

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
 Data File : VN074961.D
 Acq On : 21 Oct 2022 14:59
 Operator : JC\MD
 Sample : N5222-07
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-3

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\82N102022W.M
 Title : SW846 8260

Signal : TIC: VN074961.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.588	1102	1111	1126	rBV4	1145410	3745049	1.38%	0.299%
2	9.106	1188	1199	1206	rBV	1686325	3778079	1.40%	0.301%
3	10.571	1439	1448	1452	rBV	3851026	7010294	2.59%	0.559%
4	10.635	1452	1459	1472	rVB	16250014	29761154	11.00%	2.374%
5	11.865	1661	1668	1676	rBV	2261437	4118405	1.52%	0.329%
6	11.965	1676	1685	1694	rVV3	61956455	110787802	40.94%	8.837%
7	12.076	1694	1704	1720	rVB4	130589979	270599177	100.00%	21.585%
8	12.400	1751	1759	1770	rVB	11493965	19131053	7.07%	1.526%
9	12.700	1802	1810	1817	rVB	4073734	6847397	2.53%	0.546%
10	12.853	1828	1836	1846	rBV	3344518	5699408	2.11%	0.455%
11	13.035	1860	1867	1872	rBV	8877723	14646549	5.41%	1.168%
12	13.100	1872	1878	1881	rVV	30284103	50982296	18.84%	4.067%
13	13.129	1881	1883	1887	rVV	24066097	36358726	13.44%	2.900%
14	13.176	1887	1891	1899	rVB	26727615	41720181	15.42%	3.328%
15	13.341	1911	1919	1928	rBV	23791079	40020197	14.79%	3.192%
16	13.482	1930	1943	1951	rBV2	122635319	214945881	79.43%	17.146%
17	13.823	1990	2001	2017	rVB2	43047382	77785005	28.75%	6.205%
18	13.953	2017	2023	2025	rBV	3731975	5670190	2.10%	0.452%
19	13.994	2025	2030	2046	rVB3	41101854	82534470	30.50%	6.584%
20	14.176	2055	2061	2067	rBV2	7163007	12530952	4.63%	1.000%
21	14.247	2067	2073	2075	rVV	6662769	10561235	3.90%	0.842%
22	14.276	2075	2078	2082	rVV	5718112	8433778	3.12%	0.673%
23	14.329	2082	2087	2093	rVB	9577447	14993771	5.54%	1.196%
24	14.400	2093	2099	2102	rBV	2267723	3737173	1.38%	0.298%
25	14.447	2102	2107	2116	rVB2	9380112	15642489	5.78%	1.248%
26	14.576	2123	2129	2135	rVB	2807519	4574430	1.69%	0.365%
27	14.653	2135	2142	2145	rBV	6361667	10405255	3.85%	0.830%
28	14.694	2145	2149	2154	rVB	8842125	13361505	4.94%	1.066%
29	14.929	2183	2189	2194	rBV	7958125	13204140	4.88%	1.053%
30	15.053	2201	2210	2216	rBV2	13585502	28657708	10.59%	2.286%
31	15.117	2216	2221	2229	rVB2	1891702	3630917	1.34%	0.290%
32	15.212	2229	2237	2244	rBV2	3115343	5834928	2.16%	0.465%
33	15.317	2244	2255	2261	rBV3	2201889	5871703	2.17%	0.468%
34	15.441	2268	2276	2285	rVB3	1647351	4087368	1.51%	0.326%
35	15.641	2296	2310	2321	rVB2	30778442	61651520	22.78%	4.918%
36	15.747	2321	2328	2334	rBV	1997890	3883820	1.44%	0.310%

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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\82N102022W.M
Title : SW846 8260

