

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
 Data File : VN085234.D
 Acq On : 17 Dec 2024 19:10
 Operator : JC\MD
 Sample : P5291-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW3-20241213

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M

Title : SW846 8260

Signal : TIC: VN085234.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.165	1046	1056	1060	rBV2	118573	273577	1.36%	0.274%
2	8.224	1060	1066	1077	rVB	229481	566687	2.82%	0.567%
3	8.577	1117	1126	1138	rBV	127129	288488	1.43%	0.289%
4	8.741	1141	1154	1169	rBV10	47662	211625	1.05%	0.212%
5	9.100	1205	1215	1229	rBV	347927	766929	3.81%	0.768%
6	10.565	1456	1464	1469	rBV	487698	893766	4.44%	0.895%
7	10.630	1469	1475	1484	rVB	1381178	2515145	12.50%	2.518%
8	11.865	1677	1685	1692	rBV	427561	763469	3.79%	0.764%
9	11.965	1693	1702	1711	rVV	6789180	11616201	57.72%	11.632%
10	12.071	1711	1720	1737	rVB	10345846	20124671	100.00%	20.151%
11	12.394	1763	1775	1785	rBV	6114442	10505474	52.20%	10.519%
12	12.694	1817	1826	1833	rBV	334484	540481	2.69%	0.541%
13	12.847	1845	1852	1861	rVB	362475	621880	3.09%	0.623%
14	13.035	1877	1884	1889	rBV	676832	1125908	5.59%	1.127%
15	13.094	1889	1894	1897	rVV	1941668	3178809	15.80%	3.183%
16	13.129	1897	1900	1903	rVV	1189746	1809711	8.99%	1.812%
17	13.171	1903	1907	1915	rVB	1416475	2221846	11.04%	2.225%
18	13.335	1927	1935	1945	rVB	1935799	3187906	15.84%	3.192%
19	13.482	1945	1960	1967	rBV	8859211	14415495	71.63%	14.435%
20	13.818	2006	2017	2033	rVB	2386803	4580327	22.76%	4.586%
21	13.947	2033	2039	2041	rBV	249911	367852	1.83%	0.368%
22	13.994	2041	2047	2062	rVB	2638803	5225910	25.97%	5.233%
23	14.176	2072	2078	2084	rBV2	480948	823917	4.09%	0.825%
24	14.241	2084	2089	2092	rVV	437496	753423	3.74%	0.754%
25	14.270	2092	2094	2099	rVV	393761	507797	2.52%	0.508%
26	14.329	2099	2104	2110	rVB	584541	898055	4.46%	0.899%
27	14.394	2110	2115	2118	rBV2	144141	228082	1.13%	0.228%
28	14.441	2118	2123	2131	rVB2	570112	1000872	4.97%	1.002%
29	14.570	2140	2145	2151	rVB2	148979	237974	1.18%	0.238%
30	14.653	2151	2159	2162	rBV	437929	751883	3.74%	0.753%
31	14.688	2162	2165	2170	rVB	569141	816105	4.06%	0.817%
32	14.923	2200	2205	2210	rBV	470713	775224	3.85%	0.776%
33	15.047	2217	2226	2232	rBV2	782008	1758247	8.74%	1.761%
34	15.117	2232	2238	2246	rVB2	129716	268321	1.33%	0.269%
35	15.206	2246	2253	2261	rBV3	184217	358673	1.78%	0.359%
36	15.317	2261	2272	2277	rBV4	190536	507688	2.52%	0.508%

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ClientSampleId :
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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

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Title : SW846 8260

37	15.441	2284	2293	2300	rVB3	144482	363768	1.81%	0.364%
38	15.635	2311	2326	2337	rBV	1778901	3509449	17.44%	3.514%
39	15.741	2337	2344	2350	rVV	137161	288025	1.43%	0.288%
40	16.776	2513	2520	2522	rBV2	128491	218555	1.09%	0.219%

