

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
 Data File : VN079032.D
 Acq On : 24 Aug 2023 15:29
 Operator : JC\MD
 Sample : 04075-01 20X
 Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
 ALS Vial : 12 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: VN079032.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.847	139	152	157	rBV7	27289	81972	4.05%	0.423%
2	8.177	1046	1058	1062	rBV	209405	512322	25.34%	2.647%
3	8.229	1062	1067	1079	rVB	350363	757530	37.47%	3.914%
4	8.582	1116	1127	1141	rBV	217970	503705	24.92%	2.602%
5	9.106	1207	1216	1228	rBV	514693	1067871	52.82%	5.517%
6	10.570	1456	1465	1475	rBV	797902	1456841	72.07%	7.526%
7	11.870	1676	1686	1697	rBV	750652	1337482	66.16%	6.910%
8	11.970	1697	1703	1714	rVB	47548	80930	4.00%	0.418%
9	12.070	1714	1720	1726	rBV3	28053	53051	2.62%	0.274%
10	12.406	1771	1777	1785	rBV5	22927	52858	2.61%	0.273%
11	12.629	1795	1815	1816	rBV2	91960	301130	14.90%	1.556%
12	12.853	1844	1853	1862	rVB	602072	1040568	51.47%	5.376%
13	13.317	1912	1932	1955	rVB4	302208	1566239	77.48%	8.092%
14	13.488	1955	1961	1965	rBV2	38232	63362	3.13%	0.327%
15	13.535	1965	1969	1974	rVB2	35640	52458	2.59%	0.271%
16	13.664	1974	1991	2007	rBV3	268804	1495166	73.96%	7.724%
17	13.794	2007	2013	2022	rVB	668322	1143113	56.55%	5.906%
18	14.017	2035	2051	2061	rBV3	453656	1624069	80.34%	8.390%
19	14.129	2061	2070	2075	rBV3	133413	405098	20.04%	2.093%
20	14.476	2119	2129	2135	rBV5	78295	245693	12.15%	1.269%
21	14.564	2137	2144	2153	rVV4	135174	452283	22.37%	2.337%
22	14.647	2153	2158	2164	rVV5	29417	81709	4.04%	0.422%
23	14.700	2164	2167	2172	rVB5	18325	25258	1.25%	0.130%
24	14.794	2178	2183	2185	rBV4	24392	31455	1.56%	0.163%
25	14.853	2186	2193	2203	rVB3	63082	219145	10.84%	1.132%
26	15.076	2218	2231	2235	rBV9	66161	243790	12.06%	1.259%
27	15.123	2235	2239	2246	rVB	93534	176655	8.74%	0.913%
28	15.205	2246	2253	2260	rBV2	96069	190263	9.41%	0.983%
29	15.317	2262	2272	2279	rBV9	37578	106779	5.28%	0.552%
30	15.523	2293	2307	2319	rBV3	420189	1588158	78.56%	8.205%
31	15.647	2320	2328	2338	rVV	1002859	2021528	100.00%	10.444%
32	15.747	2341	2345	2351	rVB5	31787	70022	3.46%	0.362%
33	15.841	2355	2361	2373	rVB5	18192	50140	2.48%	0.259%
34	15.947	2373	2379	2383	rBV7	8748	22801	1.13%	0.118%
35	16.017	2383	2391	2392	rBV7	18593	28355	1.40%	0.146%
36	16.252	2419	2431	2432	rBV8	35032	79829	3.95%	0.412%

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Instrument :
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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

37	16.582	2479	2487	2503	rVB8	28138	126662	6.27%	0.654%
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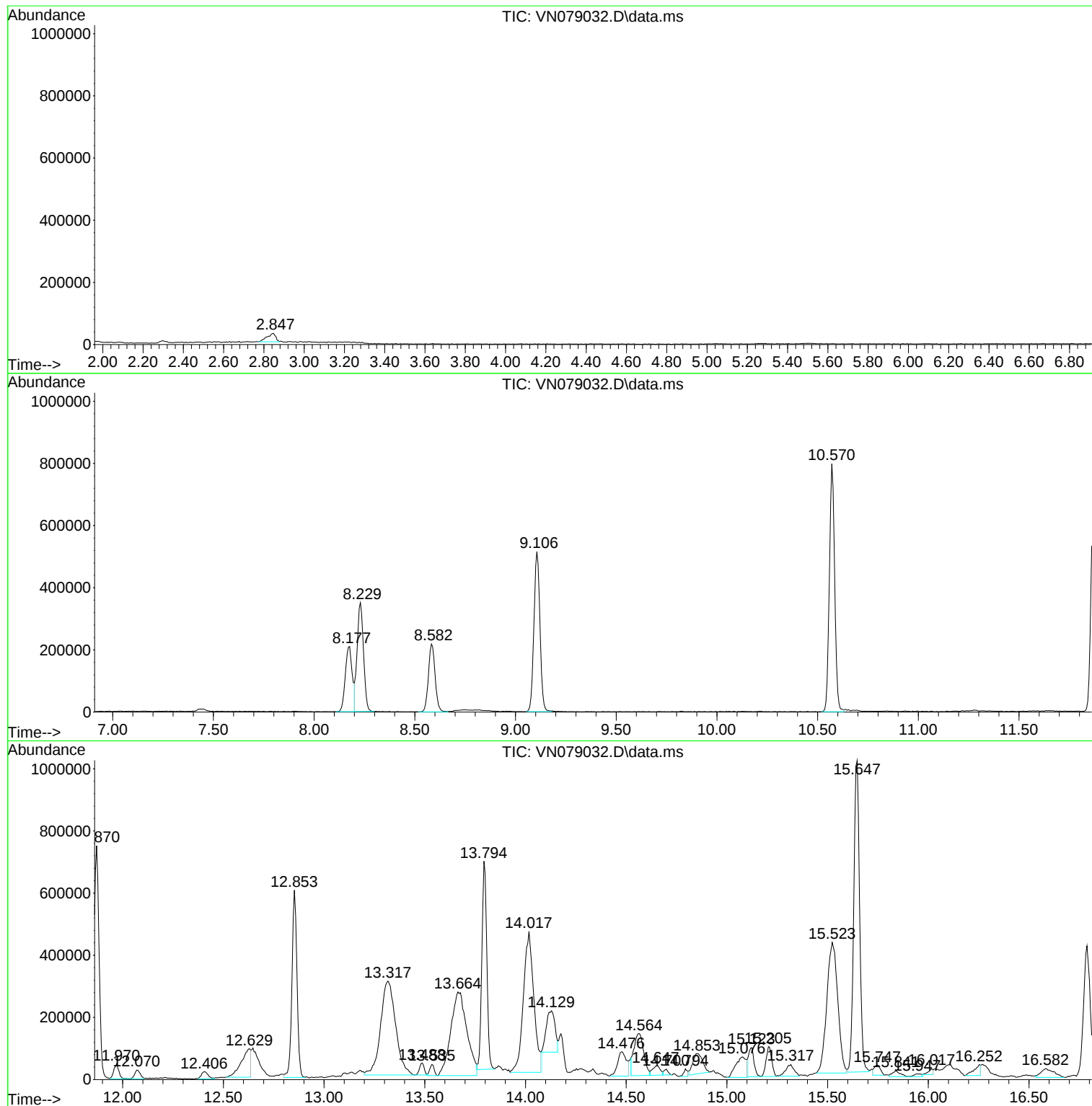
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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



