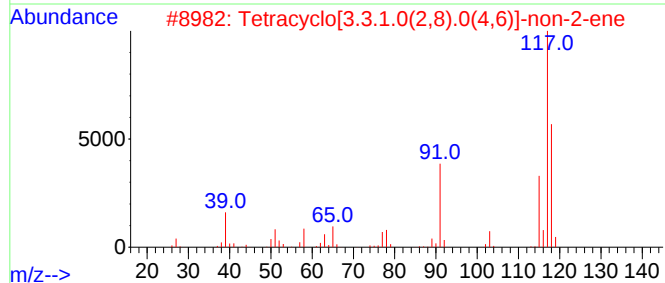
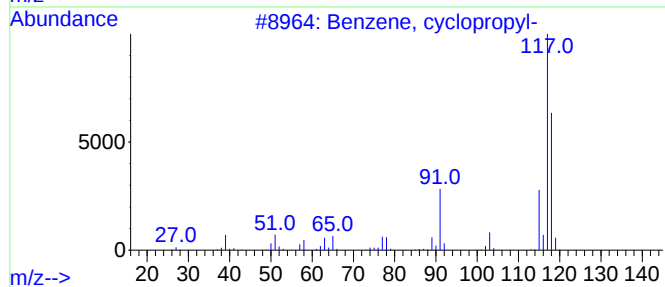
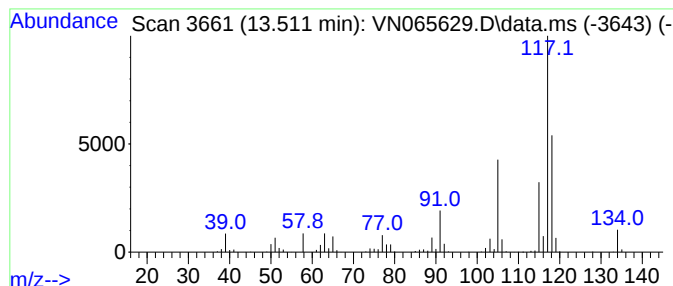
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, cyclopropyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.511	80.90 ug/l	1223860	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	93
2			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4			Indane	118	C9H10	000496-11-7	76
5			Deltacyclene	118	C9H10	007785-10-6	68



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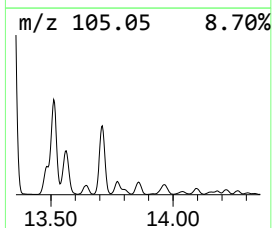
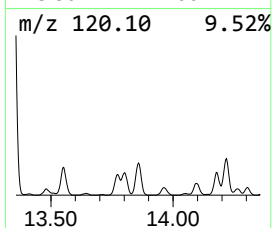
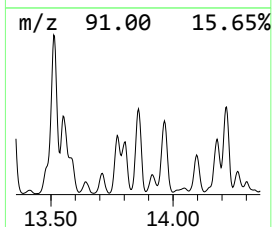
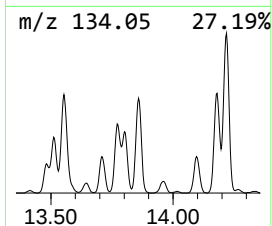
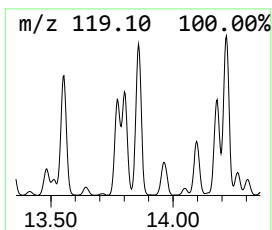
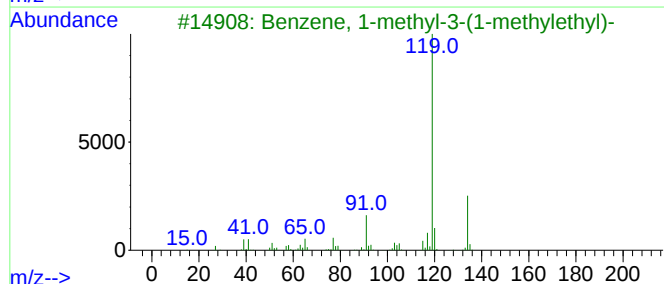
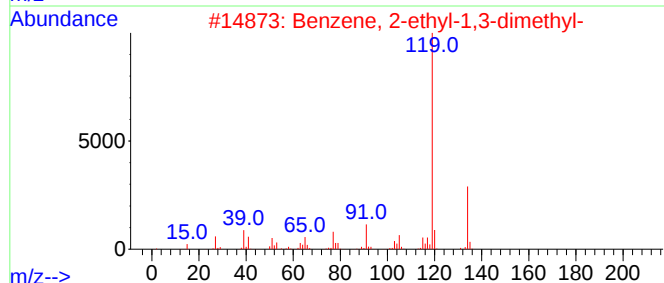
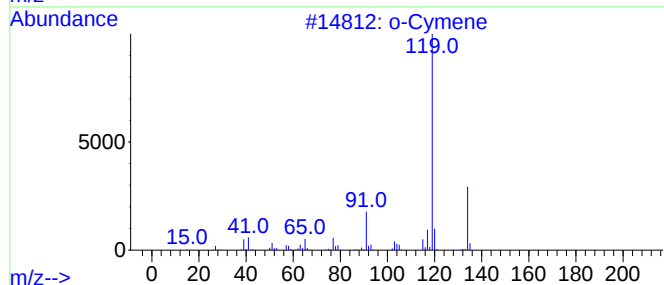
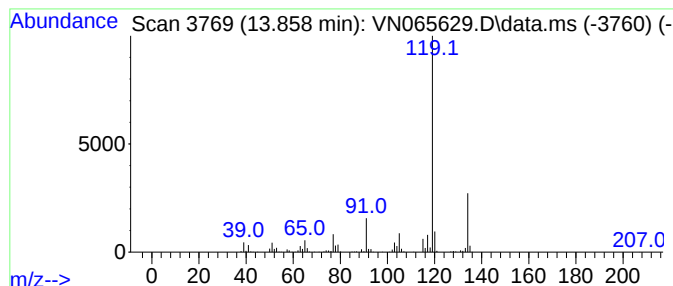
