

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
 Data File : VN079039.D
 Acq On : 24 Aug 2023 18:18
 Operator : JC\MD
 Sample : 04075-01
 Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NEVINS-SB05-Z113-114

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: VN079039.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	1061	rBV	250507	596421	1.41%	0.736%
2	8.224	1061	1066	1081	rVB	407022	909831	2.15%	1.123%
3	8.582	1117	1127	1142	rBV	265256	607253	1.43%	0.749%
4	9.100	1207	1215	1224	rBV	609406	1266134	2.99%	1.562%
5	10.570	1456	1465	1472	rBV	918475	1721133	4.06%	2.124%
6	11.870	1678	1686	1695	rBV	875845	1558183	3.68%	1.923%
7	11.970	1695	1703	1710	rVV	842790	1446856	3.42%	1.785%
8	12.076	1712	1721	1731	rVV	535549	1068448	2.52%	1.318%
9	12.406	1769	1777	1787	rBV3	490978	976022	2.30%	1.204%
10	12.853	1846	1853	1863	rBV	731934	1257709	2.97%	1.552%
11	13.176	1904	1908	1914	rVB	269428	480779	1.14%	0.593%
12	13.347	1921	1937	1944	rBV3	247119	582507	1.38%	0.719%
13	13.488	1951	1961	1965	rBV	873834	1508972	3.56%	1.862%
14	13.535	1965	1969	1974	rVV	940317	1452794	3.43%	1.793%
15	13.794	2008	2013	2022	rBV2	914506	2104659	4.97%	2.597%
16	14.000	2042	2048	2059	rVB5	326657	913600	2.16%	1.127%
17	14.176	2072	2078	2086	rVB	2486535	4243921	10.02%	5.236%
18	14.470	2120	2128	2133	rBV	639685	1112676	2.63%	1.373%
19	14.700	2163	2167	2171	rVV3	394342	593744	1.40%	0.733%
20	14.794	2178	2183	2188	rBV2	487425	800948	1.89%	0.988%
21	15.041	2218	2225	2232	rBV3	506535	1361229	3.21%	1.680%
22	15.123	2233	2239	2246	rVB	2085901	3701586	8.74%	4.567%
23	15.211	2246	2254	2262	rVB2	2176925	4066018	9.60%	5.017%
24	15.317	2262	2272	2278	rBV4	312256	723532	1.71%	0.893%
25	15.647	2320	2328	2338	rVB	22809481	42354932	100.00%	52.261%
26	15.747	2339	2345	2352	rBV	389841	736530	1.74%	0.909%
27	16.011	2383	2390	2399	rVV5	186770	599393	1.42%	0.740%
28	16.152	2408	2414	2419	rVV	301647	603159	1.42%	0.744%
29	16.282	2428	2436	2442	rBV3	338295	868462	2.05%	1.072%
30	16.576	2480	2486	2500	rVB2	293576	827812	1.95%	1.021%

