

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
 Data File : VX037050.D
 Acq On : 17 Aug 2023 09:35
 Operator : JC/MD
 Sample : 03958-03
 Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 53 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NEVINS-SB02-Z64-65

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: VX037050.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	718	rBV	72529	211671	1.15%	0.287%
2	5.544	720	731	750	rVB2	123574	355777	1.94%	0.482%
3	5.952	788	798	805	rBV	78979	203885	1.11%	0.276%
4	6.757	920	930	946	rBV	202400	481443	2.62%	0.653%
5	8.647	1234	1240	1248	rBV	423301	654407	3.56%	0.887%
6	10.055	1466	1471	1477	rBV	471528	613641	3.34%	0.832%
7	10.195	1488	1494	1500	rBV	653038	890973	4.85%	1.208%
8	10.640	1562	1567	1582	rVB	160490	226914	1.24%	0.308%
9	10.964	1614	1620	1628	rBV	139444	197237	1.07%	0.267%
10	11.085	1634	1640	1650	rBV	435128	621542	3.38%	0.842%
11	11.396	1684	1691	1695	rBV	260869	385481	2.10%	0.522%
12	11.476	1701	1704	1713	rVB	225465	277557	1.51%	0.376%
13	11.610	1722	1726	1734	rBV	232244	296766	1.62%	0.402%
14	11.750	1745	1749	1754	rVB	451503	573707	3.12%	0.778%
15	12.024	1788	1794	1800	rBV2	603213	807369	4.40%	1.094%
16	12.085	1800	1804	1809	rVB	240147	329158	1.79%	0.446%
17	12.244	1824	1830	1837	rBV	3757990	4700475	25.60%	6.371%
18	12.317	1837	1842	1848	rBV2	503879	685776	3.73%	0.929%
19	12.421	1853	1859	1864	rBV2	308590	391510	2.13%	0.531%
20	12.616	1885	1891	1894	rBV	657244	809320	4.41%	1.097%
21	12.701	1900	1905	1910	rBV2	246981	416729	2.27%	0.565%
22	12.799	1917	1921	1925	rBV	164450	237411	1.29%	0.322%
23	12.963	1944	1948	1953	rVB	305735	386010	2.10%	0.523%
24	13.049	1958	1962	1967	rVV2	195926	347282	1.89%	0.471%
25	13.170	1977	1982	1986	rBV	589109	751024	4.09%	1.018%
26	13.286	1992	2001	2006	rBV3	533453	1028385	5.60%	1.394%
27	13.341	2006	2010	2017	rVV	945859	1134818	6.18%	1.538%
28	13.427	2018	2024	2028	rVB	1396414	1881023	10.24%	2.549%
29	13.542	2039	2043	2047	rBV	305612	427341	2.33%	0.579%
30	13.579	2047	2049	2059	rVB2	105990	192212	1.05%	0.261%
31	13.676	2060	2065	2068	rBV2	157474	230872	1.26%	0.313%
32	13.780	2076	2082	2088	rVV	13713123	18363731	100.00%	24.890%
33	13.865	2090	2096	2100	rVV	394546	602490	3.28%	0.817%
34	13.920	2100	2105	2111	rVB3	191810	328948	1.79%	0.446%
35	14.073	2125	2130	2131	rBV2	153322	188741	1.03%	0.256%
36	14.097	2131	2134	2137	rVV	327923	424360	2.31%	0.575%

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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37	14.134	2137	2140	2148	rVB4	242280	485849	2.65%	0.659%
38	14.219	2149	2154	2157	rBV	484731	702638	3.83%	0.952%
39	14.256	2157	2160	2164	rVV2	211403	301958	1.64%	0.409%
40	14.317	2164	2170	2176	rVV	480552	820508	4.47%	1.112%
41	14.408	2182	2185	2192	rVB	144137	207617	1.13%	0.281%
42	14.524	2200	2204	2210	rVB2	197081	285883	1.56%	0.387%
43	14.597	2212	2216	2218	rVV	152130	195223	1.06%	0.265%
44	14.634	2218	2222	2233	rVB	4639793	6134244	33.40%	8.314%
45	14.780	2240	2246	2252	rBV	6709941	8572087	46.68%	11.618%
46	15.207	2308	2316	2320	rBV	807432	1178371	6.42%	1.597%
47	15.255	2320	2324	2331	rVB2	128055	216722	1.18%	0.294%
48	15.371	2331	2343	2347	rBV	1173697	1917737	10.44%	2.599%
49	15.408	2347	2349	2353	rVB	289035	313245	1.71%	0.425%
50	15.475	2354	2360	2365	rBV	1694653	2564410	13.96%	3.476%
51	15.609	2377	2382	2386	rBV	1794589	2803680	15.27%	3.800%
52	15.646	2386	2388	2394	rVB	812775	1088988	5.93%	1.476%
53	15.737	2394	2403	2409	rVB3	133689	253052	1.38%	0.343%
54	15.835	2409	2419	2424	rBV	477106	1287494	7.01%	1.745%
55	15.987	2437	2444	2453	rVV	297671	545110	2.97%	0.739%
56	16.085	2454	2460	2469	rVV	333745	592689	3.23%	0.803%
57	16.194	2469	2478	2484	rVB	87479	186593	1.02%	0.253%
58	16.322	2490	2499	2508	rBV2	1159343	2235836	12.18%	3.030%
59	16.652	2548	2553	2569	rVB2	78696	234364	1.28%	0.318%

