

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
 Data File : VN069918.D
 Acq On : 9 Dec 2021 18:03
 Operator : JC/MD
 Sample : M4969-03
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-1A

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\82N120221W.M

Title : SW846 8260

Signal : TIC: VN069918.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.993	724	747	769	rBV	329456	903337	1.19%	0.189%
2	5.374	1238	1262	1303	rVB2	799962	2786480	3.66%	0.582%
3	5.618	1325	1353	1393	rVB2	1464362	5147605	6.75%	1.076%
4	6.468	1642	1670	1699	rBV4	666758	2165352	2.84%	0.452%
5	6.608	1701	1722	1741	rVV2	385659	1183817	1.55%	0.247%
6	6.903	1813	1832	1865	rVB3	371095	1089835	1.43%	0.228%
7	7.147	1899	1923	1942	rBV2	1906036	5616032	7.37%	1.174%
8	7.844	2168	2183	2204	rVB	796225	1941903	2.55%	0.406%
9	8.021	2227	2249	2260	rBV	990699	2458350	3.23%	0.514%
10	8.088	2261	2274	2293	rVV3	2464492	6293837	8.26%	1.315%
11	8.177	2297	2307	2332	rVB4	463412	1210138	1.59%	0.253%
12	8.461	2386	2413	2441	rBV2	31431650	76209620	100.00%	15.925%
13	8.590	2448	2461	2473	rBV2	944073	2204570	2.89%	0.461%
14	8.968	2581	2602	2630	rBV3	3971717	9775884	12.83%	2.043%
15	9.244	2697	2705	2724	rVB	604041	1210459	1.59%	0.253%
16	9.459	2751	2785	2801	rBV2	1255515	3976085	5.22%	0.831%
17	9.802	2898	2913	2917	rBV3	491034	871859	1.14%	0.182%
18	9.883	2934	2943	2960	rVB	485807	957643	1.26%	0.200%
19	9.971	2961	2976	2986	rBV	1810487	3549375	4.66%	0.742%
20	10.202	3047	3062	3091	rBV4	437970	1243660	1.63%	0.260%
21	10.322	3092	3107	3120	rBV	1319414	2457521	3.22%	0.514%
22	10.440	3135	3151	3166	rBV	4707995	8959812	11.76%	1.872%
23	10.636	3207	3224	3237	rVB6	399987	832671	1.09%	0.174%
24	10.859	3293	3307	3327	rVV5	860899	1875295	2.46%	0.392%
25	11.130	3396	3408	3420	rBV	940265	1557669	2.04%	0.325%
26	11.744	3621	3637	3650	rBV	5109090	9306677	12.21%	1.945%
27	11.843	3662	3674	3696	rVB	4603252	8160763	10.71%	1.705%
28	11.953	3700	3715	3740	rVB	1292903	2676156	3.51%	0.559%
29	12.090	3755	3766	3789	rVB3	461632	896849	1.18%	0.187%
30	12.578	3933	3948	3965	rBV	11124199	18401589	24.15%	3.845%
31	12.731	3990	4005	4028	rVB	4167712	7417721	9.73%	1.550%
32	12.919	4060	4075	4092	rBV2	29544227	50350317	66.07%	10.521%
33	13.058	4119	4127	4142	rVB	705477	1190697	1.56%	0.249%
34	13.219	4173	4187	4208	rBV	1922958	3290305	4.32%	0.688%
35	13.366	4230	4242	4258	rVB	1208925	2093256	2.75%	0.437%
36	13.495	4272	4290	4305	rBV3	1773799	4248039	5.57%	0.888%

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

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37	13.672	4342	4356	4384	rBV2	4882096	10747119	14.10%	2.246%
38	13.838	4403	4418	4422	rBV	10830078	15769702	20.69%	3.295%
39	13.876	4423	4432	4444	rVB2	39759407	63956292	83.92%	13.365%
40	14.002	4468	4479	4492	rVB	1787137	2804370	3.68%	0.586%
41	14.131	4516	4527	4544	rBV2	398079	813703	1.07%	0.170%
42	14.217	4544	4559	4572	rBV	19907102	31439430	41.25%	6.570%
43	14.278	4572	4582	4589	rVV	2690282	4367510	5.73%	0.913%
44	14.327	4589	4600	4617	rVB2	10426618	17880282	23.46%	3.736%
45	14.538	4661	4679	4690	rBV	8996630	14686390	19.27%	3.069%
46	14.809	4767	4780	4792	rBV	7887357	12694468	16.66%	2.653%
47	14.930	4806	4825	4838	rBV3	10840576	22420232	29.42%	4.685%
48	14.986	4839	4846	4863	rVB4	658758	1361378	1.79%	0.284%
49	15.083	4870	4882	4898	rBV2	950920	1723153	2.26%	0.360%
50	15.193	4900	4923	4934	rBV6	1504461	3495900	4.59%	0.731%
51	15.308	4951	4966	4987	rVB4	1307711	3146653	4.13%	0.658%
52	15.504	5011	5039	5056	rBV	7006614	13481952	17.69%	2.817%
53	15.804	5135	5151	5170	rBV2	626051	1239567	1.63%	0.259%
54	16.614	5438	5453	5482	rVB	882035	2010012	2.64%	0.420%

