

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
 Data File : VN079037.D
 Acq On : 24 Aug 2023 17:30
 Operator : JC\MD
 Sample : 04047-04 40X
 Misc : 6.72g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NEVINS-SB05-Z83-84

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: VN079037.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	rBV	2698004	6475303	4.40%	1.941%
2	10.571	1457	1465	1470	rBV	946486	1763722	1.20%	0.529%
3	10.635	1470	1476	1489	rVB	6844655	12311383	8.37%	3.691%
4	11.870	1678	1686	1695	rBV	886829	1593845	1.08%	0.478%
5	11.970	1695	1703	1711	rVV	9590196	16446943	11.18%	4.930%
6	12.070	1712	1720	1731	rVB	5772091	11018766	7.49%	3.303%
7	12.406	1764	1777	1785	rBV2	3463600	6624760	4.50%	1.986%
8	13.100	1889	1895	1898	rBV	2027646	3428196	2.33%	1.028%
9	13.135	1898	1901	1905	rVV	2005660	3226276	2.19%	0.967%
10	13.176	1905	1908	1914	rVV	1081338	1675308	1.14%	0.502%
11	13.341	1914	1936	1951	rVB4	1410099	6697374	4.55%	2.008%
12	13.488	1951	1961	1965	rBV	3291000	5848947	3.97%	1.753%
13	13.535	1965	1969	1974	rVV	5118240	7751553	5.27%	2.324%
14	13.588	1974	1978	1982	rVV	827597	1488464	1.01%	0.446%
15	13.676	1983	1993	2008	rVV3	969112	4664732	3.17%	1.398%
16	13.800	2008	2014	2015	rVV	976537	1513346	1.03%	0.454%
17	13.823	2015	2018	2022	rVV	1284290	2138128	1.45%	0.641%
18	14.000	2034	2048	2061	rBV3	3587087	11016635	7.49%	3.302%
19	14.117	2061	2068	2072	rVV4	753009	2236468	1.52%	0.670%
20	14.176	2072	2078	2086	rVB	20026073	33937331	23.06%	10.173%
21	14.470	2119	2128	2133	rBV	1981389	3713923	2.52%	1.113%
22	14.794	2178	2183	2188	rBV2	1207399	2011990	1.37%	0.603%
23	15.041	2218	2225	2232	rBV2	903139	2426889	1.65%	0.727%
24	15.123	2232	2239	2247	rVB	5594533	9971488	6.78%	2.989%
25	15.211	2247	2254	2261	rVB	5762489	10606037	7.21%	3.179%
26	15.317	2262	2272	2278	rBV2	875880	1959814	1.33%	0.587%
27	15.523	2288	2307	2320	rBV	1471760	6890834	4.68%	2.066%
28	15.647	2320	2328	2338	rVV2	71022936	147154395	100.00%	44.112%
29	15.747	2339	2345	2353	rVB	1540528	3021910	2.05%	0.906%
30	16.282	2428	2436	2452	rVB2	656044	2367777	1.61%	0.710%
31	16.576	2480	2486	2502	rVB3	534624	1613362	1.10%	0.484%

