

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
 Data File : VX037053.D
 Acq On : 17 Aug 2023 10:47
 Operator : JC/MD
 Sample : 03958-07
 Misc : 7.94g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 56 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NEVINS-SB02-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: VX037053.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.031	804	811	825	rVB	222488	585190	1.44%	0.305%
2	6.757	920	930	944	rBV	217374	519433	1.28%	0.271%
3	8.647	1234	1240	1247	rVB	462939	708479	1.75%	0.369%
4	10.055	1467	1471	1476	rVB	506998	648859	1.60%	0.338%
5	10.195	1488	1494	1500	rBV	2506968	3257683	8.03%	1.697%
6	10.299	1503	1511	1517	rVB	835575	1184354	2.92%	0.617%
7	10.640	1562	1567	1577	rBV	610872	807370	1.99%	0.421%
8	10.963	1614	1620	1624	rBV	416034	556833	1.37%	0.290%
9	11.085	1634	1640	1650	rVB2	550492	924056	2.28%	0.481%
10	11.396	1684	1691	1695	rBV	843729	1670603	4.12%	0.870%
11	11.451	1695	1700	1703	rBV	412994	495526	1.22%	0.258%
12	11.616	1722	1727	1734	rVB	798617	1064245	2.62%	0.554%
13	11.750	1745	1749	1755	rVB	1894540	2399051	5.91%	1.250%
14	11.969	1783	1785	1789	rVV	360287	421018	1.04%	0.219%
15	12.024	1789	1794	1800	rVV2	693829	1245537	3.07%	0.649%
16	12.085	1800	1804	1809	rVV	830663	1219079	3.00%	0.635%
17	12.244	1825	1830	1837	rBV	12052588	15560036	38.34%	8.105%
18	12.317	1837	1842	1848	rBV2	1629882	2205351	5.43%	1.149%
19	12.555	1878	1881	1885	rVV	788317	949644	2.34%	0.495%
20	12.616	1886	1891	1894	rVV	1776184	2139084	5.27%	1.114%
21	12.701	1900	1905	1910	rBV	1516778	2244624	5.53%	1.169%
22	12.750	1910	1913	1917	rVV	325465	412611	1.02%	0.215%
23	12.920	1938	1941	1944	rVV	438414	537422	1.32%	0.280%
24	12.963	1944	1948	1954	rVV	976810	1427641	3.52%	0.744%
25	13.048	1954	1962	1967	rVV2	625747	1293626	3.19%	0.674%
26	13.097	1967	1970	1975	rVB	369739	479869	1.18%	0.250%
27	13.170	1977	1982	1986	rVV	3132831	3786974	9.33%	1.973%
28	13.292	1992	2002	2007	rBV2	1962698	3327919	8.20%	1.733%
29	13.341	2007	2010	2014	rVB	1227419	1365738	3.36%	0.711%
30	13.426	2019	2024	2029	rVB	4582302	5959504	14.68%	3.104%
31	13.548	2040	2044	2047	rBV	810869	1125681	2.77%	0.586%
32	13.676	2060	2065	2069	rBV3	772785	1070254	2.64%	0.557%
33	13.786	2076	2083	2088	rVV	24367187	40586688	100.00%	21.141%
34	13.872	2088	2097	2101	rVV	986251	1667864	4.11%	0.869%
35	13.926	2101	2106	2111	rVB3	834356	1245600	3.07%	0.649%
36	14.073	2125	2130	2132	rBV3	519185	753657	1.86%	0.393%

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37	14.097	2132	2134	2137	rVV	652911	655429	1.61%	0.341%
38	14.128	2137	2139	2147	rVB3	432234	829289	2.04%	0.432%
39	14.219	2149	2154	2158	rBV2	1278782	2002182	4.93%	1.043%
40	14.317	2164	2170	2176	rBV	1168500	1976468	4.87%	1.030%
41	14.371	2176	2179	2182	rVV	406045	463491	1.14%	0.241%
42	14.408	2182	2185	2192	rVB3	281597	432078	1.06%	0.225%
43	14.524	2200	2204	2211	rVB3	472936	667135	1.64%	0.348%
44	14.597	2212	2216	2218	rVV	400994	520519	1.28%	0.271%
45	14.646	2218	2224	2233	rVB	19499567	28592494	70.45%	14.894%
46	14.725	2233	2237	2240	rBV	403149	496578	1.22%	0.259%
47	14.786	2240	2247	2255	rVV	13698894	18885522	46.53%	9.837%
48	15.207	2308	2316	2320	rBV	1308425	1822914	4.49%	0.950%
49	15.255	2320	2324	2331	rVB4	287150	567740	1.40%	0.296%
50	15.371	2333	2343	2347	rBV	4560736	6921537	17.05%	3.605%
51	15.408	2347	2349	2354	rVB2	641080	733910	1.81%	0.382%
52	15.475	2354	2360	2365	rBV	3190122	4909776	12.10%	2.557%
53	15.615	2371	2383	2386	rBV	3391003	5504644	13.56%	2.867%
54	15.652	2386	2389	2395	rVB	1803061	2490577	6.14%	1.297%
55	15.835	2410	2419	2431	rVB2	766745	2335673	5.75%	1.217%
56	15.987	2438	2444	2452	rVB	482233	823233	2.03%	0.429%
57	16.085	2455	2460	2469	rVB2	245035	457103	1.13%	0.238%
58	16.322	2485	2499	2511	rBV2	1917689	4043453	9.96%	2.106%