37	16.782	2496	2504	2505	rBV	4265006	6433887	2.38%	0.513%
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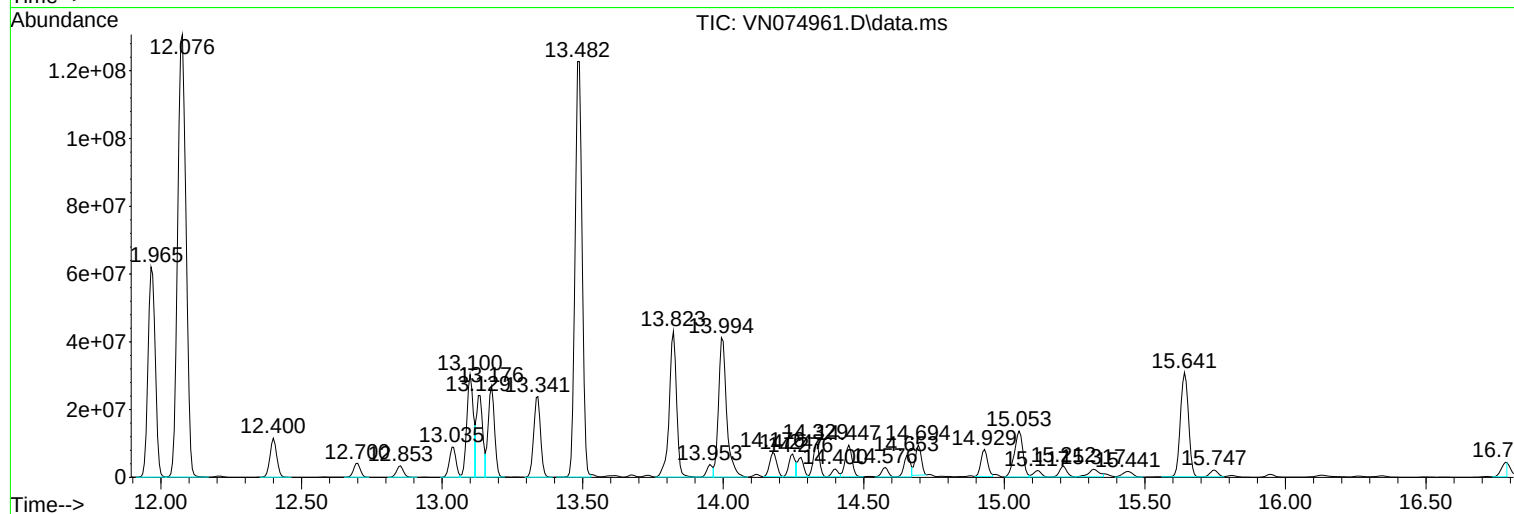
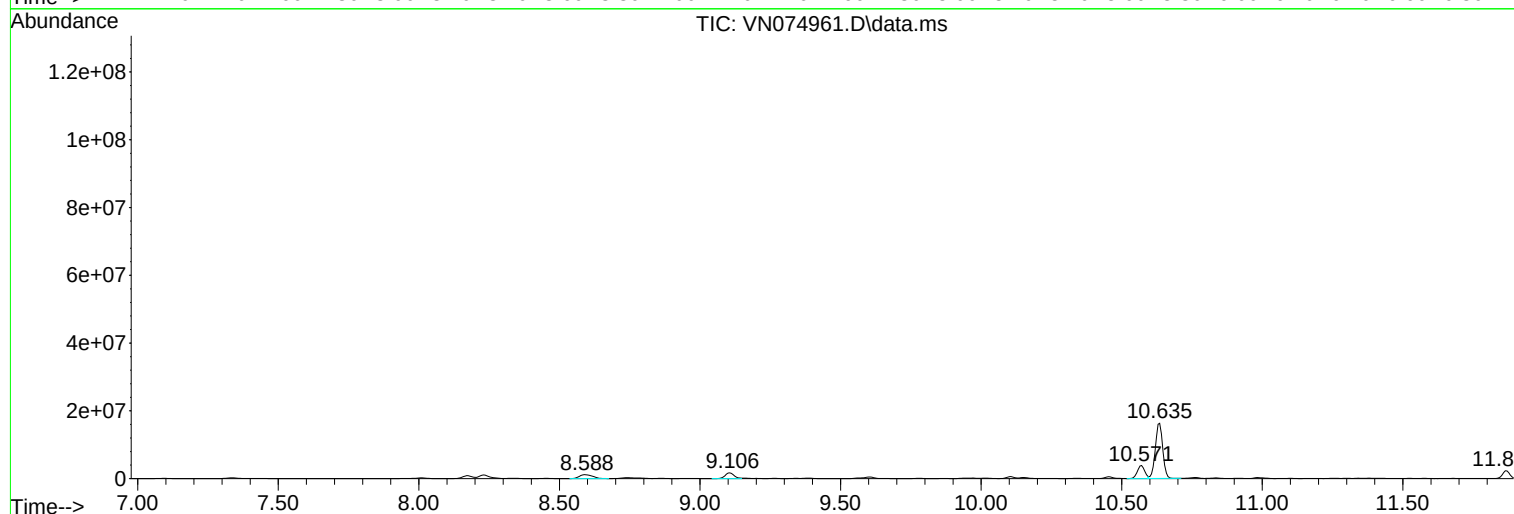
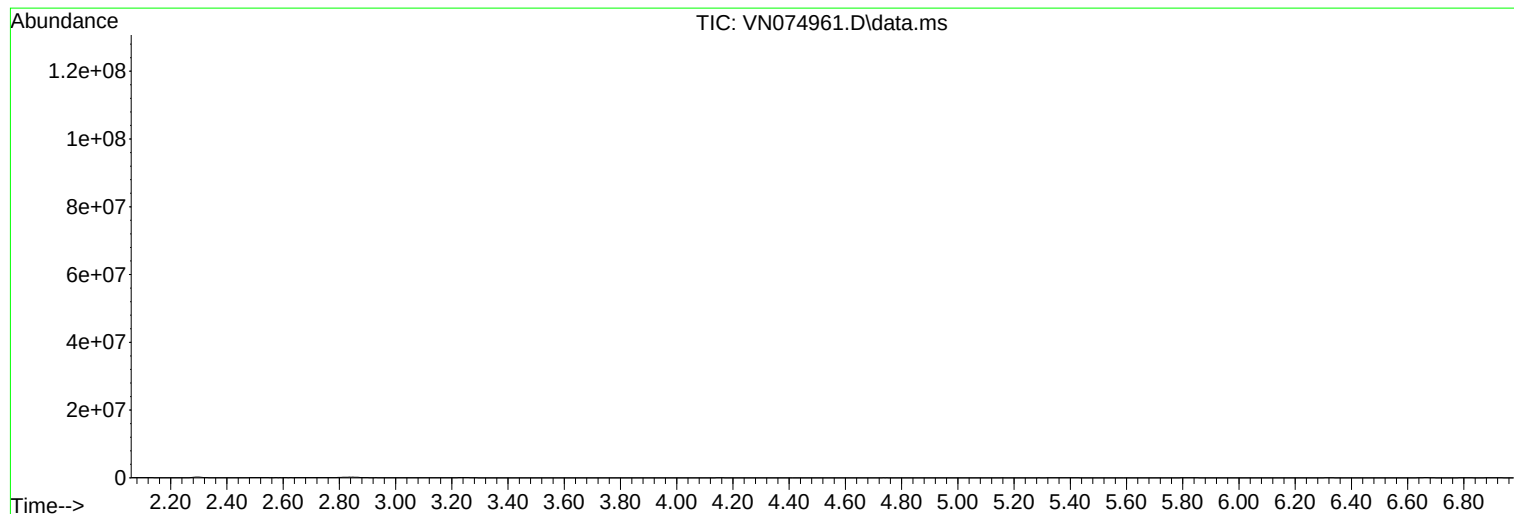
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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



