

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
 Data File : VX036996.D
 Acq On : 15 Aug 2023 18:32
 Operator : JC/MD
 Sample : 03932-02 10X
 Misc : 5.30g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NEVINS-SB-01-Z20-22

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: VX036996.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.580	560	573	585	rBV	24220	81692	1.53%	0.381%
2	5.385	694	705	717	rBV	80247	236686	4.44%	1.105%
3	5.550	720	732	751	rVB	131104	378419	7.11%	1.767%
4	5.958	788	799	806	rBV	87017	225332	4.23%	1.052%
5	6.037	806	812	824	rVB	30974	85909	1.61%	0.401%
6	6.763	921	931	944	rBV	216557	517623	9.72%	2.417%
7	8.647	1235	1240	1250	rVB	451132	708292	13.30%	3.307%
8	10.055	1466	1471	1477	rBV	477481	626448	11.76%	2.925%
9	10.195	1488	1494	1500	rBV	292353	384095	7.21%	1.793%
10	10.963	1613	1620	1624	rBV	47830	65897	1.24%	0.308%
11	11.079	1634	1639	1650	rVB	412710	555862	10.44%	2.595%
12	11.402	1685	1692	1695	rBV	56169	82141	1.54%	0.384%
13	11.451	1695	1700	1704	rVV	64814	83420	1.57%	0.389%
14	11.610	1722	1726	1734	rVB	98460	133739	2.51%	0.624%
15	11.750	1745	1749	1757	rVB	236815	298174	5.60%	1.392%
16	12.018	1788	1793	1800	rBV	489800	675594	12.69%	3.154%
17	12.085	1800	1804	1809	rVV	97115	139209	2.61%	0.650%
18	12.244	1824	1830	1837	rBV	1278543	1628467	30.58%	7.603%
19	12.317	1837	1842	1848	rVV2	158200	217930	4.09%	1.017%
20	12.555	1878	1881	1885	rVB	59174	62279	1.17%	0.291%
21	12.609	1886	1890	1894	rVB	122435	145779	2.74%	0.681%
22	12.695	1899	1904	1911	rBV	102903	179095	3.36%	0.836%
23	12.890	1932	1936	1939	rBV3	35901	60390	1.13%	0.282%
24	12.963	1944	1948	1954	rVB2	86281	141717	2.66%	0.662%
25	13.042	1954	1961	1967	rBV4	49897	93634	1.76%	0.437%
26	13.170	1974	1982	1986	rBV	189094	252223	4.74%	1.178%
27	13.292	1992	2002	2007	rBV2	206252	355943	6.68%	1.662%
28	13.341	2007	2010	2014	rVV	144234	158530	2.98%	0.740%
29	13.384	2014	2017	2020	rVV2	63261	72840	1.37%	0.340%
30	13.426	2020	2024	2029	rVB	351120	456703	8.58%	2.132%
31	13.542	2040	2043	2047	rBV	55595	70983	1.33%	0.331%
32	13.676	2060	2065	2068	rBV3	55734	88995	1.67%	0.416%
33	13.774	2076	2081	2088	rVB	4203899	5324912	100.00%	24.861%
34	13.841	2088	2092	2094	rVV3	60348	87810	1.65%	0.410%
35	13.865	2094	2096	2100	rVV	54095	63327	1.19%	0.296%
36	13.920	2100	2105	2110	rVB5	51416	92479	1.74%	0.432%

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37	14.073	2126	2130	2132	rBV2	44201	58312	1.10%	0.272%
38	14.097	2132	2134	2137	rVV2	58324	64863	1.22%	0.303%
39	14.127	2137	2139	2146	rVB4	37309	57536	1.08%	0.269%
40	14.219	2150	2154	2158	rBV3	70105	92522	1.74%	0.432%
41	14.316	2164	2170	2176	rBV	71344	119005	2.23%	0.556%
42	14.633	2214	2222	2233	rVB	1783990	2392008	44.92%	11.168%
43	14.780	2240	2246	2254	rBV	1118015	1433290	26.92%	6.692%
44	15.206	2308	2316	2320	rBV2	129940	199150	3.74%	0.930%
45	15.371	2338	2343	2347	rBV	282908	392017	7.36%	1.830%
46	15.475	2355	2360	2365	rBV	226172	342098	6.42%	1.597%
47	15.615	2377	2383	2386	rBV	271736	429870	8.07%	2.007%
48	15.645	2386	2388	2395	rVB	151157	219226	4.12%	1.024%
49	15.834	2410	2419	2429	rVB2	72720	213824	4.02%	0.998%
50	15.987	2439	2444	2453	rVB	50156	90699	1.70%	0.423%
51	16.084	2455	2460	2467	rBV	32138	57305	1.08%	0.268%
52	16.322	2491	2499	2511	rBV2	195181	424030	7.96%	1.980%