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 4 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.858	28.01 ug/l	423819	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5			p-Cymene	134	C10H14	000099-87-6	95



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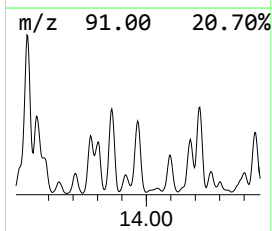
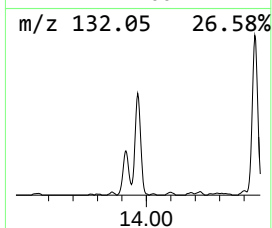
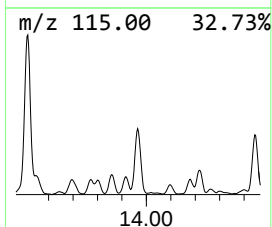
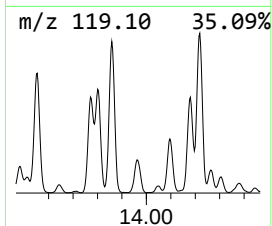
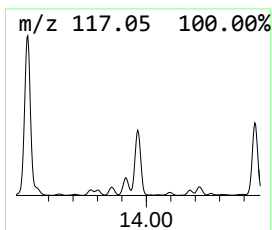
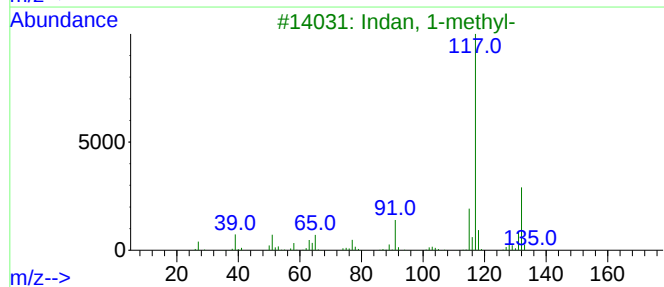
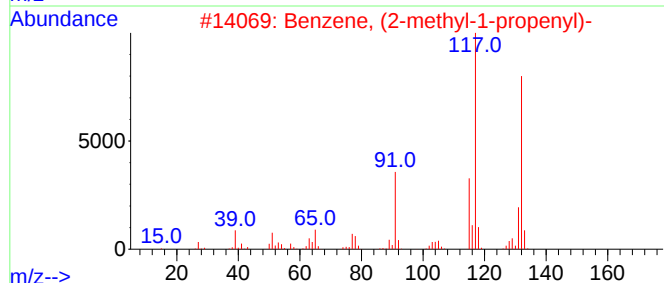
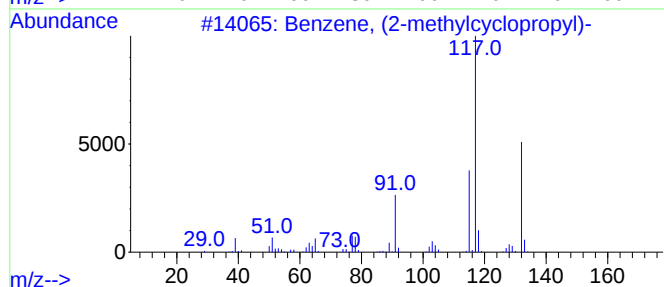
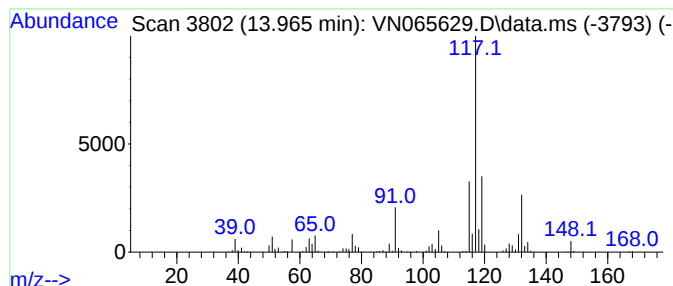
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, (2-methylcycloprop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	28.69 ug/l	433990	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	76