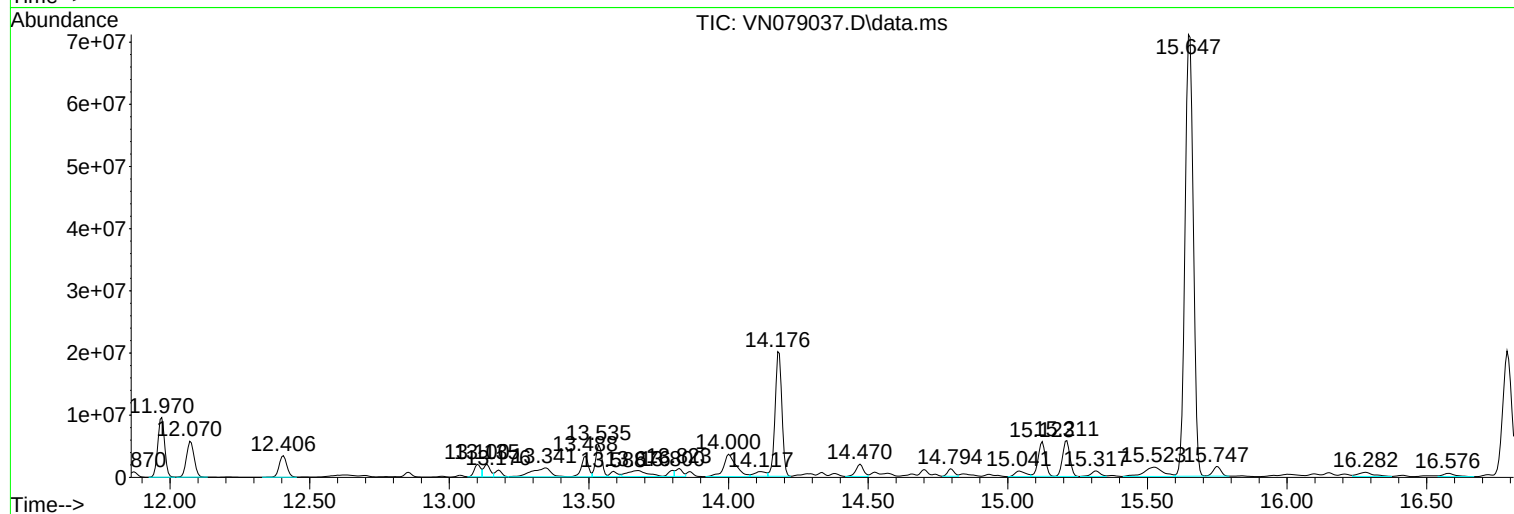
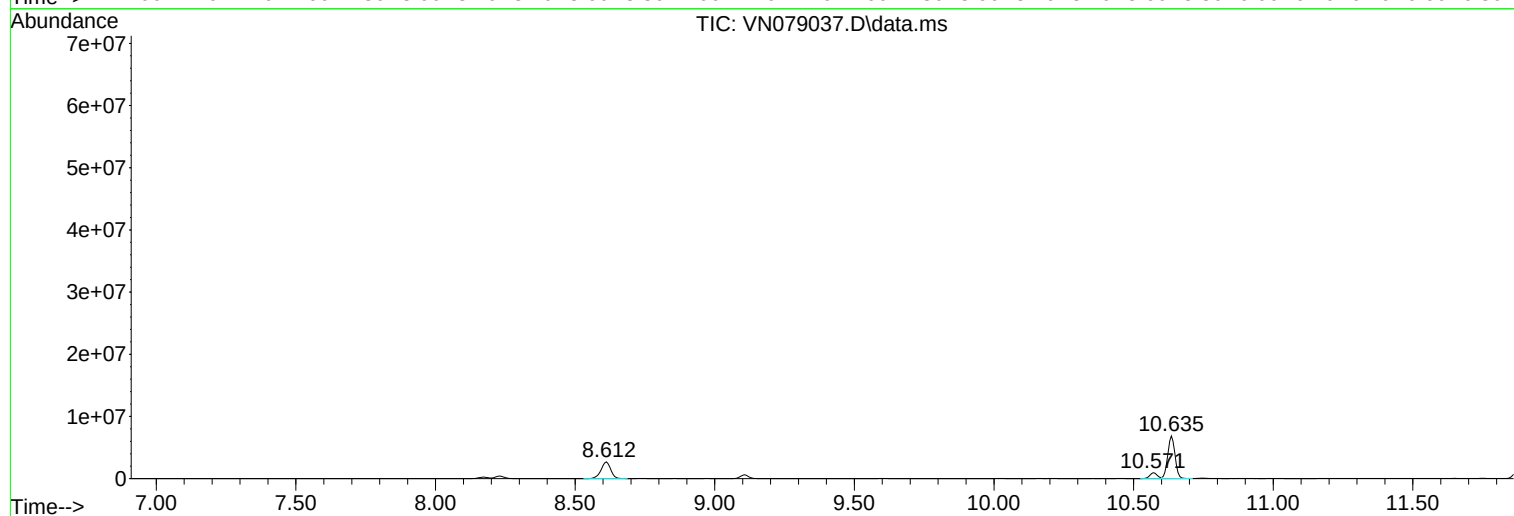
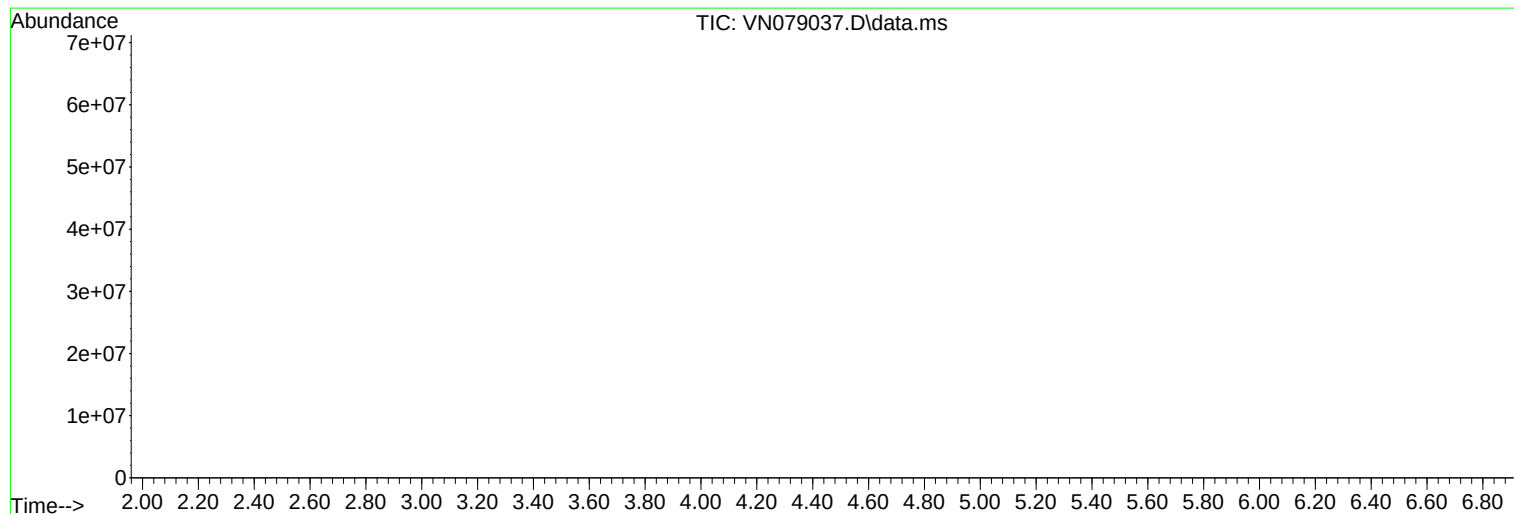
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Instrument :
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ClientSampleId :
NEVINS-SB05-Z83-84

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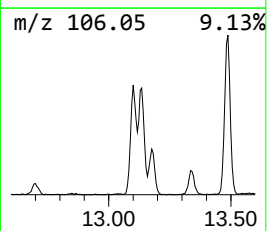
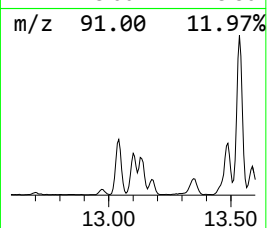
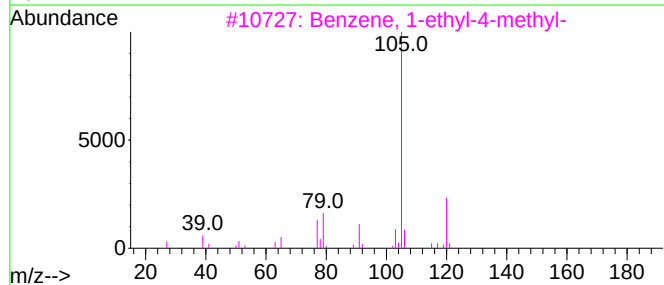
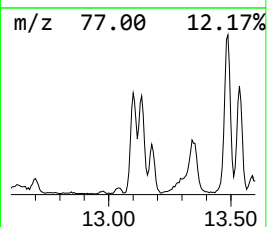
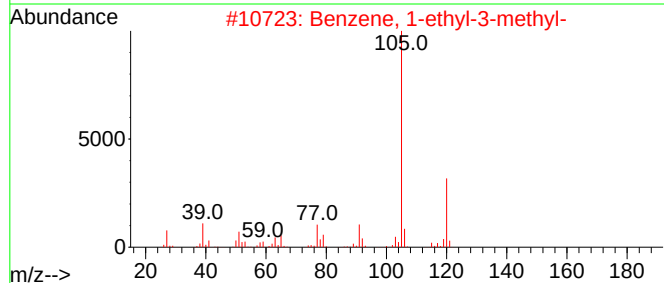
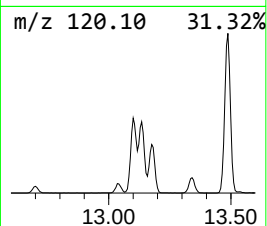
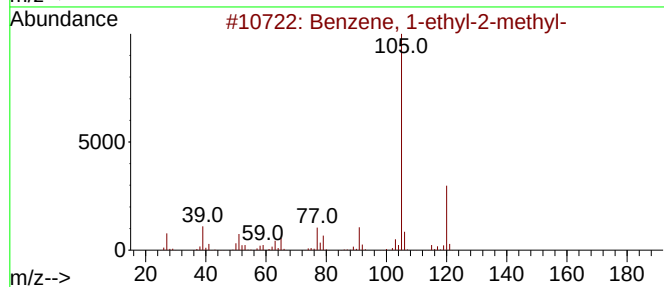
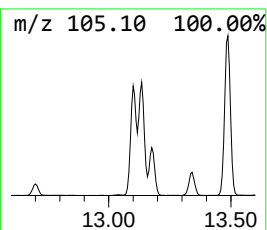
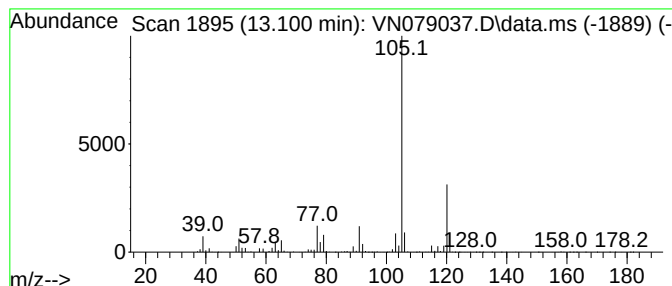
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	113.27 ug/l	3428200	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	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



