

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080923\
 Data File : VX036891.D
 Acq On : 09 Aug 2023 16:44
 Operator : JC/MD
 Sample : 03903-11 20X
 Misc : 5.63g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-11

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: VX036891.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.593	562	575	589	rBV2	5234	18791	1.61%	0.199%
2	5.385	694	705	716	rBV2	83126	239835	20.51%	2.546%
3	5.550	716	732	756	rVB	133356	418928	35.82%	4.446%
4	5.824	768	777	788	rBV4	7254	22140	1.89%	0.235%
5	5.958	788	799	816	rBV	86135	232379	19.87%	2.466%
6	6.245	836	846	856	rVB	17868	52969	4.53%	0.562%
7	6.611	897	906	914	rBV3	6360	15074	1.29%	0.160%
8	6.763	922	931	942	rBV	216826	525075	44.90%	5.573%
9	7.379	1021	1032	1043	rBV5	9236	22771	1.95%	0.242%
10	7.495	1044	1051	1057	rBV2	5680	11708	1.00%	0.124%
11	7.982	1122	1131	1140	rVB	16300	35058	3.00%	0.372%
12	8.104	1144	1151	1160	rBV2	20002	47526	4.06%	0.504%
13	8.183	1160	1164	1174	rVB4	6482	13193	1.13%	0.140%
14	8.275	1174	1179	1183	rBV	9666	16977	1.45%	0.180%
15	8.440	1201	1206	1209	rBV	10156	15991	1.37%	0.170%
16	8.647	1226	1240	1253	rBV	456143	764338	65.36%	8.112%
17	8.915	1277	1284	1290	rBV3	11844	20798	1.78%	0.221%
18	9.500	1375	1380	1386	rBV5	7946	14316	1.22%	0.152%
19	9.903	1442	1446	1452	rVB	16598	23904	2.04%	0.254%
20	10.006	1456	1463	1466	rBV	13669	19421	1.66%	0.206%
21	10.055	1466	1471	1477	rBV	476285	635770	54.36%	6.748%
22	10.195	1489	1494	1499	rVB	42110	55603	4.75%	0.590%
23	10.305	1507	1512	1517	rVB	20116	28040	2.40%	0.298%
24	10.360	1517	1521	1533	rVB3	16976	30607	2.62%	0.325%
25	10.963	1614	1620	1625	rBV	25636	34846	2.98%	0.370%
26	11.079	1634	1639	1644	rBV	408874	540798	46.24%	5.740%
27	11.189	1650	1657	1661	rBV	16045	22028	1.88%	0.234%
28	11.305	1669	1676	1682	rVB	107282	136487	11.67%	1.449%
29	11.402	1686	1692	1696	rVV	154802	202888	17.35%	2.153%
30	11.451	1696	1700	1712	rVB	187778	270484	23.13%	2.871%
31	11.616	1722	1727	1734	rBV	26421	41149	3.52%	0.437%
32	11.750	1745	1749	1759	rVB	975453	1169502	100.00%	12.413%
33	11.841	1759	1764	1766	rBV	12498	17155	1.47%	0.182%
34	11.890	1770	1772	1775	rVB	12795	12997	1.11%	0.138%
35	11.933	1775	1779	1782	rBV	17032	20810	1.78%	0.221%
36	12.024	1788	1794	1799	rBV	500668	664488	56.82%	7.053%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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

