

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
 Data File : VX037044.D
 Acq On : 17 Aug 2023 07:11
 Operator : JC/MD
 Sample : 03975-03 10X
 Misc : 7.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NEVINS-SB03-Z46-47

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_X\Method\82X072123W.M
 Title : SW846 8260

Signal : TIC: VX037044.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	694	705	721	rBV2	92148	273433	2.14%	0.760%
2	5.550	721	732	747	rVB	153096	437171	3.43%	1.215%
3	5.952	785	798	804	rBV	98001	257072	2.02%	0.715%
4	6.038	804	812	829	rVB	228479	615223	4.82%	1.710%
5	6.757	921	930	946	rBV	253392	607956	4.77%	1.690%
6	8.647	1234	1240	1248	rBV	550625	837770	6.57%	2.329%
7	10.055	1465	1471	1480	rVB	574889	776307	6.09%	2.158%
8	10.195	1488	1494	1503	rBV	1146223	1501912	11.78%	4.175%
9	10.299	1503	1511	1518	rVV	430829	579537	4.54%	1.611%
10	10.640	1562	1567	1582	rVB	346746	443458	3.48%	1.233%
11	11.079	1634	1639	1650	rVB	513886	647558	5.08%	1.800%
12	11.396	1684	1691	1696	rBV	160131	212913	1.67%	0.592%
13	11.610	1722	1726	1734	rVB	125658	160147	1.26%	0.445%
14	11.750	1740	1749	1754	rBV	411711	532640	4.18%	1.481%
15	12.018	1788	1793	1799	rBV	654172	828944	6.50%	2.304%
16	12.085	1799	1804	1808	rVV	160215	206580	1.62%	0.574%
17	12.244	1824	1830	1837	rBV	3090610	3920515	30.74%	10.898%
18	12.610	1886	1890	1894	rBV	117218	132298	1.04%	0.368%
19	12.695	1899	1904	1910	rBV	190134	272776	2.14%	0.758%
20	13.164	1977	1981	1986	rBV	261035	317791	2.49%	0.883%
21	13.286	1991	2001	2006	rBV2	161801	305473	2.40%	0.849%
22	13.341	2006	2010	2014	rVB	254509	298016	2.34%	0.828%
23	13.420	2019	2023	2029	rVB	734615	953137	7.47%	2.649%
24	13.774	2076	2081	2088	rVV	9931370	12752078	100.00%	35.446%
25	13.865	2088	2096	2100	rVB	184145	293960	2.31%	0.817%
26	14.219	2150	2154	2157	rBV2	89261	129412	1.01%	0.360%
27	14.317	2165	2170	2176	rBV	95319	147350	1.16%	0.410%
28	14.634	2218	2222	2233	rVB	896952	1166480	9.15%	3.242%
29	14.774	2240	2245	2255	rBV	1290307	1712028	13.43%	4.759%
30	15.207	2308	2316	2320	rBV	205801	304483	2.39%	0.846%
31	15.371	2332	2343	2347	rBV	635145	939329	7.37%	2.611%
32	15.475	2354	2360	2365	rBV	488942	759553	5.96%	2.111%
33	15.609	2377	2382	2386	rBV	591060	917601	7.20%	2.551%
34	15.646	2386	2388	2394	rVB	313115	399530	3.13%	1.111%
35	15.835	2409	2419	2430	rVB	145307	431798	3.39%	1.200%
36	15.981	2438	2443	2452	rVB	91685	163445	1.28%	0.454%

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ClientSampleId :
NEVINS-SB03-Z46-47

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_X\Method\82X072123W.M
Title : SW846 8260