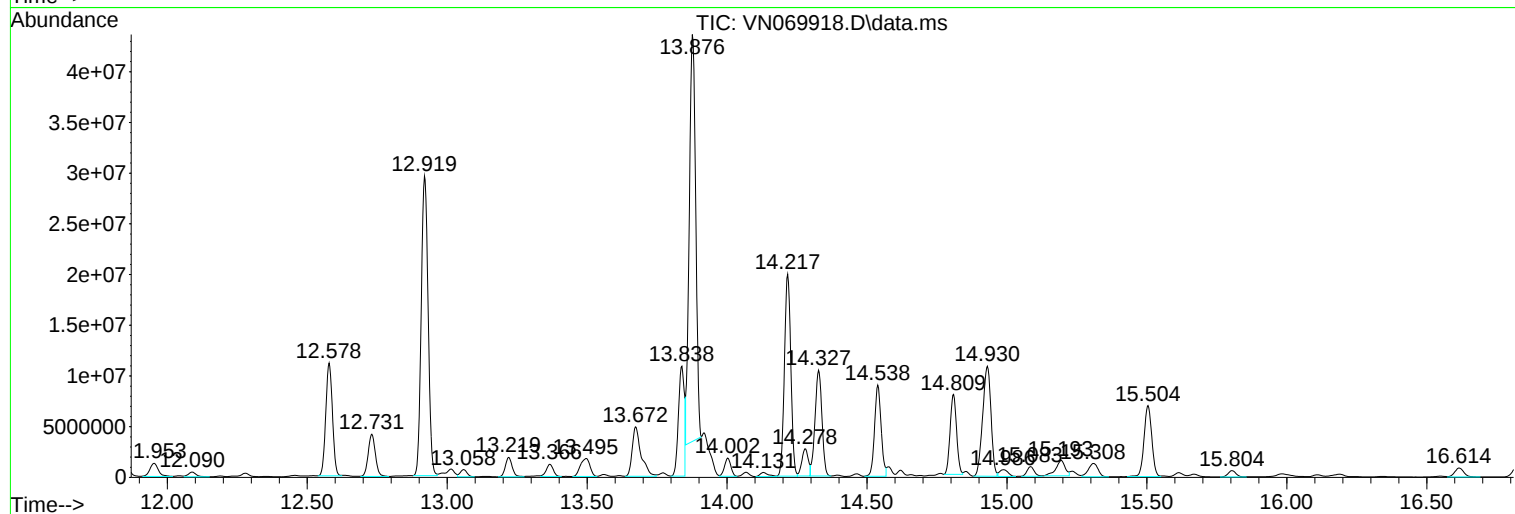
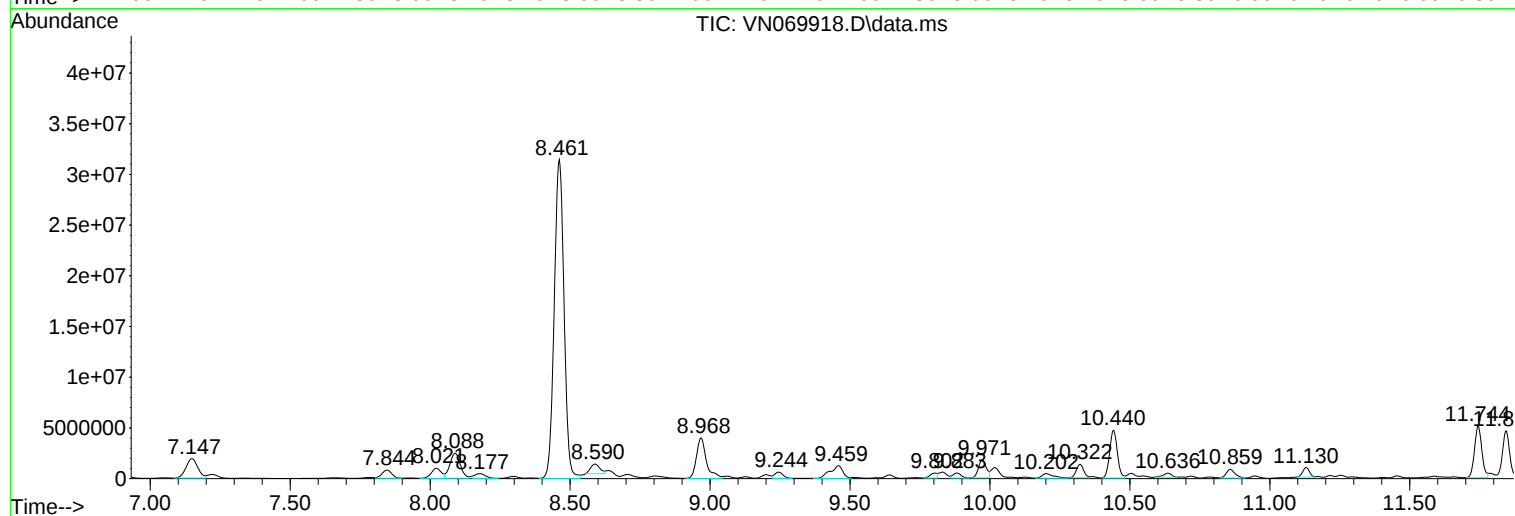
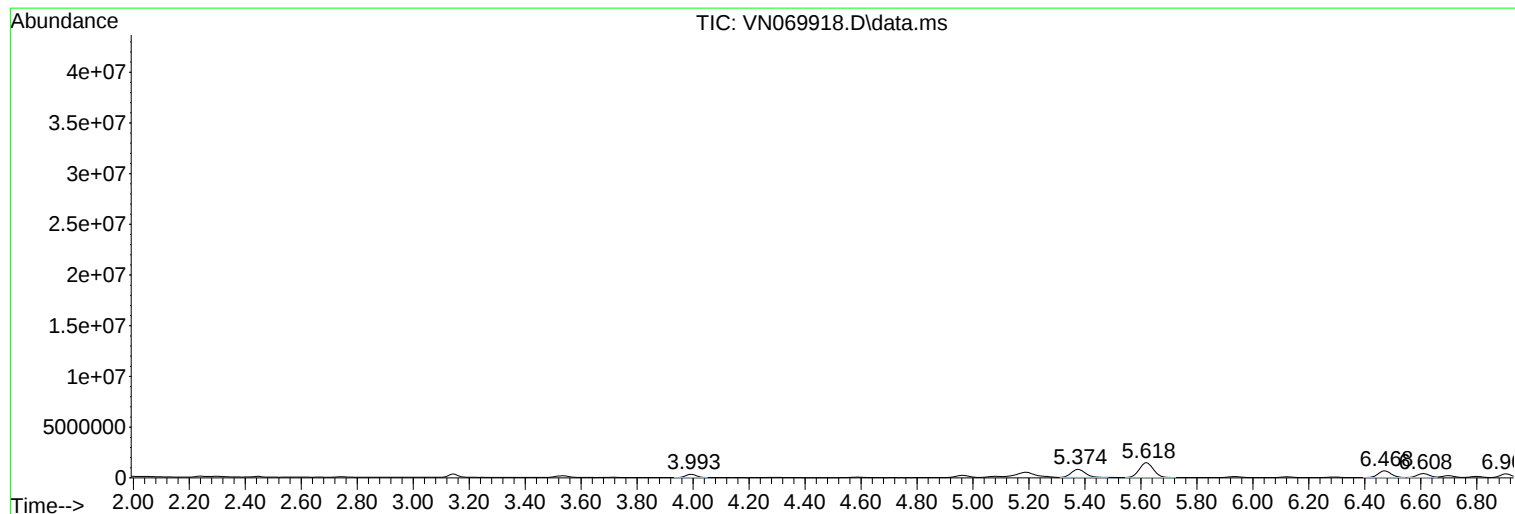
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Quant Title : SW846 8260