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	74
3			Indan, 1-methyl-	132	C10H12	000767-58-8	70
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065629.D
Acq On : 27 Jan 2021 14:59
Operator : JC/MD
Sample : M1190-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41709

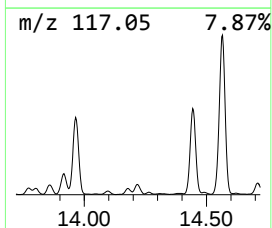
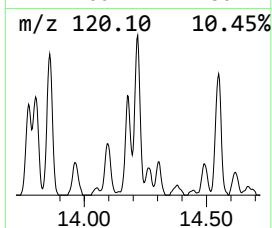
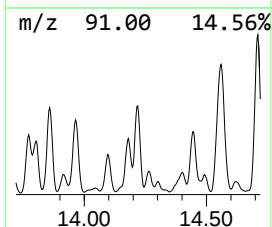
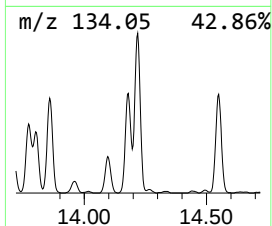
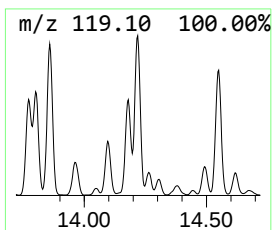
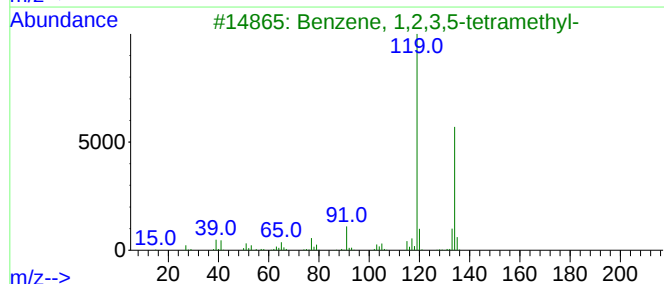
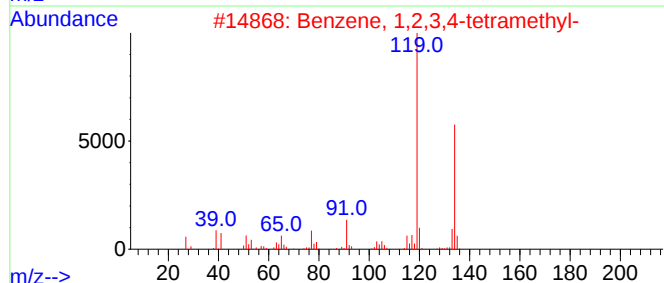
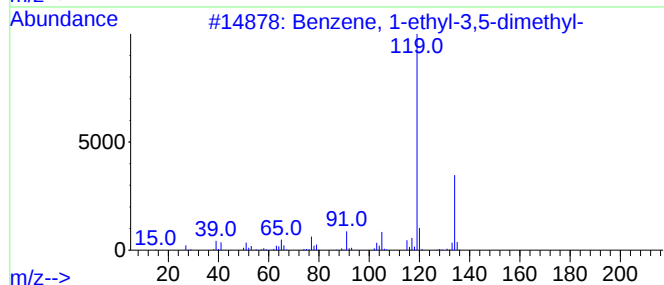
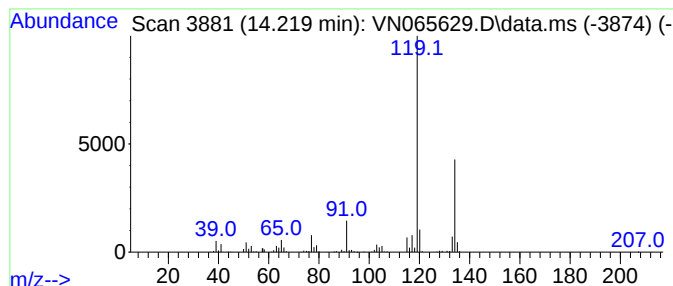
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-3,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	31.07 ug/l	470075	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	95
