

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
 Data File : VN079029.D
 Acq On : 24 Aug 2023 14:17
 Operator : JC\MD
 Sample : 04093-04
 Misc : 7.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NEVINS-SB04-Z94-95

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: VN079029.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	51	57	63	rBV3	10066	20786	1.64%	0.170%
2	2.830	136	149	150	rBV8	33124	87092	6.86%	0.710%
3	5.489	593	601	603	rBV4	9235	17616	1.39%	0.144%
4	8.171	1047	1057	1061	rBV	188918	449962	35.46%	3.670%
5	8.224	1061	1066	1076	rVB	293791	658014	51.85%	5.368%
6	8.582	1115	1127	1140	rBV	195809	464971	36.64%	3.793%
7	9.106	1206	1216	1224	rBV	453471	939485	74.03%	7.664%
8	10.571	1455	1465	1472	rBV	685496	1269047	100.00%	10.352%
9	10.635	1472	1476	1482	rVB2	50628	89009	7.01%	0.726%
10	11.870	1678	1686	1697	rBV	648475	1150483	90.66%	9.385%
11	11.965	1697	1702	1711	rVB	51447	91350	7.20%	0.745%
12	12.082	1716	1722	1729	rBV	23579	39290	3.10%	0.321%
13	12.412	1770	1778	1786	rBV4	48311	102154	8.05%	0.833%
14	12.629	1797	1815	1834	rBV3	42178	236943	18.67%	1.933%
15	12.806	1838	1845	1846	rVV7	7710	14924	1.18%	0.122%
16	12.853	1846	1853	1864	rVB	505697	879274	69.29%	7.173%
17	13.188	1904	1910	1913	rBV7	9779	20287	1.60%	0.165%
18	13.317	1914	1932	1933	rBV2	141931	404711	31.89%	3.301%
19	13.488	1956	1961	1965	rVB3	13341	24140	1.90%	0.197%
20	13.535	1965	1969	1973	rVB4	12825	18092	1.43%	0.148%
21	13.670	1973	1992	2007	rBV5	135692	734363	57.87%	5.990%
22	13.794	2007	2013	2021	rVB	594309	1004751	79.17%	8.196%
23	14.012	2035	2050	2060	rBV2	229346	837098	65.96%	6.828%
24	14.129	2062	2070	2074	rVV4	106755	349423	27.53%	2.850%
25	14.176	2074	2078	2086	rVB	172044	317741	25.04%	2.592%
26	14.488	2120	2131	2136	rBV5	34290	107691	8.49%	0.878%
27	14.559	2138	2143	2153	rVB5	56236	162993	12.84%	1.330%
28	14.847	2184	2192	2193	rBV5	28937	48912	3.85%	0.399%
29	15.082	2219	2232	2233	rBV8	19314	52663	4.15%	0.430%
30	15.123	2237	2239	2247	rVB5	23286	29274	2.31%	0.239%
31	15.206	2247	2253	2260	rBV4	23856	45905	3.62%	0.374%
32	15.317	2265	2272	2281	rVB10	11188	31216	2.46%	0.255%
33	15.529	2289	2308	2320	rBV3	200124	741691	58.44%	6.050%
34	15.647	2320	2328	2337	rVV	339678	718779	56.64%	5.863%
35	15.747	2340	2345	2352	rVB7	11707	29414	2.32%	0.240%
36	16.105	2400	2406	2414	rVB9	8556	25053	1.97%	0.204%

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NEVINS-SB04-Z94-95

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

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Title : SW846 8260

37	16.276	2433	2435	2446	rVB7	11193	22282	1.76%	0.182%
38	16.594	2479	2489	2496	rBV8	6303	22036	1.74%	0.180%