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



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Misc : 5.00mL/MSVOA_N/WATER
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Instrument :
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ClientSampleId :
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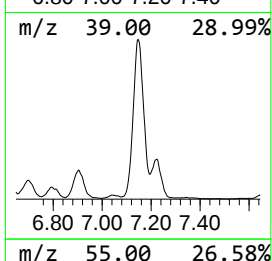
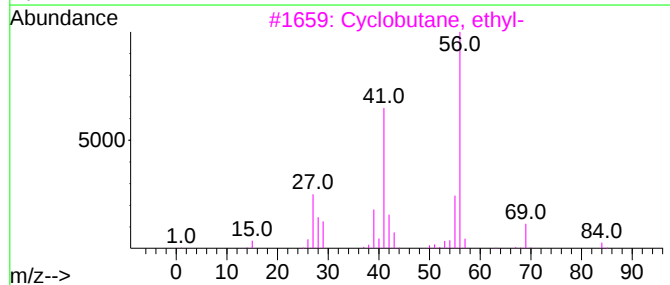
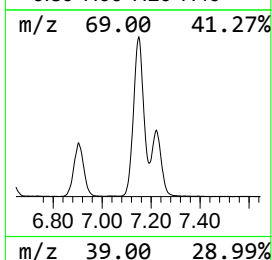
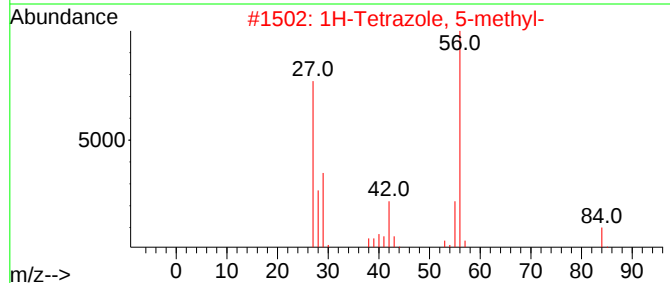
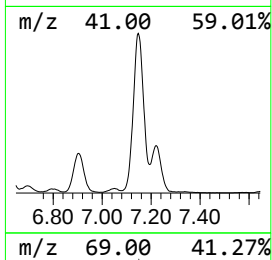
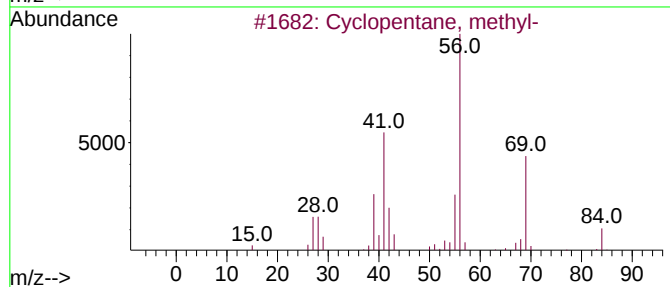
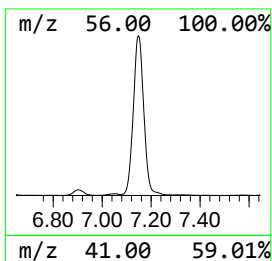
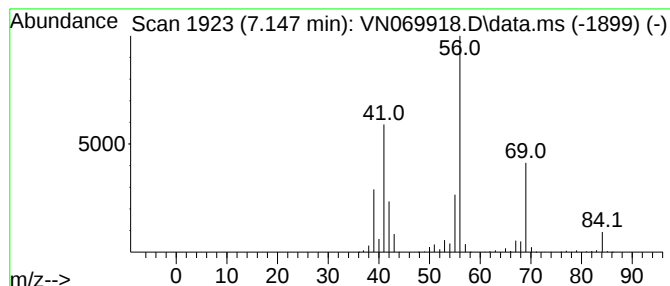
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	44.62 ug/l	5616030	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			Cyclohexane	84	C6H12	000110-82-7	64
5			Cyclobutane	56	C4H8	000287-23-0	53



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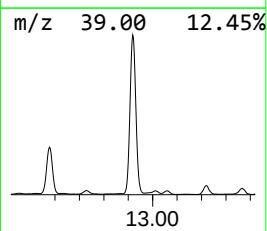
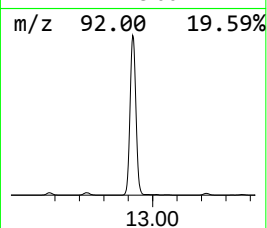
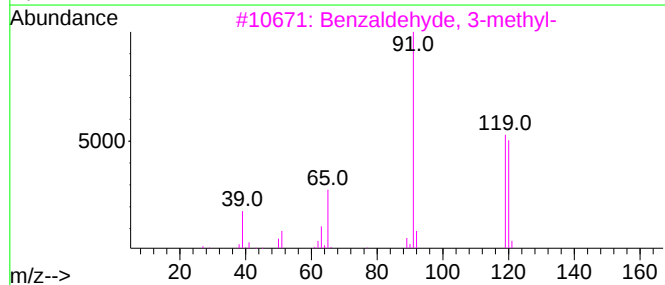
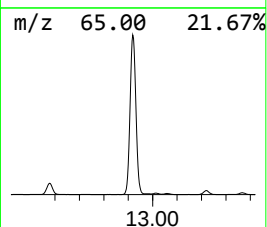
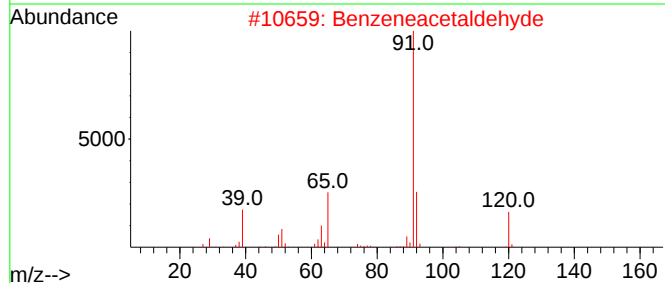
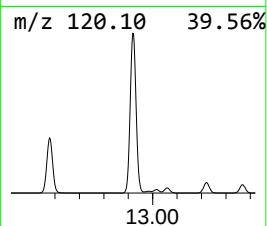
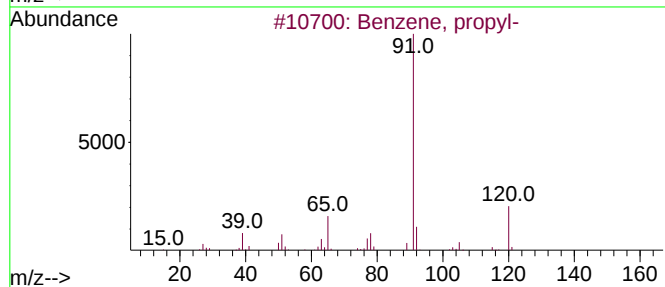
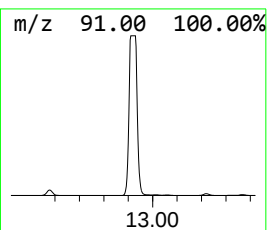
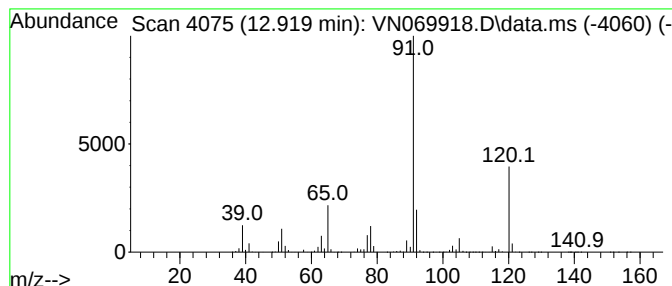
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.919	234.25 ug/l	50350300	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, propyl-	120	C9H12	000103-65-1	90
2			Benzeneacetaldehyde	120	C8H8O	000122-78-1	87
3			Benzaldehyde, 3-methyl-	120	C8H8O	000620-23-5	76
4			Propanenitrile, 3-[(phenylmethyl...]	160	C10H12N2	000706-03-6	59
5			N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	59