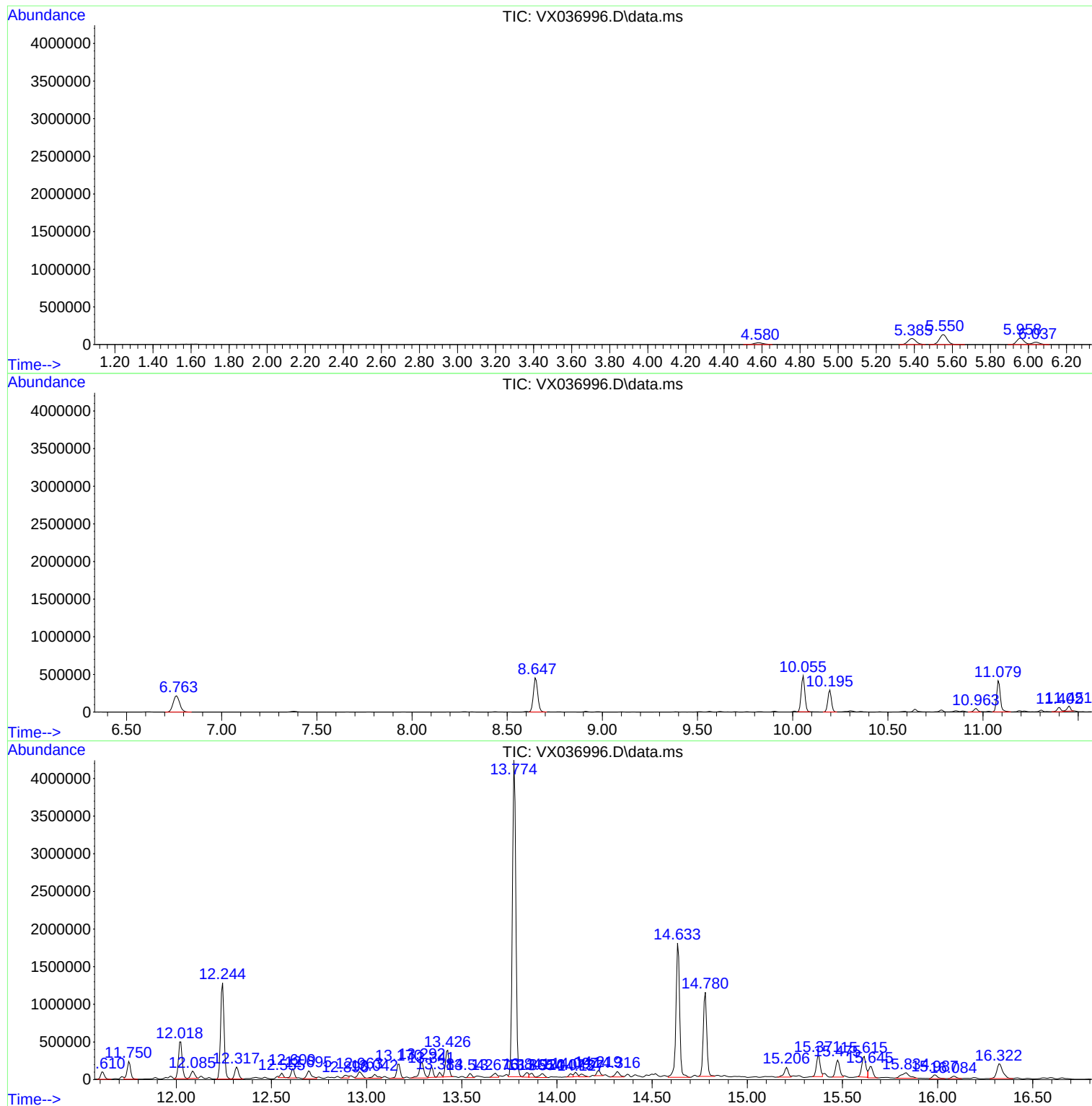
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Quant Title : SW846 8260

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



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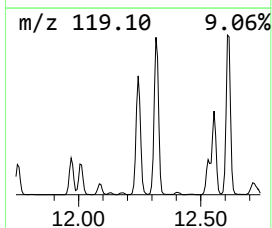
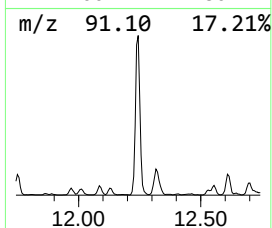
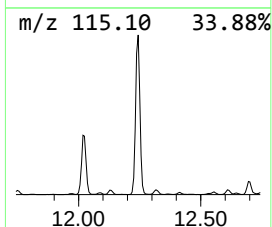
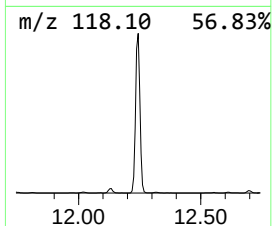
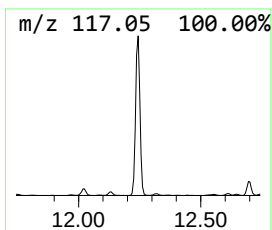
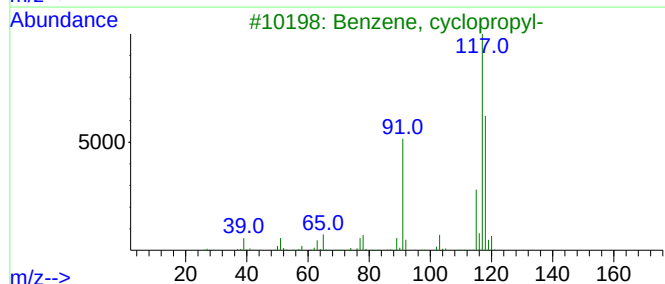
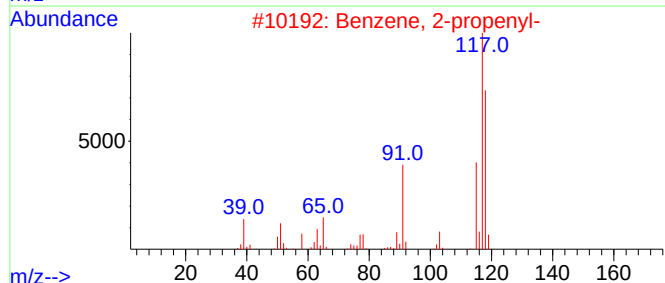
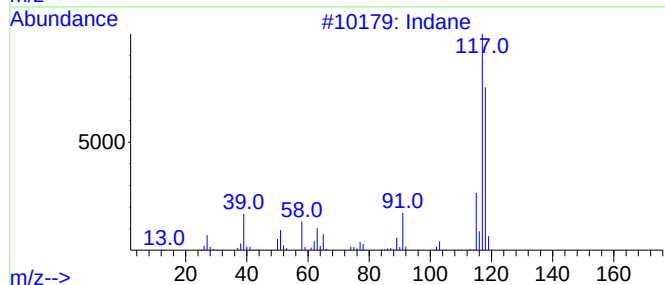
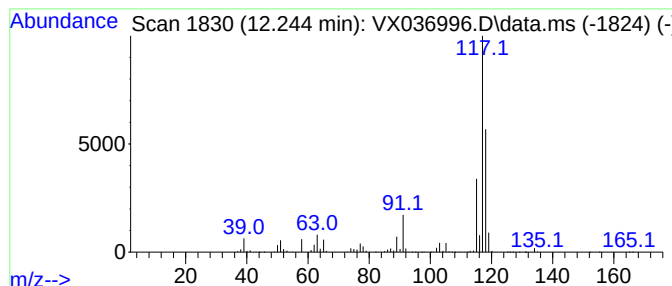
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	120.52 ug/l	1628470	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	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	80
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Deltacyclene	118	C9H10	007785-10-6	64