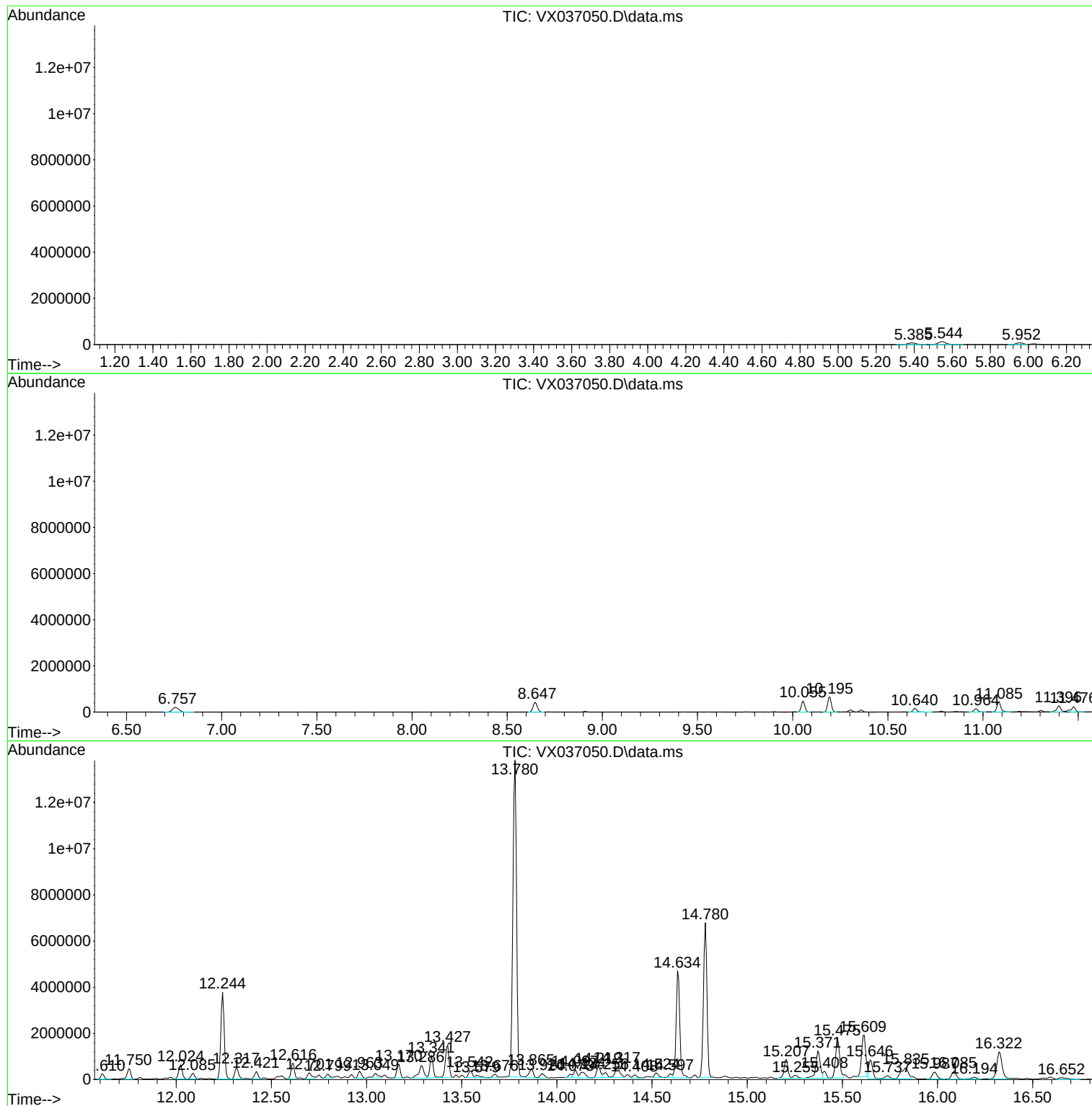
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z64-65

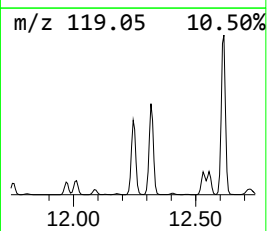
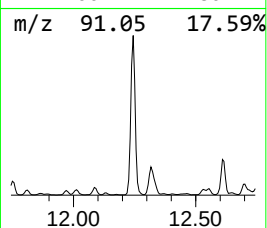
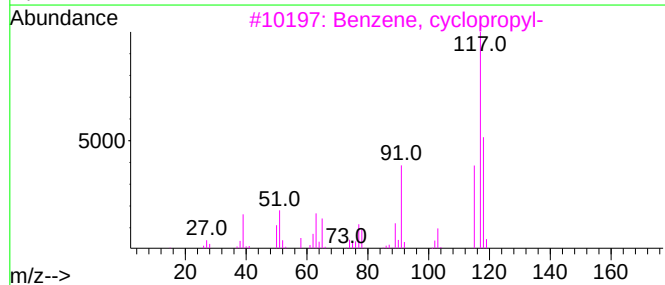
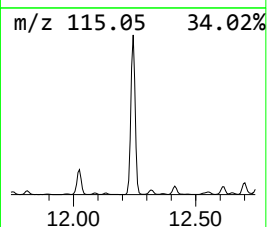
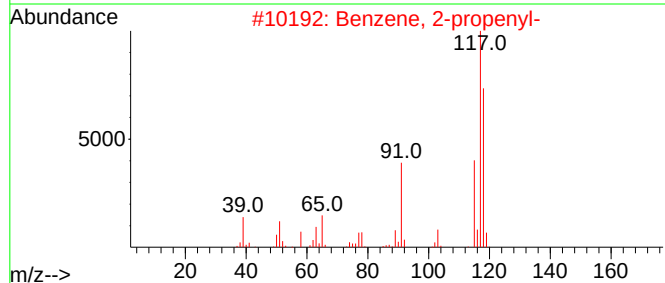
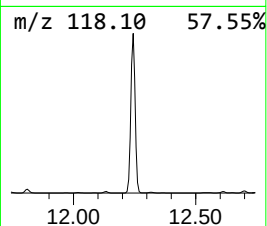
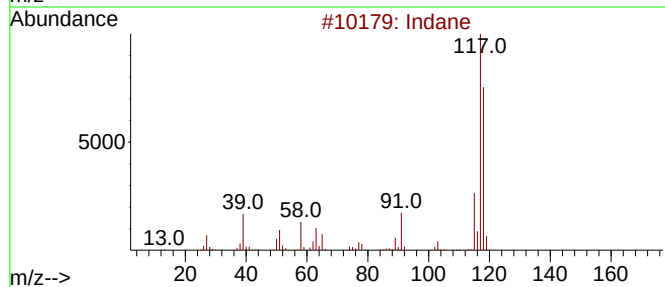
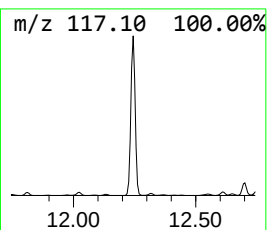
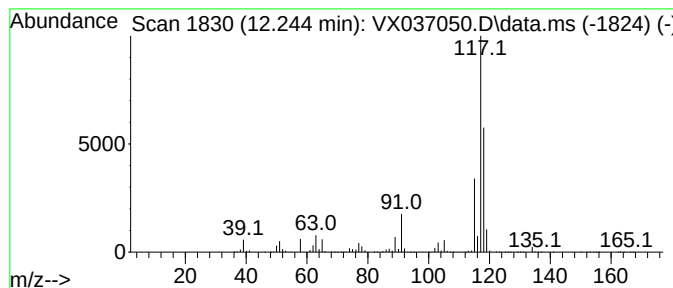
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	291.10 ug/l	4700480	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, 2-propenyl-	118	C9H10	000300-57-2	87
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Deltacyclene	118	C9H10	007785-10-6	64



