

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
 Data File : VX037047.D
 Acq On : 17 Aug 2023 08:23
 Operator : JC/MD
 Sample : 03975-01 20X
 Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 50 Sample Multiplier: 1

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

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: VX037047.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.550	722	732	749	rVB	151658	431978	1.17%	0.419%
2	6.763	921	931	945	rBV	249191	599327	1.62%	0.581%
3	8.647	1234	1240	1248	rBV	529451	824218	2.23%	0.799%
4	10.055	1465	1471	1480	rBV	572728	772291	2.09%	0.749%
5	10.195	1488	1494	1503	rBV	1569997	2066881	5.58%	2.004%
6	10.299	1503	1511	1518	rVV	812609	1075832	2.91%	1.043%
7	10.640	1562	1567	1581	rVB	476065	603949	1.63%	0.586%
8	11.079	1634	1639	1650	rVB	494772	632853	1.71%	0.614%
9	11.378	1683	1688	1696	rBV	850897	1554799	4.20%	1.508%
10	11.750	1740	1749	1754	rBV	683036	848386	2.29%	0.823%
11	12.018	1788	1793	1799	rVB	649855	864817	2.34%	0.839%
12	12.244	1824	1830	1837	rBV	6174706	7591935	20.50%	7.363%
13	12.317	1837	1842	1848	rVV2	357752	456903	1.23%	0.443%
14	12.610	1885	1890	1894	rBV	365530	442929	1.20%	0.430%
15	13.164	1977	1981	1986	rBV	826308	1033588	2.79%	1.002%
16	13.286	1992	2001	2006	rBV3	407128	730755	1.97%	0.709%
17	13.341	2006	2010	2015	rVV	886975	1046487	2.83%	1.015%
18	13.426	2019	2024	2029	rVB	2036917	2674175	7.22%	2.593%
19	13.786	2076	2083	2088	rBV	23516095	37031044	100.00%	35.913%
20	13.871	2088	2097	2101	rVB	1001494	1391216	3.76%	1.349%
21	14.219	2150	2154	2157	rBV2	342001	473329	1.28%	0.459%
22	14.317	2164	2170	2176	rBV	375454	600251	1.62%	0.582%
23	14.640	2218	2223	2232	rVB	12655770	16084311	43.43%	15.599%
24	14.780	2240	2246	2255	rVB	7733185	9844813	26.59%	9.548%
25	15.207	2308	2316	2320	rBV	938990	1303225	3.52%	1.264%
26	15.371	2331	2343	2348	rBV	1973315	2985559	8.06%	2.895%
27	15.475	2354	2360	2365	rBV	1444695	2223713	6.00%	2.157%
28	15.609	2377	2382	2386	rBV	1408580	2266440	6.12%	2.198%
29	15.646	2386	2388	2395	rVB	821188	1138302	3.07%	1.104%
30	15.835	2409	2419	2424	rBV	359195	959931	2.59%	0.931%
31	15.987	2438	2444	2454	rVB	221007	396071	1.07%	0.384%
32	16.322	2490	2499	2512	rBV2	1089716	2162800	5.84%	2.098%