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4			o-Cymene	134	C10H14	000527-84-4	94
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065629.D
Acq On : 27 Jan 2021 14:59
Operator : JC/MD
Sample : M1190-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41709

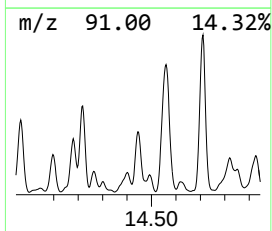
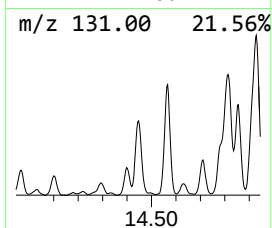
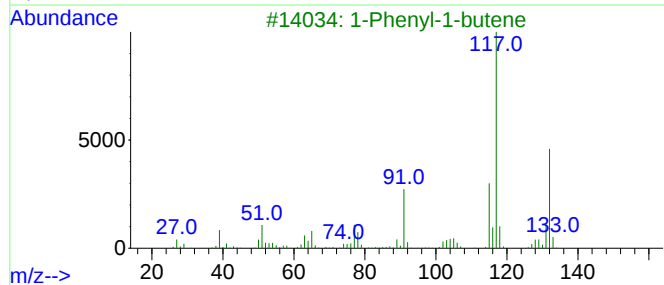
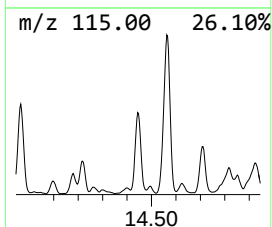
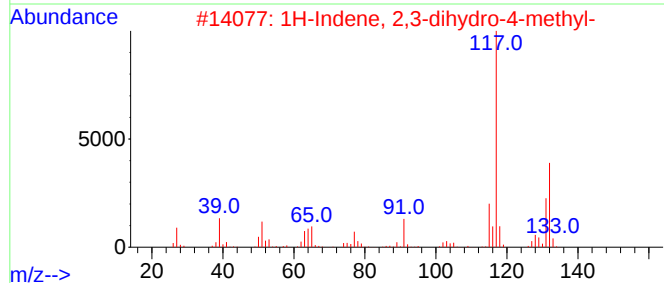
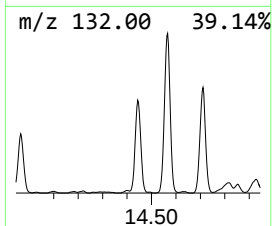
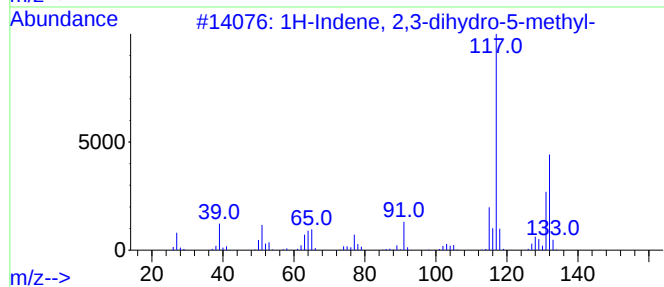
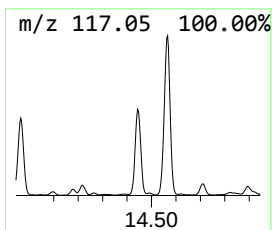
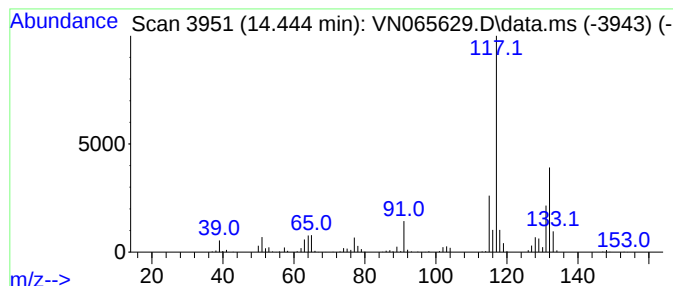
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Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.444	28.24 ug/l	427262	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
2			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	86
