

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
 Data File : VN080627.D
 Acq On : 02 Jan 2024 16:07
 Operator : JC\MD
 Sample : 06038-05 5X
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 T-803

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\82N122723W.M
 Title : SW846 8260

Signal : TIC: VN080627.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	rBV	219323	503153	2.53%	0.785%
2	8.224	1060	1066	1080	rVB	429283	986550	4.96%	1.539%
3	8.582	1117	1127	1141	rVB3	228280	701826	3.53%	1.095%
4	9.100	1204	1215	1227	rBV	666669	1350769	6.79%	2.107%
5	10.565	1455	1464	1473	rBV	843283	1589712	7.99%	2.480%
6	11.865	1677	1685	1694	rBV	1065100	1903459	9.57%	2.969%
7	11.965	1694	1702	1711	rVV	2062323	3424955	17.22%	5.342%
8	12.070	1712	1720	1731	rVB	612627	1167351	5.87%	1.821%
9	12.400	1765	1776	1786	rBV	306023	551755	2.77%	0.861%
10	12.694	1819	1826	1834	rBV	301672	507621	2.55%	0.792%
11	12.853	1846	1853	1862	rVB	744399	1299971	6.54%	2.028%
12	13.035	1878	1884	1889	rBV	128911	209527	1.05%	0.327%
13	13.100	1889	1895	1897	rVV	387188	611236	3.07%	0.953%
14	13.129	1897	1900	1904	rVV	415772	714118	3.59%	1.114%
15	13.176	1904	1908	1915	rVB	299317	499891	2.51%	0.780%
16	13.335	1928	1935	1942	rBV	317817	558809	2.81%	0.872%
17	13.482	1950	1960	1966	rBV	1238173	2024481	10.18%	3.158%
18	13.794	2007	2013	2021	rVV2	1240057	2706511	13.61%	4.221%
19	13.859	2021	2024	2032	rVB	304656	473721	2.38%	0.739%
20	13.953	2032	2040	2042	rBV	268351	452531	2.28%	0.706%
21	13.994	2042	2047	2061	rVV	4623512	8446743	42.48%	13.175%
22	14.329	2099	2104	2110	rBV	375295	594516	2.99%	0.927%
23	14.447	2113	2124	2133	rVV2	346111	741003	3.73%	1.156%
24	14.659	2150	2160	2163	rBV2	113734	256688	1.29%	0.400%
25	14.694	2163	2166	2170	rVV	191004	269148	1.35%	0.420%
26	14.929	2200	2206	2217	rVB	846132	1493145	7.51%	2.329%
27	15.053	2217	2227	2233	rBV2	580156	1265871	6.37%	1.974%
28	15.117	2233	2238	2246	rVB	371522	683889	3.44%	1.067%
29	15.206	2246	2253	2261	rVB2	820990	1514075	7.61%	2.362%
30	15.311	2262	2271	2279	rBV2	218773	493988	2.48%	0.770%
31	15.641	2319	2327	2338	rVB	10090353	19885514	100.00%	31.016%
32	15.747	2339	2345	2355	rVB2	118113	240229	1.21%	0.375%
33	16.147	2402	2413	2418	rBV2	115302	305060	1.53%	0.476%
34	16.276	2427	2435	2440	rBV3	102215	245034	1.23%	0.382%
35	16.782	2512	2521	2522	rBV2	3580413	5440275	27.36%	8.485%

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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\82N122723W.M
Title : SW846 8260