37	16.322	2490	2499	2511	rBV2	372961	740385	5.81%	2.058%
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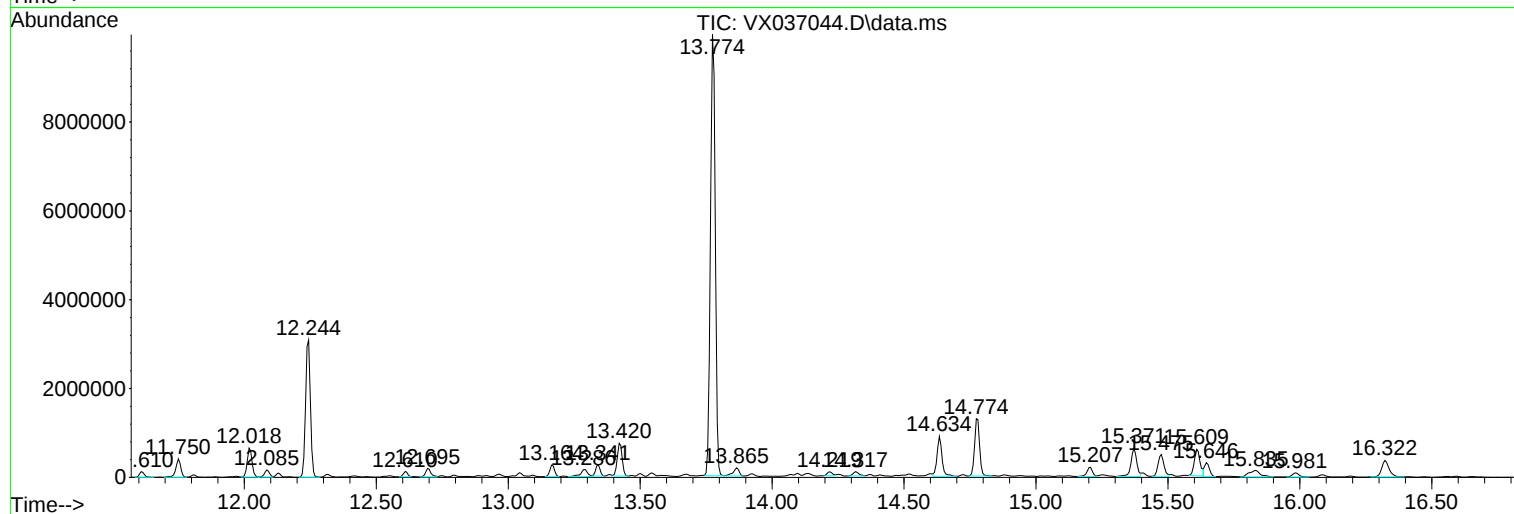
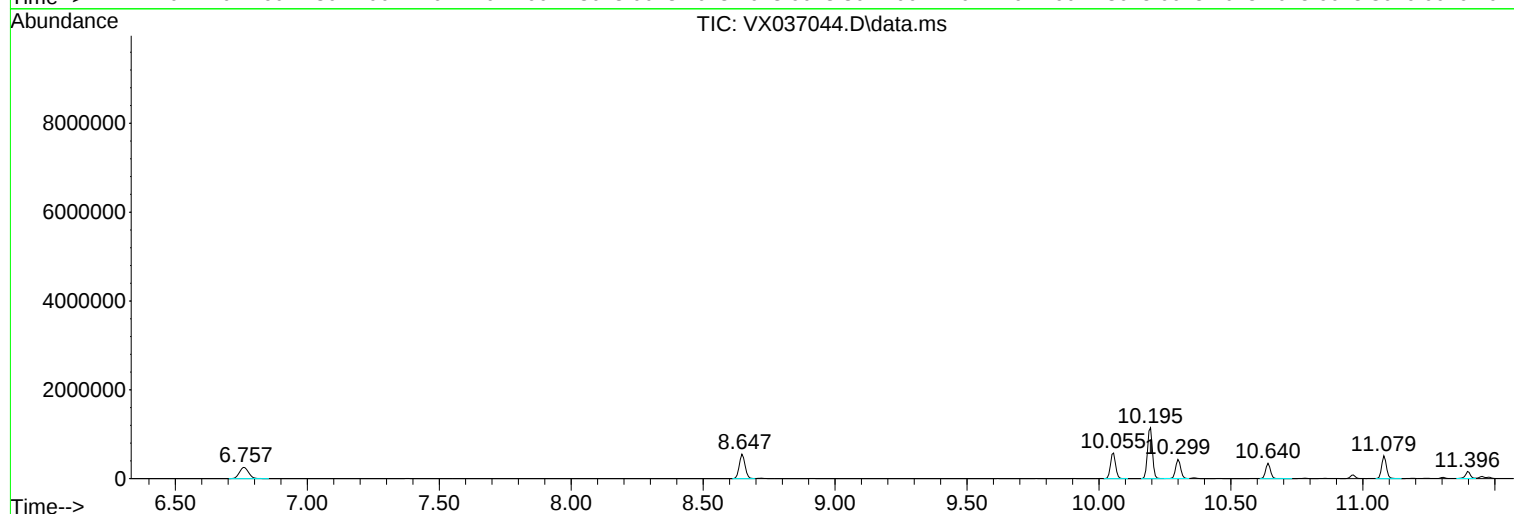
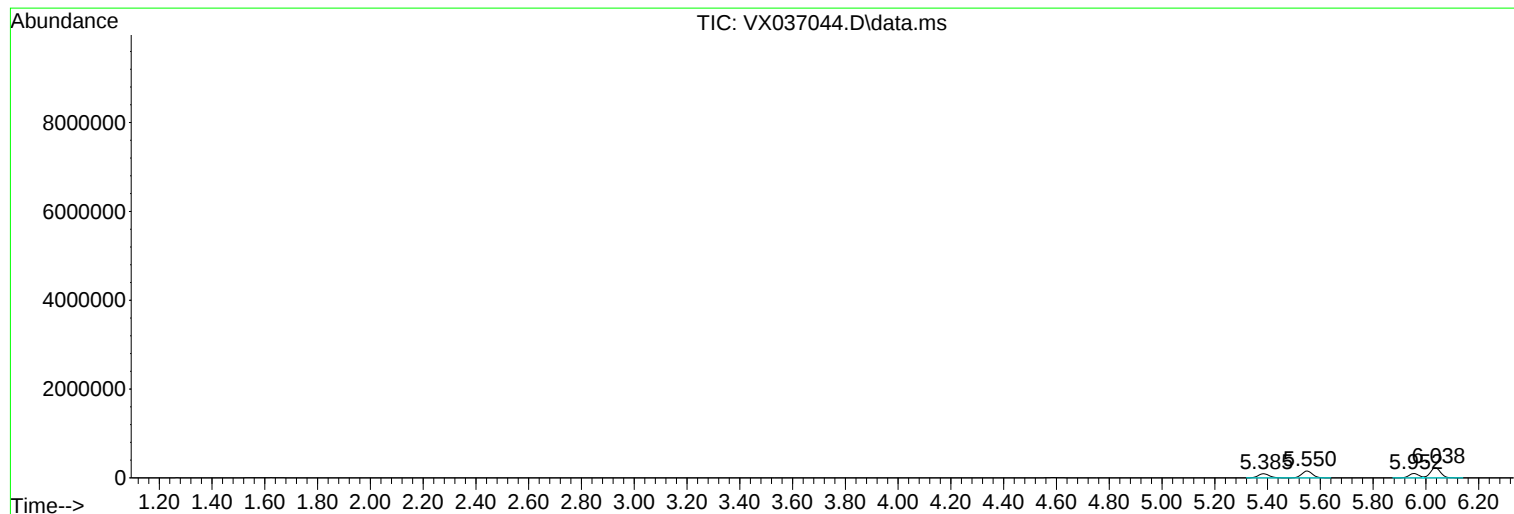
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
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NEVINS-SB03-Z46-47