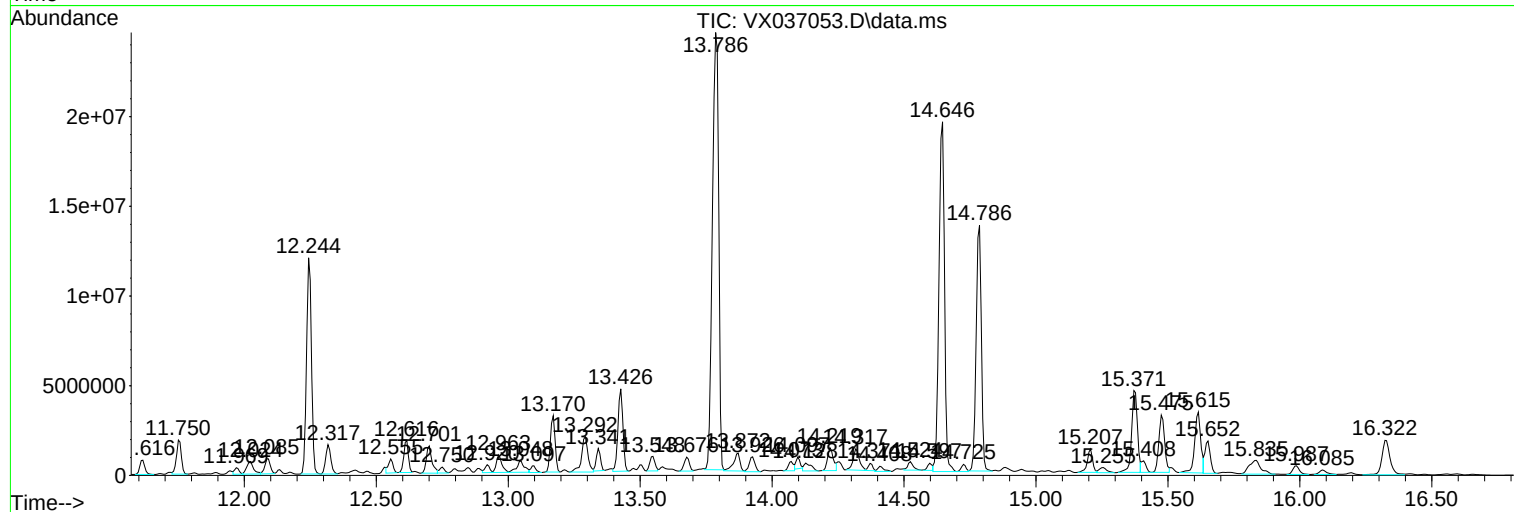
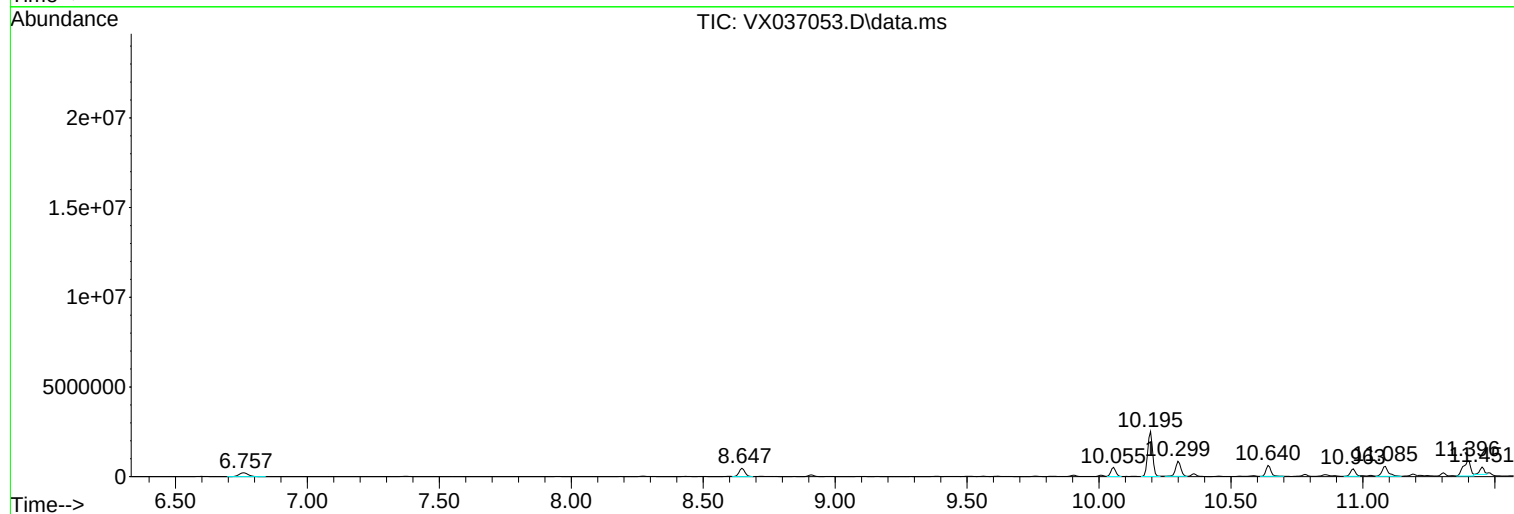
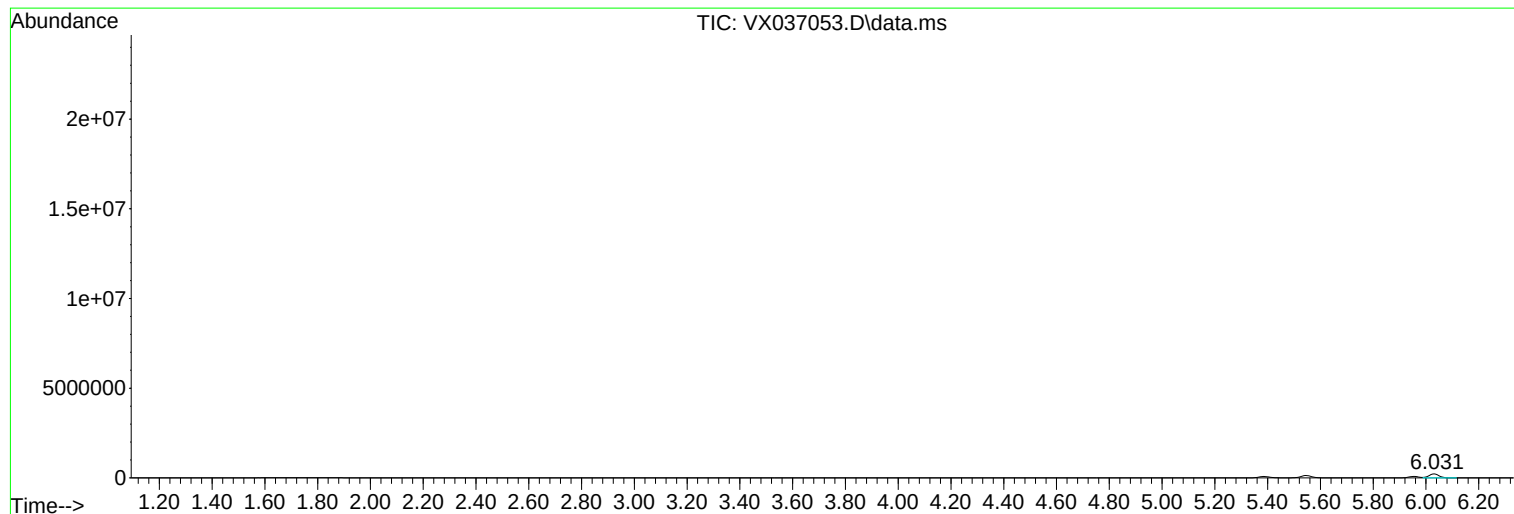
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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z10-12