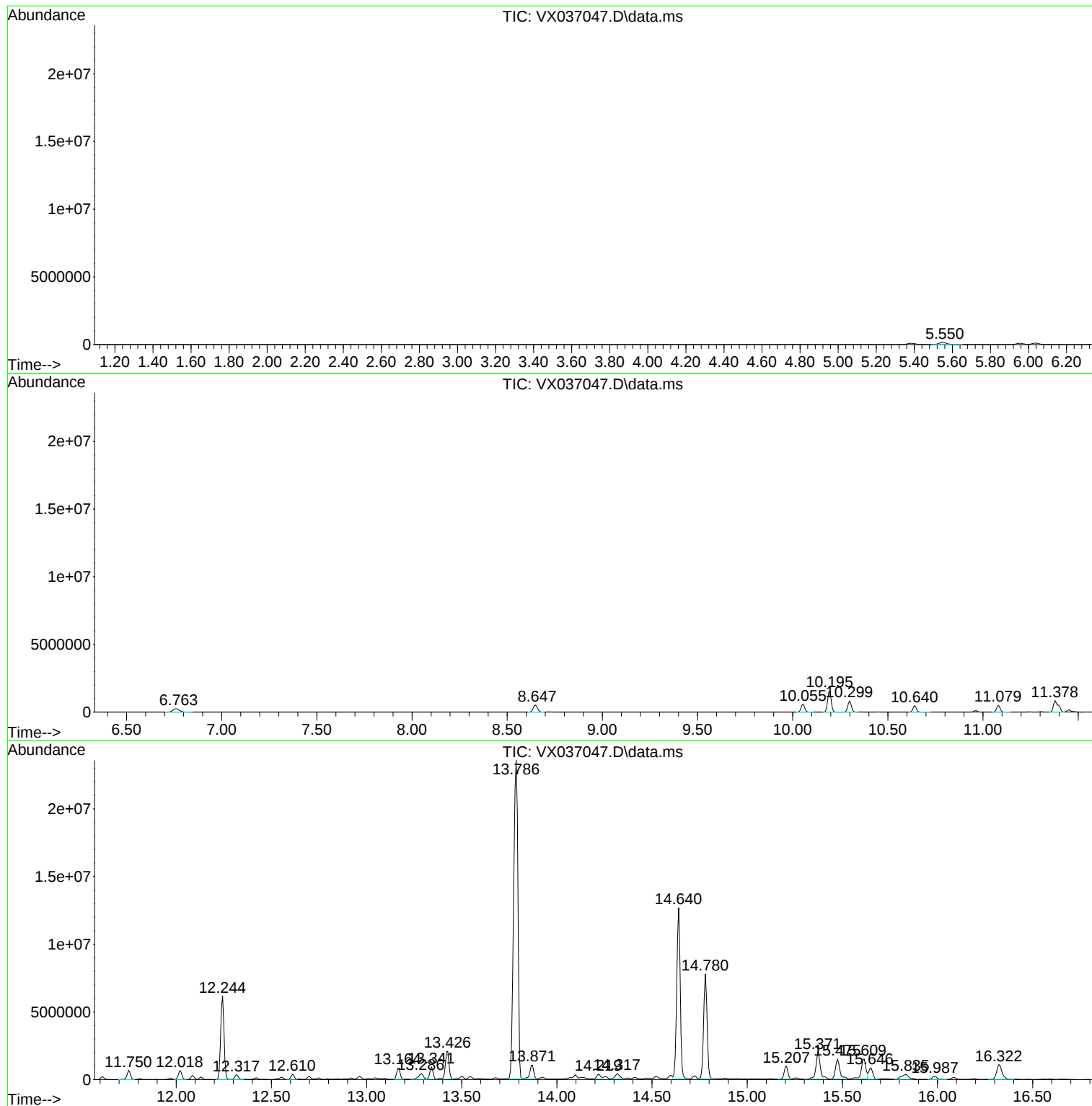
Sum of corrected areas: 103113108

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

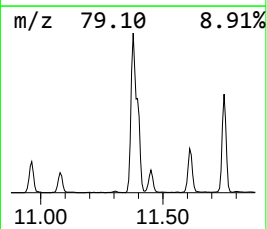
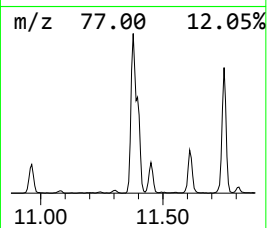
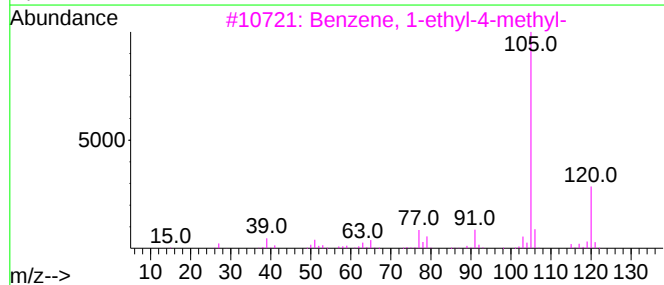
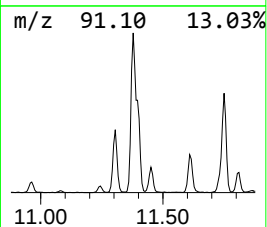
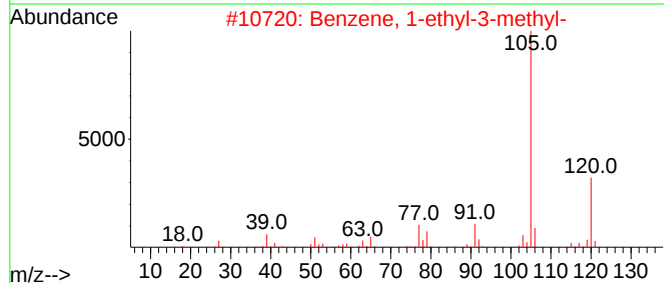
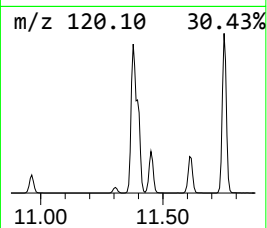
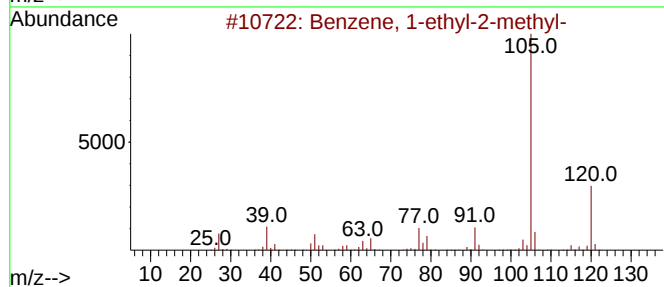
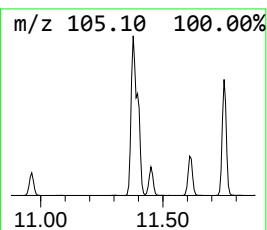
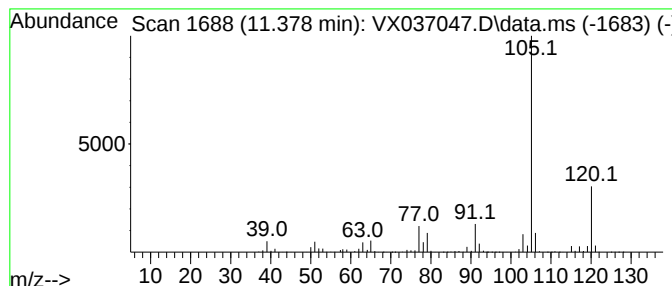
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	89.89 ug/l	1554800	1,4-Dichlorobenzene-d4	12.024