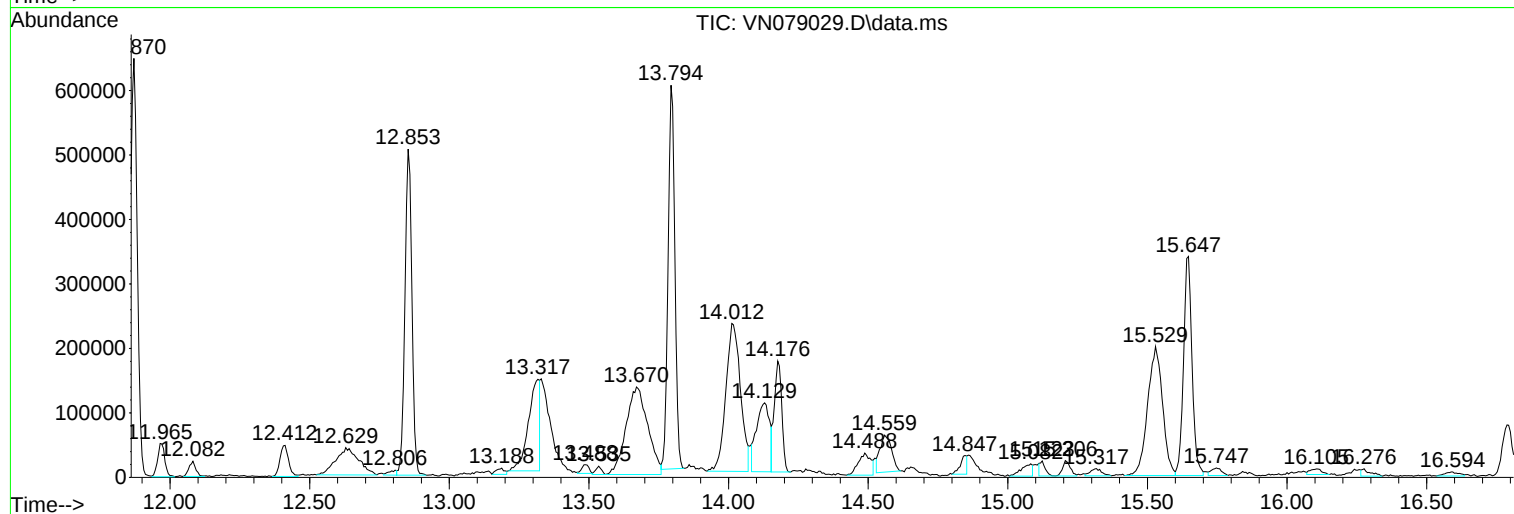
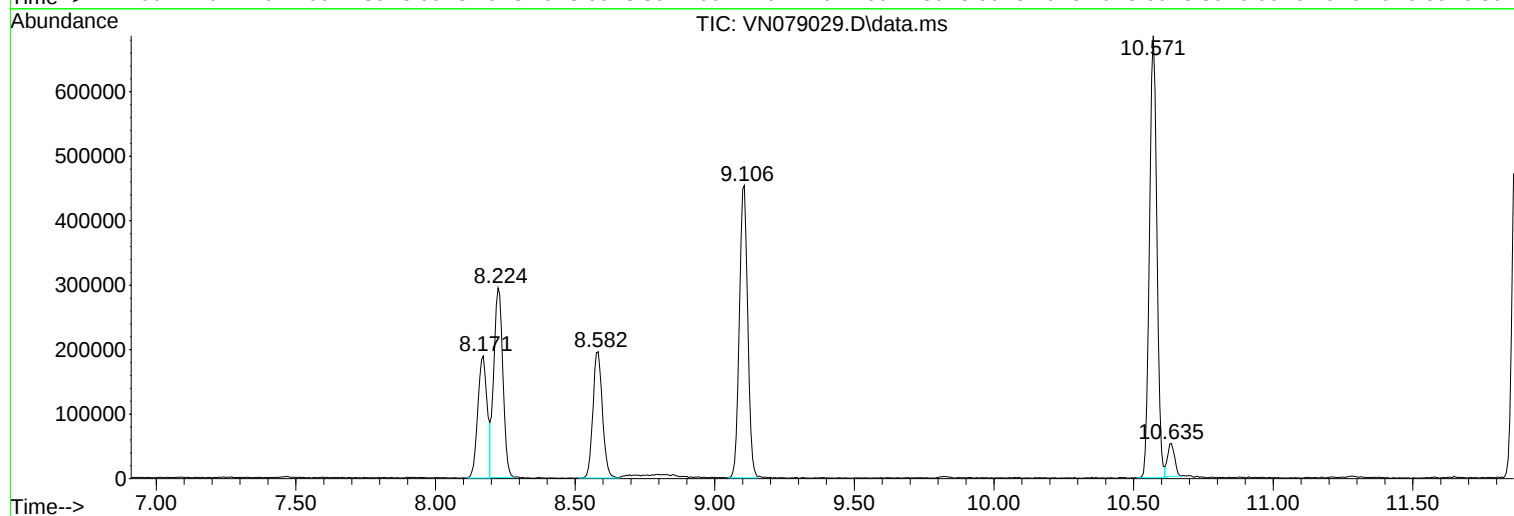
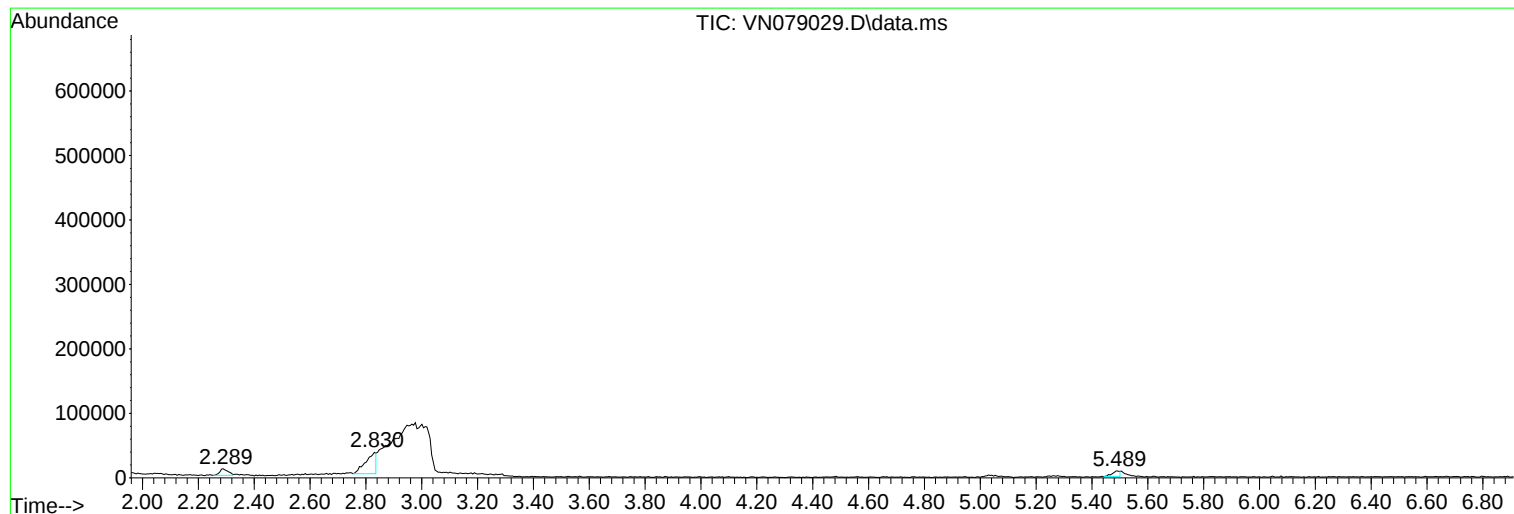
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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