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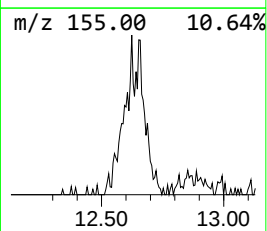
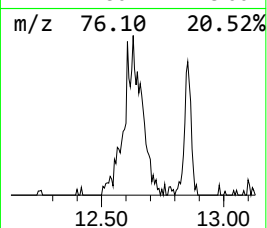
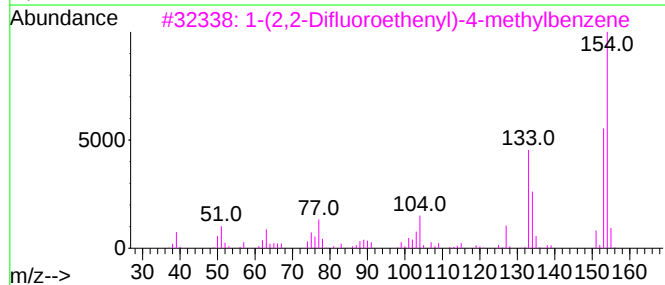
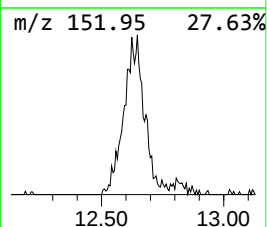
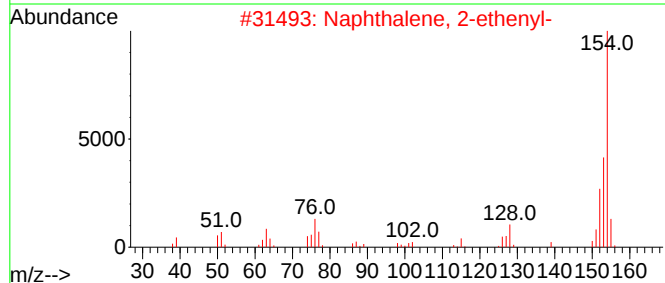
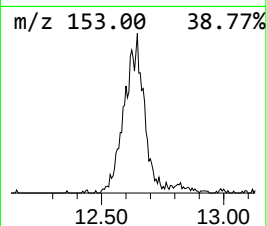
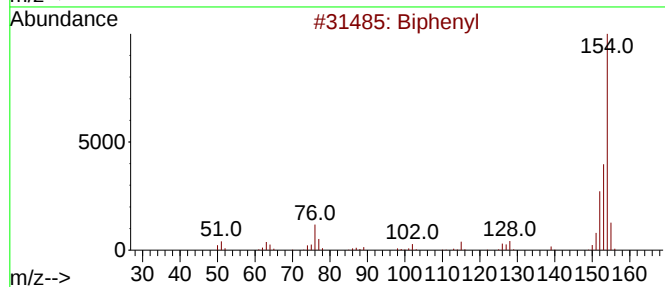
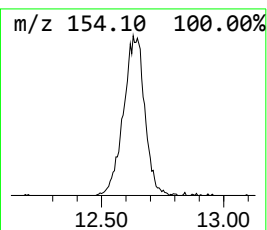
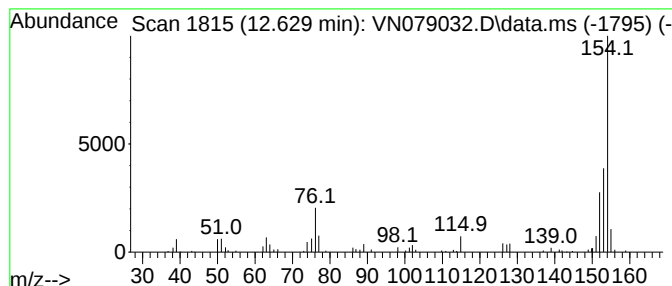
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 1 Naphthalene, 2-ethenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.629	11.26 ug/l	301130	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	93
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	76
3			1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	53
4			Acenaphthene	154	C12H10	000083-32-9	49
5			6-Cyanoquinoline	154	C10H6N2	023395-72-4	37



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ALS Vial : 12 Sample Multiplier: 1