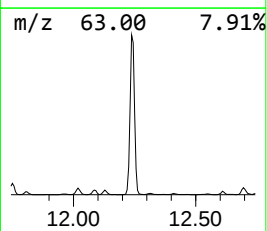
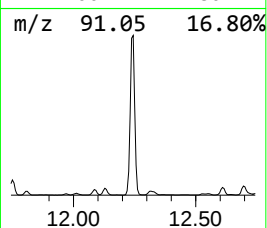
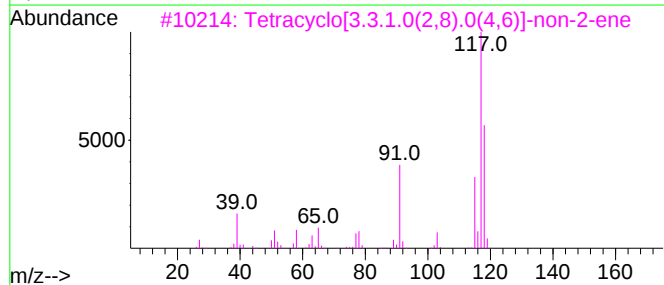
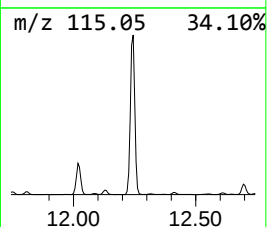
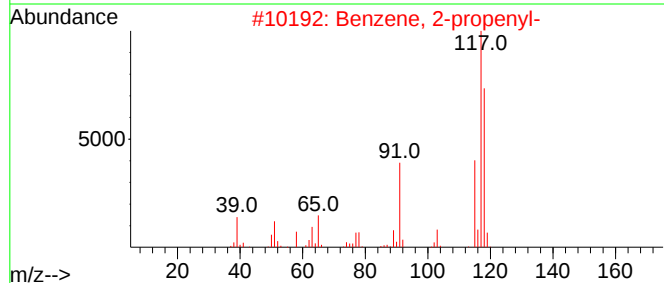
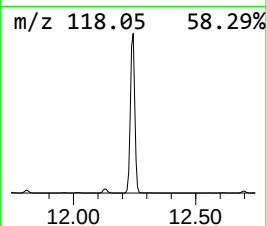
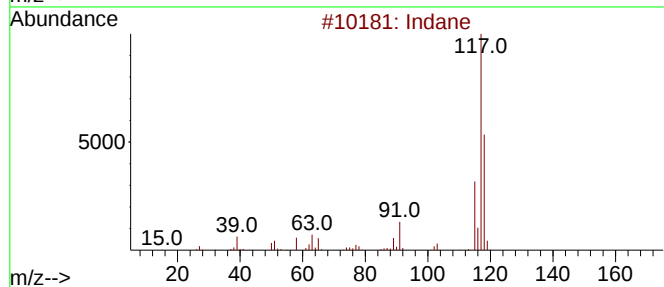
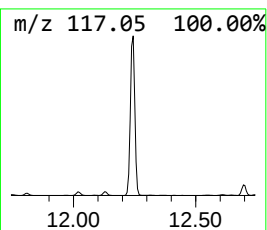
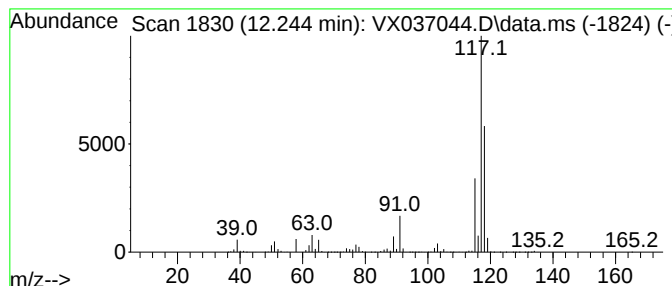
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	236.48 ug/l	3920520	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	80
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	74



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ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z46-47

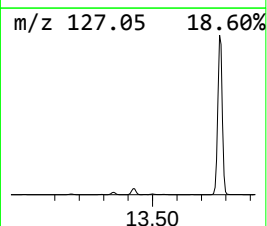
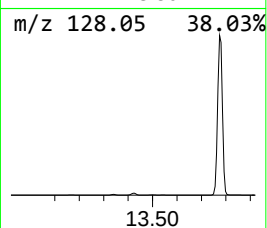
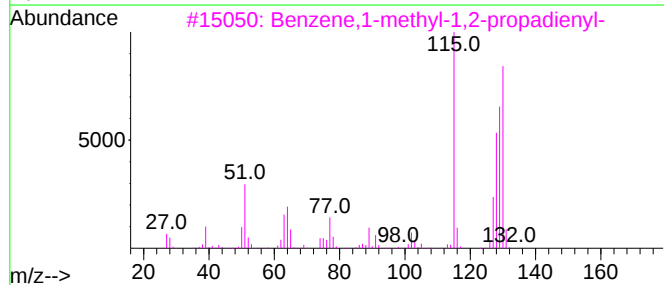
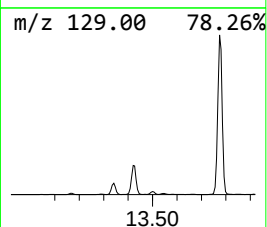
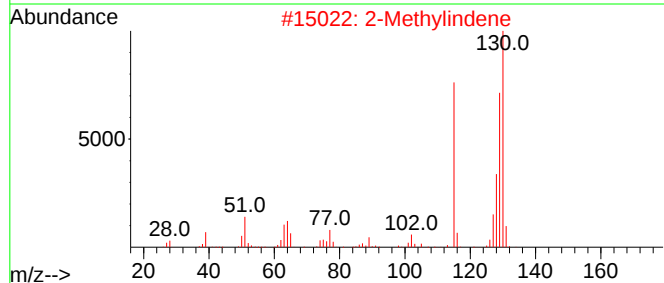
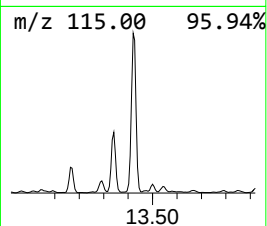
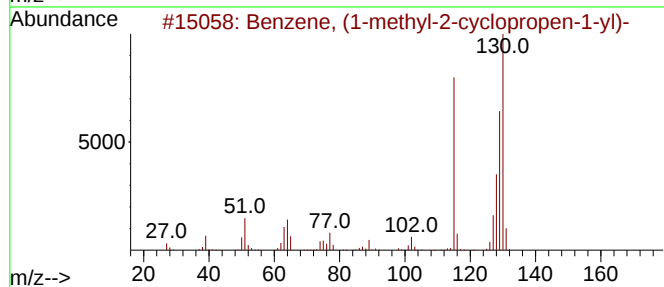
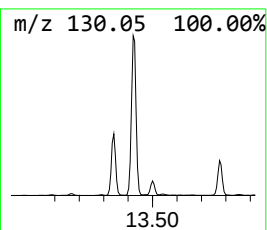
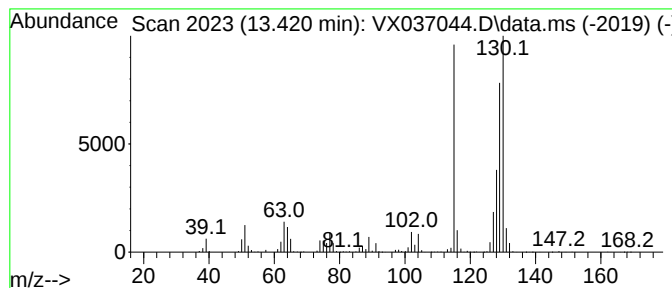
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, (1-methyl-2-cyclop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	57.49 ug/l	953137	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
2			2-Methylindene	130	C10H10	002177-47-1	95
3			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	95
4			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	94
5			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94



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Misc : 7.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z46-47