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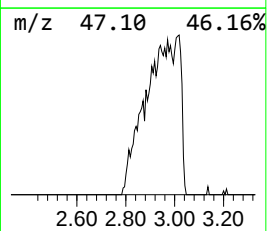
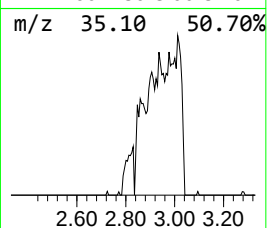
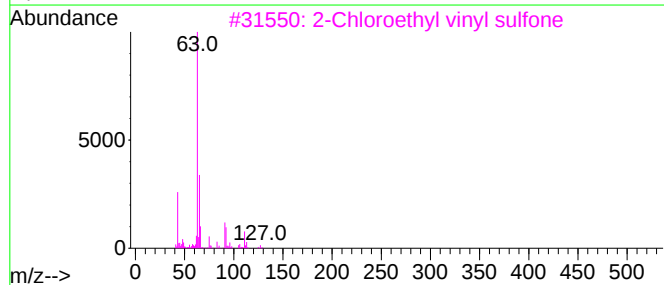
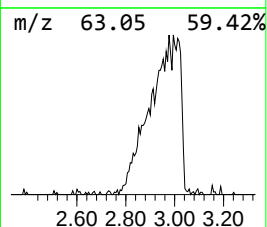
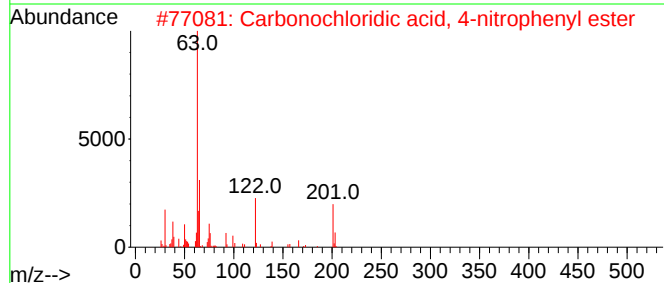
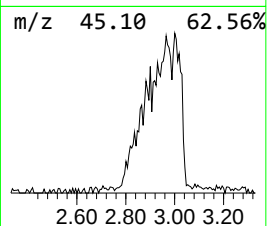
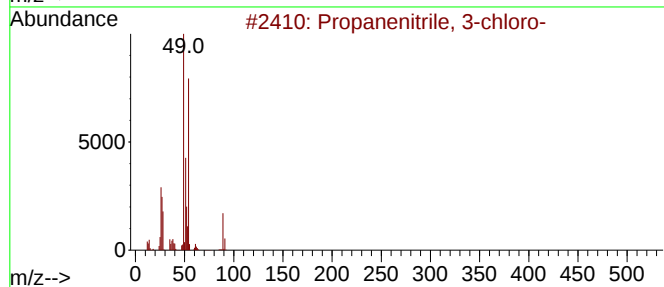
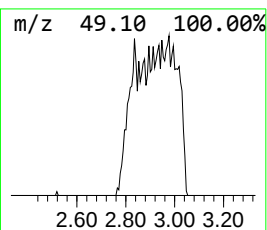
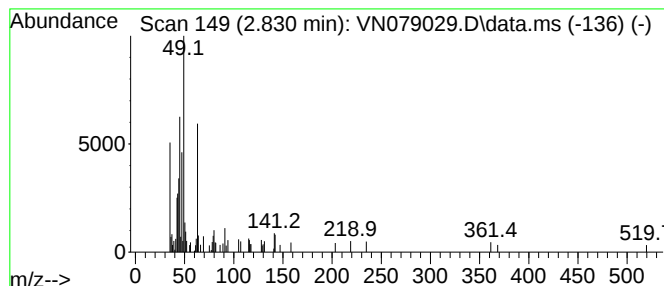
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.830 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.830	6.62 ug/l	87092	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanenitrile, 3-chloro-	89	C3H4ClN	000542-76-7	17
2			Carbonochloridic acid, 4-nitroph...	201	C7H4ClNO4	007693-46-1	9
3			2-Chloroethyl vinyl sulfone	154	C4H7ClO2S	007327-58-4	9
4			Ethene, (2-chloroethoxy)-	106	C4H7ClO	000110-75-8	9
5			1-Ethanol, 2-[(3,5-dinitrophenyl...	244	C8H8N2O5S	1000337-27-1	9



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z94-95

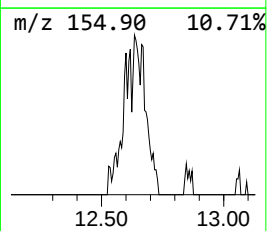
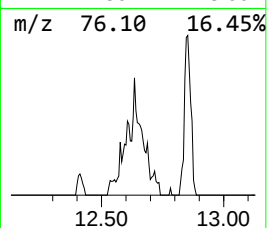
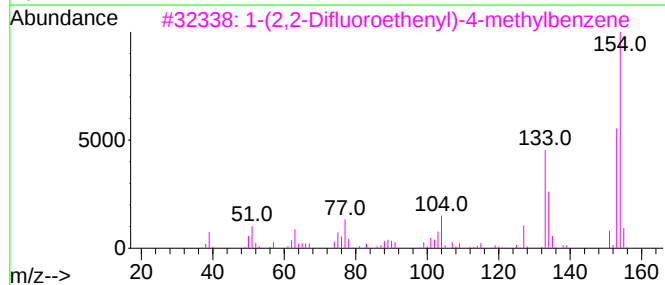
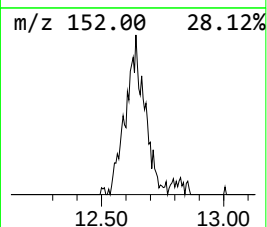
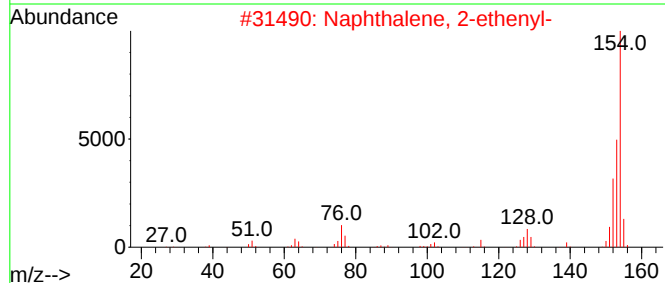
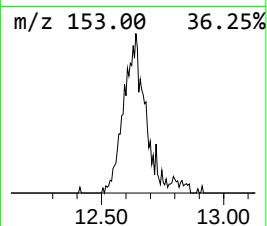
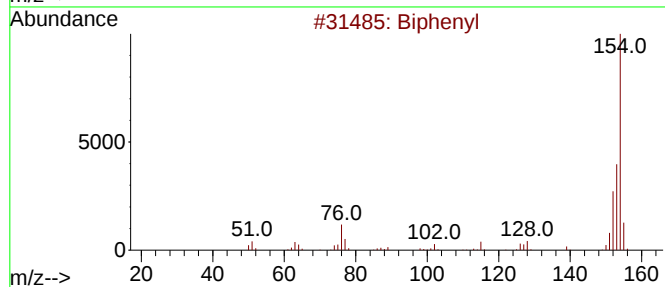
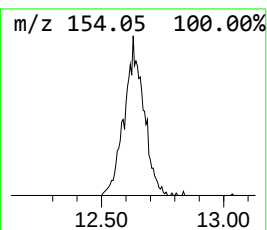
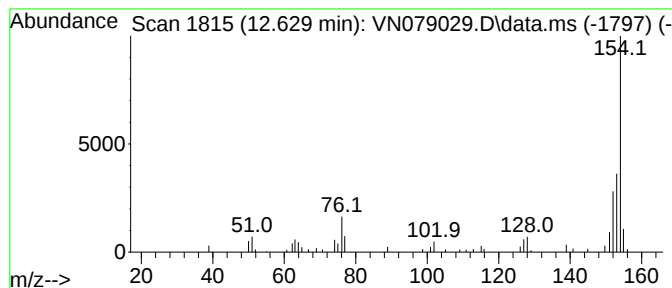
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, 2-ethenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.629	10.30 ug/l	236943	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	87
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	81
3			1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	53
4			Propanedinitrile, 2,4,6-cyclohep...	154	C10H6N2	002860-54-0	50
5			Acenaphthene	154	C12H10	000083-32-9	50