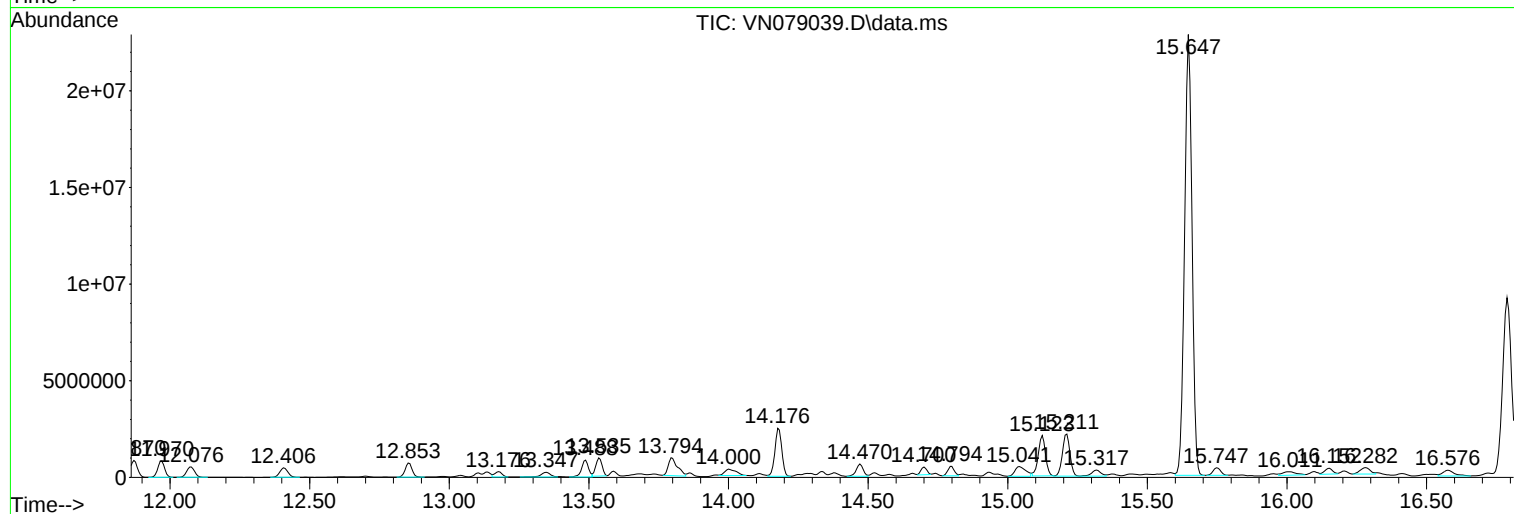
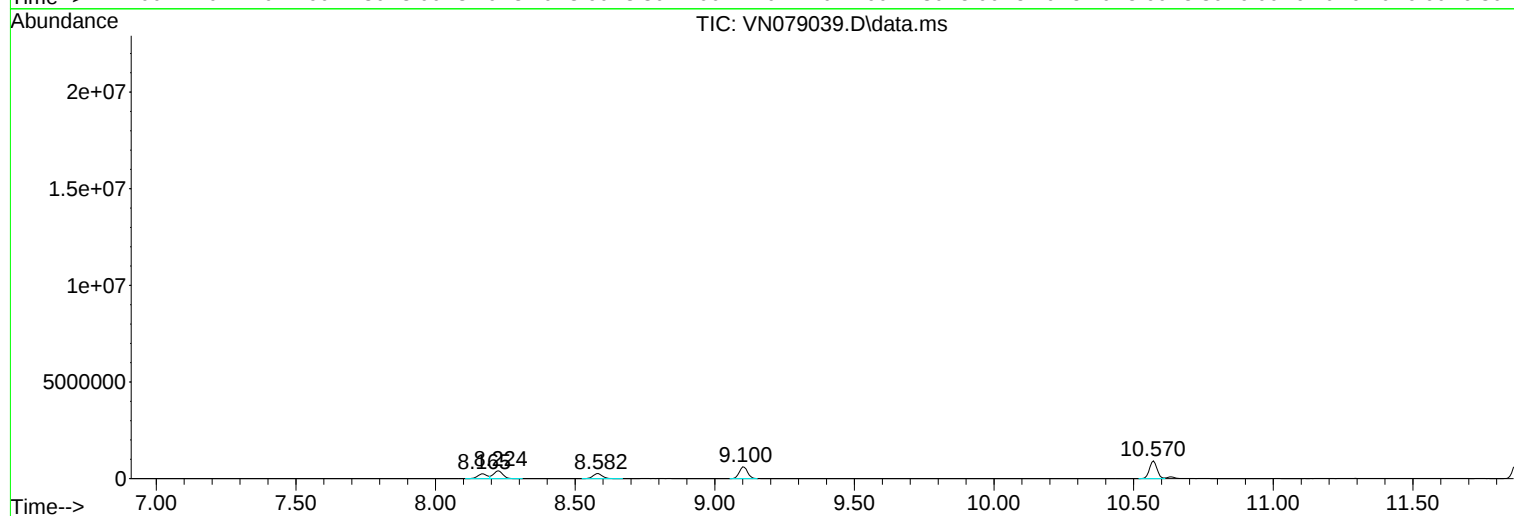
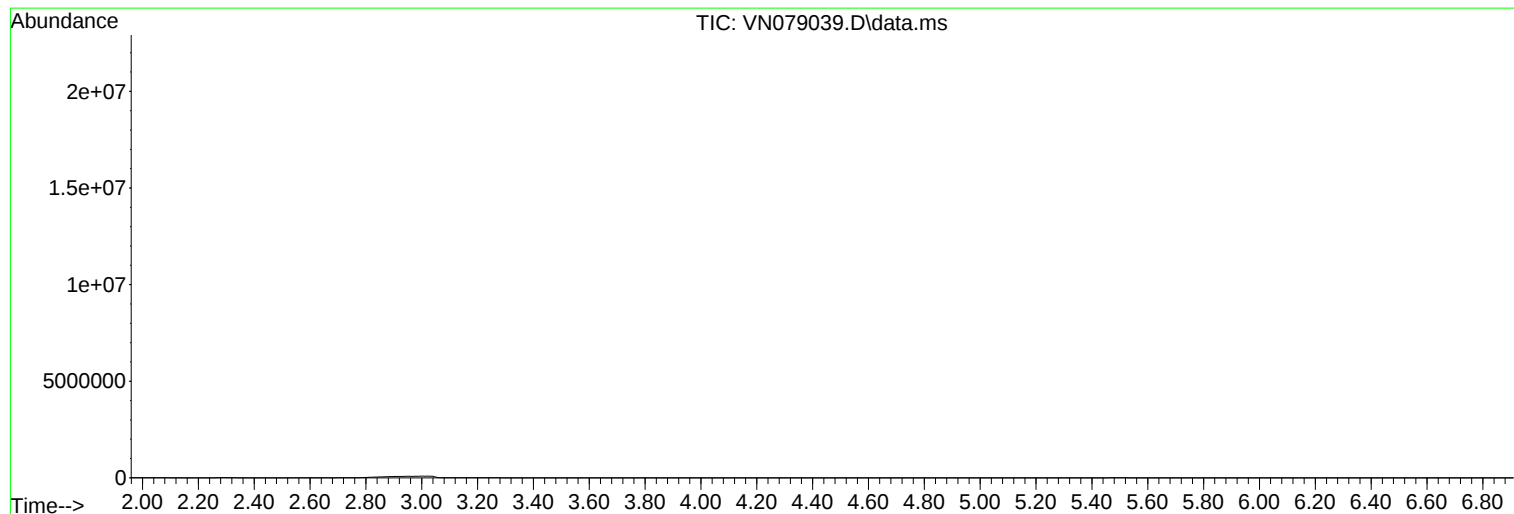
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NEVINS-SB05-Z113-114

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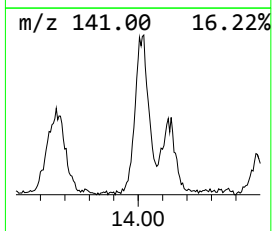
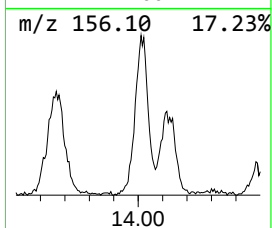
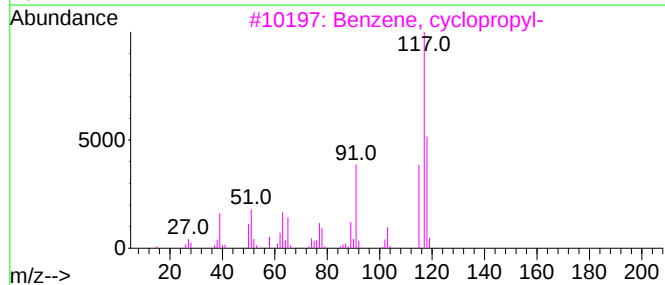
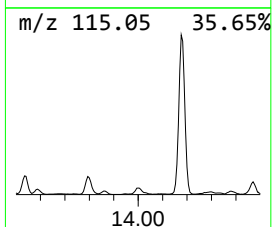
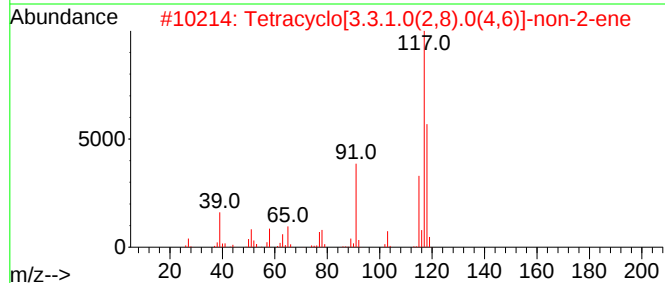
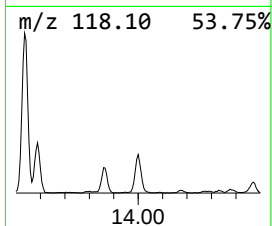
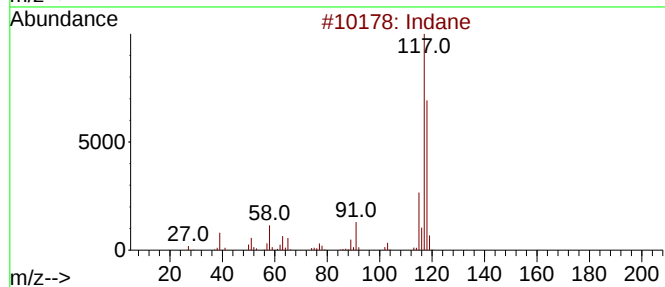
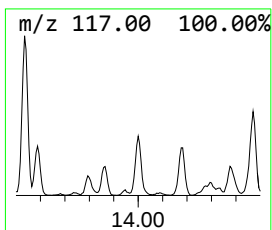
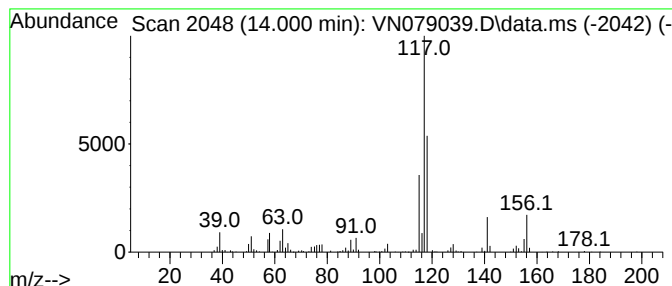
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	21.70 ug/l	913600	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	70
2			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	52
4			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	49
5			Deltacyclene	118	C9H10	007785-10-6	47



