

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
 Data File : VN079036.D
 Acq On : 24 Aug 2023 17:06
 Operator : JC\MD
 Sample : 04093-02 20X
 Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NEVINS-SB04-Z52-53

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\82N081523W.M

Title : SW846 8260

Signal : TIC: VN079036.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.612	1118	1132	1145	rBV2	1476609	3799287	2.76%	1.257%
2	10.571	1457	1465	1472	rBV	868870	1649337	1.20%	0.546%
3	11.870	1679	1686	1695	rBV	844209	1514625	1.10%	0.501%
4	11.970	1695	1703	1712	rVV	11254324	18787245	13.65%	6.218%
5	12.070	1712	1720	1730	rVB	3998603	7864729	5.72%	2.603%
6	12.400	1764	1776	1786	rBV	3206333	5606645	4.07%	1.856%
7	12.700	1821	1827	1835	rVB	979348	1704555	1.24%	0.564%
8	13.100	1889	1895	1898	rBV	2141223	3691738	2.68%	1.222%
9	13.135	1898	1901	1905	rVV	3223566	5048182	3.67%	1.671%
10	13.176	1905	1908	1914	rVB	1291542	2011831	1.46%	0.666%
11	13.341	1920	1936	1951	rVB3	1452379	4046623	2.94%	1.339%
12	13.488	1951	1961	1966	rBV	4198125	7342106	5.34%	2.430%
13	13.676	1975	1993	1999	rBV3	1056942	3350208	2.43%	1.109%
14	13.823	2015	2018	2022	rVV	1367979	2317113	1.68%	0.767%
15	13.953	2034	2040	2042	rBV	1451709	2195479	1.60%	0.727%
16	14.000	2042	2048	2061	rVV	28844985	52351812	38.04%	17.326%
17	14.335	2099	2105	2114	rVB	2015953	3212615	2.33%	1.063%
18	14.453	2114	2125	2133	rBV2	1275741	3560241	2.59%	1.178%
19	14.929	2201	2206	2219	rVB	2604216	4754818	3.46%	1.574%
20	15.047	2219	2226	2233	rBV2	1140770	3200481	2.33%	1.059%
21	15.123	2233	2239	2246	rVB	3078167	5479298	3.98%	1.813%
22	15.211	2246	2254	2262	rVB	6197968	11208348	8.15%	3.709%
23	15.317	2262	2272	2280	rBV2	1241623	2879776	2.09%	0.953%
24	15.523	2299	2307	2319	rVV	638554	2361330	1.72%	0.781%
25	15.647	2319	2328	2338	rVV2	67441205	137608176	100.00%	45.542%
26	15.753	2339	2346	2358	rVB	1175472	2488716	1.81%	0.824%
27	15.988	2381	2386	2401	rVB2	679078	2119141	1.54%	0.701%

