

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080223\
 Data File : VX036779.D
 Acq On : 02 Aug 2023 18:41
 Operator : JC/MD
 Sample : 03815-03 10X
 Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DUP-01

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: VX036779.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	692	705	720	rBV	85035	248502	1.14%	0.339%
2	5.550	722	732	747	rVB	140702	396166	1.81%	0.541%
3	5.958	789	799	805	rBV	89825	244310	1.12%	0.333%
4	6.038	805	812	829	rVB	272743	721618	3.30%	0.985%
5	6.763	920	931	946	rBV	226981	541411	2.48%	0.739%
6	8.647	1233	1240	1246	rBV	479221	771928	3.53%	1.054%
7	8.720	1246	1252	1268	rVB	484985	763113	3.49%	1.042%
8	10.055	1465	1471	1487	rBV	482672	658871	3.01%	0.899%
9	10.195	1488	1494	1504	rBV	499819	640468	2.93%	0.874%
10	10.299	1504	1511	1519	rBV	527056	701758	3.21%	0.958%
11	10.646	1562	1568	1580	rVB3	322389	546706	2.50%	0.746%
12	11.079	1634	1639	1653	rBV	416274	517201	2.37%	0.706%
13	11.378	1683	1688	1695	rBV	182445	332592	1.52%	0.454%
14	11.750	1741	1749	1754	rBV	378412	465202	2.13%	0.635%
15	11.805	1754	1758	1762	rBV	248538	300369	1.37%	0.410%
16	12.018	1788	1793	1799	rVB	516943	660225	3.02%	0.901%
17	12.244	1821	1830	1838	rBV	311195	421889	1.93%	0.576%
18	12.414	1852	1858	1864	rVB	2052820	2587465	11.83%	3.532%
19	13.341	2005	2010	2016	rVB	673961	799741	3.66%	1.092%
20	13.426	2016	2024	2029	rBV	752164	993627	4.54%	1.356%
21	13.780	2075	2082	2087	rBV	16165669	21868487	100.00%	29.850%
22	13.865	2091	2096	2103	rVB	675373	859329	3.93%	1.173%
23	14.597	2211	2216	2218	rBV	348677	416347	1.90%	0.568%
24	14.640	2218	2223	2232	rVV	9882654	13121173	60.00%	17.910%
25	14.725	2232	2237	2241	rVV	277812	370899	1.70%	0.506%
26	14.780	2241	2246	2258	rVB	7260152	9310570	42.58%	12.709%
27	15.207	2308	2316	2321	rBV	1290208	1739591	7.95%	2.375%
28	15.347	2331	2339	2340	rBV	232767	297118	1.36%	0.406%
29	15.371	2340	2343	2347	rVV	432264	662453	3.03%	0.904%
30	15.475	2354	2360	2364	rVV	1440051	2353013	10.76%	3.212%
31	15.511	2364	2366	2371	rVV	307892	419114	1.92%	0.572%
32	15.578	2371	2377	2378	rVV2	239745	393355	1.80%	0.537%
33	15.615	2378	2383	2386	rVV	1777079	2964578	13.56%	4.047%
34	15.652	2386	2389	2396	rVV	908229	1333314	6.10%	1.820%
35	15.737	2396	2403	2410	rVV2	300051	504328	2.31%	0.688%
36	15.835	2410	2419	2430	rVB	412457	1119194	5.12%	1.528%

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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	15.987	2437	2444	2453	rVB	242988	440354	2.01%	0.601%
38	16.084	2453	2460	2467	rBV	647495	1123153	5.14%	1.533%
39	16.322	2484	2499	2506	rBV	306114	651795	2.98%	0.890%

