

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
 Data File : VX037039.D
 Acq On : 17 Aug 2023 05:12
 Operator : JC/MD
 Sample : 03958-03 10X
 Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 42 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: VX037039.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	693	705	721	rBV2	86627	253090	13.29%	2.525%
2	5.550	721	732	747	rVB	140809	401204	21.06%	4.002%
3	5.952	788	798	809	rBV	89831	244620	12.84%	2.440%
4	6.757	921	930	946	rBV	232096	555519	29.17%	5.541%
5	8.647	1234	1240	1262	rVB	485492	761079	39.96%	7.592%
6	10.055	1465	1471	1487	rBV	515756	700508	36.78%	6.988%
7	10.195	1489	1494	1500	rVV	68012	90919	4.77%	0.907%
8	10.640	1561	1567	1575	rBV	15881	22255	1.17%	0.222%
9	11.079	1634	1639	1652	rBV	431165	549245	28.84%	5.479%
10	11.396	1684	1691	1697	rBV	22788	36164	1.90%	0.361%
11	11.610	1722	1726	1734	rVB	21324	28274	1.48%	0.282%
12	11.750	1745	1749	1755	rVB	44178	54258	2.85%	0.541%
13	12.018	1788	1793	1800	rBV	539015	676831	35.54%	6.752%
14	12.085	1800	1804	1809	rVB	23867	31928	1.68%	0.318%
15	12.244	1824	1830	1837	rBV	356610	448254	23.54%	4.471%
16	12.317	1837	1842	1848	rVV	42490	61731	3.24%	0.616%
17	12.421	1853	1859	1863	rBV2	32162	39927	2.10%	0.398%
18	12.610	1885	1890	1895	rBV	55760	67516	3.54%	0.673%
19	12.695	1899	1904	1910	rBV2	22697	37247	1.96%	0.372%
20	12.963	1944	1948	1953	rVB	25144	35615	1.87%	0.355%
21	13.042	1958	1961	1967	rVV2	15071	20686	1.09%	0.206%
22	13.164	1977	1981	1986	rBV	51061	64644	3.39%	0.645%
23	13.268	1992	1998	1999	rBV2	31668	42901	2.25%	0.428%
24	13.286	1999	2001	2006	rVV2	46906	62699	3.29%	0.625%
25	13.341	2006	2010	2014	rVB	62469	74906	3.93%	0.747%
26	13.426	2019	2024	2028	rVB	108607	144006	7.56%	1.436%
27	13.542	2039	2043	2047	rBV	24480	32524	1.71%	0.324%
28	13.676	2060	2065	2068	rBV2	12255	19965	1.05%	0.199%
29	13.774	2076	2081	2088	rVV	1574862	1904607	100.00%	18.999%
30	13.865	2088	2096	2100	rVV2	33299	58991	3.10%	0.588%
31	13.920	2101	2105	2111	rVB3	14013	22136	1.16%	0.221%
32	14.134	2137	2140	2146	rVB4	17361	31036	1.63%	0.310%
33	14.219	2150	2154	2157	rBV2	32146	42555	2.23%	0.424%
34	14.256	2157	2160	2164	rVB2	14988	21520	1.13%	0.215%
35	14.317	2164	2170	2176	rBV2	37260	63513	3.33%	0.634%
36	14.518	2200	2203	2208	rVB3	14650	20704	1.09%	0.207%

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NEVINS-SB02-Z64-65

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37	14.603	2212	2217	2218	rVV	15140	21030	1.10%	0.210%
38	14.634	2218	2222	2233	rVB	383085	481527	25.28%	4.803%
39	14.780	2240	2246	2255	rBV	570811	752792	39.52%	7.509%
40	15.207	2308	2316	2320	rBV	63833	94869	4.98%	0.946%
41	15.255	2320	2324	2332	rVB6	9981	22236	1.17%	0.222%
42	15.371	2332	2343	2347	rBV	82282	133716	7.02%	1.334%
43	15.408	2347	2349	2354	rVB	22514	24994	1.31%	0.249%
44	15.475	2354	2360	2365	rBV	102280	164166	8.62%	1.638%
45	15.609	2377	2382	2386	rBV	138931	209820	11.02%	2.093%
46	15.646	2386	2388	2394	rVB	54275	73914	3.88%	0.737%
47	15.835	2409	2419	2424	rBV2	32725	91984	4.83%	0.918%
48	15.987	2437	2444	2454	rVB	21277	37573	1.97%	0.375%
49	16.085	2454	2460	2469	rBV2	11040	19287	1.01%	0.192%
50	16.322	2491	2499	2510	rBV	90175	173309	9.10%	1.729%