4			Indan, 1-methyl-	132	C10H12	000767-58-8	81
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065629.D
Acq On : 27 Jan 2021 14:59
Operator : JC/MD
Sample : M1190-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41709

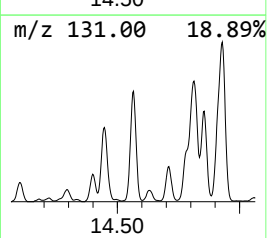
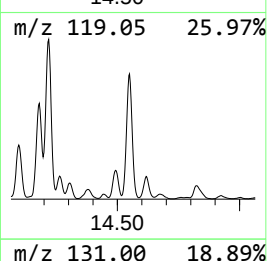
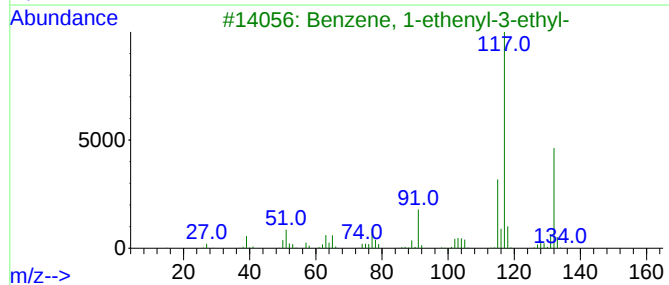
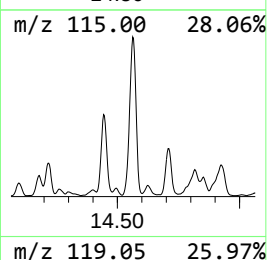
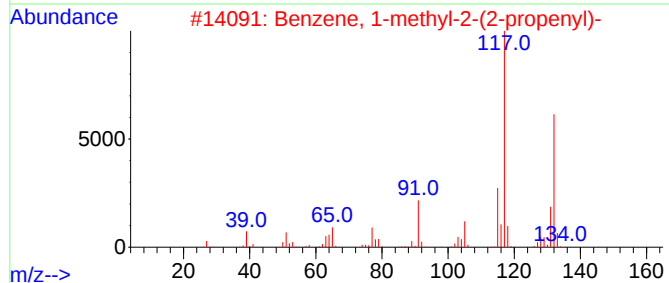
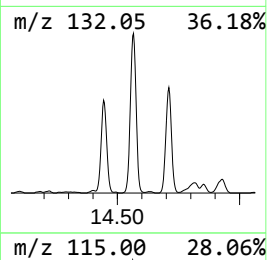
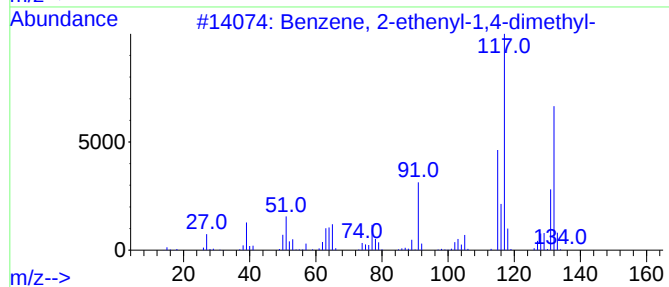
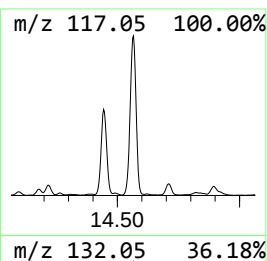
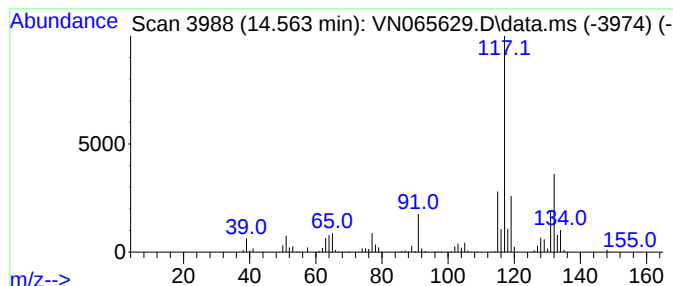
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.563	76.75 ug/l	1161060	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			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	81
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065629.D
Acq On : 27 Jan 2021 14:59