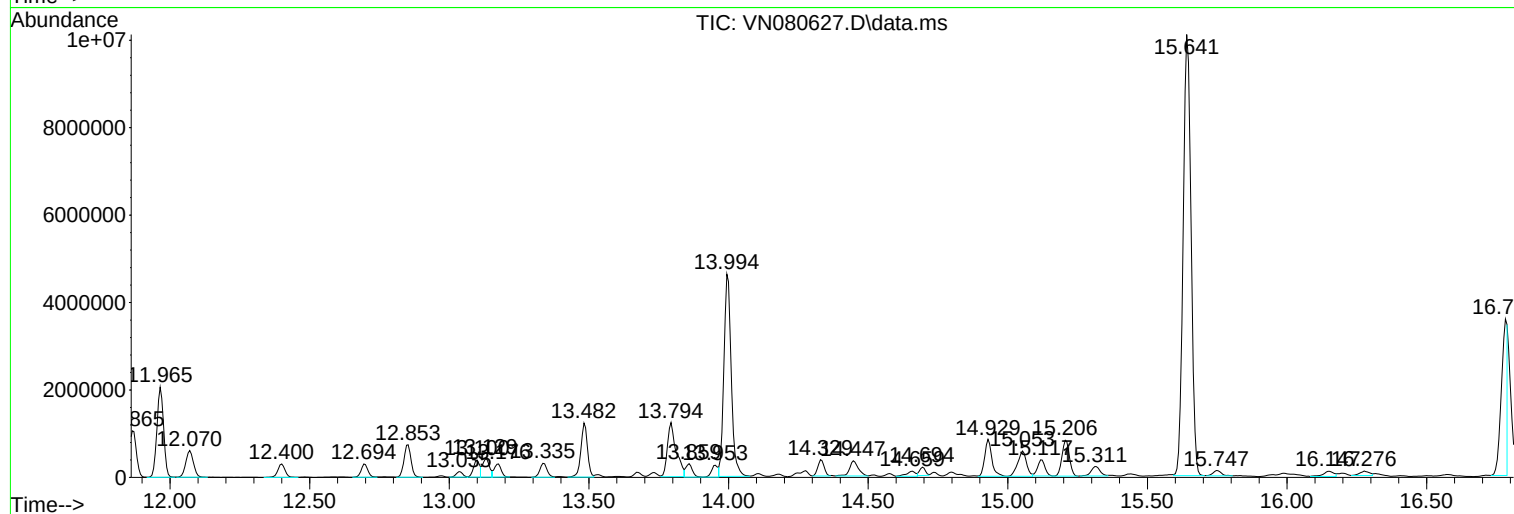
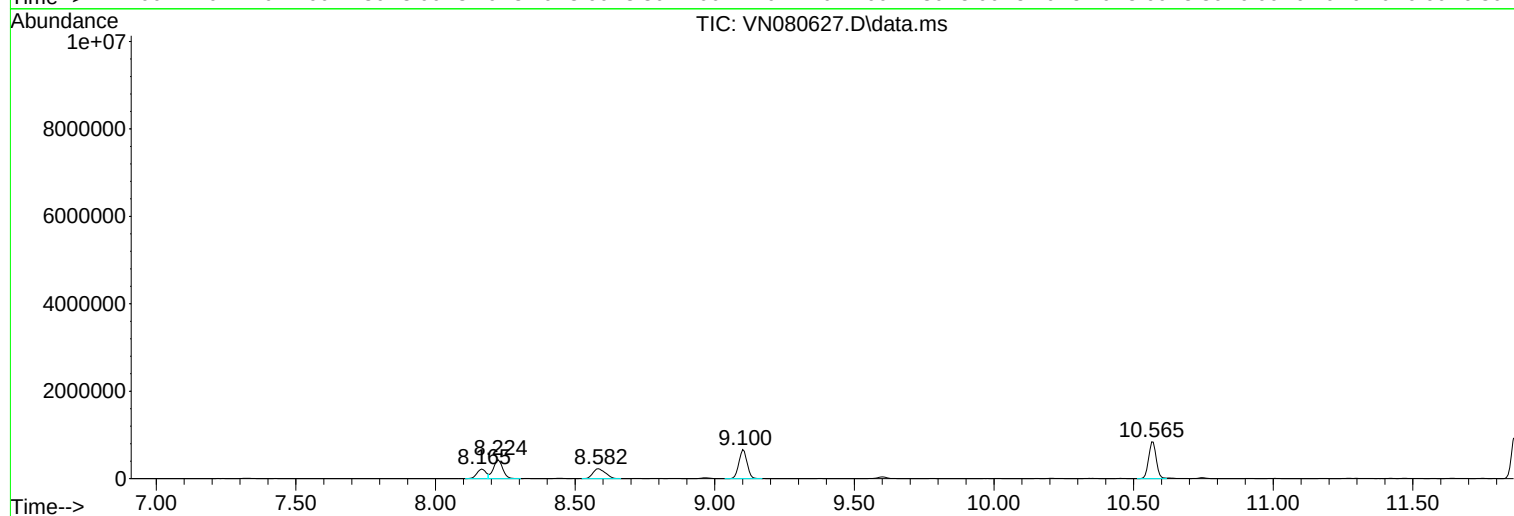
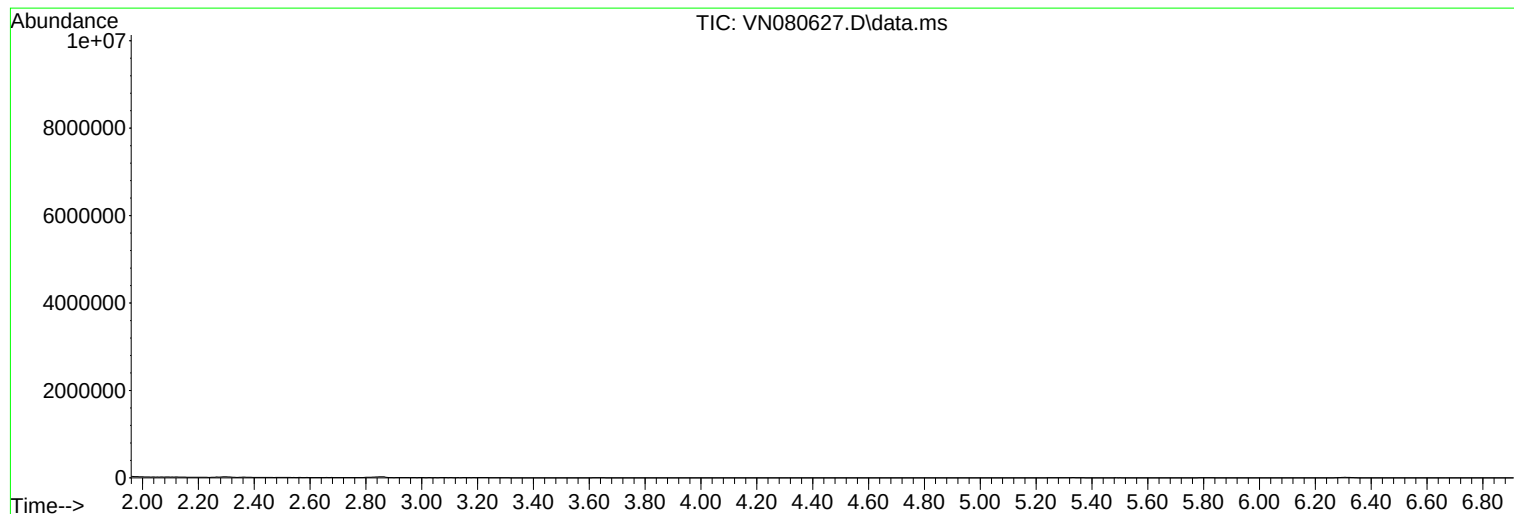
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_N
ClientSampleId :
T-803