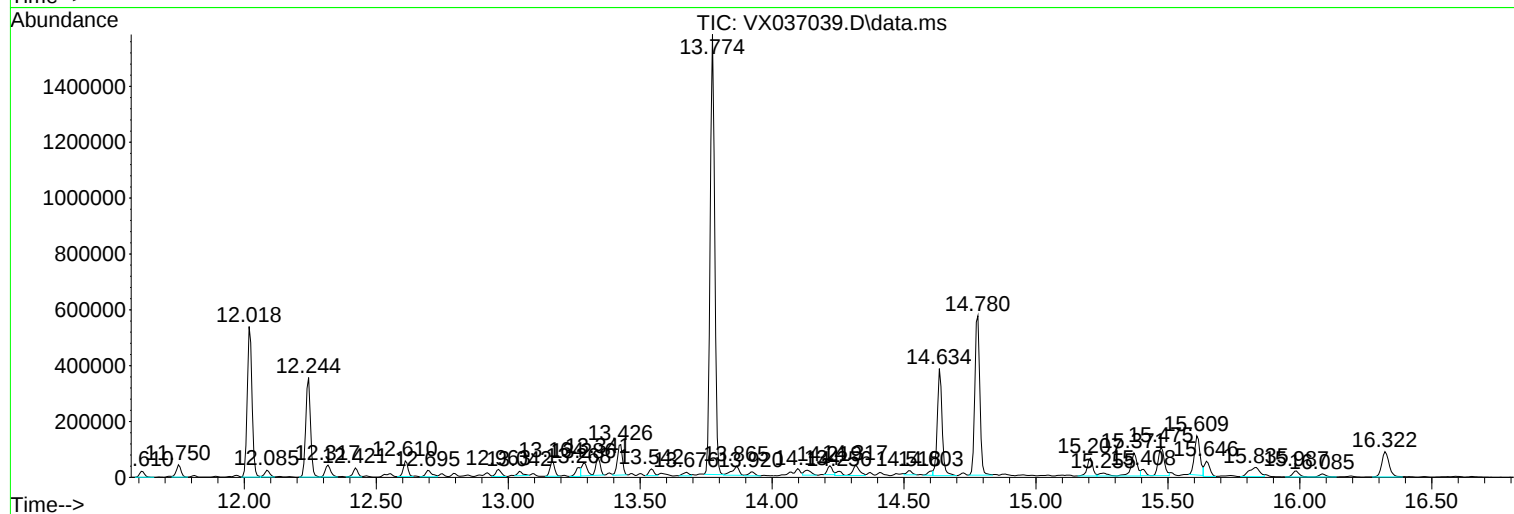
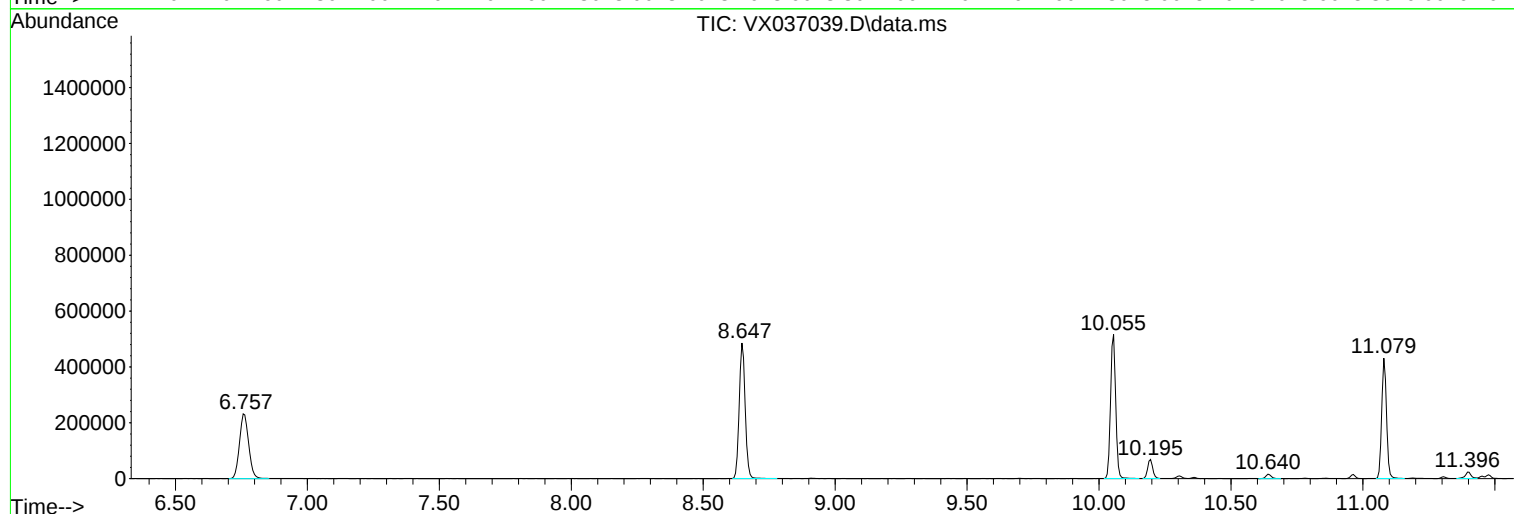
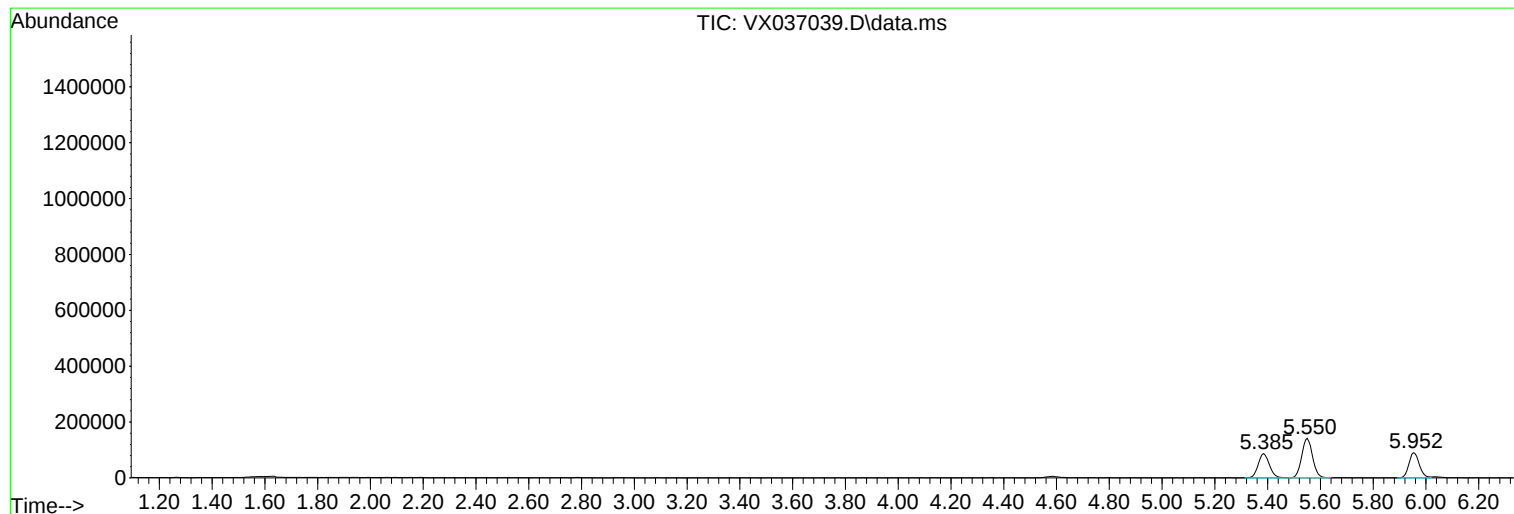
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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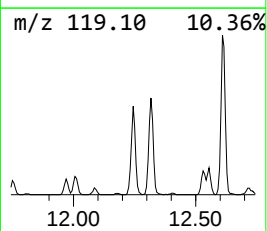
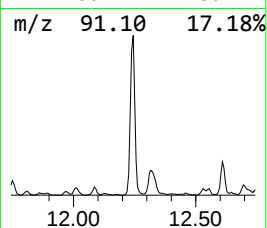
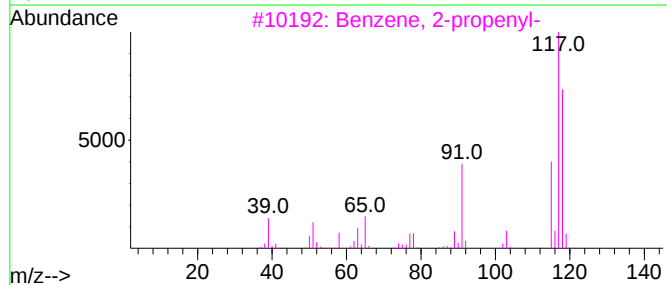
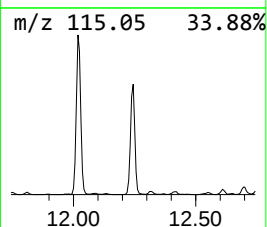
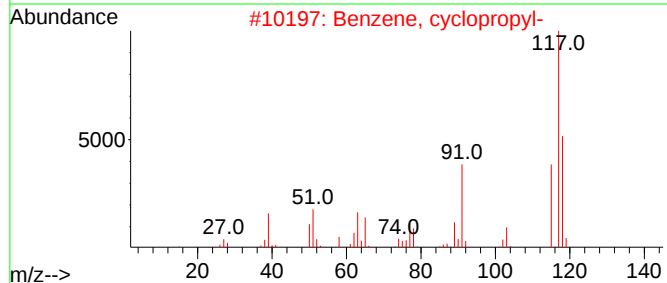
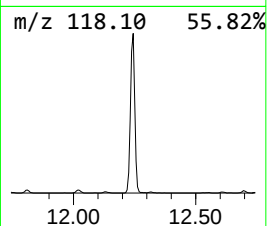
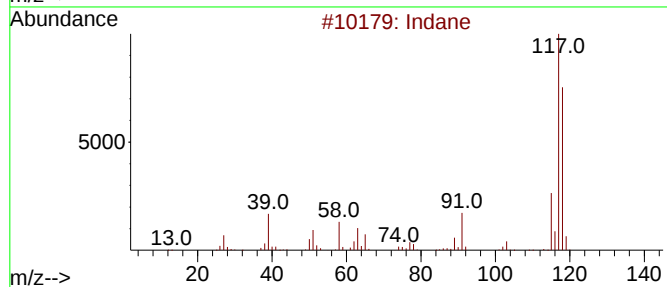
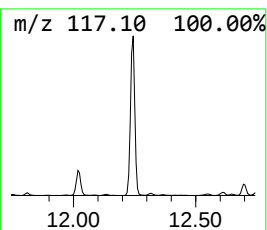
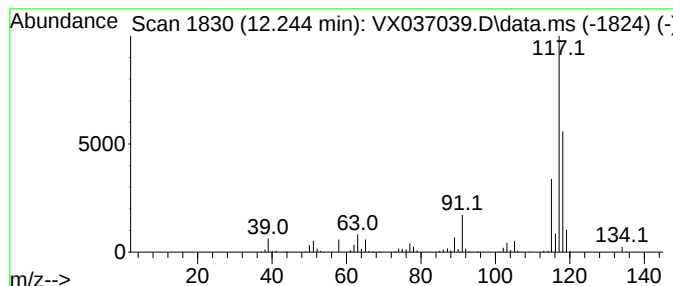
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	33.11 ug/l	448254	1,4-Dichlorobenzene-d4	12.018