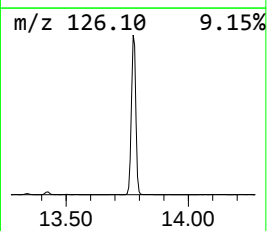
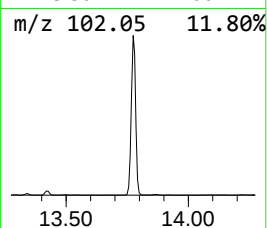
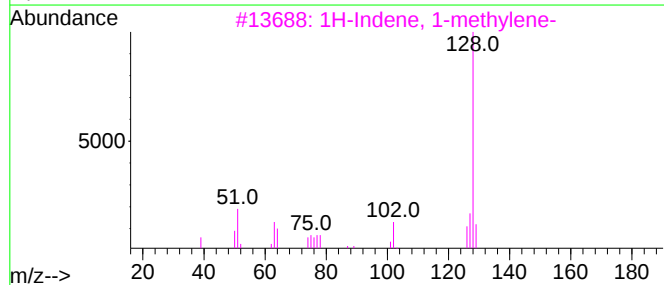
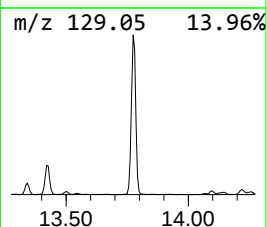
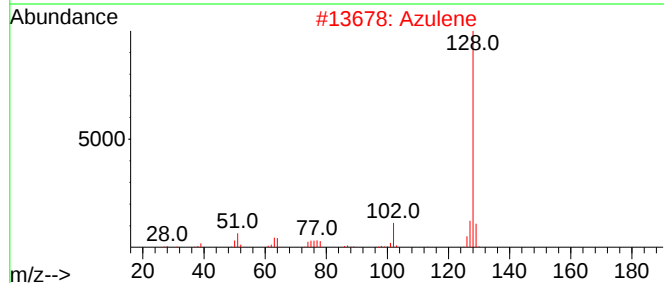
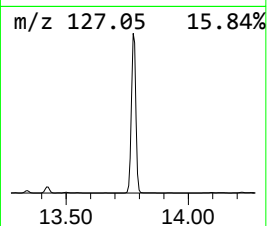
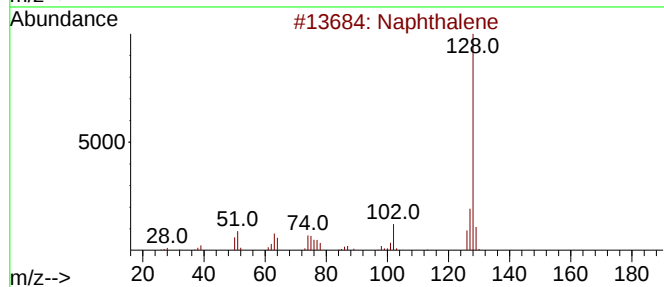
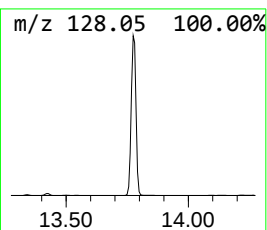
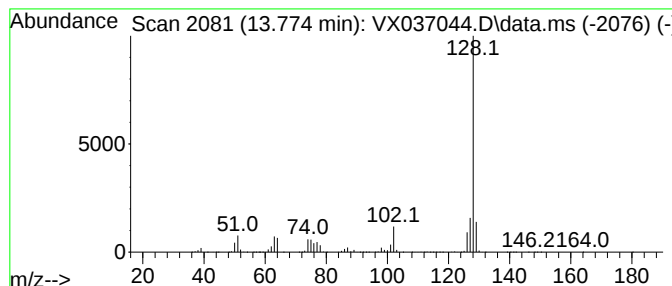
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	769.18 ug/l	12752100	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Azulene	128	C10H8	000275-51-4	94
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
4			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	53



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Instrument :
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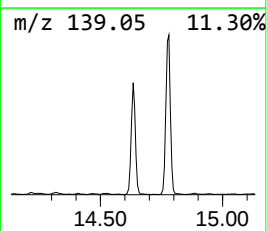
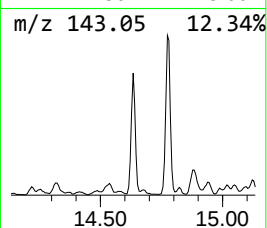
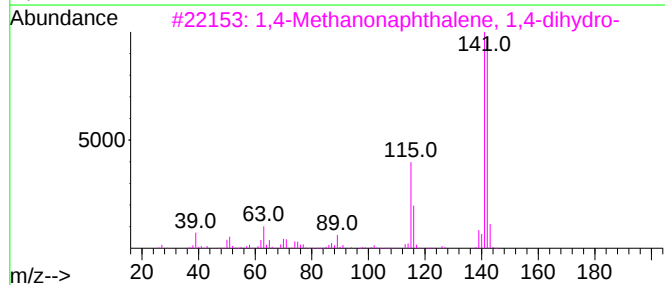
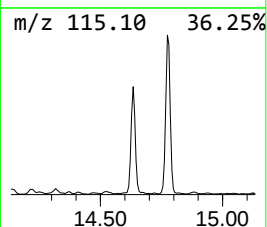
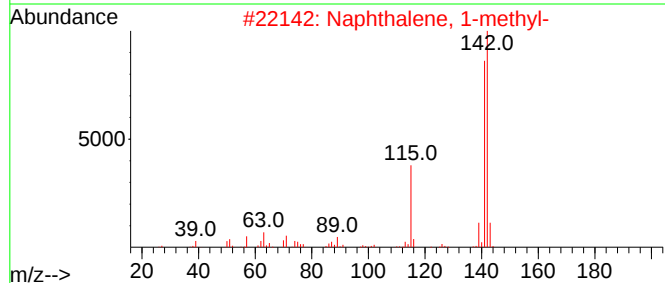
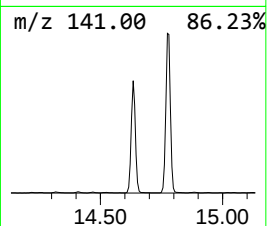
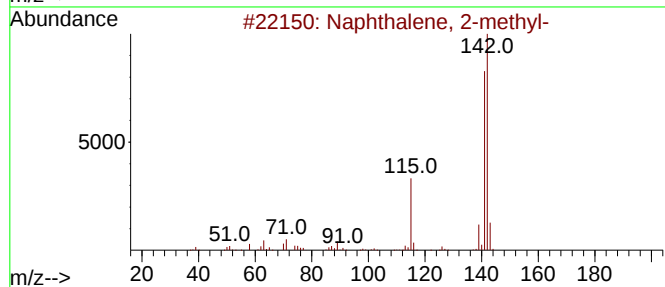
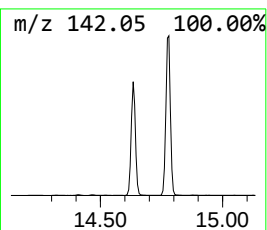
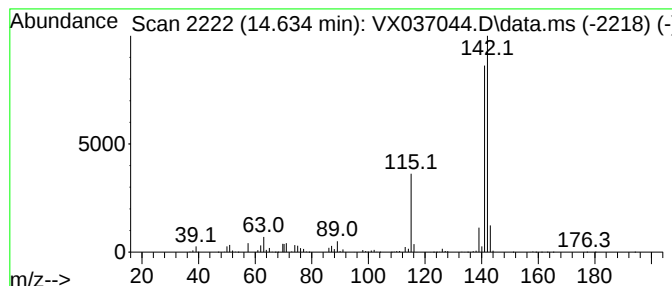
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Quant Title : SW846 8260