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Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z113-114

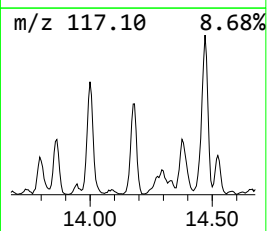
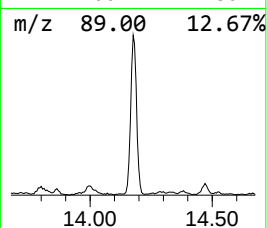
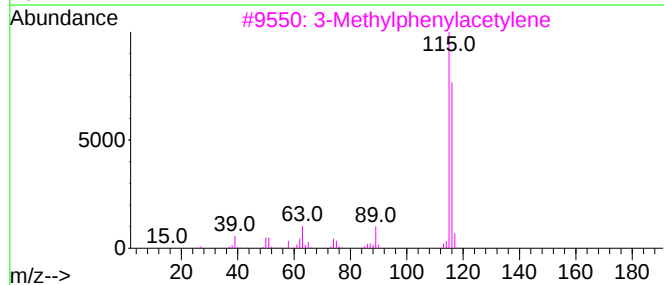
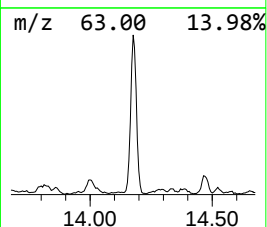
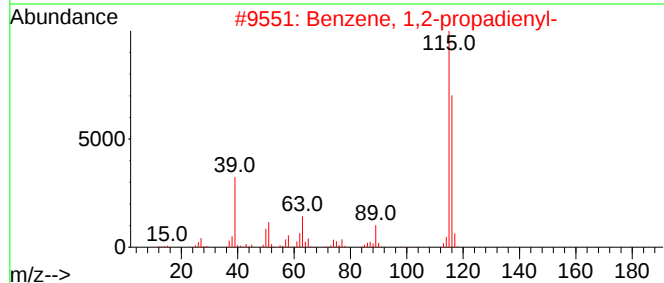
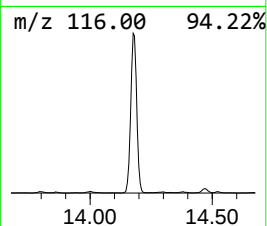
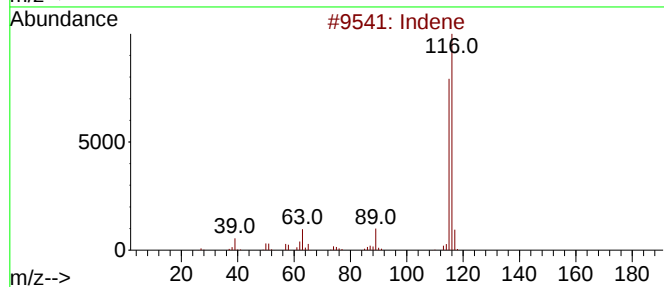
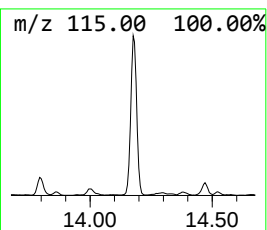
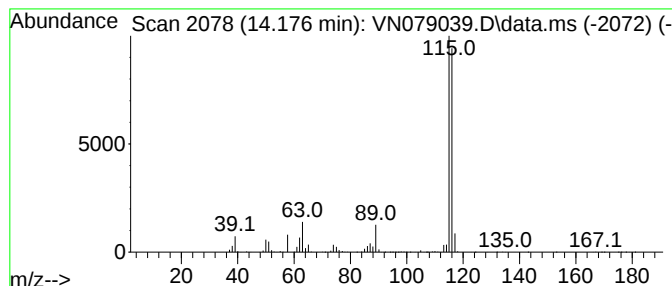
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 2 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	100.82 ug/l	4243920	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90