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	81
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
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 : 42 Sample Multiplier: 1

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

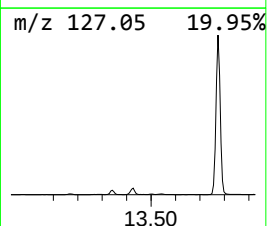
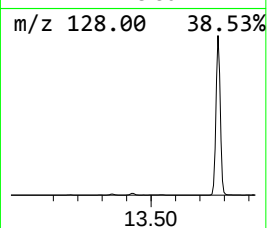
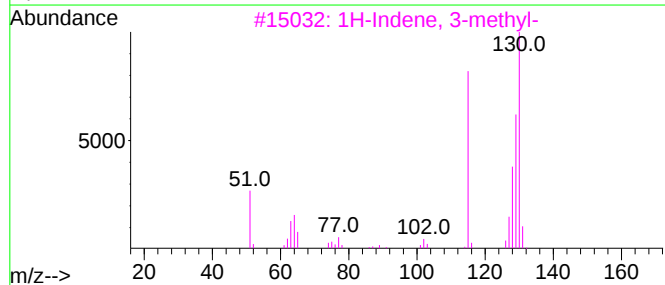
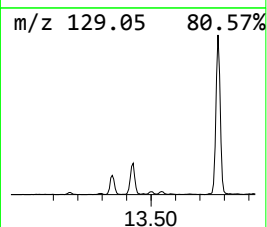
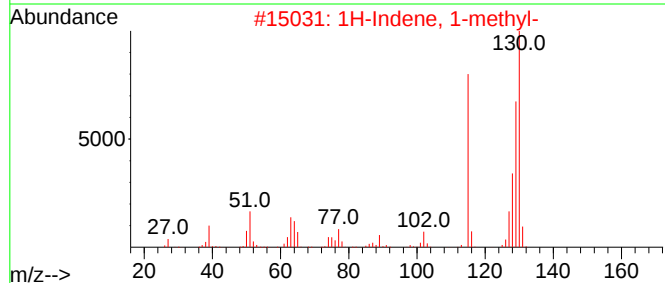
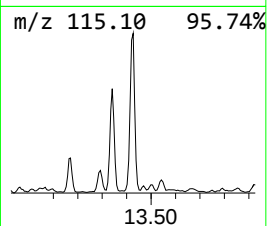
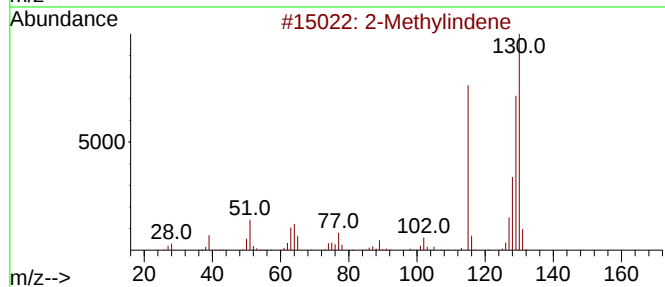
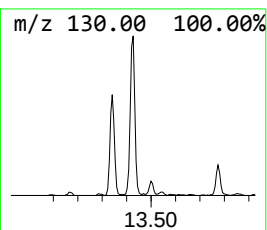
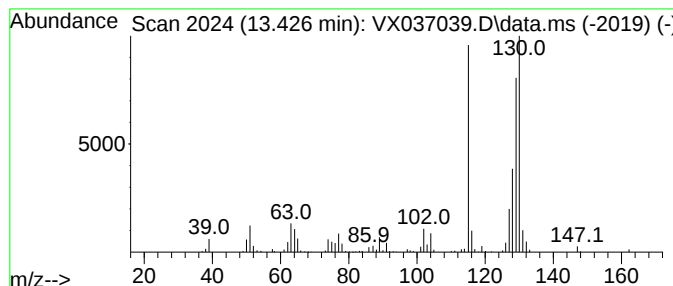
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Methylindene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	10.64 ug/l	144006	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			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
3			1H-Indene, 3-methyl-	130	C10H10	000767-60-2	94
4			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
5			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
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Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