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

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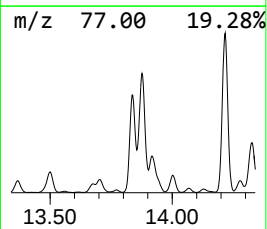
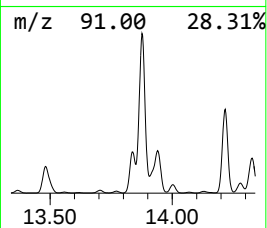
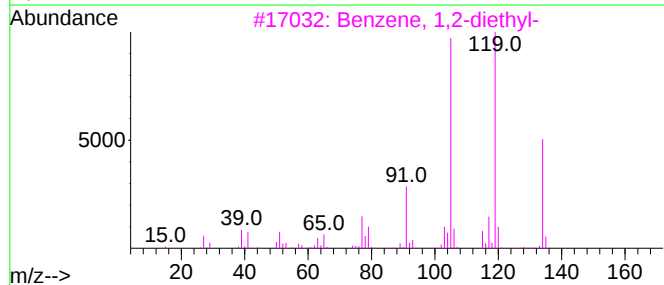
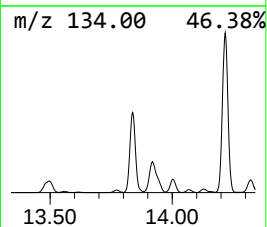
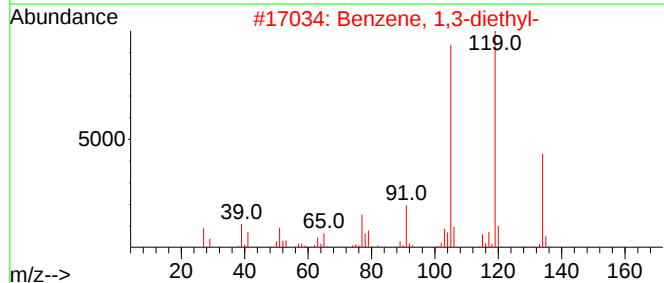
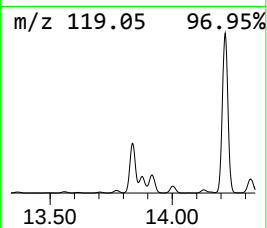
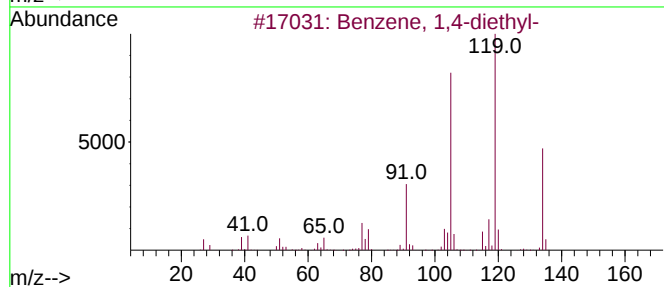
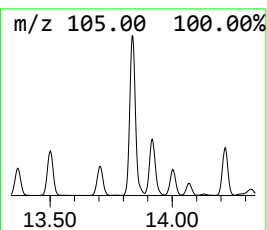
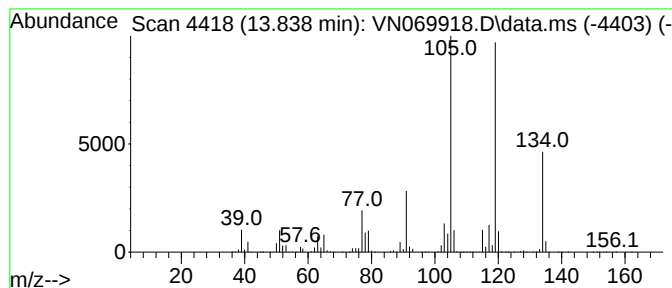
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,4-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	73.37 ug/l	15769700	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	97
2			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	96
3			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	87
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	81