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

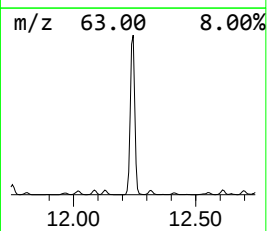
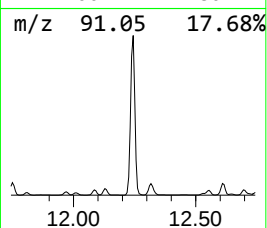
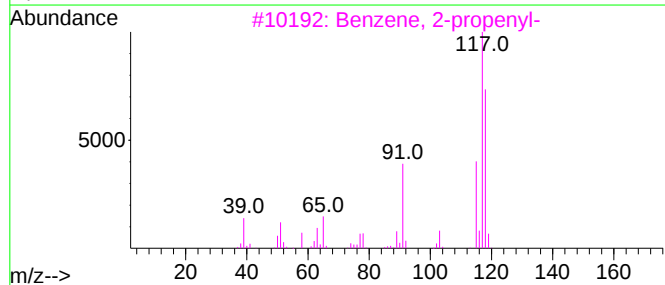
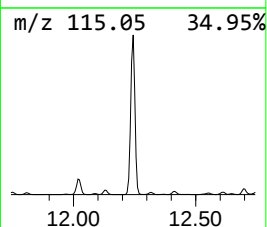
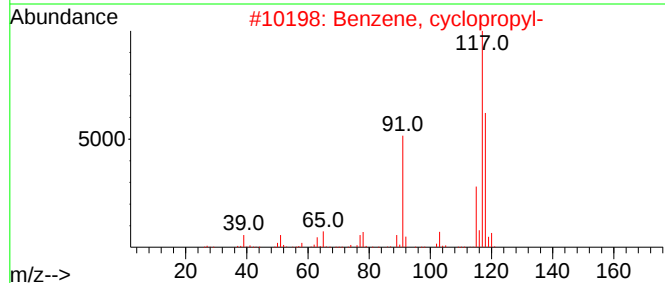
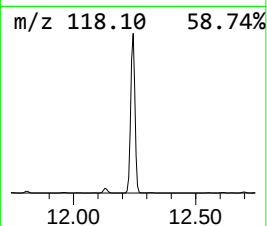
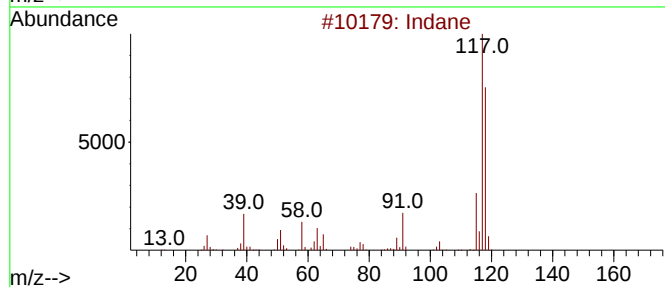
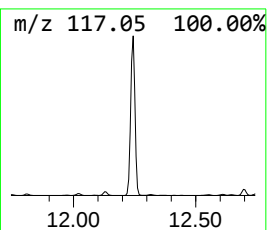
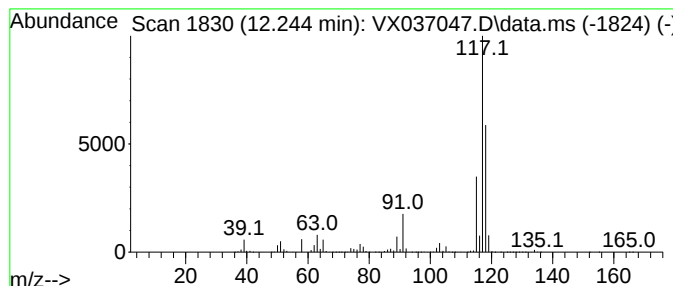
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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	438.93 ug/l	7591940	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Deltacyclene	118	C9H10	007785-10-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

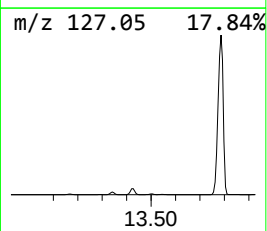
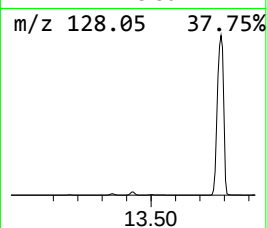
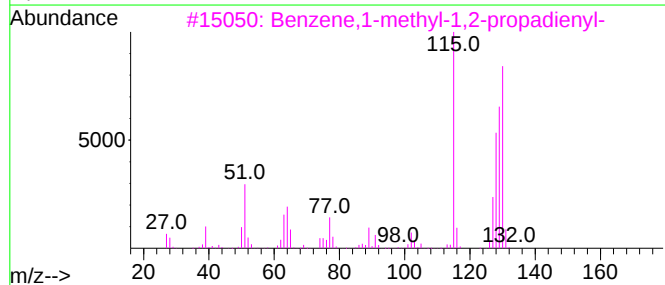
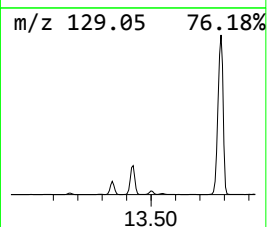
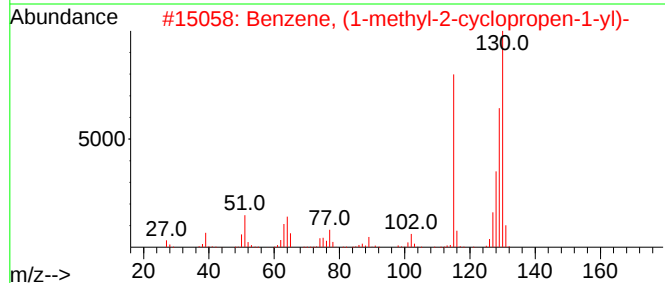
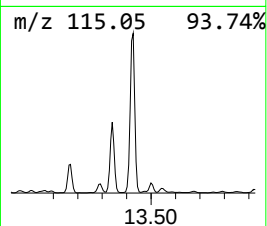
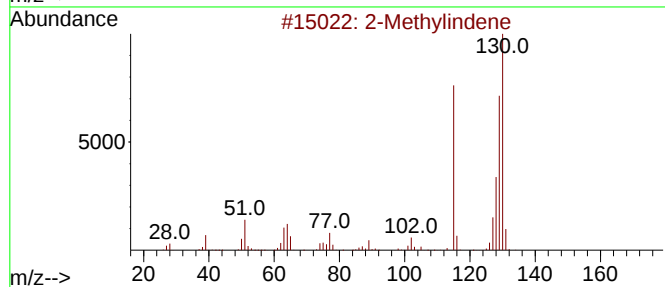
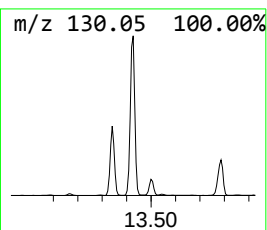
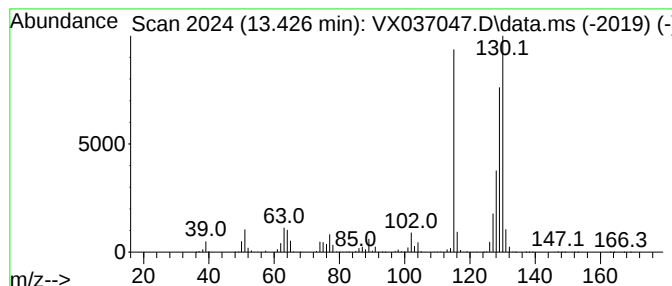
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, (1-methyl-2-cyclop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	154.61 ug/l	2674180	1,4-Dichlorobenzene-d4	12.024