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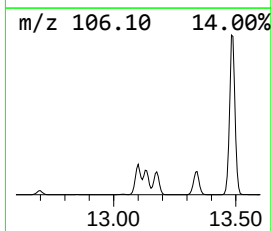
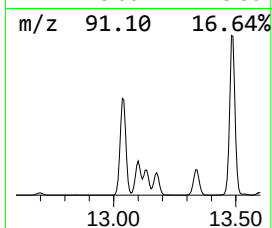
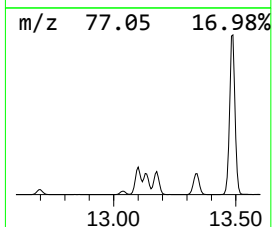
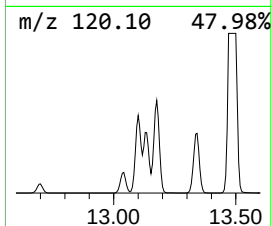
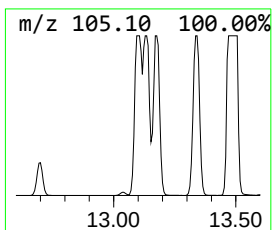
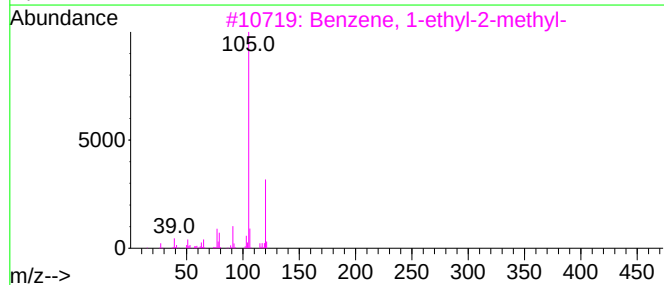
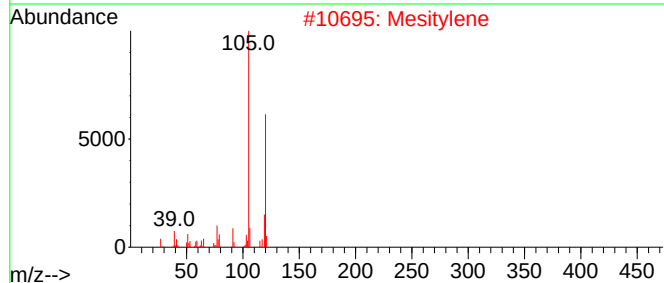
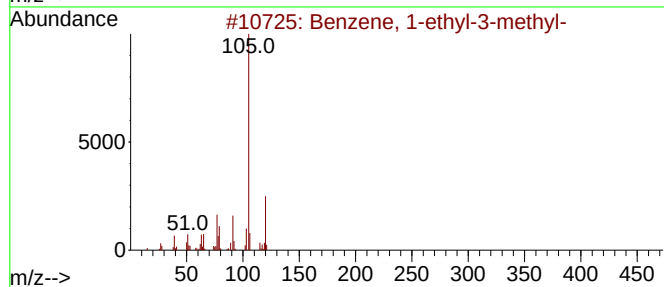
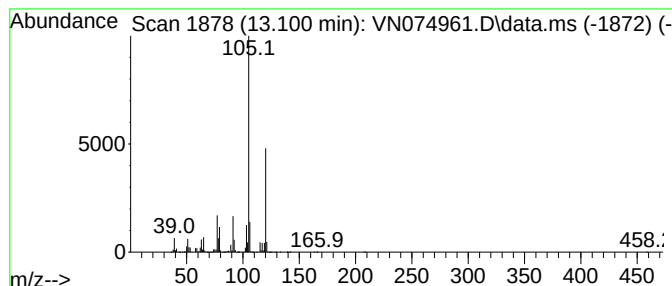
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	32.77 ug/l	50982300	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	93
2			Mesitylene	120	C9H12	000108-67-8	91
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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Instrument :
MSVOA_N
ClientSampleId :
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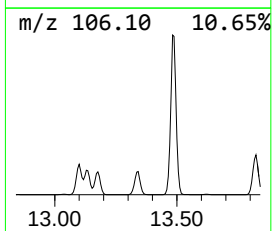
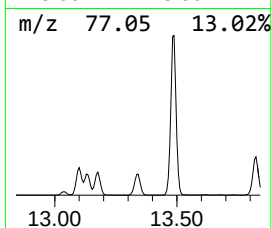
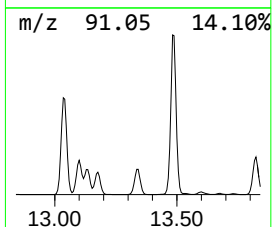
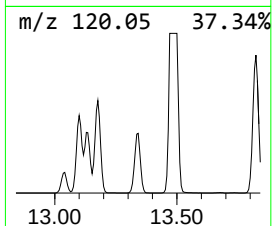
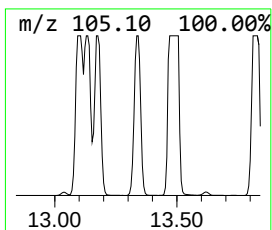
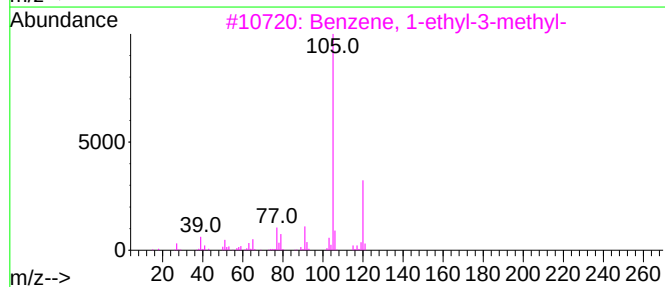
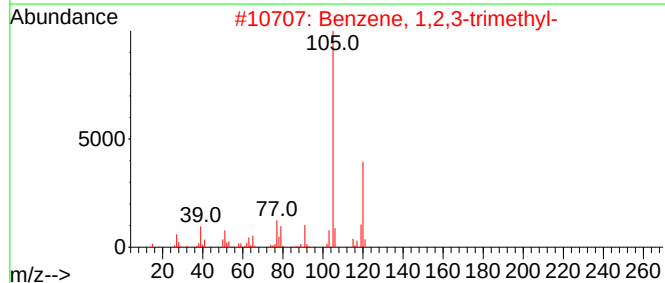
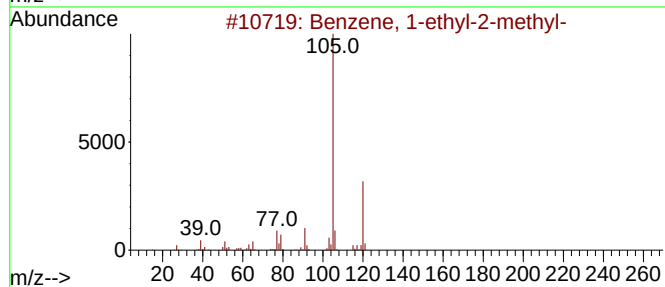
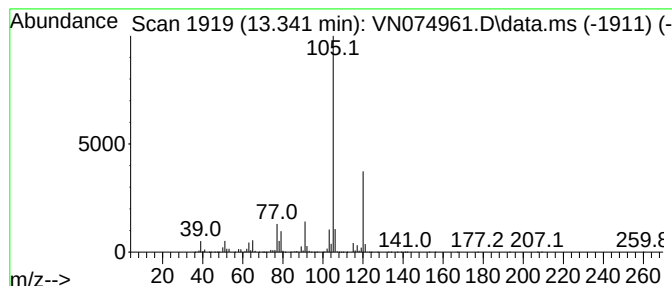
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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.
13.341	25.72 ug/l	40020200	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			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