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z94-95

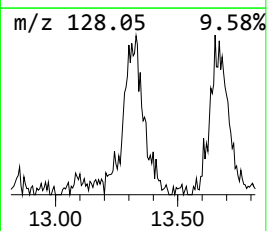
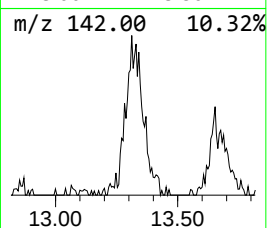
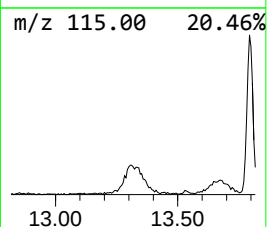
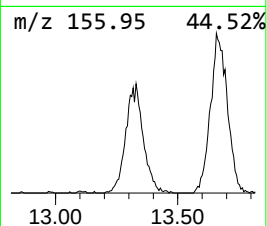
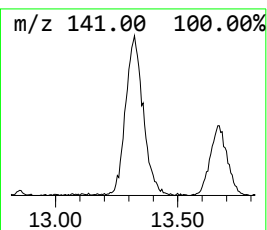
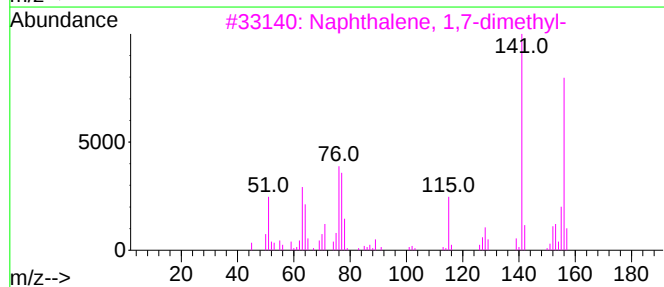
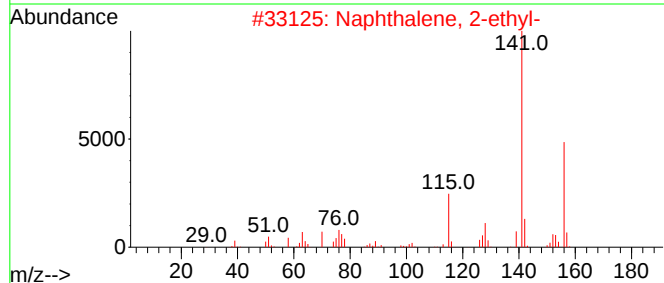
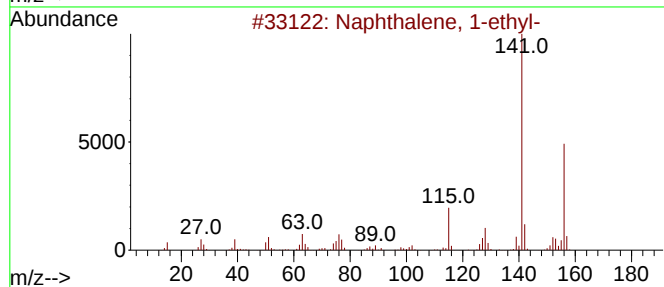
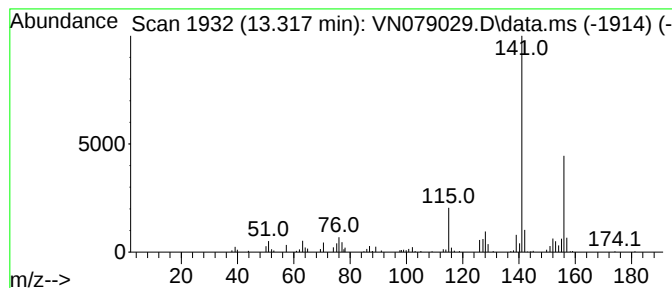
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.318	20.14 ug/l	404711	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	97
2			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	96
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	87
4			2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	59
5			2,4-Difluoromesitylene	156	C9H10F2	000392-61-0	59



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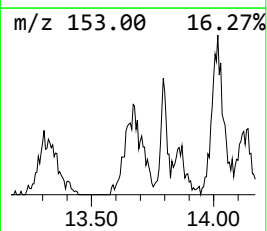
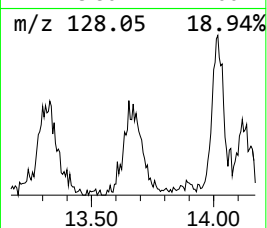
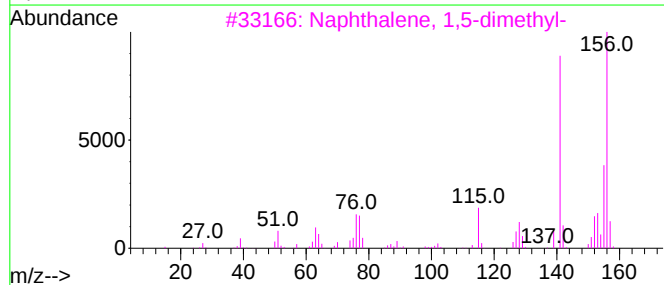
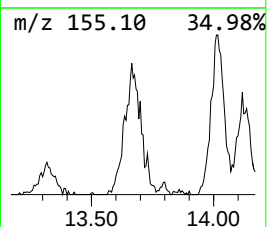
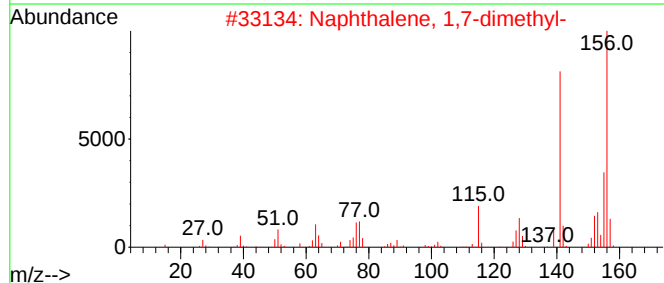
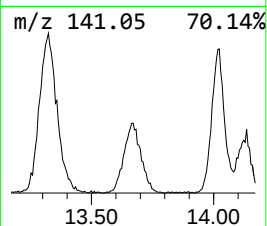
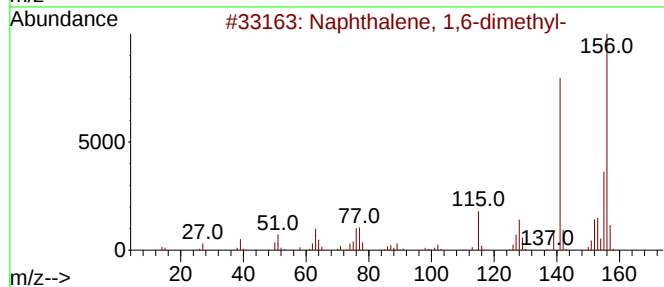
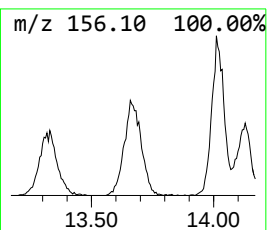
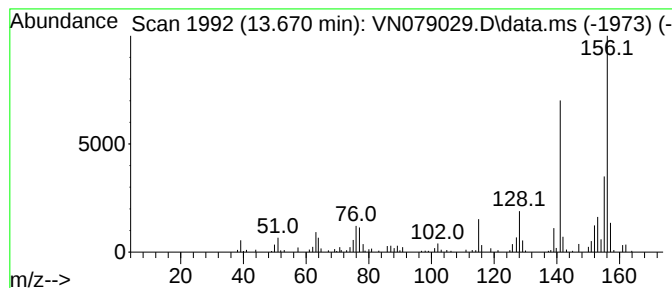
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Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.670	36.54 ug/l	734363	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	96
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95