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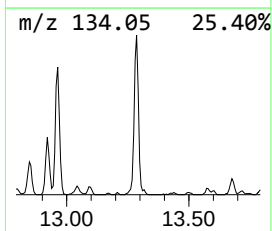
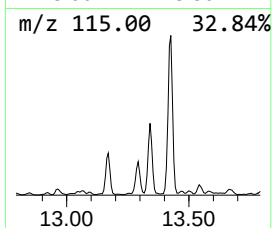
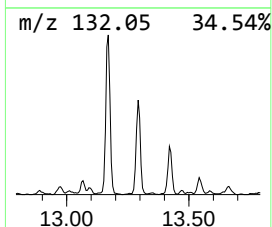
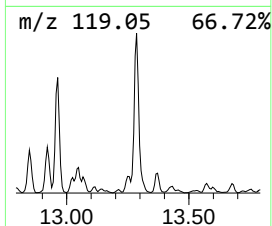
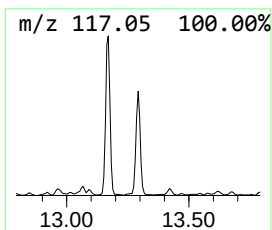
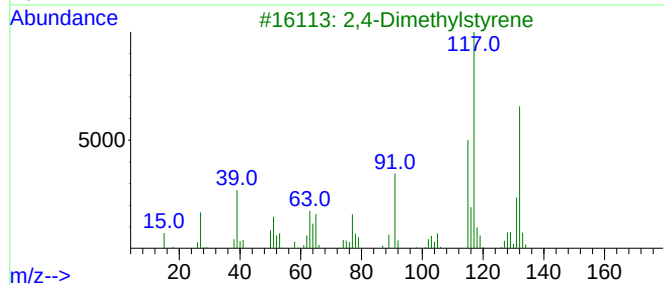
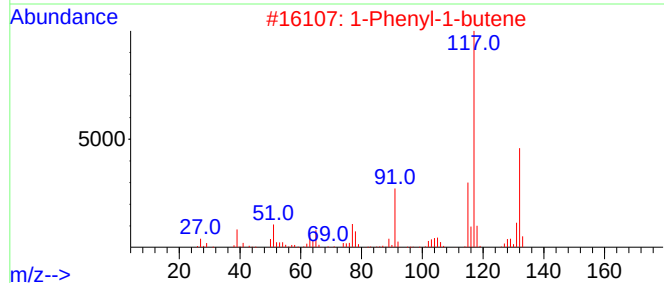
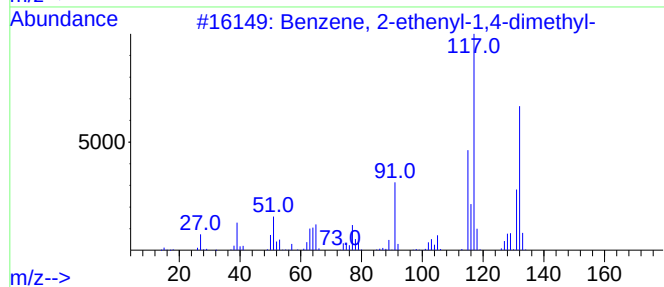
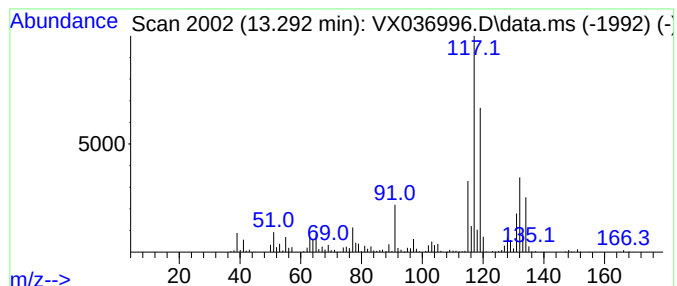
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	26.34 ug/l	355943	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	95
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	95
3			2,4-Dimethylstyrene	132	C10H12	002234-20-0	87
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70



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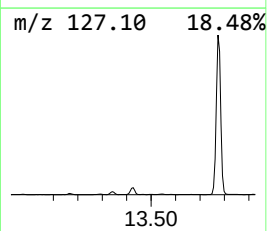
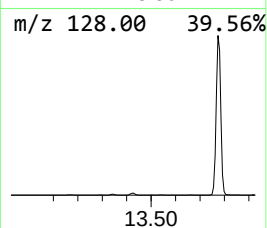
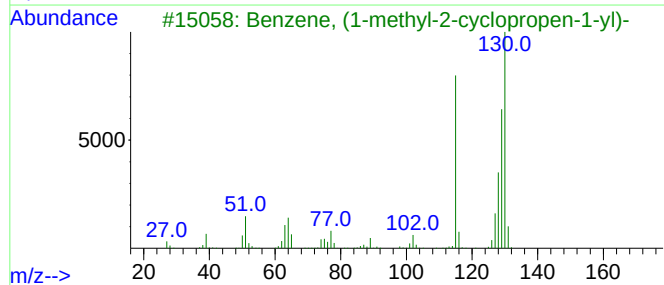
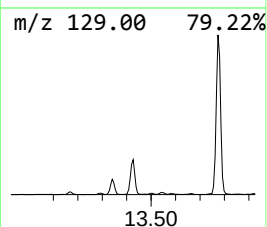
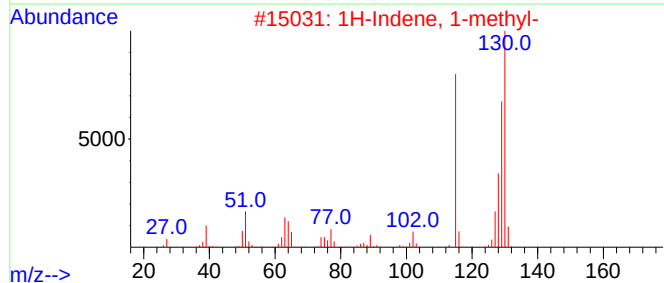
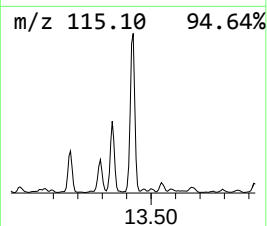
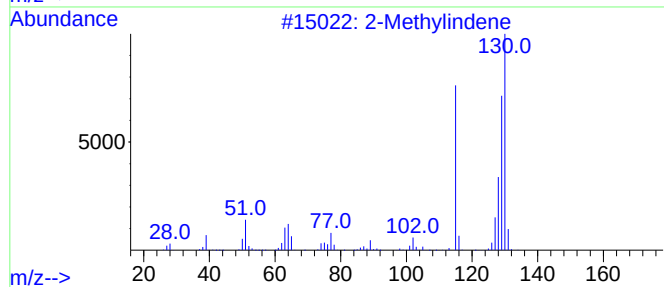
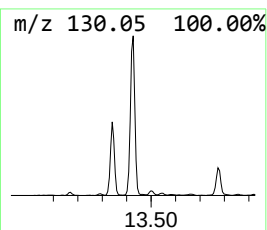
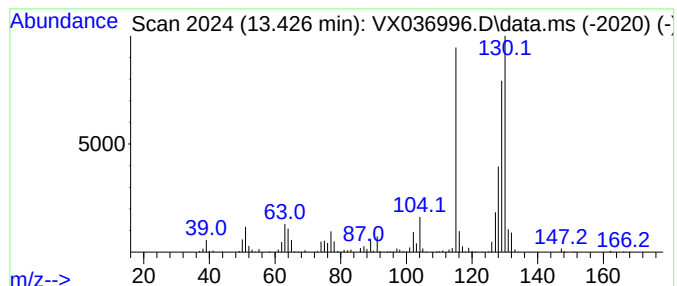
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Quant Title : SW846 8260