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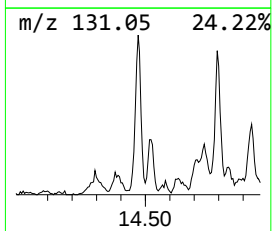
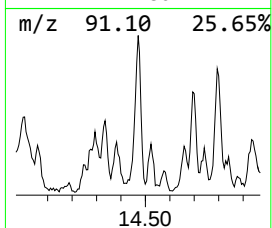
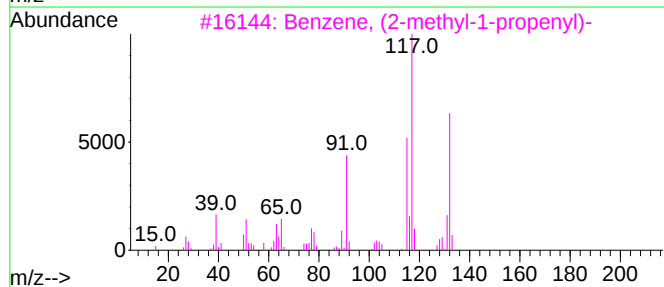
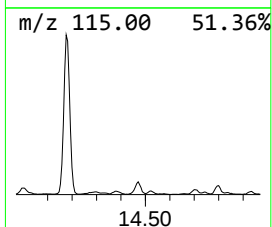
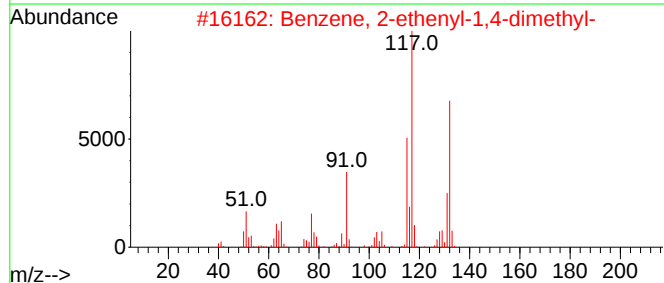
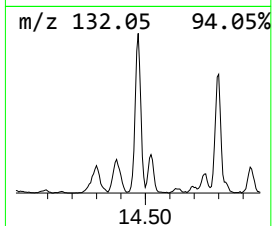
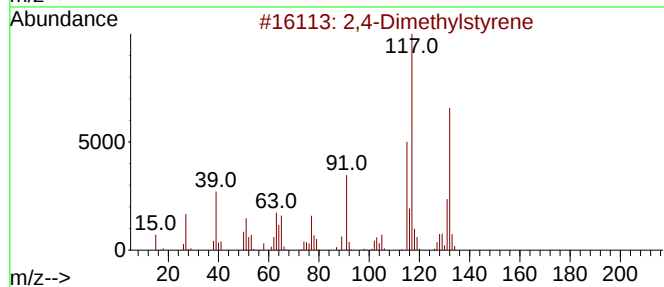
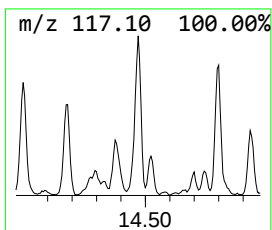
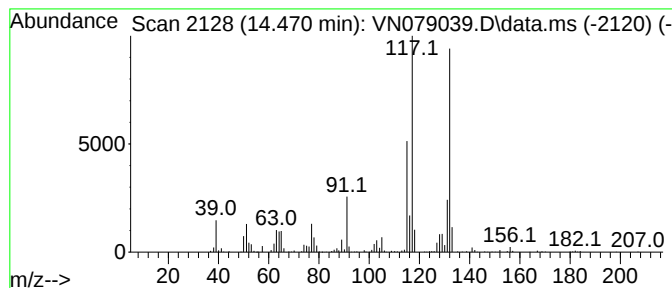
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Quant Title : SW846 8260

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

Peak Number 3 2,4-Dimethylstyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.470	26.43 ug/l	1112680	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dimethylstyrene	132	C10H12	002234-20-0	96
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	95
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	94
5			o-Isopropenyltoluene	132	C10H12	007399-49-7	94



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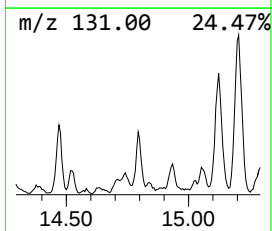
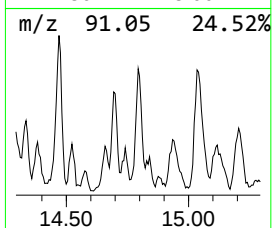
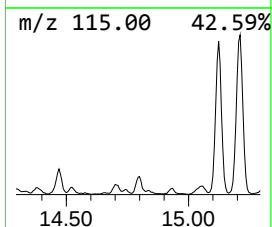
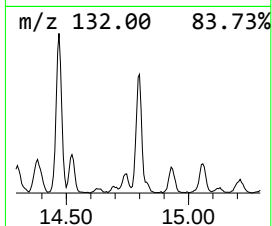
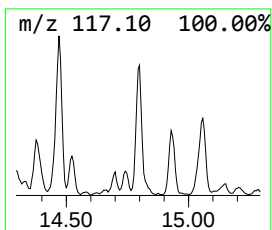
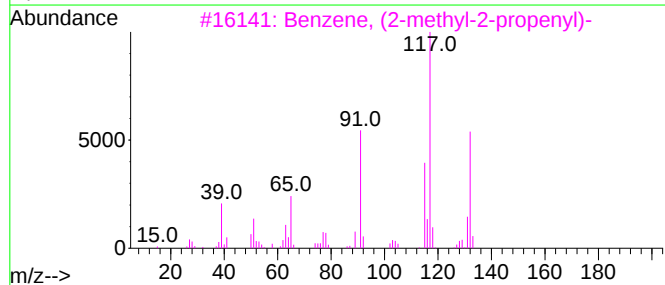
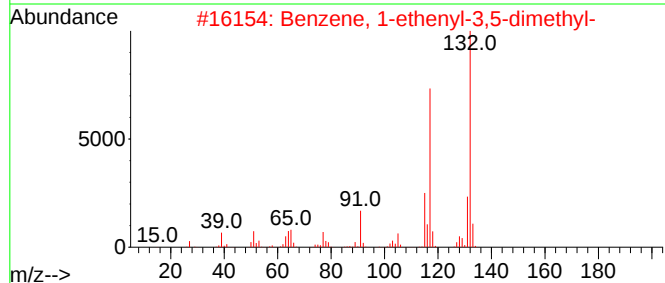
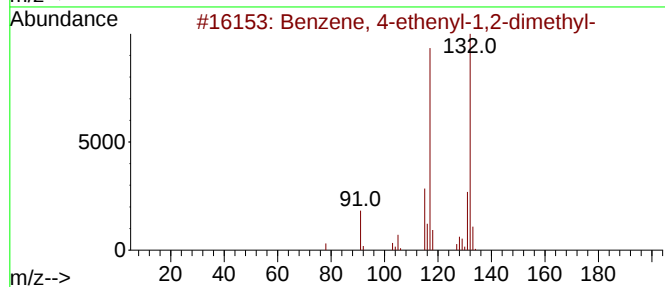
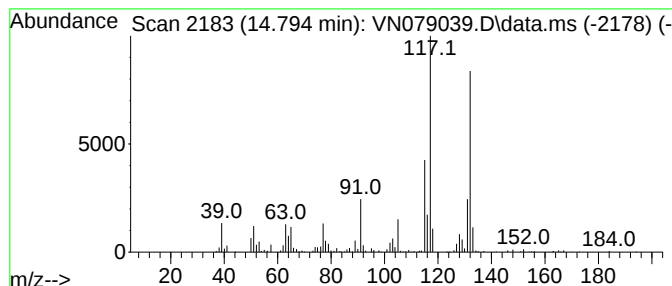
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 4-ethenyl-1,2-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.794	19.03 ug/l	800948	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethenyl-1,2-dimethyl-	132	C10H12	027831-13-6	97
2			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	95
3			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	95
4			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	95
5			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	94