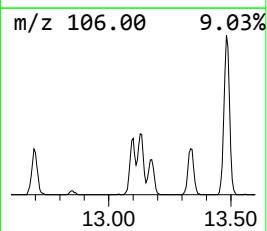
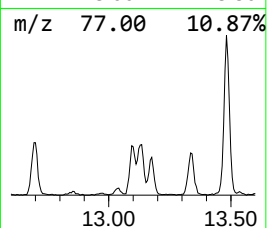
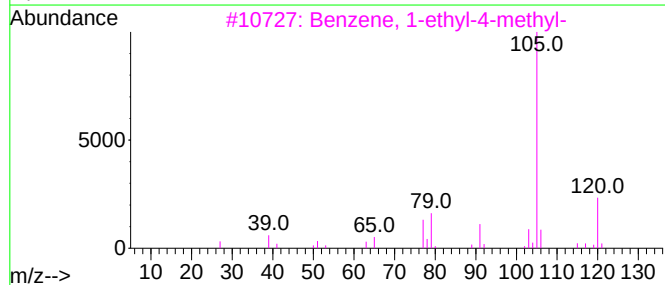
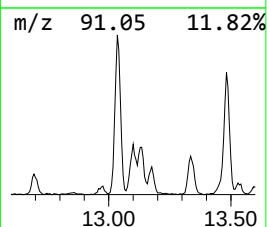
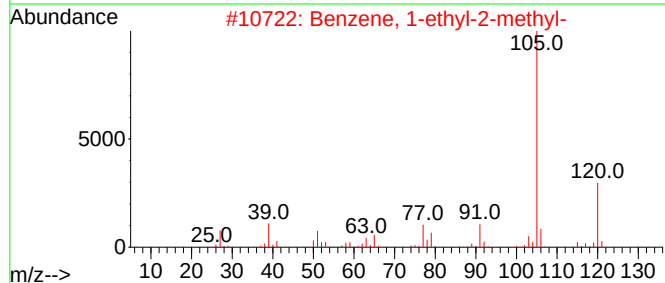
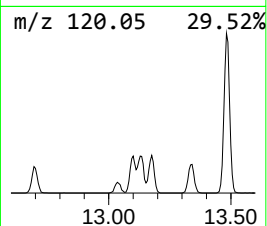
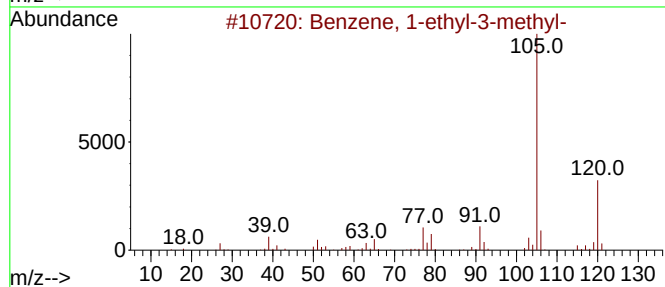
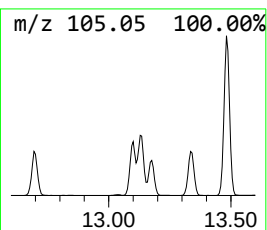
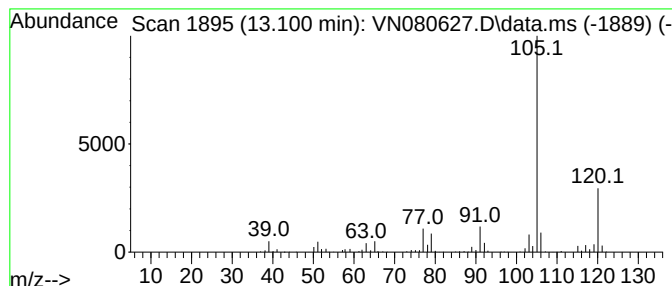
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	11.29 ug/l	611236	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	90



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Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-803

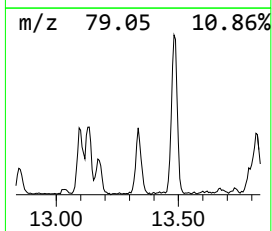
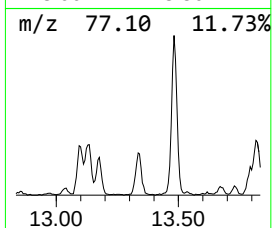
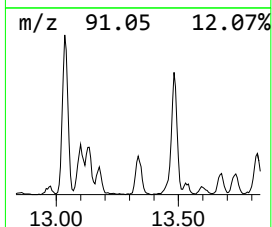
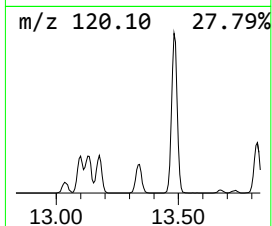
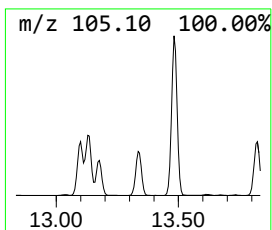
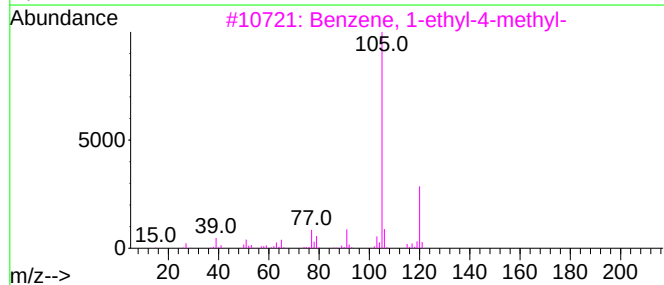
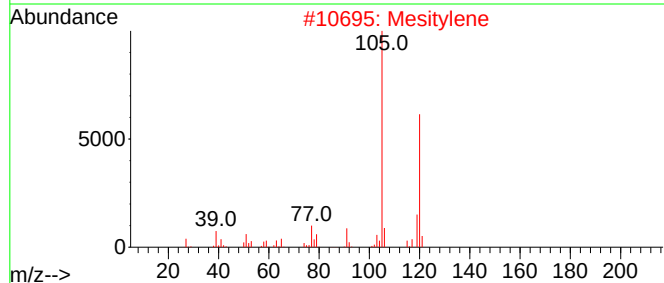
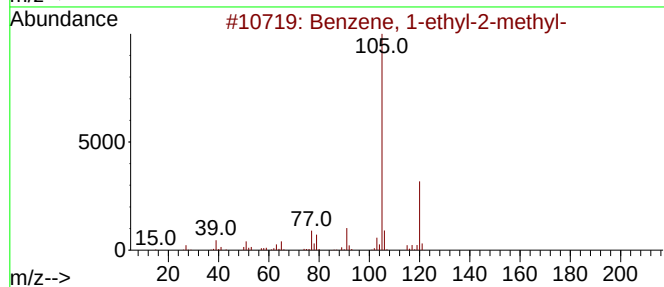
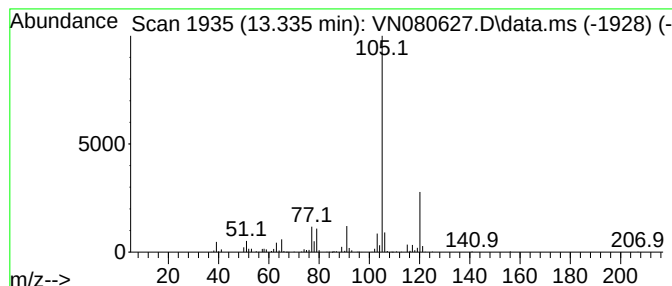
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	10.32 ug/l	558809	1,4-Dichlorobenzene-d4	13.794

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



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Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-803