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

Peak Number 3 2-Methylindene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	33.80 ug/l	456703	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindene	130	C10H10	002177-47-1	96
2			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
3			Benzene, (1-methyl-2-cyclopropen-1-yl)-	130	C10H10	065051-83-4	94
4			Benzene, 1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93
5			1H-Indene, 3-methyl-	130	C10H10	000767-60-2	93



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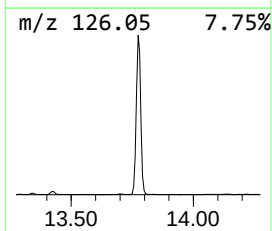
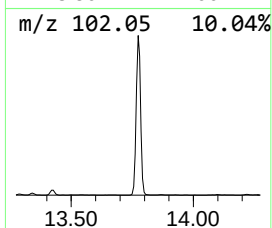
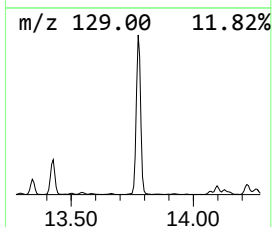
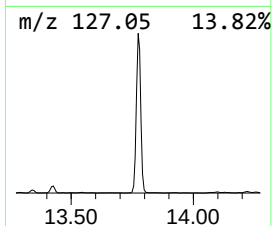
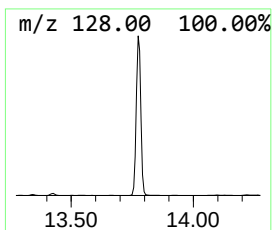
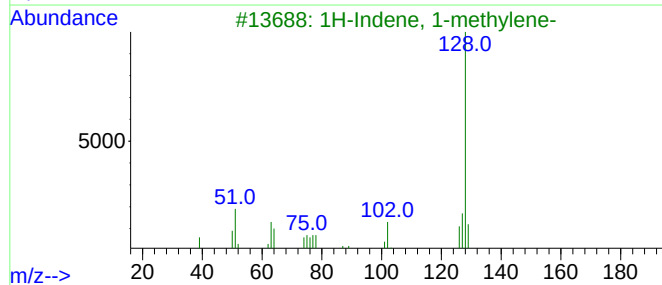
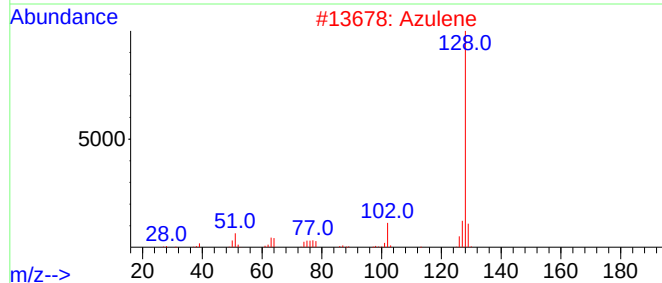
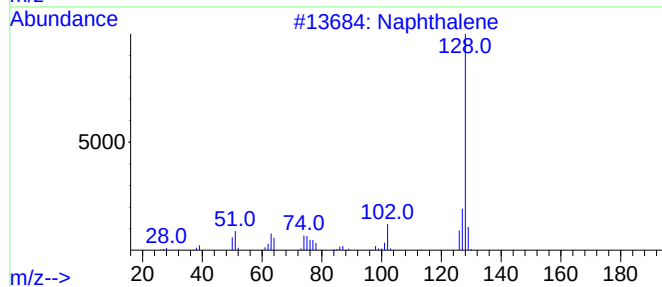
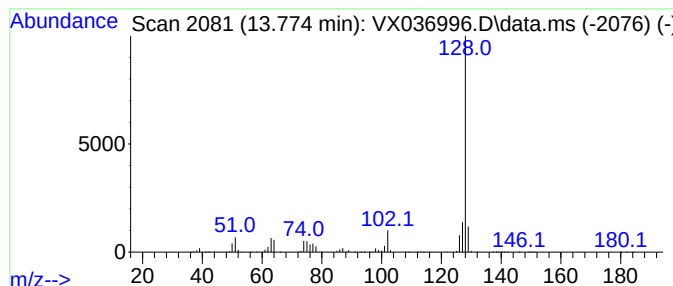
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Quant Title : SW846 8260

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

Peak Number 4 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	394.09 ug/l	5324910	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Azulene	128	C10H8	000275-51-4	94
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	83
4			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	50
5			1H-Cyclopenta[c]thiophene, hexah...	128	C7H12S	053907-80-5	47