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



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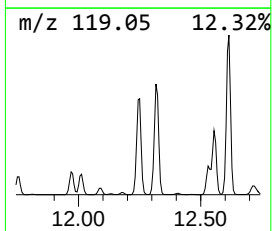
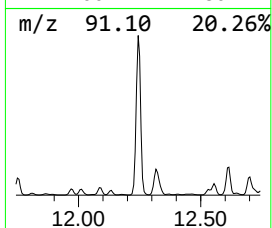
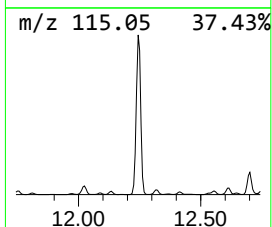
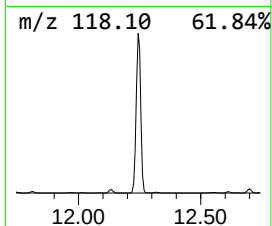
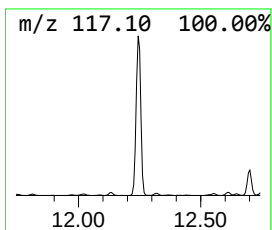
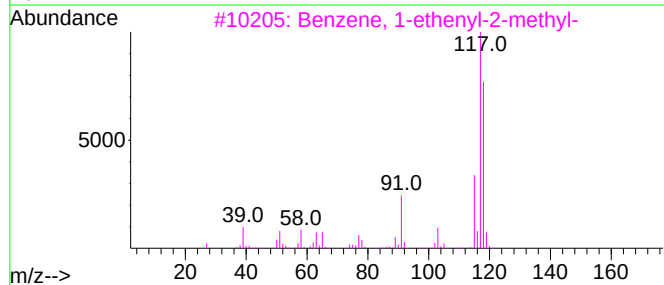
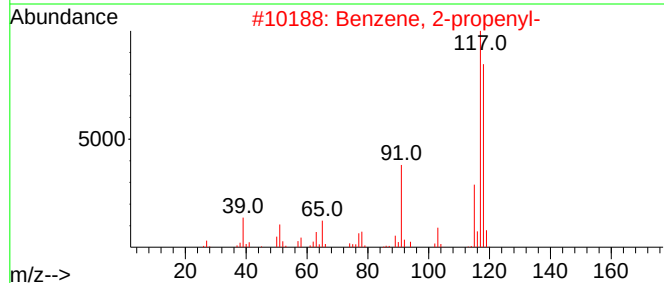
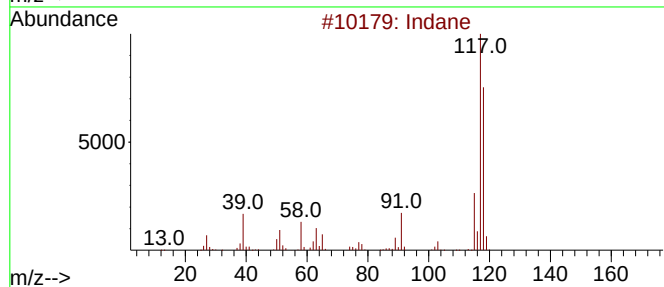
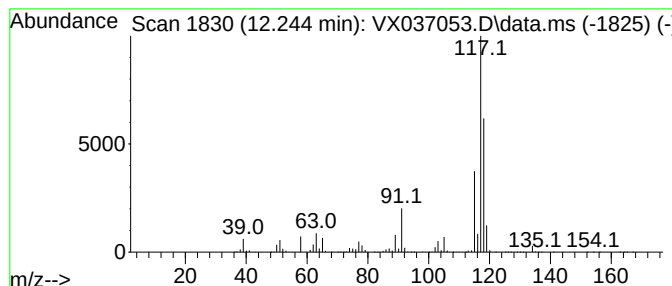
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	624.63 ug/l	15560000	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	81
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64



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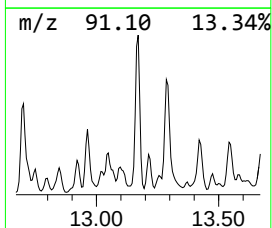
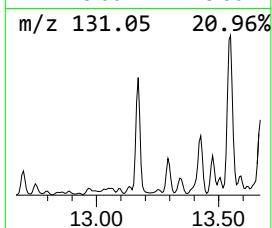
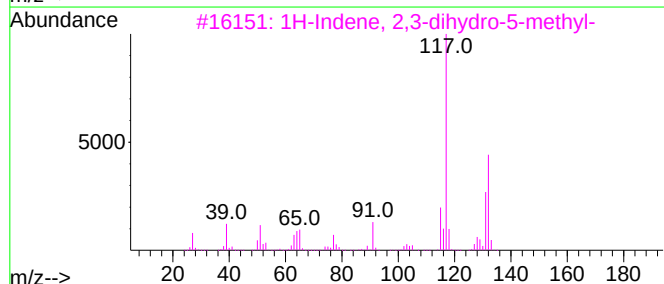
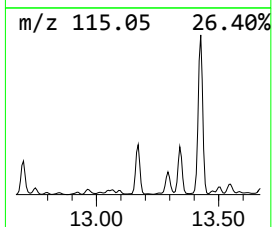
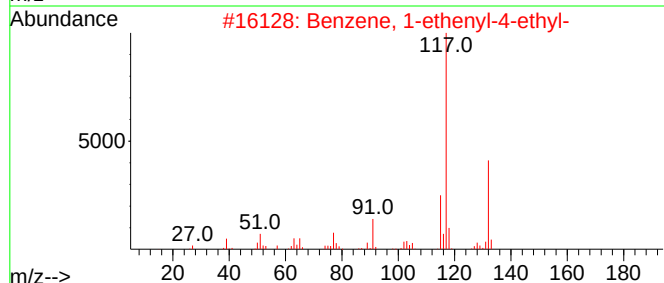
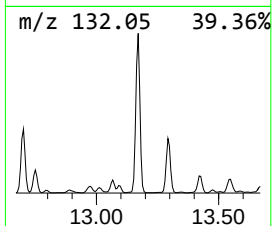
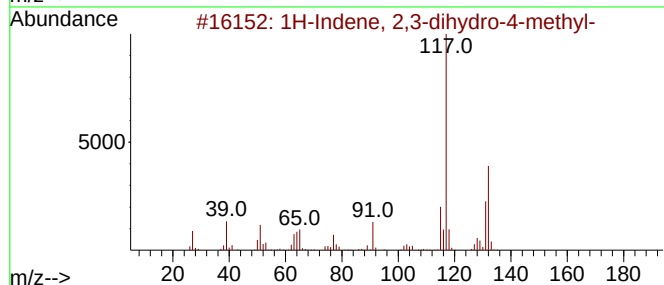
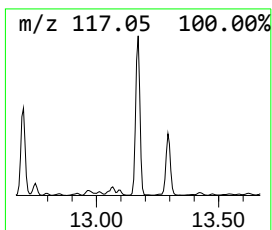
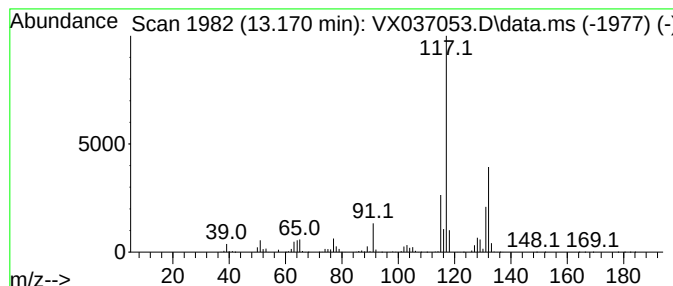
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	152.02 ug/l	3786970	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95	
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94	
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93	
4	Indan, 1-methyl-	132	C10H12	000767-58-8	90	
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90	