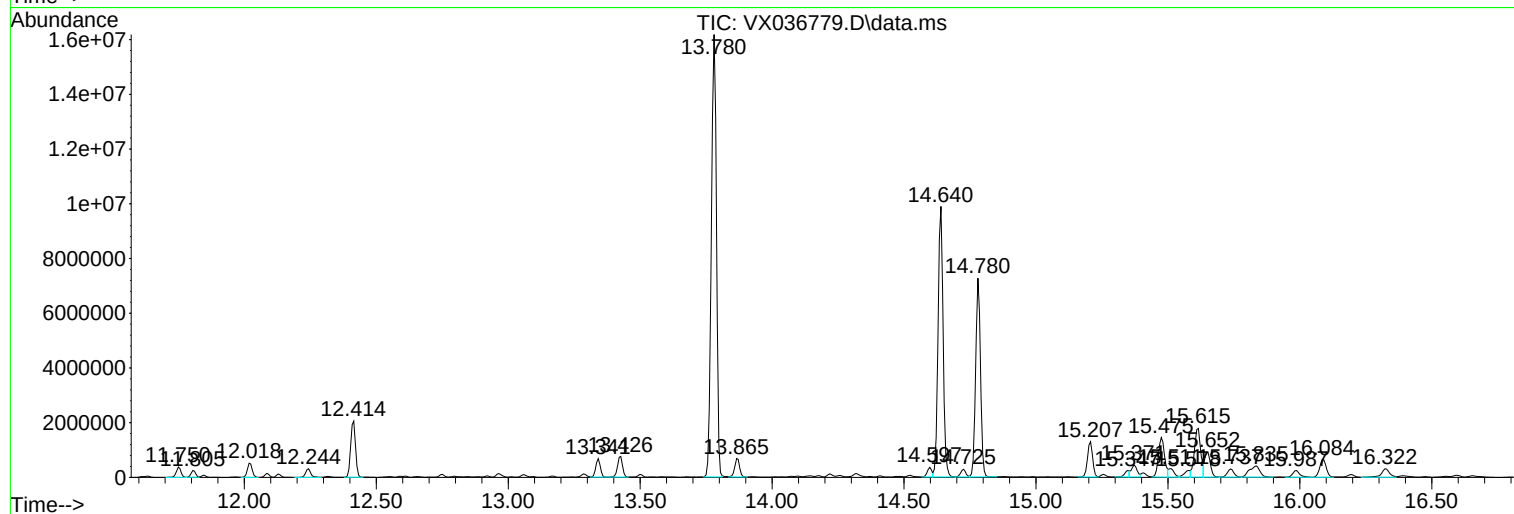
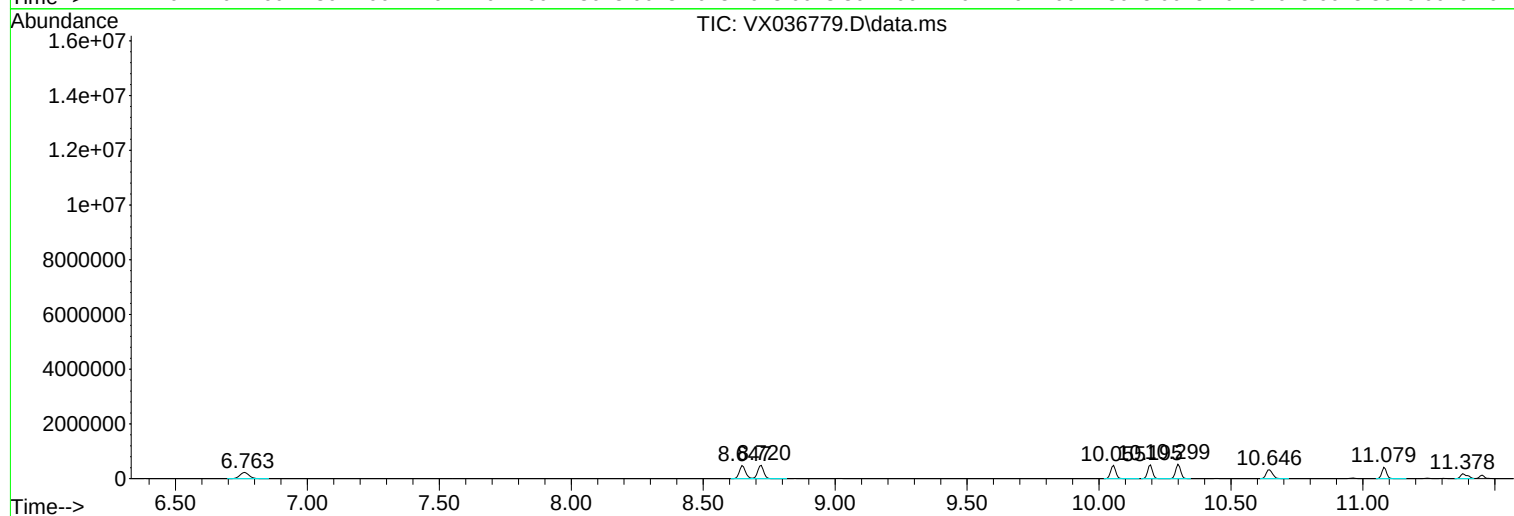
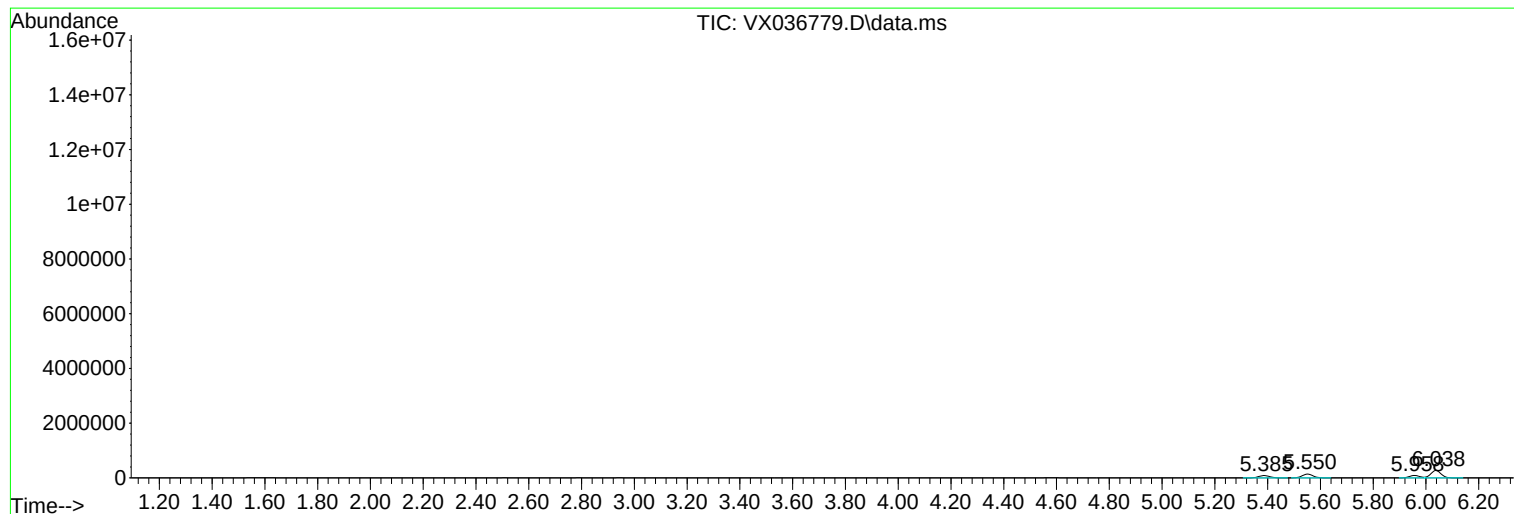
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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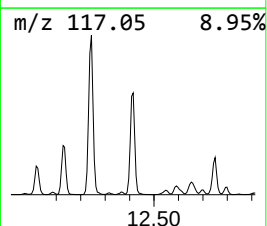
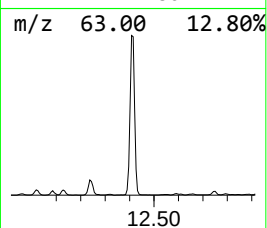
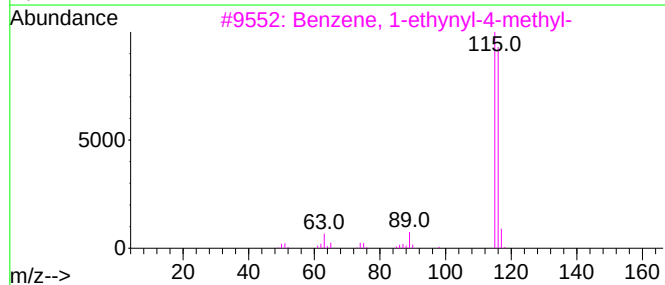
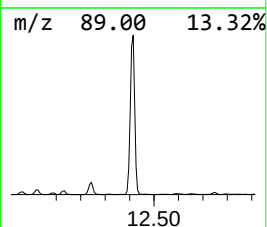
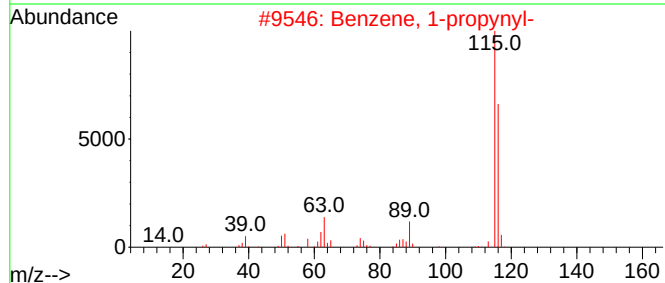
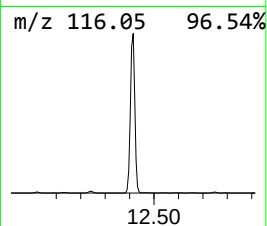
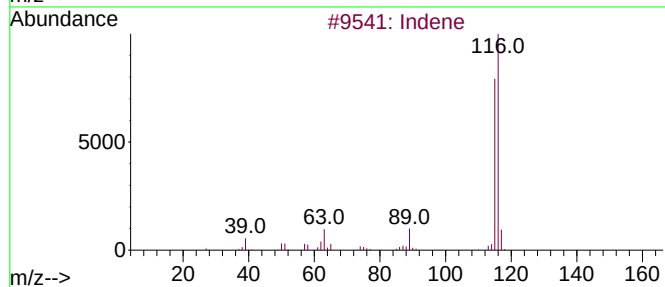
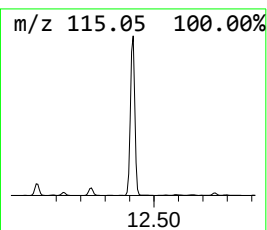
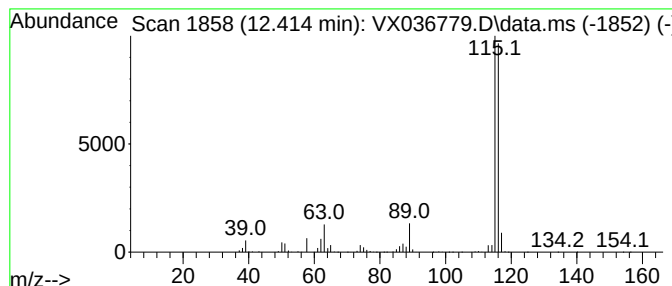
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	195.95 ug/l	2587470	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5			2-Methylphenylacetylene	116	C9H8	000766-47-2	90