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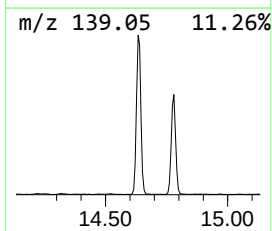
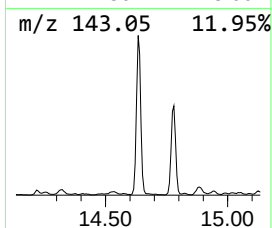
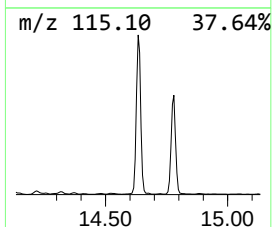
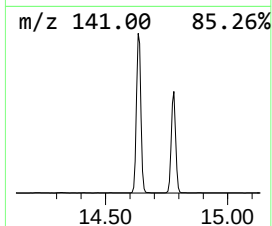
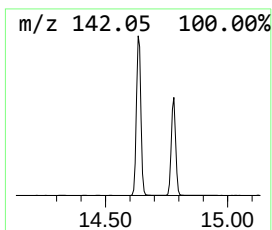
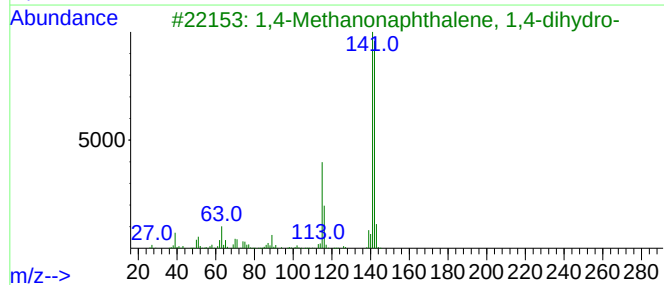
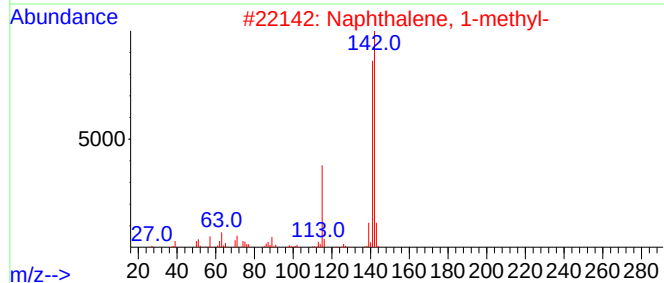
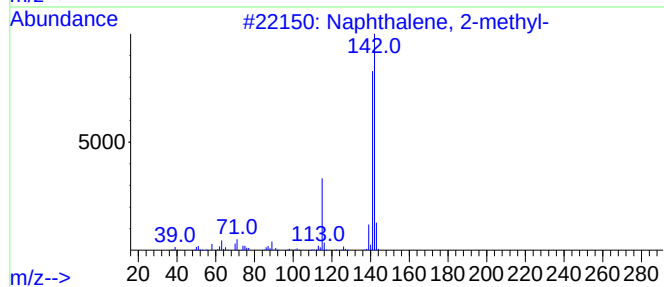
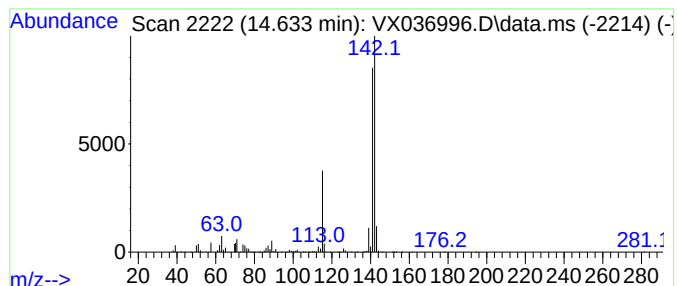
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Quant Title : SW846 8260

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

Peak Number 5 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	177.03 ug/l	2392010	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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX036996.D
Acq On : 15 Aug 2023 18:32
Operator : JC/MD
Sample : 03932-02 10X
Misc : 5.30g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z20-22

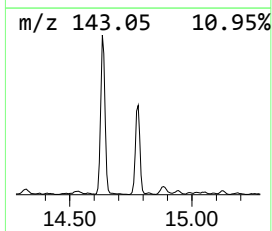
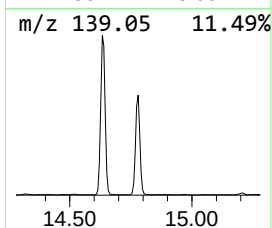
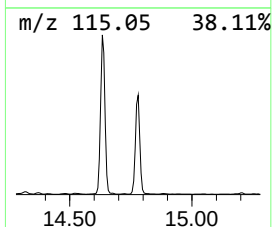
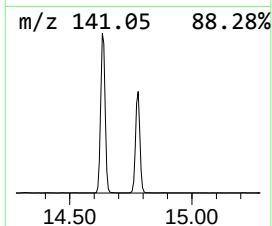
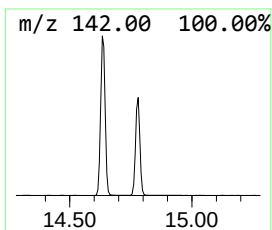
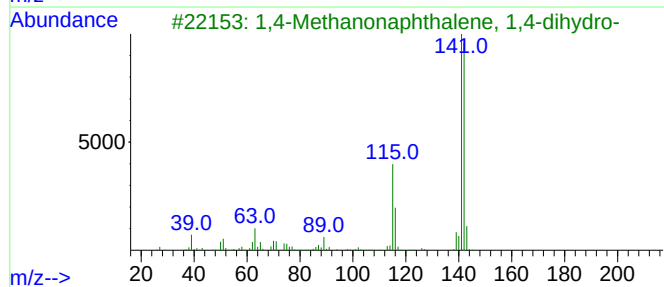
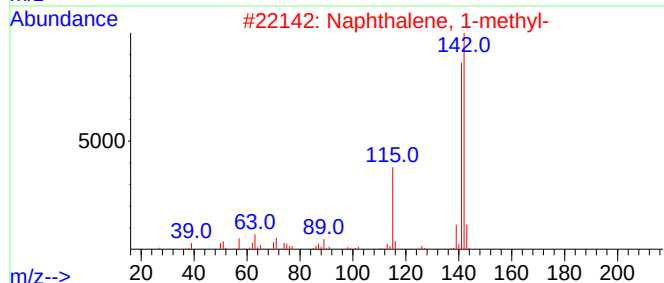
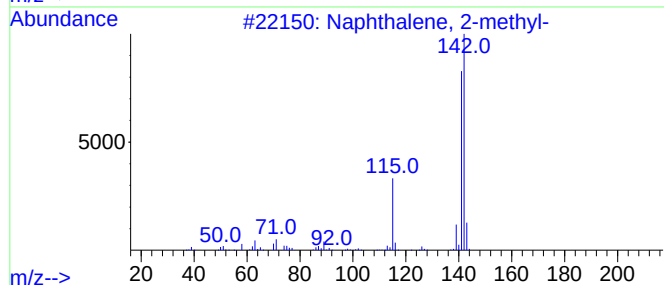
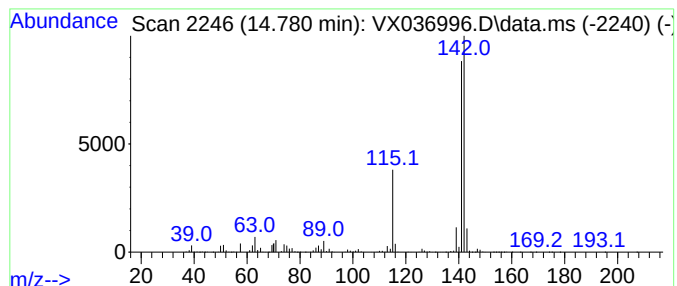
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Quant Title : SW846 8260