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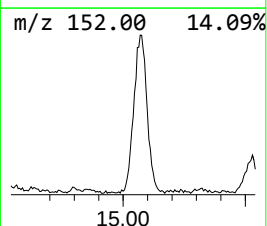
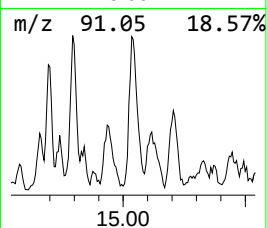
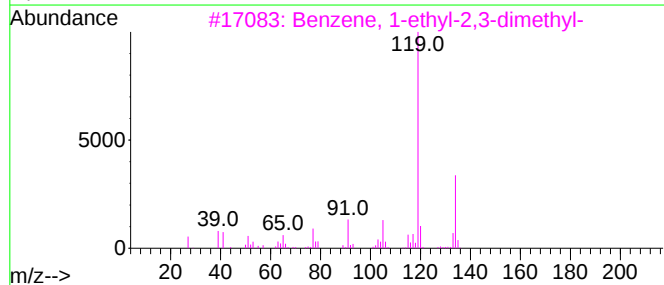
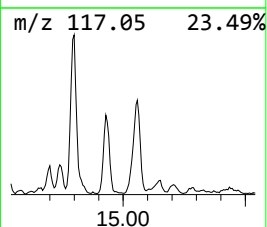
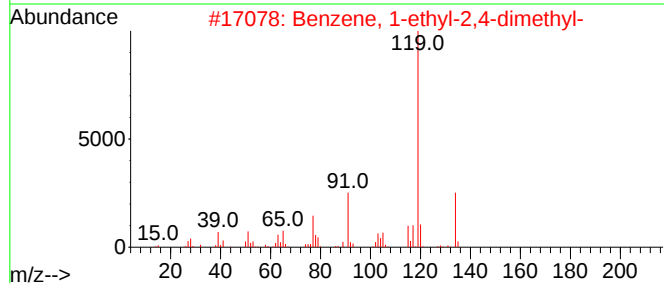
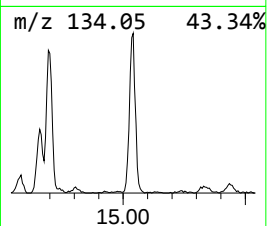
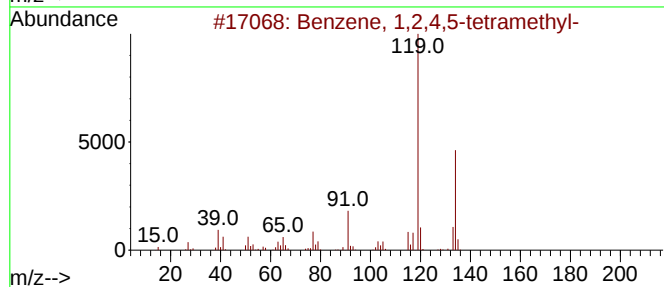
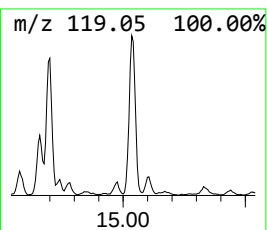
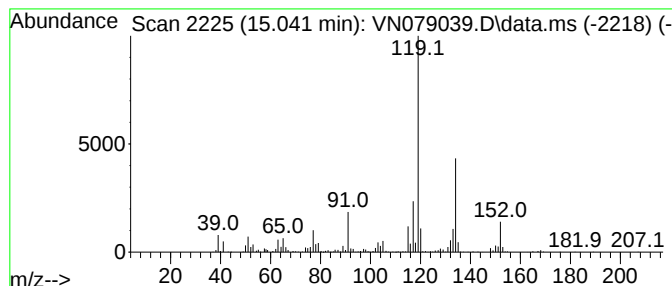
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	32.34 ug/l	1361230	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
2			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	87
4			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	87
5			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079039.D
Acq On : 24 Aug 2023 18:18
Operator : JC\MD
Sample : 04075-01
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z113-114

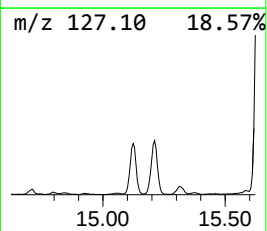
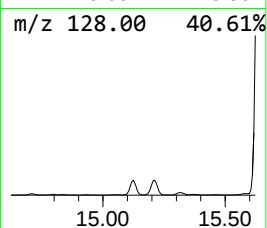
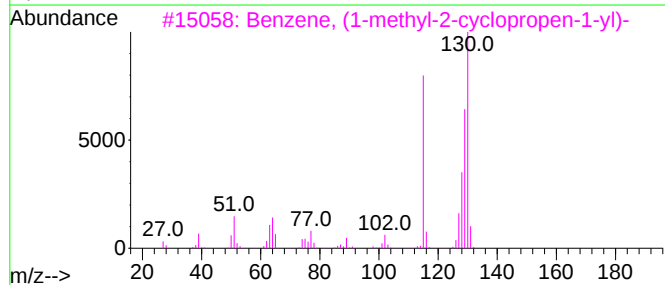
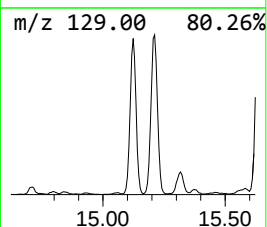
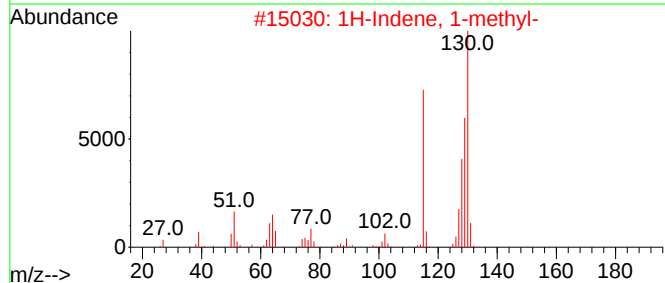
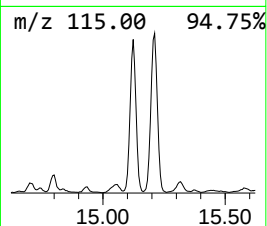
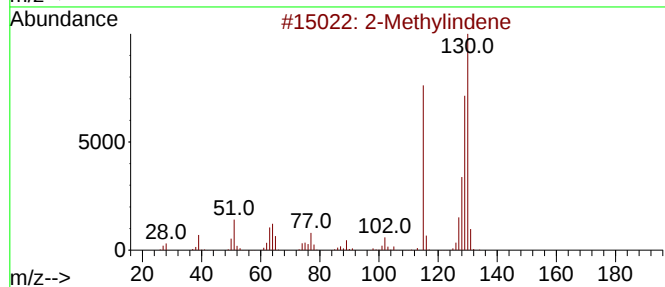
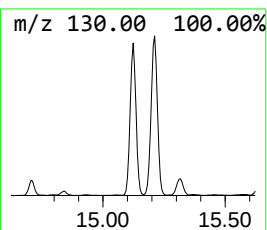
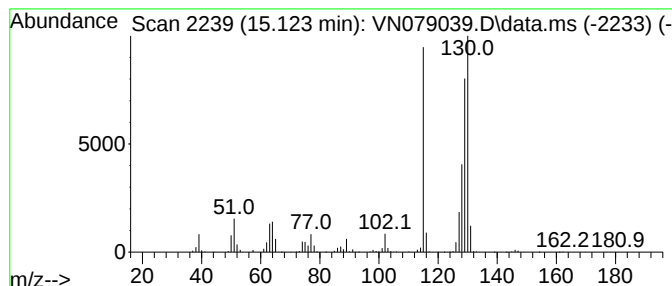
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Quant Title : SW846 8260