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ALS Vial : 53 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NEVINS-SB02-Z64-65

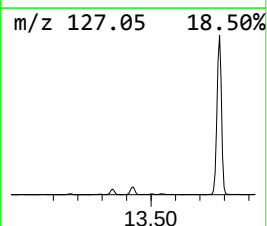
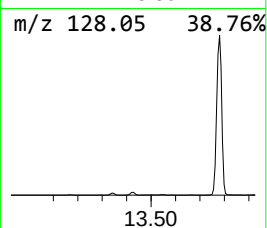
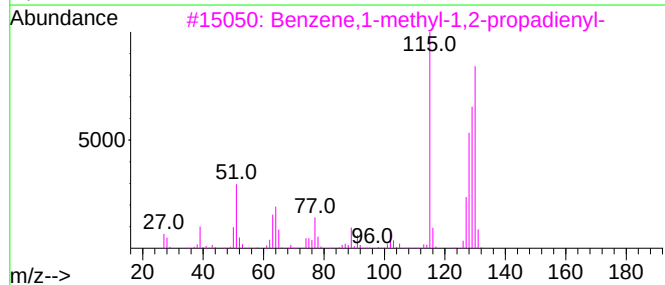
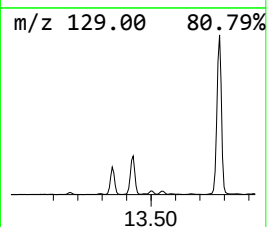
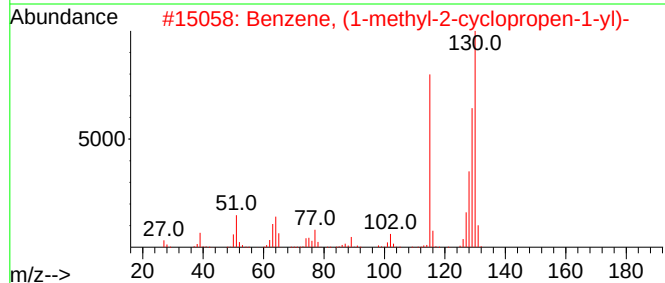
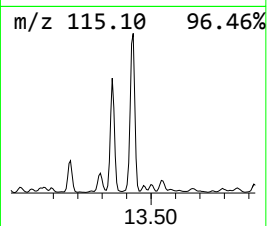
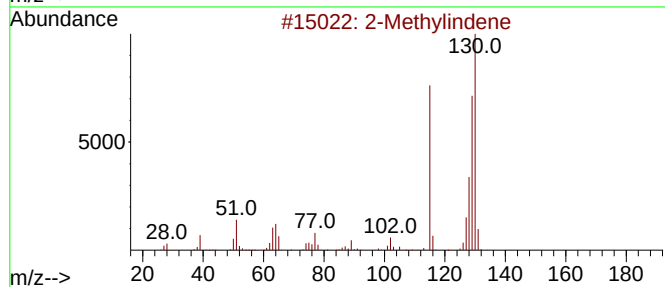
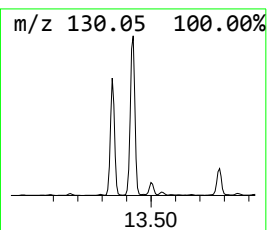
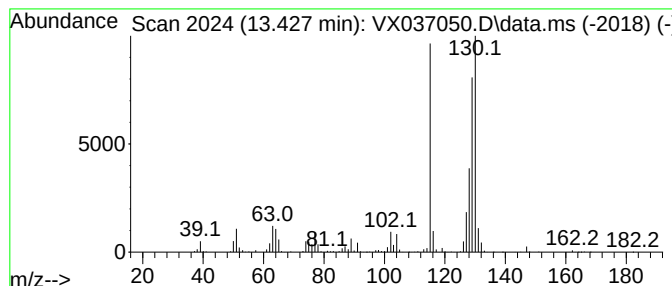
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, (1-methyl-2-cyclop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	116.49 ug/l	1881020	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	1H-Indene, 1-methyl-			130	C10H10	000767-59-9	94
5	Cycloprop[a]indene, 1,1a,6,6a-te...			130	C10H10	015677-15-3	93



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ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z64-65