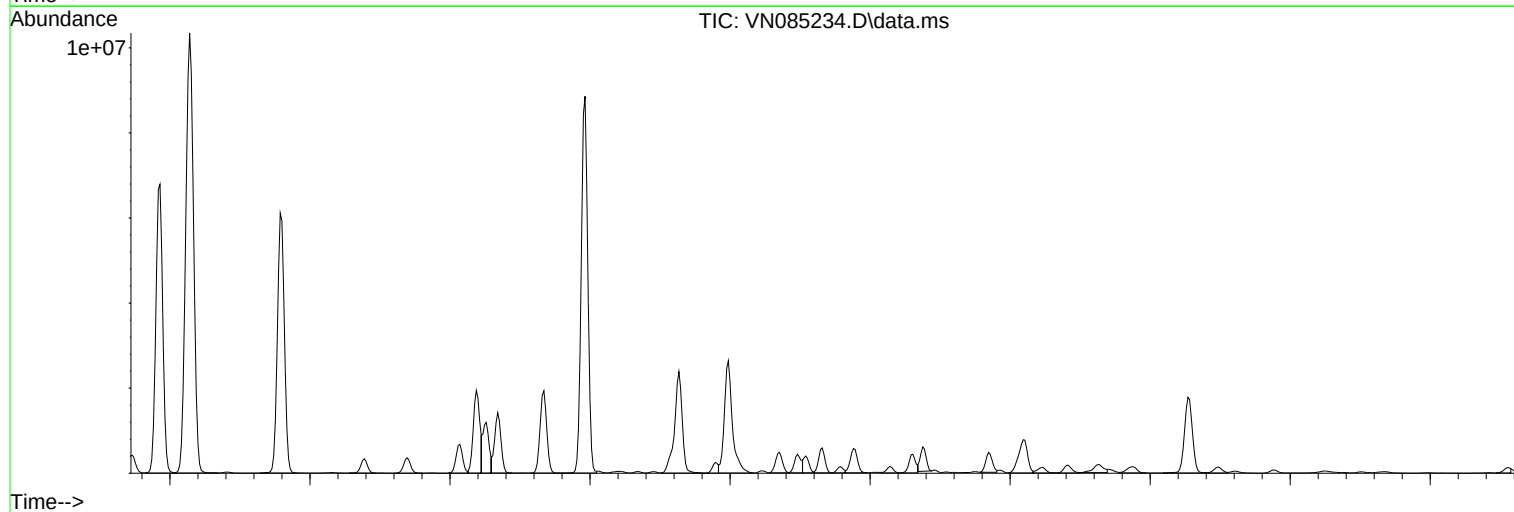
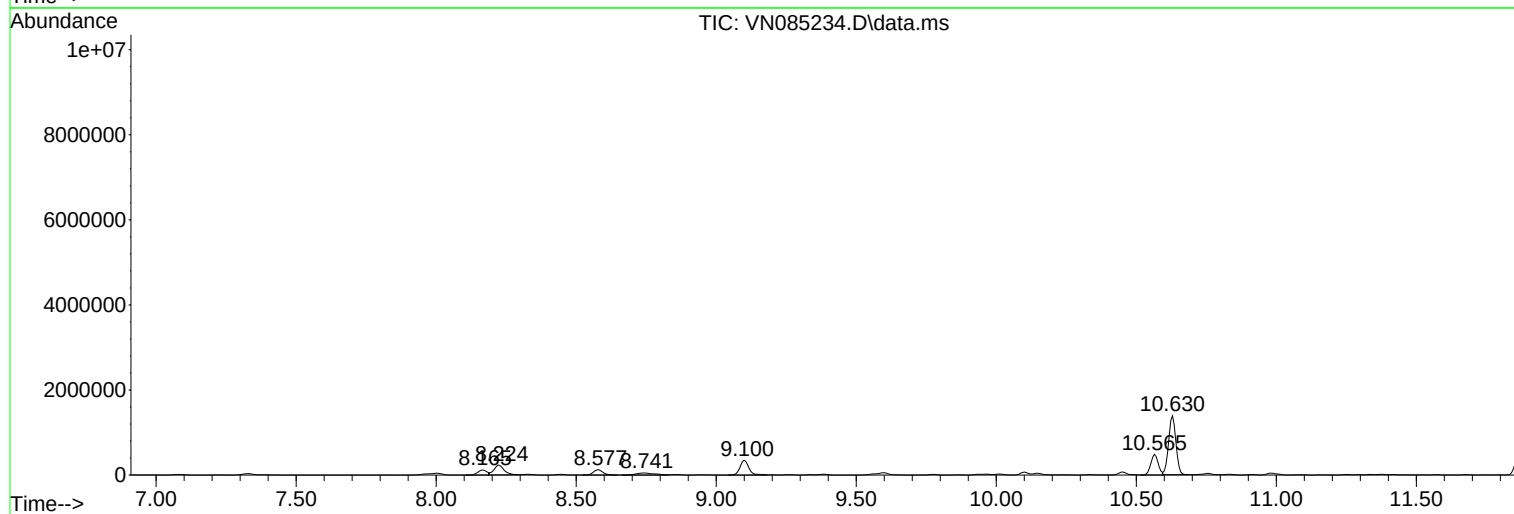
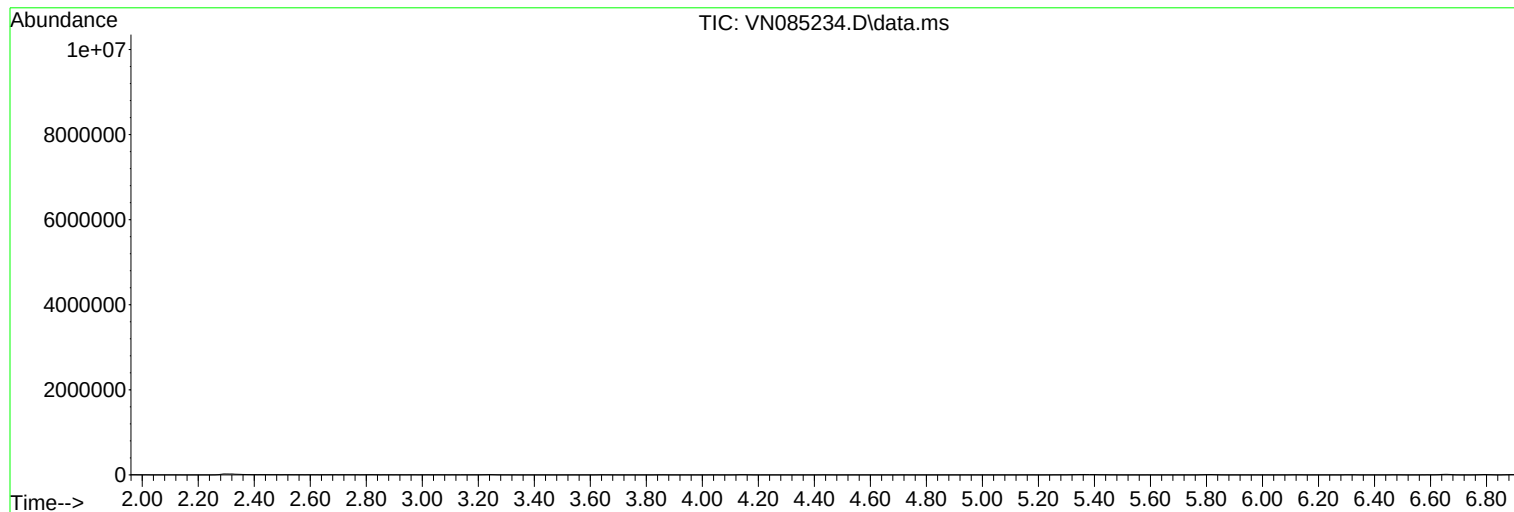
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_N
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MW3-20241213