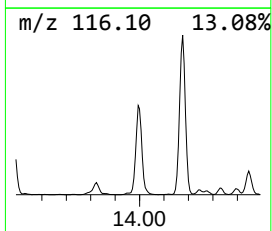
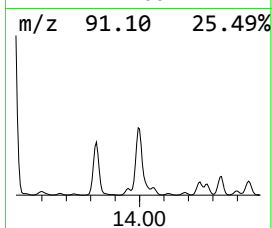
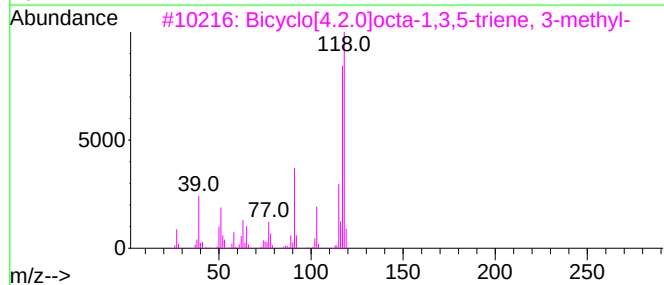
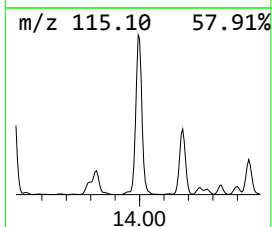
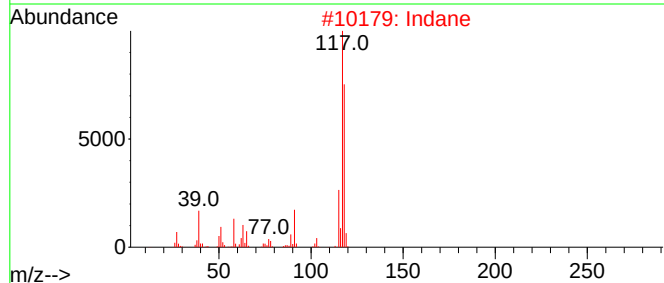
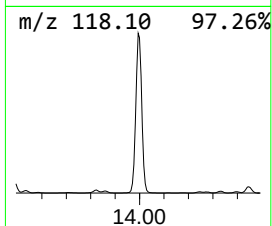
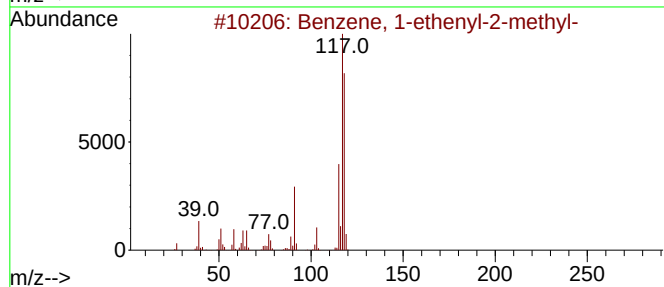
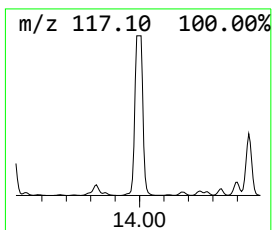
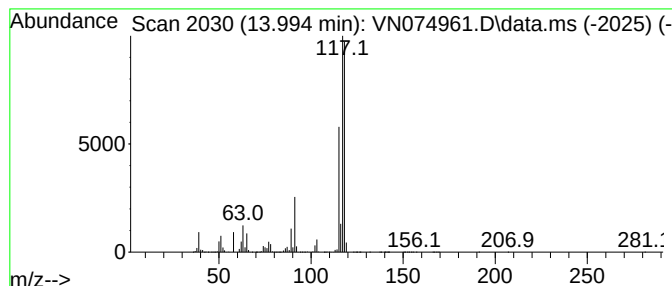
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethenyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	53.05 ug/l	82534500	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	89
2			Indane	118	C9H10	000496-11-7	81
3			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	022250-74-4	72
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	72
5			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	70



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

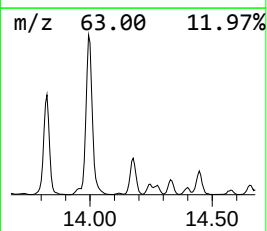
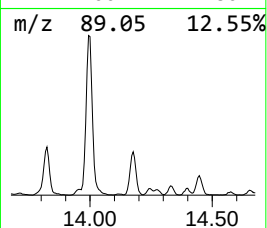
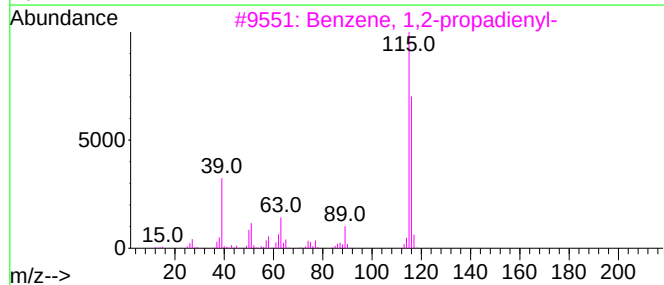
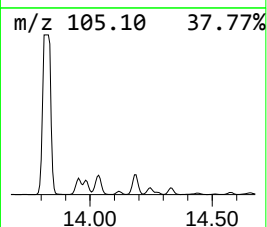
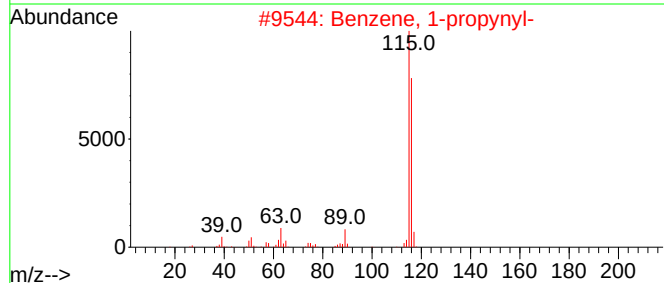
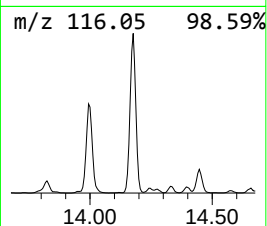
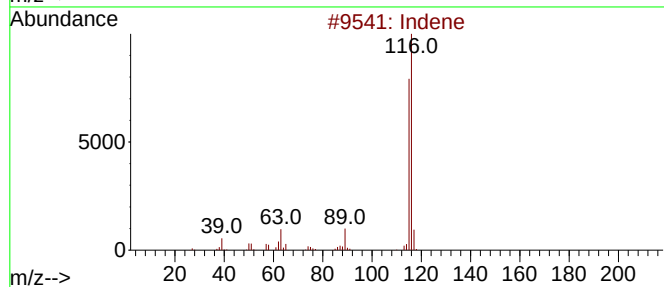
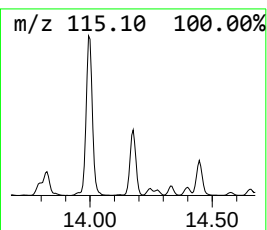
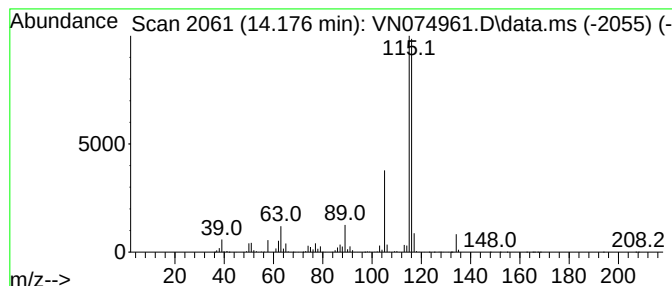
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Quant Title : SW846 8260