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ClientSampleId :
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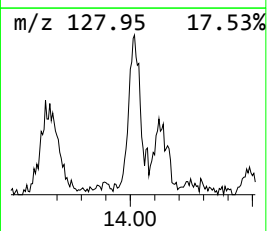
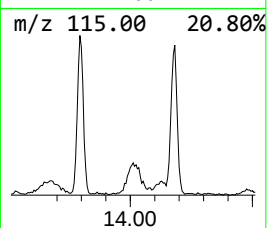
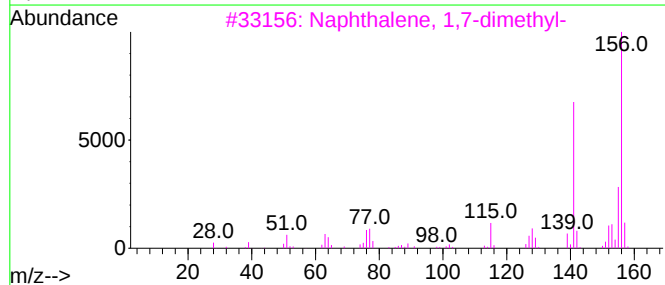
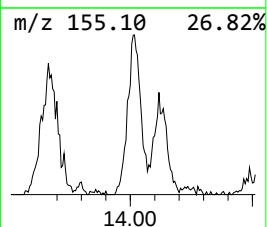
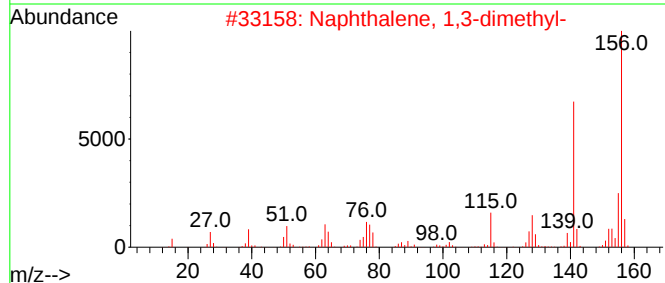
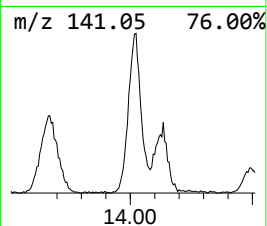
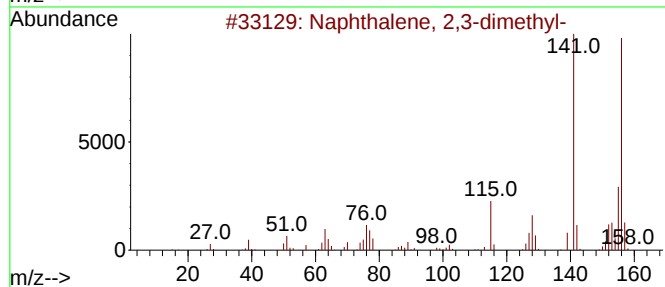
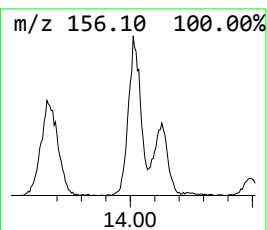
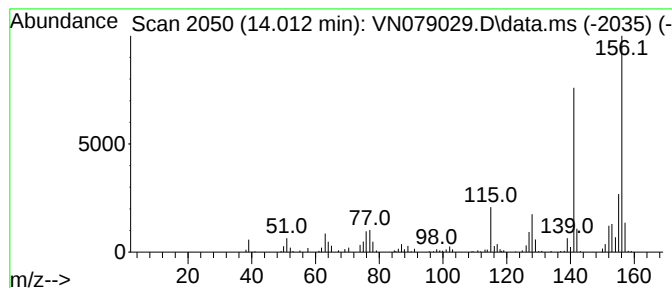
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.012	41.66 ug/l	837098	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079029.D
Acq On : 24 Aug 2023 14:17
Operator : JC\MD
Sample : 04093-04
Misc : 7.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z94-95