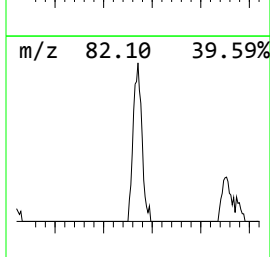
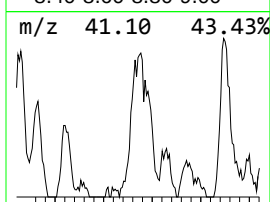
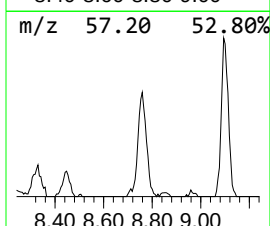
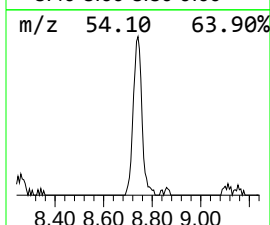
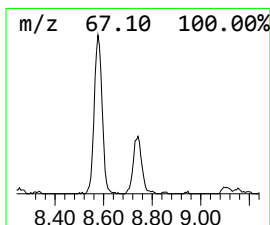
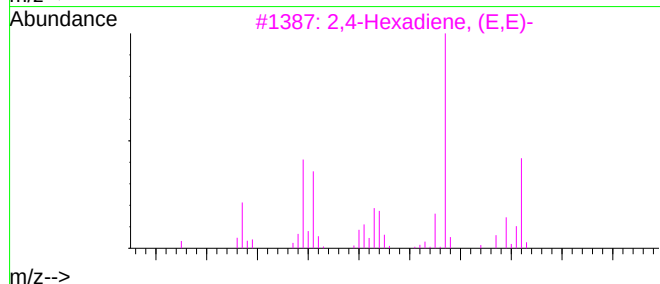
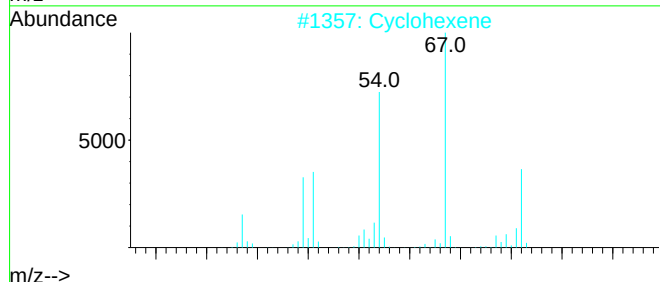
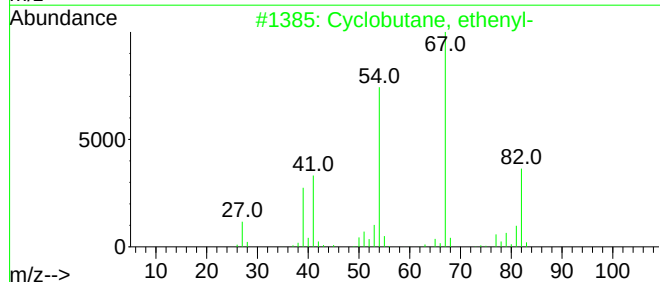
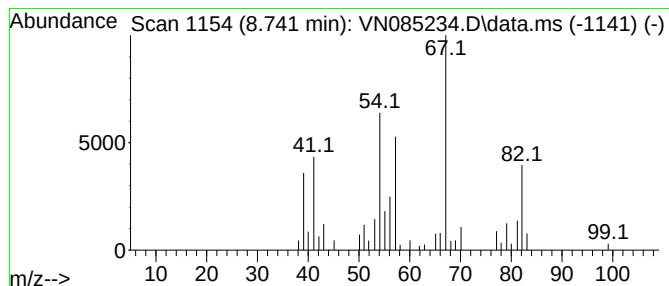
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclobutane, ethenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.741	13.80 ug/l	211625	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	68
2	Cyclohexene	82	C6H10	000110-83-8	64
3	2,4-Hexadiene, (E,E)-	82	C6H10	005194-51-4	60
4	1,3-Pentadiene, 2-methyl-, (E)-	82	C6H10	000926-54-5	60
5	1,3-Pentadiene, 2-methyl-	82	C6H10	001118-58-7	60



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3-20241213

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

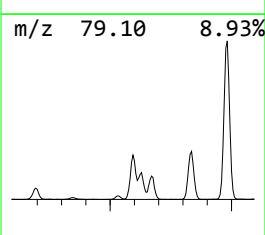
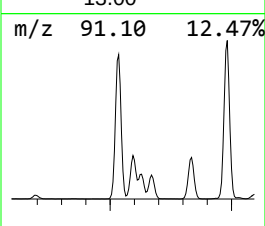
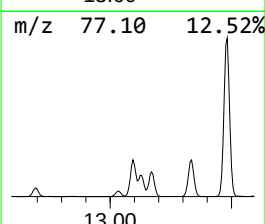
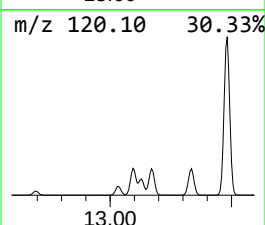
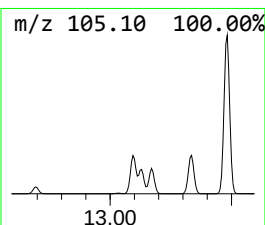
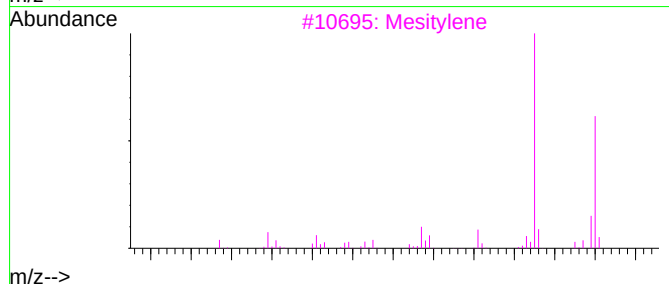
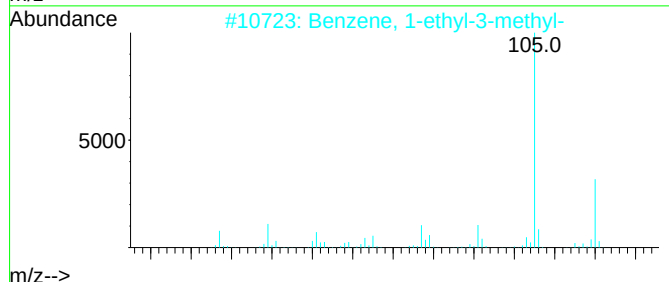
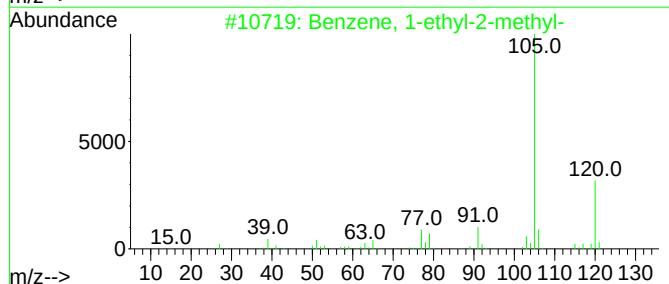
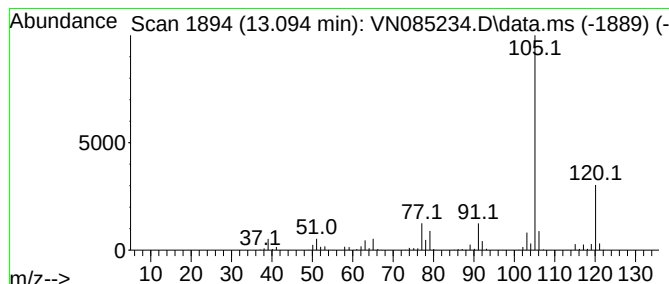
TIC Library : C:\Database\NIST20.L