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Instrument :
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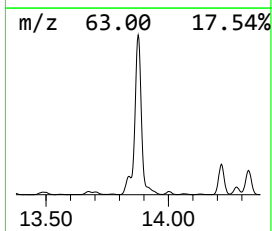
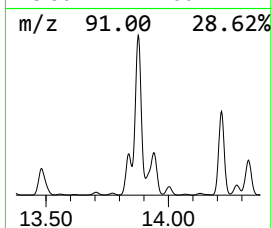
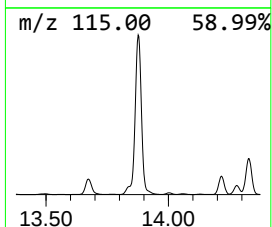
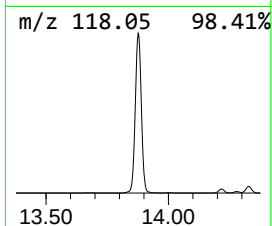
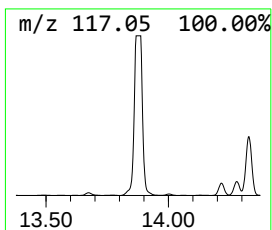
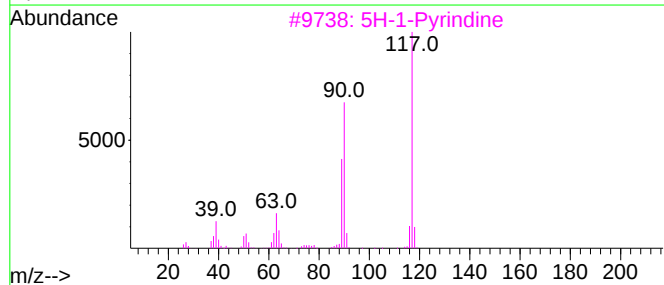
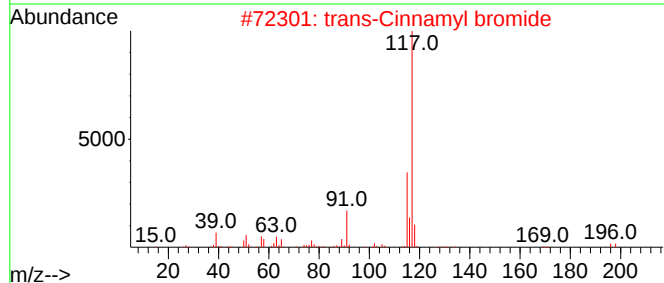
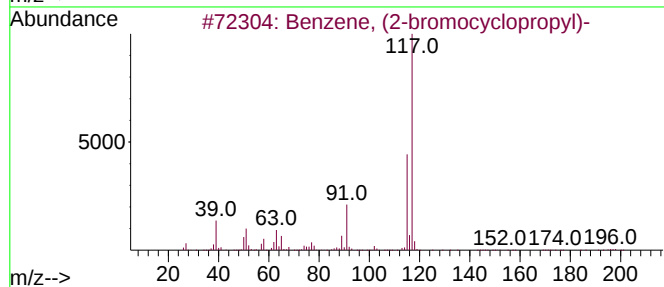
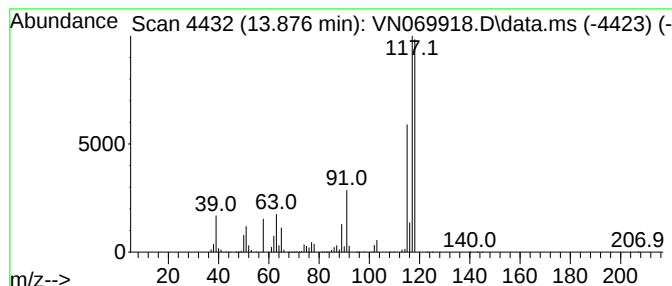
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, (2-bromocyclopropyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	297.55 ug/l	63956300	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	52
2			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	47
3			5H-1-Pyridine	117	C8H7N	000270-91-7	38
4			Indolizine	117	C8H7N	000274-40-8	35
5			Indole	117	C8H7N	000120-72-9	35



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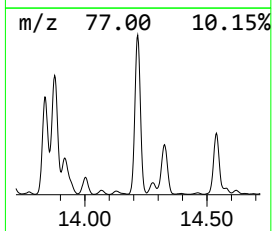
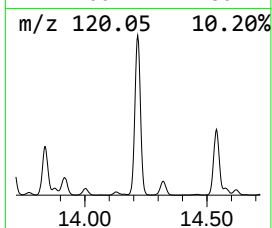
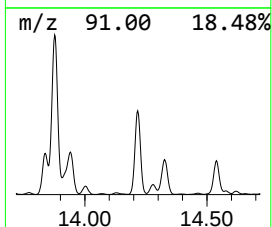
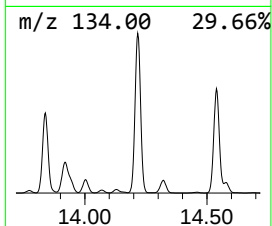
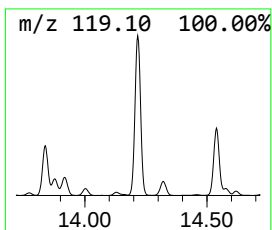
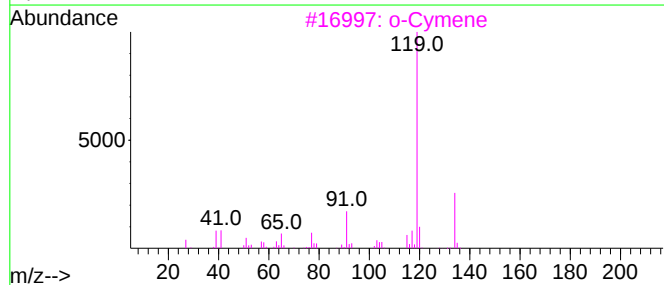
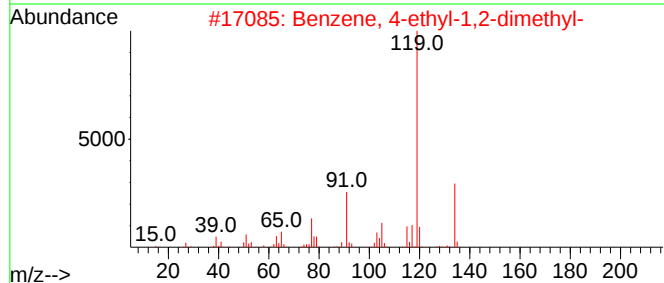
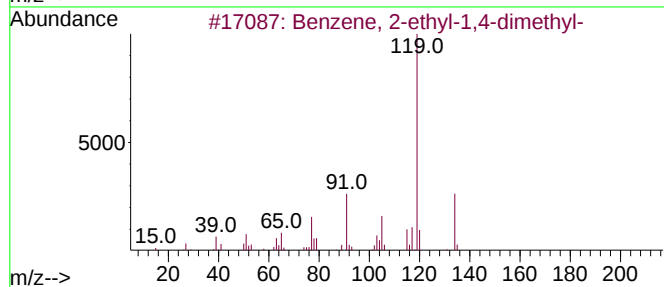
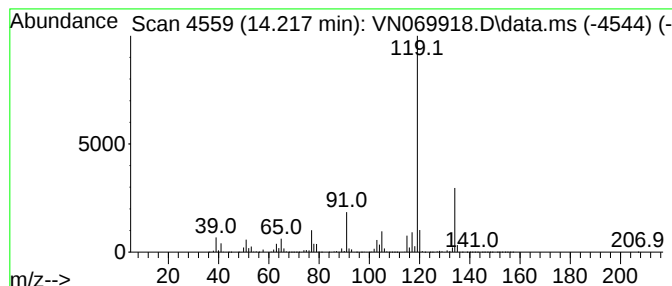
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	146.27 ug/l	31439400	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5			p-Cymene	134	C10H14	000099-87-6	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069918.D
Acq On : 9 Dec 2021 18:03
Operator : JC/MD
Sample : M4969-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1A