Operator : JC/MD
Sample : M1190-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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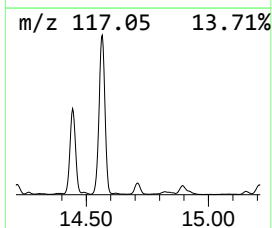
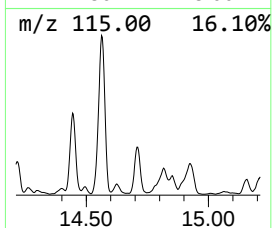
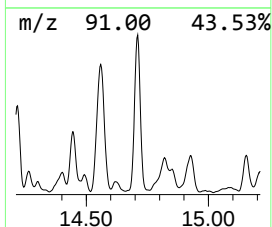
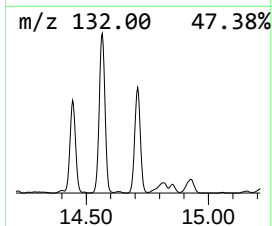
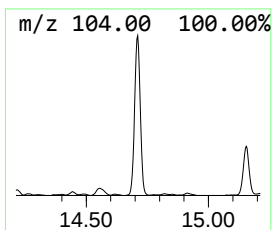
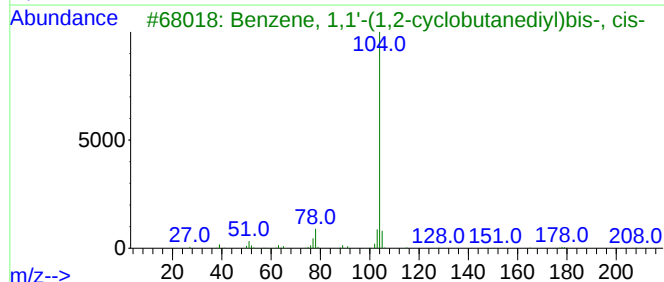
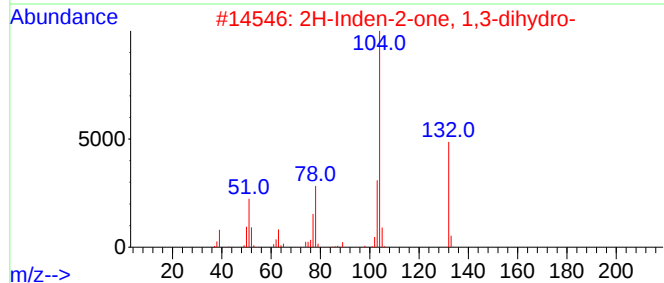
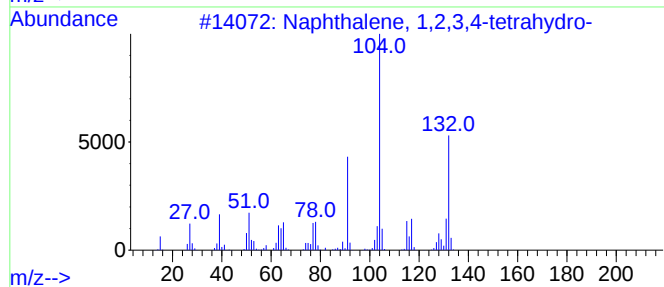
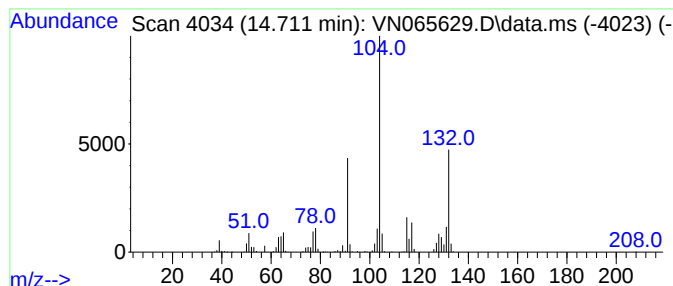
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.711	29.66 ug/l	448723	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	50
3			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	43
4			Isoquinoline, 1,2,3,4-tetrahydro-	133	C9H11N	000091-21-4	43
5			N-Ethylbenzimidoyl bromide	211	C9H10BrN	041182-87-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065629.D