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

Peak Number 4 1,4-Methanonaphthalene, 1,4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	70.36 ug/l	1166480	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



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Instrument :
MSVOA_X
ClientSampleId :
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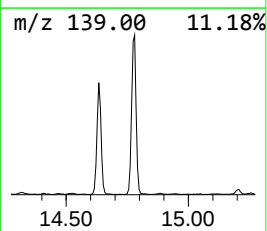
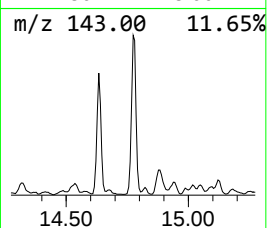
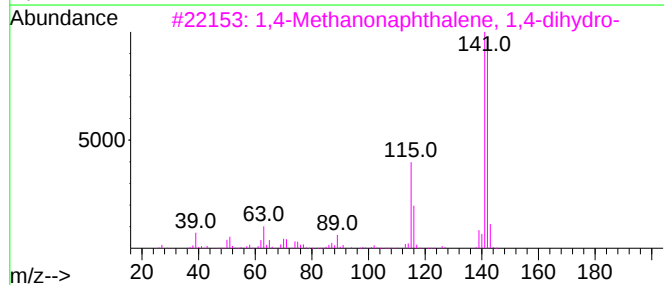
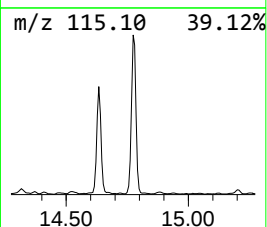
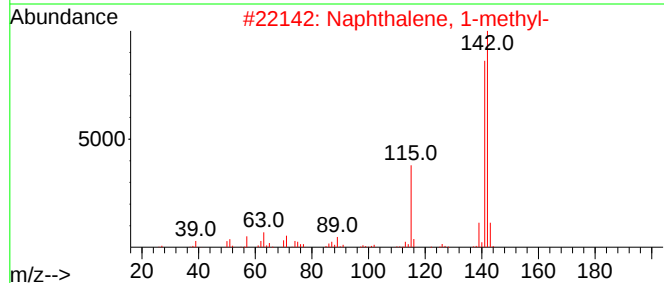
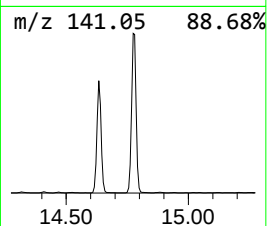
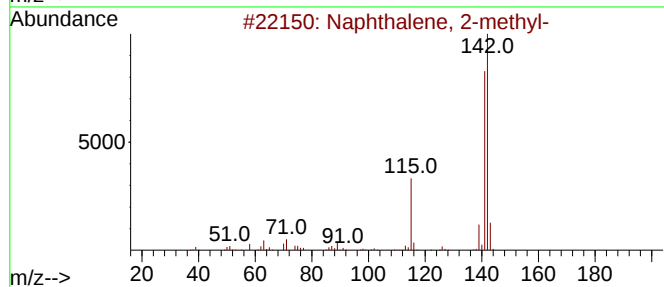
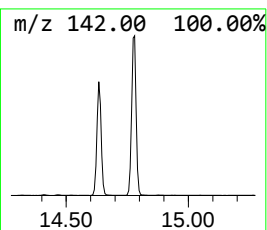
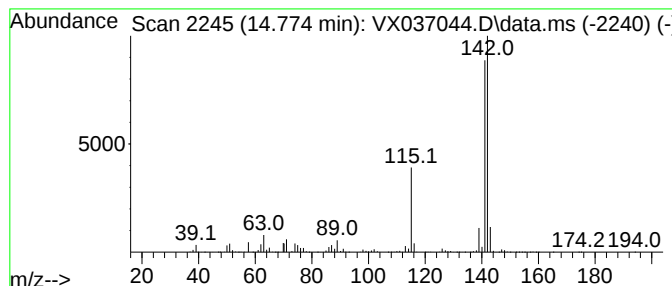
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Quant Title : SW846 8260

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

Peak Number 5 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	103.27 ug/l	1712030	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037044.D
Acq On : 17 Aug 2023 07:11
Operator : JC/MD
Sample : 03975-03 10X
Misc : 7.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z46-47