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	Cycloprop[a]indene, 1,1a,6,6a-te...			130	C10H10	015677-15-3	94
5	1,4-Dihydronaphthalene			130	C10H10	000612-17-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

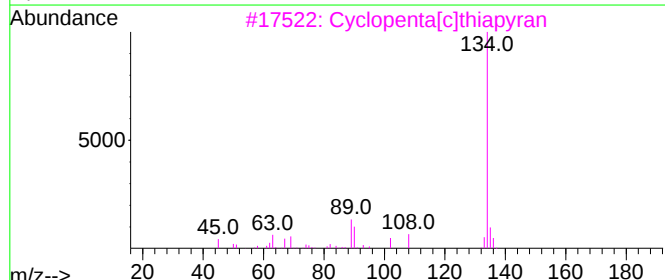
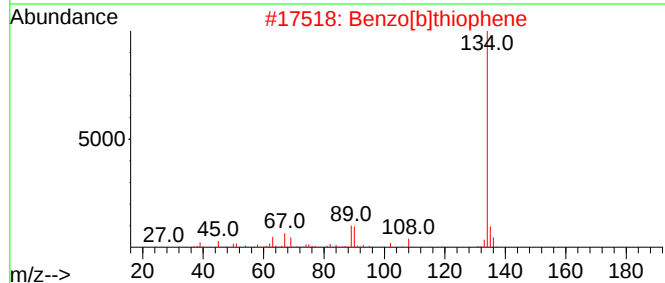
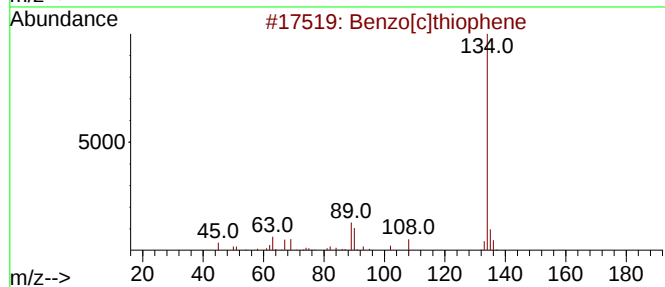
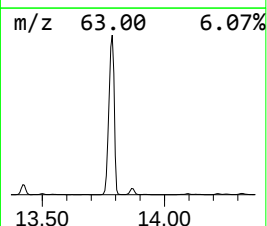
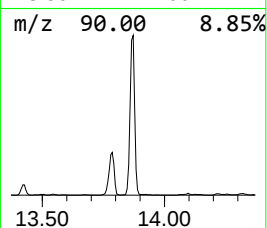
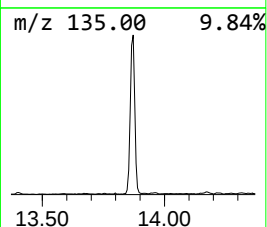
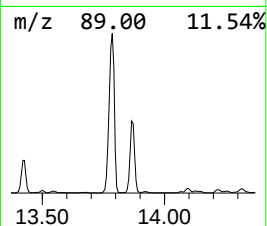
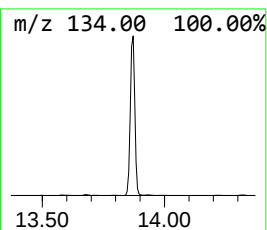
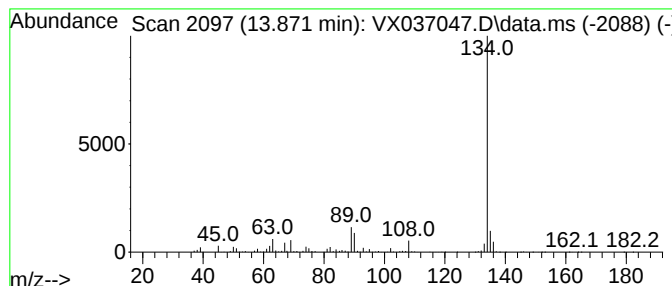
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzo[c]thiophene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	80.43 ug/l	1391220	1,4-Dichlorobenzene-d4	12.024