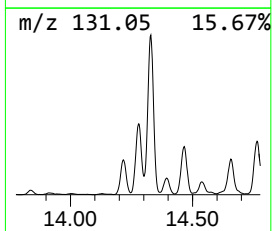
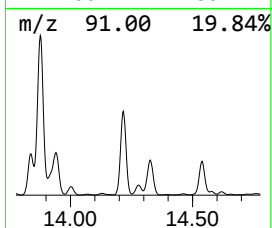
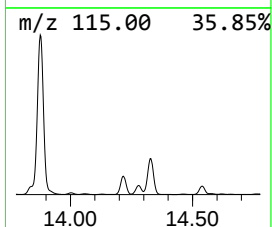
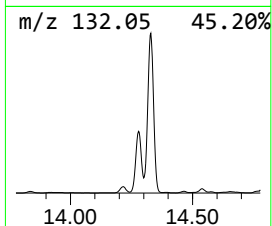
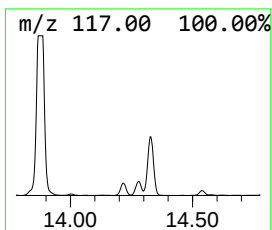
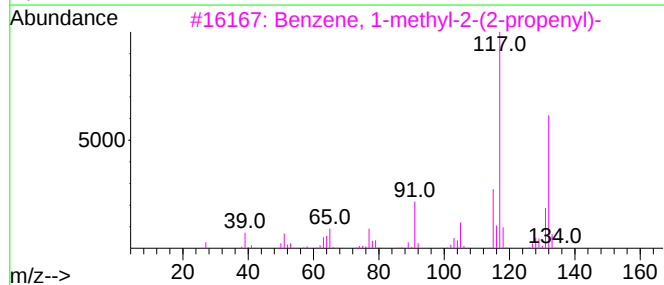
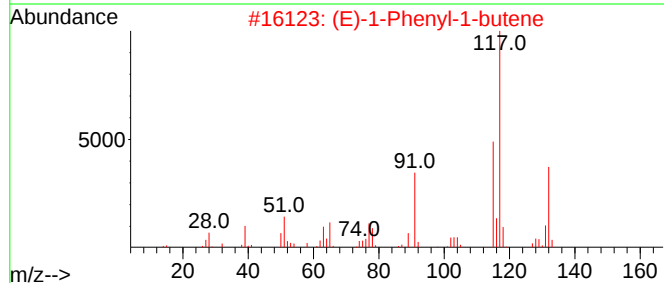
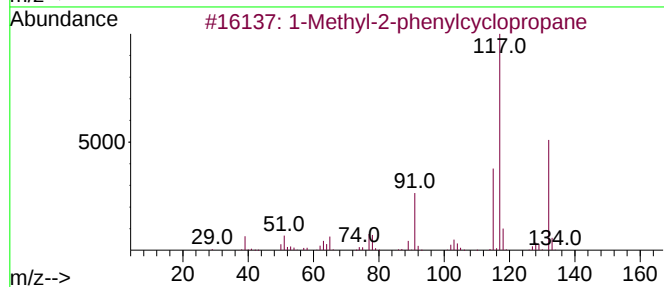
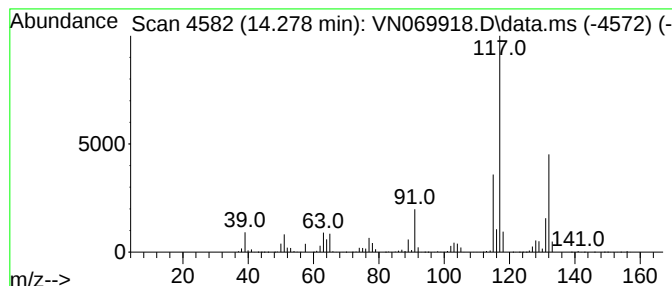
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Quant Title : SW846 8260

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

Peak Number 6 1-Methyl-2-phenylcyclopropane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.278	20.32 ug/l	4367510	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	95
2			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	95
3			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	94
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	94
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069918.D
Acq On : 9 Dec 2021 18:03
Operator : JC/MD
Sample : M4969-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1A

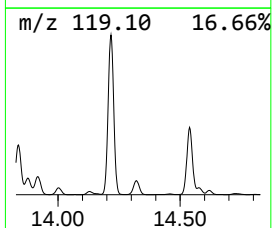
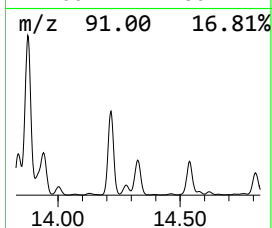
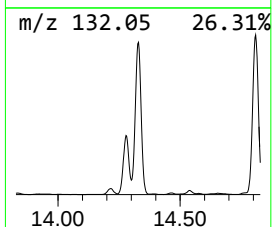
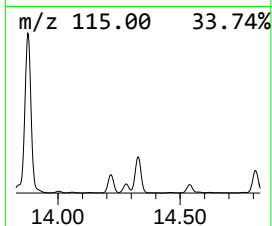
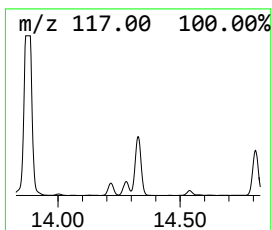
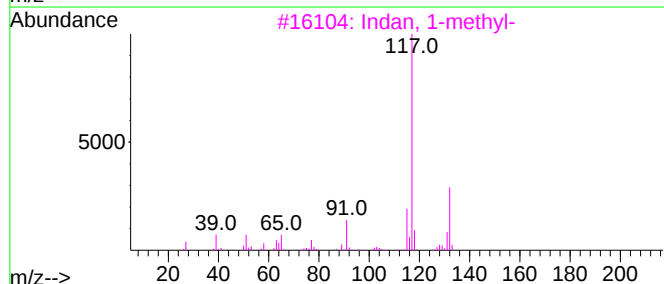
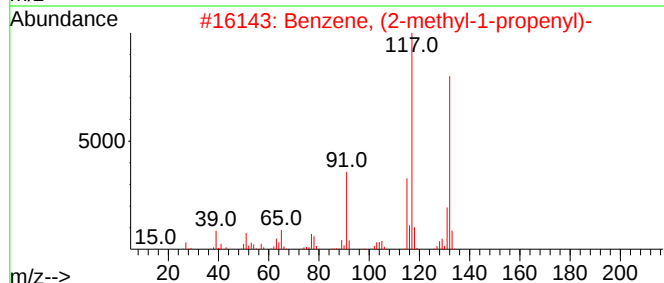
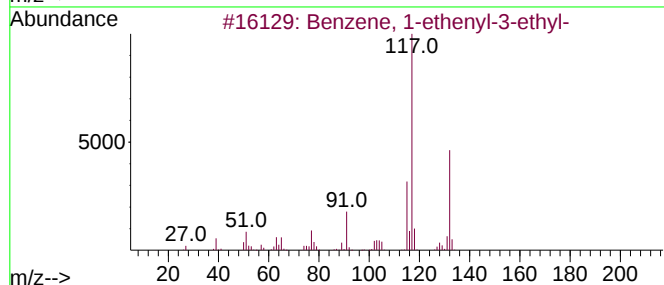
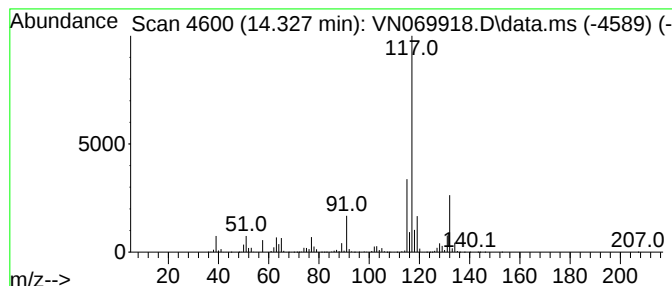
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	83.19 ug/l	17880300	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	83
3			Indan, 1-methyl-	132	C10H12	000767-58-8	81
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069918.D
Acq On : 9 Dec 2021 18:03
Operator : JC/MD
Sample : M4969-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1A