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.
13.094	34.70 ug/l	3178810	1,4-Dichlorobenzene-d4	13.788

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-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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ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

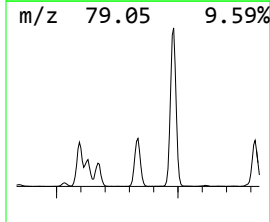
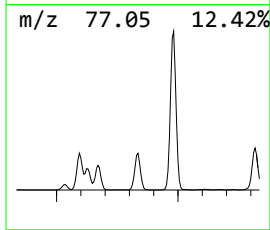
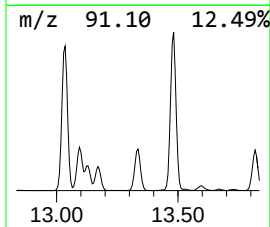
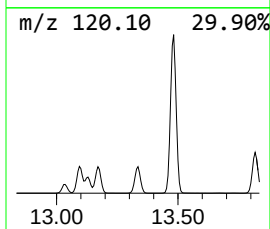
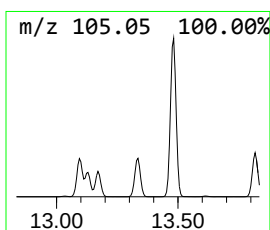
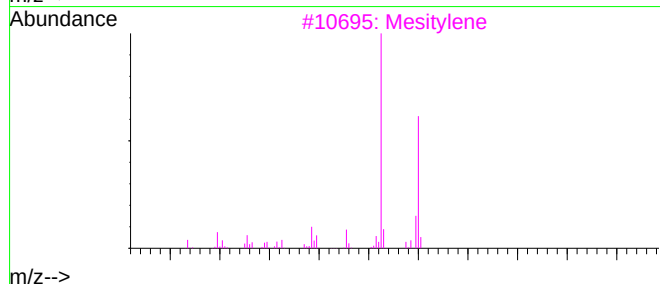
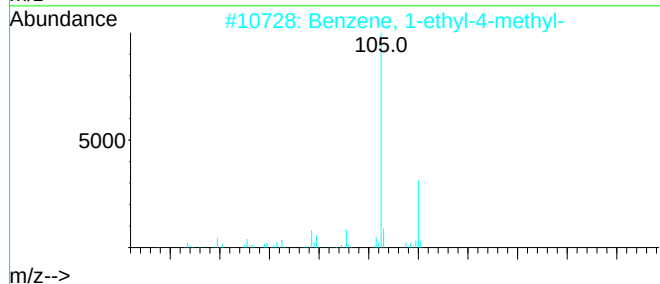
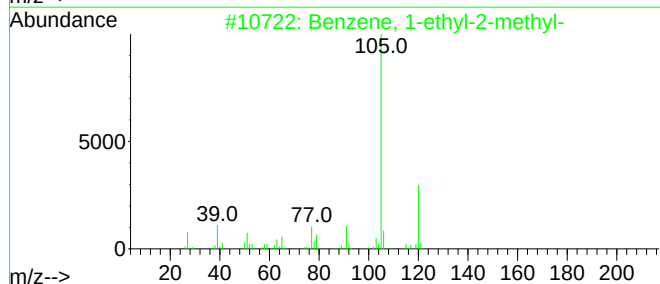
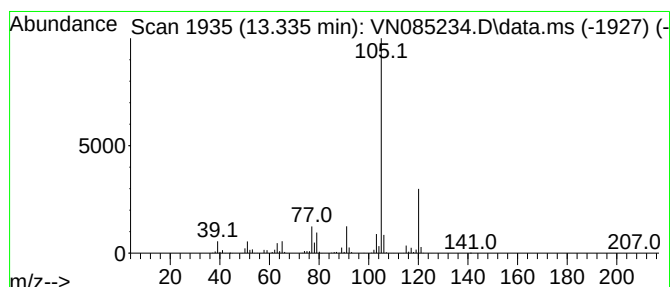
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	34.80 ug/l	3187910	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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Instrument :
MSVOA_N
ClientSampleId :
MW3-20241213