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Instrument :
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ClientSampleId :
NEVINS-SB05-Z83-84

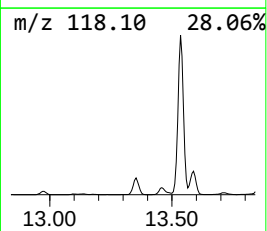
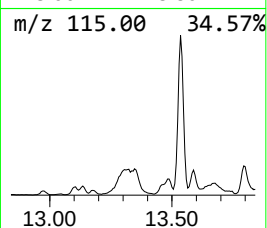
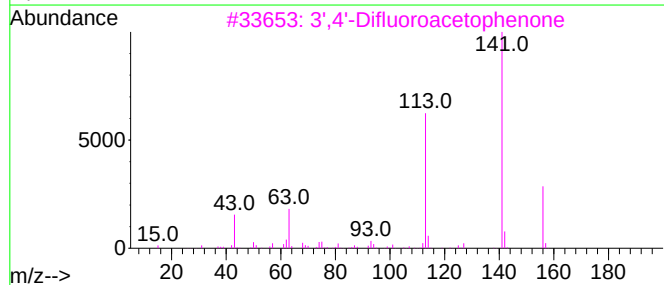
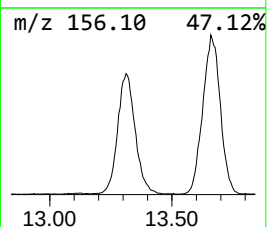
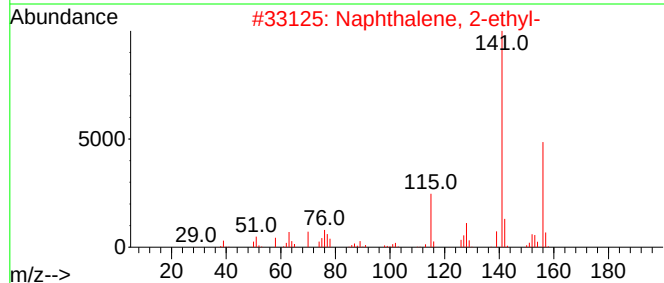
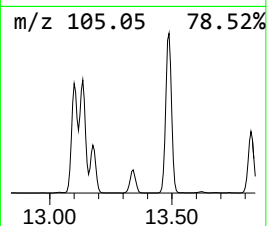
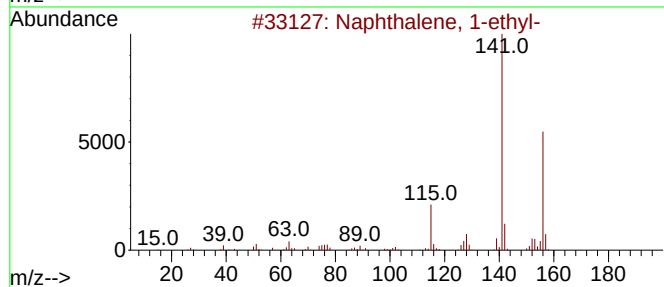
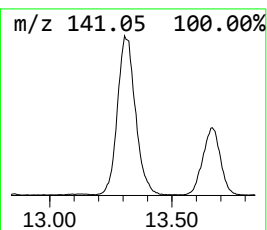
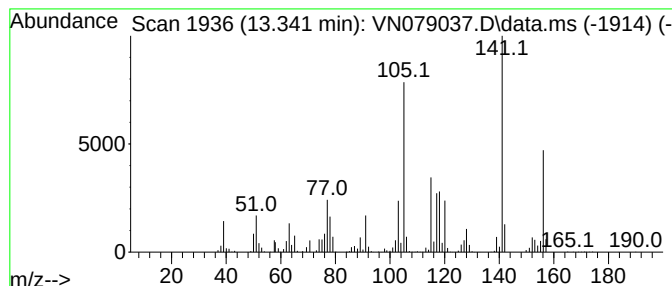
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, 1-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	221.28 ug/l	6697370	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	91
2			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	91
3			3',4'-Difluoroacetophenone	156	C8H6F2O	000369-33-5	43
4			2,5-Dimethoxyfluorobenzene	156	C8H9FO2	082830-49-7	38
5			2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	38



