

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
 Data File : VX037048.D
 Acq On : 17 Aug 2023 08:47
 Operator : JC/MD
 Sample : 03975-02 20X
 Misc : 7.22g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NEVINS-SB03-Z10-12-Q

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: VX037048.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.037	804	812	830	rVB	299416	801759	1.29%	0.377%
2	8.647	1234	1240	1247	rBV	516484	801021	1.29%	0.377%
3	10.055	1466	1471	1477	rBV	562598	749789	1.20%	0.353%
4	10.195	1488	1494	1504	rBV	5638898	7295431	11.71%	3.435%
5	10.299	1504	1511	1518	rVV	2859616	3743158	6.01%	1.762%
6	10.640	1562	1567	1581	rVB	1509401	1926229	3.09%	0.907%
7	11.079	1634	1639	1650	rVB	505161	643680	1.03%	0.303%
8	11.378	1683	1688	1690	rBV	3046193	3941781	6.33%	1.856%
9	11.451	1696	1700	1707	rVB	592197	745041	1.20%	0.351%
10	11.610	1721	1726	1734	rBV	727701	912801	1.47%	0.430%
11	11.750	1740	1749	1754	rBV	2153019	2749394	4.41%	1.294%
12	12.018	1788	1793	1799	rVV2	741884	1078999	1.73%	0.508%
13	12.085	1799	1804	1808	rVV	849483	1046750	1.68%	0.493%
14	12.244	1824	1830	1837	rBV	14319392	19053060	30.59%	8.970%
15	12.317	1837	1842	1848	rVV2	1340867	1711575	2.75%	0.806%
16	12.555	1873	1881	1885	rBV	580936	913747	1.47%	0.430%
17	12.609	1885	1890	1894	rBV	1248361	1540014	2.47%	0.725%
18	12.695	1900	1904	1910	rBV	624699	1001394	1.61%	0.471%
19	12.963	1944	1948	1953	rBV	601286	759543	1.22%	0.358%
20	13.164	1977	1981	1986	rVB	2177554	2721805	4.37%	1.281%
21	13.286	1992	2001	2006	rBV2	1039219	1706529	2.74%	0.803%
22	13.341	2006	2010	2016	rVV	2160416	2573540	4.13%	1.212%
23	13.426	2016	2024	2029	rVB	4864975	6396378	10.27%	3.011%
24	13.500	2029	2036	2040	rBV2	501422	715209	1.15%	0.337%
25	13.548	2040	2044	2048	rBV	493189	696314	1.12%	0.328%
26	13.798	2076	2085	2089	rBV2	28370885	62295316	100.00%	29.329%
27	13.871	2089	2097	2102	rVV	2413116	3242601	5.21%	1.527%
28	14.097	2131	2134	2137	rVV	718258	873701	1.40%	0.411%
29	14.219	2149	2154	2157	rBV	811794	1152355	1.85%	0.543%
30	14.316	2164	2170	2177	rVV	820684	1363228	2.19%	0.642%
31	14.597	2211	2216	2218	rVV	573126	733285	1.18%	0.345%
32	14.646	2218	2224	2233	rVB	21059139	30763736	49.38%	14.484%
33	14.786	2241	2247	2255	rVB	14115664	19522375	31.34%	9.191%
34	15.207	2308	2316	2320	rBV	1994711	2655278	4.26%	1.250%
35	15.371	2331	2343	2348	rBV	4071650	6278101	10.08%	2.956%
36	15.475	2354	2360	2365	rBV	2762235	4427095	7.11%	2.084%

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Title : SW846 8260

37	15.615	2377	2383	2386	rVV	2800165	4678621	7.51%	2.203%
38	15.652	2386	2389	2395	rVB	1561010	2193753	3.52%	1.033%
39	15.835	2409	2419	2424	rBV	661124	1756271	2.82%	0.827%
40	15.987	2438	2444	2454	rVB	398981	692825	1.11%	0.326%
41	16.322	2491	2499	2509	rBV2	1750250	3545895	5.69%	1.669%