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

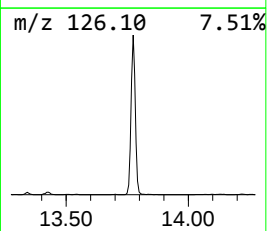
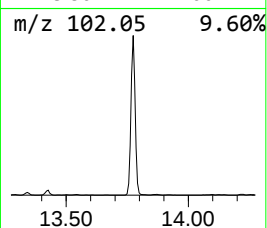
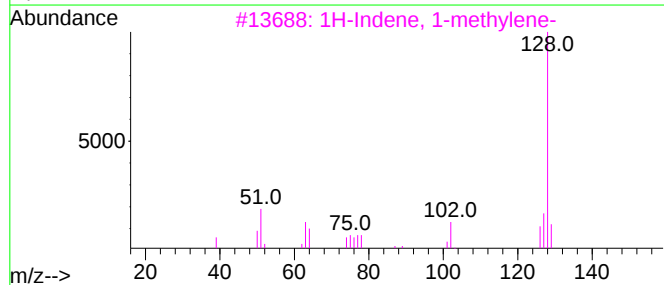
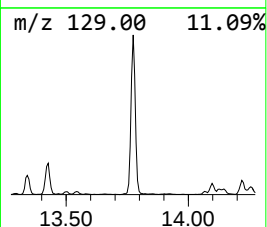
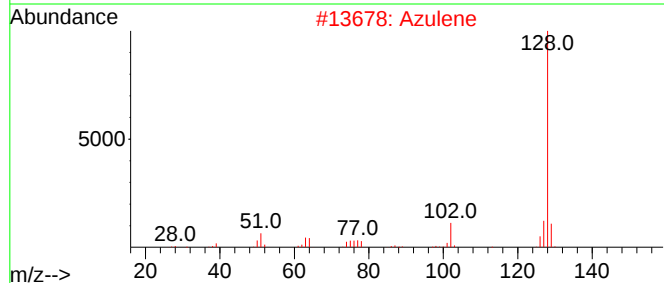
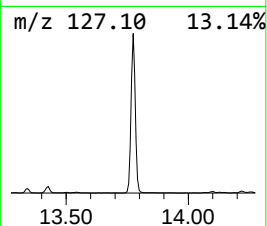
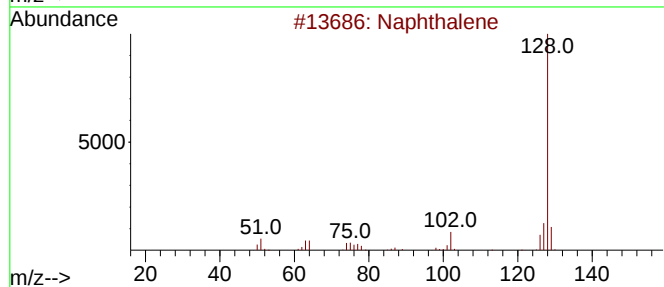
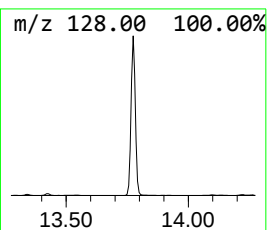
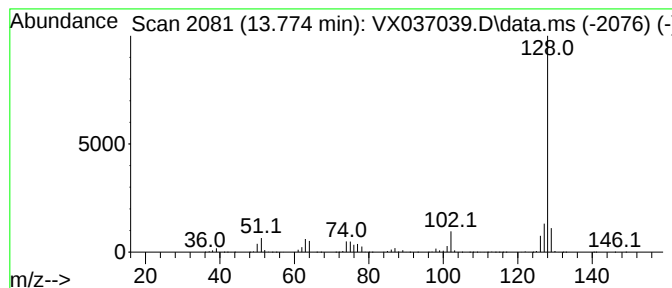
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	140.70 ug/l	1904610	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	94
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	78
4			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	53



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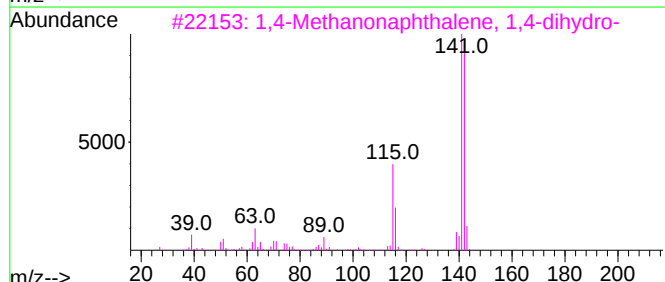
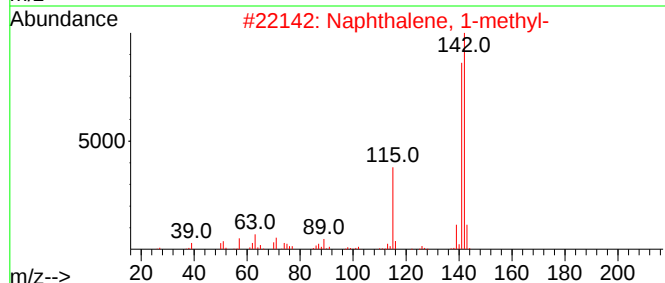
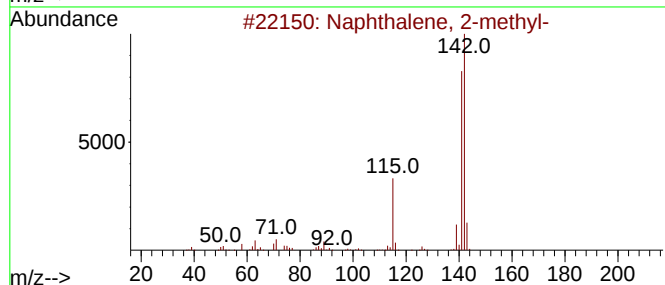
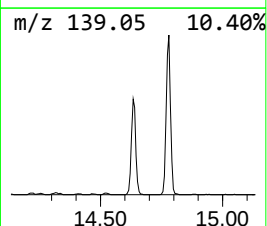
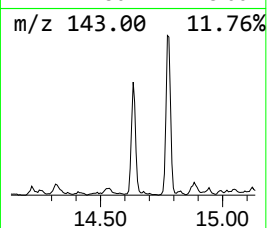
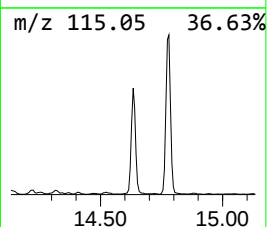
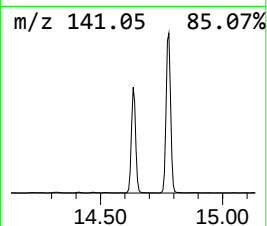
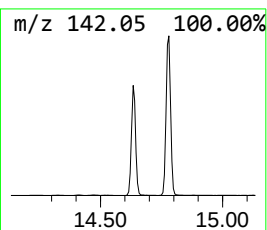
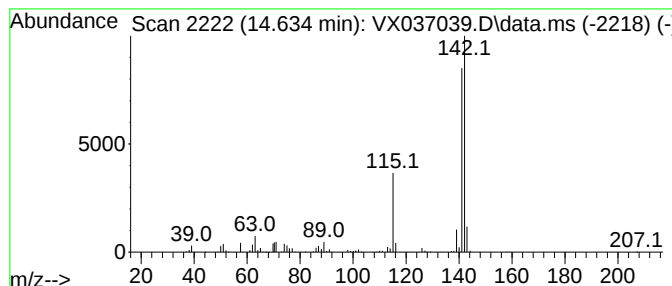
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	35.57 ug/l	481527	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	50