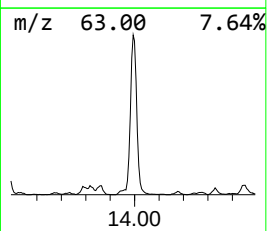
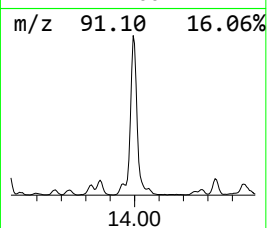
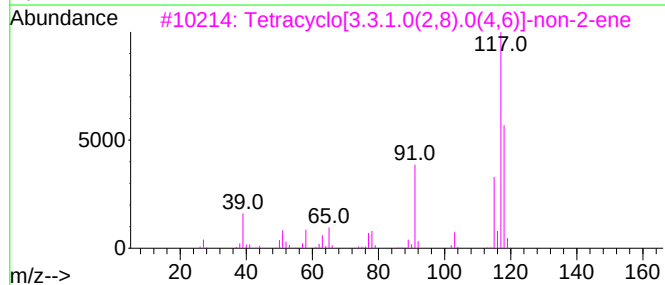
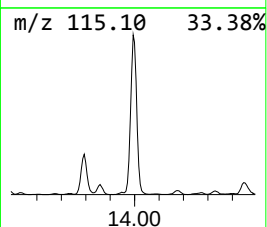
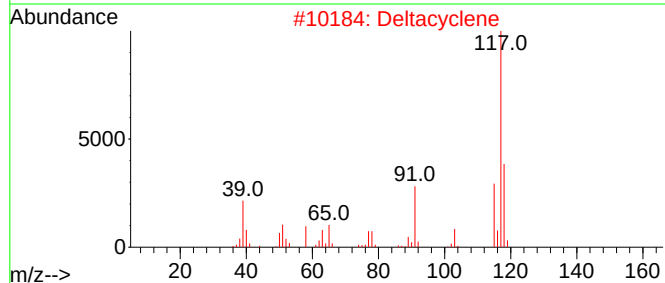
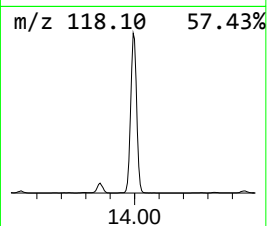
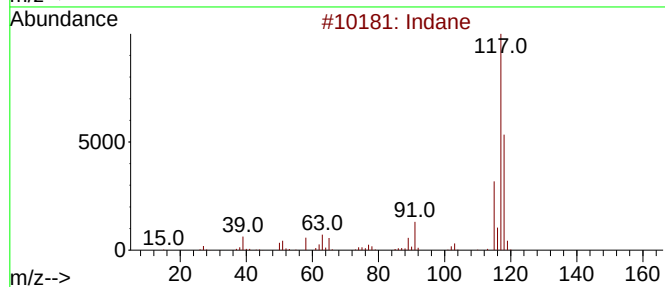
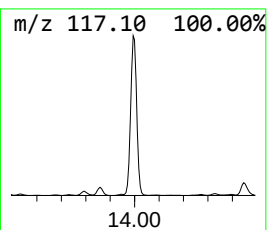
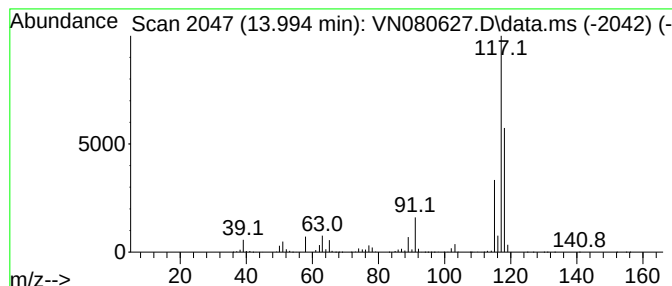
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

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

Peak Number 3 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	156.04 ug/l	8446740	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Deltacyclene	118	C9H10	007785-10-6	72
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	59
5			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-803

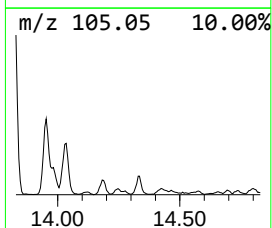
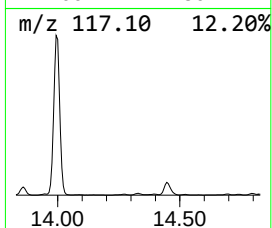
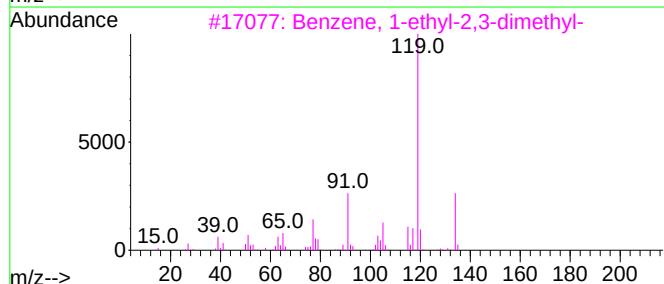
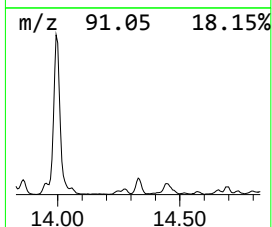
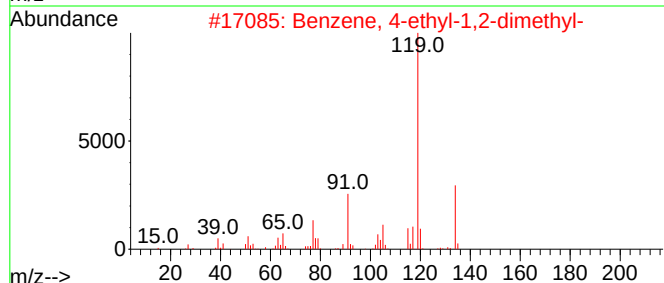
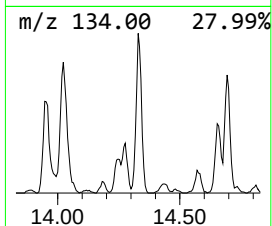
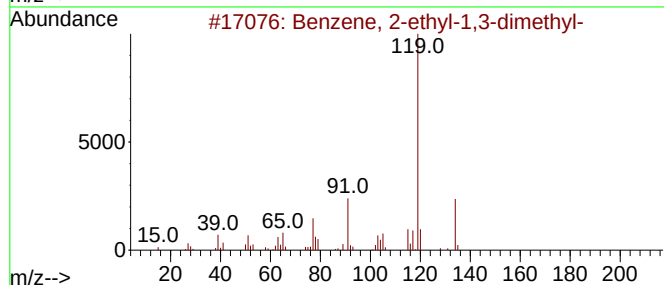
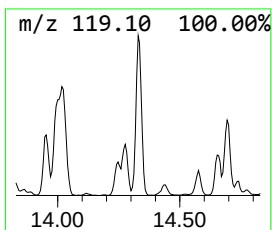
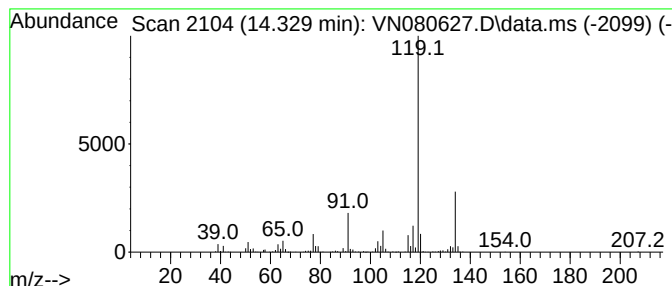
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 2-ethyl-1,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	10.98 ug/l	594516	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4			o-Cymene	134	C10H14	000527-84-4	94
5			p-Cymene	134	C10H14	000099-87-6	94