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01

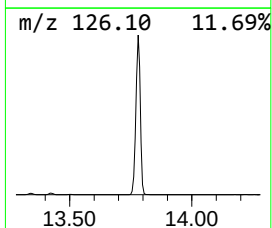
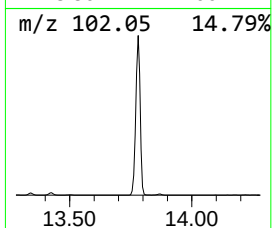
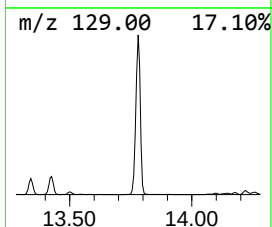
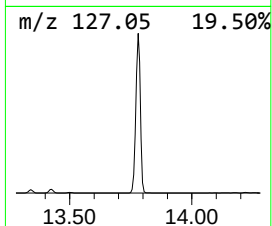
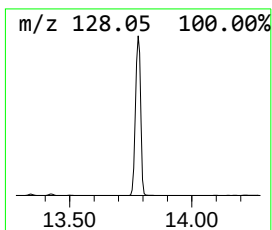
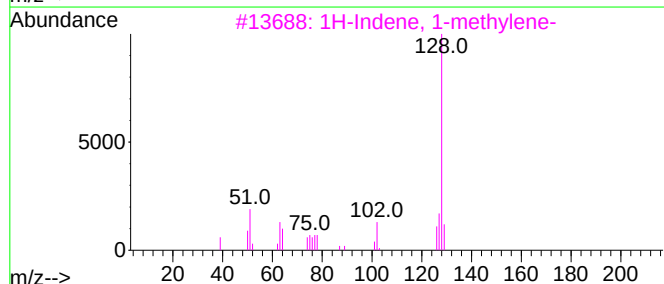
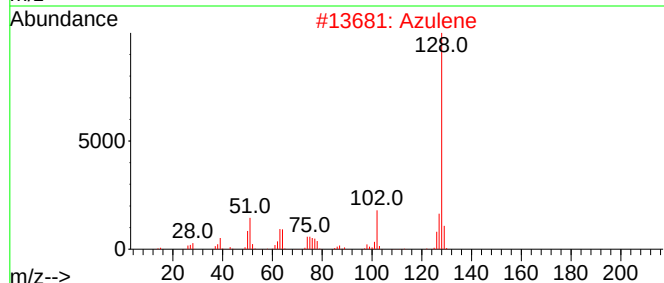
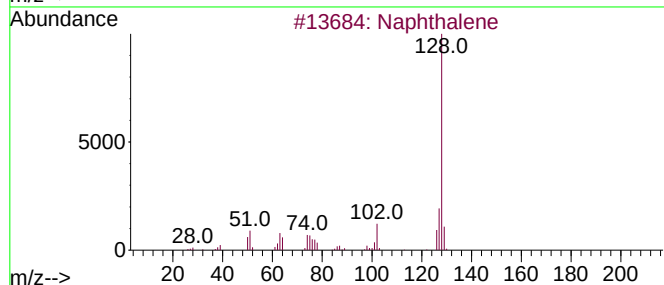
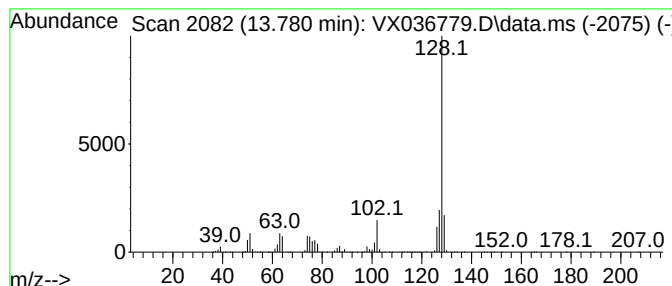
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	1656.14 ug/l	21868500	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	91
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	72
5			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	59



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Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01