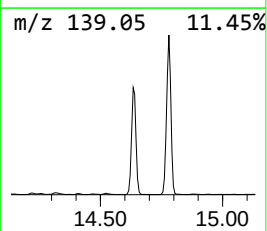
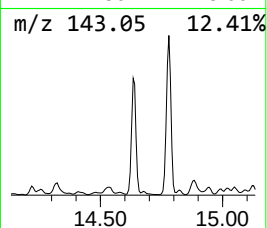
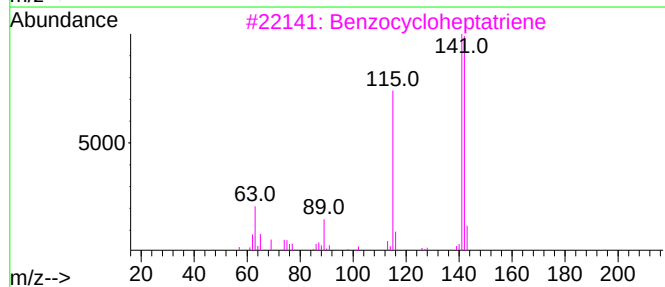
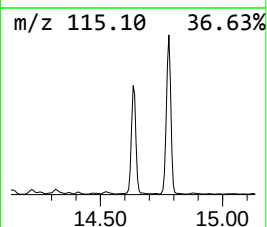
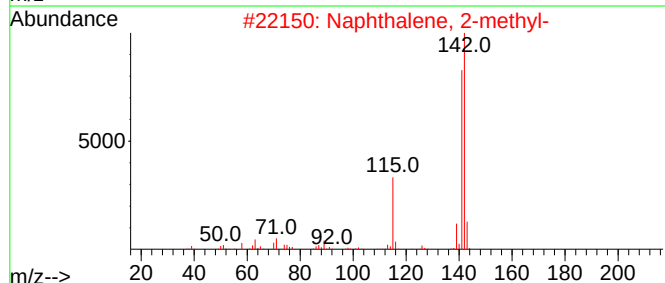
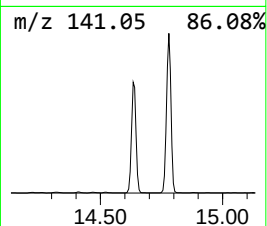
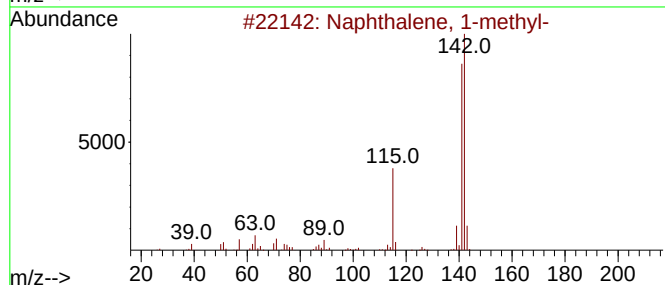
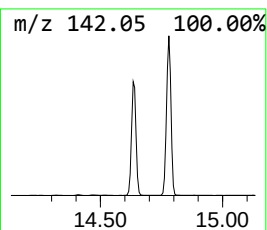
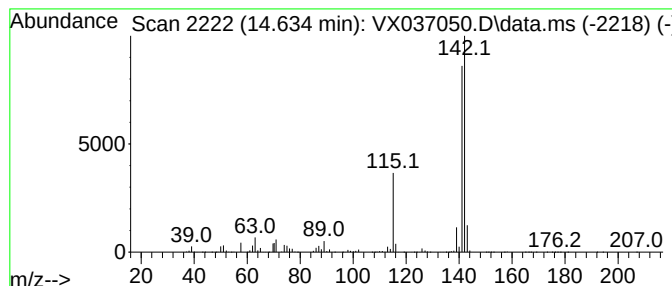
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	379.89 ug/l	6134240	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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



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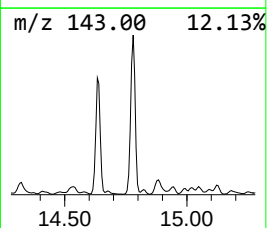
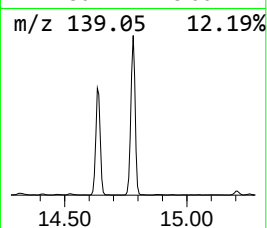
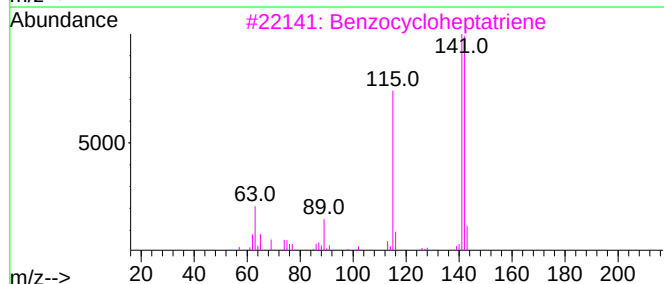
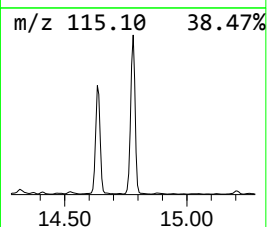
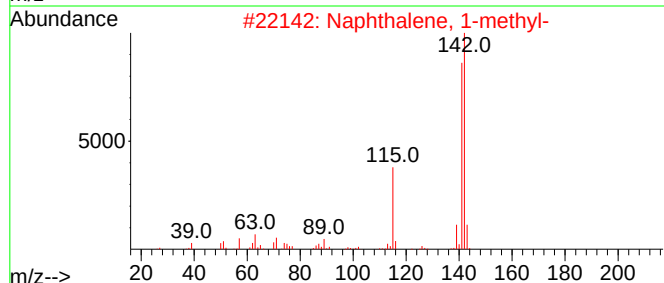
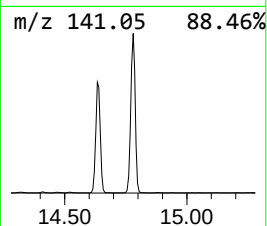
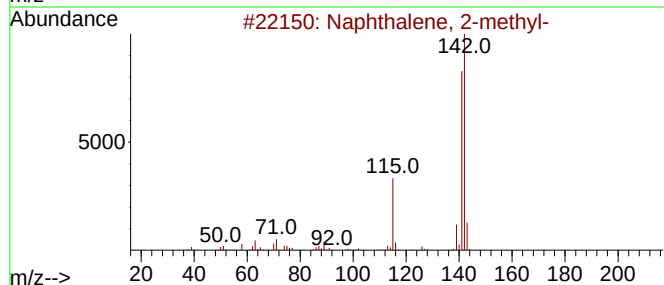
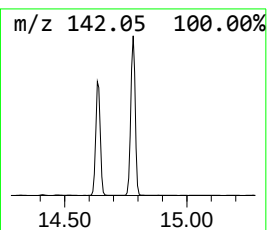
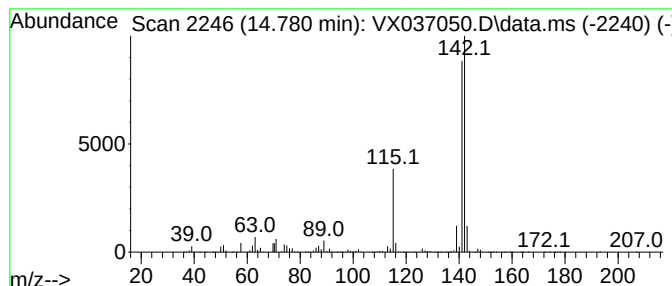
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzocycloheptatriene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	530.87 ug/l	8572090	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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91