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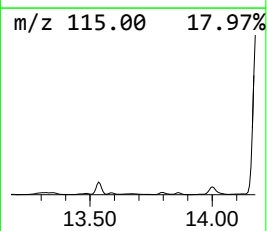
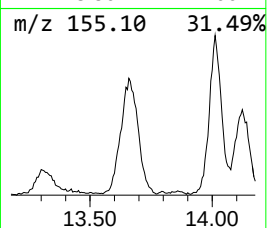
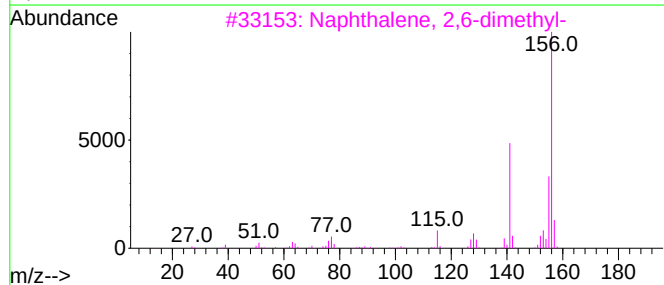
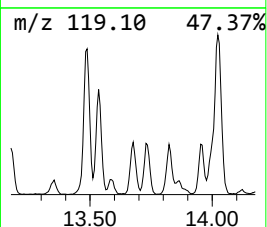
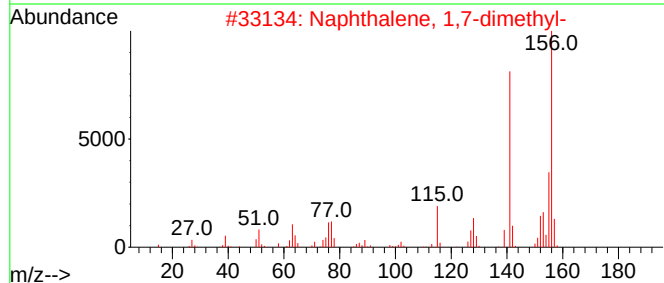
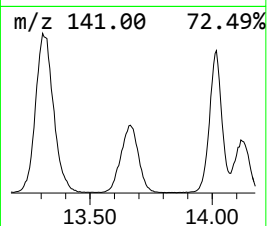
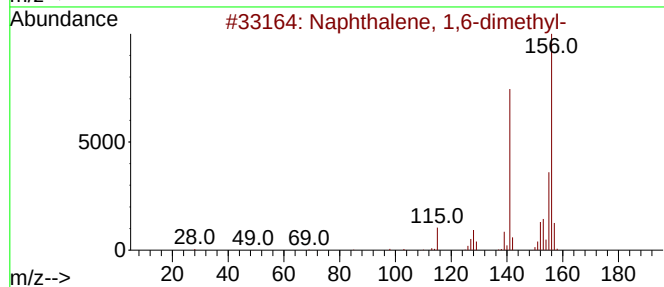
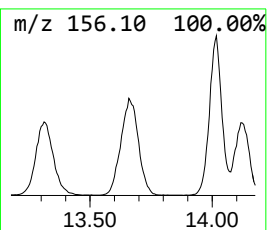
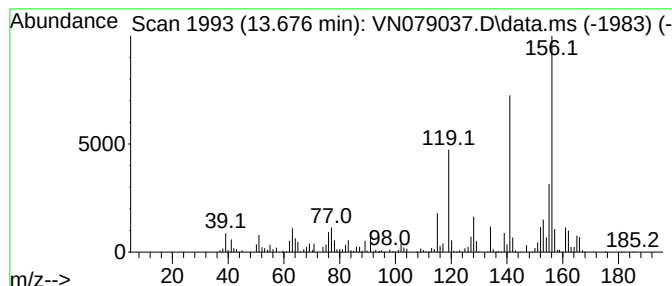
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Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	154.12 ug/l	4664730	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	94
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	93
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	93



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Instrument :
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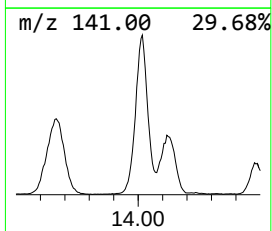
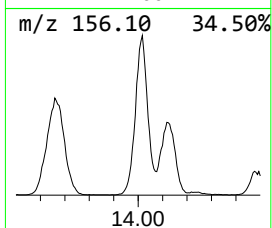
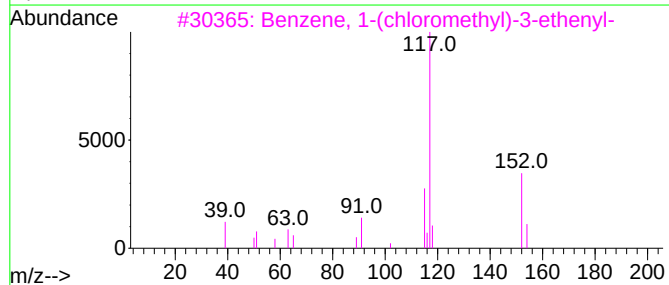
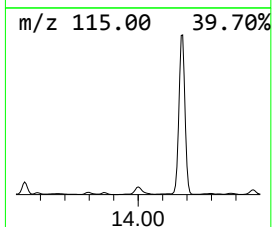
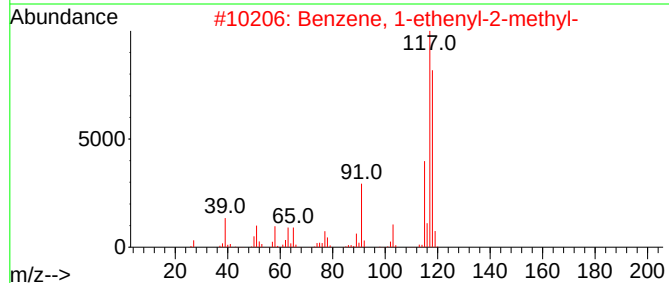
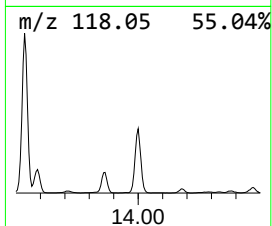
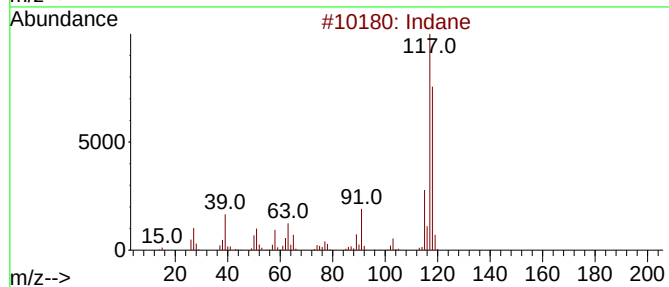
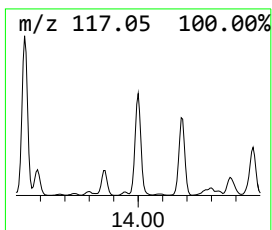
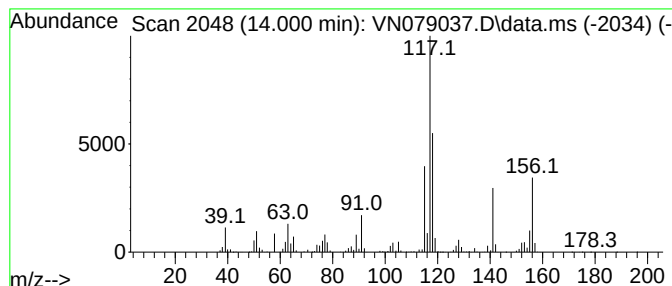
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	363.98 ug/l	11016600	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	90
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
3			Benzene, 1-(chloromethyl)-3-ethe...	152	C9H9Cl	039833-65-3	55
4			Deltacyclene	118	C9H10	007785-10-6	50
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	50