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

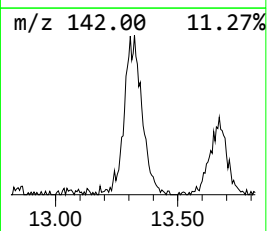
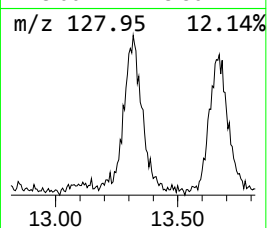
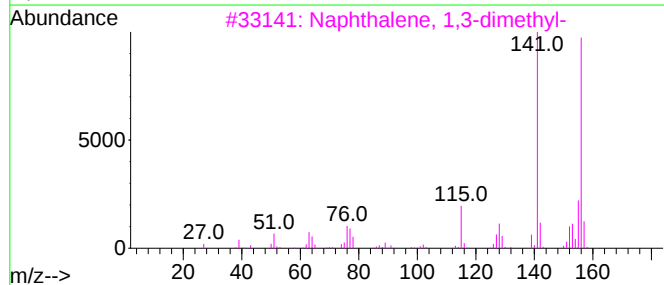
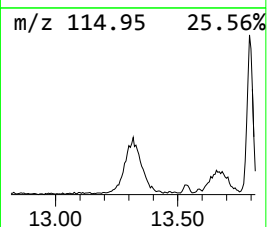
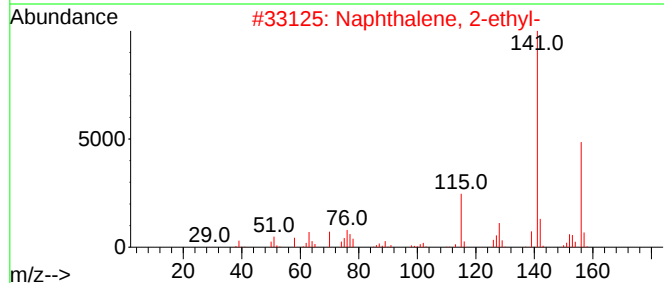
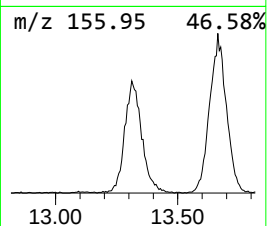
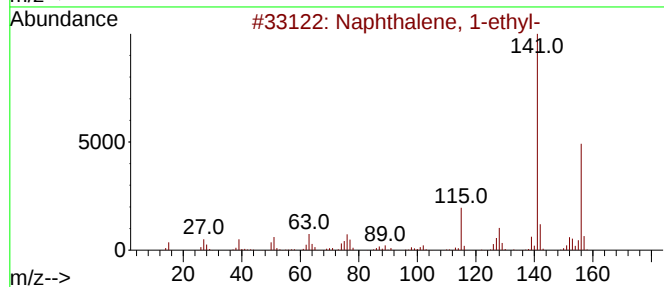
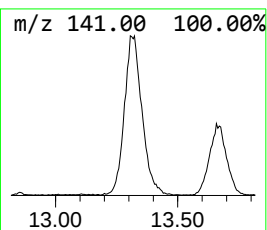
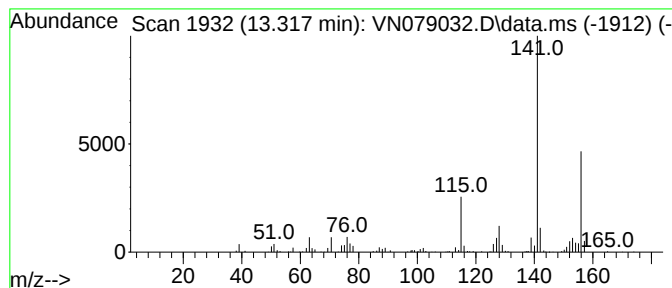
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Naphthalene, 1-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.317	68.51 ug/l	1566240	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	96
2			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	94
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91
4			2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	64
5			2,4-Difluoromesitylene	156	C9H10F2	000392-61-0	59



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ALS Vial : 12 Sample Multiplier: 1

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

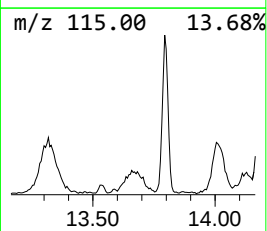
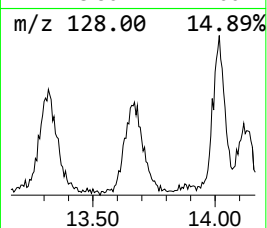
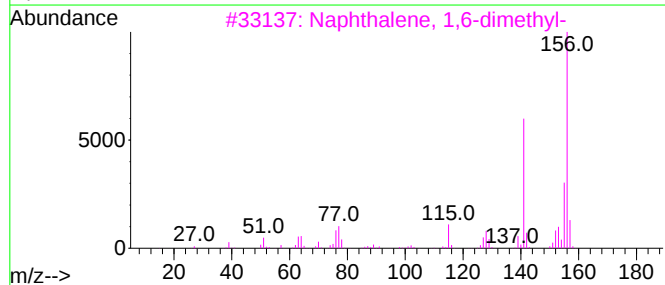
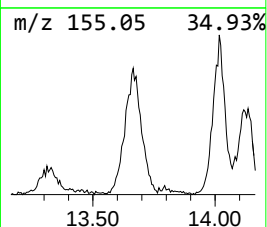
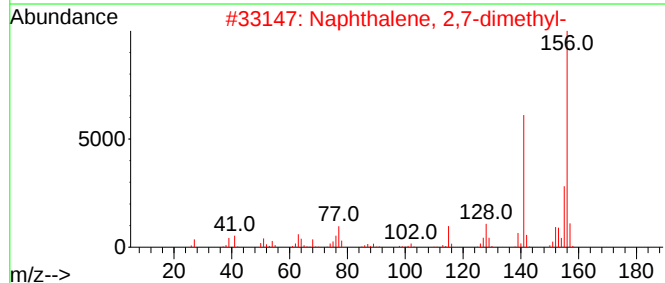
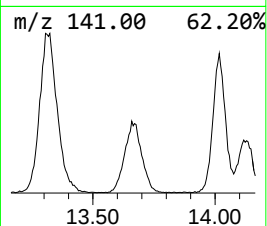
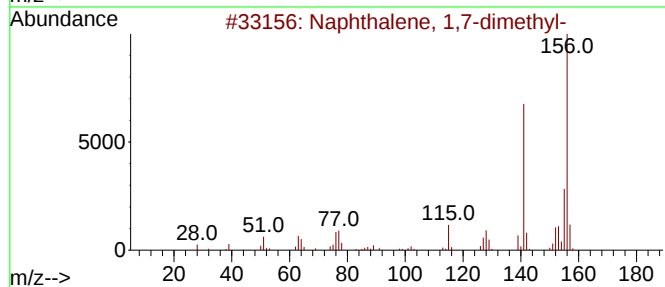
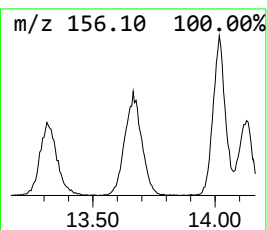
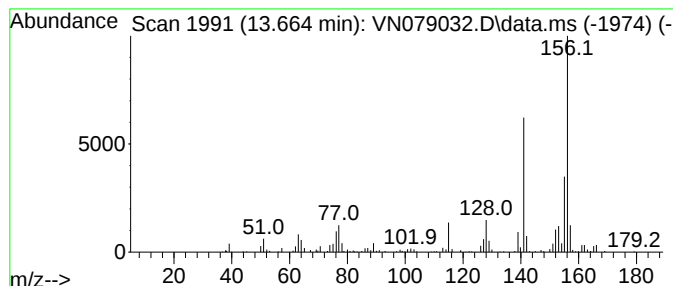
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1,7-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.664	65.40 ug/l	1495170	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96