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NEVINS-SB02-Z64-65

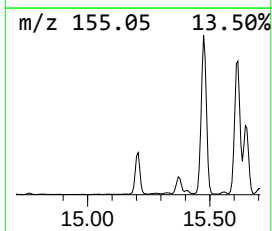
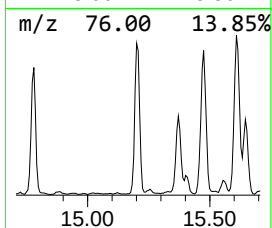
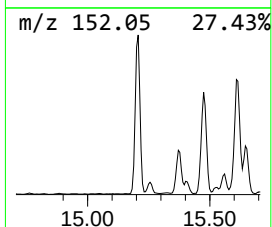
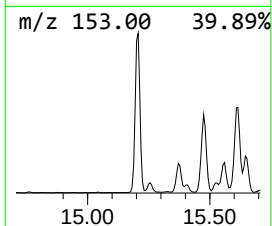
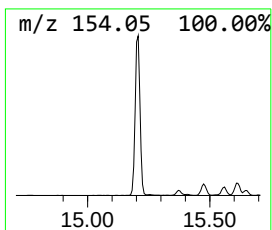
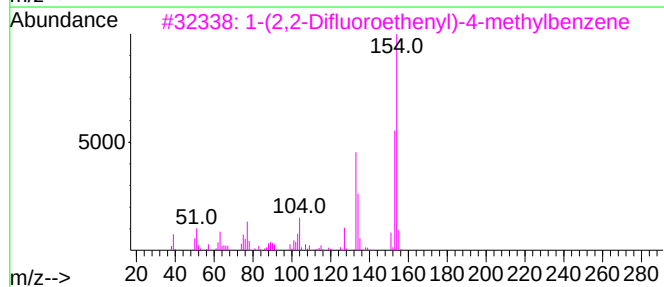
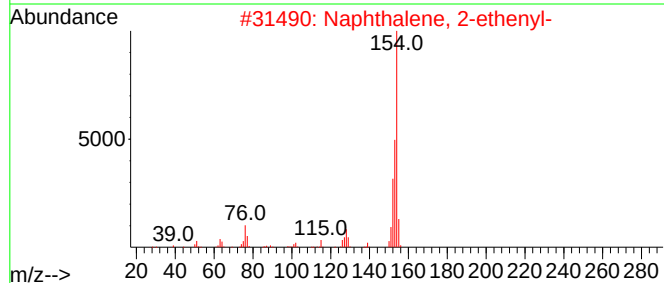
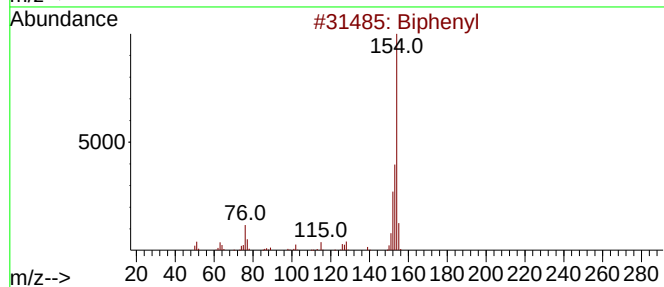
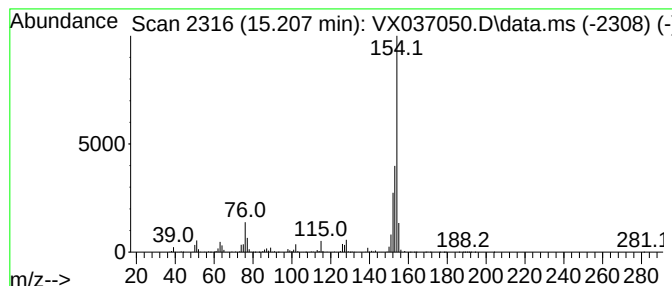
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Quant Title : SW846 8260

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

Peak Number 5 Biphenyl Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.207	72.98 ug/l	1178370	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	94
3			1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	53
4			6-Cyanoquinoline	154	C10H6N2	023395-72-4	49
5			1-Isoquinolinecarbonitrile	154	C10H6N2	001198-30-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037050.D
Acq On : 17 Aug 2023 09:35
Operator : JC/MD
Sample : 03958-03
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z64-65

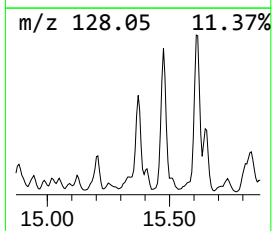
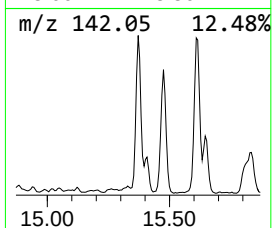
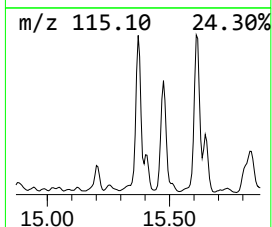
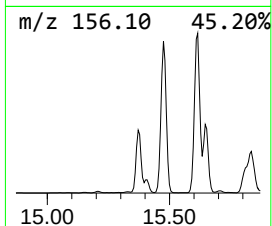
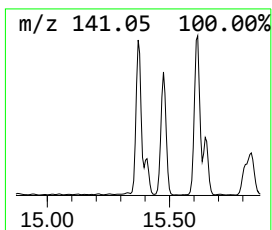
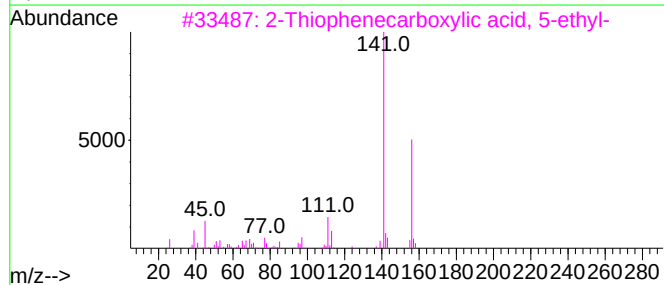
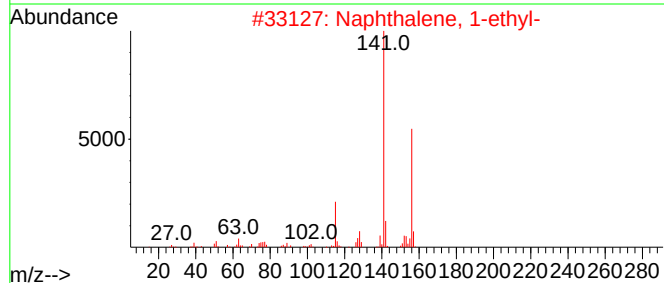
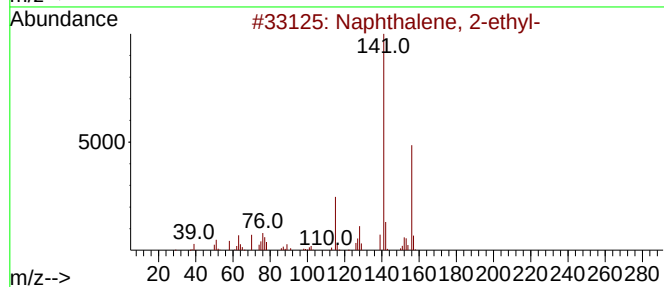
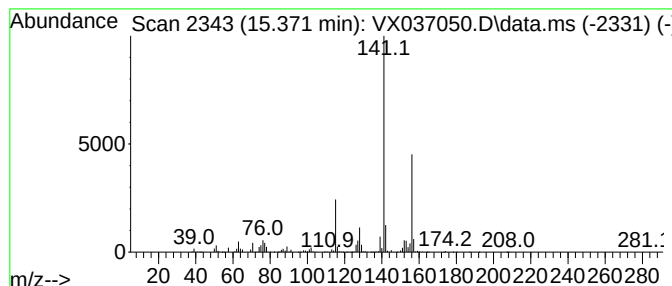
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	118.77 ug/l	1917740	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	96
2			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	96
3			2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	64
4			2,4-Difluoromesitylene	156	C9H10F2	000392-61-0	59
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037050.D
Acq On : 17 Aug 2023 09:35
Operator : JC/MD
Sample : 03958-03
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z64-65