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ALS Vial : 56 Sample Multiplier: 1

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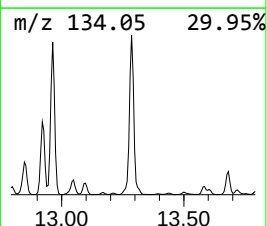
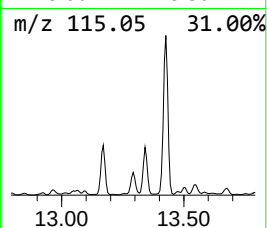
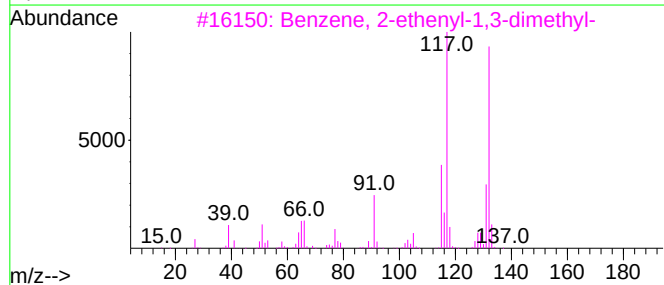
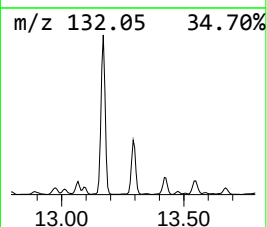
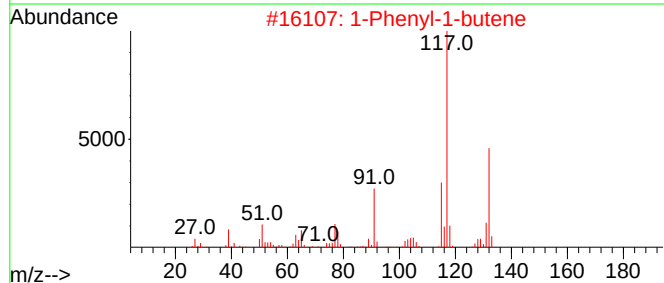
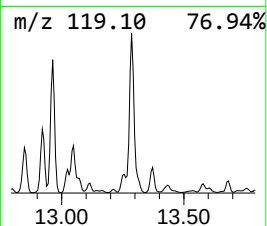
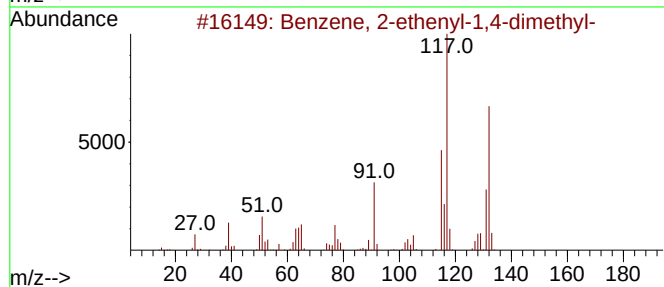
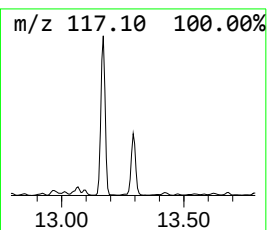
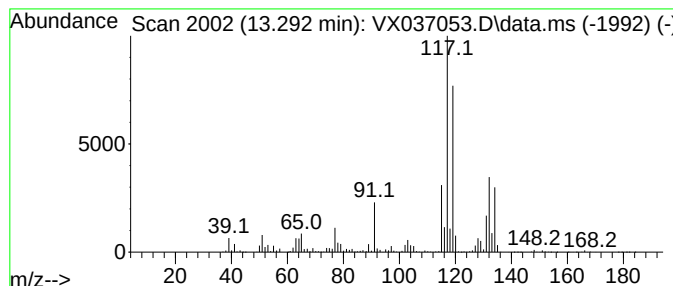
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	133.59 ug/l	3327920	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	94
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	92
3			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	78
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	78
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	60



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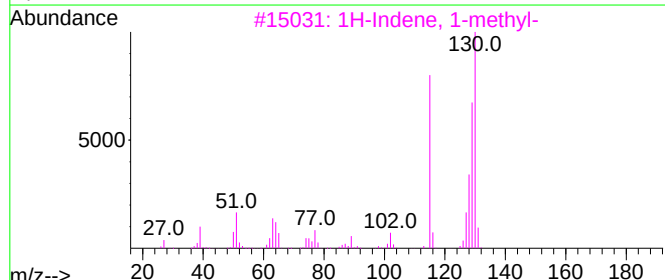
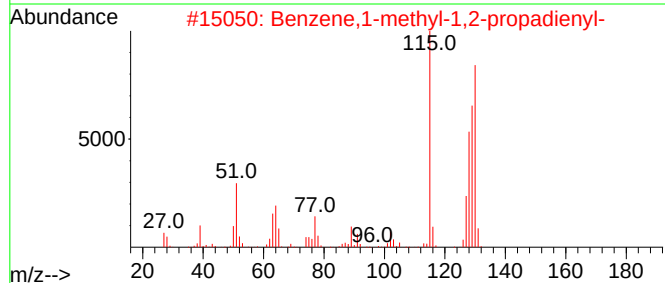
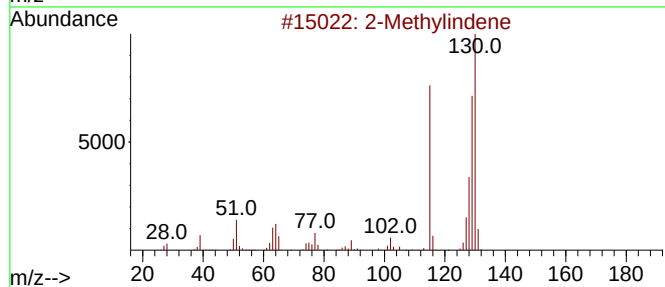
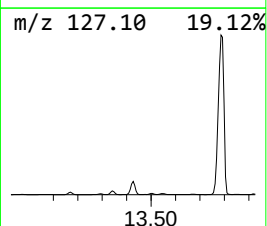
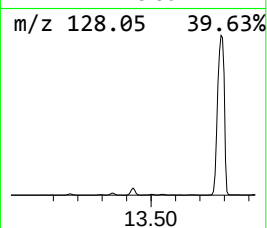
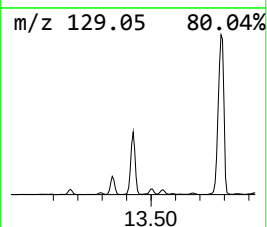
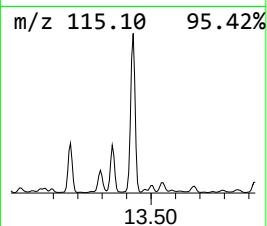
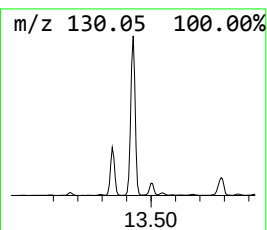
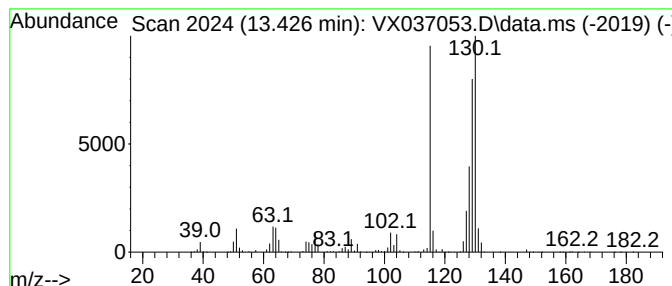
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene,1-methyl-1,2-propad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	239.23 ug/l	5959500	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-1,2-propadienyl-	130	C10H10	022433-39-2	94
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
4			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
5			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	93