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

Peak Number 6 Benzocycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	106.08 ug/l	1433290	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX036996.D
Acq On : 15 Aug 2023 18:32
Operator : JC/MD
Sample : 03932-02 10X
Misc : 5.30g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z20-22

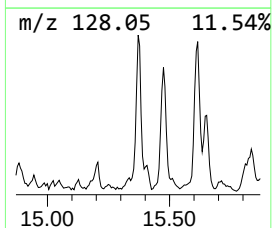
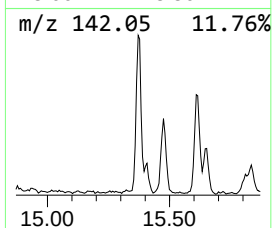
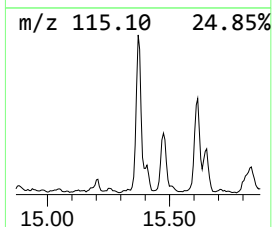
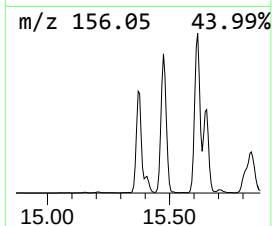
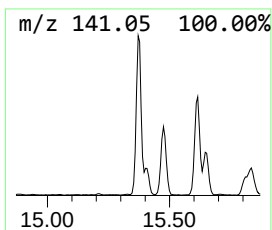
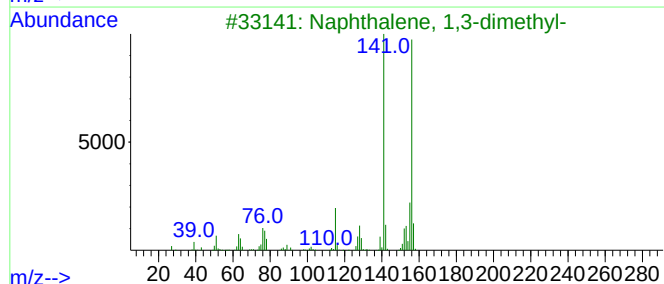
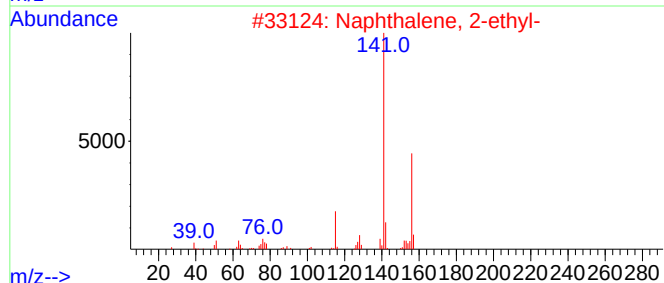
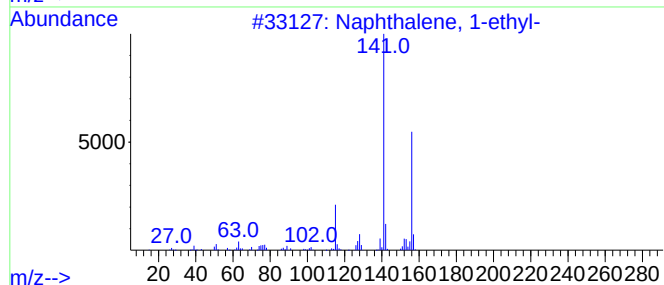
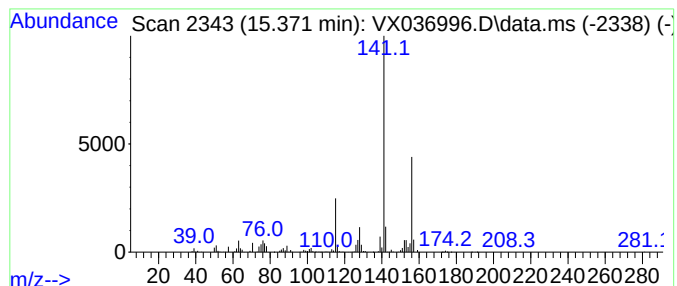
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	29.01 ug/l	392017	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	95
2			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	95
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	58
5			5-Acetyl-2-amino-4-methylthiazole	156	C6H8N2OS	030748-47-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX036996.D
Acq On : 15 Aug 2023 18:32
Operator : JC/MD
Sample : 03932-02 10X
Misc : 5.30g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z20-22