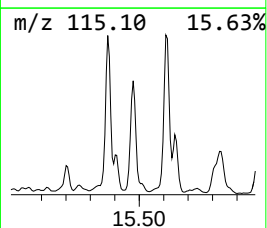
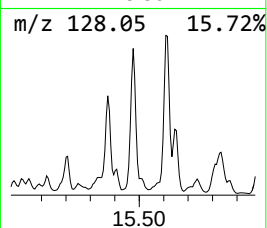
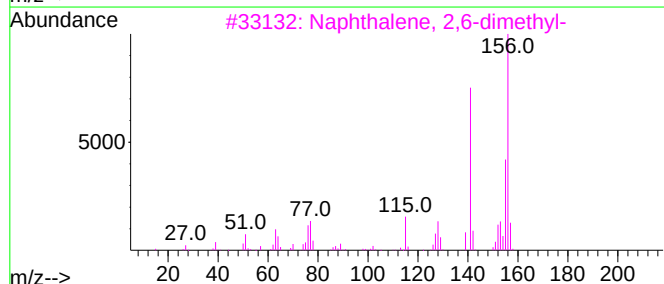
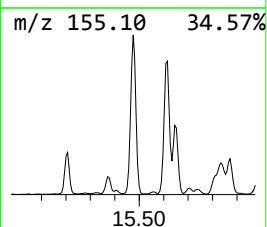
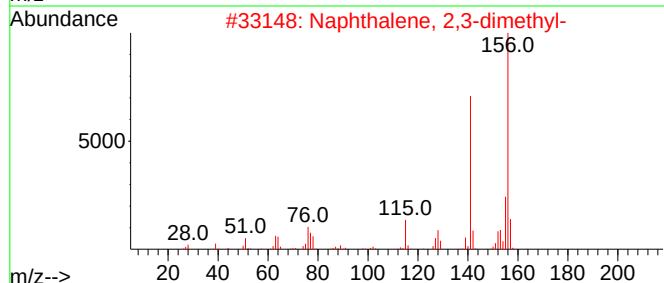
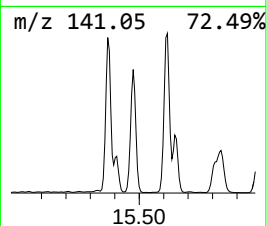
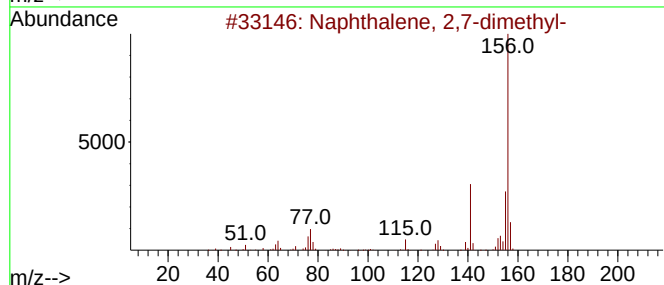
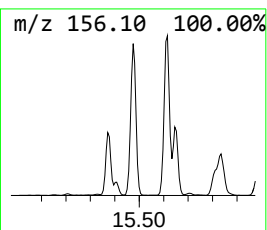
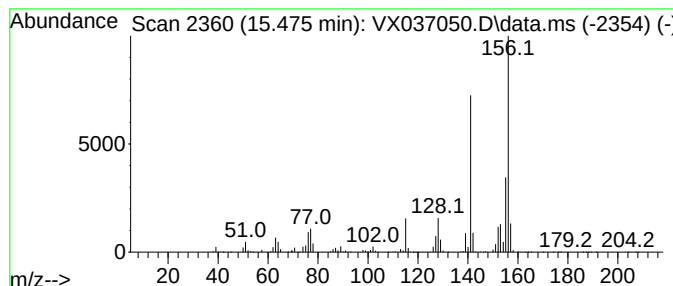
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	158.81 ug/l	2564410	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	97
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037050.D
Acq On : 17 Aug 2023 09:35
Operator : JC/MD
Sample : 03958-03
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z64-65