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NEVINS-SB02-Z64-65

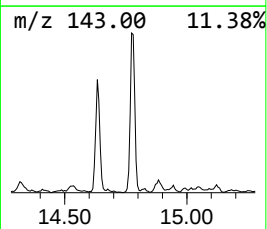
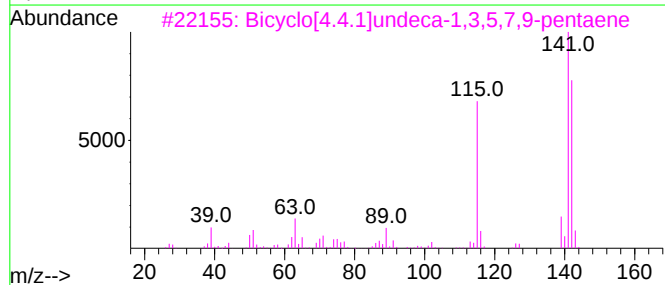
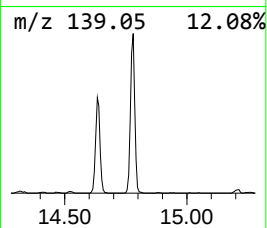
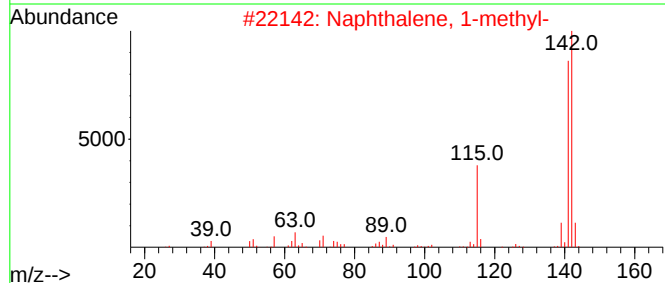
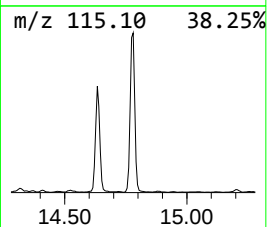
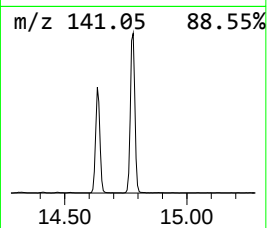
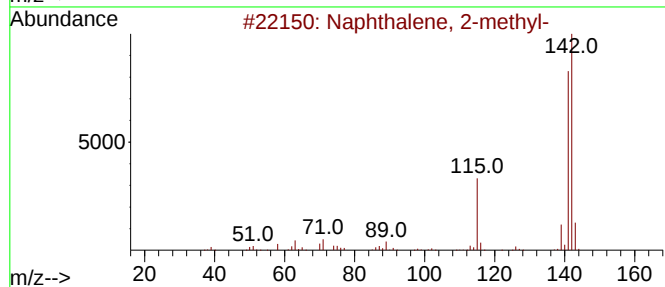
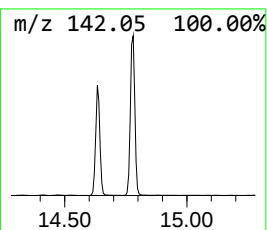
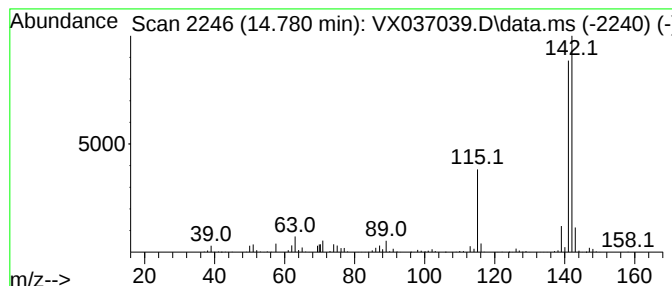
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	55.61 ug/l	752792	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 : VX037039.D
Acq On : 17 Aug 2023 05:12
Operator : JC/MD
Sample : 03958-03 10X
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