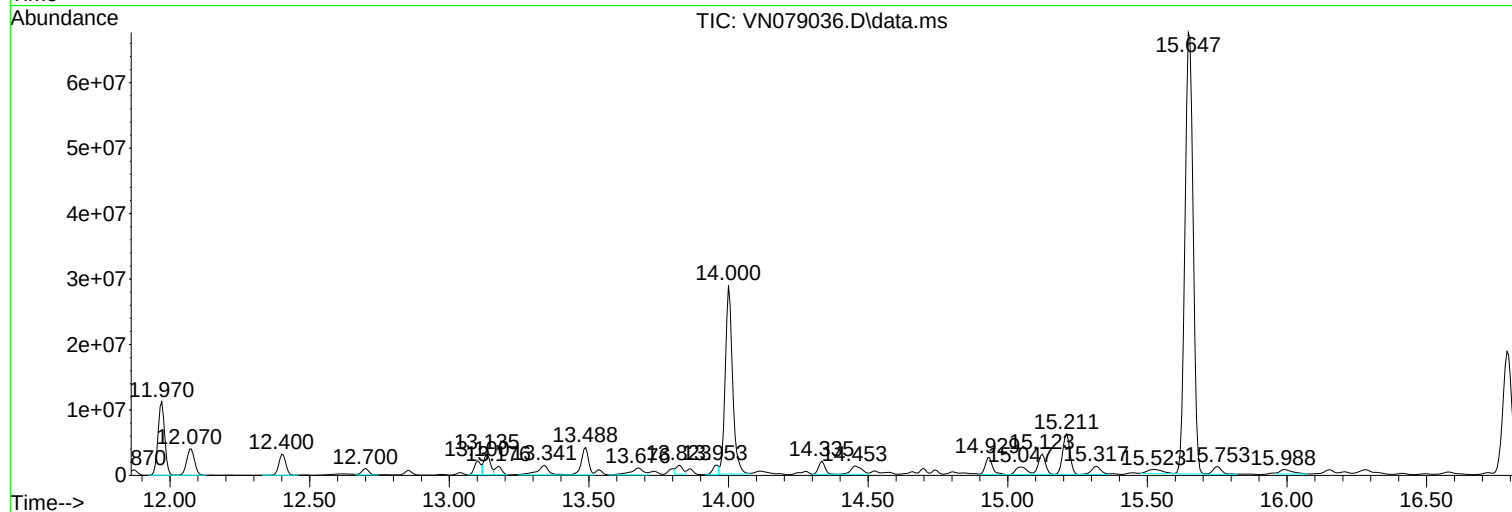
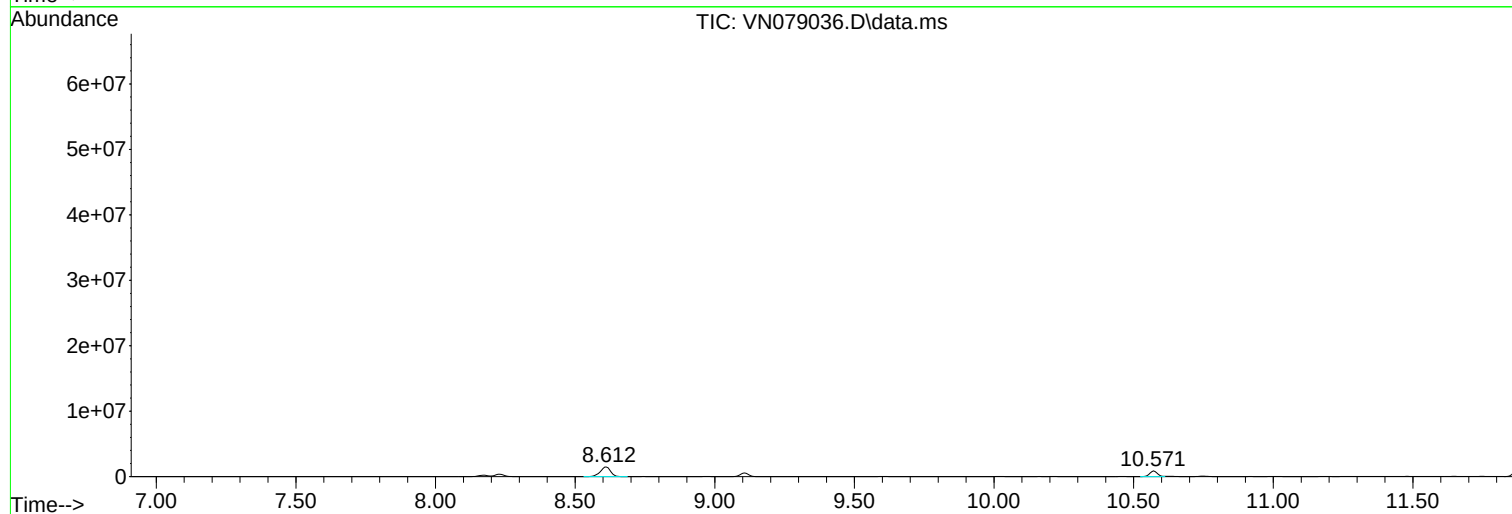
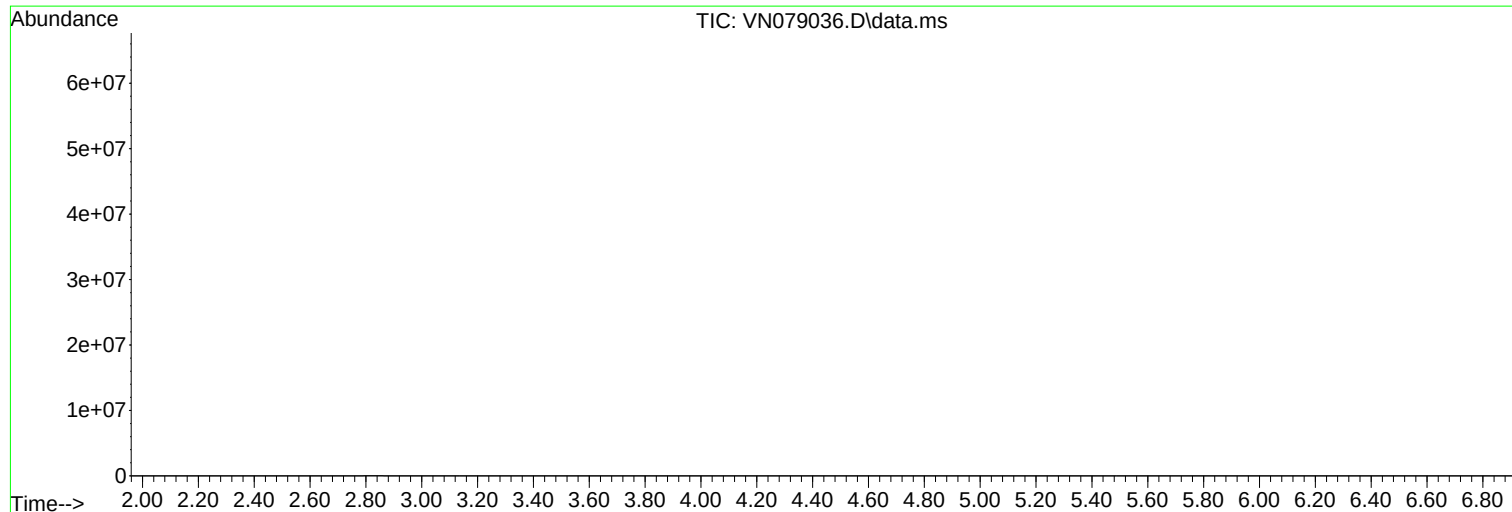
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Instrument :
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ClientSampleId :
NEVINS-SB04-Z52-53

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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



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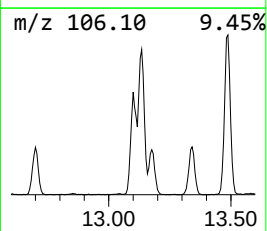
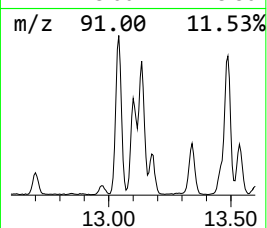
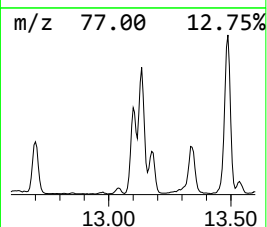
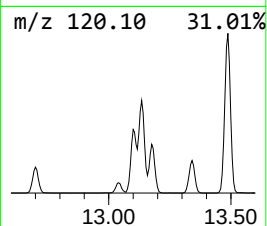
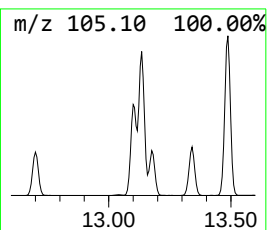
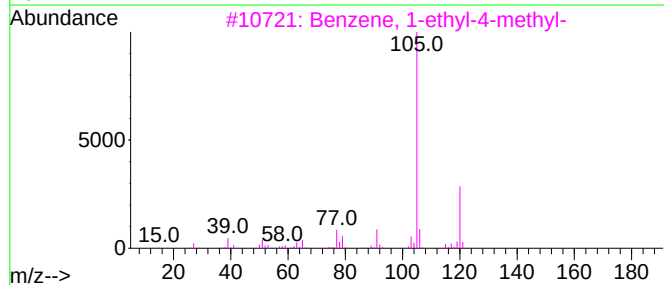
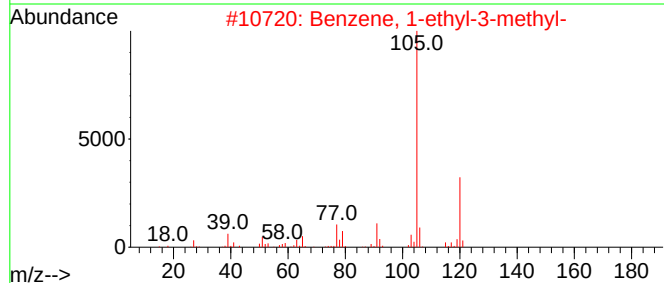
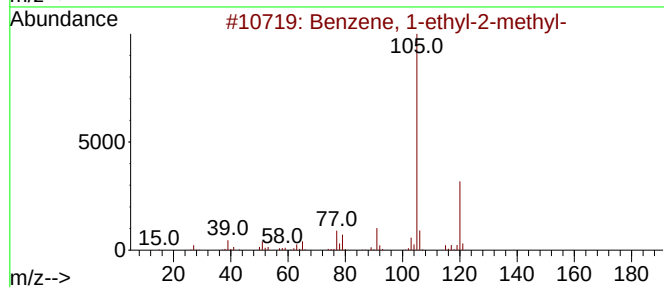
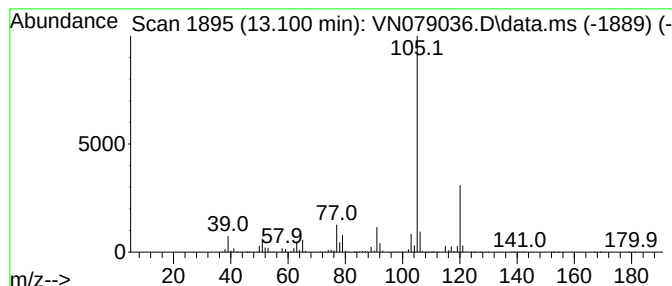
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Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	79.66 ug/l	3691740	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	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	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	91