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

Peak Number 4 Indene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	8.05 ug/l	12531000	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	93
3			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	83
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	81
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	81



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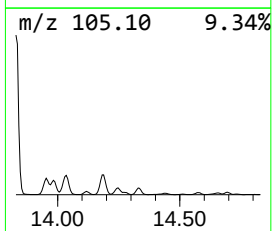
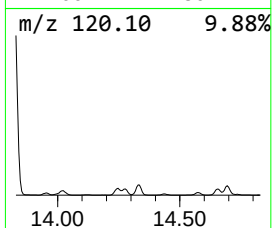
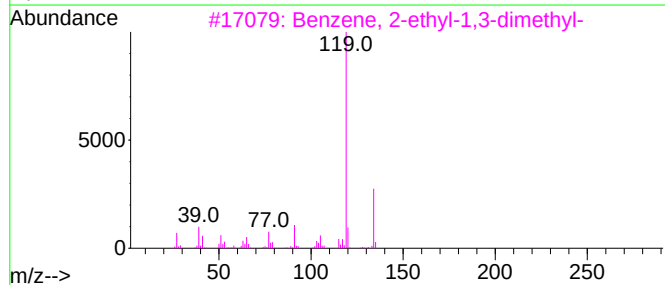
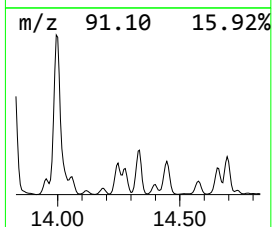
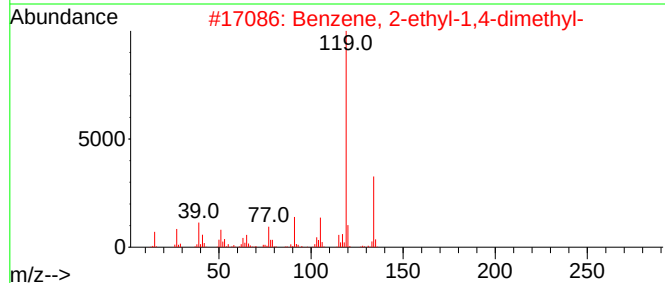
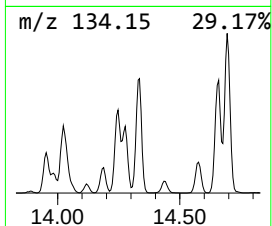
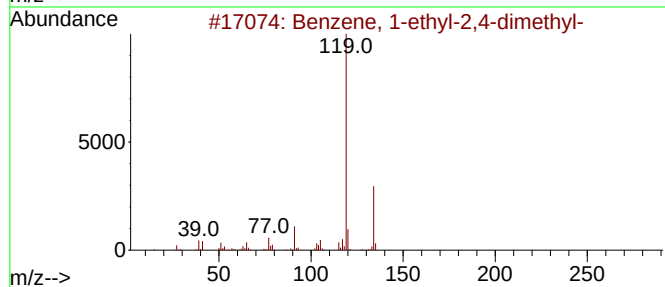
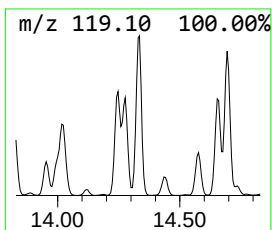
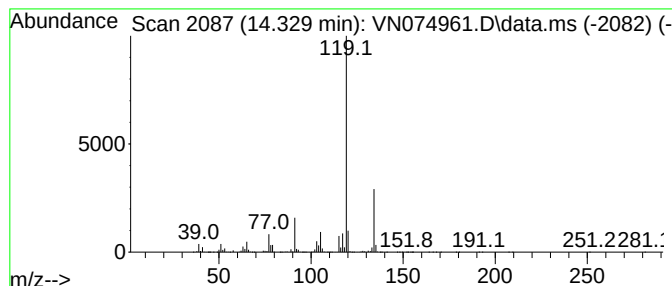
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	9.64 ug/l	14993800	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
3			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074961.D
Acq On : 21 Oct 2022 14:59
Operator : JC\MD
Sample : N5222-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