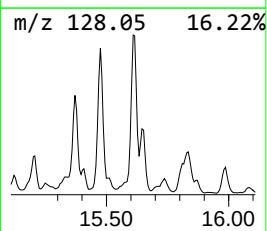
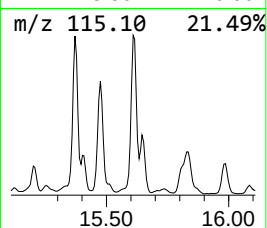
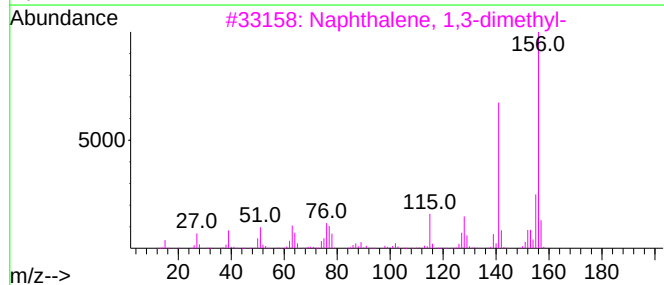
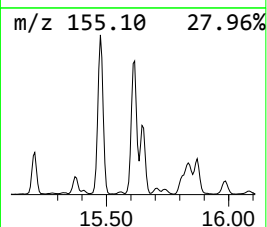
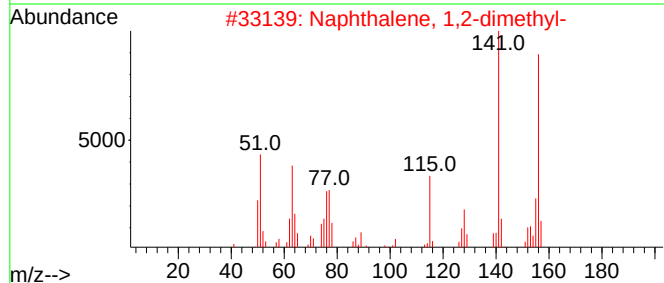
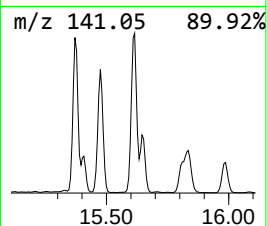
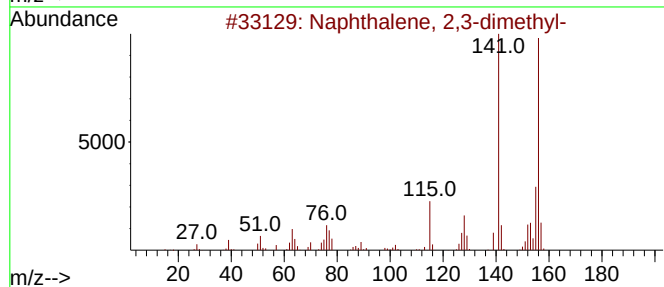
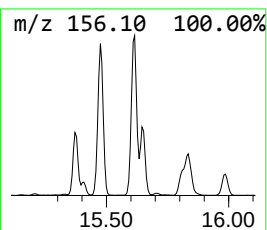
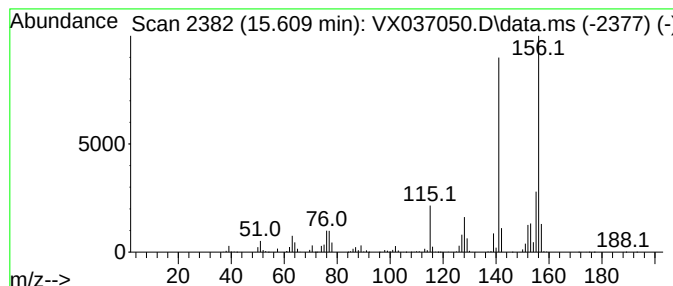
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	173.63 ug/l	2803680	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	97
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037050.D
Acq On : 17 Aug 2023 09:35
Operator : JC/MD
Sample : 03958-03
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z64-65

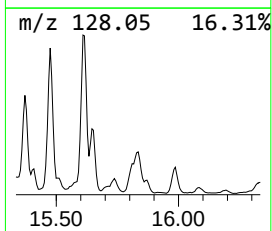
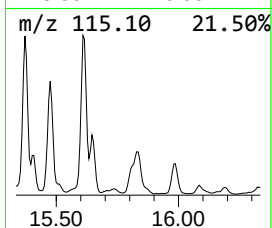
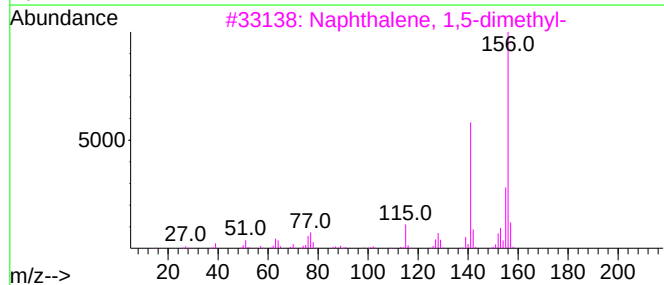
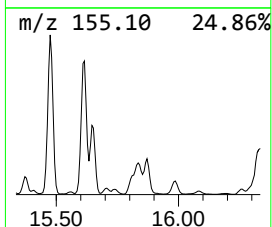
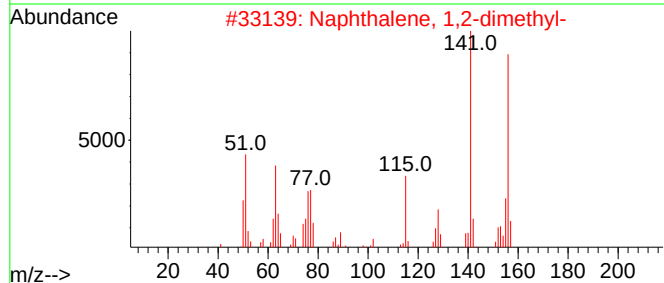
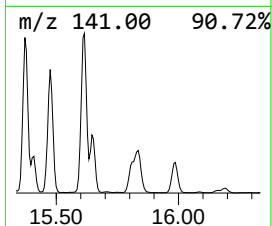
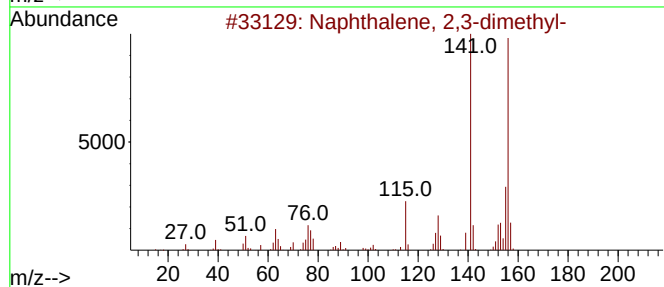
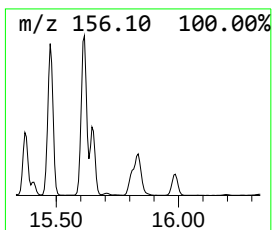
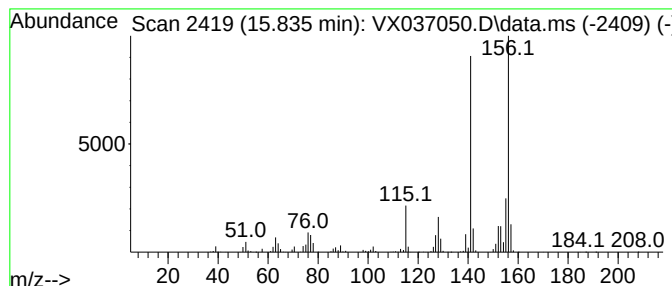
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	79.73 ug/l	1287490	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, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037050.D
Acq On : 17 Aug 2023 09:35
Operator : JC/MD
Sample : 03958-03
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z64-65