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MSVOA_N
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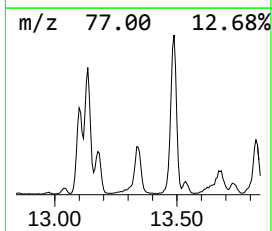
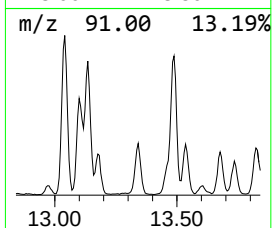
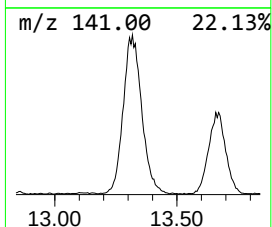
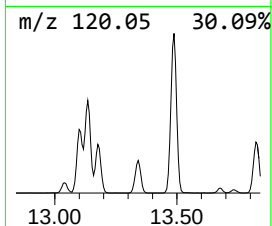
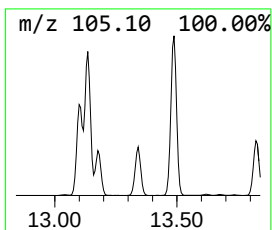
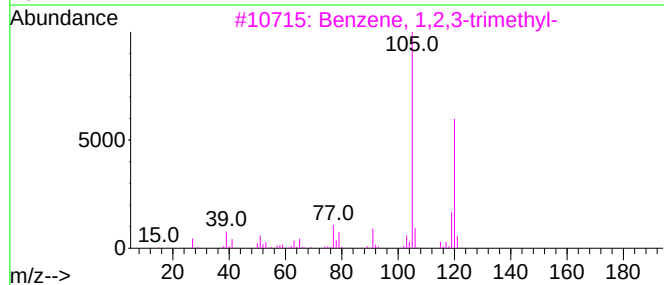
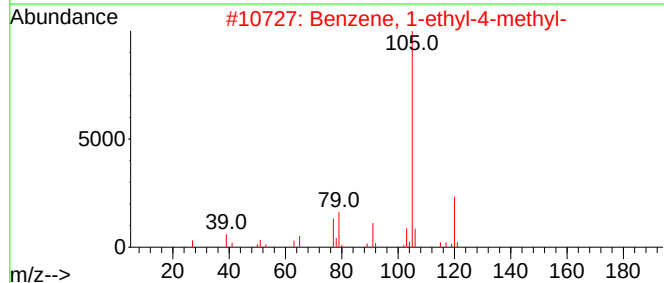
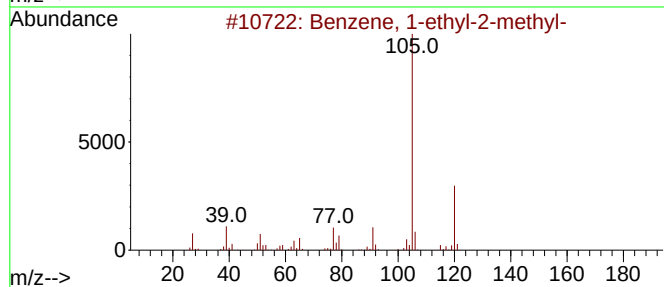
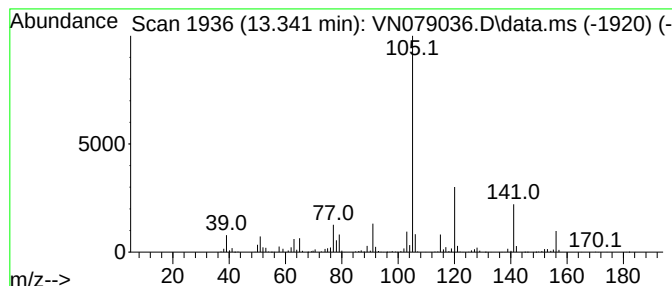
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	87.32 ug/l	4046620	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	91
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	83
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	64
4			Mesitylene	120	C9H12	000108-67-8	64
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	64