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

Peak Number 6 2-Methylindene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.123	87.94 ug/l	3701590	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			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3			Benzene, (1-methyl-2-cyclopropen-1-yl)-	130	C10H10	065051-83-4	96
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
5			Benzene, 1-butylnyl-	130	C10H10	000622-76-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079039.D
Acq On : 24 Aug 2023 18:18
Operator : JC\MD
Sample : 04075-01
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z113-114

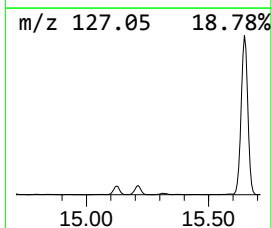
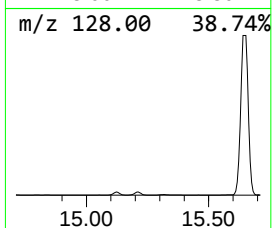
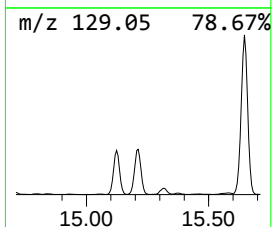
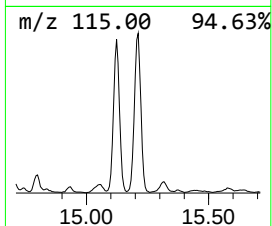
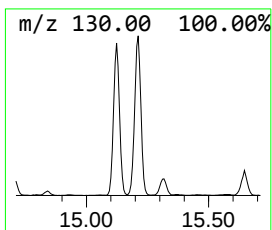
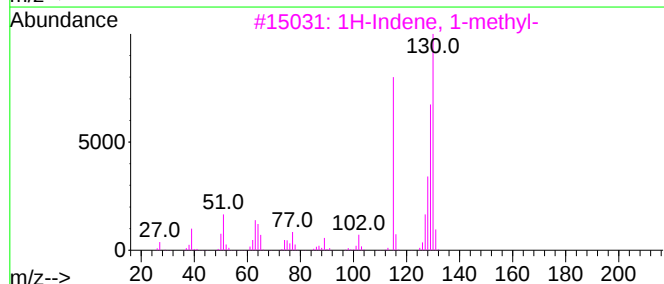
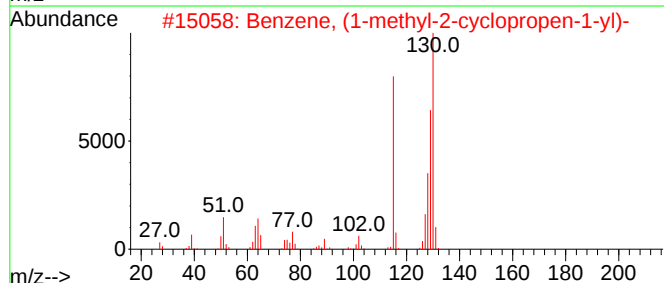
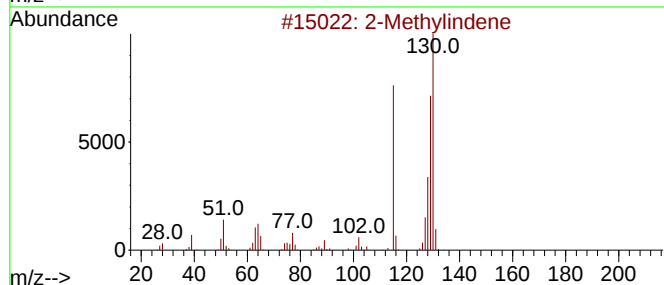
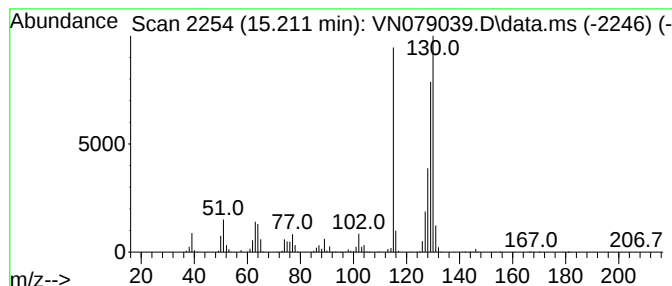
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, (1-methyl-2-cyclop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.211	96.60 ug/l	4066020	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	97
3	1H-Indene, 1-methyl-			130	C10H10	000767-59-9	96
4	Benzene, 1-butynyl-			130	C10H10	000622-76-4	95
5	Benzene,1-methyl-1,2-propadienyl-			130	C10H10	022433-39-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079039.D
Acq On : 24 Aug 2023 18:18
Operator : JC\MD
Sample : 04075-01
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z113-114