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NEVINS-SB05-Z113-114

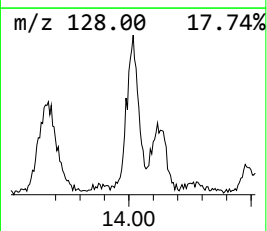
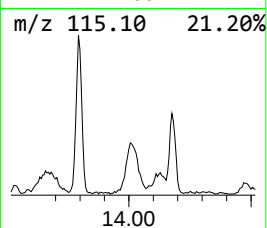
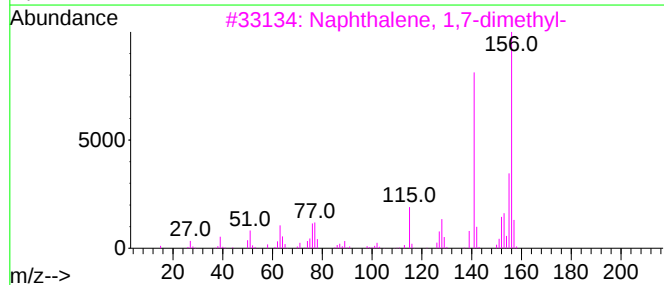
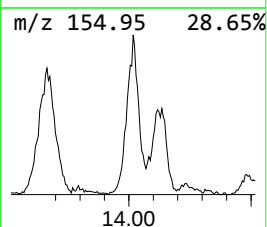
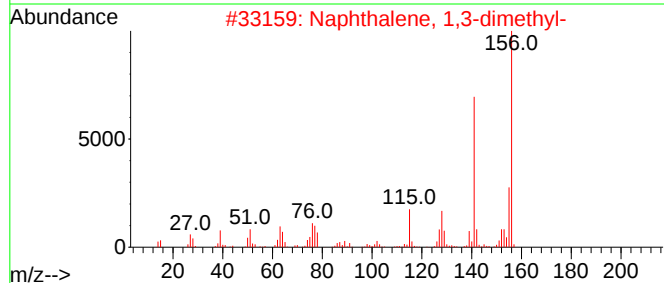
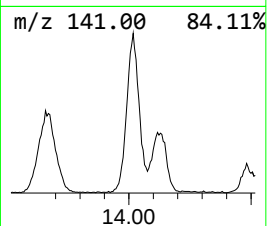
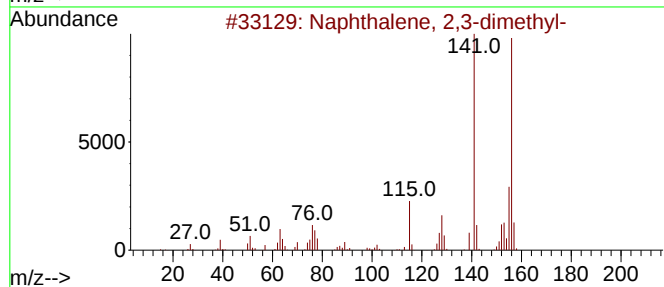
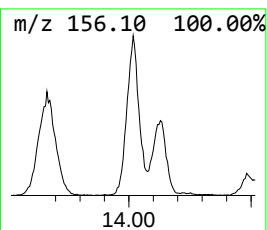
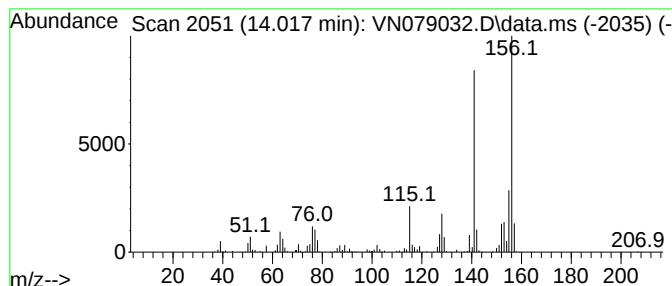
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.017	71.04 ug/l	1624070	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, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96