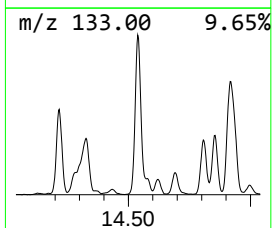
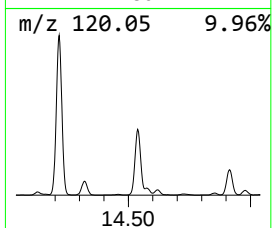
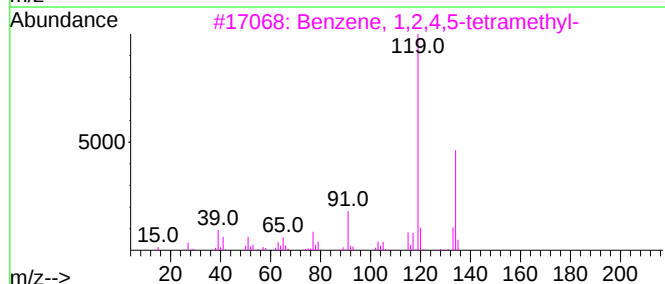
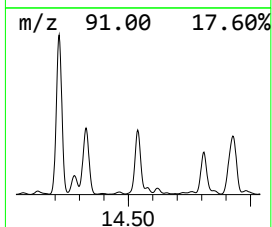
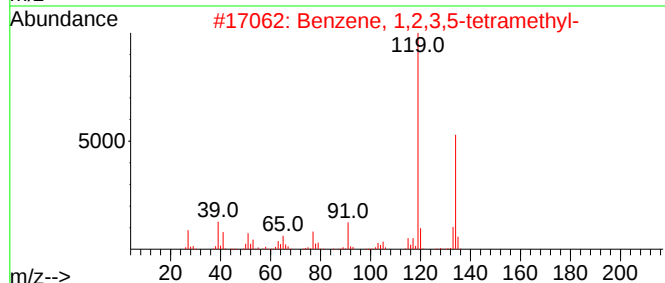
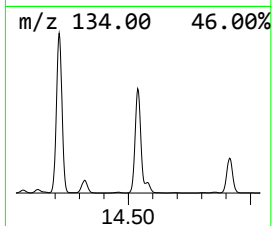
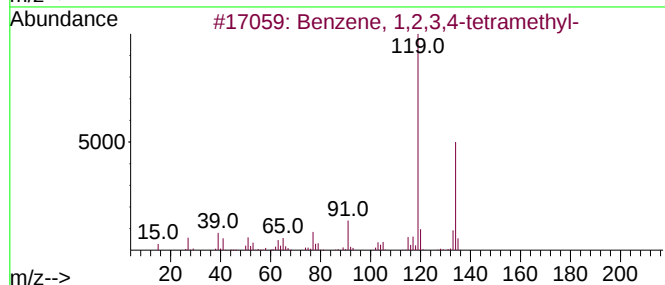
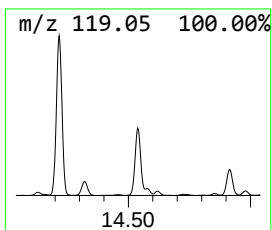
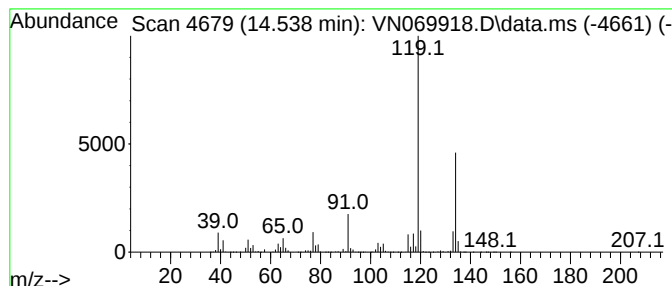
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	68.33 ug/l	14686400	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069918.D
Acq On : 9 Dec 2021 18:03
Operator : JC/MD
Sample : M4969-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1A

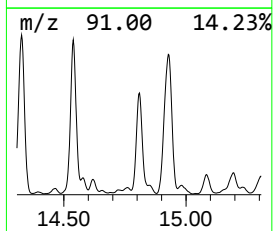
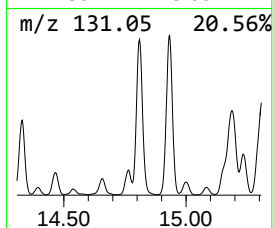
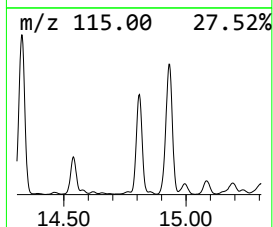
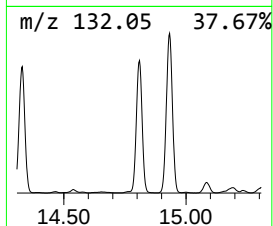
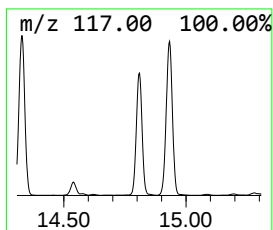
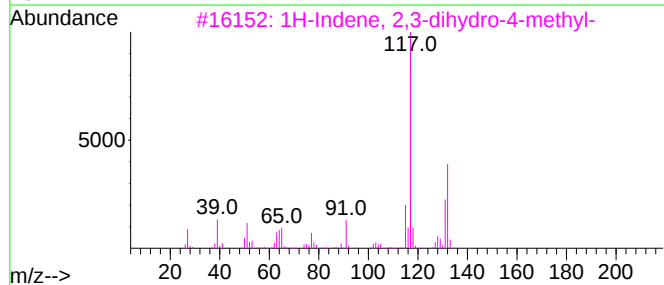
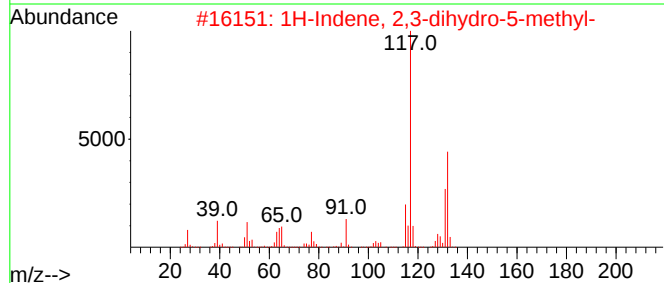
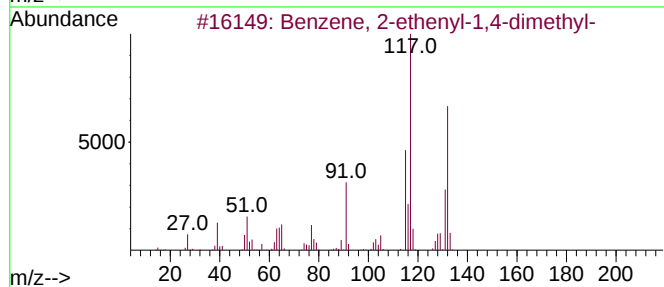
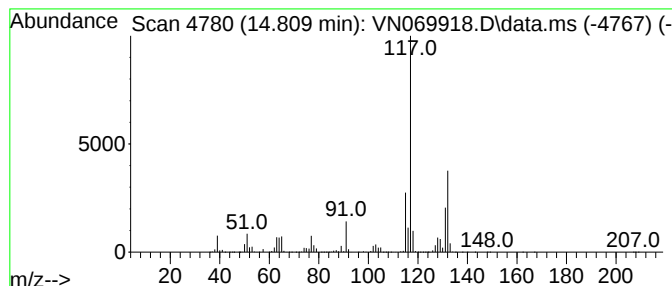
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.809	59.06 ug/l	12694500	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	96
3			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069918.D
Acq On : 9 Dec 2021 18:03
Operator : JC/MD
Sample : M4969-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1A