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NEVINS-SB04-Z52-53

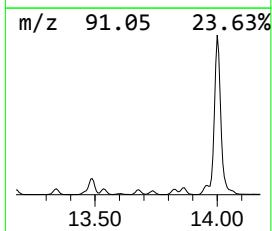
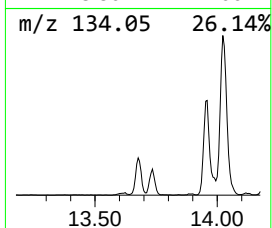
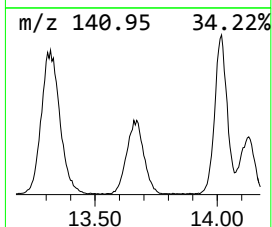
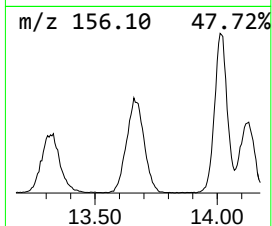
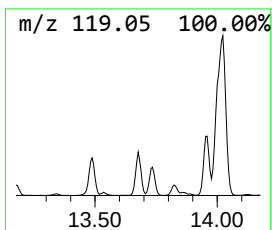
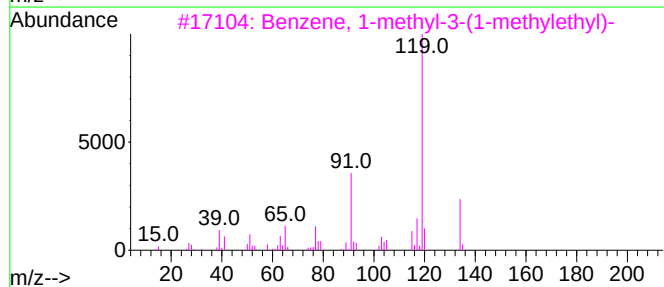
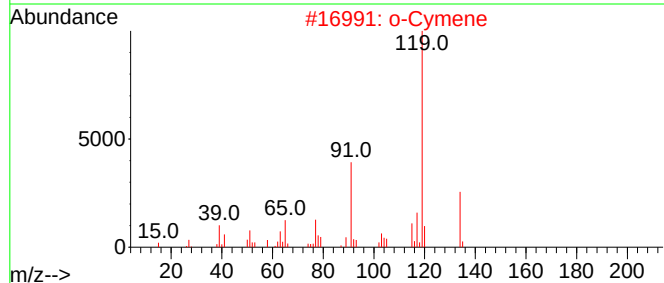
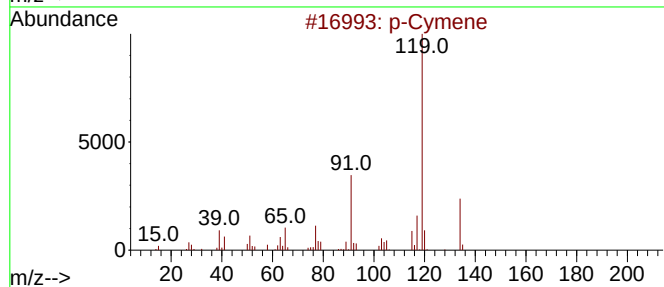
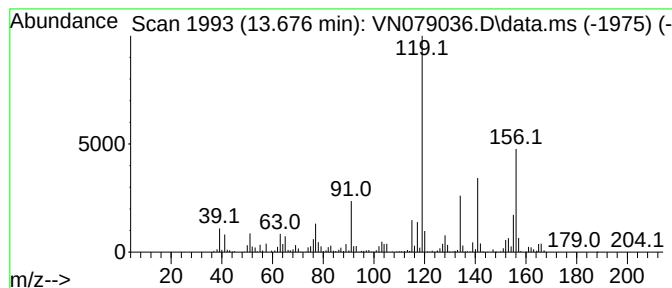
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 3 p-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	72.29 ug/l	3350210	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cymene	134	C10H14	000099-87-6	89
2			o-Cymene	134	C10H14	000527-84-4	89
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	87
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	70
5			1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	55



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ALS Vial : 16 Sample Multiplier: 1

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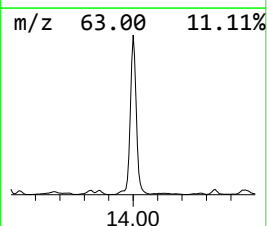
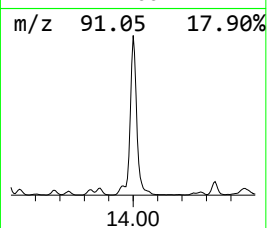
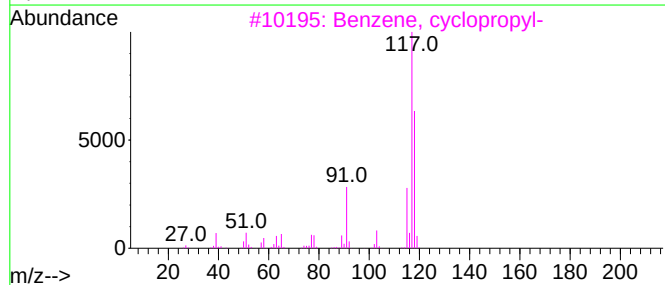
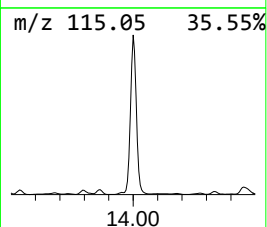
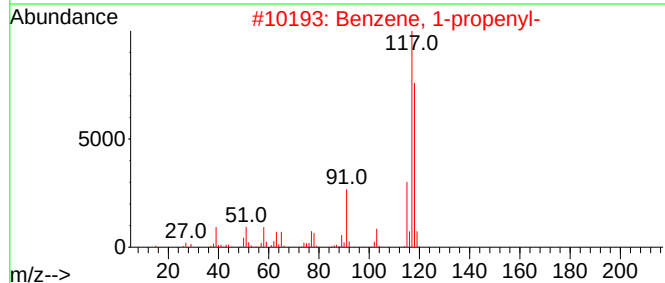
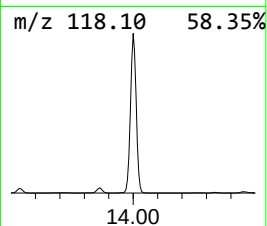
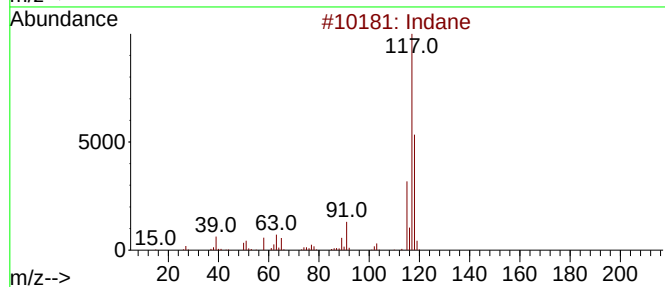
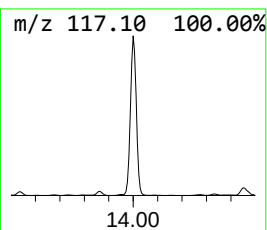
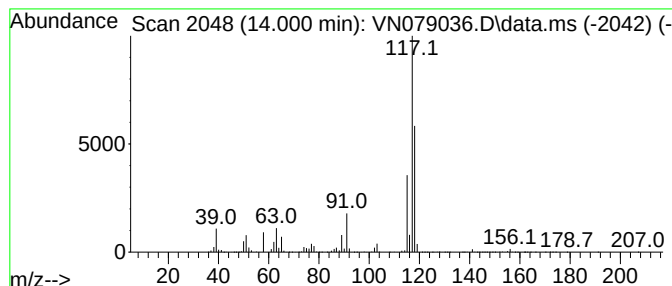
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	1129.68 ug/l	52351800	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	59
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	58
4			Benzene, 1-(chloromethyl)-3-ethe...	152	C9H9Cl	039833-65-3	53
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	49