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Data File : VX037053.D
Acq On : 17 Aug 2023 10:47
Operator : JC/MD
Sample : 03958-07
Misc : 7.94g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z10-12

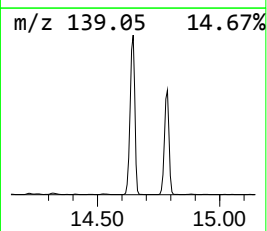
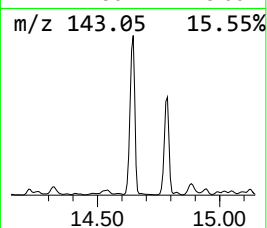
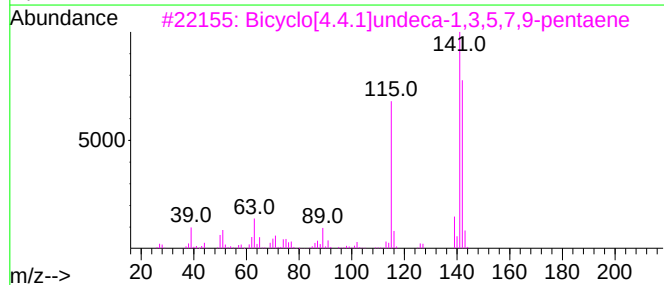
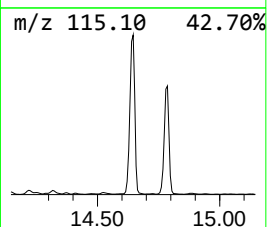
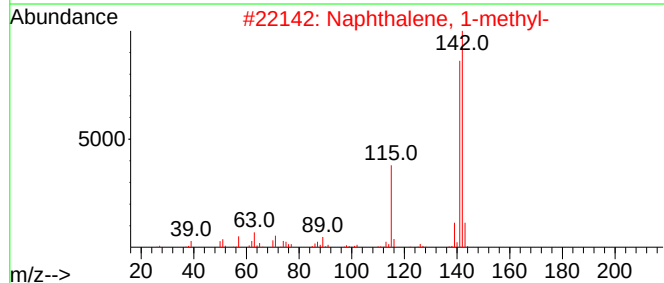
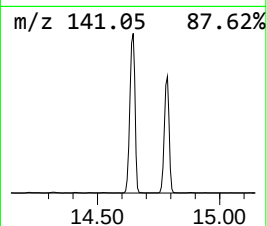
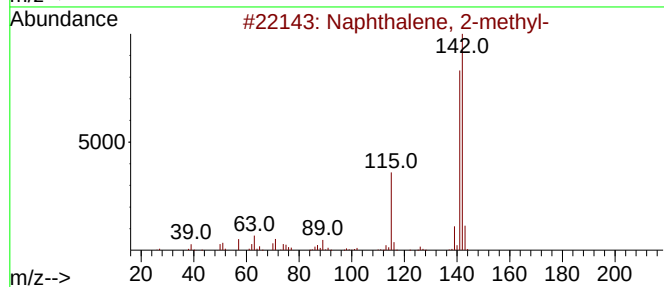
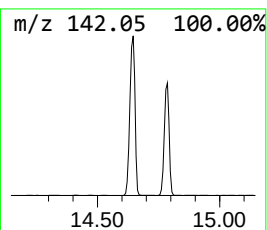
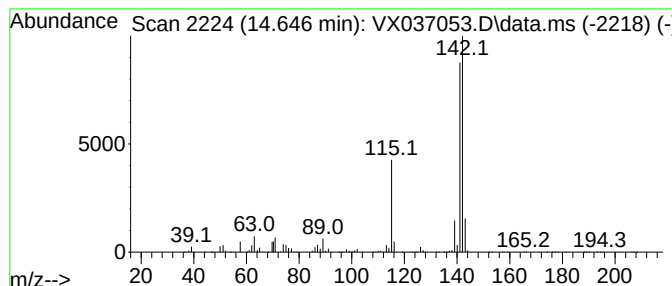
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.646	1147.80 ug/l	28592500	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			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037053.D
Acq On : 17 Aug 2023 10:47
Operator : JC/MD
Sample : 03958-07
Misc : 7.94g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z10-12