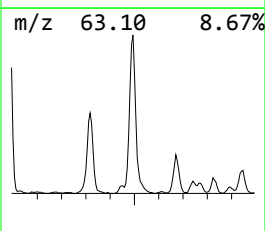
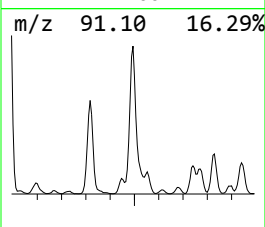
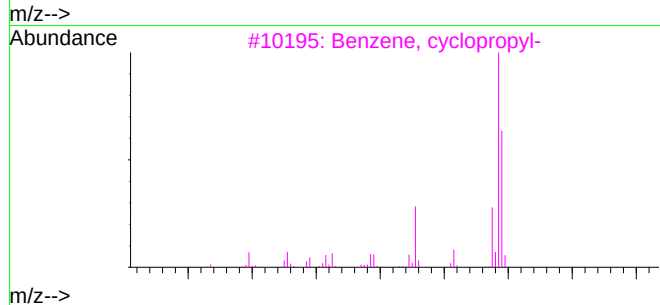
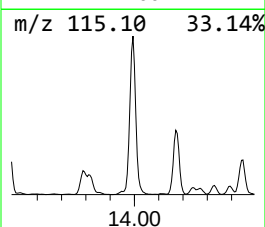
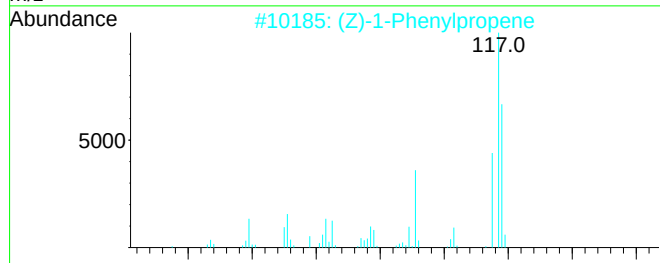
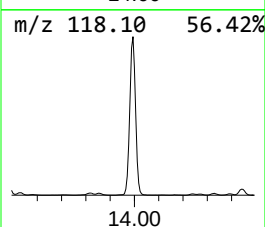
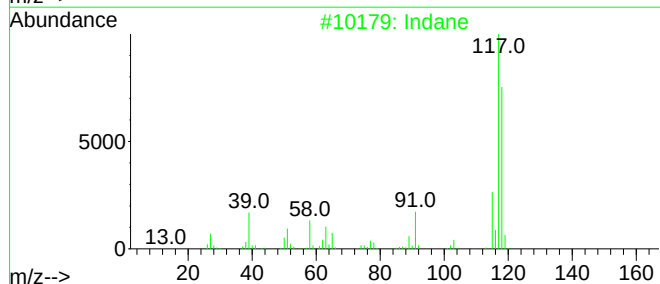
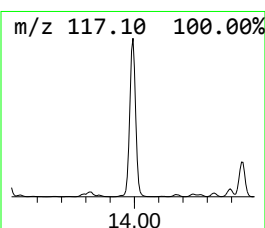
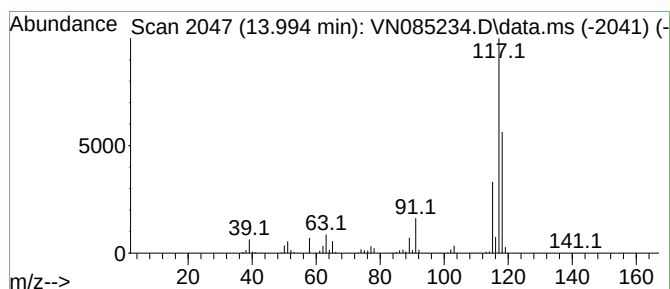
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

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

Peak Number 4 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	57.05 ug/l	5225910	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	72
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	59
4	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59



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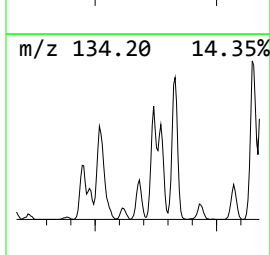
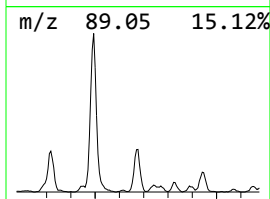
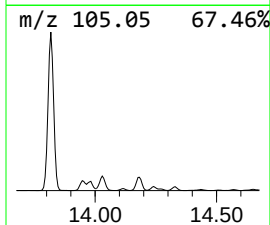
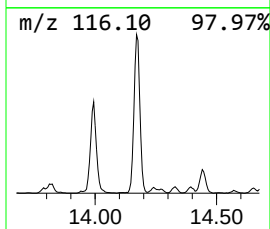
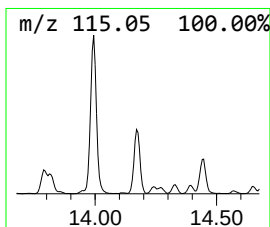
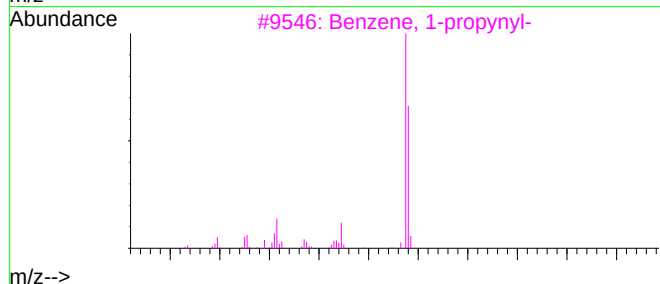
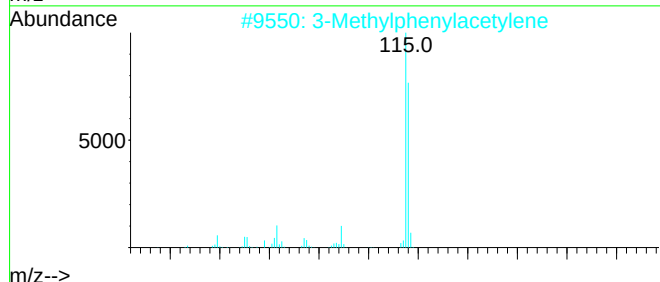
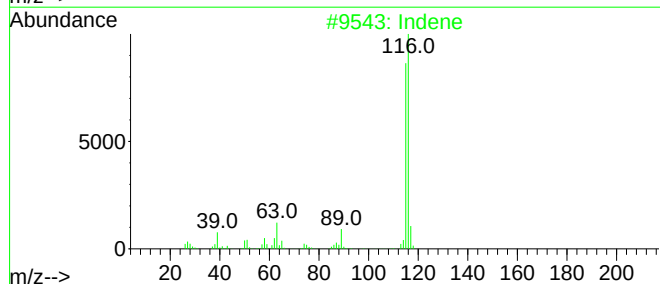
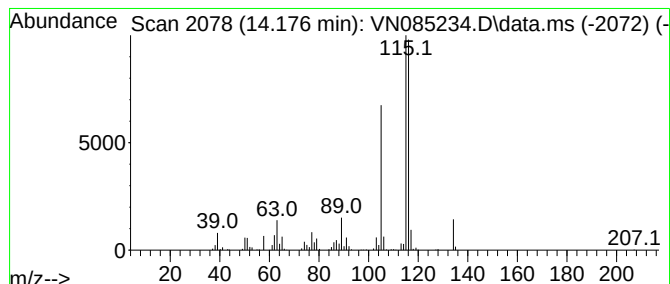
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Quant Title : SW846 8260