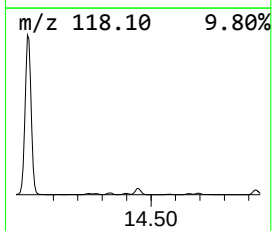
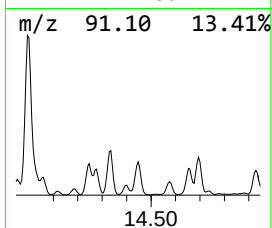
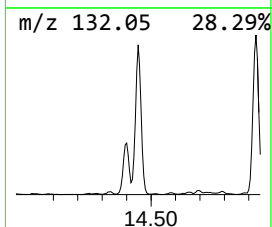
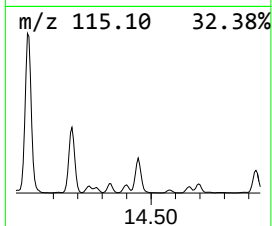
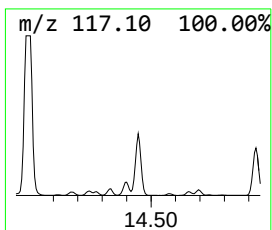
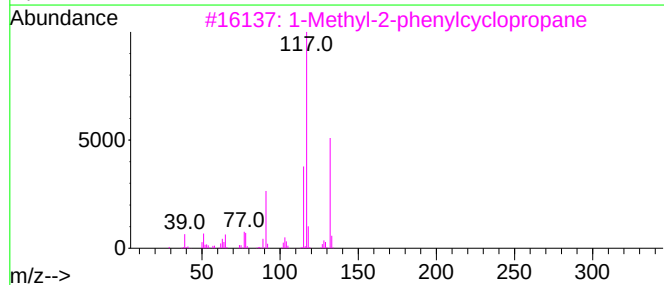
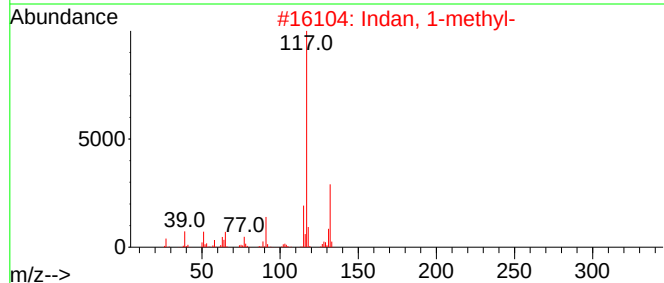
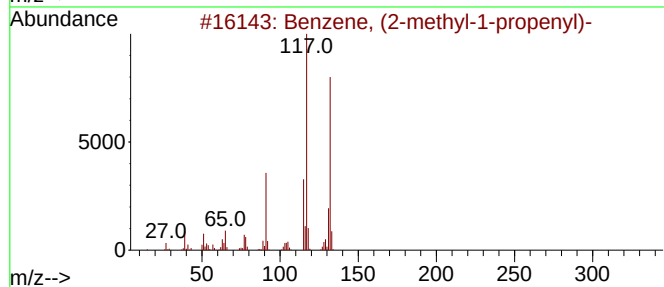
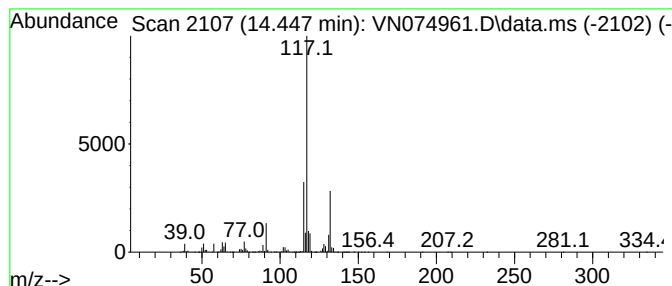
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	10.06 ug/l	15642500	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			Indan, 1-methyl-	132	C10H12	000767-58-8	87
3			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	83
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	80
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074961.D
Acq On : 21 Oct 2022 14:59
Operator : JC\MD
Sample : N5222-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

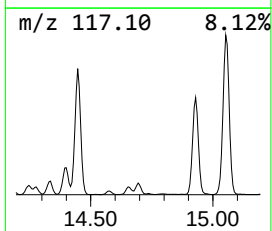
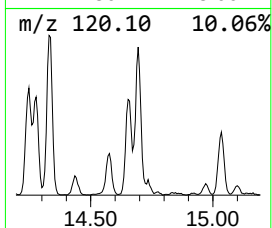
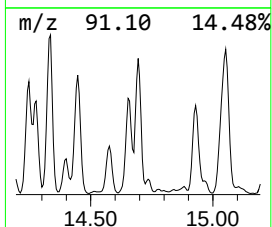
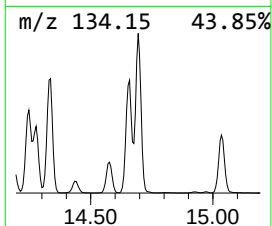
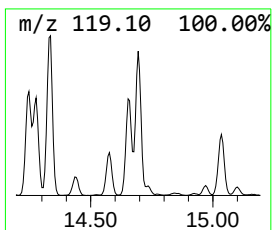
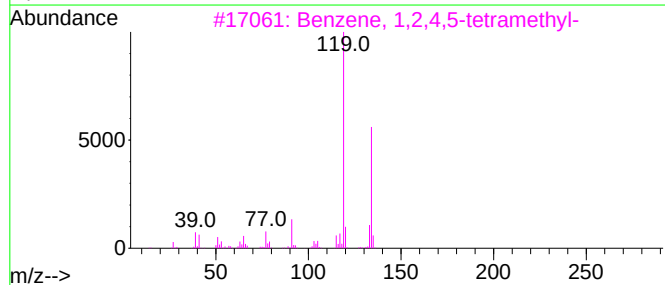
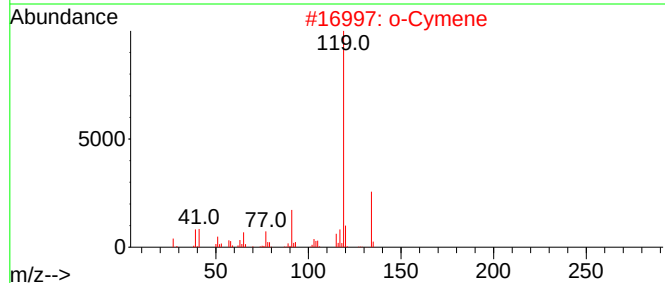
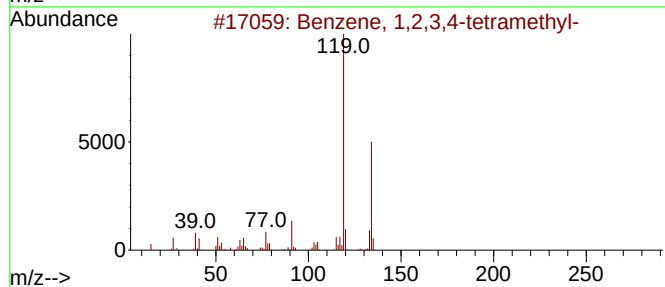
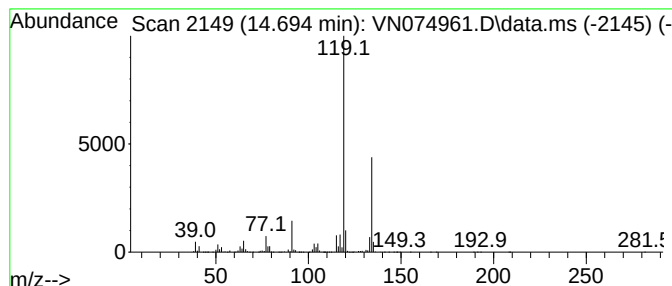
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.694	8.59 ug/l	13361500	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			o-Cymene	134	C10H14	000527-84-4	96
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074961.D
Acq On : 21 Oct 2022 14:59
Operator : JC\MD
Sample : N5222-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