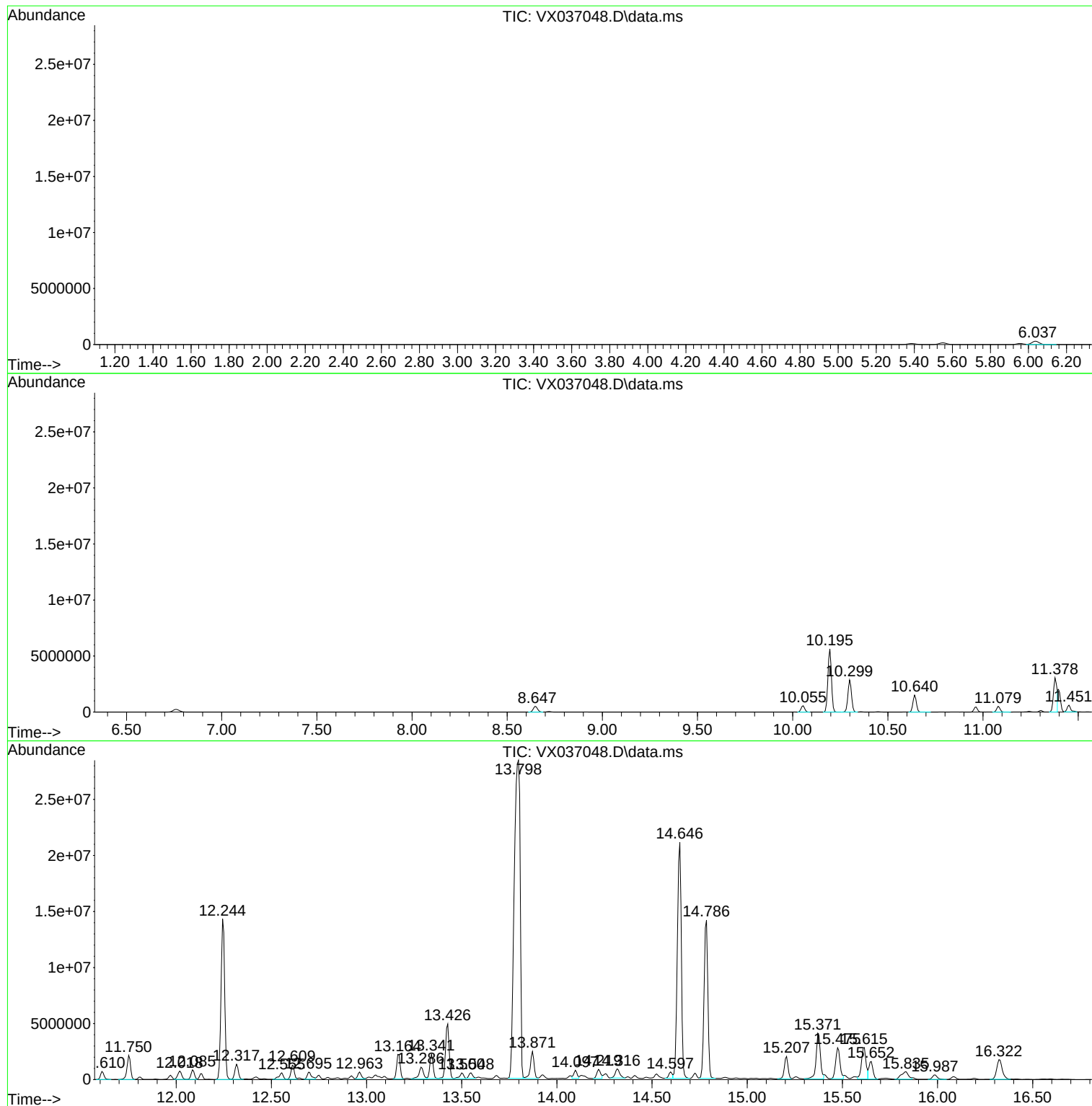
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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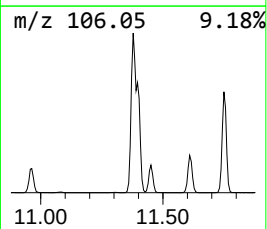
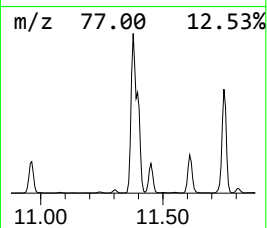
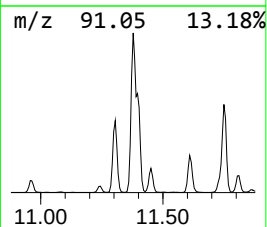
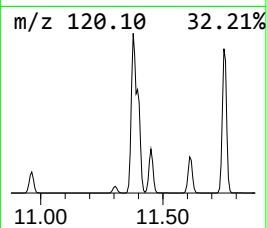
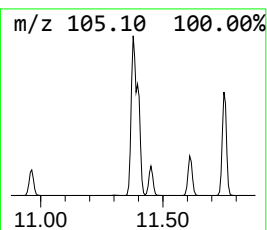
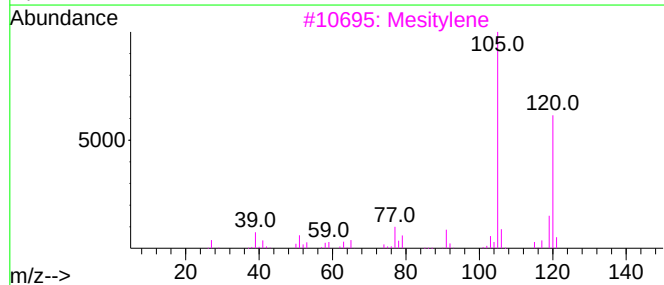
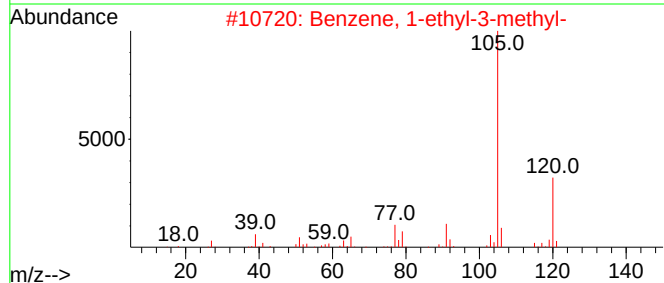
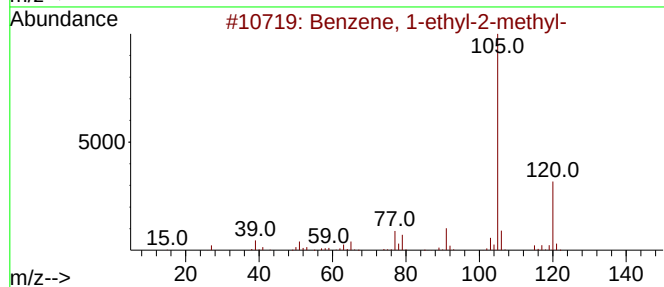
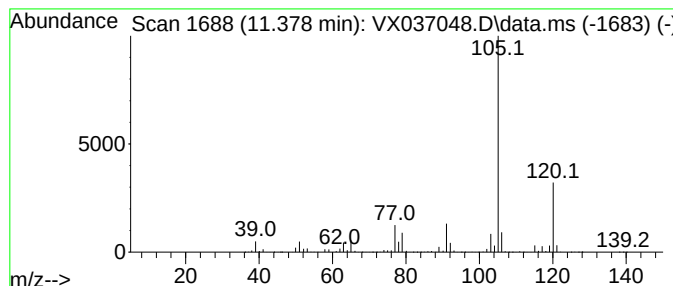
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	182.66 ug/l	3941780	1,4-Dichlorobenzene-d4	12.018

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	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z10-12-Q