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-803

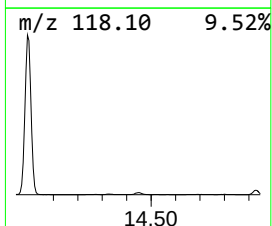
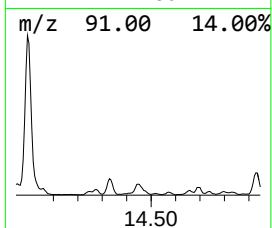
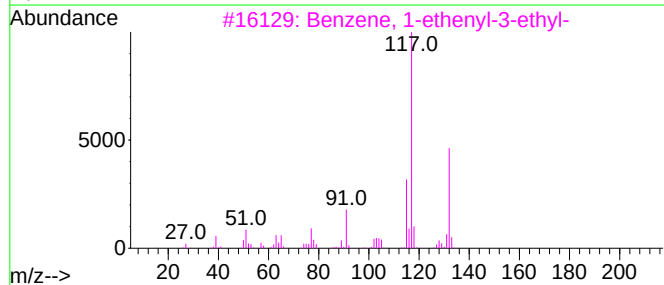
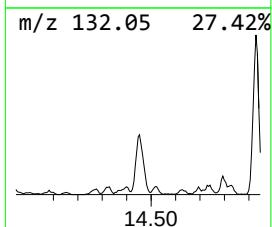
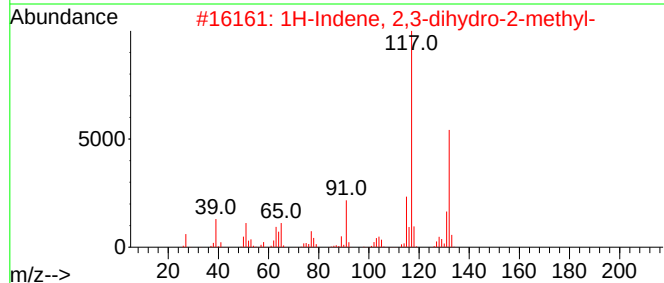
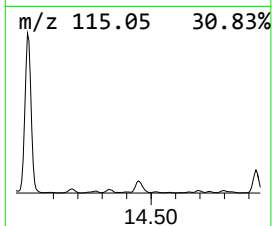
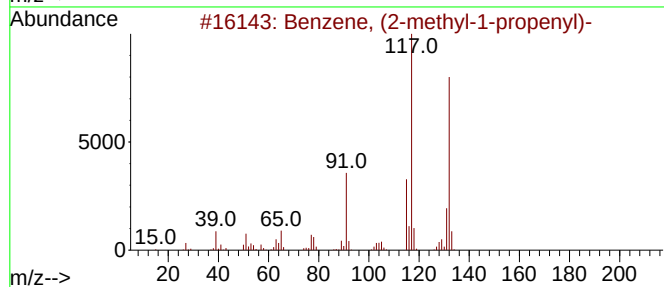
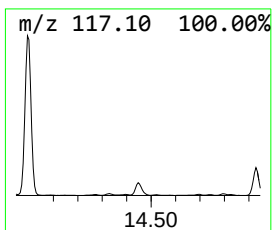
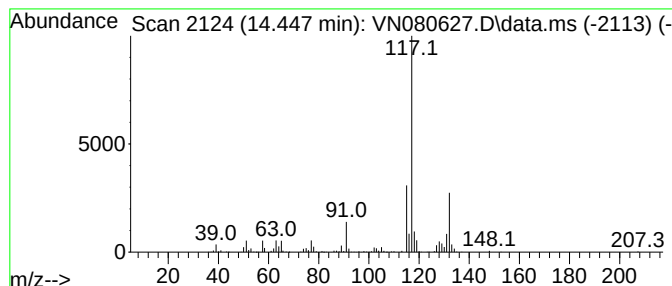
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, (2-methyl-1-propen... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	13.69 ug/l	741003	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
2			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	87
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
4			Indan, 1-methyl-	132	C10H12	000767-58-8	87
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080627.D
Acq On : 02 Jan 2024 16:07
Operator : JC\MD
Sample : 06038-05 5X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-803