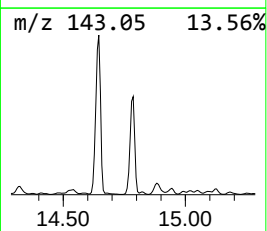
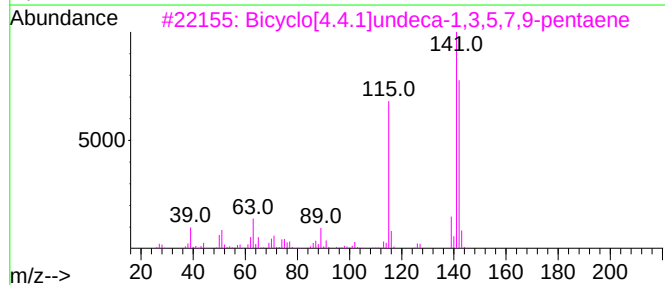
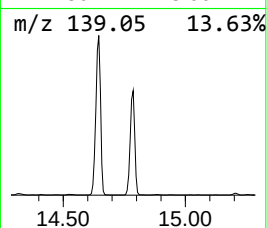
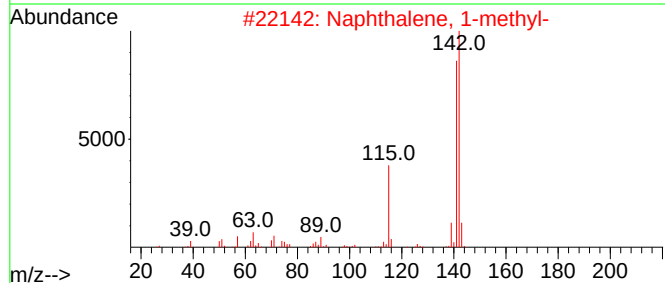
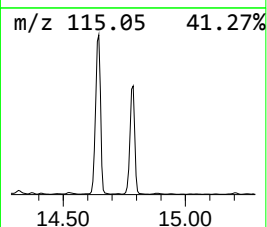
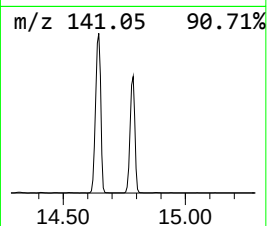
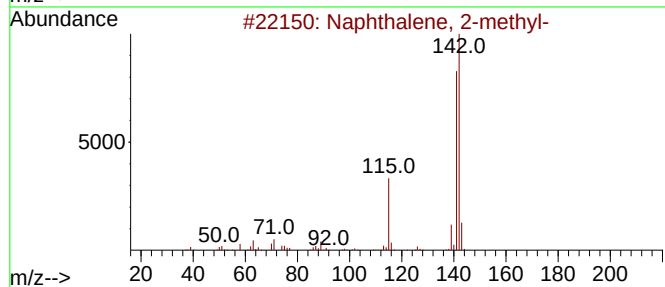
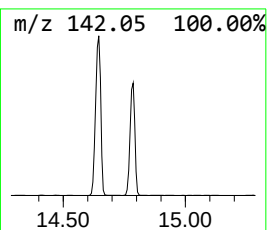
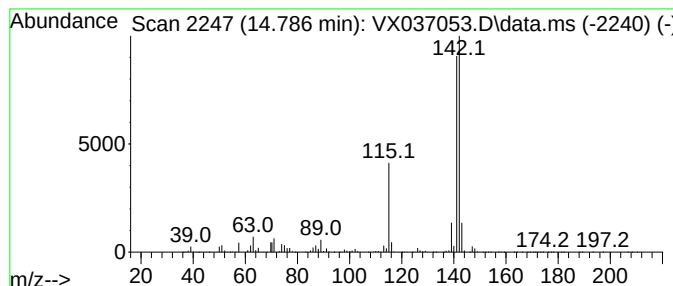
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	758.13 ug/l	18885500	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			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037053.D
Acq On : 17 Aug 2023 10:47
Operator : JC/MD
Sample : 03958-07
Misc : 7.94g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z10-12

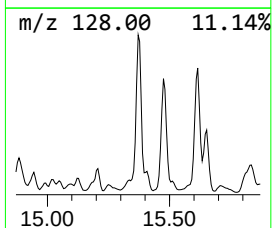
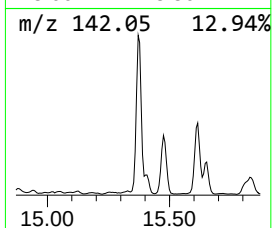
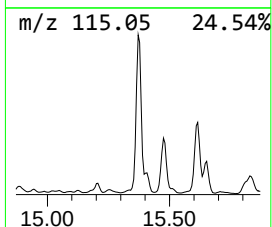
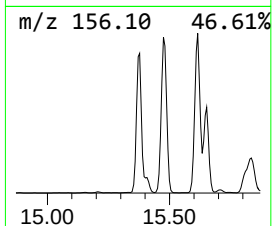
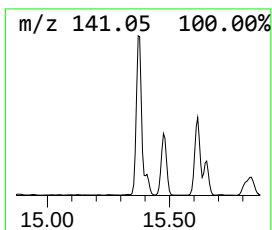
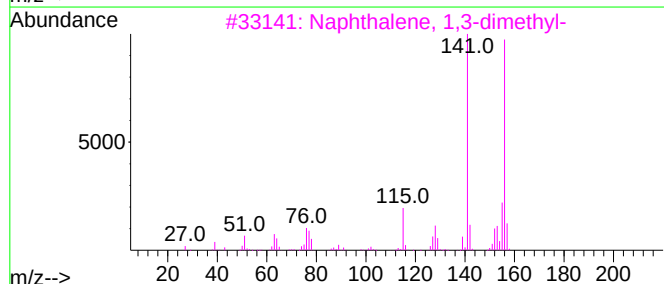
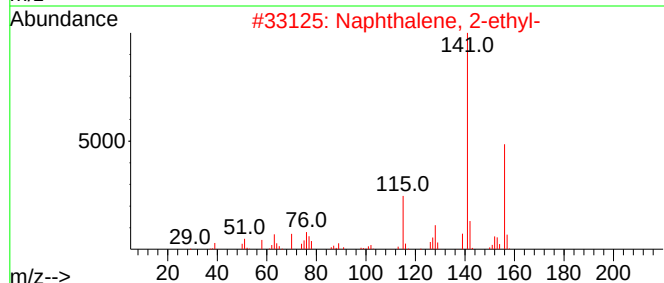
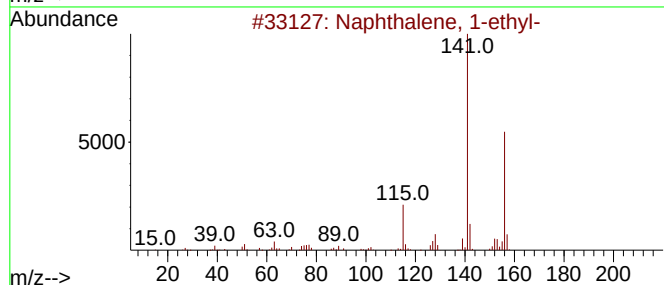
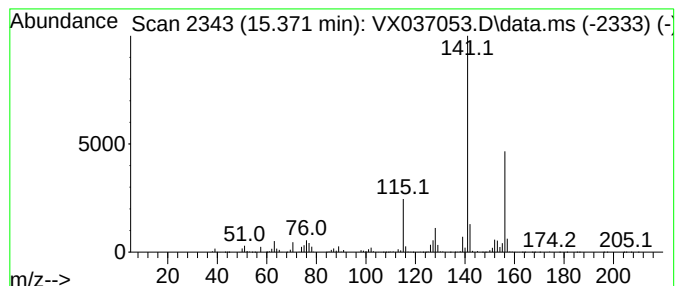
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	277.85 ug/l	6921540	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			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91
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 : VX037053.D
Acq On : 17 Aug 2023 10:47
Operator : JC/MD
Sample : 03958-07
Misc : 7.94g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z10-12