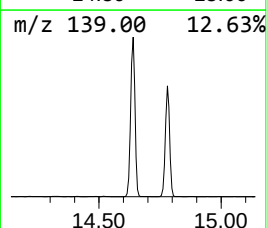
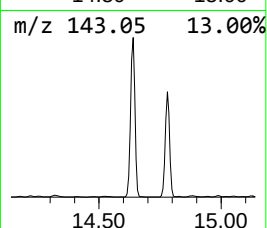
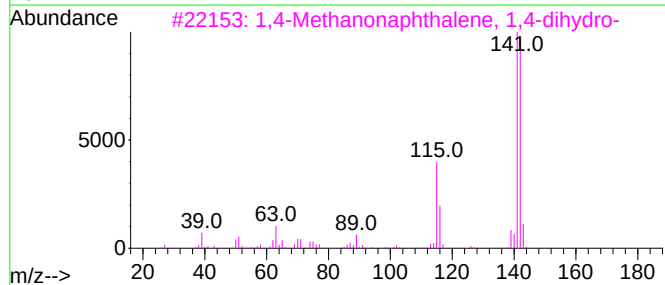
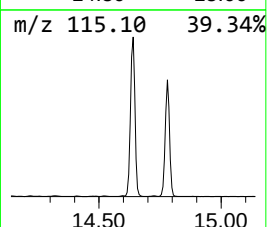
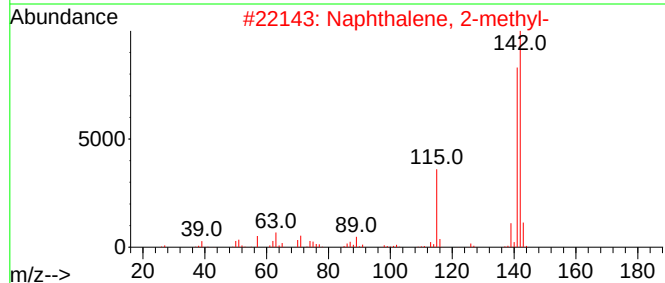
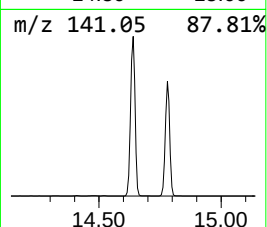
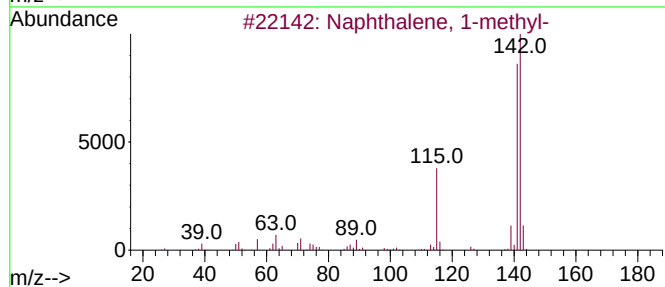
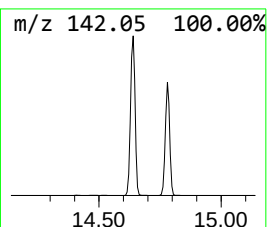
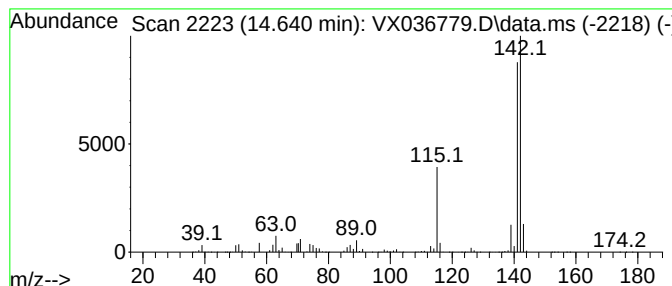
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 3 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	993.69 ug/l	13121200	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			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91



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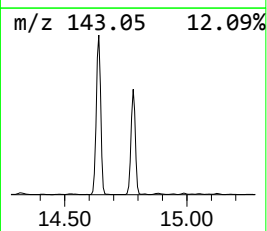
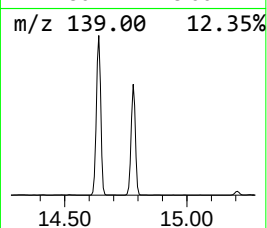
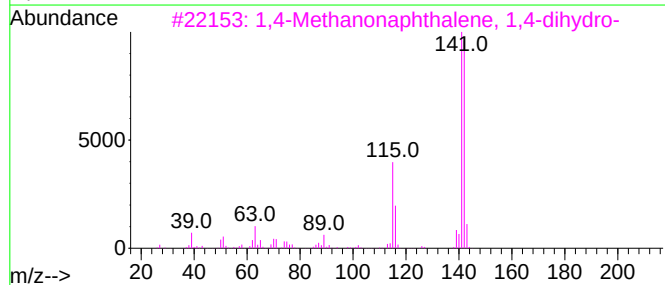
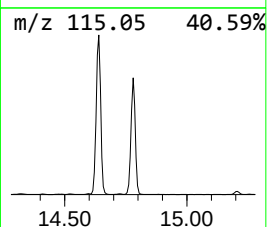
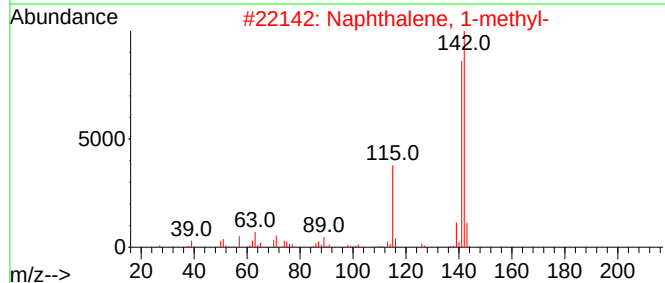
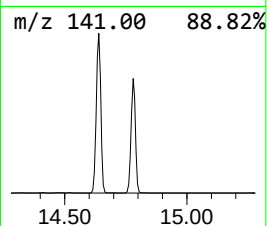
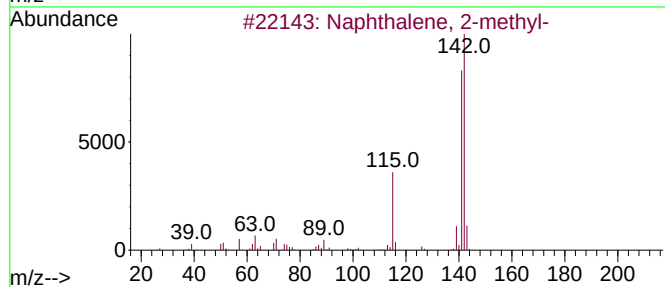
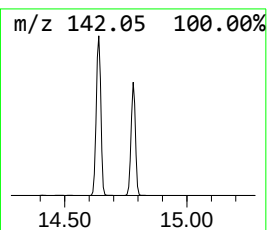
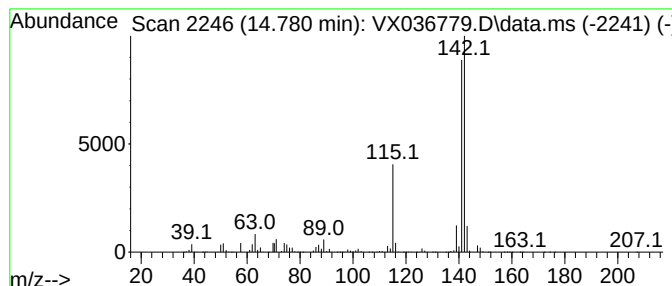
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 4 Bicyclo[4.4.1]undeca-1,3,5,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	705.11 ug/l	9310570	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	94
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