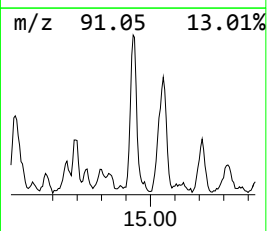
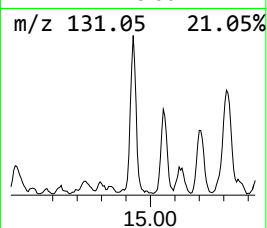
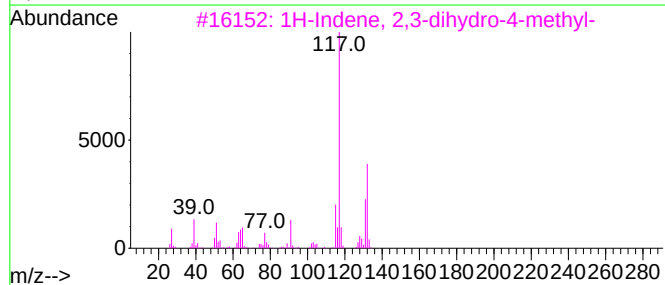
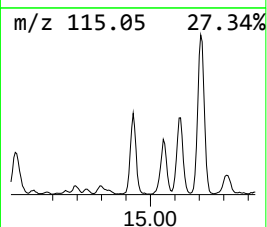
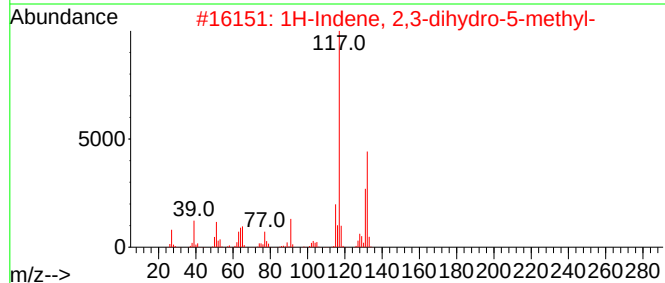
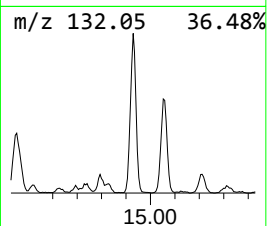
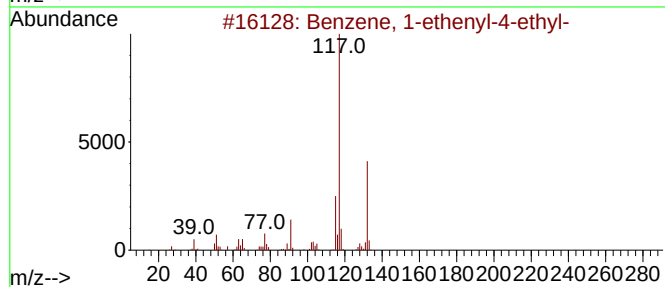
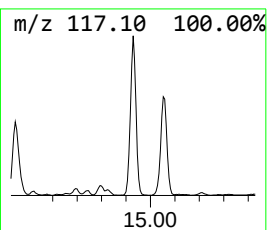
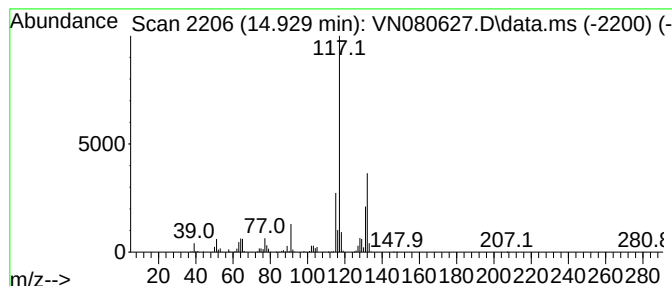
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	27.58 ug/l	1493150	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
3			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080627.D
Acq On : 02 Jan 2024 16:07
Operator : JC\MD
Sample : 06038-05 5X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-803

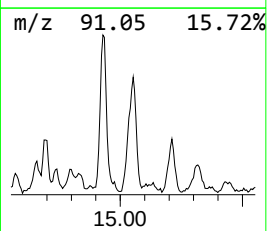
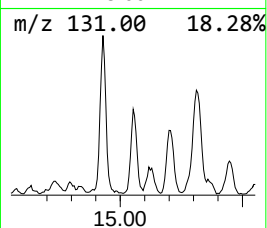
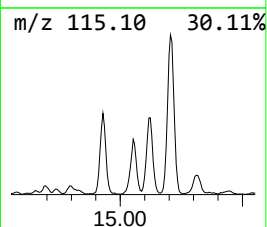
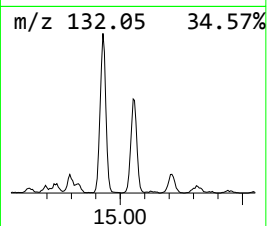
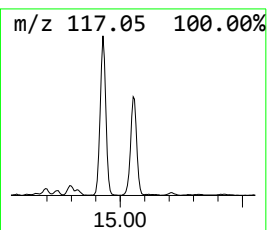
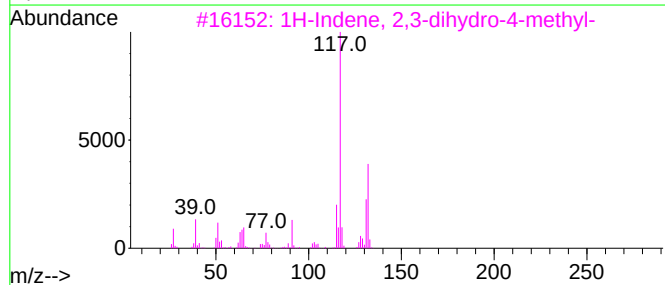
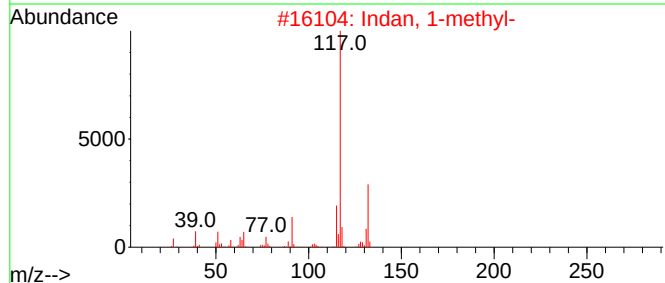