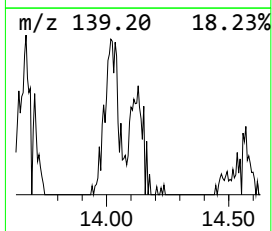
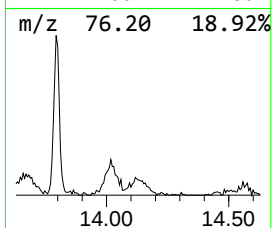
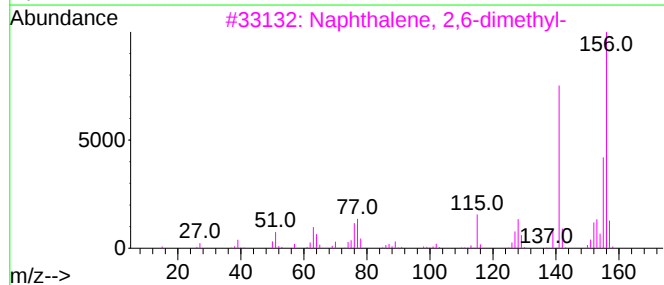
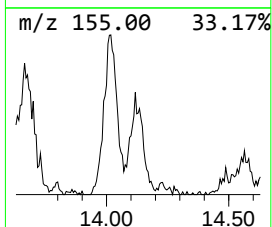
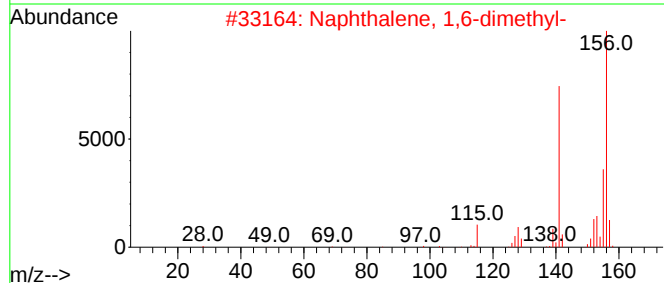
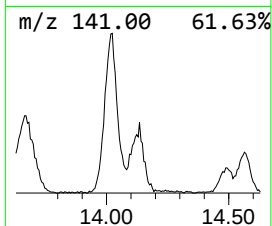
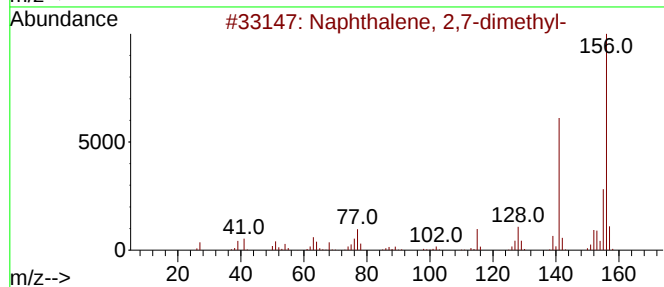
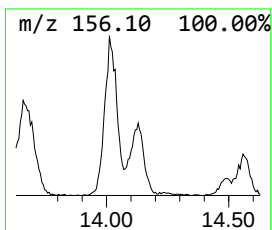
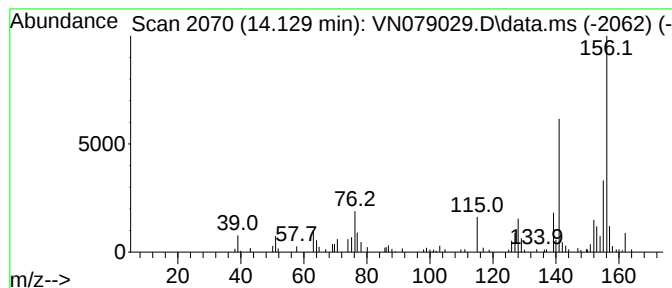
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 2,7-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.129	17.39 ug/l	349423	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	94
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	93
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	91
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079029.D
Acq On : 24 Aug 2023 14:17
Operator : JC\MD
Sample : 04093-04
Misc : 7.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z94-95

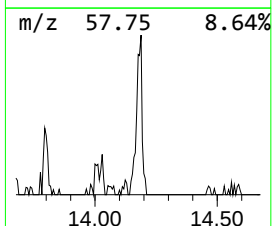
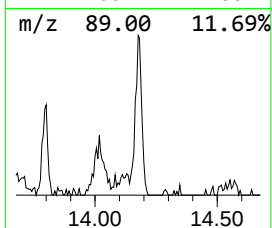
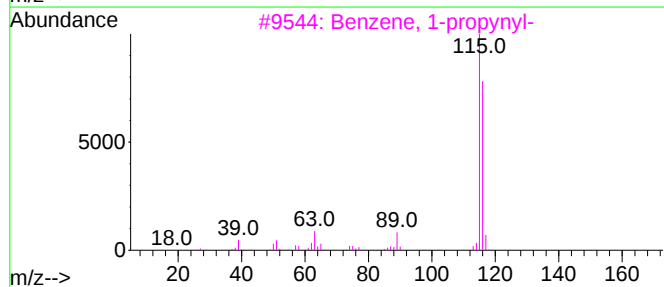
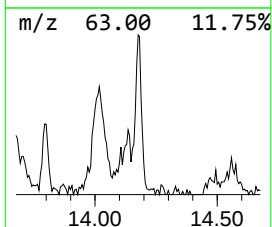
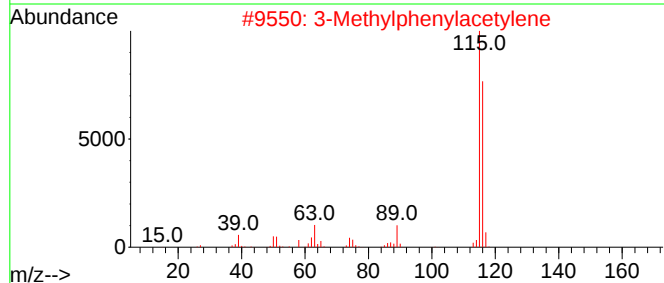
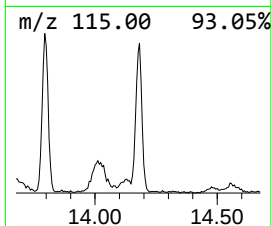
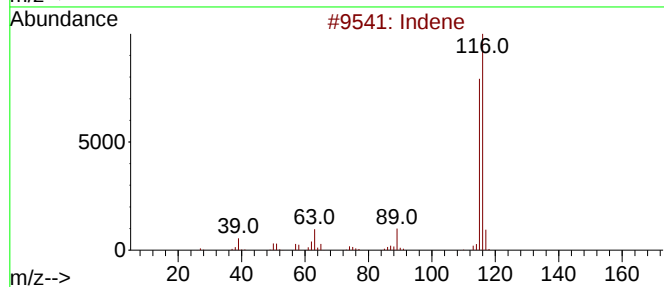
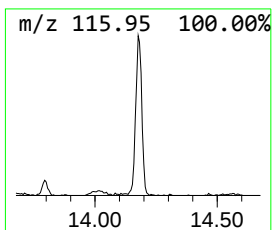
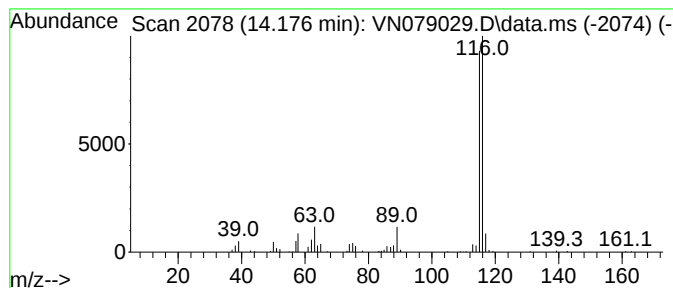
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Quant Title : SW846 8260

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

Peak Number 7 Indene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	15.81 ug/l	317741	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	94
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90
5			1-Phenyl-1-pentyn-4-ol	160	C11H12O	016330-23-7	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079029.D
Acq On : 24 Aug 2023 14:17
Operator : JC\MD
Sample : 04093-04
Misc : 7.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z94-95