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

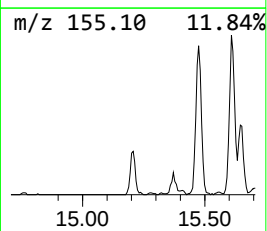
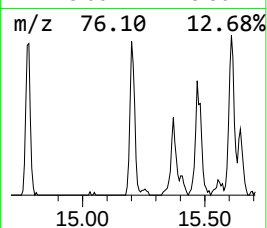
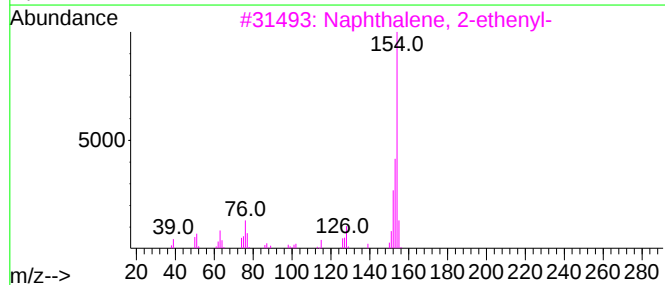
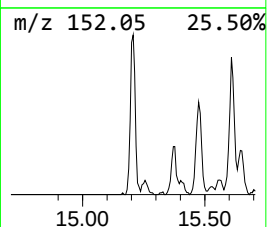
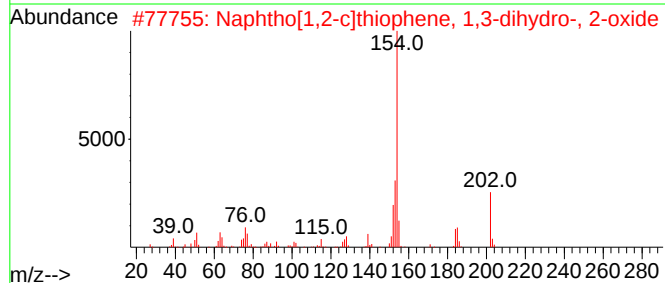
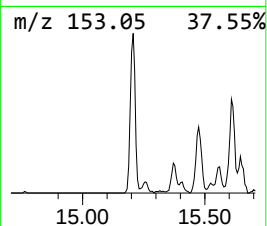
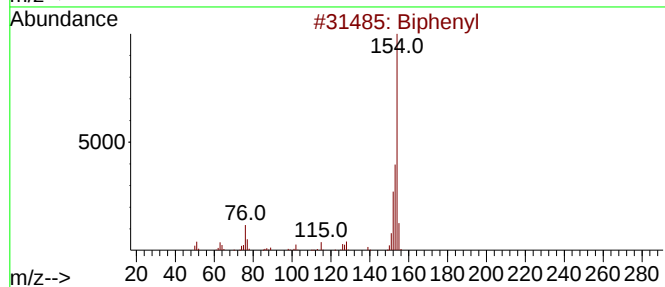
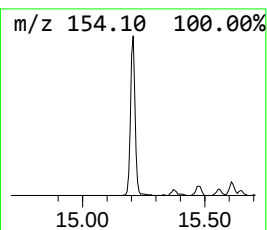
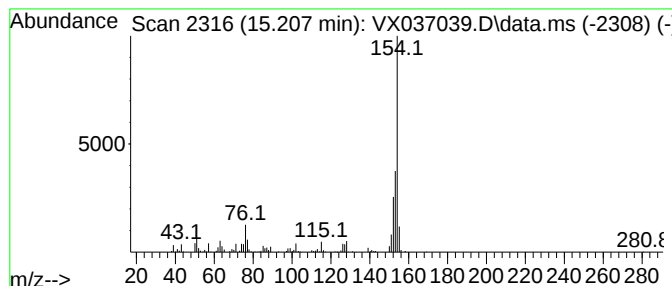
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Quant Title : SW846 8260

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

Peak Number 6 Naphtho[1,2-c]thiophene, 1,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.207	7.01 ug/l	94869	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	95
2			Naphtho[1,2-c]thiophene, 1,3-dih...	202	C12H10OS	031739-49-8	78
3			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	72
4			Naphthalene, 1,4-bis(bromomethyl)-	312	C12H10Br2	058791-49-4	59
5			3-Quinolinecarbonitrile	154	C10H6N2	034846-64-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037039.D
Acq On : 17 Aug 2023 05:12
Operator : JC/MD
Sample : 03958-03 10X
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

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

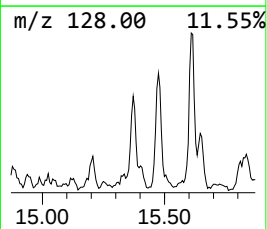
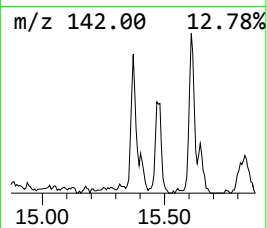
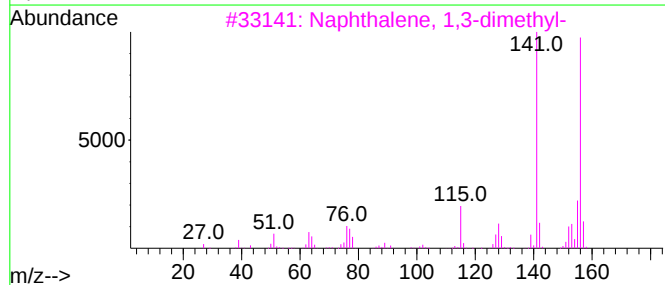
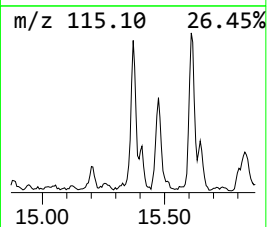
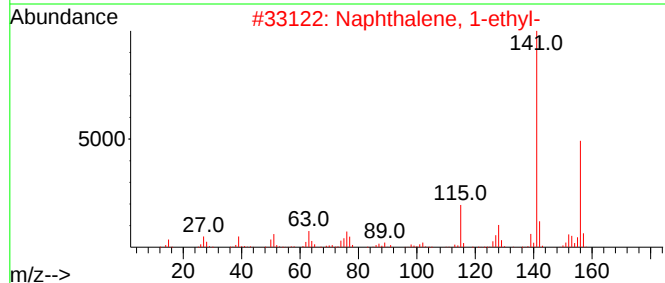
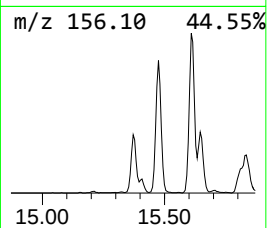
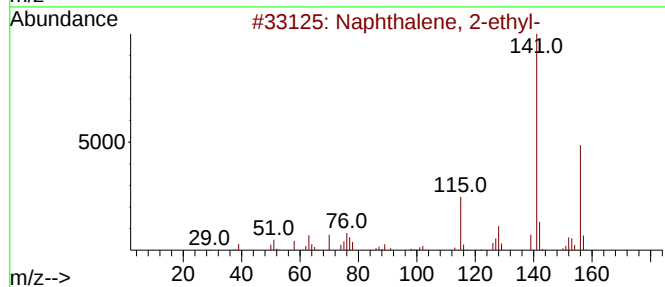
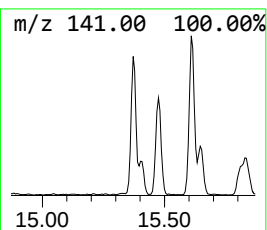
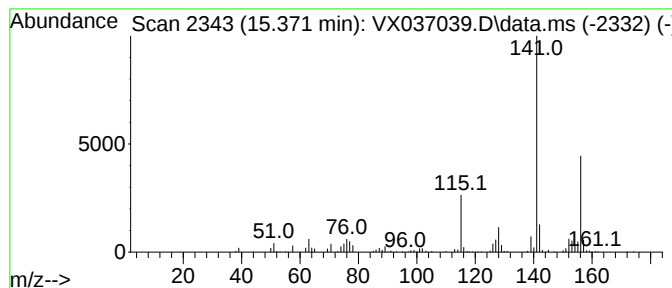
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	9.88 ug/l	133716	1,4-Dichlorobenzene-d4	12.018