37	12.085	1799	1804	1809	rBV	109281	157035	13.43%	1.667%
38	12.171	1817	1818	1822	rVB2	15532	14152	1.21%	0.150%
39	12.244	1825	1830	1837	rVV2	144710	200304	17.13%	2.126%
40	12.317	1837	1842	1849	rVB4	124377	196607	16.81%	2.087%
41	12.421	1849	1859	1863	rBV2	39804	62629	5.36%	0.665%
42	12.463	1863	1866	1873	rVB	36070	46316	3.96%	0.492%
43	12.530	1873	1877	1879	rBV	91586	113387	9.70%	1.203%
44	12.555	1879	1881	1885	rVV	79542	92251	7.89%	0.979%
45	12.610	1887	1890	1894	rVV	142334	186064	15.91%	1.975%
46	12.646	1894	1896	1900	rVV2	26709	33956	2.90%	0.360%
47	12.701	1900	1905	1915	rVB2	70775	120193	10.28%	1.276%
48	12.799	1916	1921	1926	rBV7	5788	12453	1.06%	0.132%
49	12.847	1926	1929	1933	rVV	32882	38604	3.30%	0.410%
50	12.920	1933	1941	1944	rVV	103320	139002	11.89%	1.475%
51	12.963	1944	1948	1953	rVB	142441	186199	15.92%	1.976%
52	13.042	1953	1961	1971	rBV5	30105	70796	6.05%	0.751%
53	13.170	1978	1982	1986	rVB	89719	109254	9.34%	1.160%
54	13.213	1986	1989	1992	rVB2	10841	12283	1.05%	0.130%
55	13.268	1992	1998	1999	rBV3	53482	74674	6.39%	0.793%
56	13.292	1999	2002	2007	rVV2	191333	249178	21.31%	2.645%
57	13.341	2007	2010	2012	rVV3	12194	15711	1.34%	0.167%
58	13.378	2012	2016	2020	rVV2	16942	29484	2.52%	0.313%
59	13.420	2020	2023	2028	rVV	24946	33642	2.88%	0.357%
60	13.506	2032	2037	2040	rBV2	16326	24461	2.09%	0.260%
61	13.542	2040	2043	2046	rBV	26822	33432	2.86%	0.355%
62	13.585	2046	2050	2056	rVV2	33313	60402	5.16%	0.641%
63	13.664	2060	2063	2071	rVB3	27053	46640	3.99%	0.495%
64	13.774	2077	2081	2088	rVB	139217	180313	15.42%	1.914%
65	13.841	2088	2092	2099	rVB5	15564	34303	2.93%	0.364%
66	13.926	2099	2106	2110	rBV3	17758	29998	2.57%	0.318%
67	13.969	2110	2113	2117	rBV2	12614	16760	1.43%	0.178%
68	14.073	2127	2130	2137	rBV	29957	38897	3.33%	0.413%
69	14.213	2149	2153	2164	rVB2	25967	45757	3.91%	0.486%
70	14.317	2167	2170	2176	rVV	11171	17074	1.46%	0.181%
71	14.371	2176	2179	2183	rVB	18682	21534	1.84%	0.229%
72	14.481	2192	2197	2206	rVB9	6172	17018	1.46%	0.181%
73	14.634	2213	2222	2233	rVB	121795	173804	14.86%	1.845%
74	14.780	2240	2246	2255	rBV	56475	72382	6.19%	0.768%