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

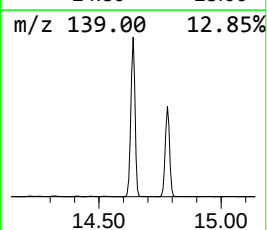
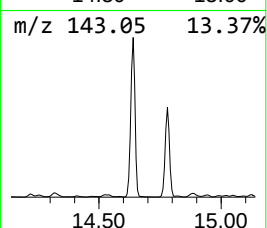
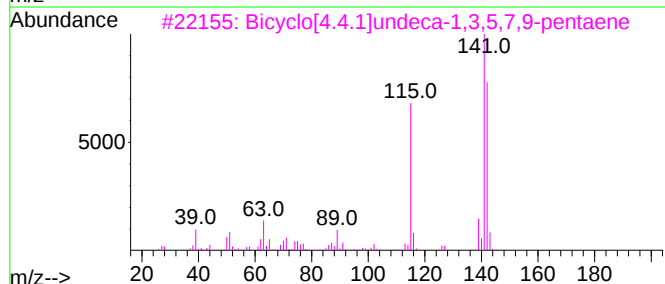
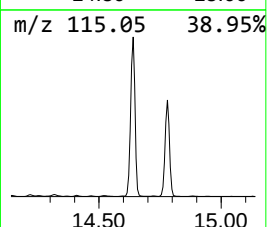
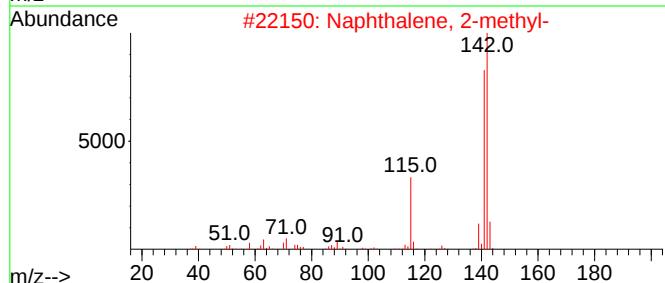
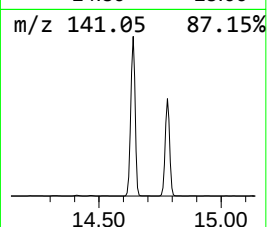
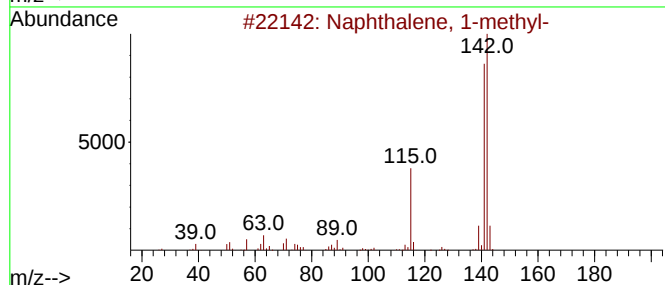
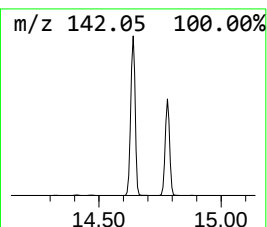
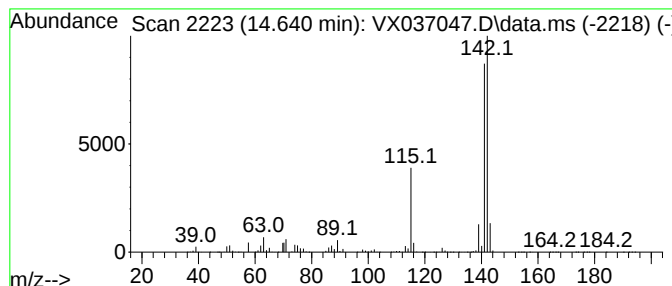
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	929.93 ug/l	16084300	1,4-Dichlorobenzene-d4	12.024

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			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

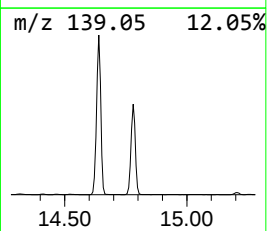
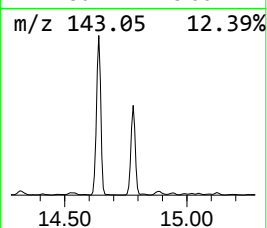
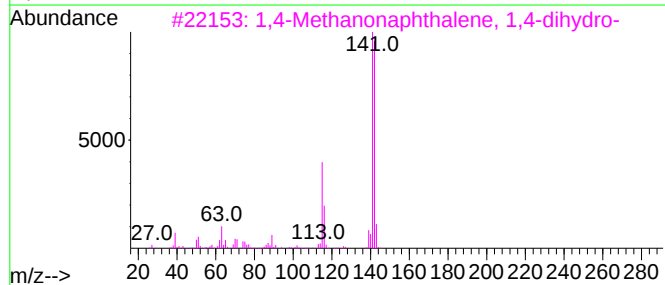
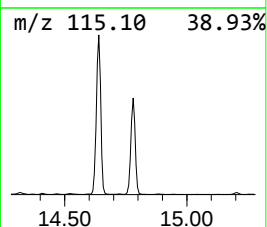
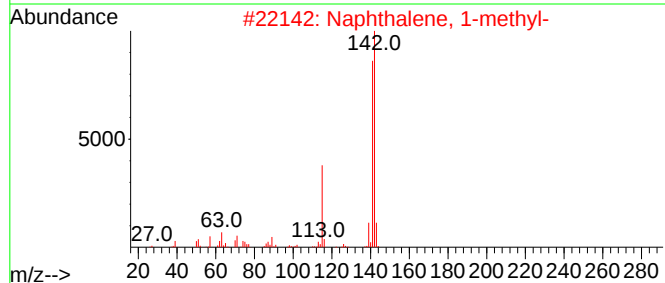
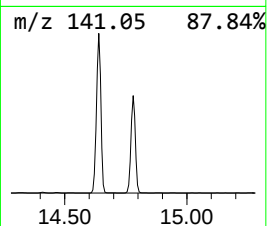
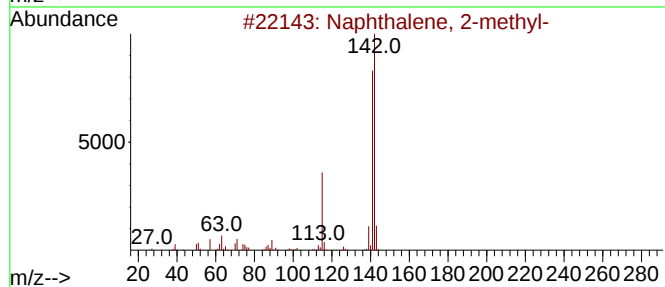
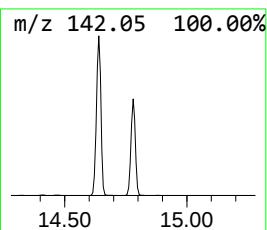
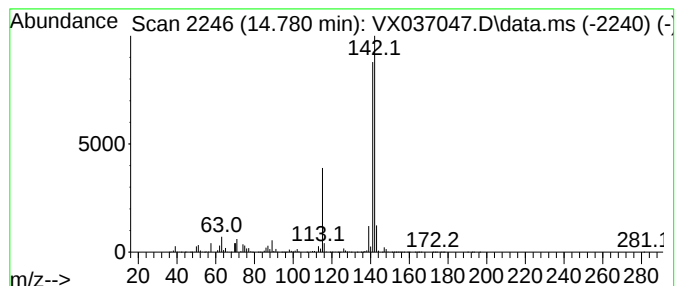
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 6 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	569.18 ug/l	9844810	1,4-Dichlorobenzene-d4	12.024