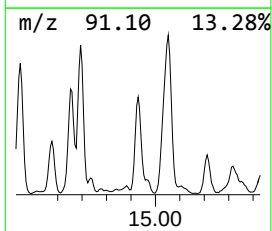
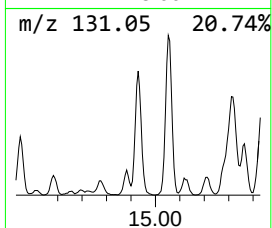
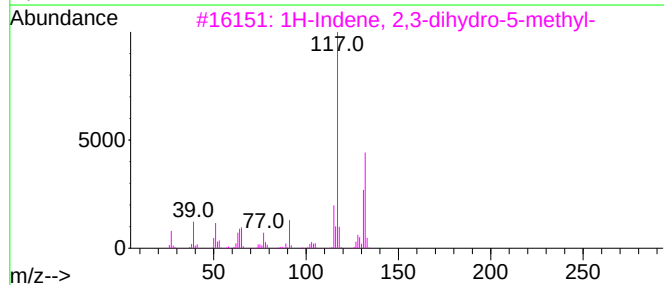
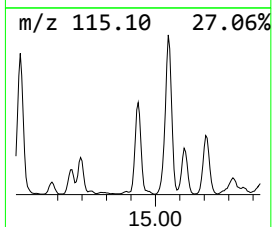
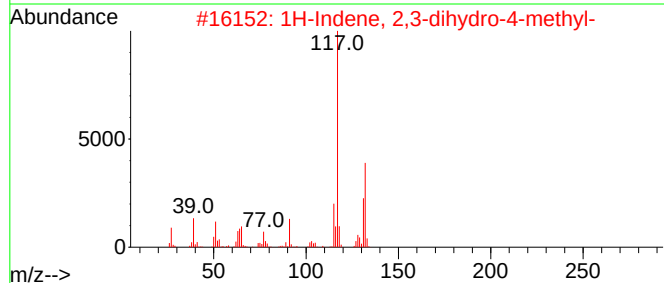
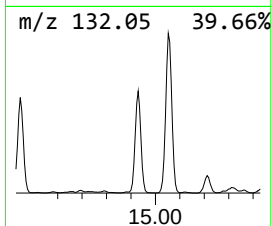
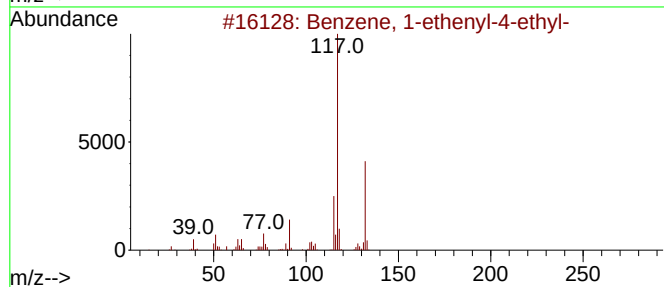
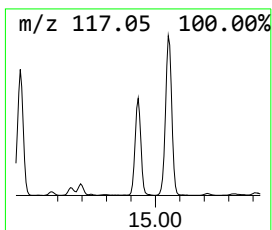
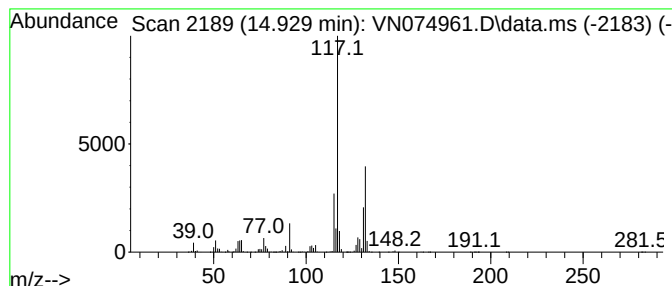
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	8.49 ug/l	13204100	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-4-methyl-	132	C10H12	000824-22-6	94
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074961.D
Acq On : 21 Oct 2022 14:59
Operator : JC\MD
Sample : N5222-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

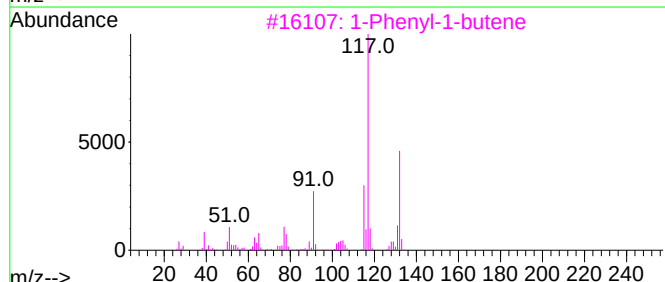
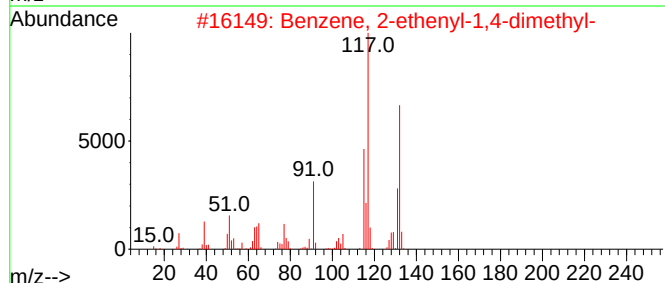
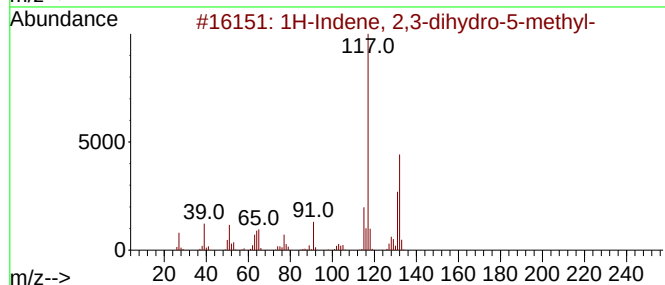
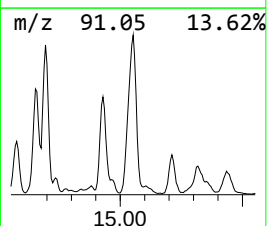
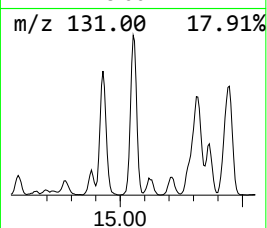
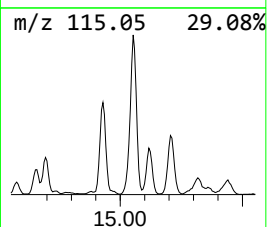
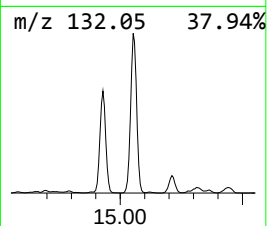
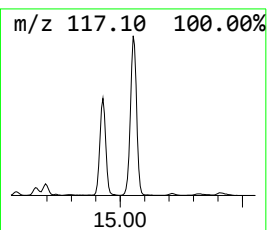
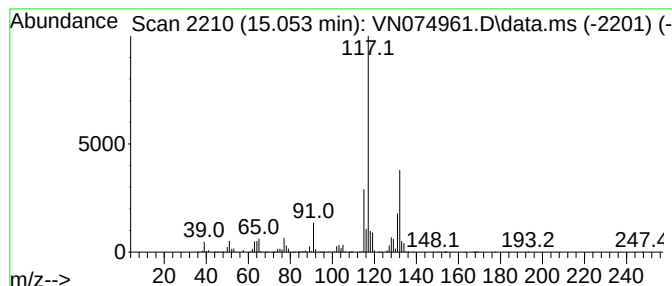
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Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	18.42 ug/l	28657700	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91	
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91	
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	90	
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90	
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074961.D
Acq On : 21 Oct 2022 14:59
Operator : JC\MD
Sample : N5222-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