Sum of corrected areas: 9421793

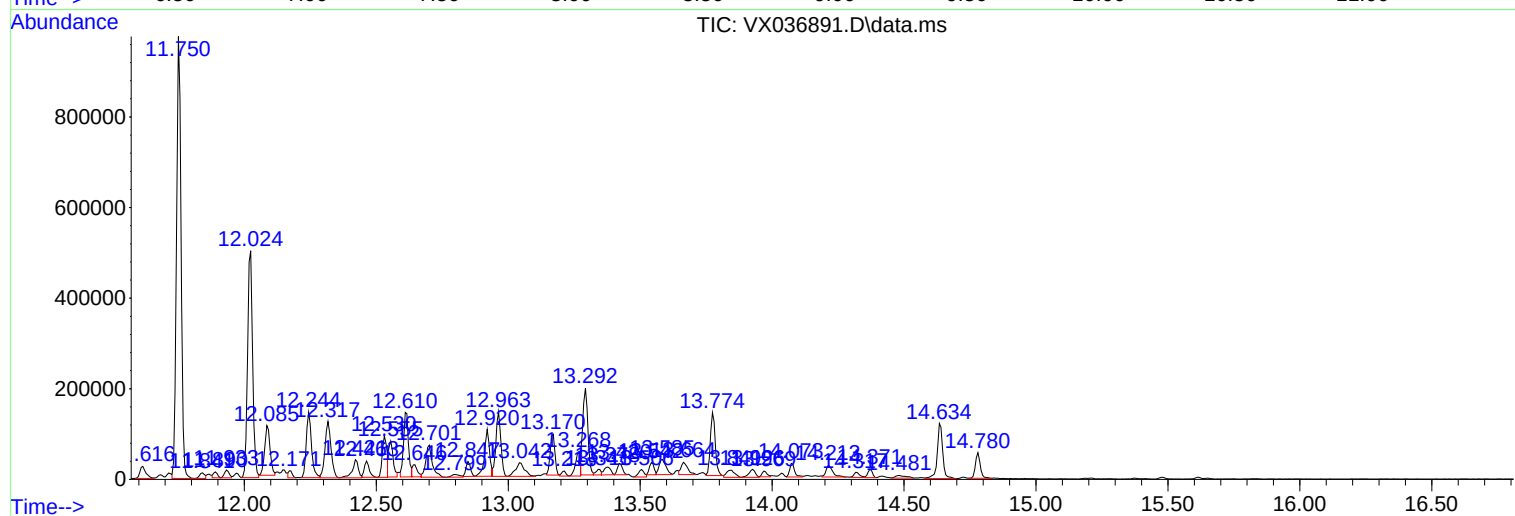
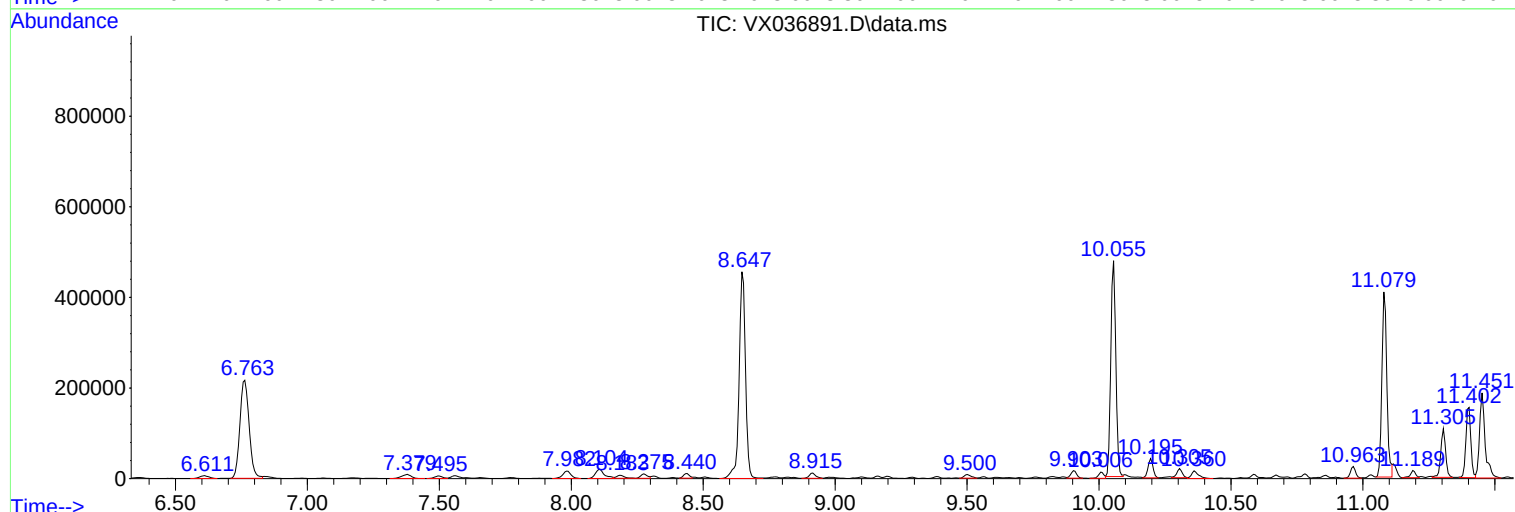
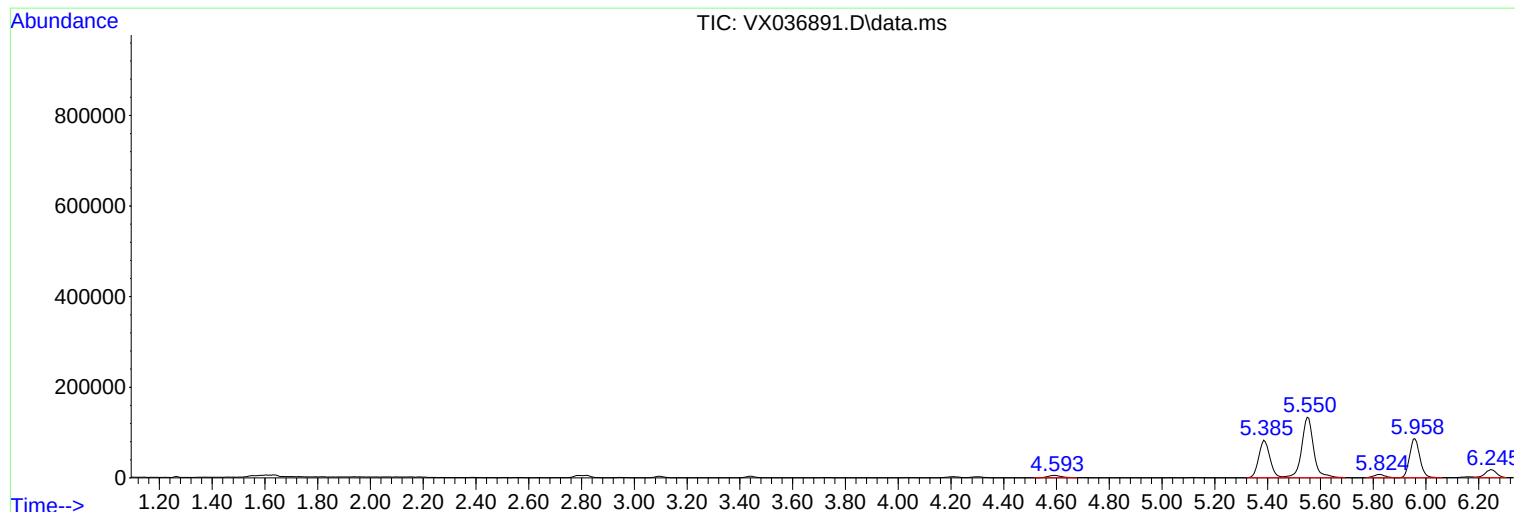
Instrument :
MSVOA_X
ClientSampleId :
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Instrument :
MSVOA_X
ClientSampleId :
MW-11