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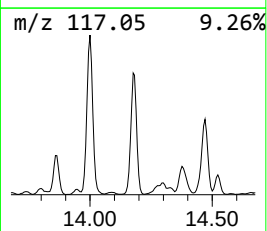
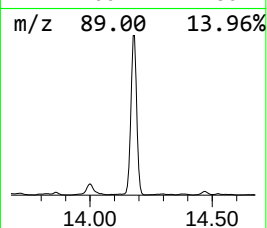
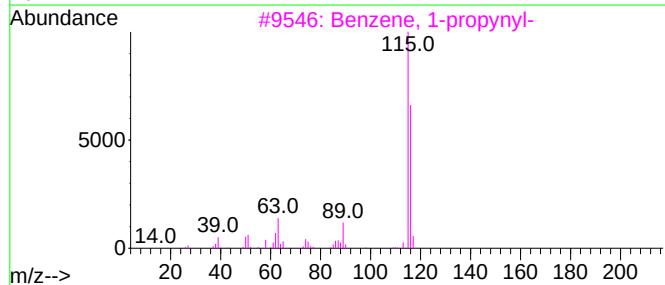
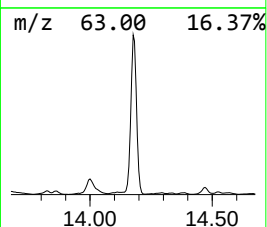
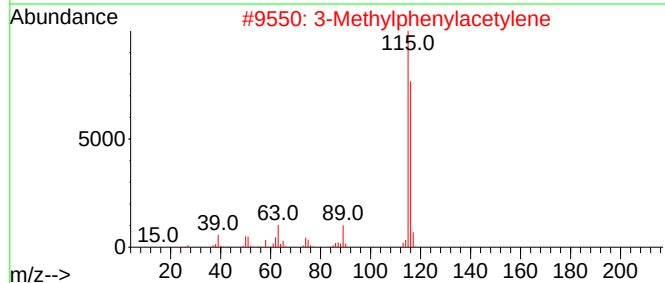
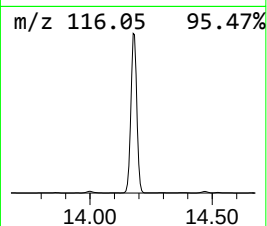
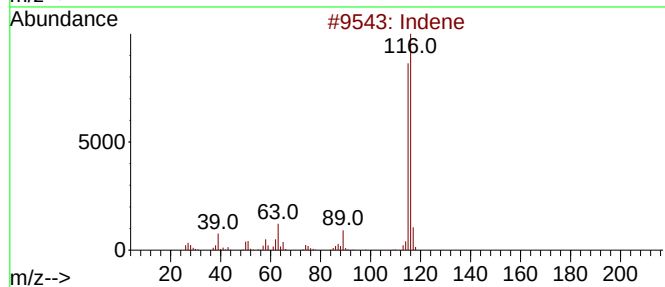
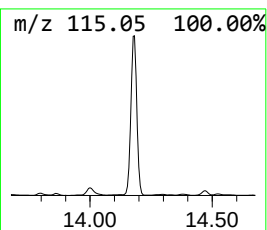
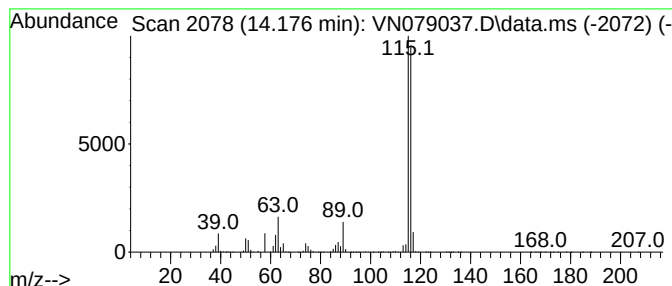
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Quant Title : SW846 8260

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

Peak Number 5 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	1121.27 ug/l	33937300	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	96
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	91



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MSVOA_N
ClientSampleId :
NEVINS-SB05-Z83-84