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			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 : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

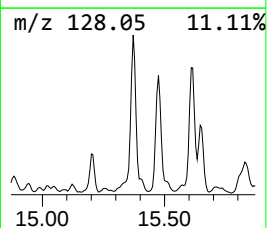
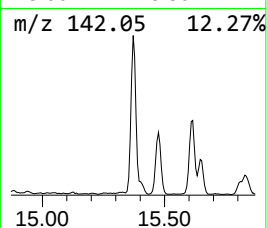
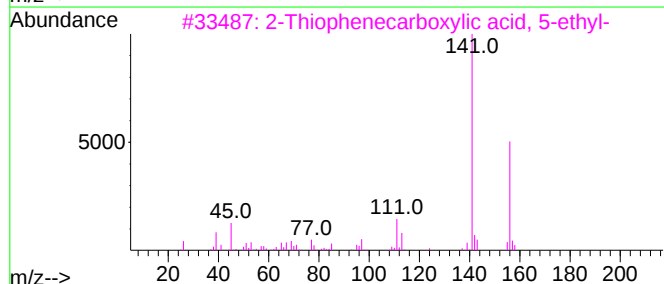
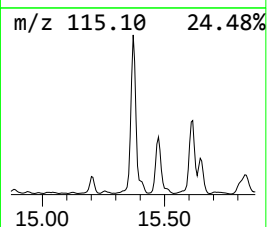
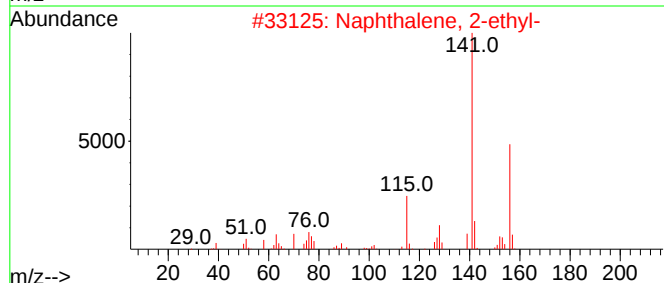
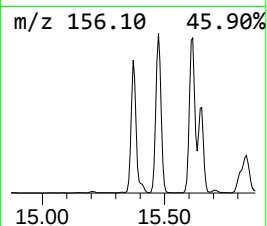
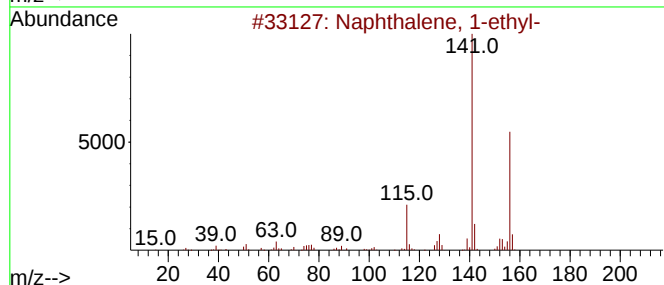
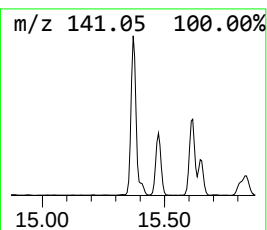
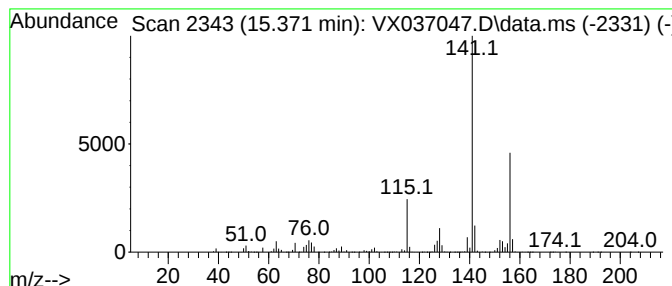
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 7 2-Thiophenecarboxylic acid,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	172.61 ug/l	2985560	1,4-Dichlorobenzene-d4	12.024

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			2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	64
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	58
5			2-Pyrimidinethiol, 4,5-dihydro-4...	156	C7H12N2S	1000319-31-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