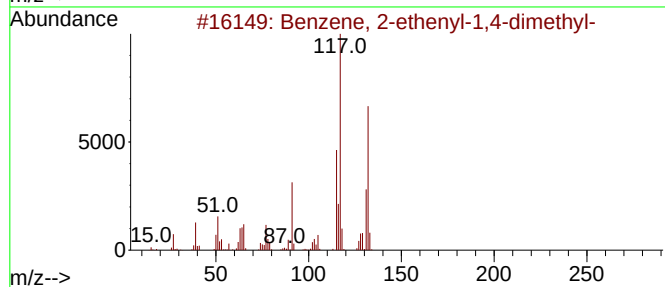
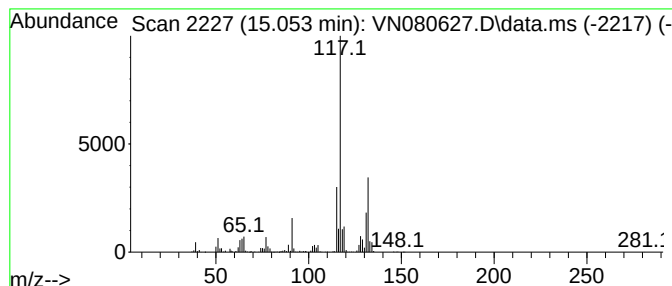
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	23.39 ug/l	1265870	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			Indan, 1-methyl-	132	C10H12	000767-58-8	93
3			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080627.D
Acq On : 02 Jan 2024 16:07
Operator : JC\MD
Sample : 06038-05 5X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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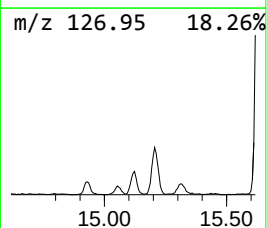
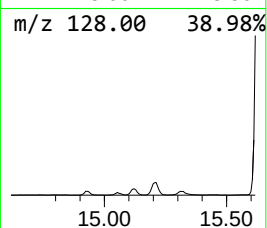
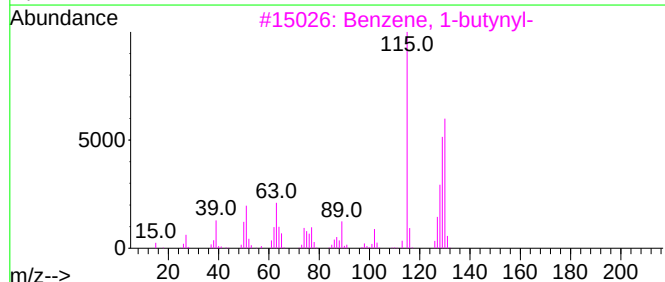
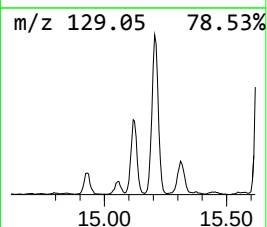
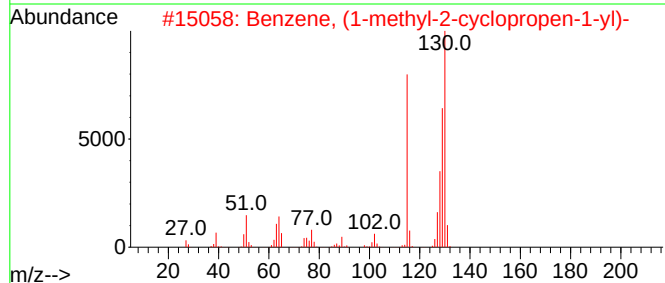
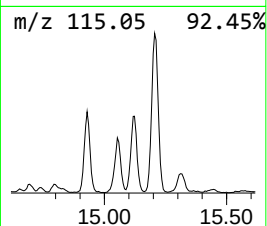
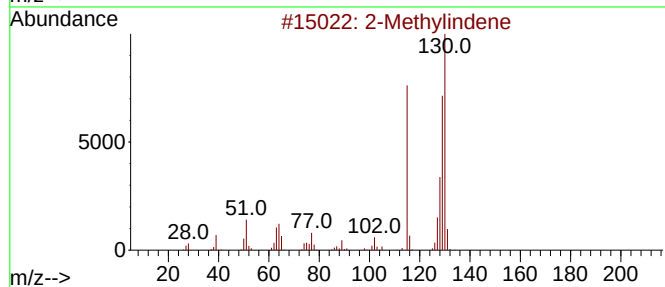
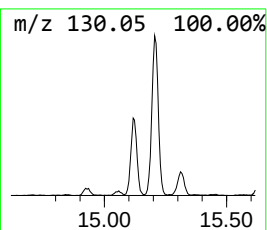
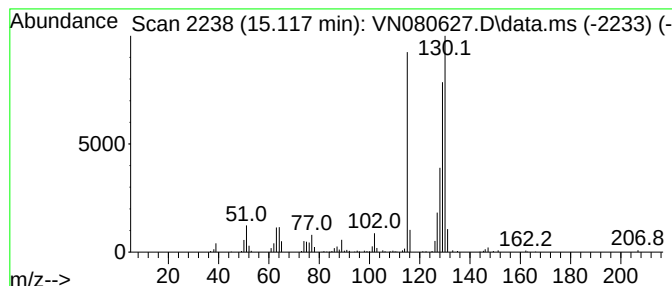
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Quant Title : SW846 8260