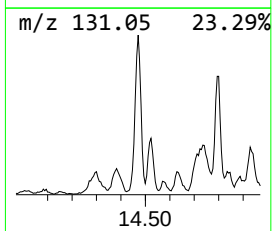
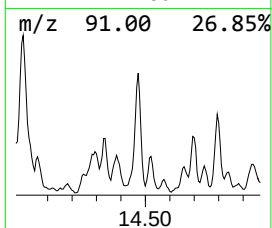
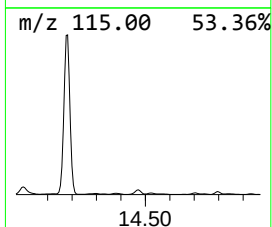
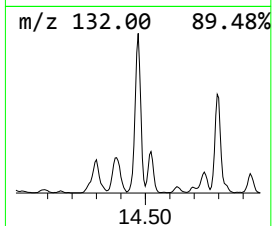
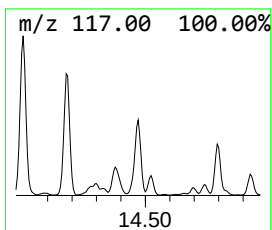
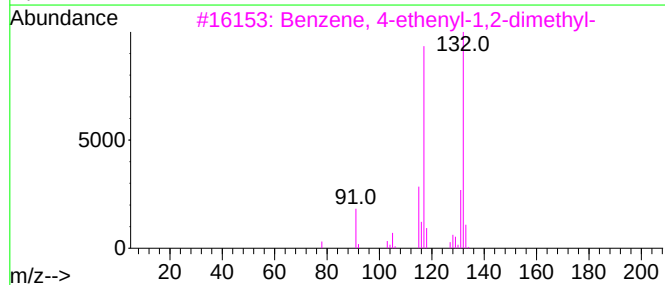
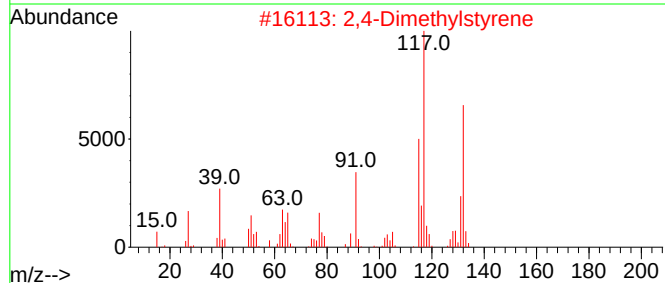
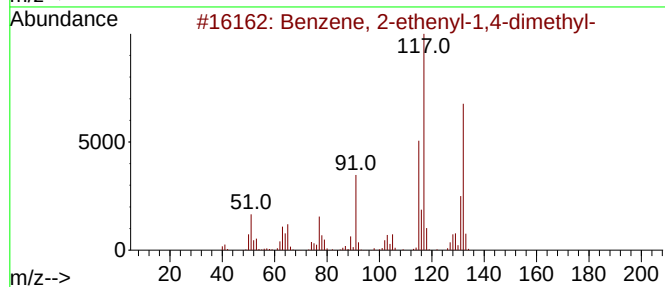
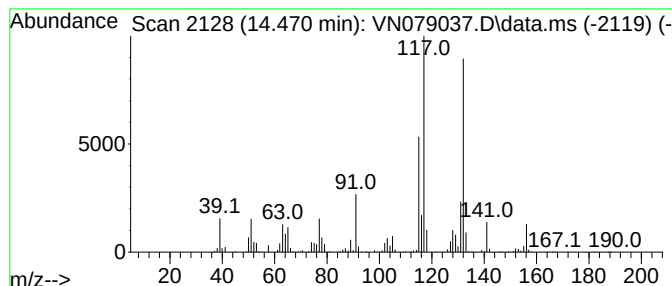
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.470	122.71 ug/l	3713920	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	95
2			2,4-Dimethylstyrene	132	C10H12	002234-20-0	95
3			Benzene, 4-ethenyl-1,2-dimethyl-	132	C10H12	027831-13-6	95
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	94
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079037.D
Acq On : 24 Aug 2023 17:30
Operator : JC\MD
Sample : 04047-04 40X
Misc : 6.72g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z83-84

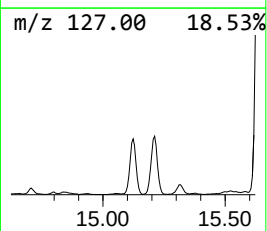
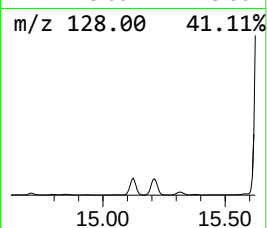
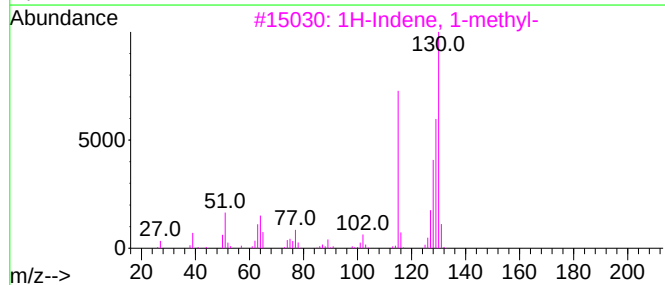
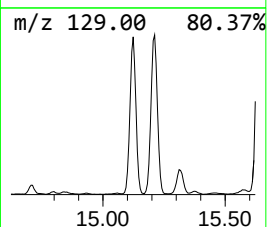
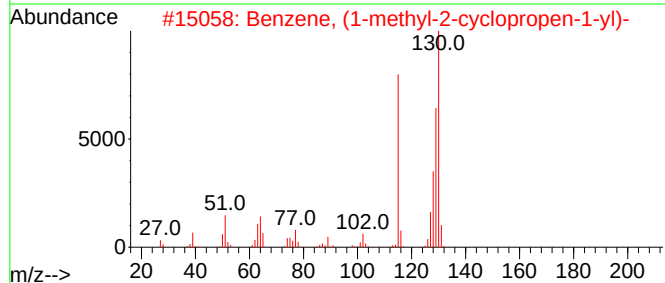
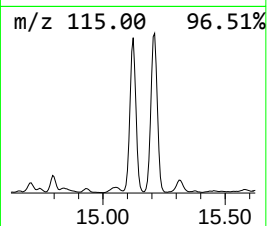
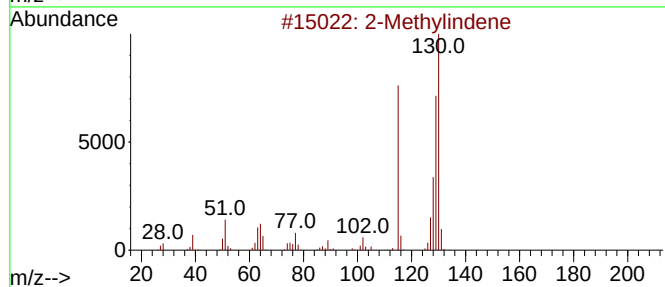
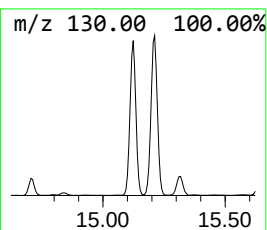
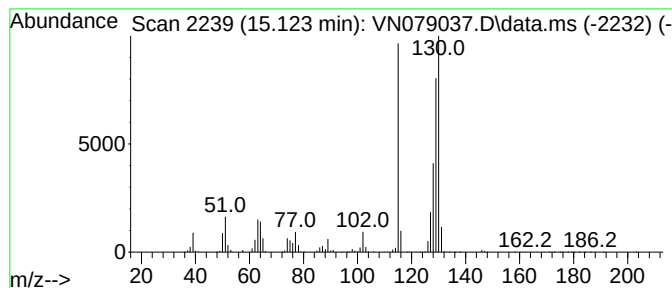
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Quant Title : SW846 8260

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

Peak Number 7 2-Methylindene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.123	329.45 ug/l	9971490	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-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93
5			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079037.D
Acq On : 24 Aug 2023 17:30
Operator : JC\MD
Sample : 04047-04 40X
Misc : 6.72g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z83-84