Acq On : 27 Jan 2021 14:59
Operator : JC/MD
Sample : M1190-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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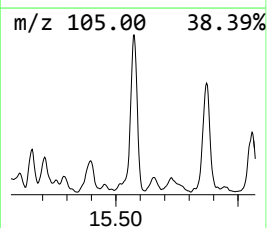
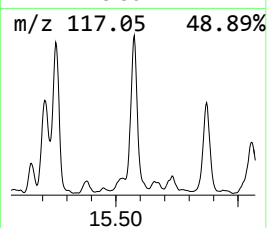
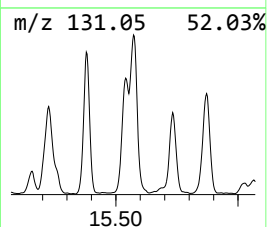
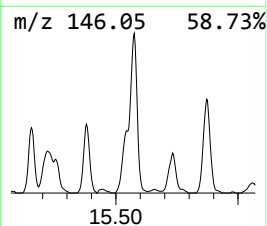
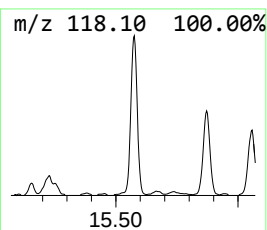
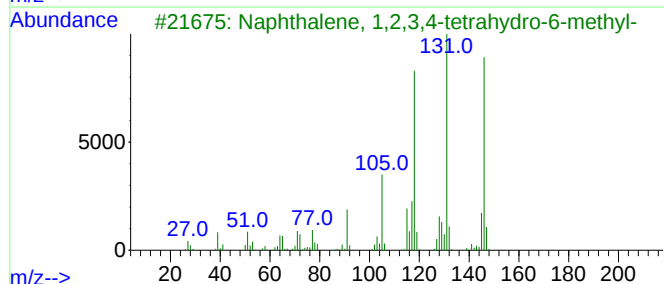
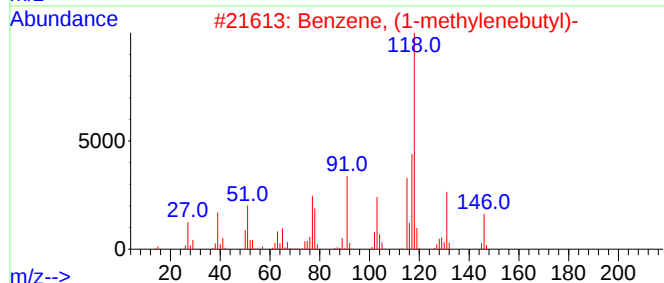
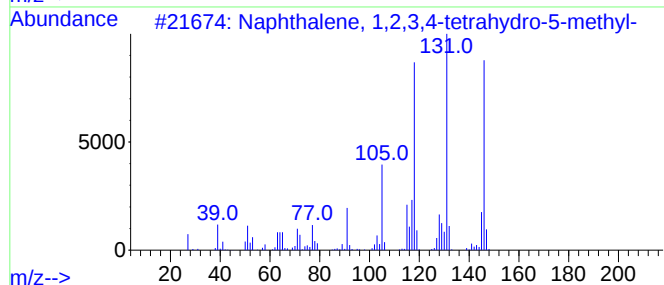
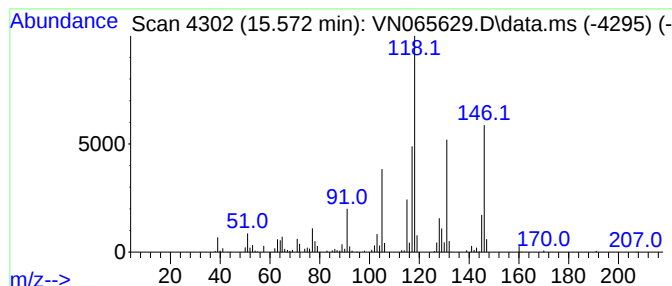
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.572	26.88 ug/l	406721	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
2			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	80
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	64
4			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	55
5			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065629.D
Acq On : 27 Jan 2021 14:59
Operator : JC/MD
Sample : M1190-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41709

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
Benzene, 1-ethy...	12.624	105.3	ug/l	1592890	4	13.315	756424	50.0
Benzene, 1,2,3-...	12.862	53.4	ug/l	807399	4	13.315	756424	50.0
Benzene, cyclop...	13.511	80.9	ug/l	1223860	4	13.315	756424	50.0
o-Cymene	13.858	28.0	ug/l	423819	4	13.315	756424	50.0
Benzene, (2-met...	13.965	28.7	ug/l	433990	4	13.315	756424	50.0
Benzene, 1-ethy...	14.219	31.1	ug/l	470075	4	13.315	756424	50.0
1H-Indene, 2,3-...	14.444	28.2	ug/l	427262	4	13.315	756424	50.0
Benzene, 2-ethe...	14.563	76.8	ug/l	1161060	4	13.315	756424	50.0
Naphthalene, 1,...	14.711	29.7	ug/l	448723	4	13.315	756424	50.0
Naphthalene, 1,...	15.572	26.9	ug/l	406721	4	13.315	756424	50.0