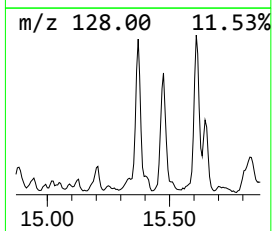
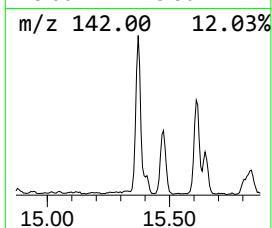
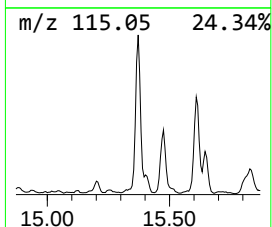
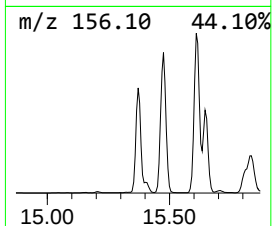
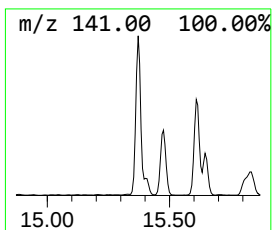
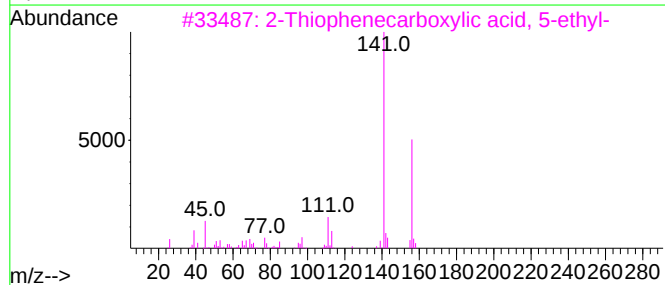
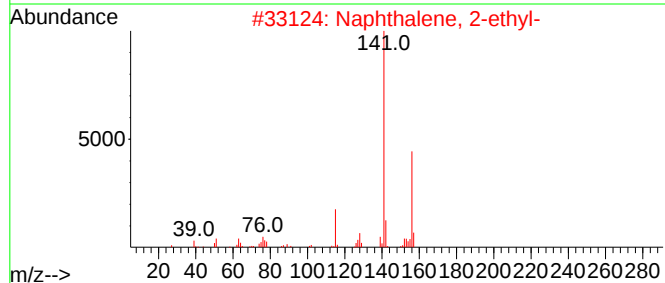
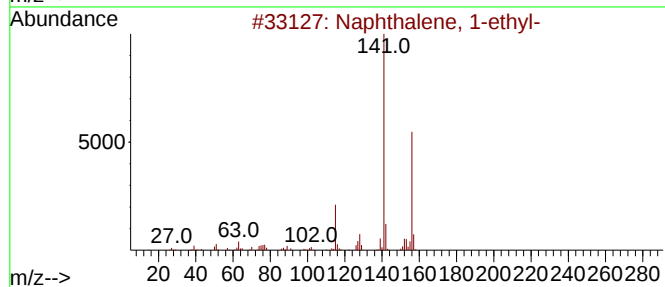
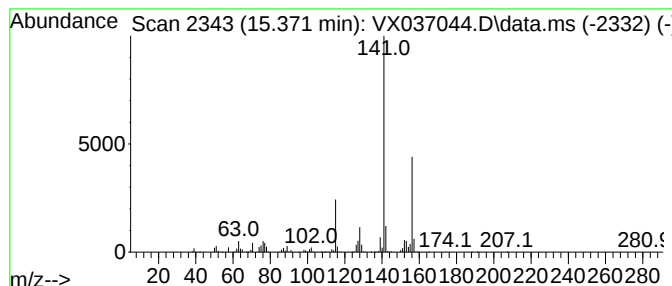
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	56.66 ug/l	939329	1,4-Dichlorobenzene-d4	12.018

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	95
3			2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	59
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	58
5			5-Acetyl-2-amino-4-methylthiazole	156	C6H8N2OS	030748-47-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037044.D
Acq On : 17 Aug 2023 07:11
Operator : JC/MD
Sample : 03975-03 10X
Misc : 7.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z46-47

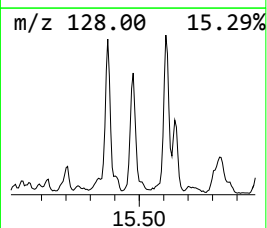
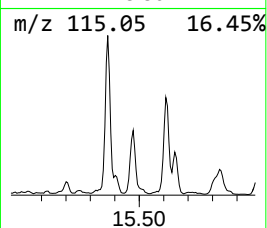
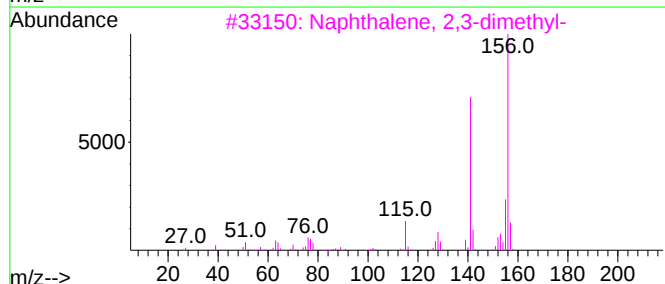
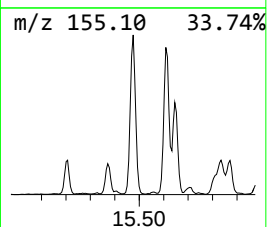
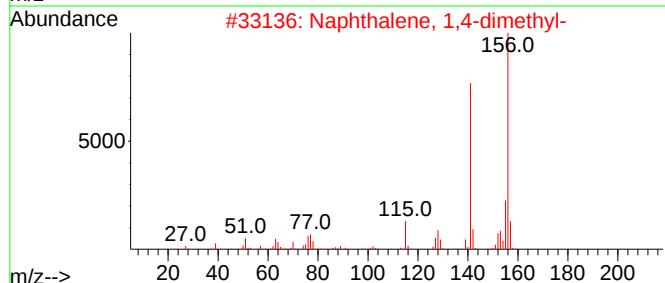
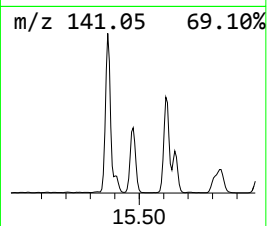
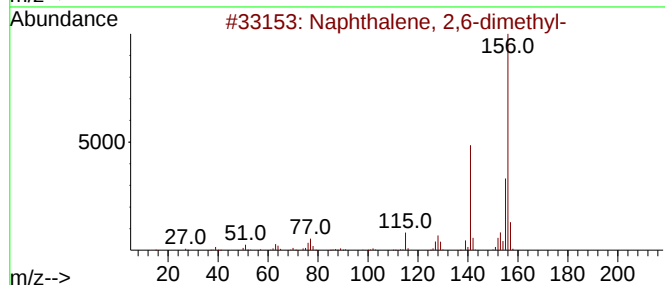
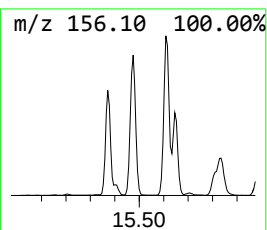
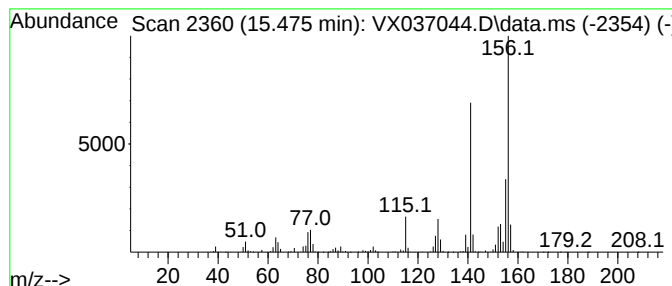
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	45.81 ug/l	759553	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037044.D
Acq On : 17 Aug 2023 07:11
Operator : JC/MD
Sample : 03975-03 10X
Misc : 7.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z46-47