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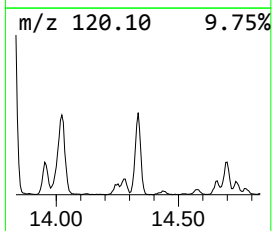
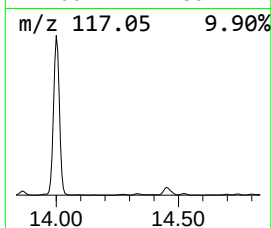
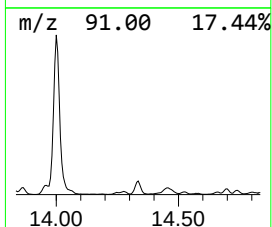
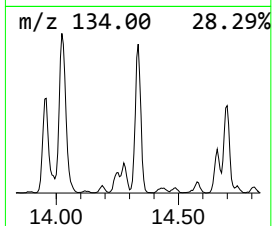
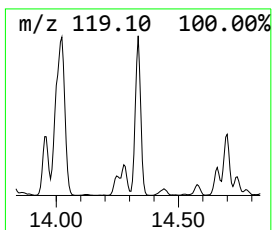
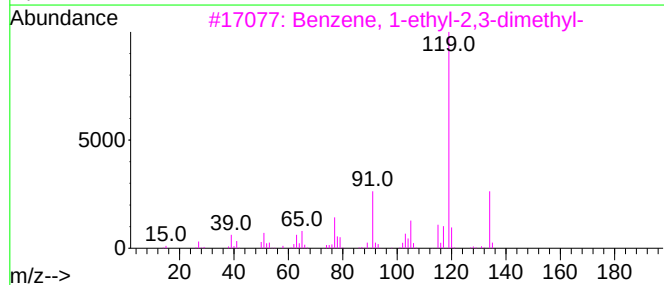
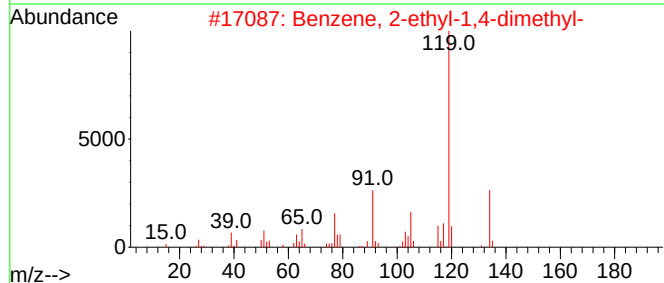
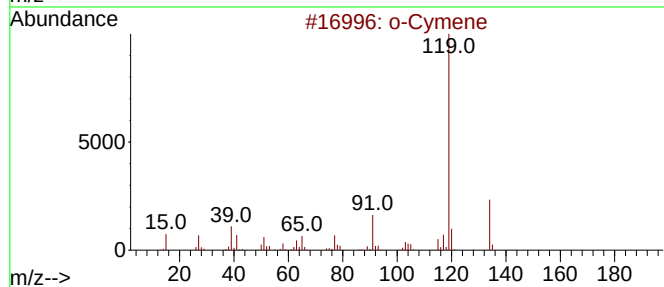
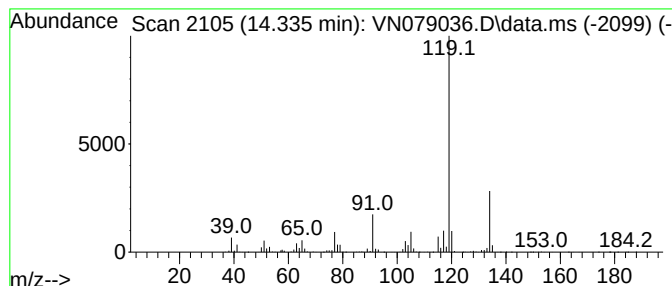
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Quant Title : SW846 8260

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

Peak Number 5 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.335	69.32 ug/l	3212620	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	95
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



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NEVINS-SB04-Z52-53

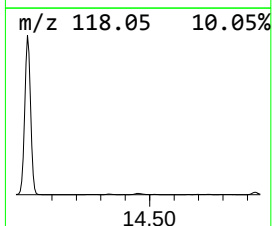
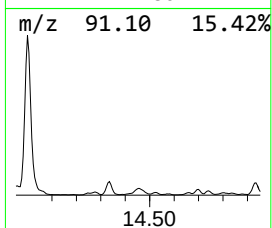
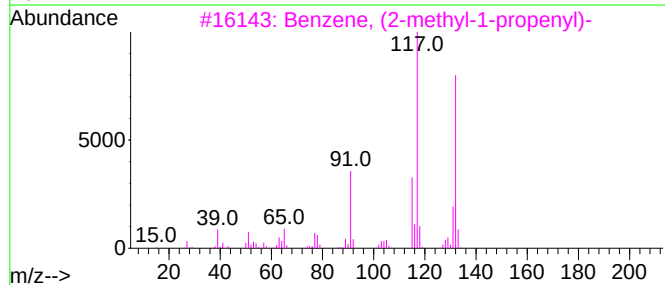
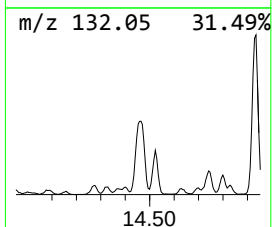
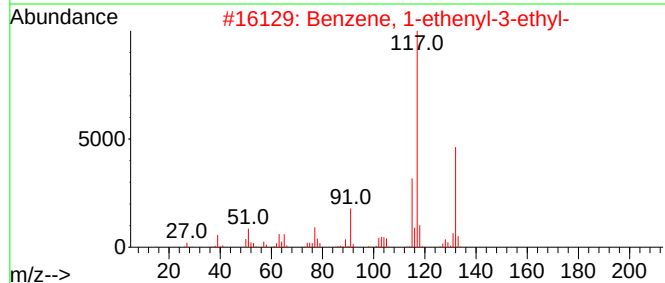
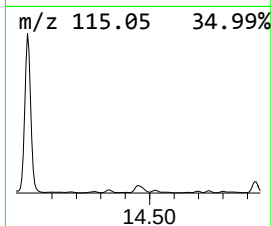
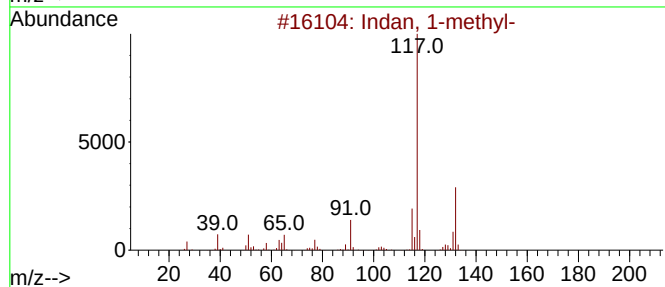
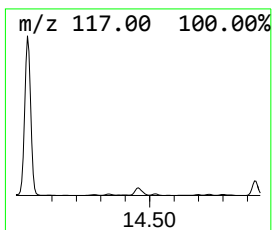
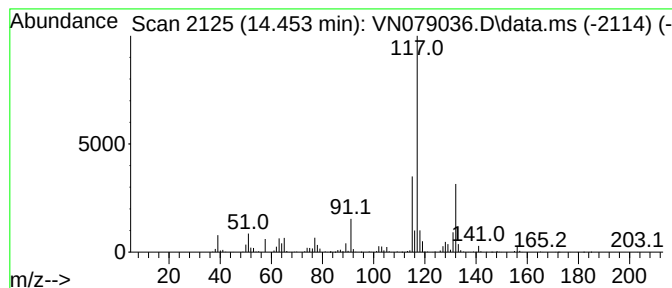
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Quant Title : SW846 8260