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

Peak Number 8 2-Methylindene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.117	12.63 ug/l	683889	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindene	130	C10H10	002177-47-1	97
2			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
3			Benzene, 1-butynyl-	130	C10H10	000622-76-4	94
4			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
5			1H-Indene, 3-methyl-	130	C10H10	000767-60-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080627.D
Acq On : 02 Jan 2024 16:07
Operator : JC\MD
Sample : 06038-05 5X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-803

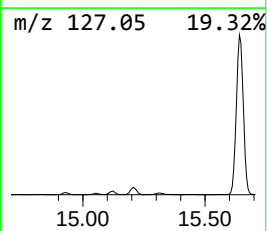
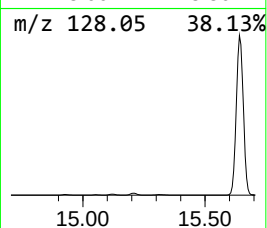
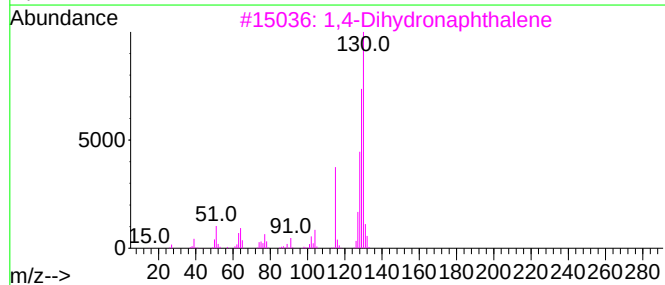
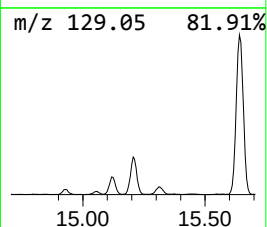
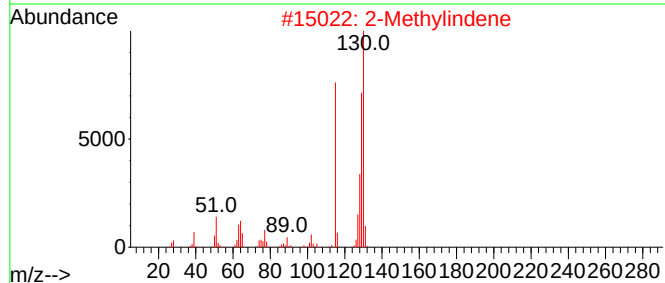
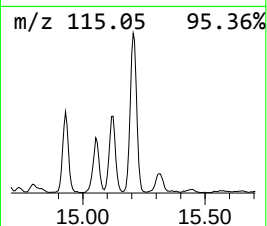
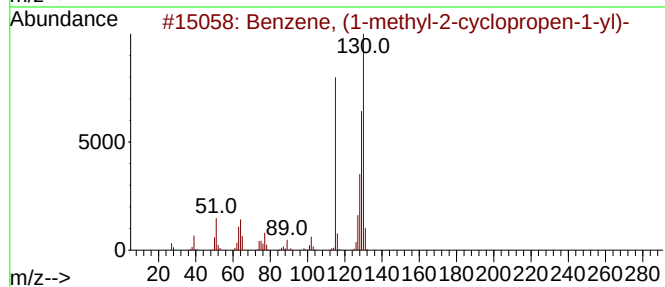
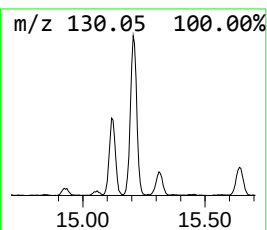
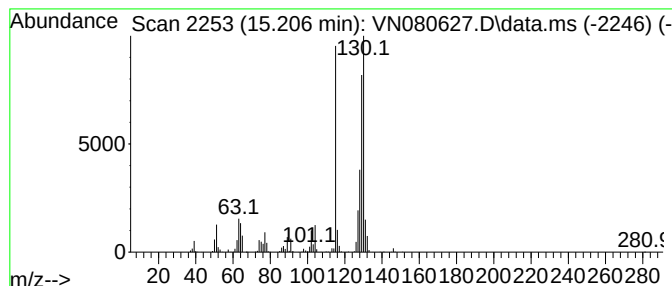
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, (1-methyl-2-cyclop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.206	27.97 ug/l	1514080	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
2			2-Methylindene	130	C10H10	002177-47-1	95
3			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	93
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93
5			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080627.D
Acq On : 02 Jan 2024 16:07
Operator : JC\MD
Sample : 06038-05 5X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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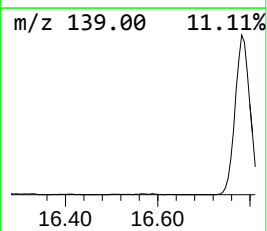
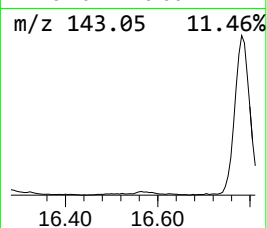
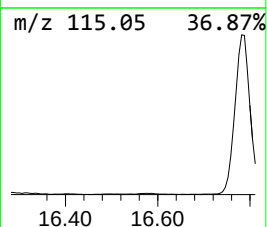
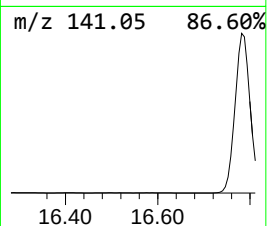
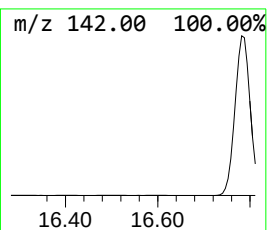
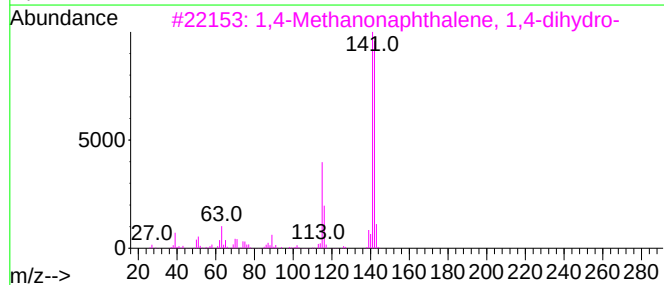
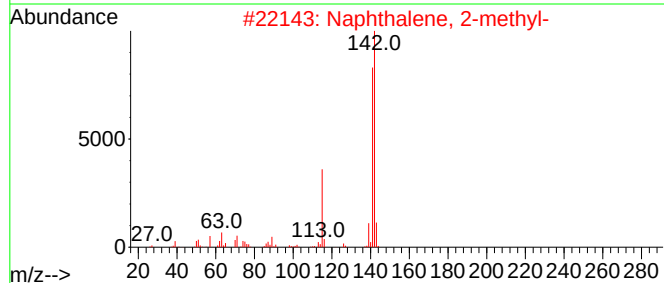
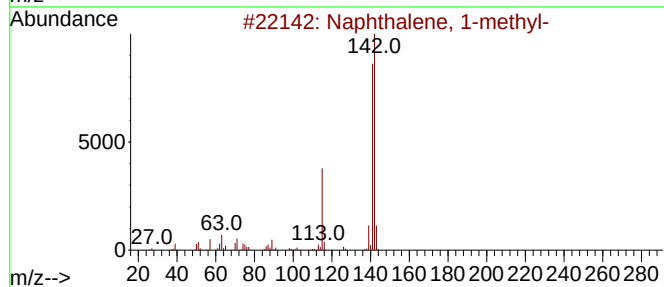
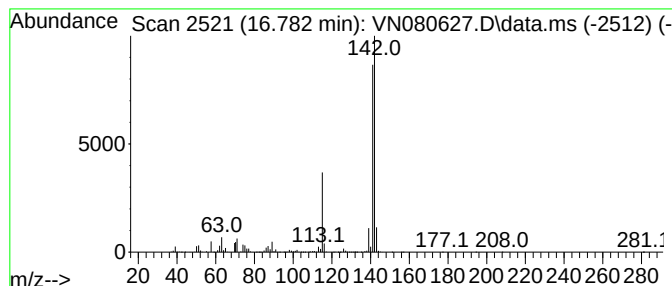
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	100.50 ug/l	5440280	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080627.D
Acq On : 02 Jan 2024 16:07
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Sample : 06038-05 5X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-803

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.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, 1-ethy...	13.335	10.3	ug/l	558809	4	13.794	2706510	50.0
Indane	13.994	156.0	ug/l	8446740	4	13.794	2706510	50.0
Benzene, 2-ethy...	14.329	11.0	ug/l	594516	4	13.794	2706510	50.0
Benzene, (2-met...	14.447	13.7	ug/l	741003	4	13.794	2706510	50.0
Benzene, 1-ethe...	14.929	27.6	ug/l	1493150	4	13.794	2706510	50.0
Benzene, 2-ethe...	15.053	23.4	ug/l	1265870	4	13.794	2706510	50.0
2-Methylindene	15.117	12.6	ug/l	683889	4	13.794	2706510	50.0
Benzene, (1-met...	15.206	28.0	ug/l	1514080	4	13.794	2706510	50.0
Naphthalene, 1-...	16.782	100.5	ug/l	5440280	4	13.794	2706510	50.0