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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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11

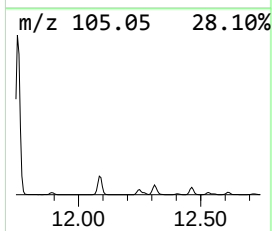
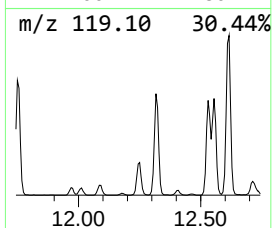
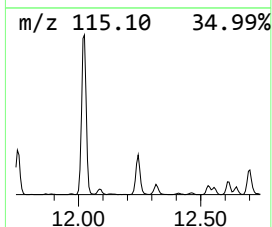
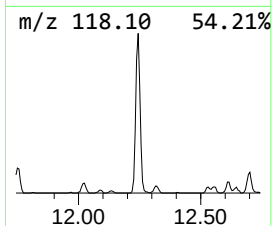
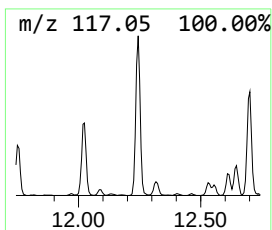
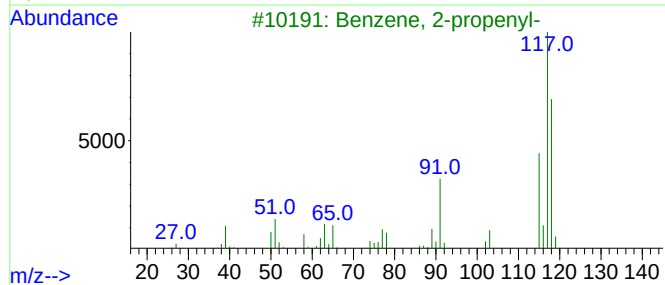
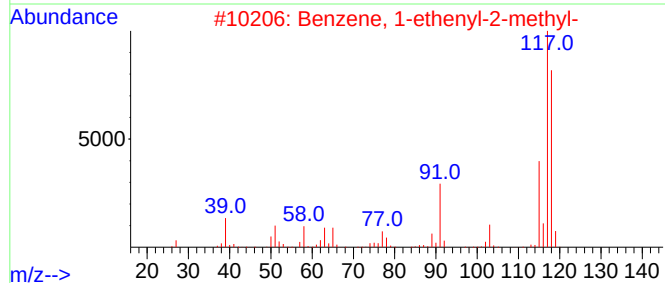
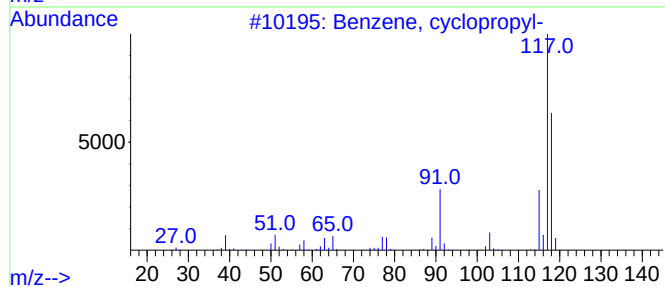
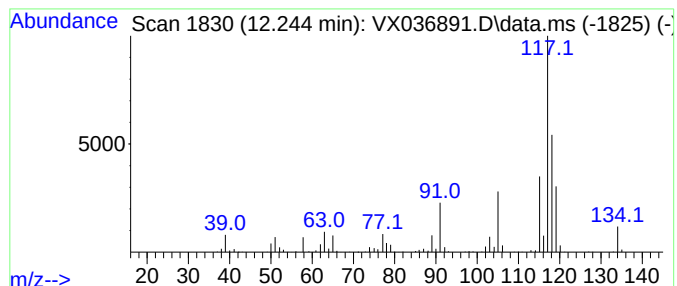
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, cyclopropyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	15.07 ug/l	200304	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	91
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	86
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
4			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64
5			Indane	118	C9H10	000496-11-7	64



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Misc : 5.63g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