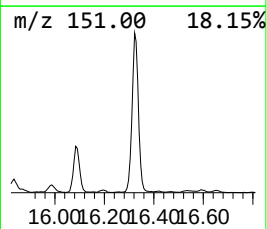
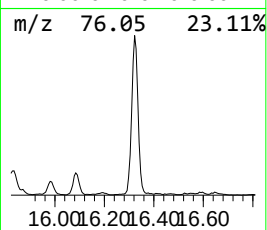
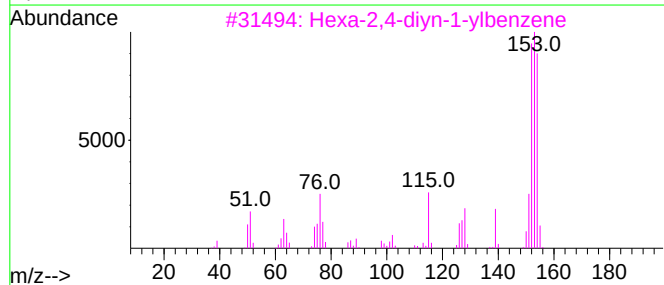
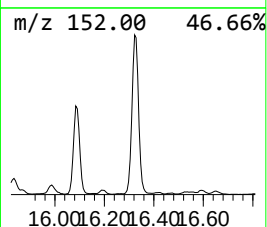
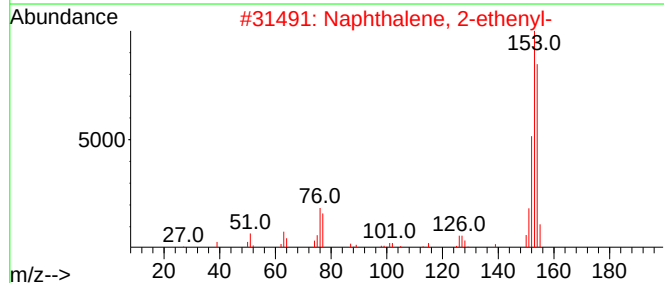
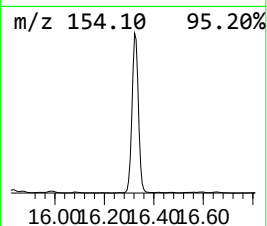
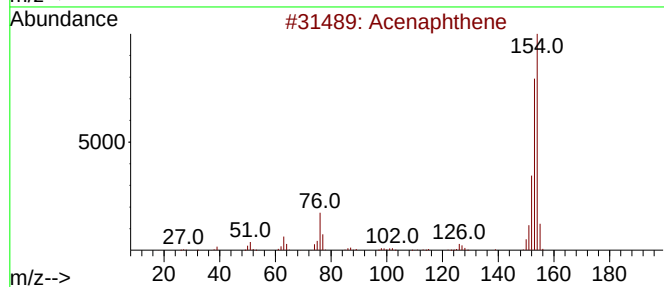
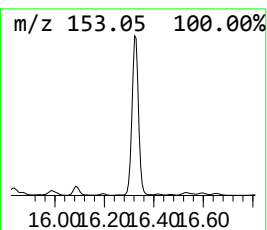
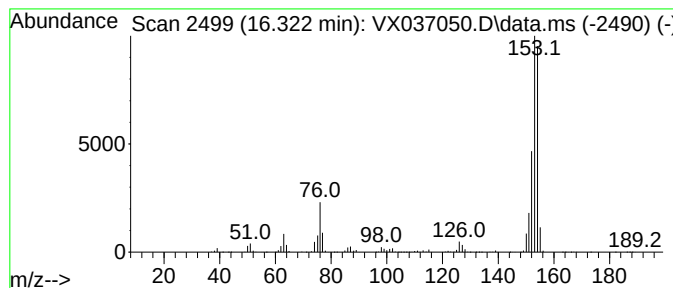
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 2-ethenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	138.46 ug/l	2235840	1,4-Dichlorobenzene-d4	12.024

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	50
5			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037050.D
Acq On : 17 Aug 2023 09:35
Operator : JC/MD
Sample : 03958-03
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z64-65

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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Benzene, (1-met...	13.427	116.5	ug/l	1881020	4	12.024	807369	50.0
Naphthalene, 1-...	14.634	379.9	ug/l	6134240	4	12.024	807369	50.0
Benzocyclohepta...	14.780	530.9	ug/l	8572090	4	12.024	807369	50.0
Biphenyl	15.207	73.0	ug/l	1178370	4	12.024	807369	50.0
Naphthalene, 1-...	15.371	118.8	ug/l	1917740	4	12.024	807369	50.0
Naphthalene, 2,...	15.475	158.8	ug/l	2564410	4	12.024	807369	50.0
Naphthalene, 2,...	15.609	173.6	ug/l	2803680	4	12.024	807369	50.0
Naphthalene, 1,...	15.835	79.7	ug/l	1287490	4	12.024	807369	50.0
Naphthalene, 2-...	16.322	138.5	ug/l	2235840	4	12.024	807369	50.0