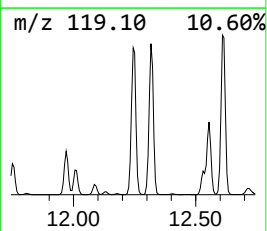
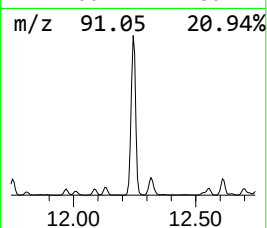
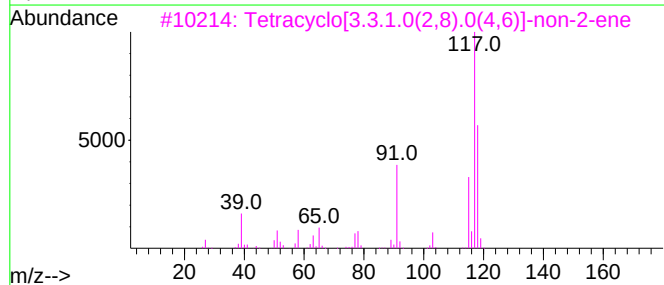
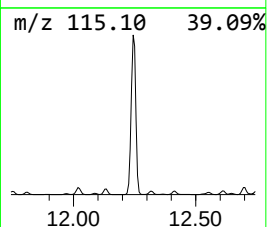
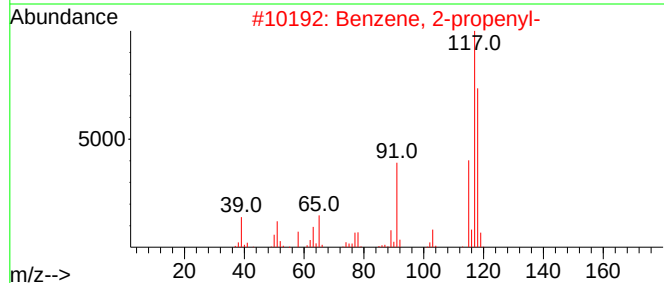
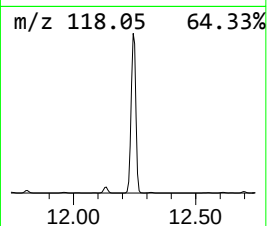
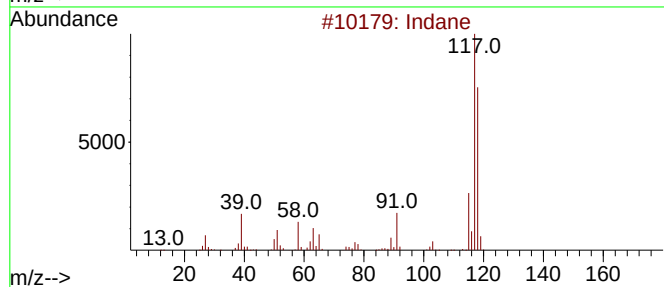
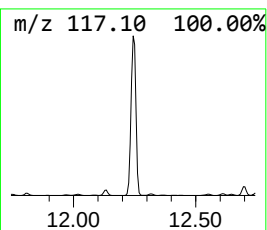
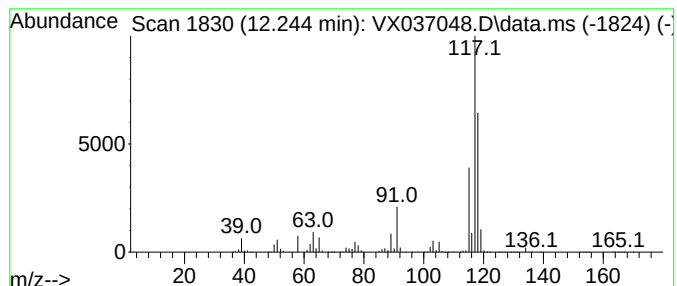
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	882.90 ug/l	19053100	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	90
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	62
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	62



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Misc : 7.22g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 51 Sample Multiplier: 1

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MSVOA_X
ClientSampleId :
NEVINS-SB03-Z10-12-Q

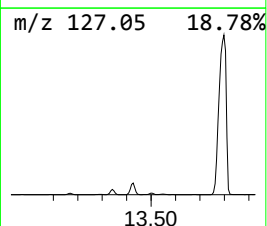
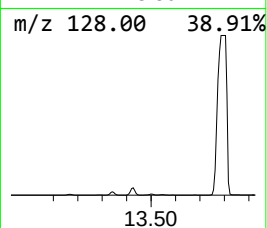
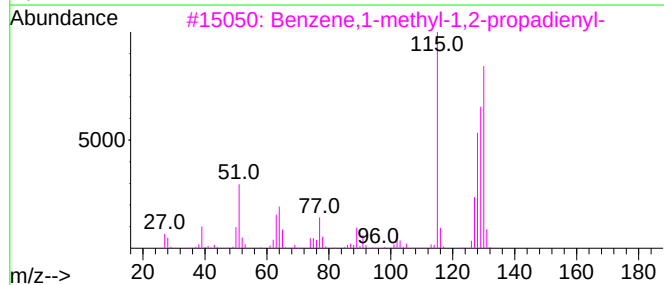
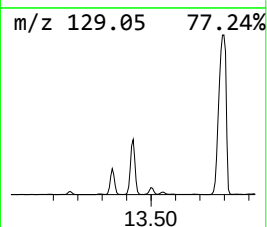
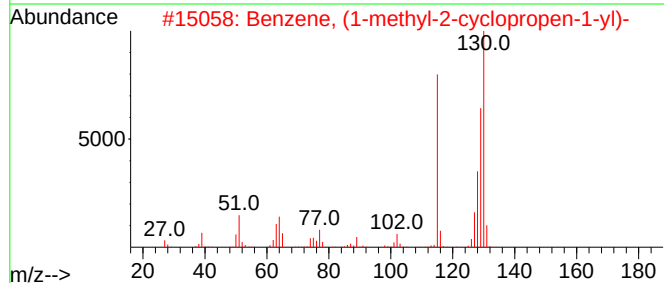
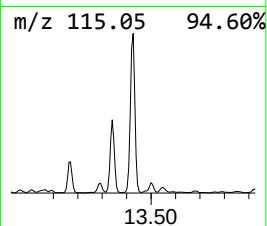
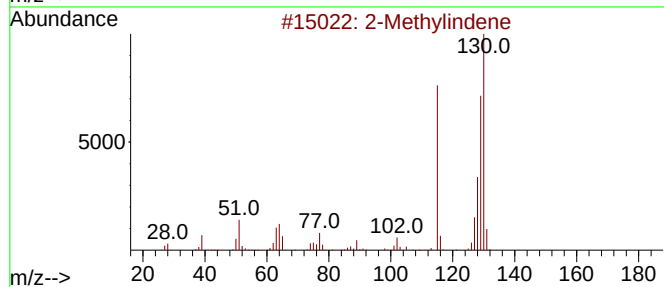
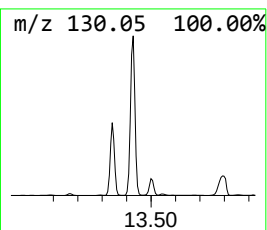
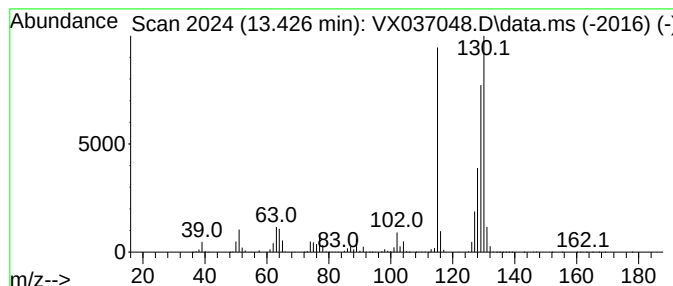
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, (1-methyl-2-cyclop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	296.40 ug/l	6396380	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene			130	C10H10	002177-47-1	95
2	Benzene, (1-methyl-2-cyclopropen...			130	C10H10	065051-83-4	95
3	Benzene,1-methyl-1,2-propadienyl-			130	C10H10	022433-39-2	94
4	1H-Indene, 1-methyl-			130	C10H10	000767-59-9	94
5	Benzene, 1-butylnyl-			130	C10H10	000622-76-4	94