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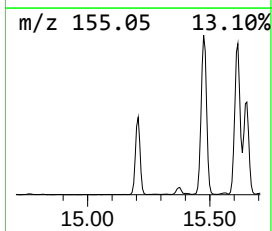
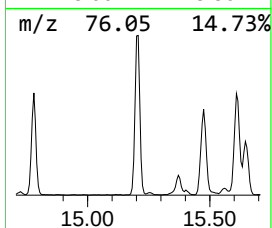
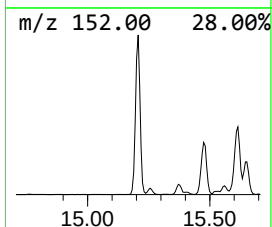
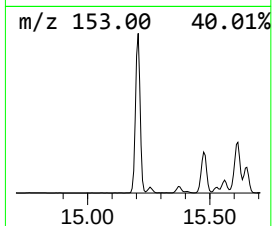
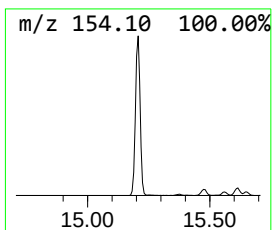
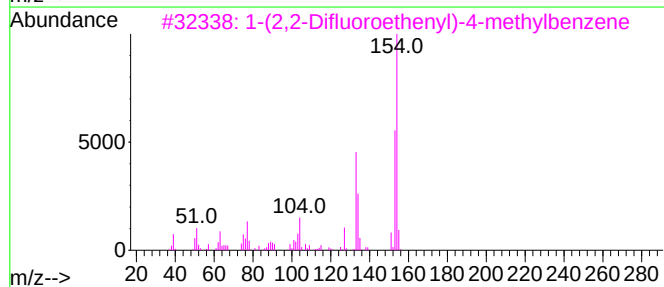
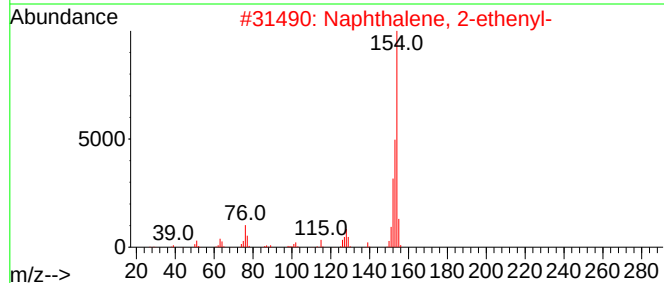
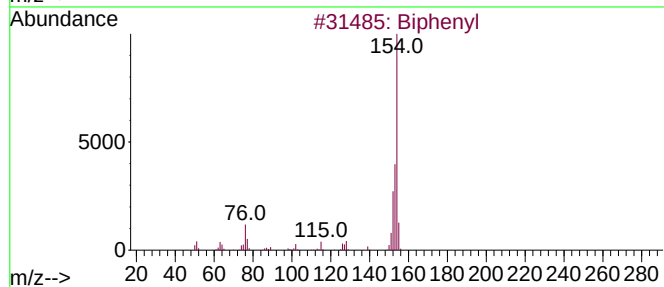
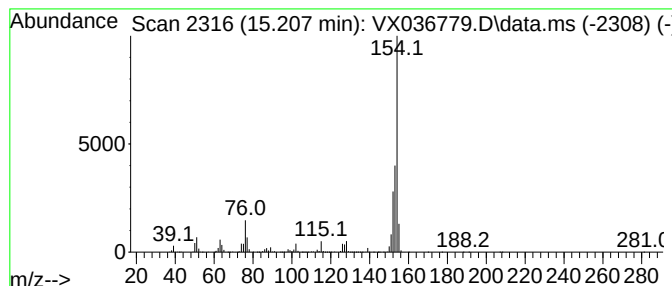
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 2-ethenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.207	131.74 ug/l	1739590	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	95
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	87
3			1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	53
4			Acenaphthene	154	C12H10	000083-32-9	49
5			3-Quinolinecarbonitrile	154	C10H6N2	034846-64-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080223\
Data File : VX036779.D
Acq On : 02 Aug 2023 18:41
Operator : JC/MD
Sample : 03815-03 10X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01