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

Peak Number 6 Indan, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.453	76.82 ug/l	3560240	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	91
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	91
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	91
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079036.D
Acq On : 24 Aug 2023 17:06
Operator : JC\MD
Sample : 04093-02 20X
Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z52-53

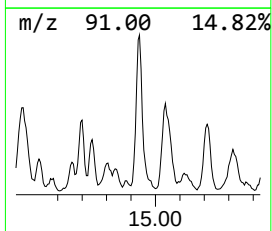
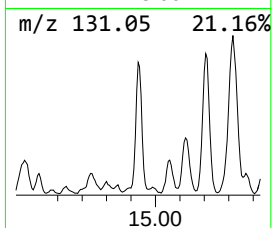
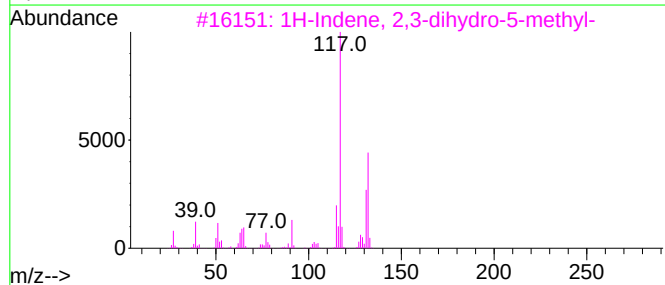
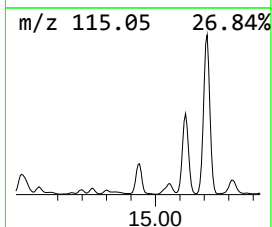
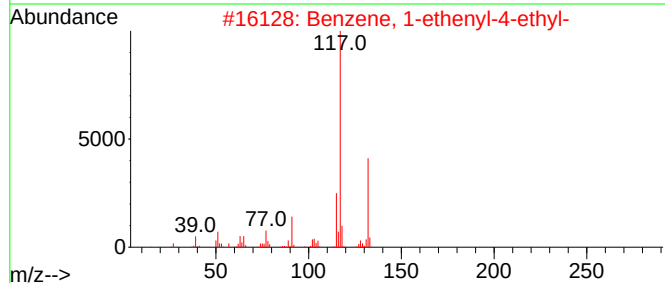
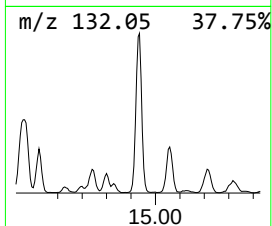
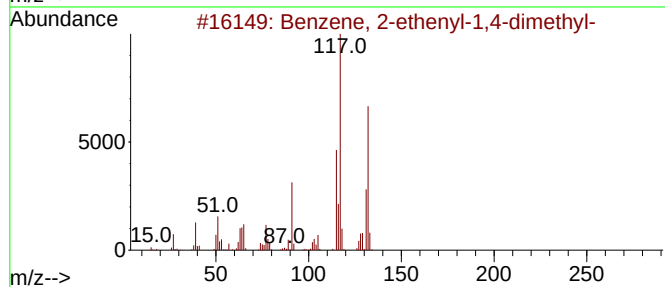
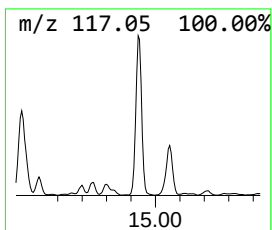
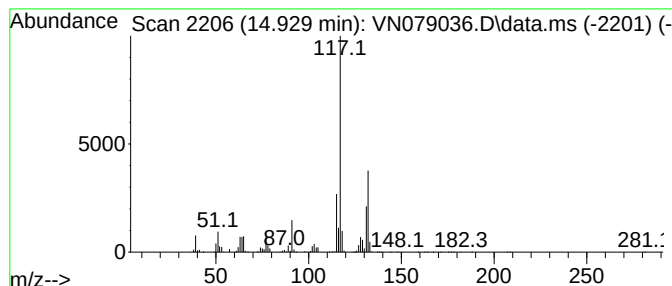
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Quant Title : SW846 8260

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.
14.929	102.60 ug/l	4754820	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			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			3-Phenylbut-1-ene	132	C10H12	000934-10-1	94
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079036.D
Acq On : 24 Aug 2023 17:06
Operator : JC\MD
Sample : 04093-02 20X
Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z52-53