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ClientSampleId :
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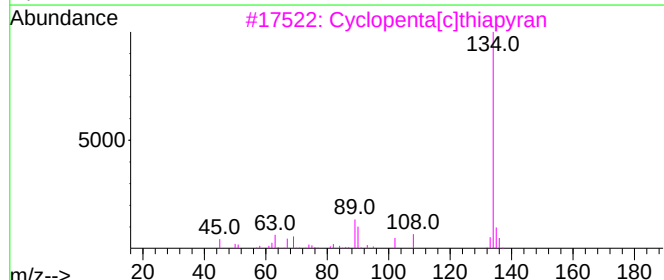
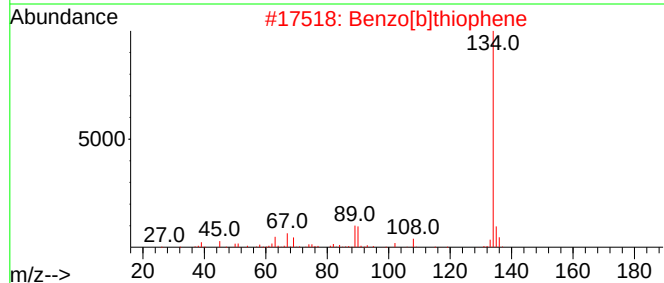
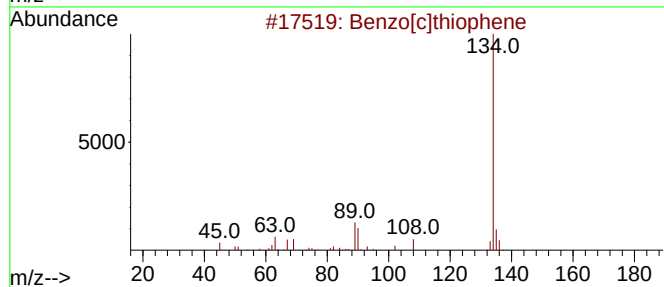
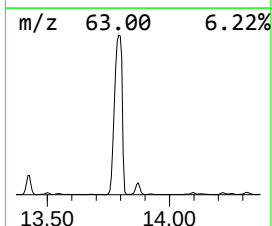
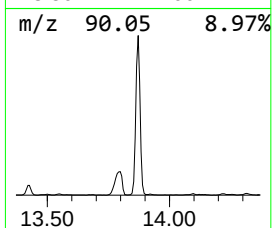
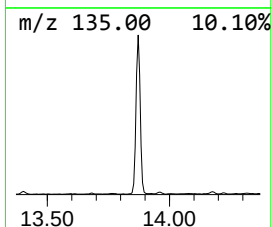
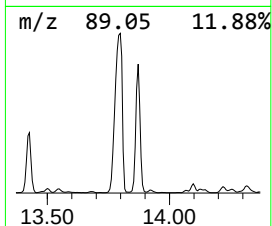
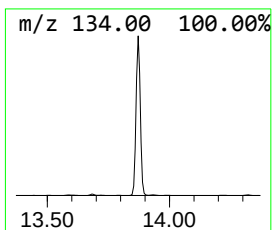
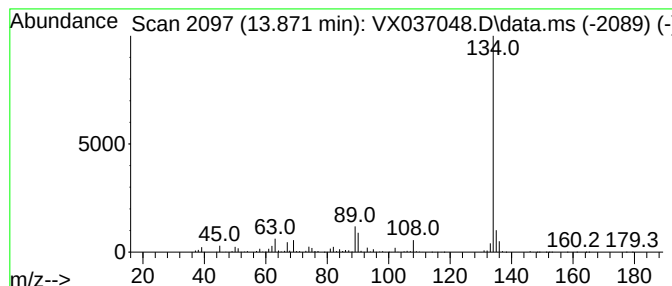
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Quant Title : SW846 8260

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

Peak Number 4 Benzo[c]thiophene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	150.26 ug/l	3242600	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	94
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4			[1]Benzo[thieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	64
5			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	45