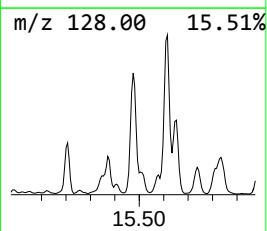
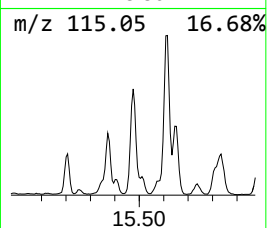
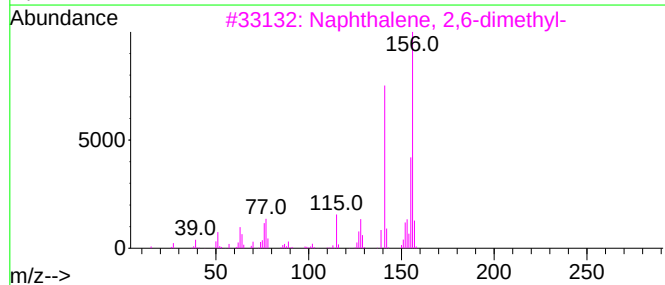
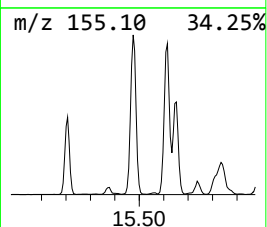
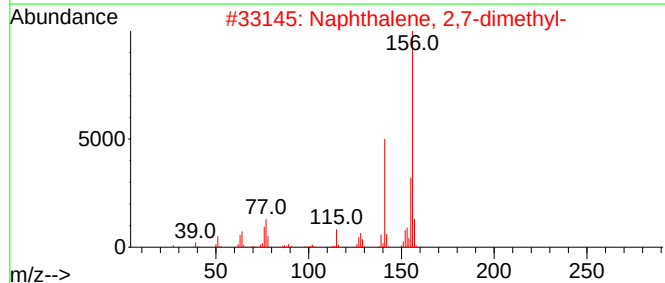
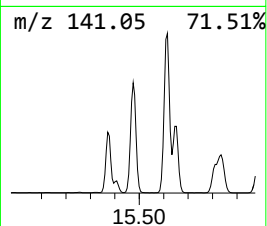
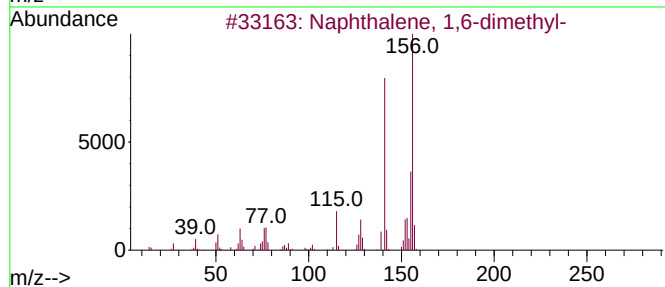
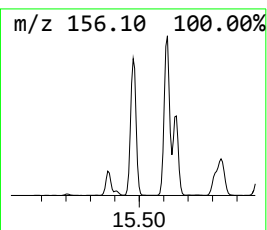
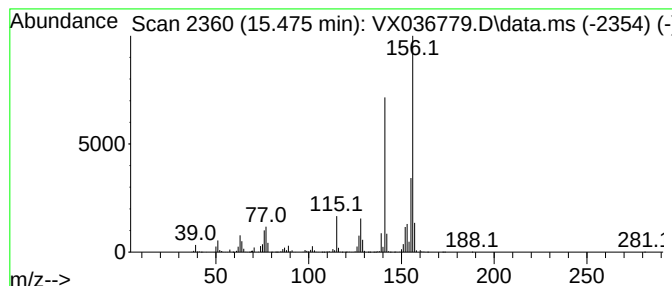
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	178.20 ug/l	2353010	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	98
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080223\
Data File : VX036779.D
Acq On : 02 Aug 2023 18:41
Operator : JC/MD
Sample : 03815-03 10X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01

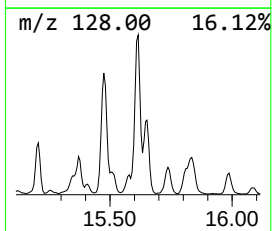
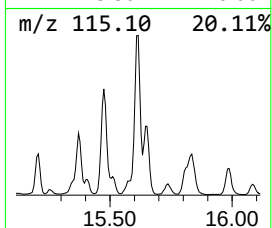
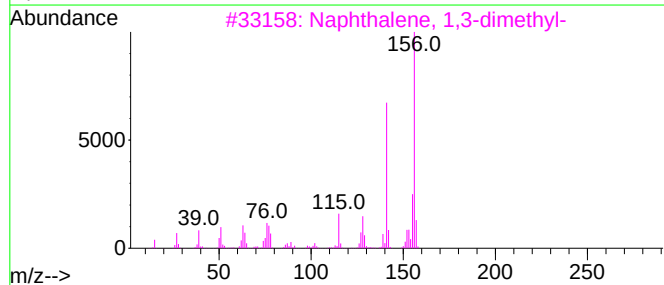
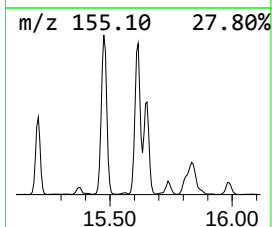
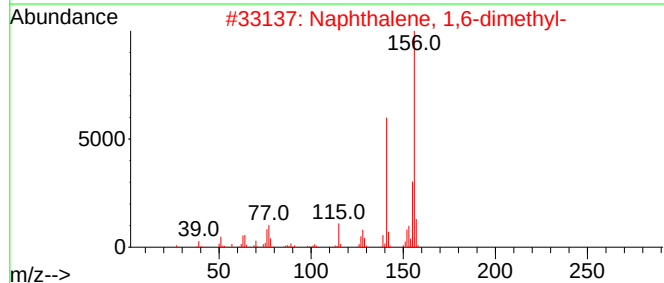
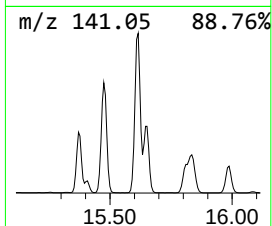
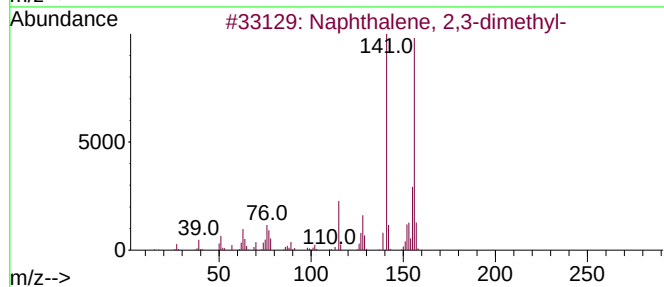
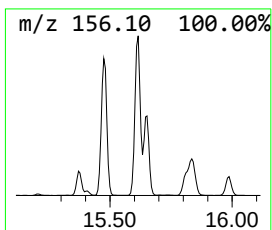
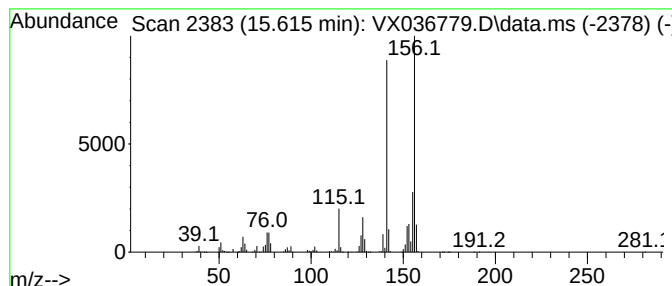
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	224.51 ug/l	2964580	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\VX080223\
Data File : VX036779.D
Acq On : 02 Aug 2023 18:41
Operator : JC/MD
Sample : 03815-03 10X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01