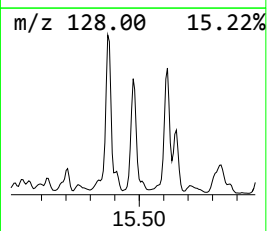
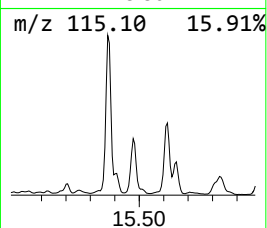
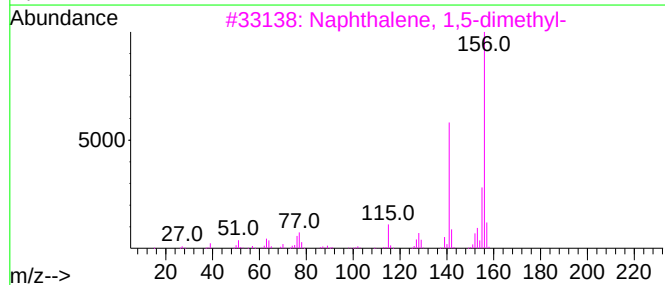
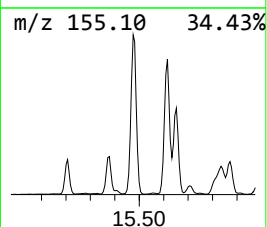
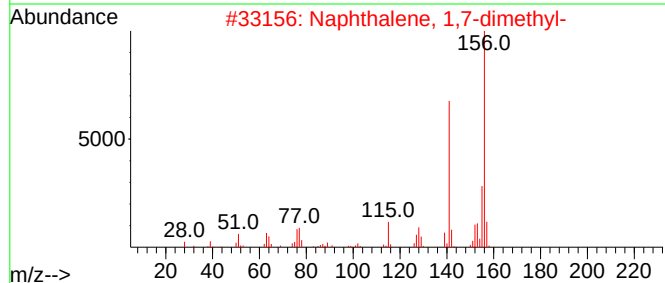
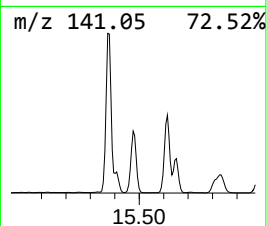
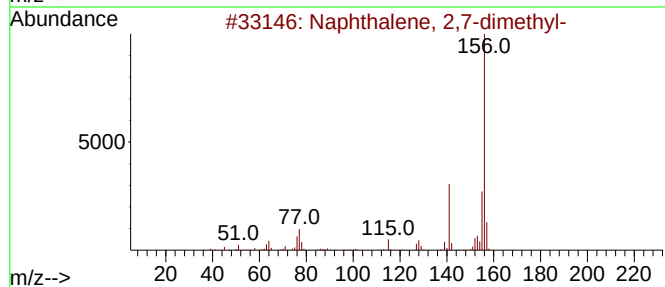
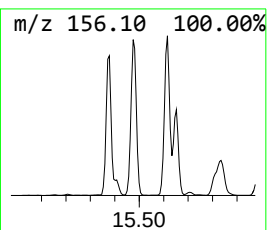
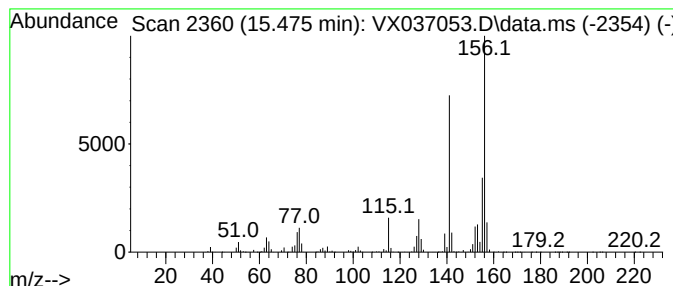
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Quant Title : SW846 8260

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	197.10 ug/l	4909780	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, 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 : VX037053.D
Acq On : 17 Aug 2023 10:47
Operator : JC/MD
Sample : 03958-07
Misc : 7.94g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z10-12

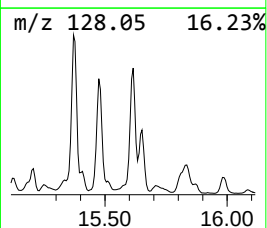
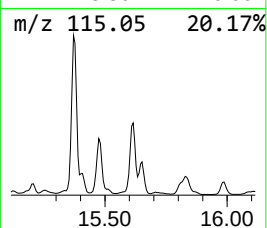
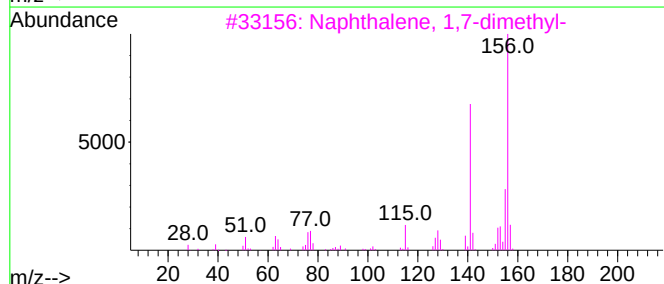
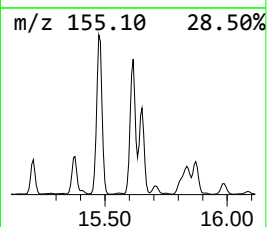
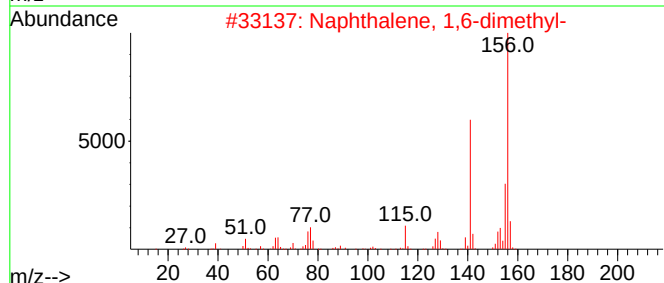
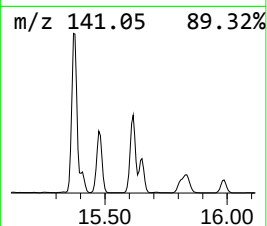
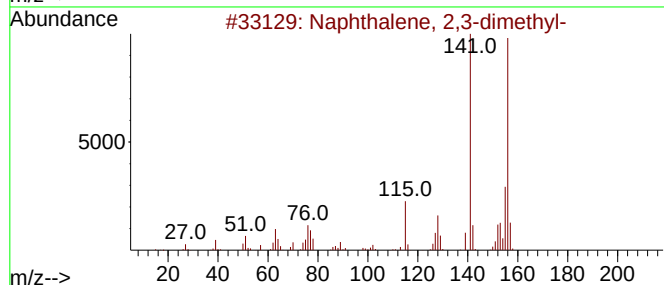
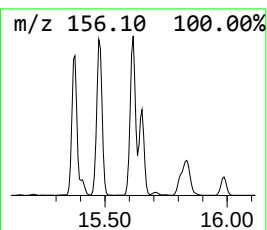
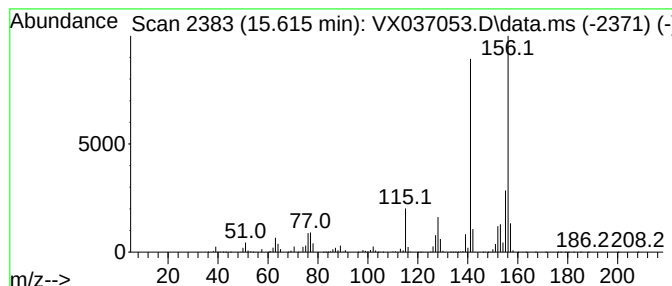
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Quant Title : SW846 8260