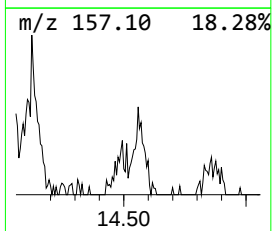
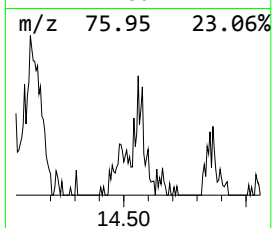
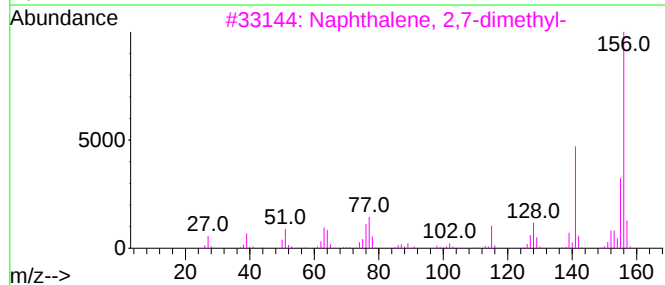
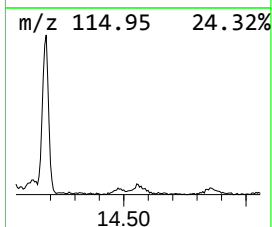
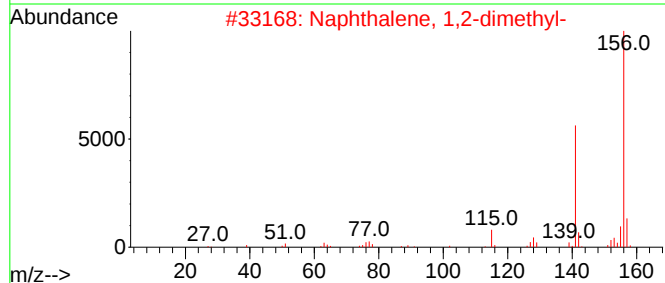
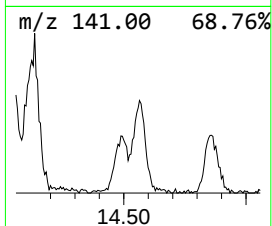
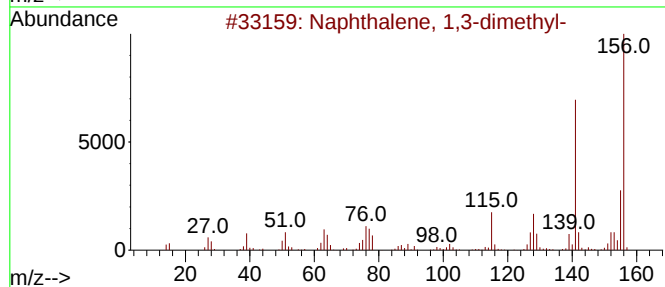
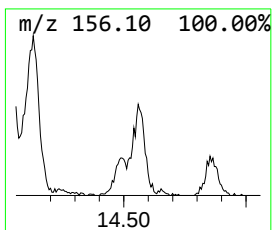
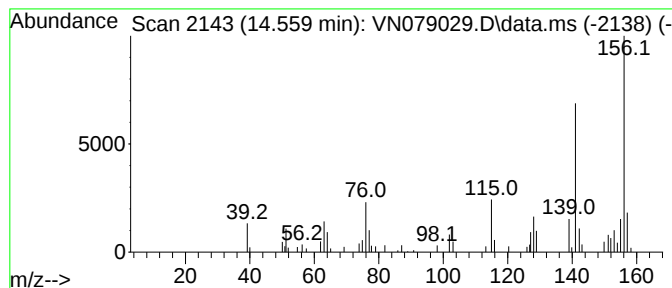
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.559	8.11 ug/l	162993	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91
2			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	90
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	90
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	90
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079029.D
Acq On : 24 Aug 2023 14:17
Operator : JC\MD
Sample : 04093-04
Misc : 7.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z94-95

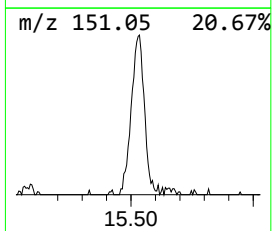
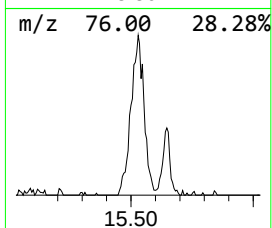
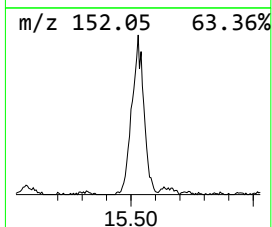
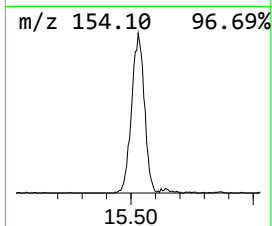
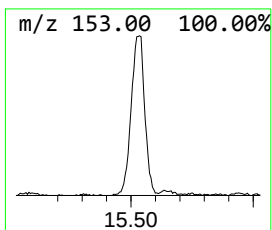
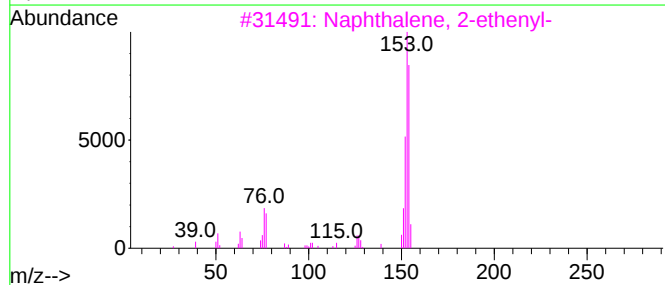
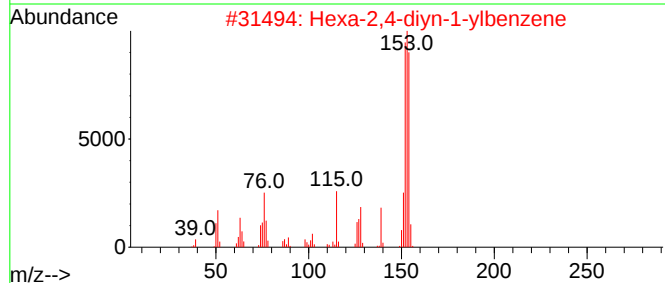
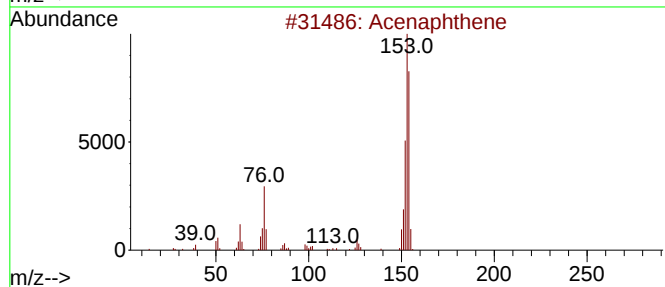
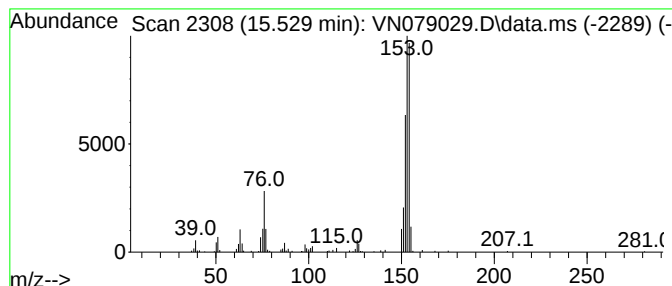
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Quant Title : SW846 8260