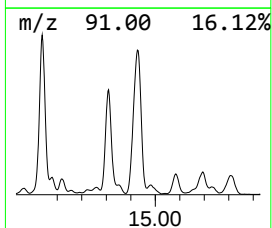
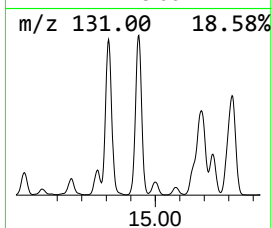
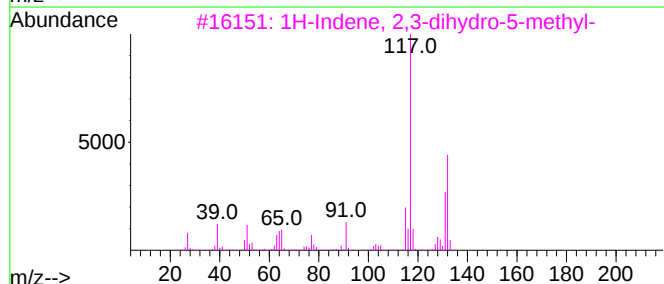
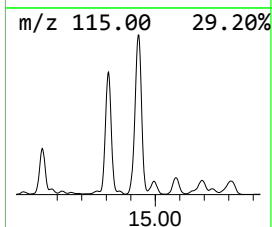
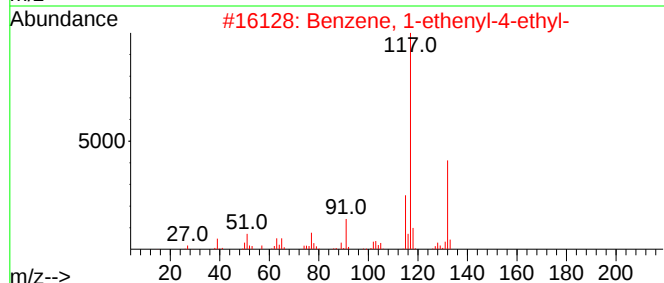
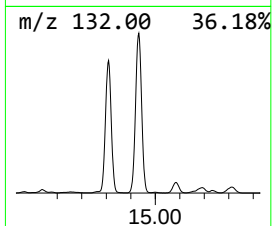
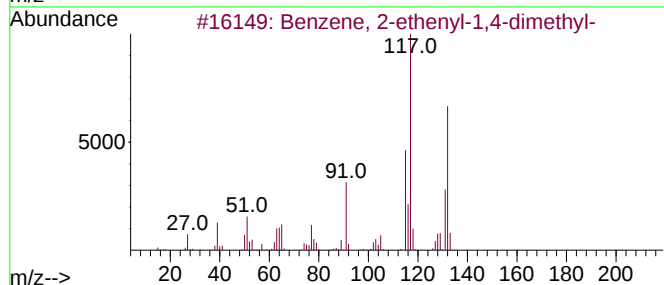
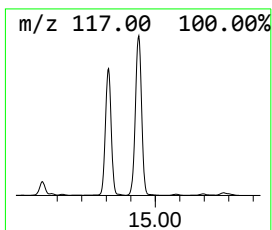
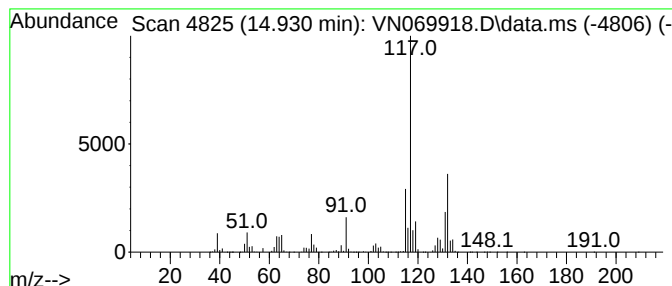
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	104.31 ug/l	22420200	1,4-Dichlorobenzene-d4	13.672

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069918.D
Acq On : 9 Dec 2021 18:03
Operator : JC/MD
Sample : M4969-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.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
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Benzene, propyl-	12.919	234.3	ug/l	50350300	4	13.672	10747100	50.0
Benzene, 1,4-di...	13.839	73.4	ug/l	15769700	4	13.672	10747100	50.0
Benzene, (2-bro...	13.876	297.6	ug/l	63956300	4	13.672	10747100	50.0
Benzene, 2-ethy...	14.217	146.3	ug/l	31439400	4	13.672	10747100	50.0
1-Methyl-2-phen...	14.278	20.3	ug/l	4367510	4	13.672	10747100	50.0
Benzene, 1-ethe...	14.327	83.2	ug/l	17880300	4	13.672	10747100	50.0
Benzene, 1,2,3,...	14.539	68.3	ug/l	14686400	4	13.672	10747100	50.0
Benzene, 2-ethe...	14.809	59.1	ug/l	12694500	4	13.672	10747100	50.0
Benzene, 1-ethe...	14.930	104.3	ug/l	22420200	4	13.672	10747100	50.0