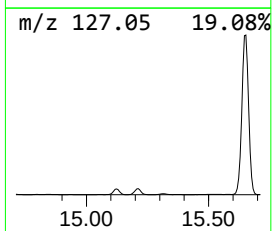
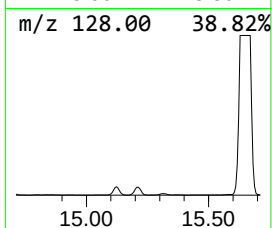
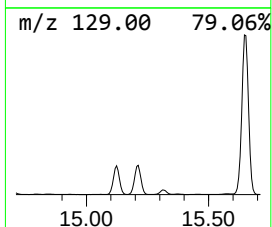
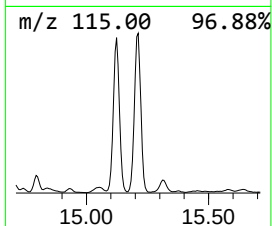
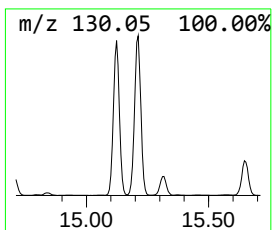
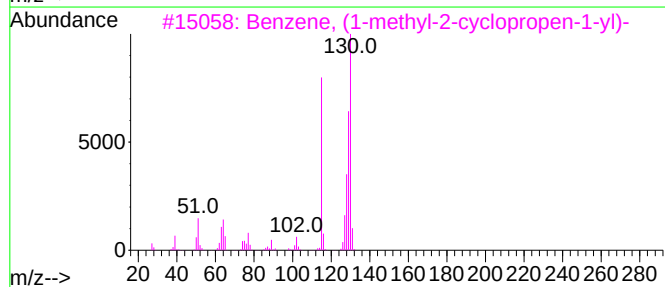
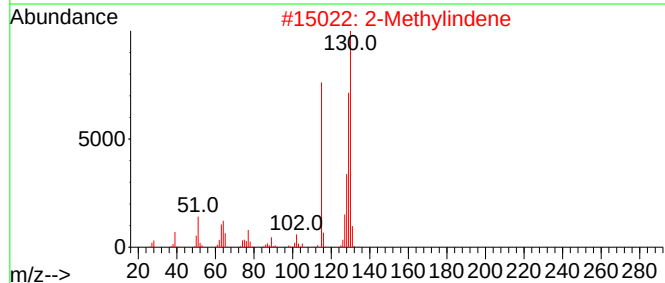
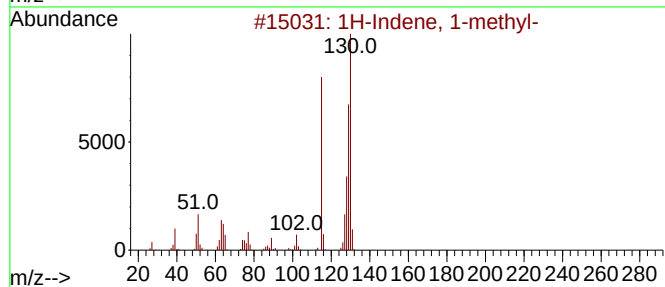
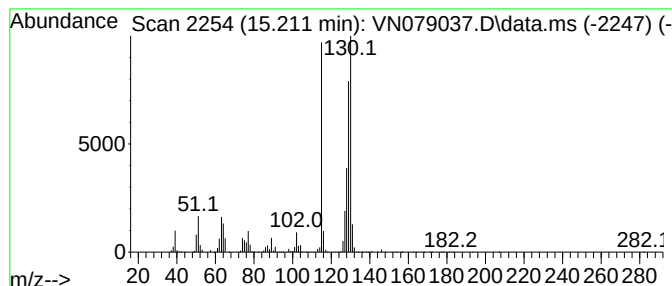
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.211	350.42 ug/l	10606000	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			2-Methylindene	130	C10H10	002177-47-1	96
3			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	95
5			Benzene, 1-butylnyl-	130	C10H10	000622-76-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079037.D
Acq On : 24 Aug 2023 17:30
Operator : JC\MD
Sample : 04047-04 40X
Misc : 6.72g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z83-84

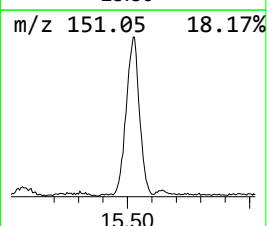
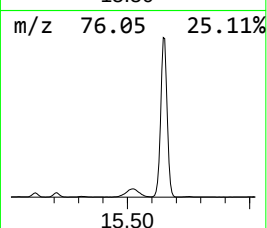
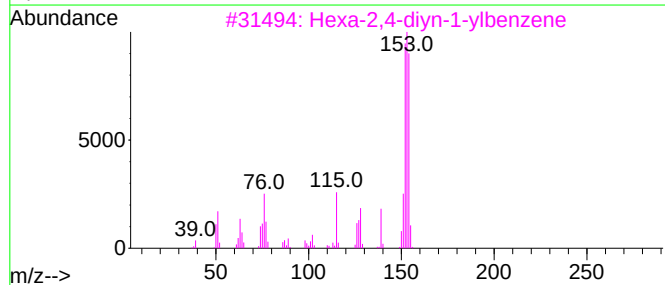
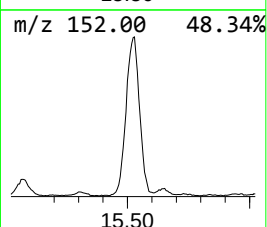
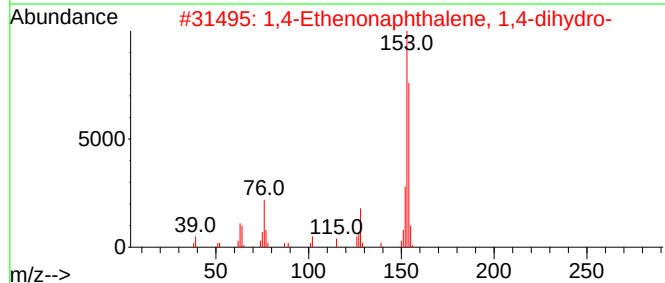
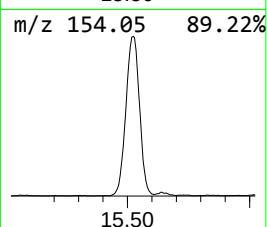
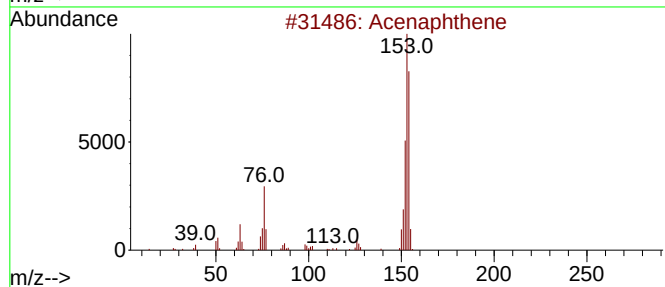
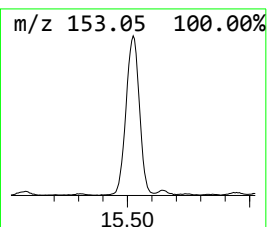
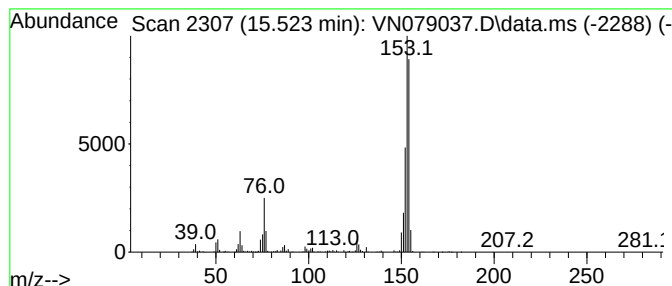
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Quant Title : SW846 8260