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

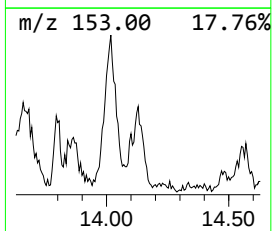
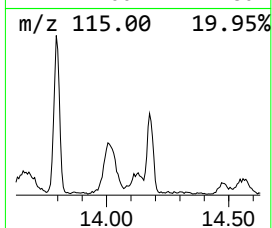
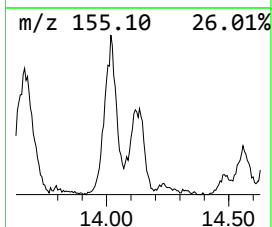
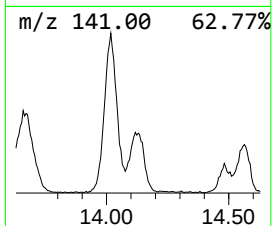
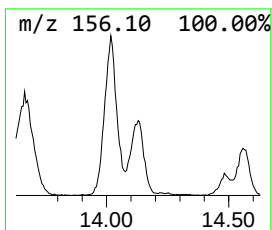
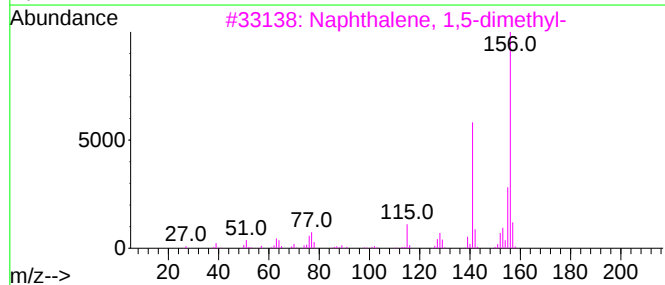
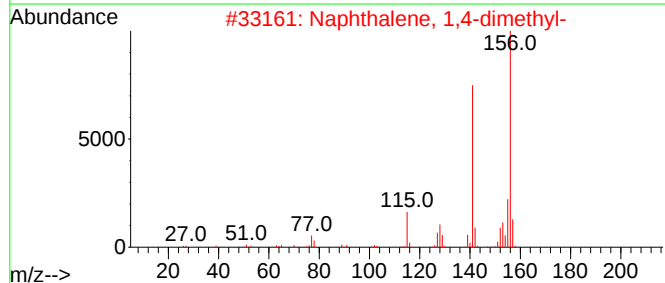
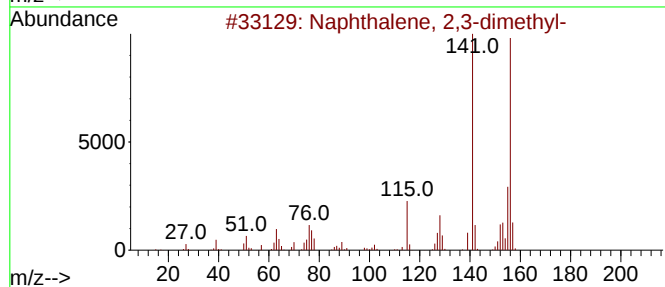
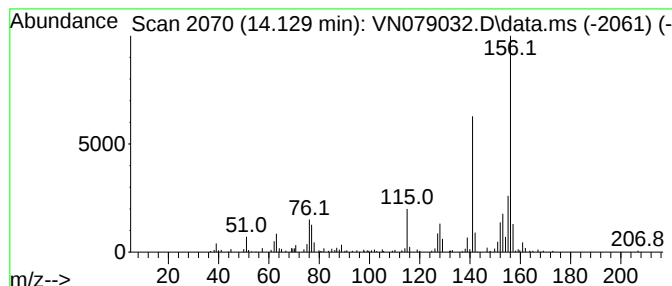
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.129	17.72 ug/l	405098	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	96
2			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	94
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	94
4			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	93
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079032.D
Acq On : 24 Aug 2023 15:29
Operator : JC\MD
Sample : 04075-01 20X
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

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

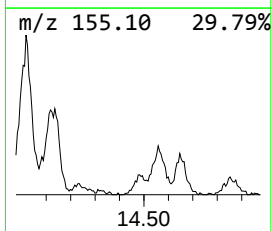
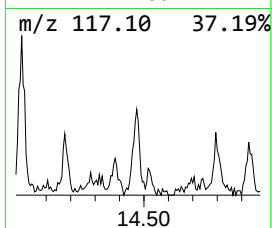
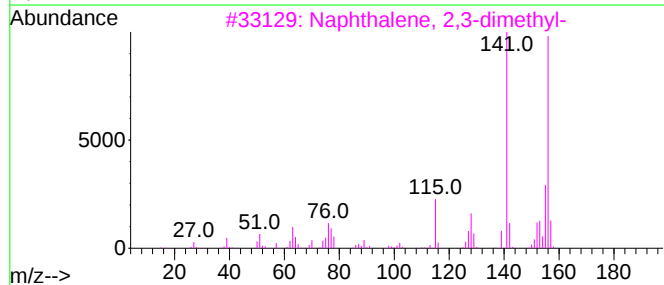
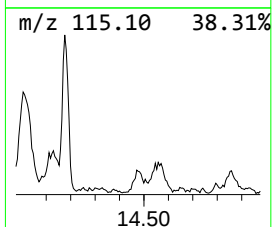
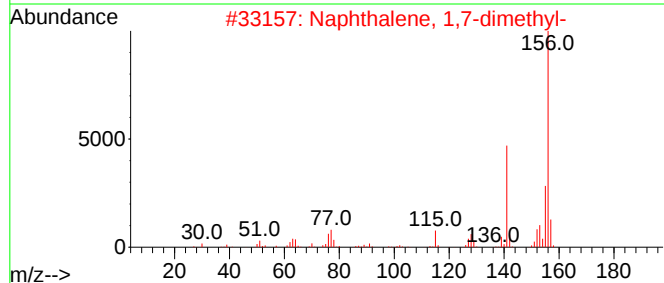
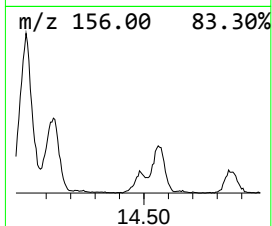
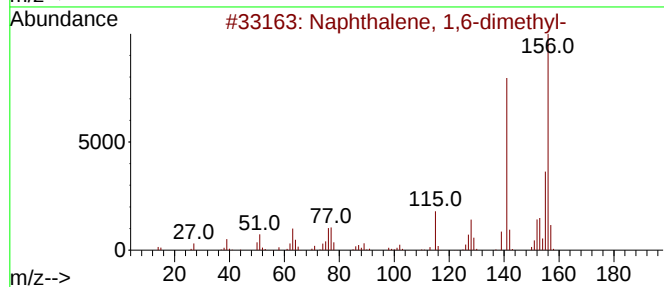
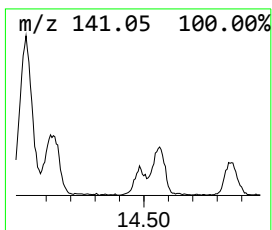
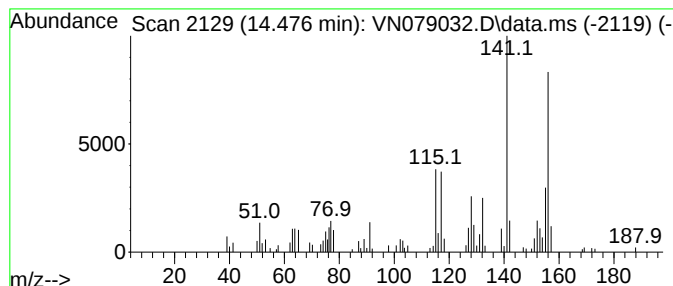
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.476	10.75 ug/l	245693	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, 2,3-dimethyl-	156	C12H12	000581-40-8	96
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	95
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079032.D
Acq On : 24 Aug 2023 15:29
Operator : JC\MD
Sample : 04075-01 20X
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