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

Peak Number 5 3-Methylphenylacetylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	8.99 ug/l	823917	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	91
2	3-Methylphenylacetylene	116	C9H8	000766-82-5	87
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	87
4	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	83
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085234.D
Acq On : 17 Dec 2024 19:10
Operator : JC\MD
Sample : P5291-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3-20241213

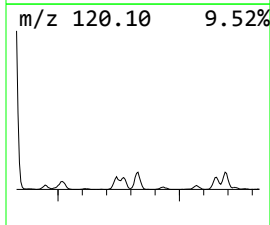
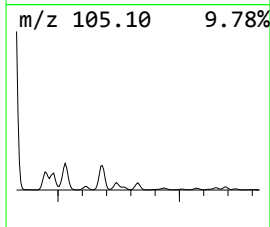
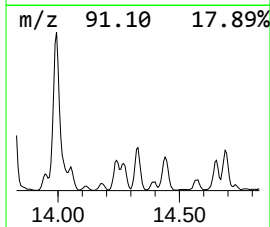
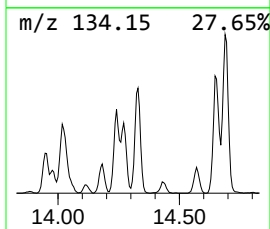
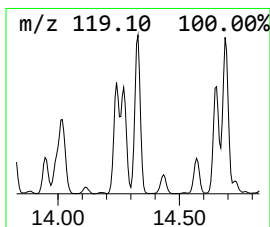
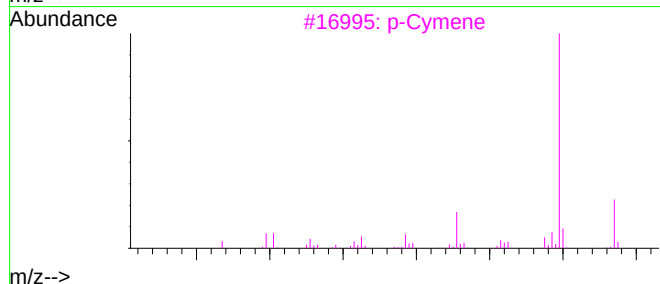
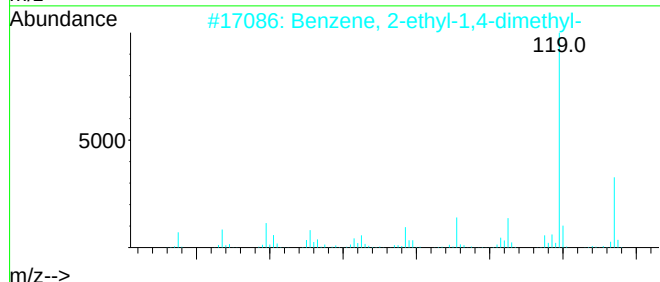
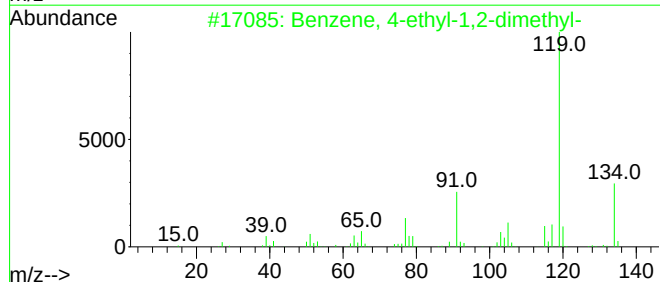
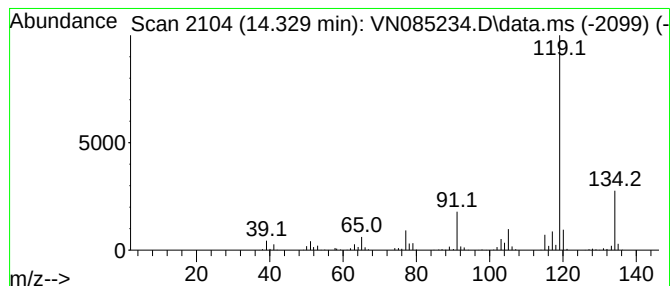
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.329	9.80 ug/l	898055	1,4-Dichlorobenzene-d4		13.788	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-		134	C10H14	000934-80-5	96
2	Benzene, 2-ethyl-1,4-dimethyl-		134	C10H14	001758-88-9	95
3	p-Cymene		134	C10H14	000099-87-6	95
4	o-Cymene		134	C10H14	000527-84-4	95
5	Benzene, 1-methyl-3-(1-methyleth...		134	C10H14	000535-77-3	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085234.D
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Operator : JC\MD
Sample : P5291-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3-20241213