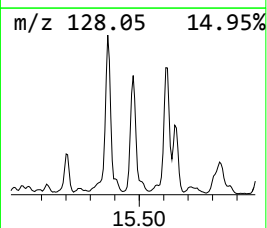
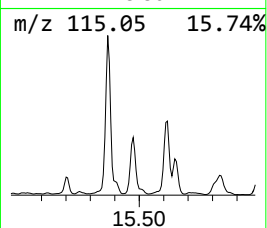
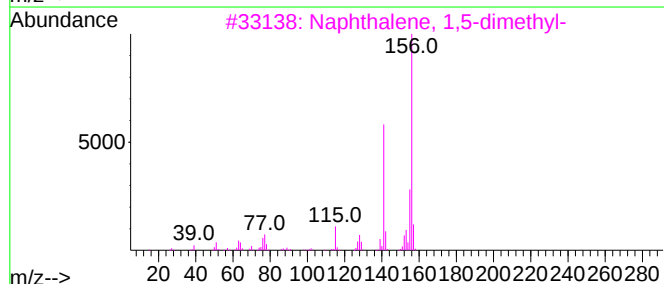
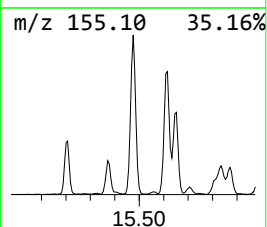
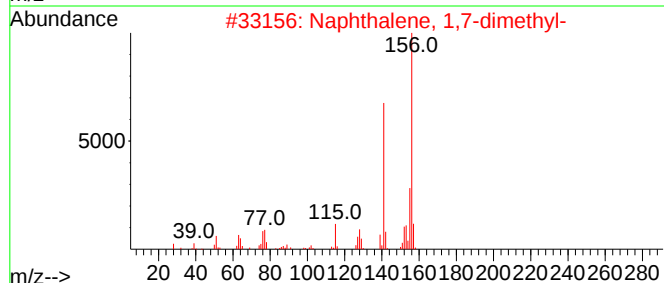
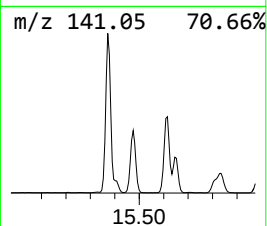
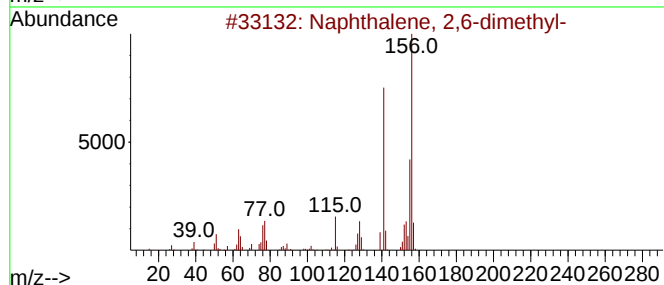
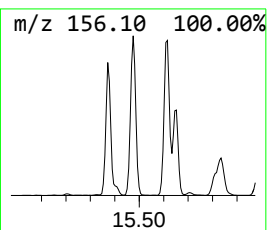
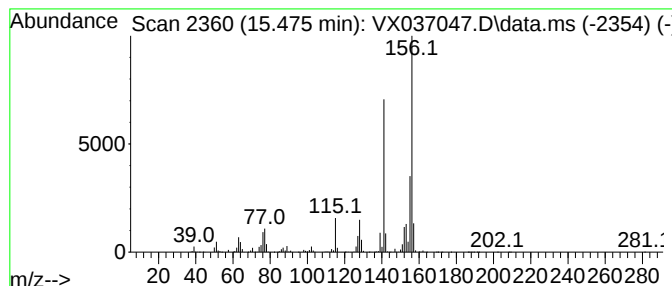
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	128.57 ug/l	2223710	1,4-Dichlorobenzene-d4	12.024

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, 1,4-dimethyl-	156	C12H12	000571-58-4	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

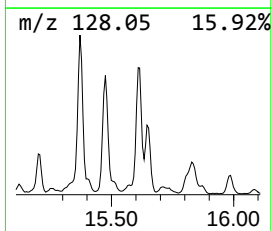
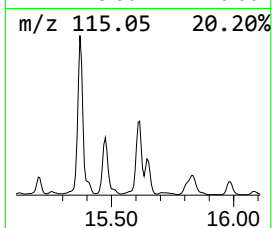
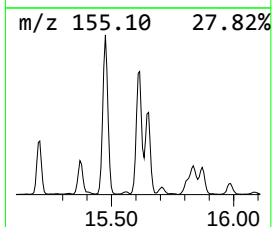
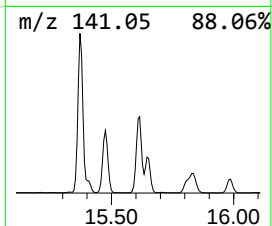
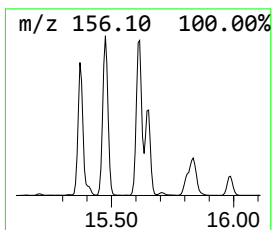
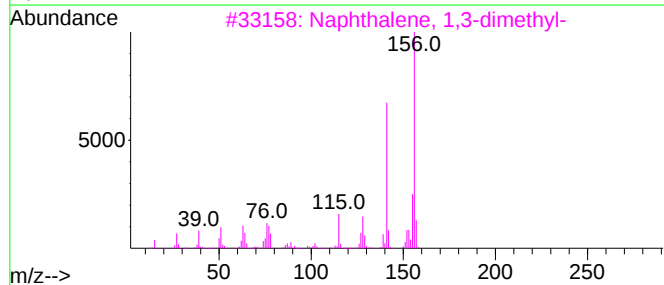
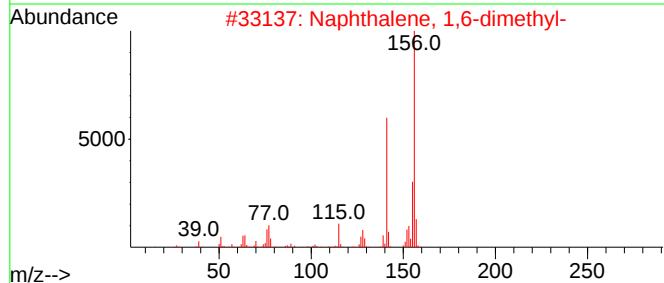
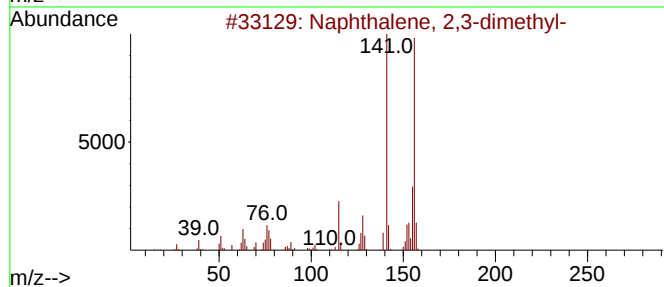
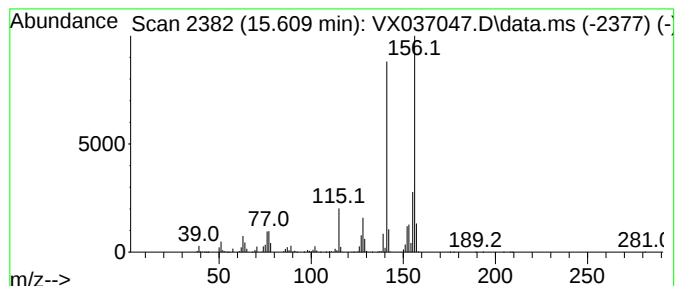
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	131.04 ug/l	2266440	1,4-Dichlorobenzene-d4	12.024