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NEVINS-SB03-Z10-12-Q

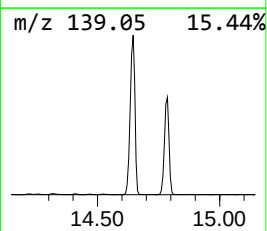
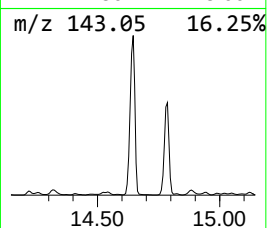
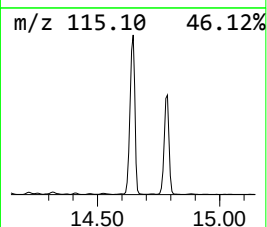
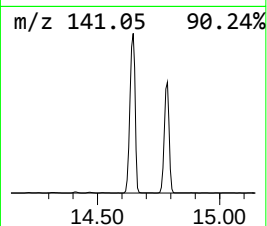
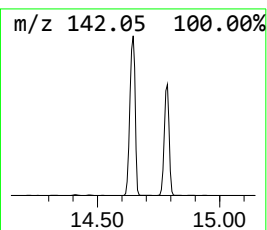
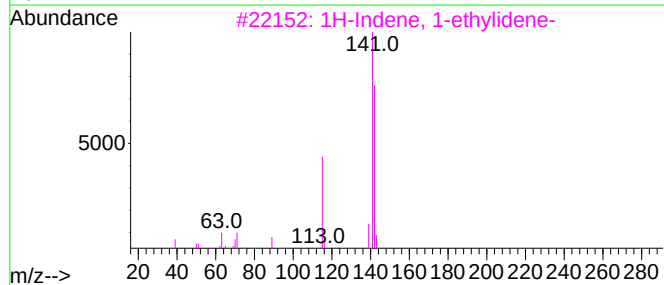
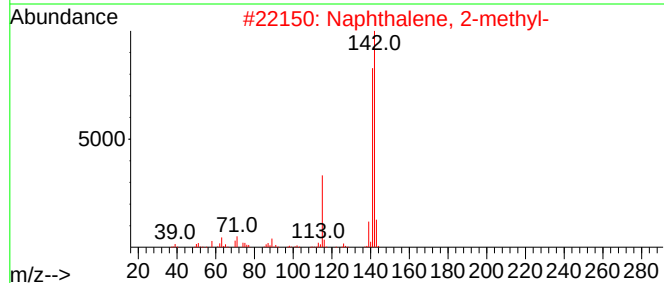
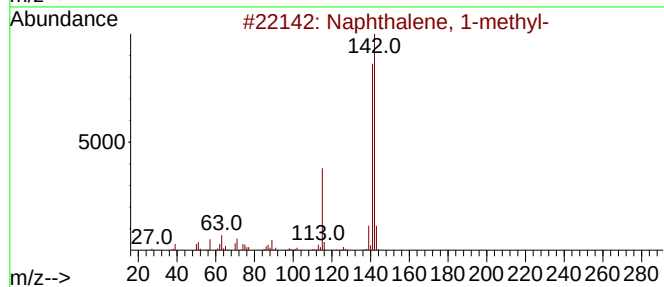
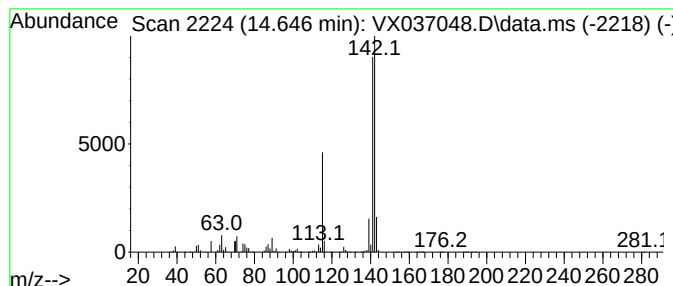
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.646	1425.57 ug/l	30763700	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91
4			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5			Benzocycloheptatriene	142	C11H10	000264-09-5	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037048.D
Acq On : 17 Aug 2023 08:47
Operator : JC/MD
Sample : 03975-02 20X
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z10-12-Q

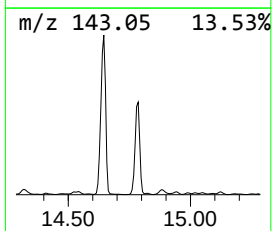
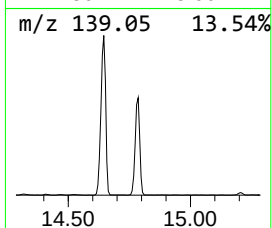
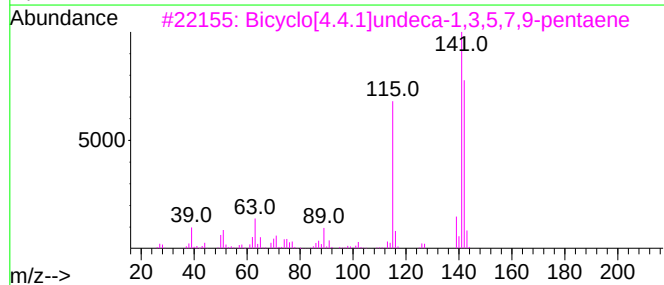
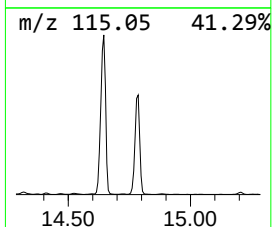
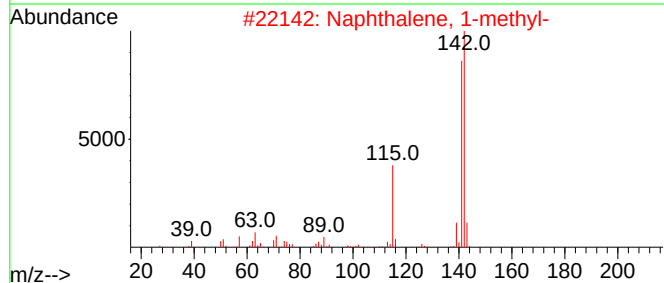
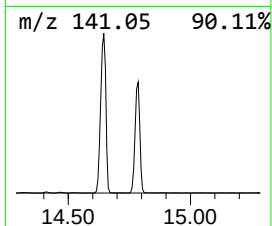
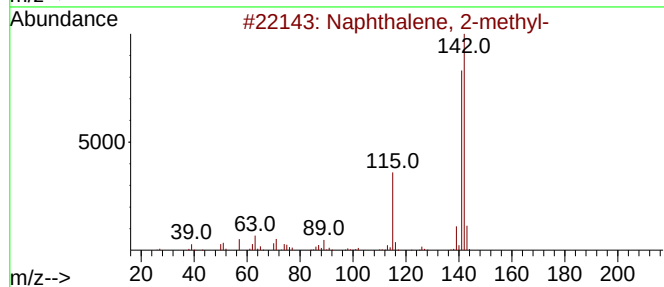
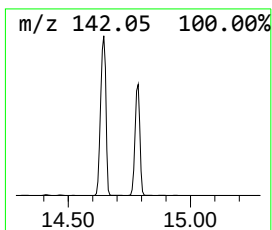
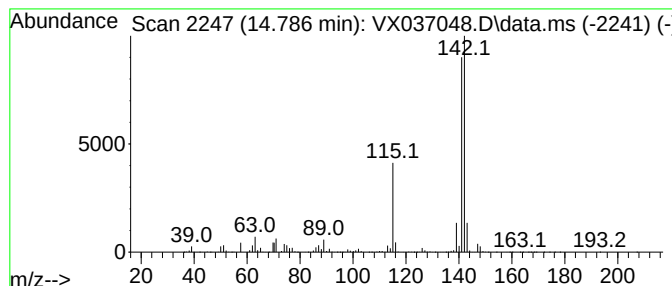
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Quant Title : SW846 8260