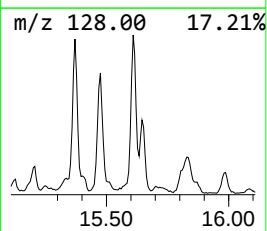
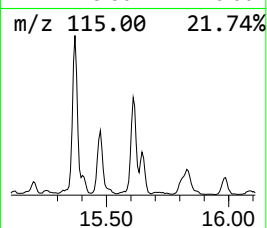
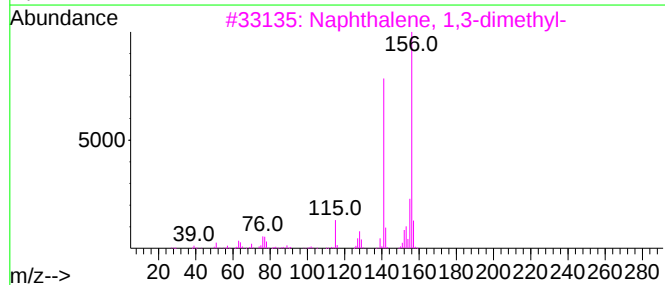
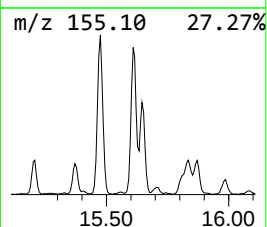
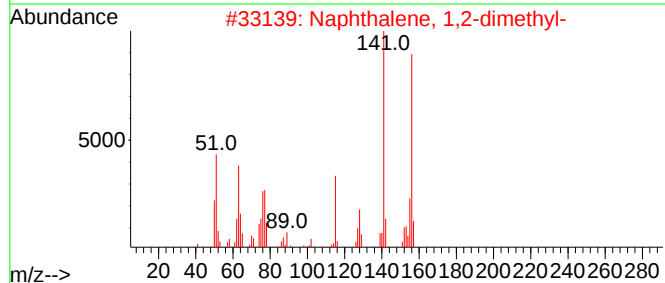
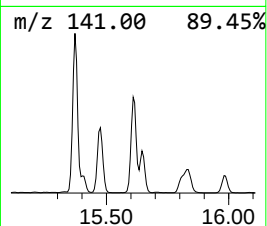
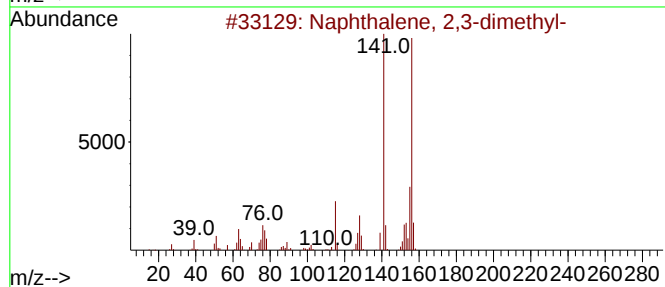
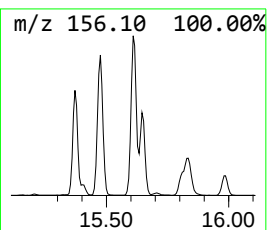
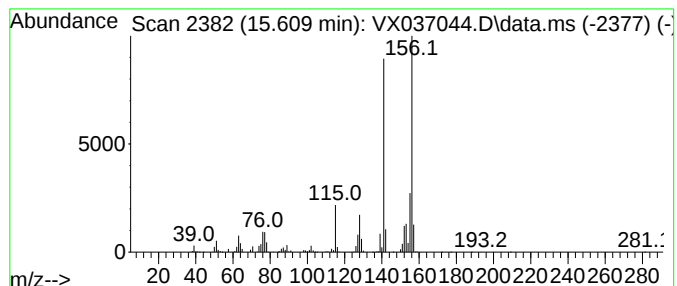
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	55.35 ug/l	917601	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037044.D
Acq On : 17 Aug 2023 07:11
Operator : JC/MD
Sample : 03975-03 10X
Misc : 7.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z46-47

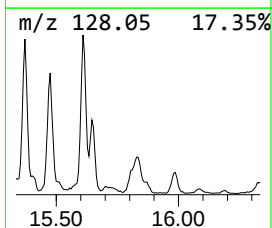
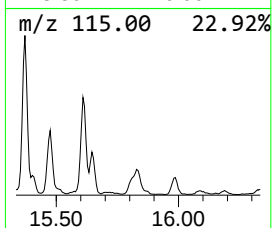
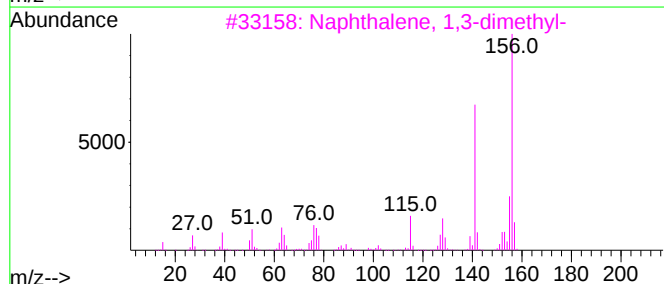
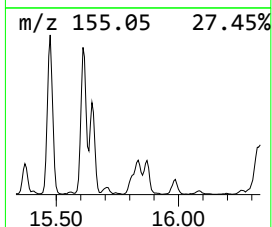
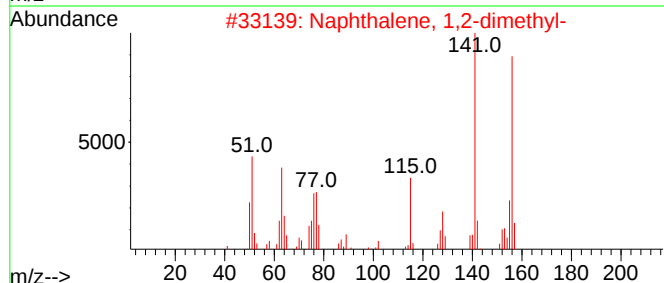
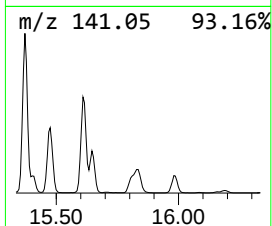
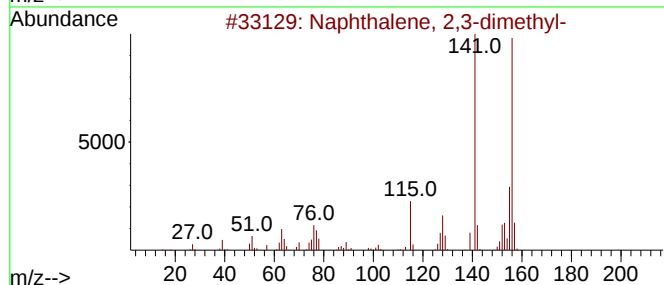
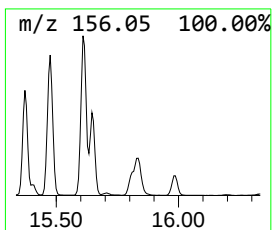
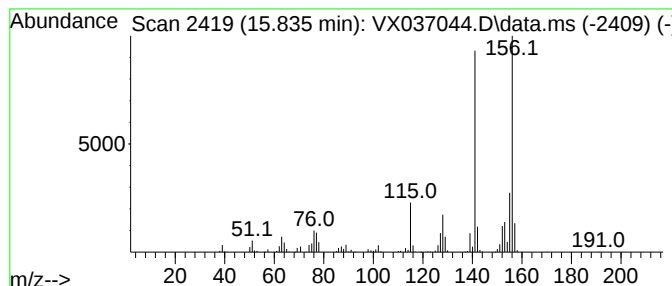
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	26.05 ug/l	431798	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037044.D
Acq On : 17 Aug 2023 07:11
Operator : JC/MD
Sample : 03975-03 10X
Misc : 7.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z46-47