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	95
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91
4			Naphthalene, 1-propyl-	170	C13H14	002765-18-6	59
5			2,4-Difluoromesitylene	156	C9H10F2	000392-61-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037039.D
Acq On : 17 Aug 2023 05:12
Operator : JC/MD
Sample : 03958-03 10X
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

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

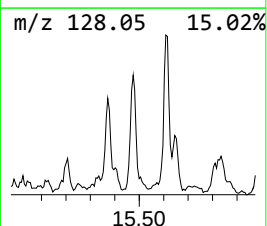
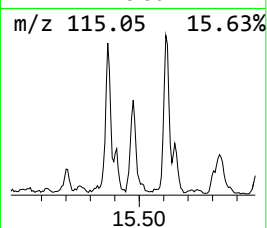
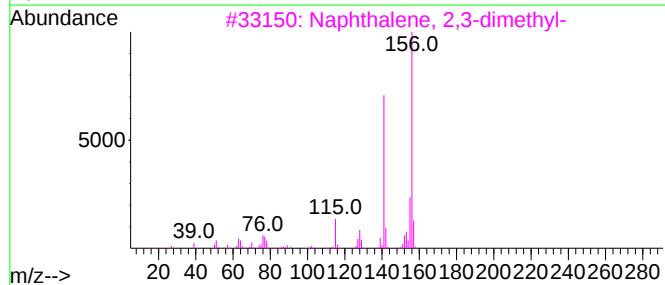
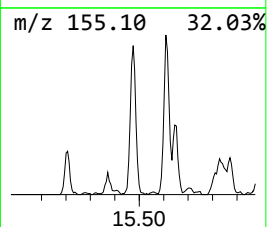
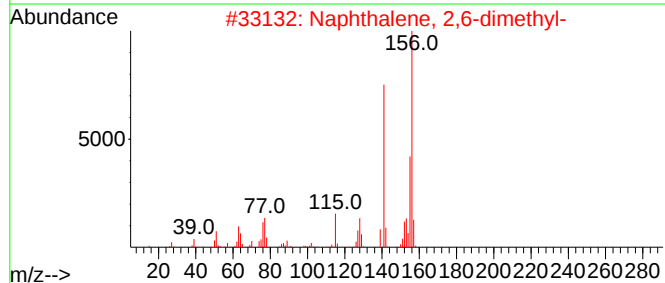
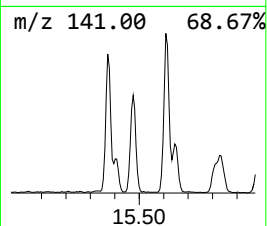
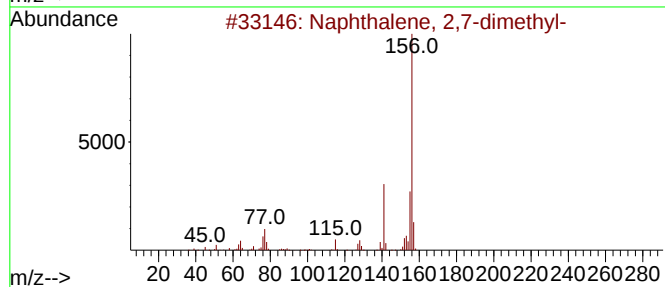
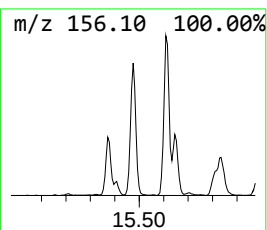
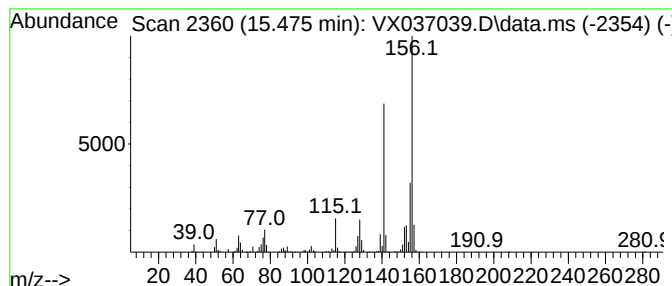
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	12.13 ug/l	164166	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037039.D
Acq On : 17 Aug 2023 05:12
Operator : JC/MD
Sample : 03958-03 10X
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

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

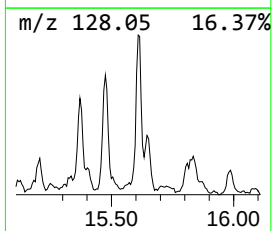
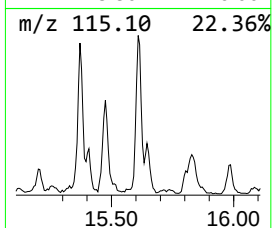
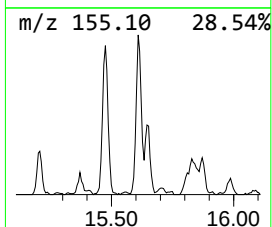
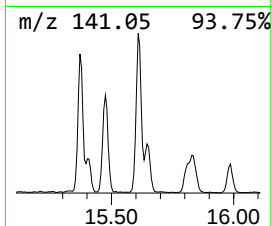
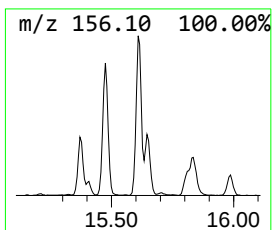
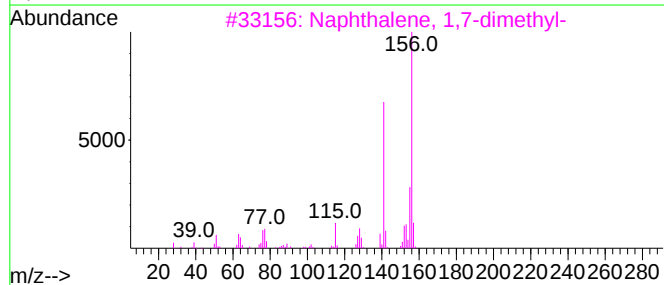
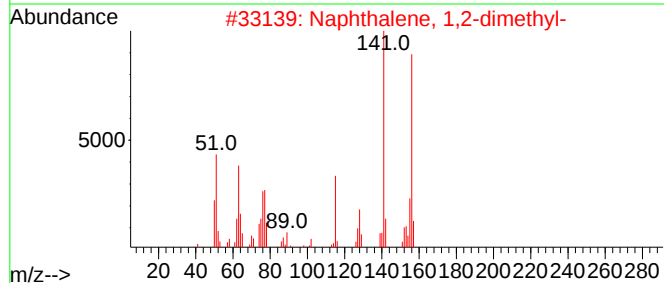
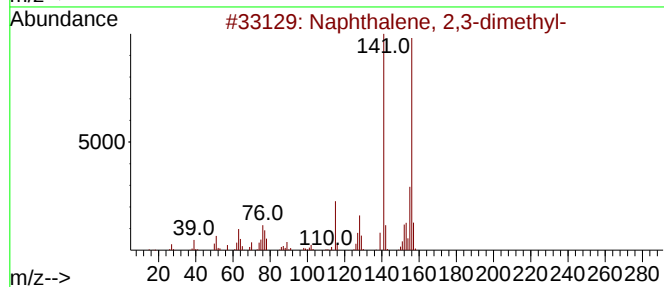
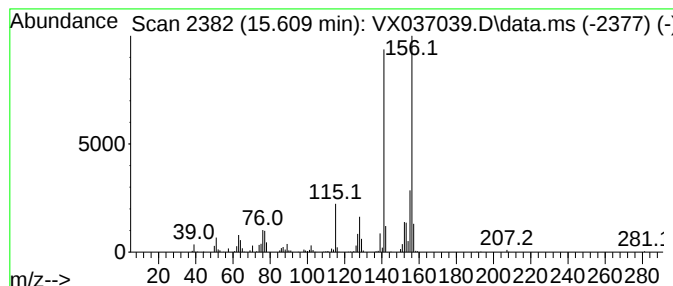
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	15.50 ug/l	209820	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037039.D
Acq On : 17 Aug 2023 05:12
Operator : JC/MD
Sample : 03958-03 10X
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