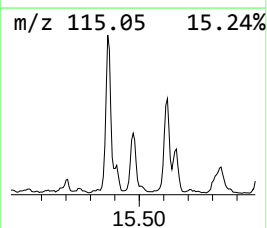
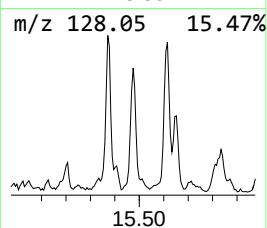
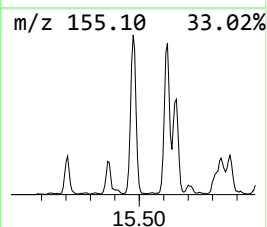
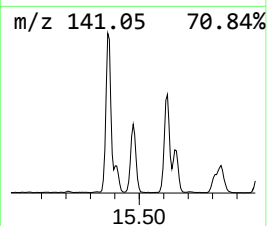
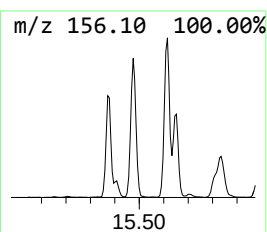
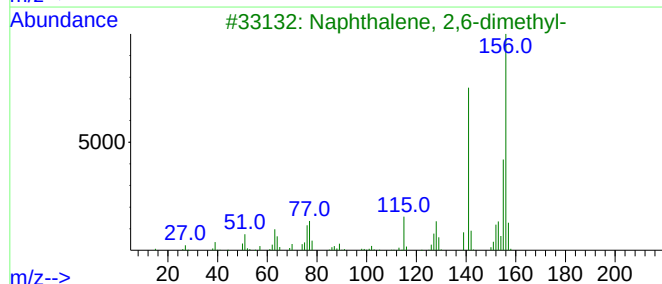
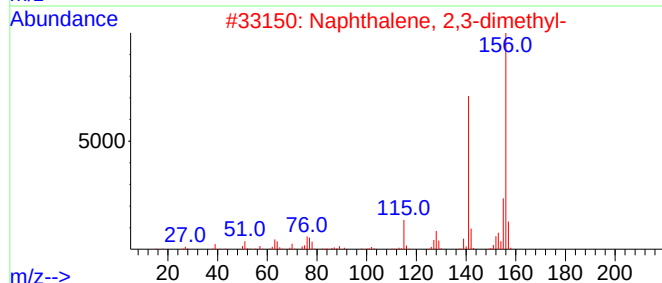
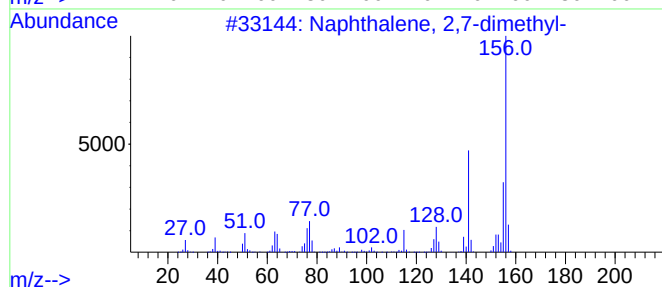
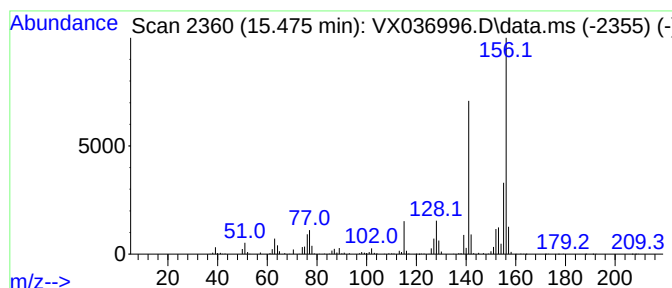
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,7-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	25.32 ug/l	342098	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, 1,6-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\VX081523\
Data File : VX036996.D
Acq On : 15 Aug 2023 18:32
Operator : JC/MD
Sample : 03932-02 10X
Misc : 5.30g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z20-22

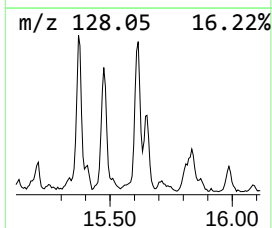
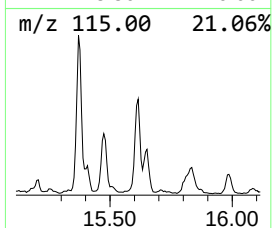
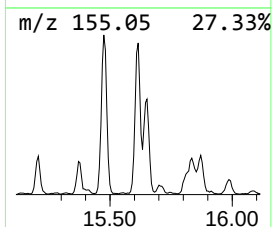
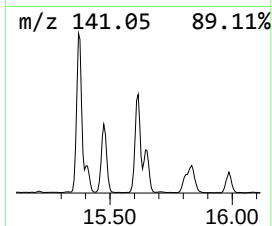
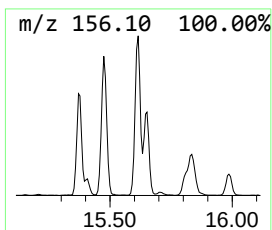
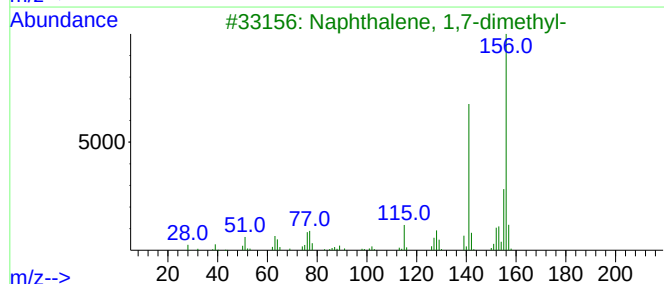
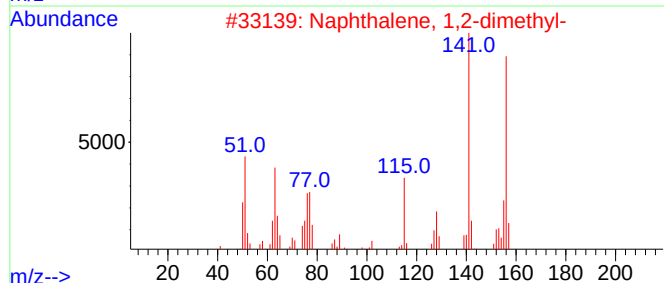
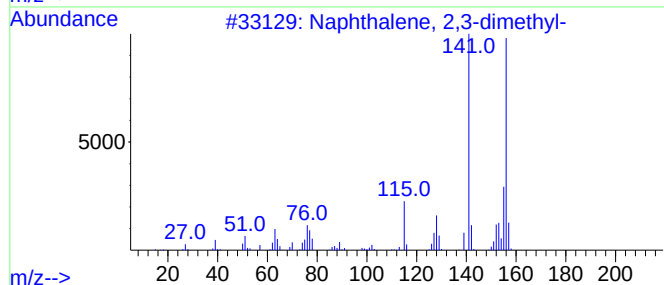
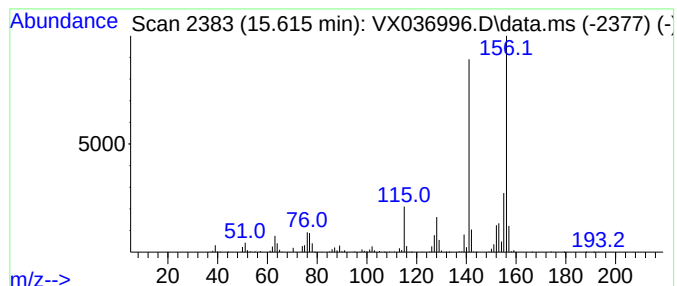
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	31.81 ug/l	429870	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, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX036996.D
Acq On : 15 Aug 2023 18:32
Operator : JC/MD
Sample : 03932-02 10X
Misc : 5.30g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