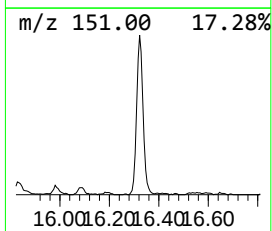
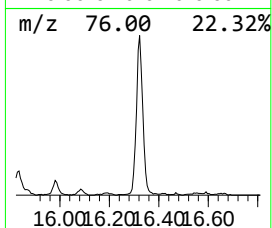
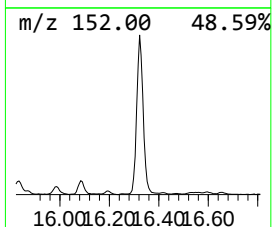
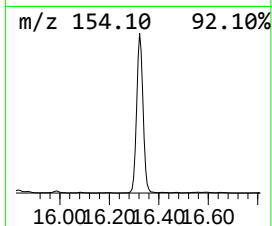
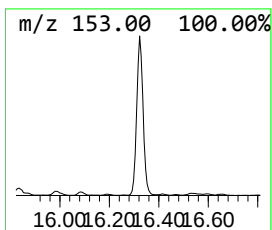
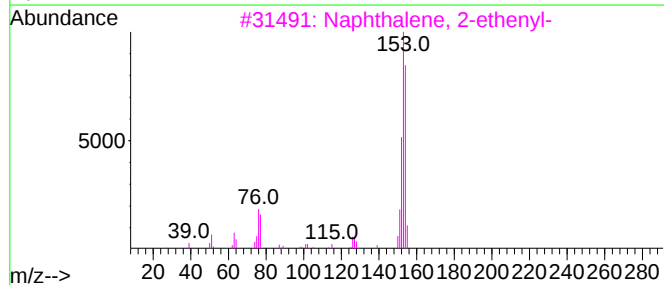
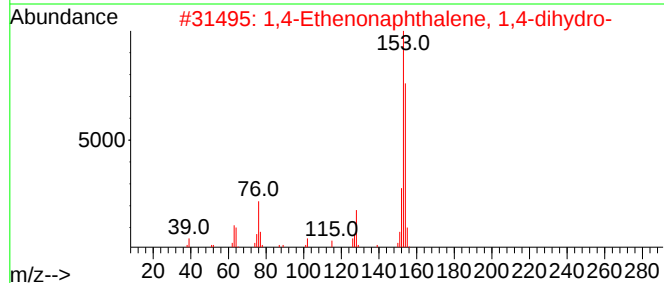
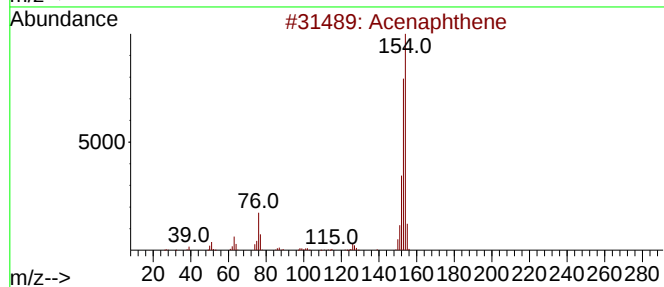
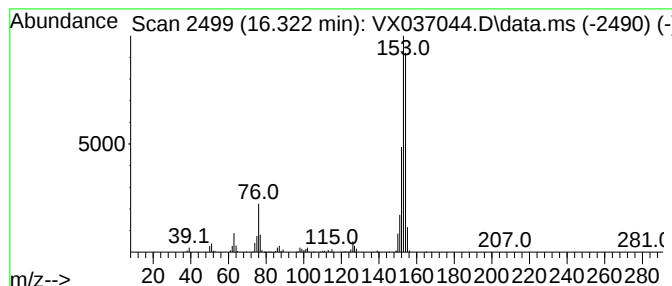
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Quant Title : SW846 8260

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

Peak Number 10 1,4-Ethenonaphthalene, 1,4-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	44.66 ug/l	740385	1,4-Dichlorobenzene-d4	12.018

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	72
3		Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	59
4		Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
5		Biphenyl	154	C12H10	000092-52-4	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037044.D
Acq On : 17 Aug 2023 07:11
Operator : JC/MD
Sample : 03975-03 10X
Misc : 7.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z46-47

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.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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Benzene, (1-met...	13.420	57.5	ug/l	953137	4	12.018	828944	50.0
Azulene	13.774	769.2	ug/l	12752100	4	12.018	828944	50.0
1,4-Methanonaph...	14.634	70.4	ug/l	1166480	4	12.018	828944	50.0
Benzocyclohepta...	14.774	103.3	ug/l	1712030	4	12.018	828944	50.0
Naphthalene, 1-...	15.371	56.7	ug/l	939329	4	12.018	828944	50.0
Naphthalene, 2,...	15.475	45.8	ug/l	759553	4	12.018	828944	50.0
Naphthalene, 2,...	15.609	55.4	ug/l	917601	4	12.018	828944	50.0
Naphthalene, 1,...	15.835	26.1	ug/l	431798	4	12.018	828944	50.0
1,4-Ethenonaph...	16.322	44.7	ug/l	740385	4	12.018	828944	50.0