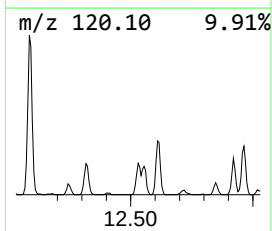
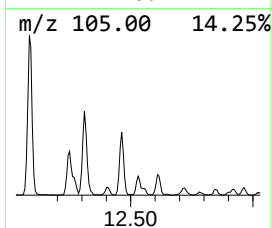
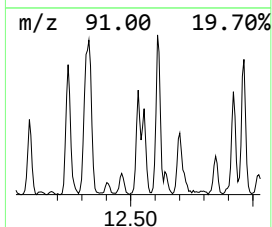
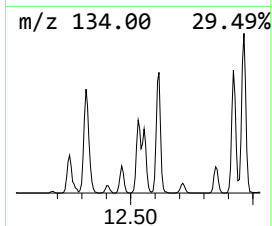
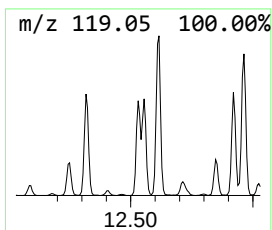
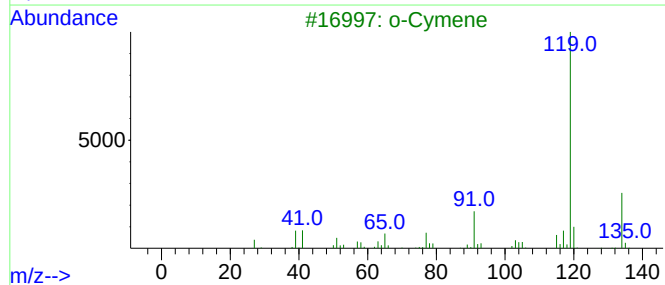
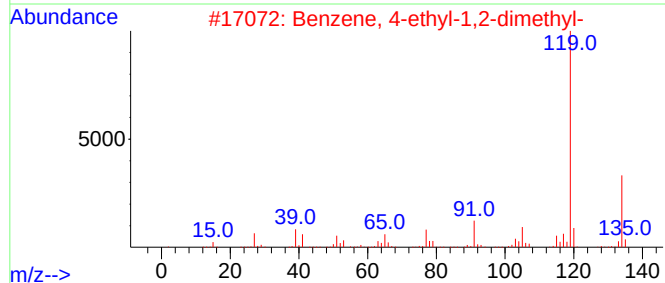
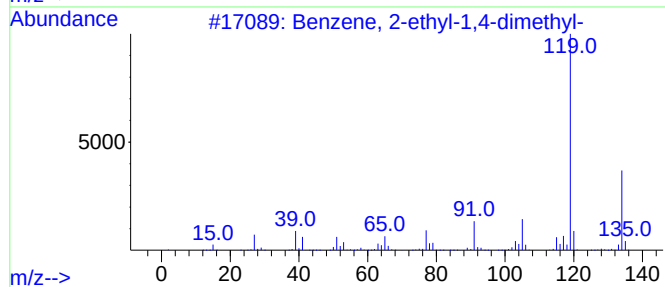
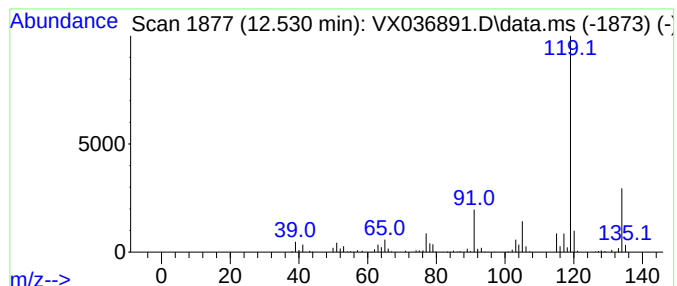
Instrument :
MSVOA_X
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MW-11

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-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.530	8.53 ug/l	113387	1,4-Dichlorobenzene-d4			12.024
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-		134	C10H14	001758-88-9	95
2	Benzene, 4-ethyl-1,2-dimethyl-		134	C10H14	000934-80-5	95
3	o-Cymene		134	C10H14	000527-84-4	95
4	Benzene, 1-ethyl-2,3-dimethyl-		134	C10H14	000933-98-2	94
5	Benzene, 2-ethyl-1,3-dimethyl-		134	C10H14	002870-04-4	94