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

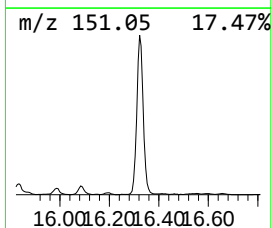
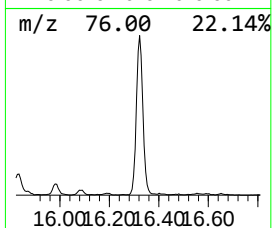
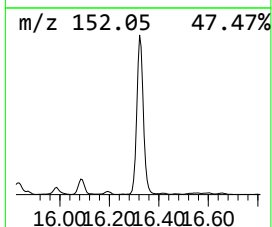
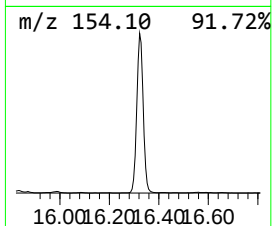
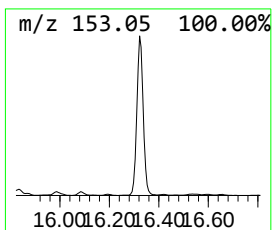
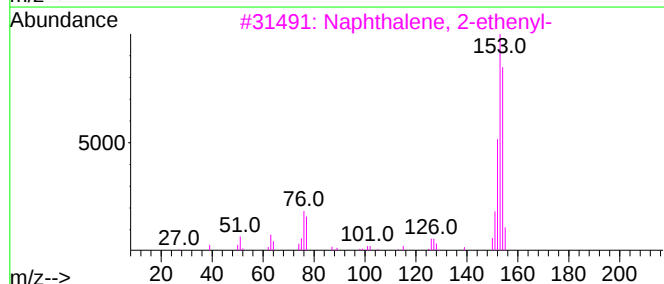
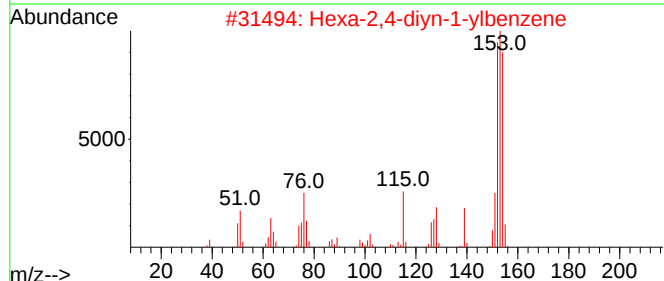
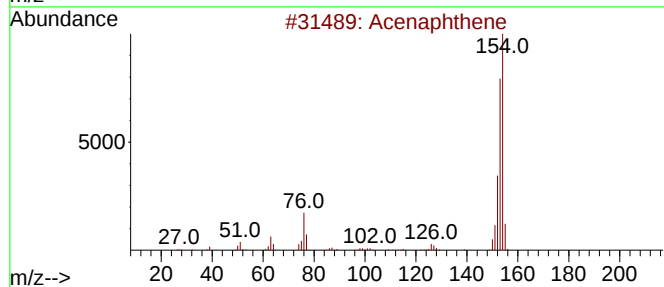
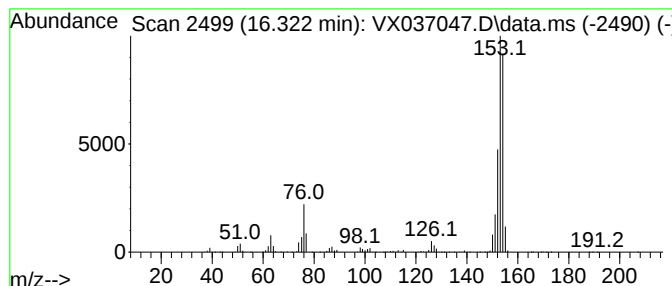
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 10 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	125.04 ug/l	2162800	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acenaphthene	154	C12H10	000083-32-9	94
2		Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
3		Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	59
4		3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5		2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037047.D
Acq On : 17 Aug 2023 08:23
Operator : JC/MD
Sample : 03975-01 20X
Misc : 5.59g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 50 Sample Multiplier: 1

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

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
Benzene, 1-ethy...	11.378	89.9	ug/l	1554800	4	12.024	864817	50.0
Indane	12.244	438.9	ug/l	7591940	4	12.024	864817	50.0
Benzene, (1-met...	13.426	154.6	ug/l	2674180	4	12.024	864817	50.0
Benzo[c]thiophene	13.871	80.4	ug/l	1391220	4	12.024	864817	50.0
Naphthalene, 1-...	14.640	929.9	ug/l	16084300	4	12.024	864817	50.0
1,4-Methanonaph...	14.780	569.2	ug/l	9844810	4	12.024	864817	50.0
2-Thiophenecarb...	15.371	172.6	ug/l	2985560	4	12.024	864817	50.0
Naphthalene, 2,...	15.475	128.6	ug/l	2223710	4	12.024	864817	50.0
Naphthalene, 2,...	15.609	131.0	ug/l	2266440	4	12.024	864817	50.0
Hexa-2,4-diyne-1...	16.322	125.0	ug/l	2162800	4	12.024	864817	50.0