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.
15.615	220.97 ug/l	5504640	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, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037053.D
Acq On : 17 Aug 2023 10:47
Operator : JC/MD
Sample : 03958-07
Misc : 7.94g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z10-12

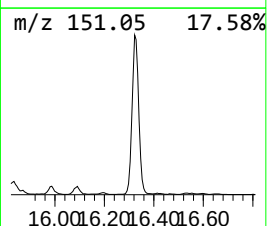
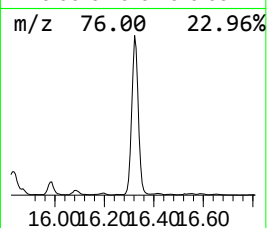
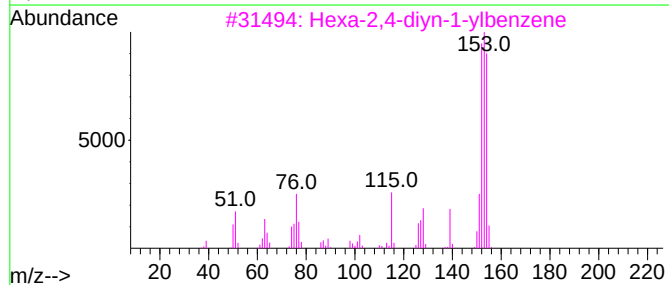
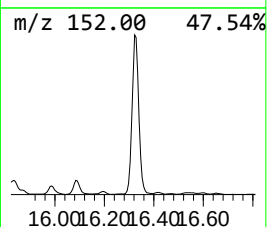
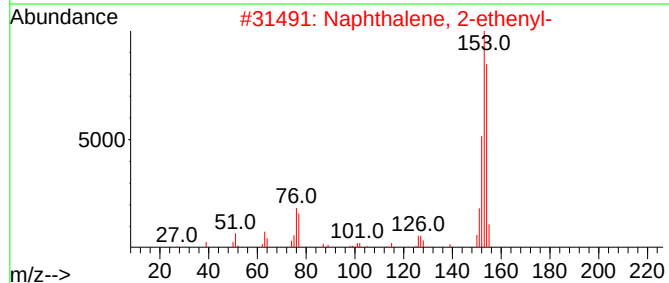
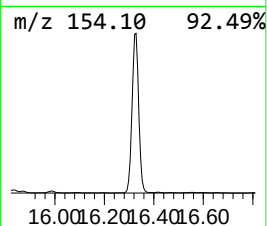
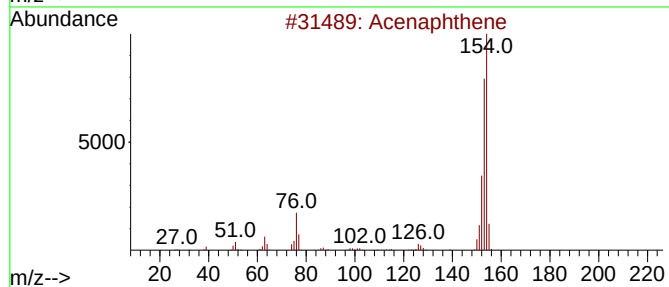
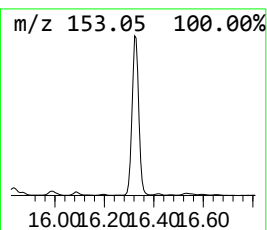
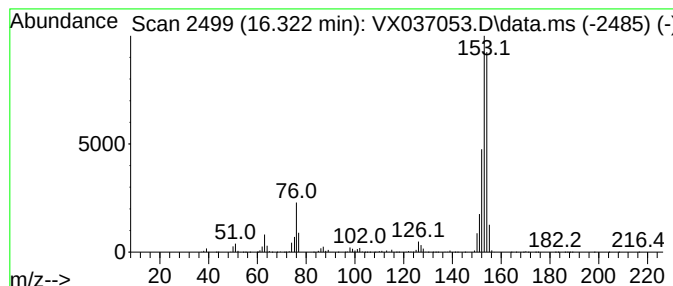
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 2-ethenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	162.32 ug/l	4043450	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	59
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			2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037053.D
Acq On : 17 Aug 2023 10:47
Operator : JC/MD
Sample : 03958-07
Misc : 7.94g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-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
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1H-Indene, 2,3-...	13.170	152.0	ug/l	3786970	4	12.024	1245540	50.0
Benzene, 2-ethe...	13.292	133.6	ug/l	3327920	4	12.024	1245540	50.0
Benzene,1-methy...	13.427	239.2	ug/l	5959500	4	12.024	1245540	50.0
Naphthalene, 1-...	14.646	1147.8	ug/l	28592500	4	12.024	1245540	50.0
Bicyclo[4.4.1]u...	14.786	758.1	ug/l	18885500	4	12.024	1245540	50.0
Naphthalene, 1,...	15.371	277.9	ug/l	6921540	4	12.024	1245540	50.0
Naphthalene, 2,...	15.475	197.1	ug/l	4909780	4	12.024	1245540	50.0
Naphthalene, 2,...	15.615	221.0	ug/l	5504640	4	12.024	1245540	50.0
Naphthalene, 2-...	16.322	162.3	ug/l	4043450	4	12.024	1245540	50.0