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

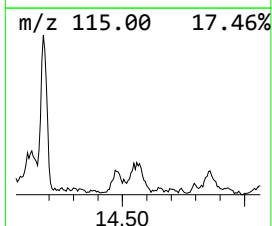
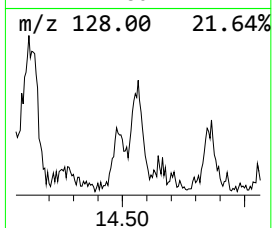
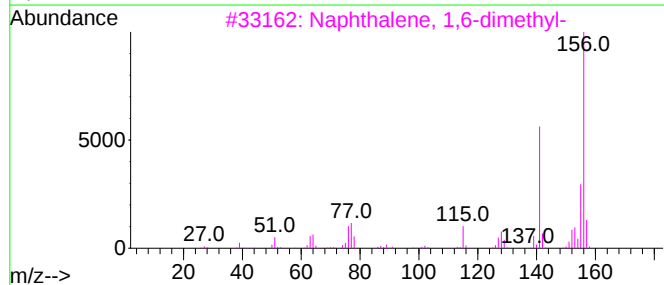
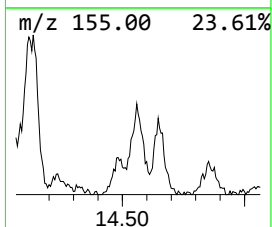
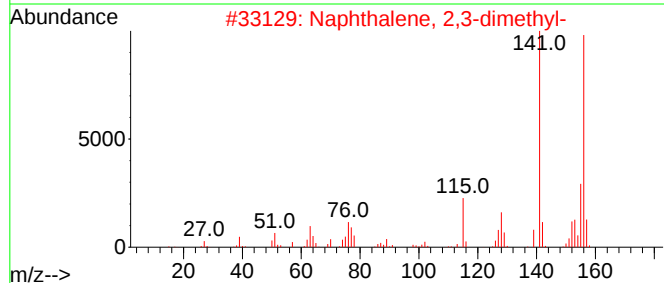
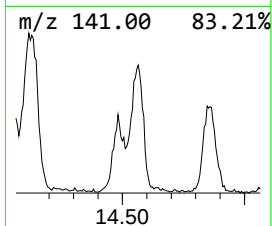
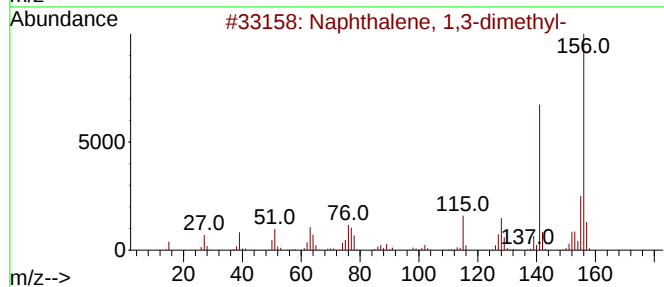
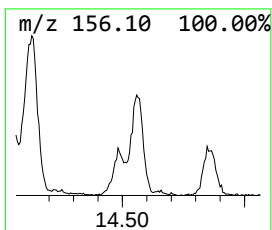
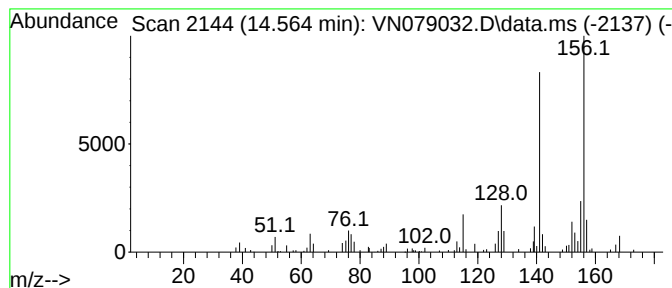
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.564	19.78 ug/l	452283	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	96
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	94
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079032.D
Acq On : 24 Aug 2023 15:29
Operator : JC\MD
Sample : 04075-01 20X
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