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

Peak Number 6 Bicyclo[4.4.1]undeca-1,3,5,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	904.65 ug/l	19522400	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			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Benzocycloheptatriene	142	C11H10	000264-09-5	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037048.D
Acq On : 17 Aug 2023 08:47
Operator : JC/MD
Sample : 03975-02 20X
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z10-12-Q

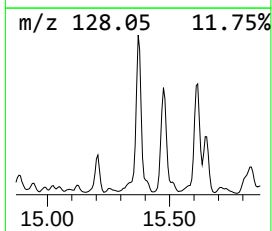
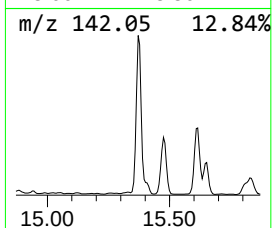
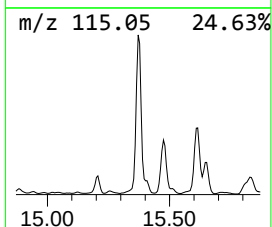
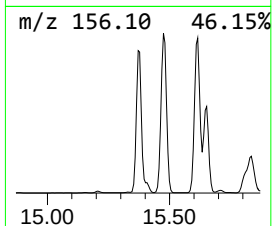
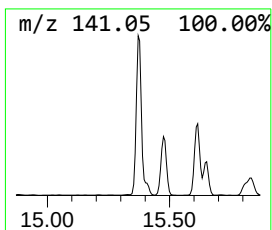
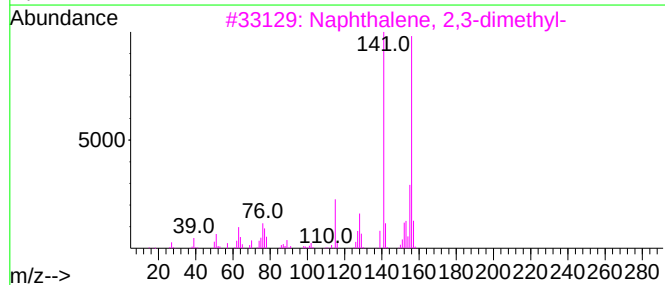
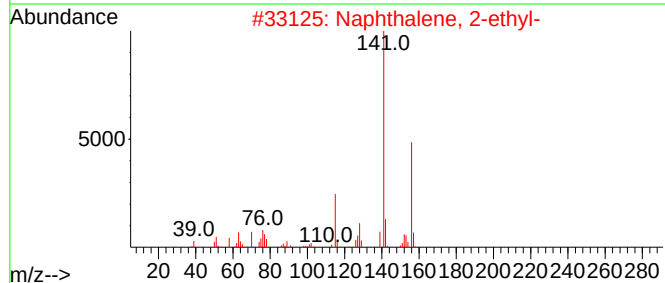
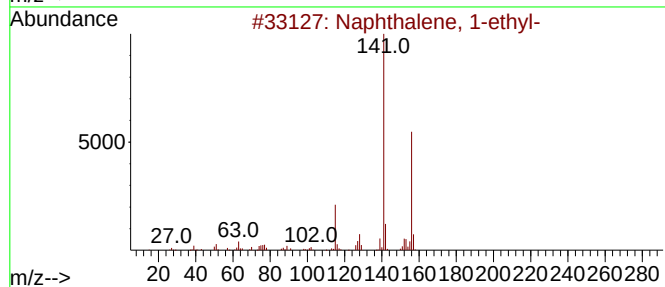
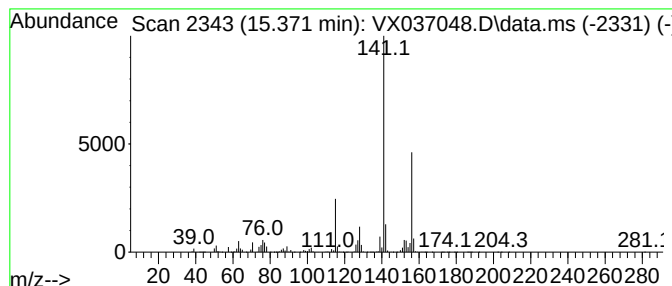
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	290.92 ug/l	6278100	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	96
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	58
4			5-Acetyl-2-amino-4-methylthiazole	156	C6H8N2OS	030748-47-1	53
5			7-Methyl-trans-8-thiabicyclo[4.3...	156	C9H16S	060133-10-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037048.D
Acq On : 17 Aug 2023 08:47
Operator : JC/MD
Sample : 03975-02 20X
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z10-12-Q