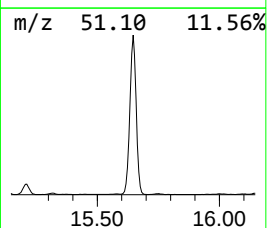
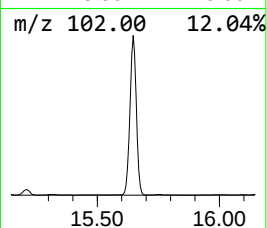
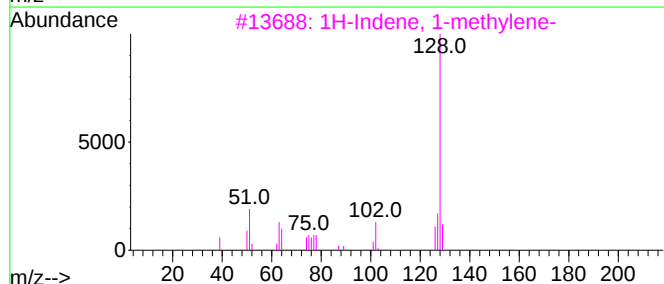
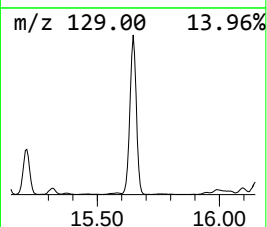
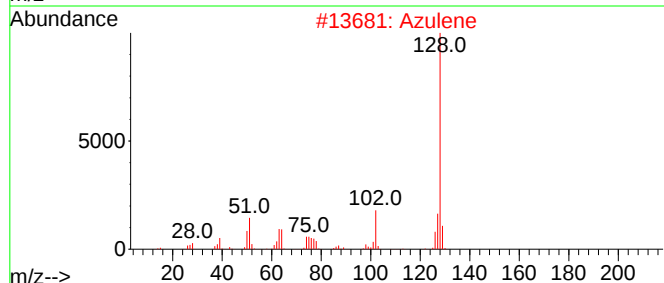
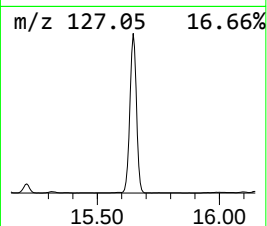
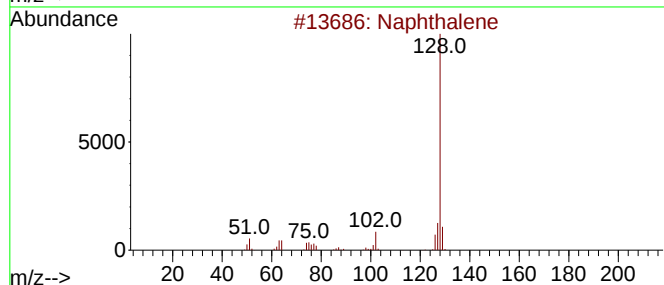
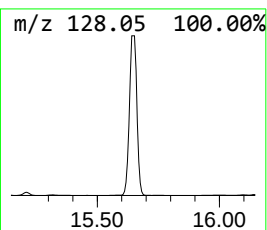
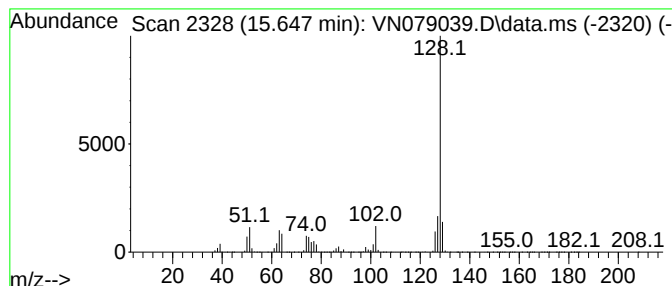
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Quant Title : SW846 8260

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

Peak Number 8 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	1006.22 ug/l	42354900	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	96
2			Azulene	128	C10H8	000275-51-4	93
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	72
5			Tetracyanoethylene	128	C6N4	000670-54-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079039.D
Acq On : 24 Aug 2023 18:18
Operator : JC\MD
Sample : 04075-01
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z113-114

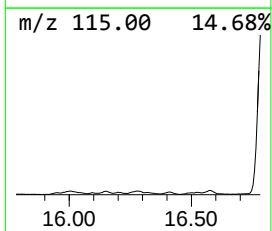
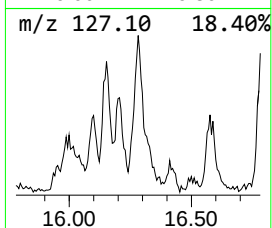
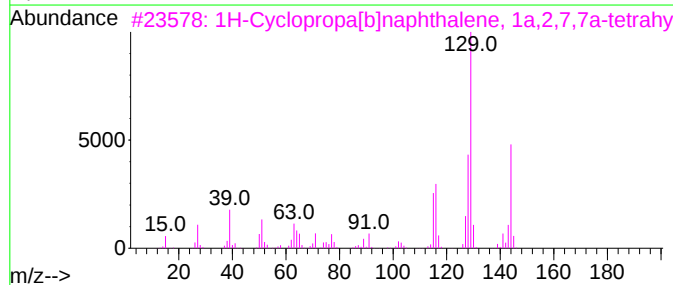
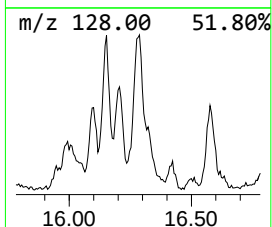
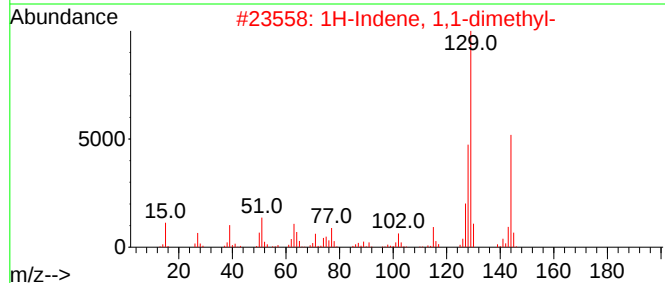
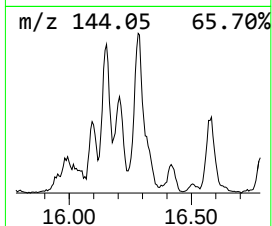
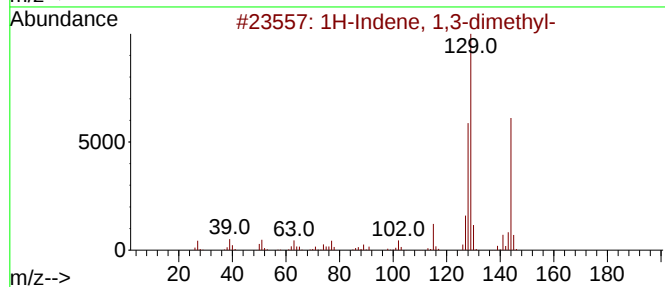
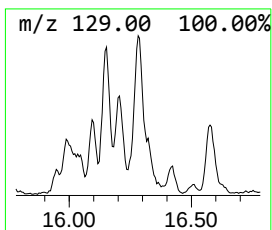
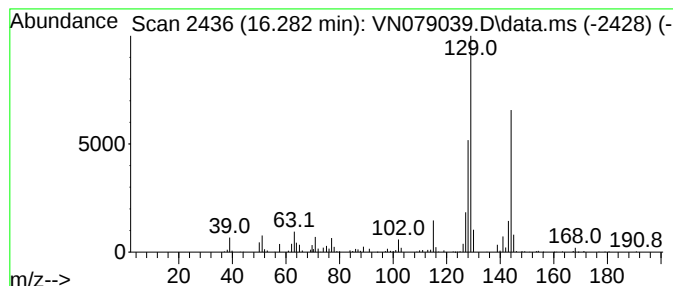
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Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, 1,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.282	20.63 ug/l	868462	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1,3-dimethyl-	144	C11H12	002177-48-2	96		
2	1H-Indene, 1,1-dimethyl-	144	C11H12	018636-55-0	94		
3	1H-Cyclopropa[b]naphthalene, 1a,...	144	C11H12	006571-72-8	93		
4	Naphthalene, 1,2-dihydro-4-methyl-	144	C11H12	004373-13-1	91		
5	1H-Indene, 4,7-dimethyl-	144	C11H12	006974-97-6	91		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079039.D
Acq On : 24 Aug 2023 18:18
Operator : JC\MD
Sample : 04075-01
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z113-114