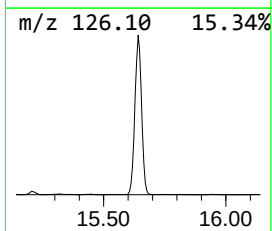
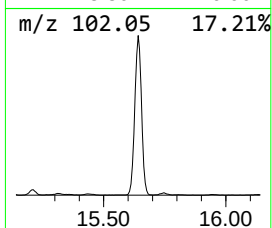
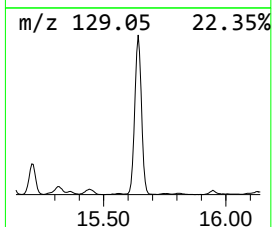
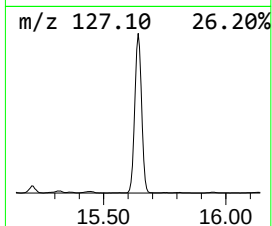
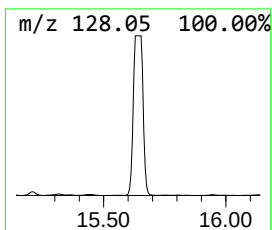
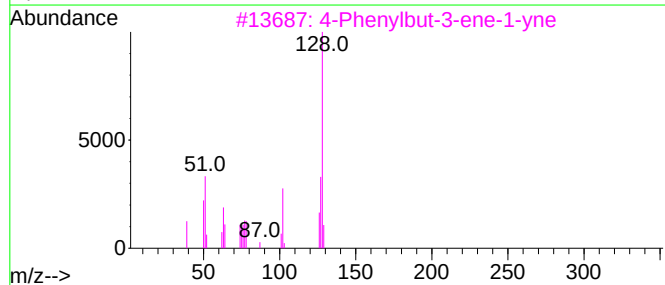
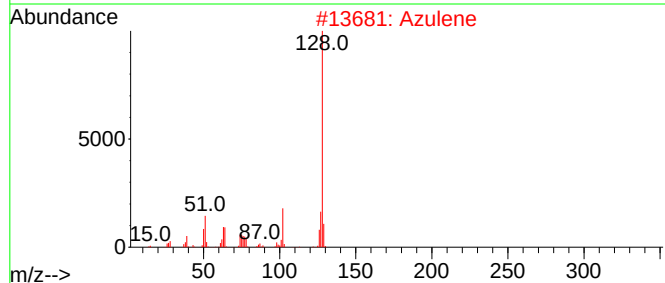
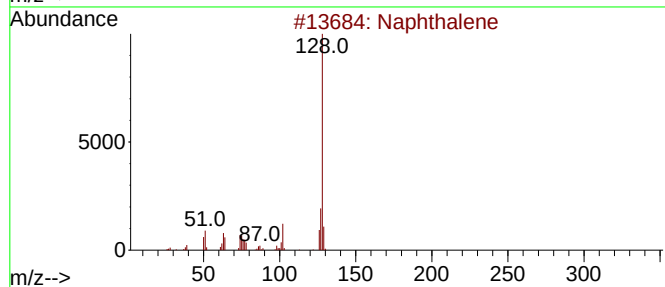
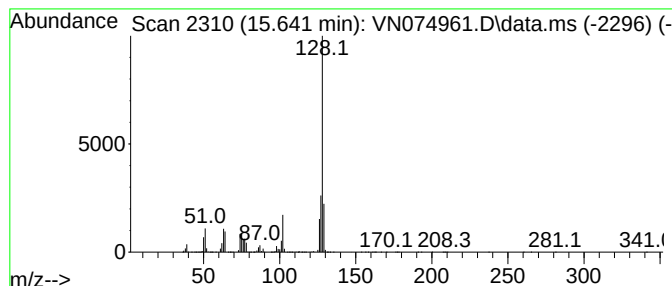
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Quant Title : SW846 8260

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

Peak Number 10 4-Phenylbut-3-ene-1-yne Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.641	39.63 ug/l	61651500	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	93
2			Azulene	128	C10H8	000275-51-4	87
3			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	74
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	72
5			Tetracyanoethylene	128	C6N4	000670-54-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074961.D
Acq On : 21 Oct 2022 14:59
Operator : JC\MD
Sample : N5222-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.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...	13.341	25.7	ug/l	40020200	4	13.794	77785000	50.0
Benzene, 1-ethe...	13.994	53.0	ug/l	82534500	4	13.794	77785000	50.0
Indene	14.176	8.1	ug/l	12531000	4	13.794	77785000	50.0
Benzene, 1-ethy...	14.329	9.6	ug/l	14993800	4	13.794	77785000	50.0
Benzene, (2-met...	14.447	10.1	ug/l	15642500	4	13.794	77785000	50.0
Benzene, 1,2,3,...	14.694	8.6	ug/l	13361500	4	13.794	77785000	50.0
Benzene, 1-ethe...	14.929	8.5	ug/l	13204100	4	13.794	77785000	50.0
1H-Indene, 2,3-...	15.053	18.4	ug/l	28657700	4	13.794	77785000	50.0
4-Phenylbut-3-e...	15.641	39.6	ug/l	61651500	4	13.794	77785000	50.0