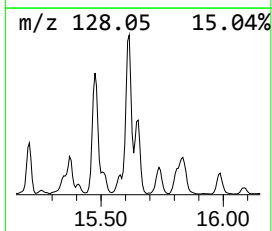
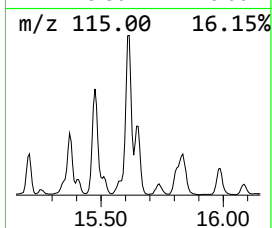
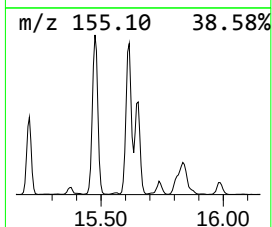
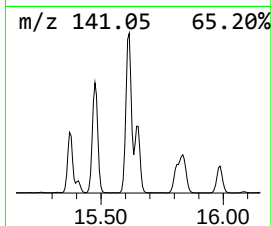
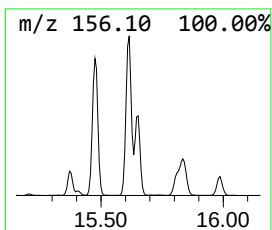
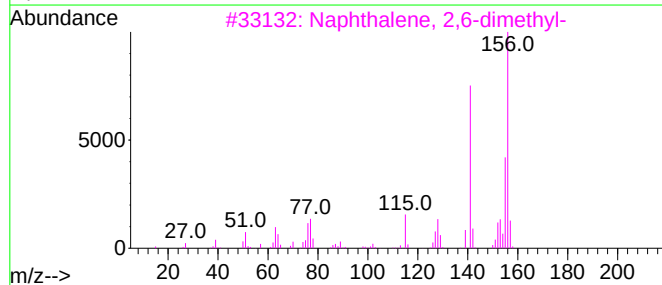
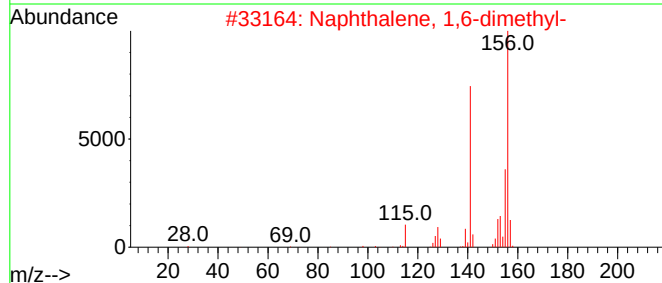
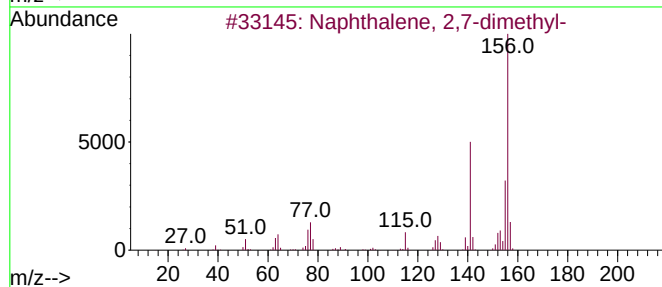
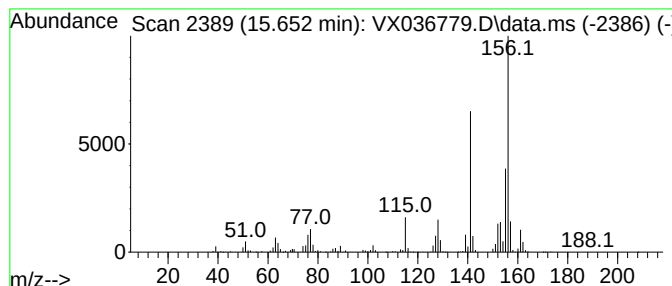
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.652	100.97 ug/l	1333310	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080223\
Data File : VX036779.D
Acq On : 02 Aug 2023 18:41
Operator : JC/MD
Sample : 03815-03 10X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01

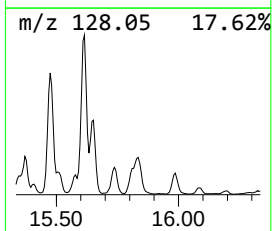
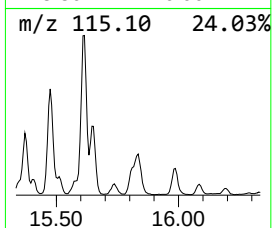
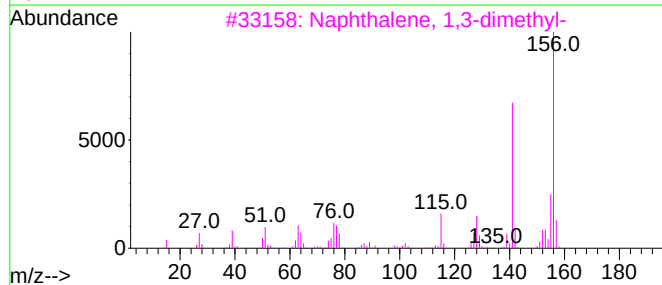
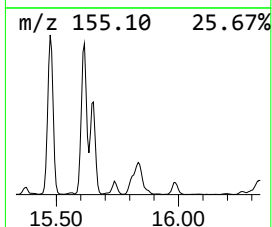
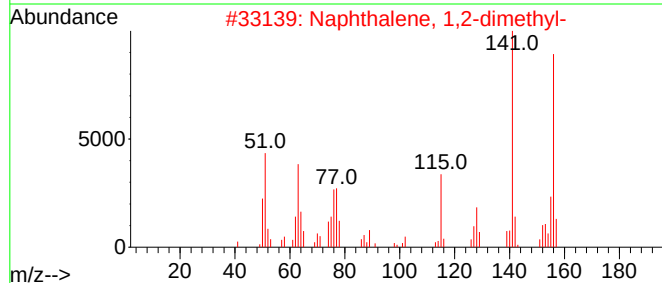
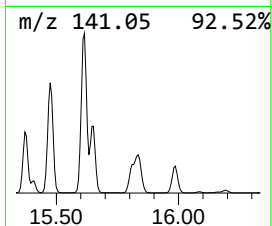
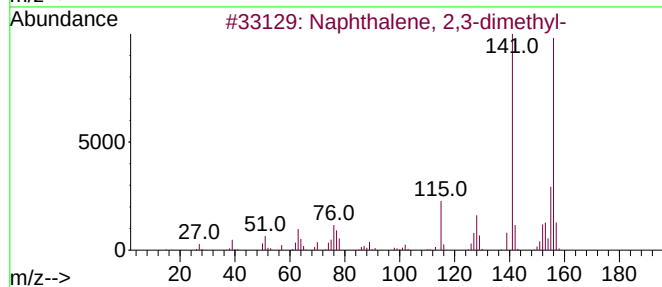
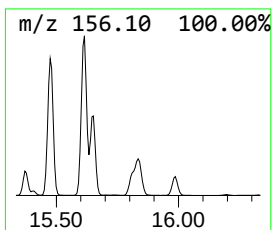
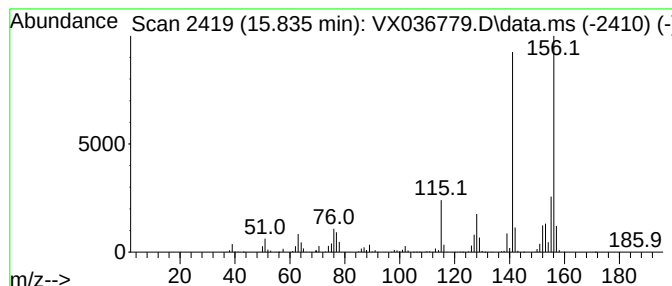
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Quant Title : SW846 8260