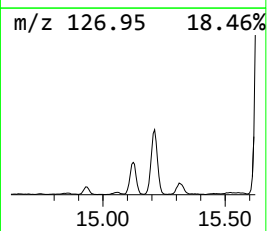
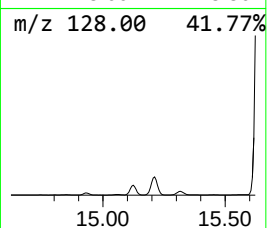
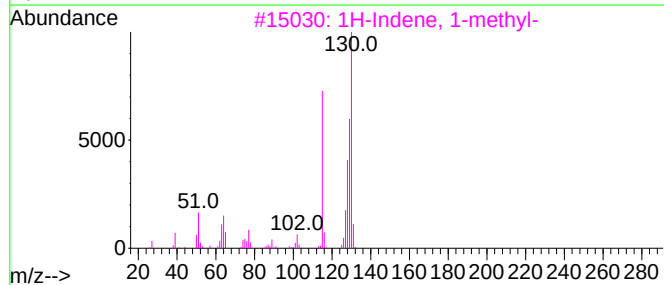
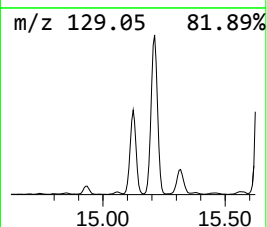
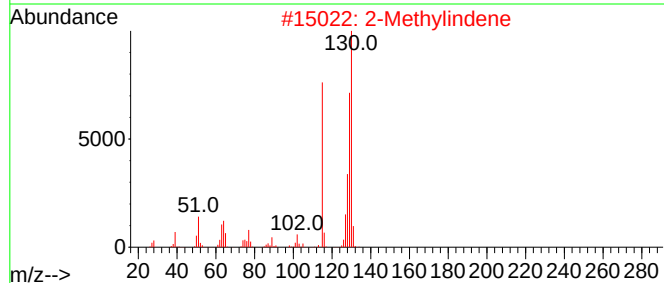
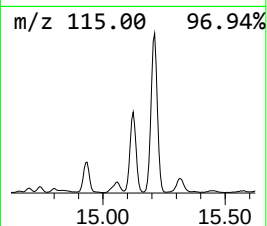
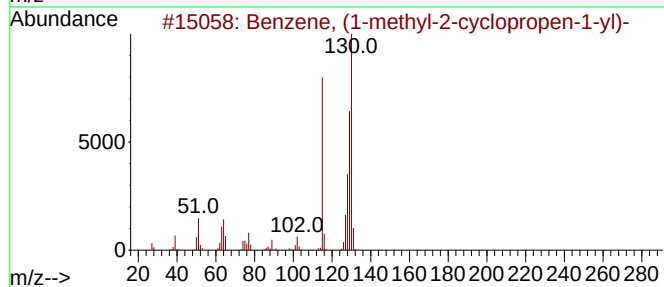
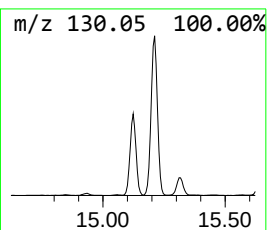
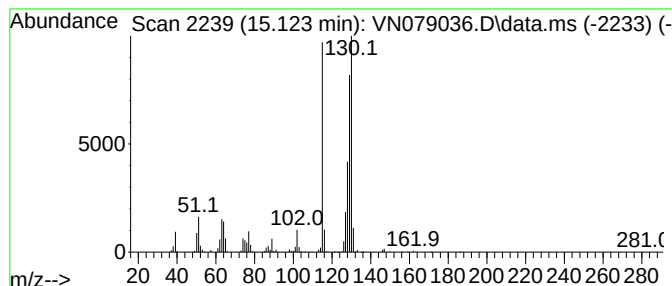
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, (1-methyl-2-cyclop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.123	118.24 ug/l	5479300	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	97
2			2-Methylindene	130	C10H10	002177-47-1	97
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
4			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
5			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079036.D
Acq On : 24 Aug 2023 17:06
Operator : JC\MD
Sample : 04093-02 20X
Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z52-53

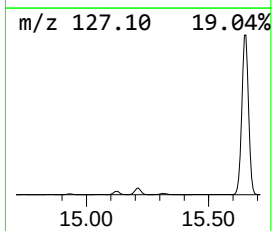
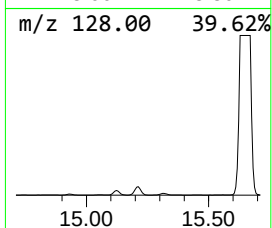
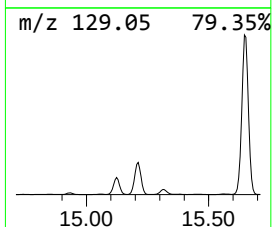
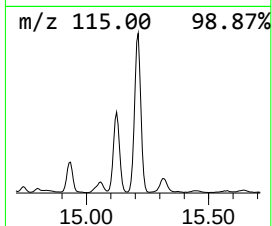
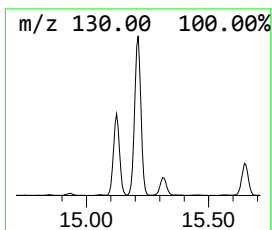
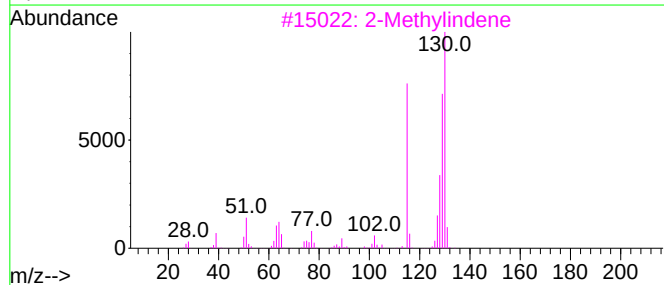
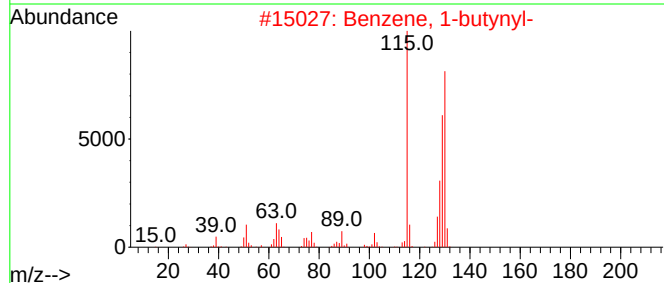
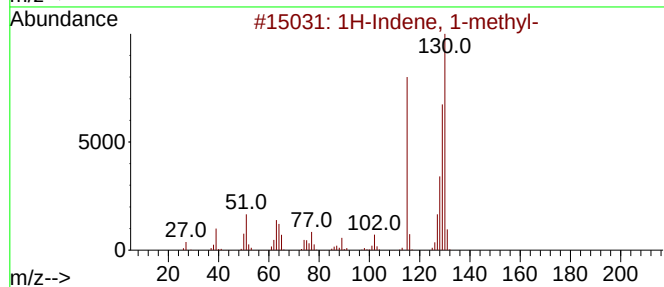
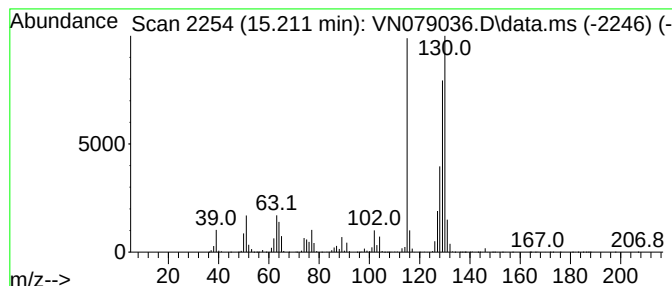
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Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.211	241.86 ug/l	11208300	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
2			Benzene, 1-butyryl-	130	C10H10	000622-76-4	95
3			2-Methylindene	130	C10H10	002177-47-1	95
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
5			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079036.D
Acq On : 24 Aug 2023 17:06
Operator : JC\MD
Sample : 04093-02 20X
Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z52-53