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

Peak Number 9 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.529	36.91 ug/l	741691	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	95
2			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	64
3			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	62
4			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	42
5			.beta.-(1-Naphthyl)acrylic acid	198	C13H10O2	013026-12-5	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079029.D
Acq On : 24 Aug 2023 14:17
Operator : JC\MD
Sample : 04093-04
Misc : 7.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z94-95

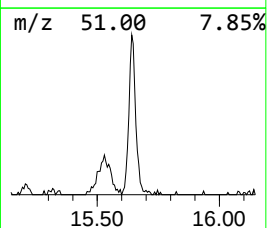
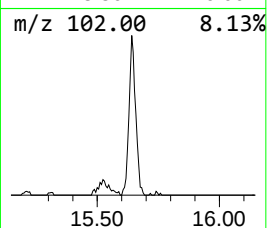
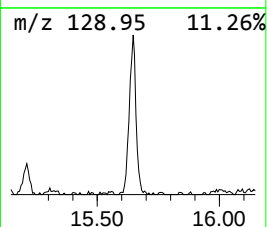
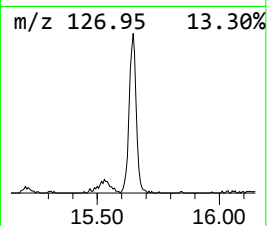
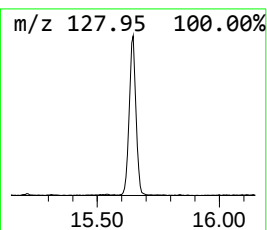
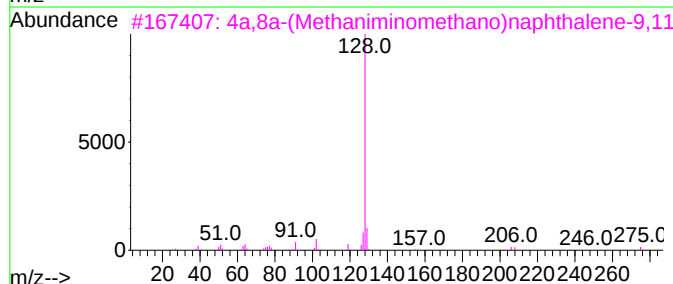
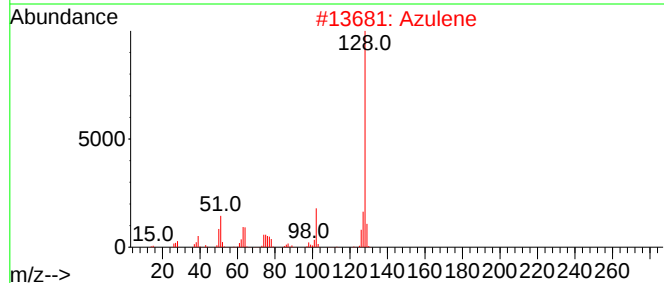
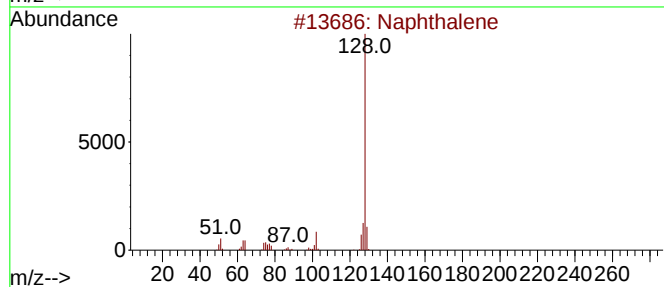
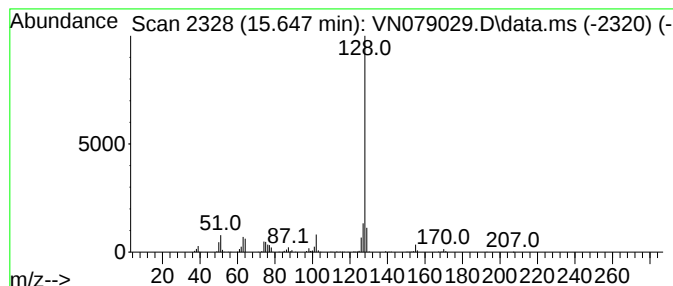
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Quant Title : SW846 8260

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

Peak Number 10 Azulene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	35.77 ug/l	718779	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	94
2			Azulene	128	C10H8	000275-51-4	90
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
4			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59
5			m-Fluorothiophenol	128	C6H5FS	002557-77-9	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079029.D
Acq On : 24 Aug 2023 14:17
Operator : JC\MD
Sample : 04093-04
Misc : 7.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z94-95

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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Naphthalene, 1-...	13.318	20.1	ug/l	404711	4	13.794	1004750	50.0
Naphthalene, 1,...	13.670	36.5	ug/l	734363	4	13.794	1004750	50.0
Naphthalene, 2,...	14.012	41.7	ug/l	837098	4	13.794	1004750	50.0
Naphthalene, 2,...	14.129	17.4	ug/l	349423	4	13.794	1004750	50.0
Indene	14.176	15.8	ug/l	317741	4	13.794	1004750	50.0
Naphthalene, 1,...	14.559	8.1	ug/l	162993	4	13.794	1004750	50.0
Hexa-2,4-diyne-1...	15.529	36.9	ug/l	741691	4	13.794	1004750	50.0
Azulene	15.647	35.8	ug/l	718779	4	13.794	1004750	50.0