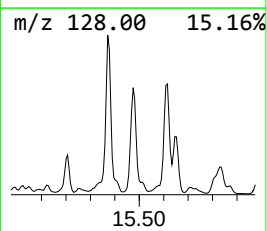
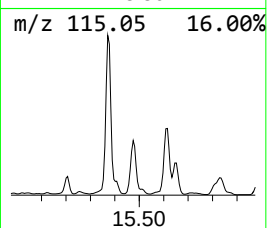
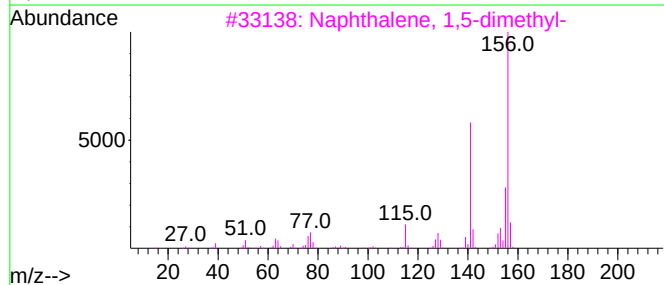
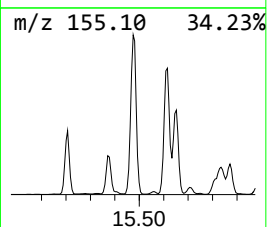
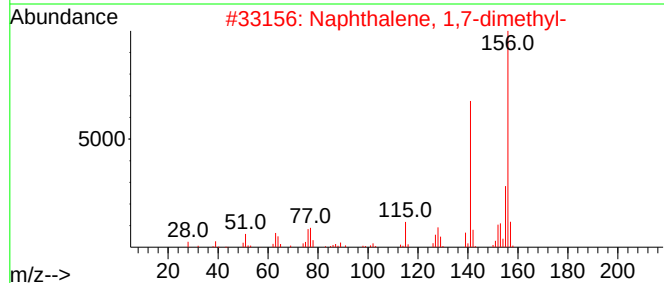
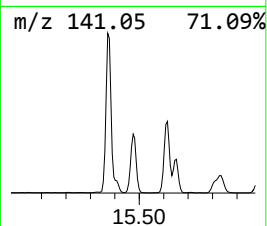
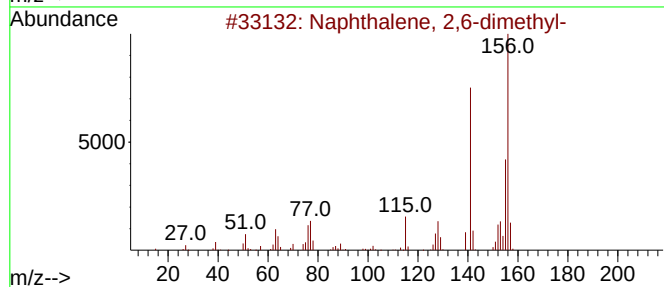
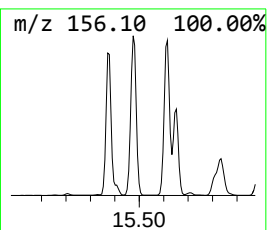
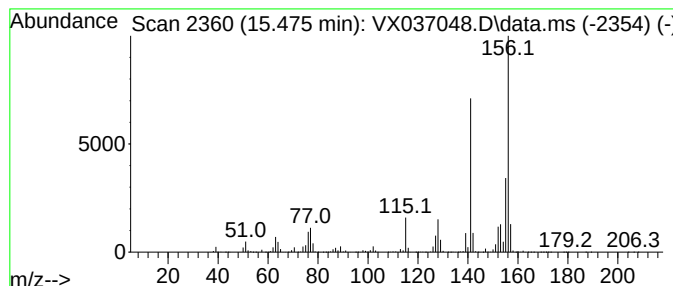
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	205.15 ug/l	4427100	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, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037048.D
Acq On : 17 Aug 2023 08:47
Operator : JC/MD
Sample : 03975-02 20X
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z10-12-Q

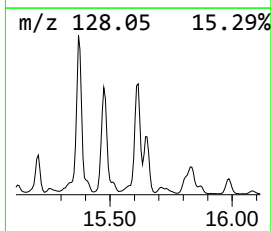
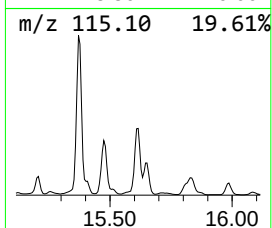
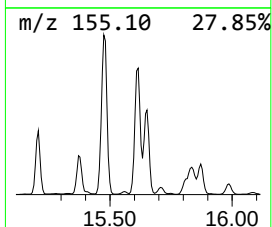
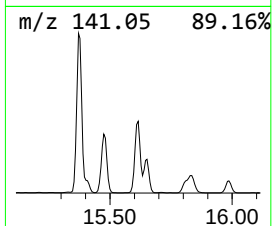
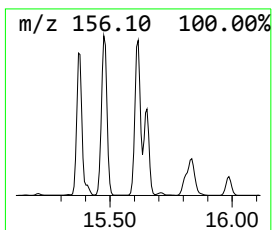
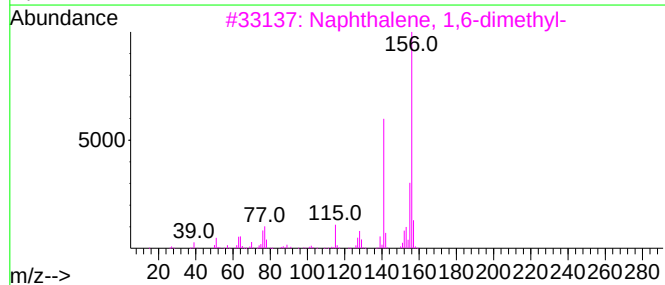
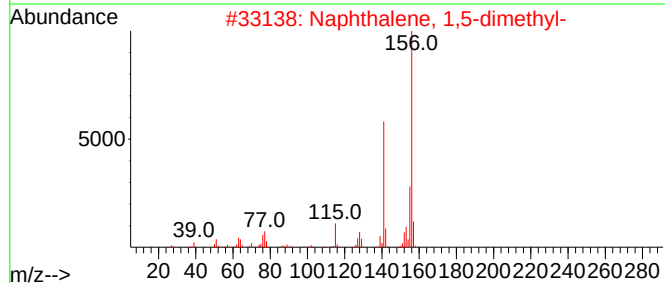
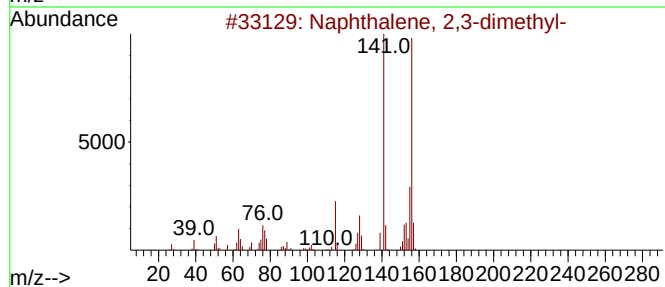
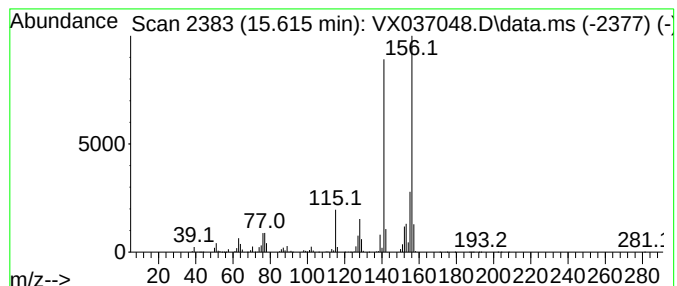
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	216.80 ug/l	4678620	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, 1,5-dimethyl-	156	C12H12	000571-61-9	97
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037048.D
Acq On : 17 Aug 2023 08:47
Operator : JC/MD
Sample : 03975-02 20X
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z10-12-Q