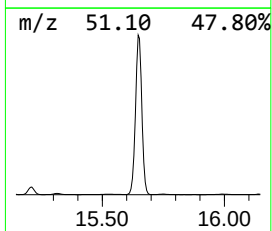
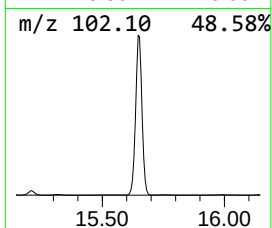
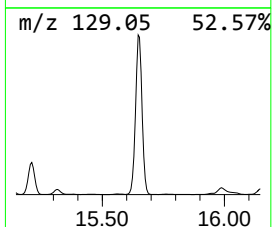
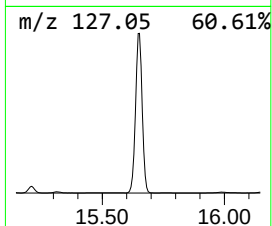
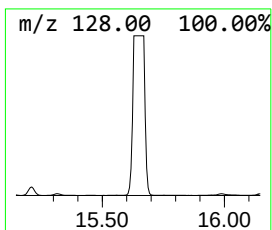
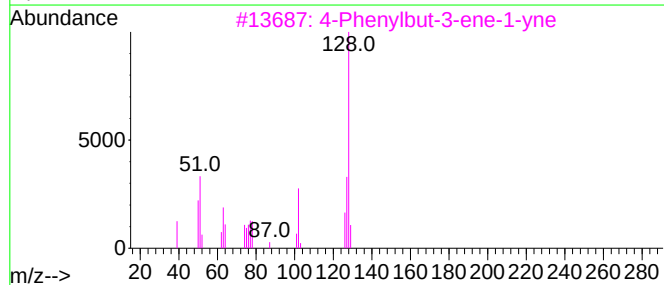
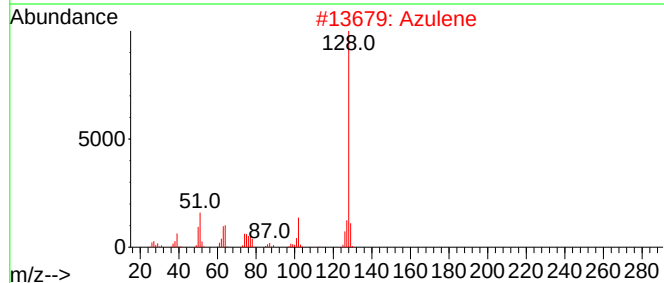
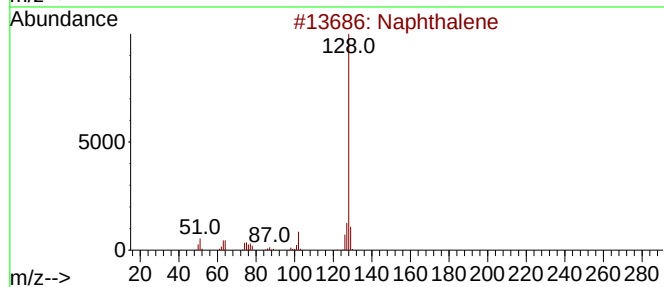
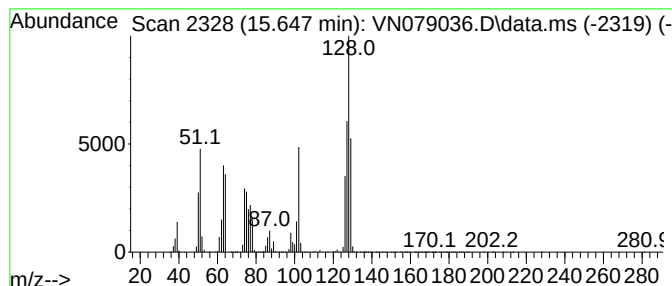
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Quant Title : SW846 8260

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

Peak Number 10 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	2969.39 ug/l	137608000	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	95
3			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	74
4			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	68
5			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079036.D
Acq On : 24 Aug 2023 17:06
Operator : JC\MD
Sample : 04093-02 20X
Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z52-53

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.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
Benzene, 1-ethy...	13.100	79.7	ug/l	3691740	4	13.794	2317110	50.0
Benzene, 1-ethy...	13.341	87.3	ug/l	4046620	4	13.794	2317110	50.0
p-Cymene	13.676	72.3	ug/l	3350210	4	13.794	2317110	50.0
Indane	14.000	1129.7	ug/l	52351800	4	13.794	2317110	50.0
o-Cymene	14.335	69.3	ug/l	3212620	4	13.794	2317110	50.0
Indan, 1-methyl-	14.453	76.8	ug/l	3560240	4	13.794	2317110	50.0
Benzene, 2-ethe...	14.929	102.6	ug/l	4754820	4	13.794	2317110	50.0
Benzene, (1-met...	15.123	118.2	ug/l	5479300	4	13.794	2317110	50.0
1H-Indene, 1-me...	15.211	241.9	ug/l	11208300	4	13.794	2317110	50.0
Azulene	15.647	2969.4	ug/l	137608000	4	13.794	2317110	50.0