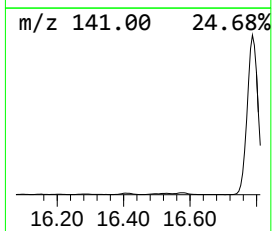
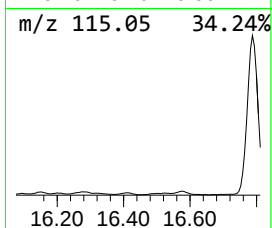
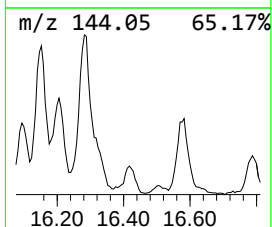
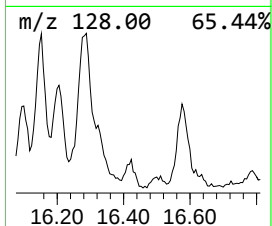
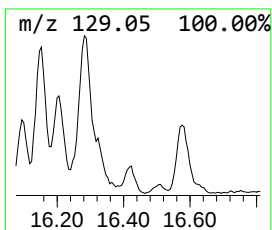
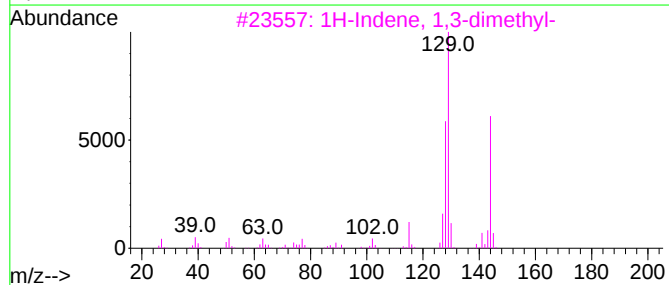
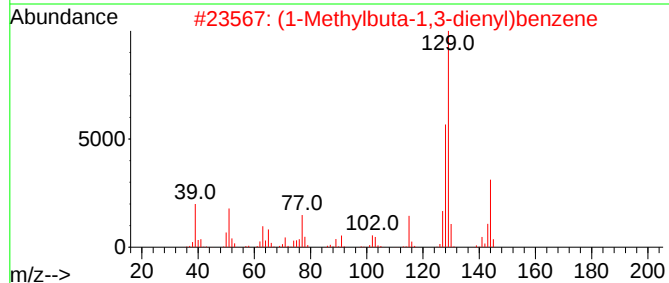
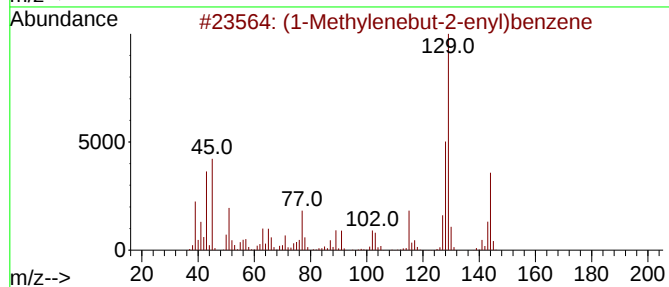
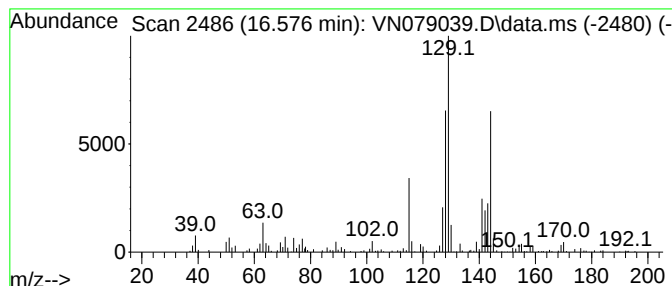
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Quant Title : SW846 8260

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

Peak Number 10 (1-Methylenebut-2-enyl)benzene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.576	19.67 ug/l	827812	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1-Methylenebut-2-enyl)benzene	144	C11H12	070588-46-4	81
2			(1-Methylbuta-1,3-dienyl)benzene	144	C11H12	054758-36-0	81
3			1H-Indene, 1,3-dimethyl-	144	C11H12	002177-48-2	76
4			1H-Cyclopropa[b]naphthalene, 1a,...	144	C11H12	006571-72-8	74
5			5H-Benzocycloheptene, 6,7-dihydro-	144	C11H12	007125-62-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079039.D
Acq On : 24 Aug 2023 18:18
Operator : JC\MD
Sample : 04075-01
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z113-114

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

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					#	RT	Resp	Conc
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Indene	14.176	100.8	ug/l	4243920	4	13.794	2104660	50.0
2,4-Dimethylsty...	14.470	26.4	ug/l	1112680	4	13.794	2104660	50.0
Benzene, 4-ethe...	14.794	19.0	ug/l	800948	4	13.794	2104660	50.0
Benzene, 1,2,4,...	15.041	32.3	ug/l	1361230	4	13.794	2104660	50.0
2-Methylindene	15.123	87.9	ug/l	3701590	4	13.794	2104660	50.0
Benzene, (1-met...	15.211	96.6	ug/l	4066020	4	13.794	2104660	50.0
Azulene	15.647	1006.2	ug/l	42354900	4	13.794	2104660	50.0
1H-Indene, 1,3-...	16.282	20.6	ug/l	868462	4	13.794	2104660	50.0
(1-Methylenebut...	16.576	19.7	ug/l	827812	4	13.794	2104660	50.0