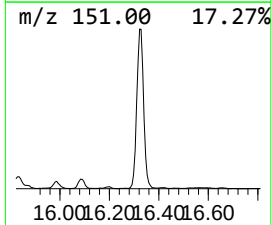
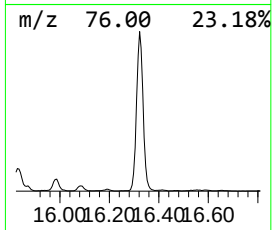
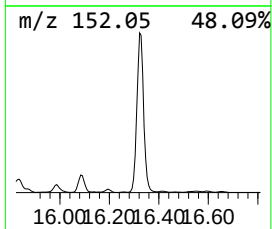
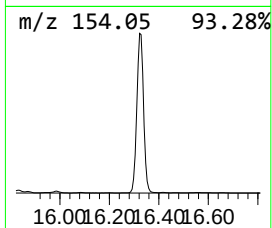
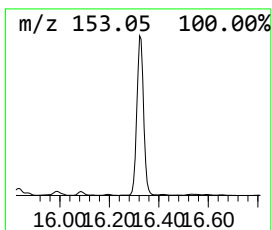
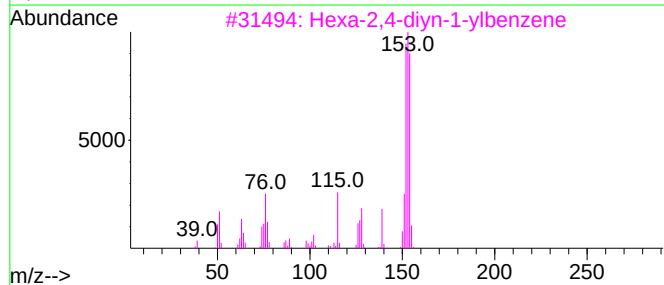
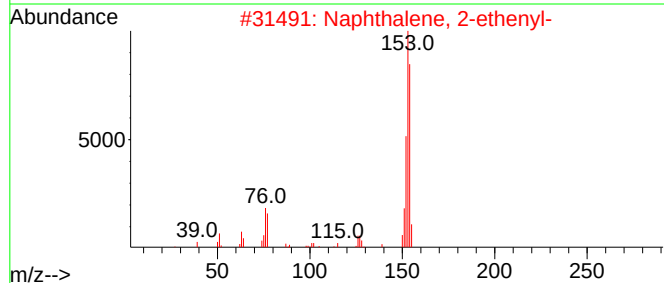
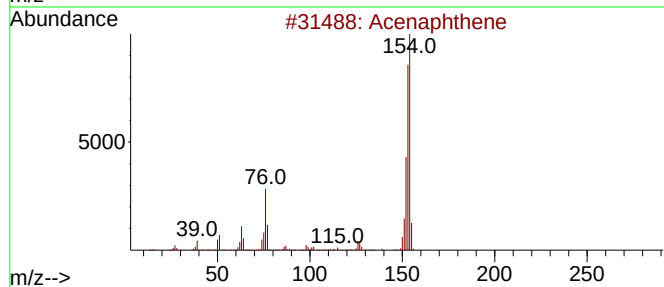
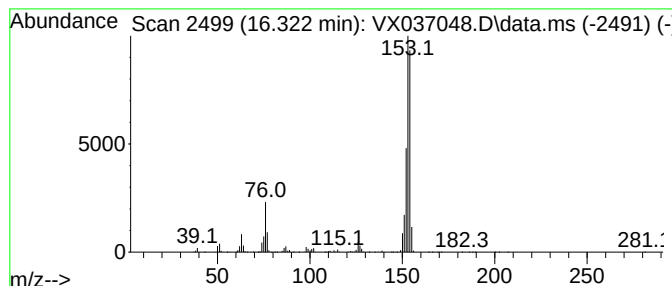
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 2-ethenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	164.31 ug/l	3545900	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acenaphthene	154	C12H10	000083-32-9	94
2		Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	64
3		Hexa-2,4-diyne-1-ylbenzene	154	C12H10	000520-74-1	59
4		3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	53
5		Biphenyl	154	C12H10	000092-52-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037048.D
Acq On : 17 Aug 2023 08:47
Operator : JC/MD
Sample : 03975-02 20X
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z10-12-Q

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Indane	12.244	882.9	ug/l	19053100	4	12.018	1079000	50.0
Benzene, (1-met...	13.426	296.4	ug/l	6396380	4	12.018	1079000	50.0
Benzo[c]thiophene	13.871	150.3	ug/l	3242600	4	12.018	1079000	50.0
Naphthalene, 1-...	14.646	1425.6	ug/l	30763700	4	12.018	1079000	50.0
Bicyclo[4.4.1]u...	14.786	904.6	ug/l	19522400	4	12.018	1079000	50.0
Naphthalene, 2,...	15.371	290.9	ug/l	6278100	4	12.018	1079000	50.0
Naphthalene, 2,...	15.475	205.2	ug/l	4427100	4	12.018	1079000	50.0
Naphthalene, 1,...	15.615	216.8	ug/l	4678620	4	12.018	1079000	50.0
Naphthalene, 2-...	16.322	164.3	ug/l	3545900	4	12.018	1079000	50.0