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	84.76 ug/l	1119190	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, 1,2-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	96
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080223\
Data File : VX036779.D
Acq On : 02 Aug 2023 18:41
Operator : JC/MD
Sample : 03815-03 10X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01

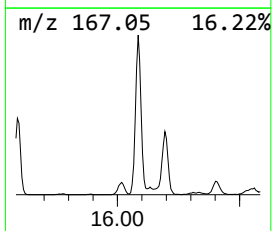
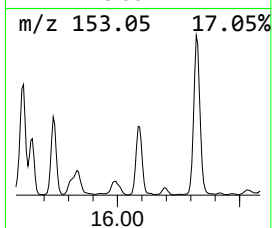
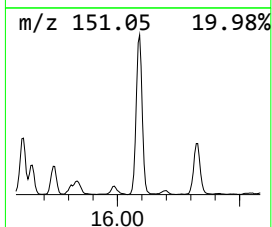
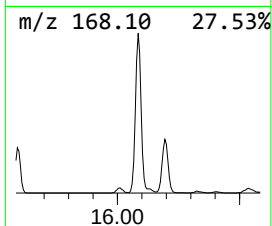
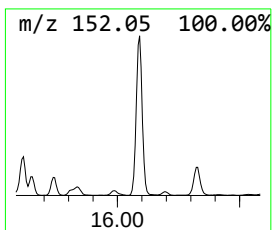
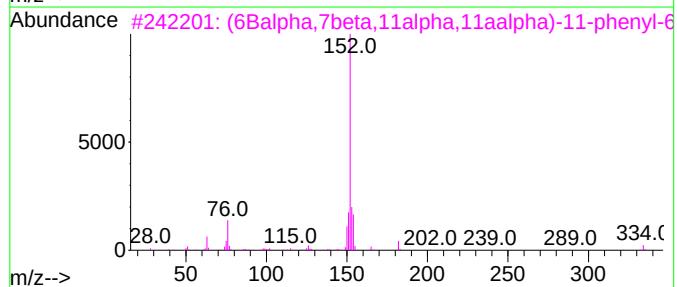
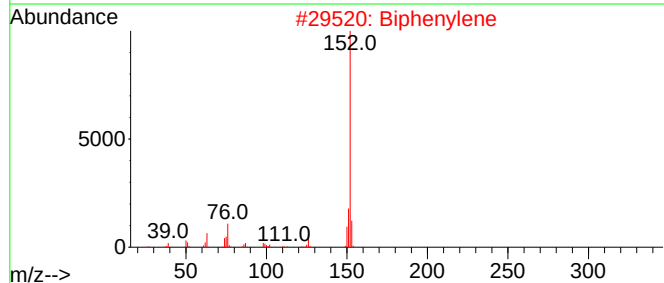
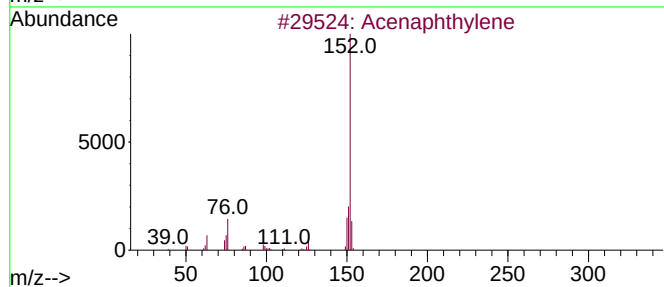
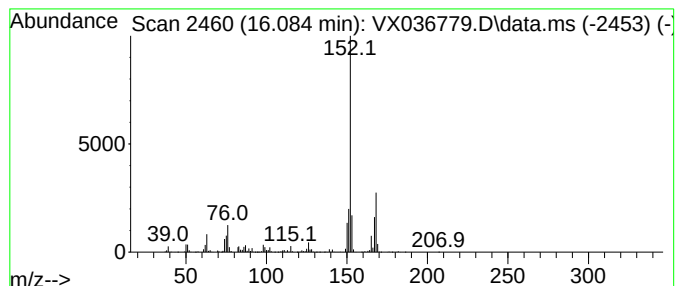
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Quant Title : SW846 8260

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

Peak Number 10 1-acenaphthenol, trifluoroa... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.084	85.06 ug/l	1123150	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthylene	152	C12H8	000208-96-8	95
2			Biphenylene	152	C12H8	000259-79-0	93
3			(6Balpha,7beta,11alpha,11aalpha)...	334	C25H18O	1000241-69-8	59
4			1-acenaphthenol, trifluoroacetat...	266	C14H9F3O2	1000376-45-2	58
5			1-Aza-2-sila-5-boracyclopent-3-e...	167	C8H18BNSi	125212-69-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080223\
Data File : VX036779.D
Acq On : 02 Aug 2023 18:41
Operator : JC/MD
Sample : 03815-03 10X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01

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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Azulene	13.780	1656.1	ug/l	21868500	4	12.024	660225	50.0
1,4-Methanonaph...	14.640	993.7	ug/l	13121200	4	12.024	660225	50.0
Bicyclo[4.4.1]u...	14.780	705.1	ug/l	9310570	4	12.024	660225	50.0
Naphthalene, 2-...	15.207	131.7	ug/l	1739590	4	12.024	660225	50.0
Naphthalene, 1,...	15.475	178.2	ug/l	2353010	4	12.024	660225	50.0
Naphthalene, 2,...	15.615	224.5	ug/l	2964580	4	12.024	660225	50.0
Naphthalene, 2,...	15.652	101.0	ug/l	1333310	4	12.024	660225	50.0
Naphthalene, 1,...	15.835	84.8	ug/l	1119190	4	12.024	660225	50.0
1-acenaphthenol...	16.084	85.1	ug/l	1123150	4	12.024	660225	50.0