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

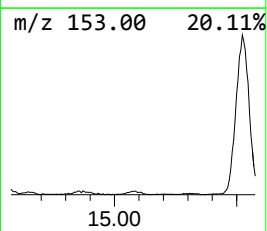
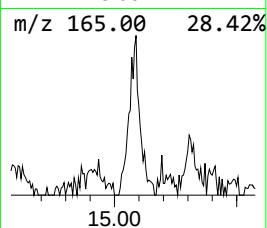
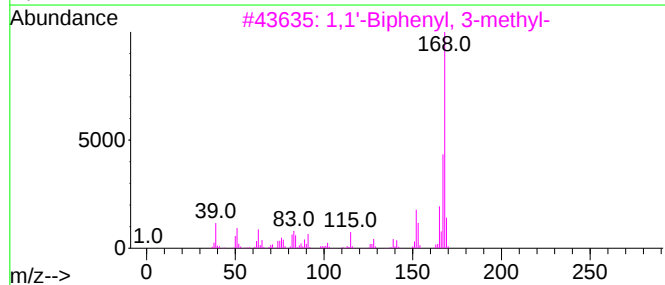
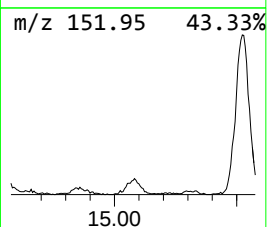
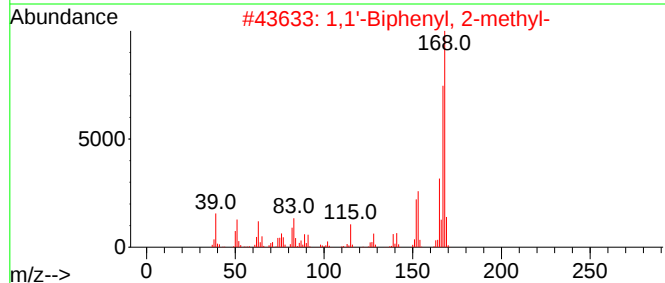
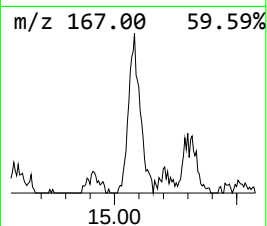
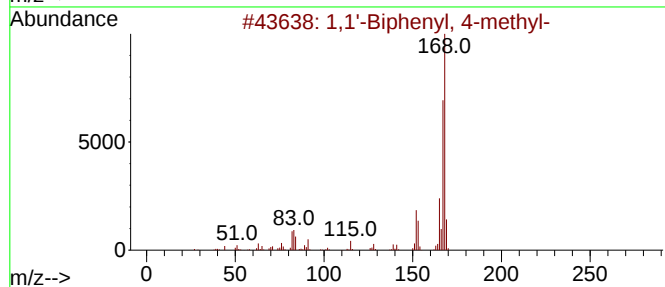
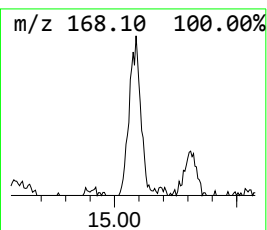
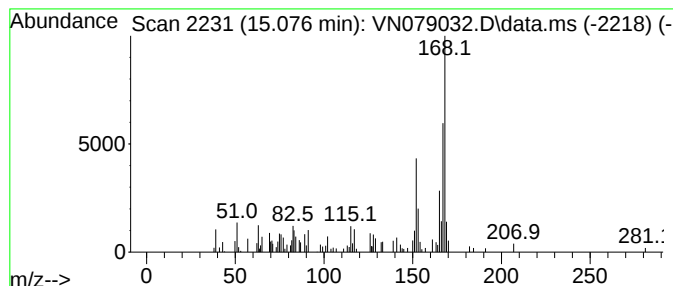
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Quant Title : SW846 8260

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

Peak Number 8 1,1'-Biphenyl, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.076	10.66 ug/l	243790	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	95
2			1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	93
3			1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	91
4			Diphenylmethane	168	C13H12	000101-81-5	49
5			Fluorene, 2,4a-dihydro-	168	C13H12	059247-36-8	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079032.D
Acq On : 24 Aug 2023 15:29
Operator : JC\MD
Sample : 04075-01 20X
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

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

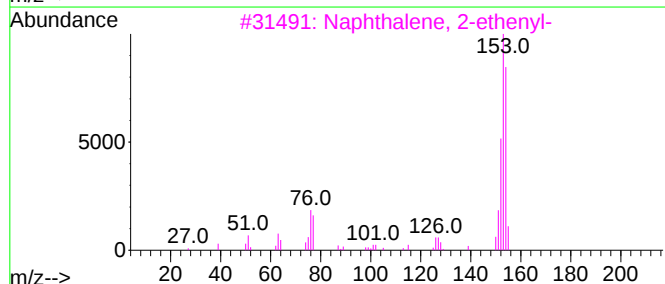
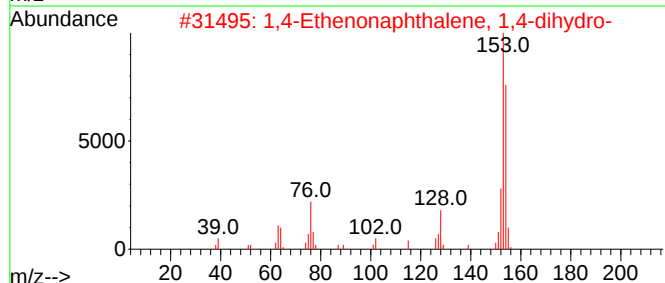
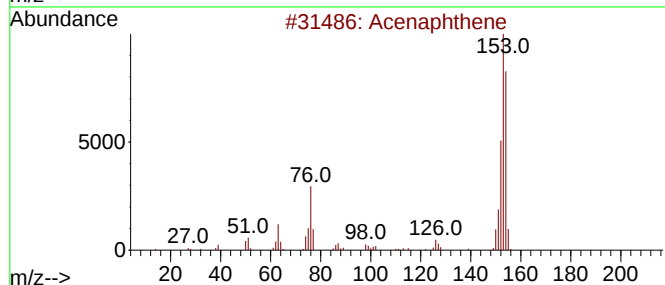
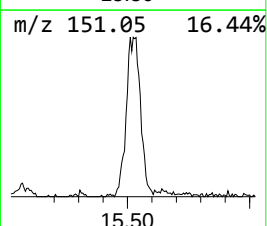
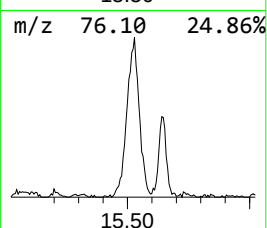
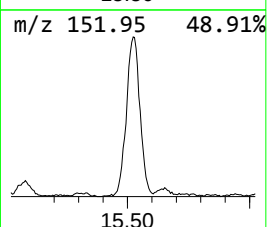
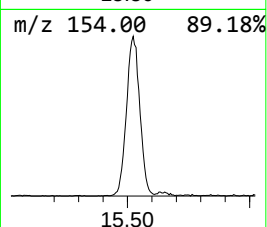
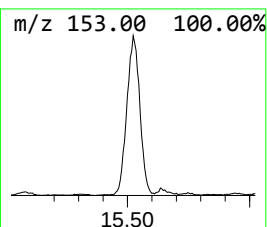
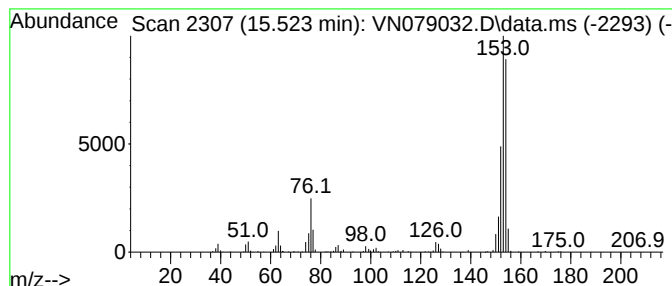
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Quant Title : SW846 8260