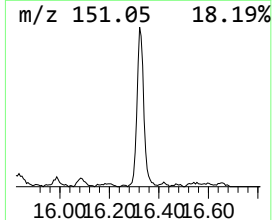
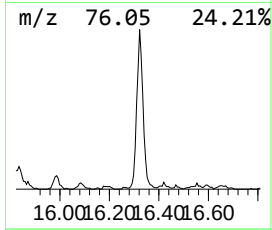
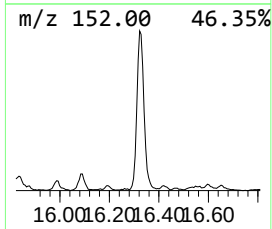
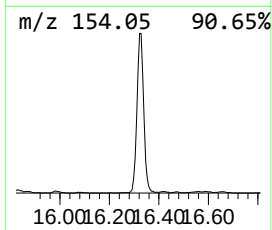
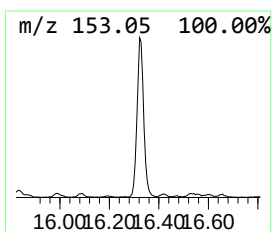
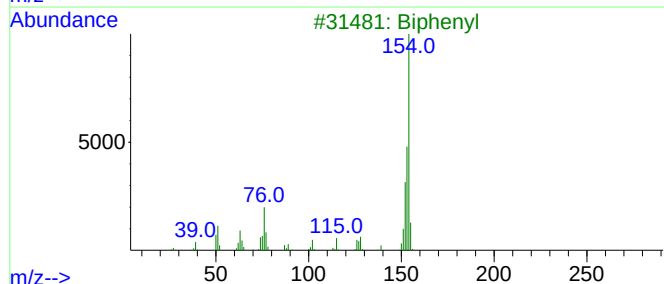
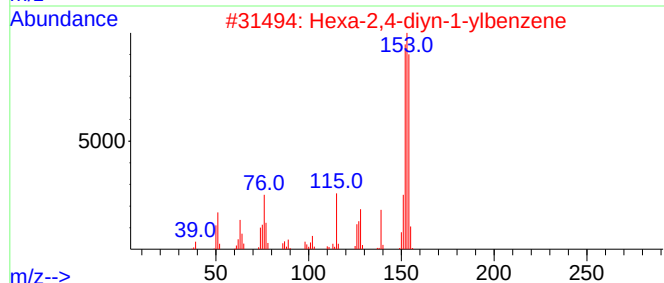
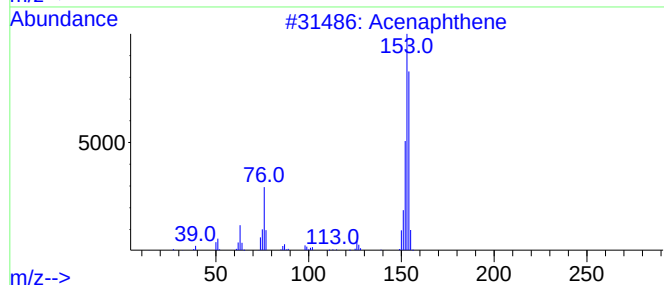
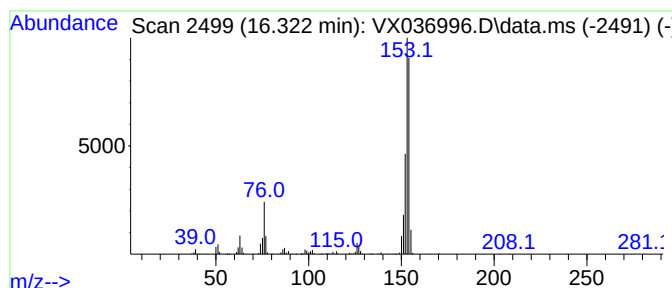
Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z20-22

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

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

Peak Number 10 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.322	31.38 ug/l	424030	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	93
2	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
3	Biphenyl	154	C12H10	000092-52-4	52
4	3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5	2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX036996.D
Acq On : 15 Aug 2023 18:32
Operator : JC/MD
Sample : 03932-02 10X
Misc : 5.30g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z20-22

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, 2-ethe...	13.292	26.3	ug/l	355943	4	12.024	675594	50.0
2-Methylindene	13.426	33.8	ug/l	456703	4	12.024	675594	50.0
Azulene	13.774	394.1	ug/l	5324910	4	12.024	675594	50.0
1,4-Methanonaph...	14.633	177.0	ug/l	2392010	4	12.024	675594	50.0
Benzocyclohepta...	14.780	106.1	ug/l	1433290	4	12.024	675594	50.0
Naphthalene, 1-...	15.371	29.0	ug/l	392017	4	12.024	675594	50.0
Naphthalene, 2,...	15.475	25.3	ug/l	342098	4	12.024	675594	50.0
Naphthalene, 2,...	15.615	31.8	ug/l	429870	4	12.024	675594	50.0
Hexa-2,4-diyne-1...	16.322	31.4	ug/l	424030	4	12.024	675594	50.0