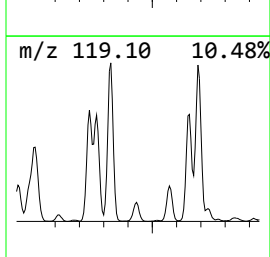
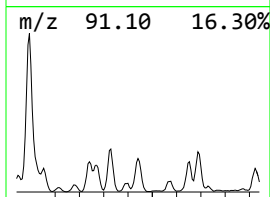
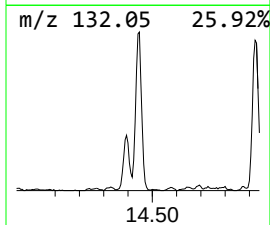
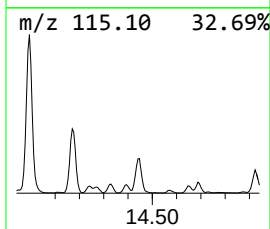
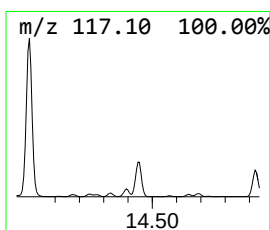
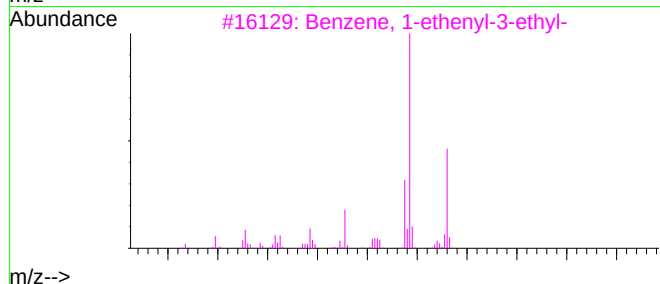
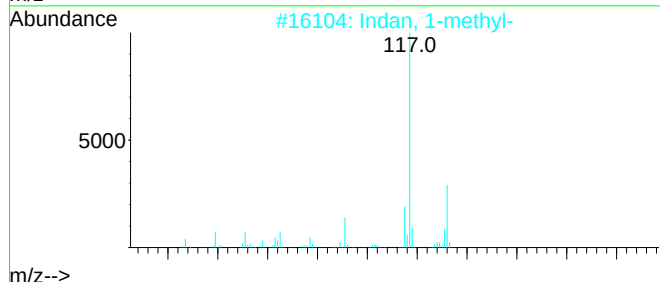
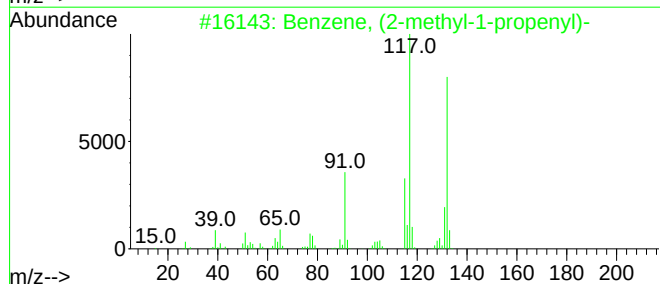
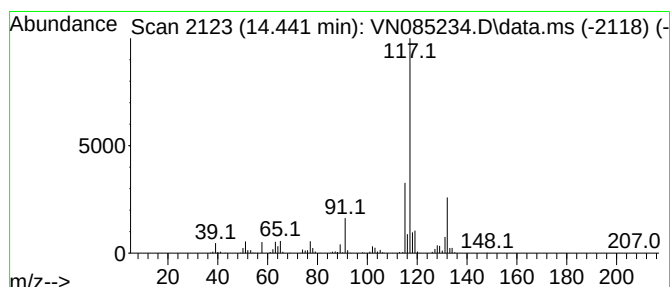
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, (2-methyl-1-propen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.441	10.93 ug/l	1000870	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
2	Indan, 1-methyl-	132	C10H12	000767-58-8	87
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	80
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085234.D
Acq On : 17 Dec 2024 19:10
Operator : JC\MD
Sample : P5291-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3-20241213

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

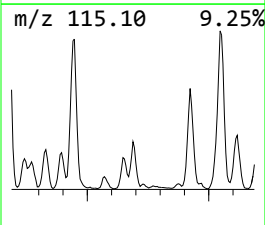
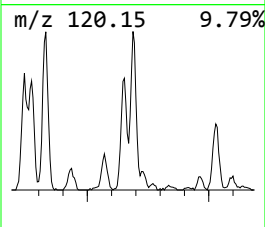
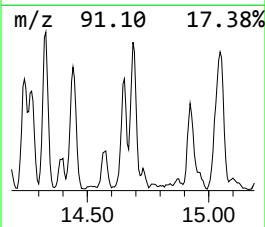
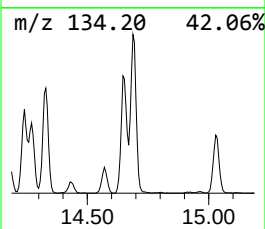
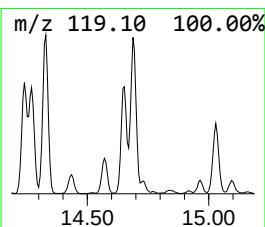
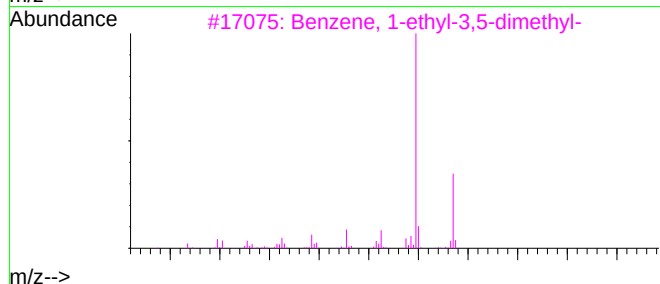
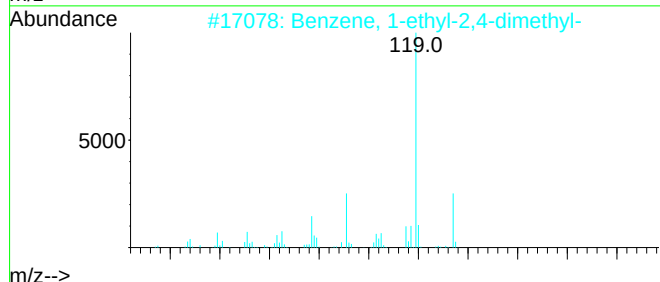
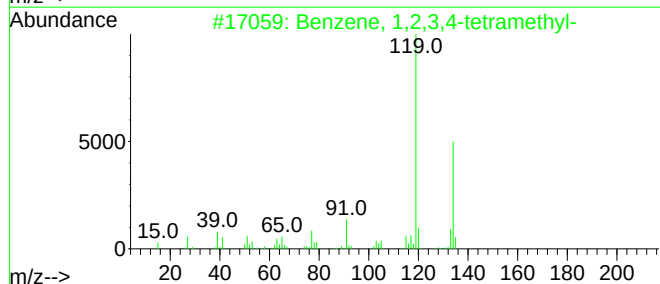
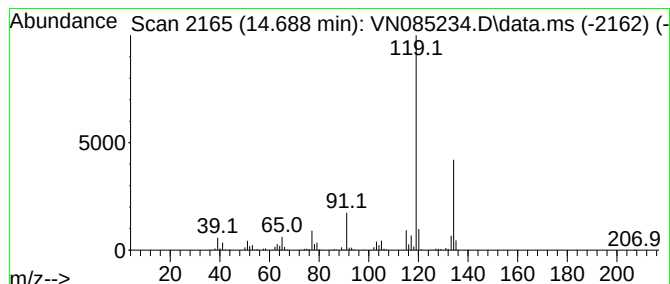
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.688	8.91 ug/l	816105	1,4-Dichlorobenzene-d4	13.788