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

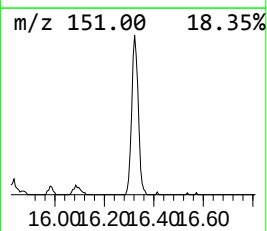
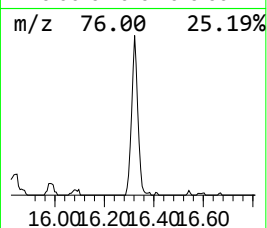
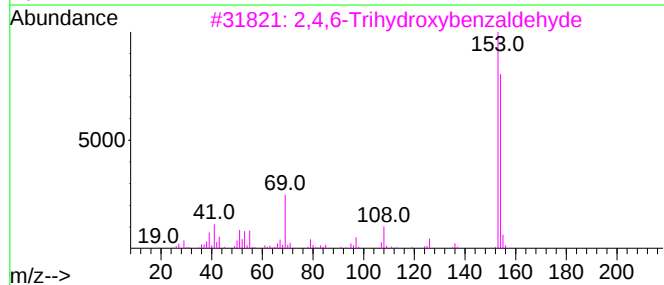
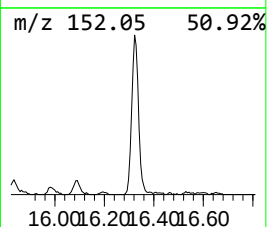
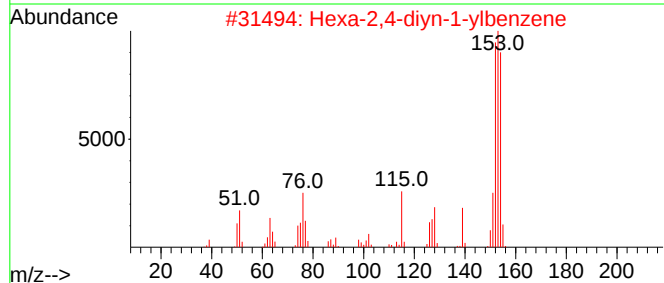
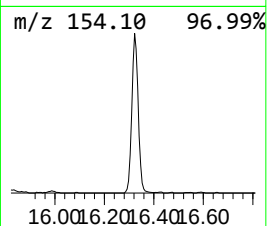
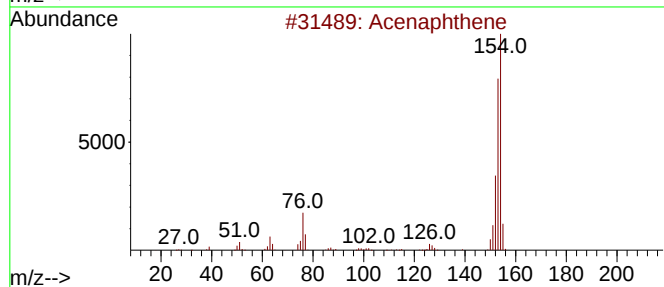
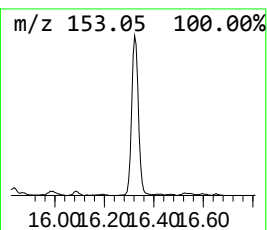
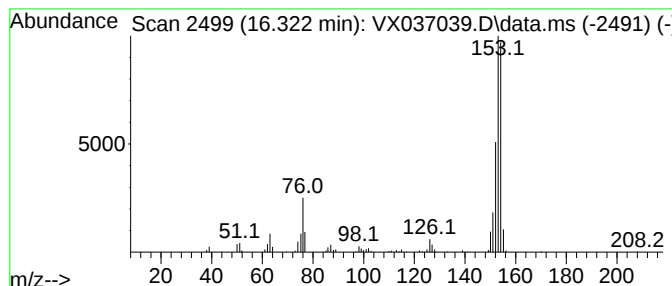
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Quant Title : SW846 8260

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

Peak Number 10 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	12.80 ug/l	173309	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	81
2			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	64
3			2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50
4			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	42
5			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037039.D
Acq On : 17 Aug 2023 05:12
Operator : JC/MD
Sample : 03958-03 10X
Misc : 6.30g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 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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2-Methylindene	13.427	10.6	ug/l	144006	4	12.018	676831	50.0
Azulene	13.774	140.7	ug/l	1904610	4	12.018	676831	50.0
1,4-Methanonaph...	14.634	35.6	ug/l	481527	4	12.018	676831	50.0
Bicyclo[4.4.1]u...	14.780	55.6	ug/l	752792	4	12.018	676831	50.0
Naphtho[1,2-c]t...	15.207	7.0	ug/l	94869	4	12.018	676831	50.0
Naphthalene, 2-...	15.371	9.9	ug/l	133716	4	12.018	676831	50.0
Naphthalene, 2,...	15.475	12.1	ug/l	164166	4	12.018	676831	50.0
Naphthalene, 2,...	15.609	15.5	ug/l	209820	4	12.018	676831	50.0
Hexa-2,4-diyne-1...	16.322	12.8	ug/l	173309	4	12.018	676831	50.0