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

Peak Number 9 1,4-Ethenonaphthalene, 1,4-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.523	69.47 ug/l	1588160	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	93
2			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	64
3			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	59
4			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	58
5			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079032.D
Acq On : 24 Aug 2023 15:29
Operator : JC\MD
Sample : 04075-01 20X
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

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

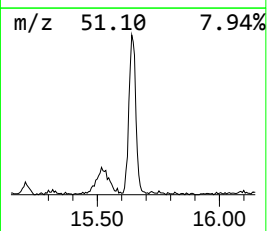
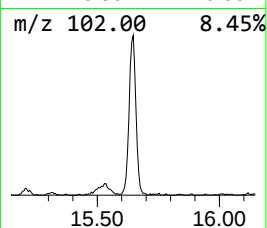
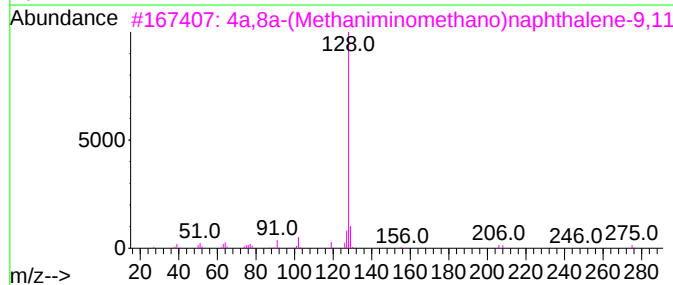
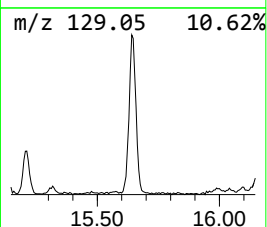
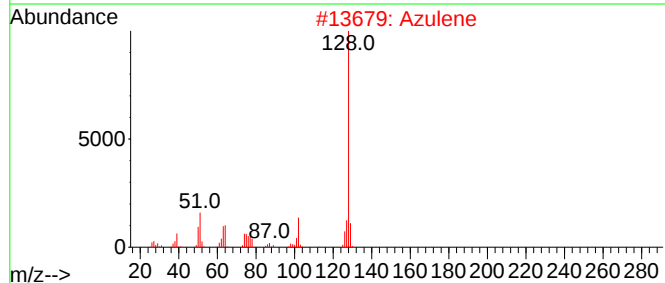
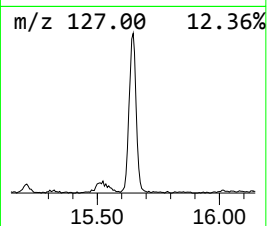
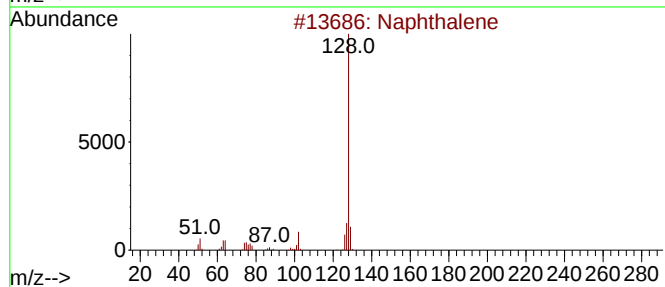
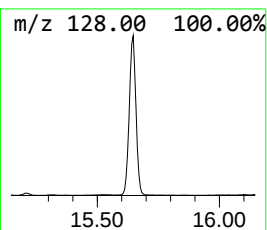
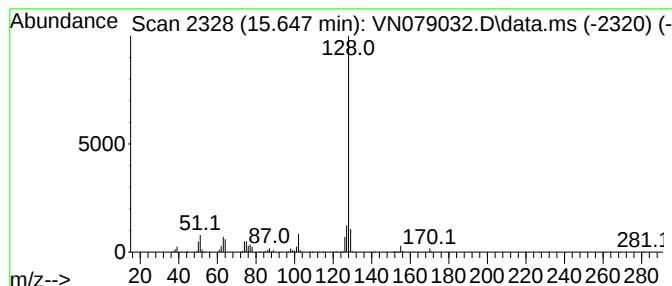
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Quant Title : SW846 8260

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

Peak Number 10 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	88.42 ug/l	2021530	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	78
4			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	64
5			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079032.D
Acq On : 24 Aug 2023 15:29
Operator : JC\MD
Sample : 04075-01 20X
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 12 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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Naphthalene, 1-...	13.317	68.5	ug/l	1566240	4	13.794	1143110	50.0
Naphthalene, 1,...	13.664	65.4	ug/l	1495170	4	13.794	1143110	50.0
Naphthalene, 2,...	14.017	71.0	ug/l	1624070	4	13.794	1143110	50.0
Naphthalene, 1,...	14.129	17.7	ug/l	405098	4	13.794	1143110	50.0
Naphthalene, 1,...	14.476	10.8	ug/l	245693	4	13.794	1143110	50.0
Naphthalene, 1,...	14.564	19.8	ug/l	452283	4	13.794	1143110	50.0
1,1'-Biphenyl, ...	15.076	10.7	ug/l	243790	4	13.794	1143110	50.0
1,4-Ethenonapht...	15.523	69.5	ug/l	1588160	4	13.794	1143110	50.0
Azulene	15.647	88.4	ug/l	2021530	4	13.794	1143110	50.0