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-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
3	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
5	o-Cymene	134	C10H14	000527-84-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085234.D
Acq On : 17 Dec 2024 19:10
Operator : JC\MD
Sample : P5291-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3-20241213

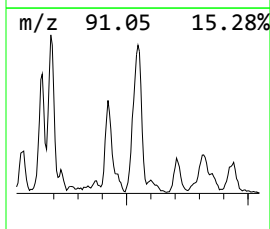
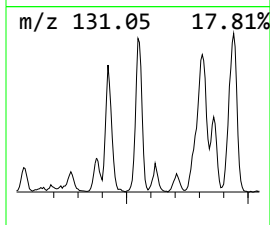
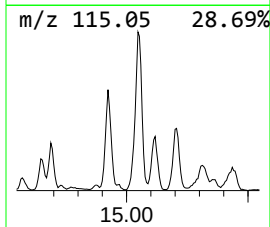
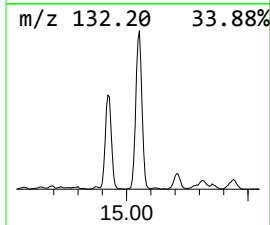
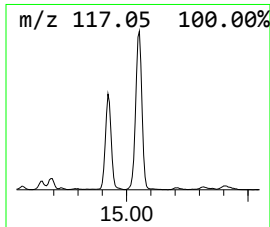
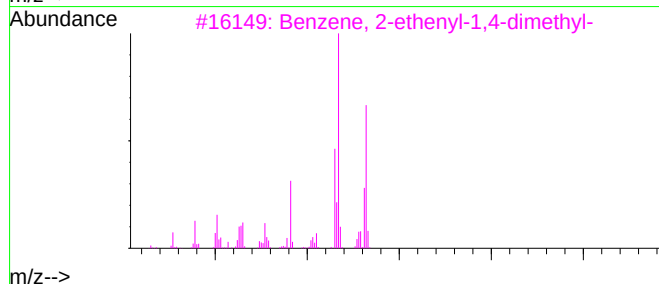
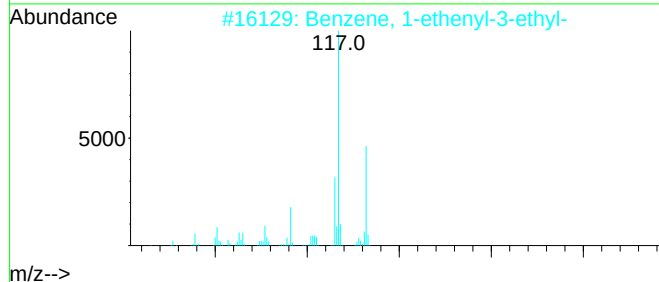
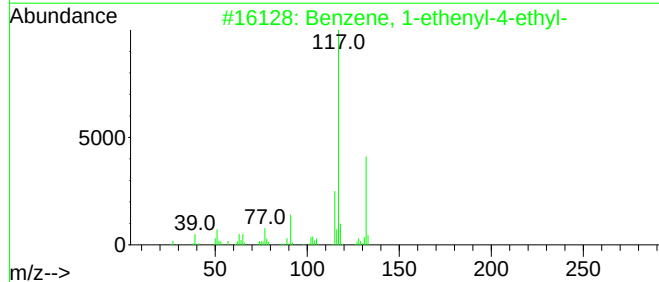
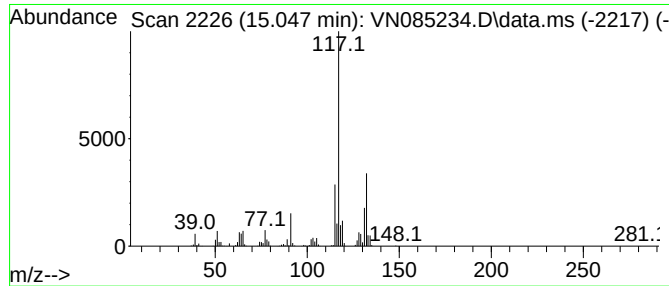
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	19.19 ug/l	1758250	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
4	Indan, 1-methyl-	132	C10H12	000767-58-8	90
5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085234.D
Acq On : 17 Dec 2024 19:10
Operator : JC\MD
Sample : P5291-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3-20241213

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclobutane, et...	8.741	13.8	ug/l	211625	2	9.100	766929	50.0
Benzene, 1-ethy...	13.094	34.7	ug/l	3178810	4	13.788	4580330	50.0
Benzene, 1-ethy...	13.335	34.8	ug/l	3187910	4	13.788	4580330	50.0
Indane	13.994	57.0	ug/l	5225910	4	13.788	4580330	50.0
3-Methylphenyla...	14.176	9.0	ug/l	823917	4	13.788	4580330	50.0
Benzene, 4-ethy...	14.329	9.8	ug/l	898055	4	13.788	4580330	50.0
Benzene, (2-met...	14.441	10.9	ug/l	1000870	4	13.788	4580330	50.0
Benzene, 1,2,3,...	14.688	8.9	ug/l	816105	4	13.788	4580330	50.0
Benzene, 1-ethe...	15.047	19.2	ug/l	1758250	4	13.788	4580330	50.0