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

Peak Number 9 1,4-Ethenonaphthalene, 1,4-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.523	227.67 ug/l	6890830	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	89
2			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	64
3			Hexa-2,4-diyne-1-ylbenzene	154	C12H10	000520-74-1	59
4			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079037.D
Acq On : 24 Aug 2023 17:30
Operator : JC\MD
Sample : 04047-04 40X
Misc : 6.72g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z83-84

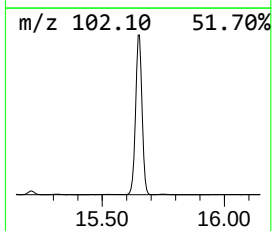
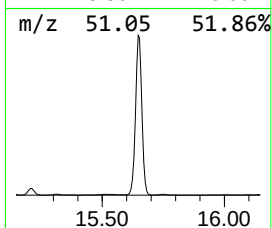
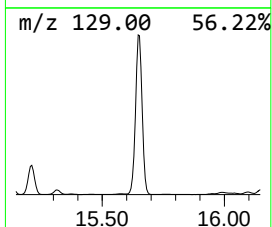
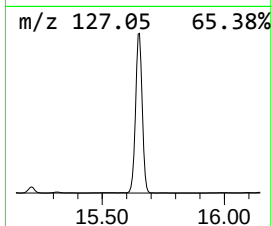
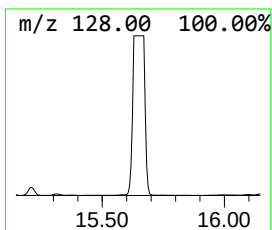
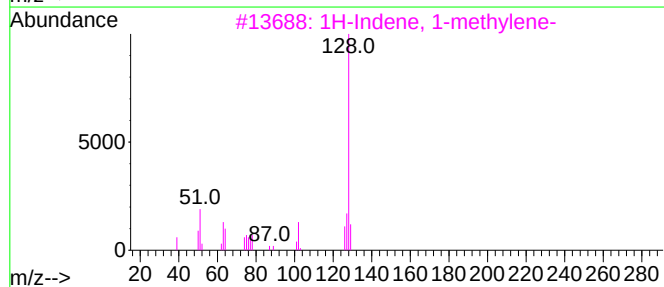
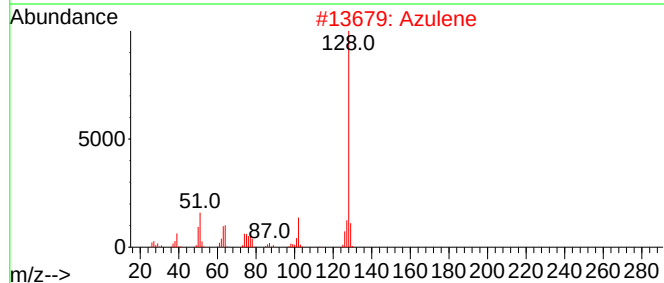
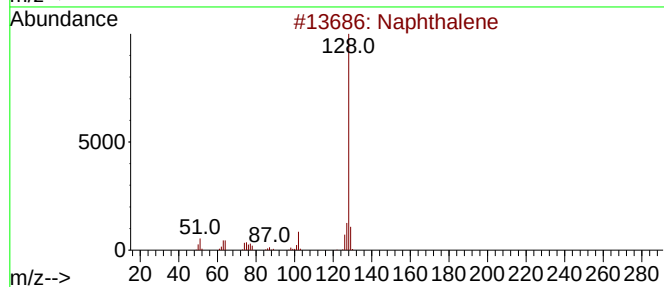
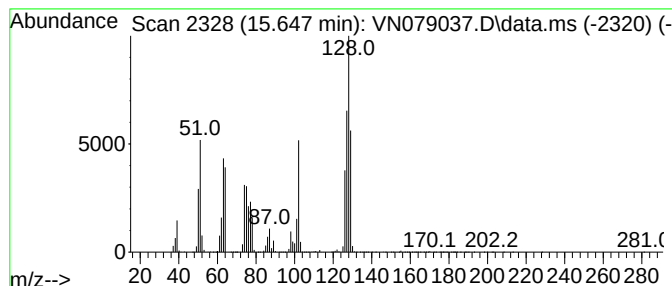
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 10 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	4861.89 ug/l	147154000	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		1H-Indene, 1-methylene-	128	C10H8	002471-84-3	74
4		4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	58
5		Phenol, 2-chloro-	128	C6H5ClO	000095-57-8	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079037.D
Acq On : 24 Aug 2023 17:30
Operator : JC\MD
Sample : 04047-04 40X
Misc : 6.72g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z83-84

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
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Naphthalene, 1-...	13.341	221.3	ug/l	6697370	4	13.794	1513350	50.0
Naphthalene, 1,...	13.676	154.1	ug/l	4664730	4	13.794	1513350	50.0
Indane	14.000	364.0	ug/l	11016600	4	13.794	1513350	50.0
Indene	14.176	1121.3	ug/l	33937300	4	13.794	1513350	50.0
Benzene, 2-ethe...	14.470	122.7	ug/l	3713920	4	13.794	1513350	50.0
2-Methylindene	15.123	329.4	ug/l	9971490	4	13.794	1513350	50.0
1H-Indene, 1-me...	15.211	350.4	ug/l	10606000	4	13.794	1513350	50.0
1,4-Ethenonapht...	15.523	227.7	ug/l	6890830	4	13.794	1513350	50.0
Azulene	15.647	4861.9	ug/l	147154000	4	13.794	1513350	50.0