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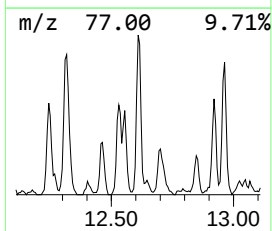
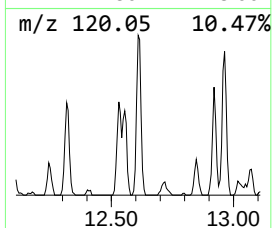
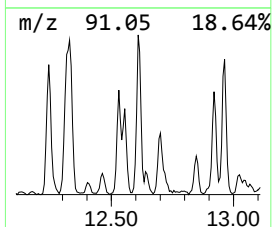
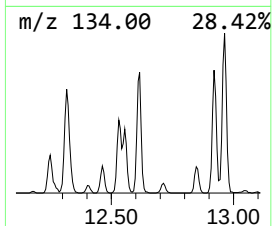
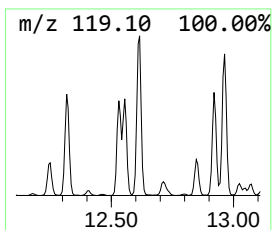
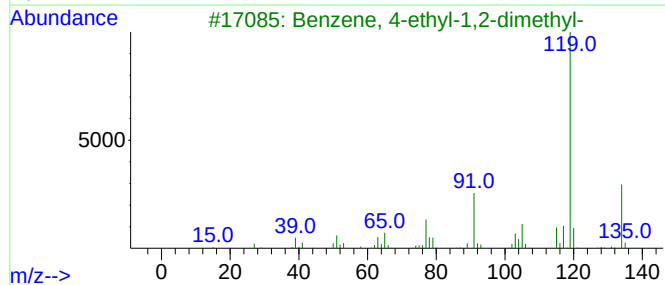
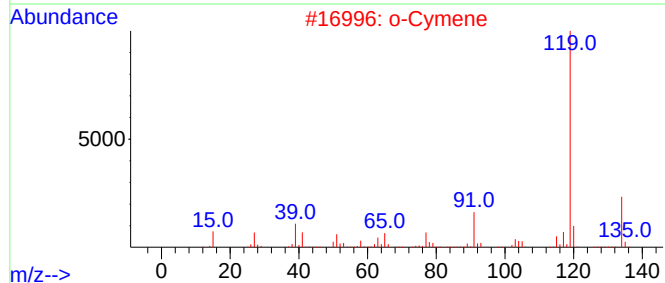
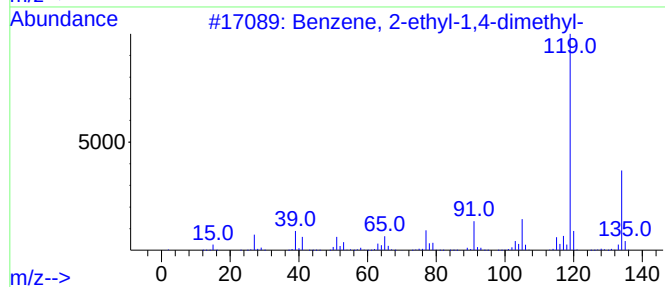
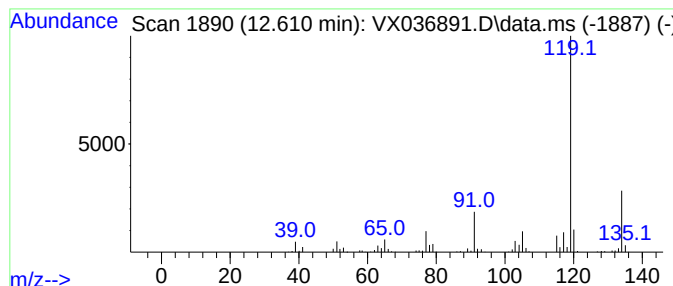
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	14.00 ug/l	186064	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
2			o-Cymene	134	C10H14	000527-84-4	95
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4			p-Cymene	134	C10H14	000099-87-6	94
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94



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Instrument :
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ClientSampleId :
MW-11

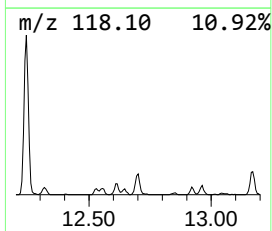
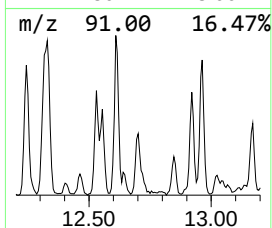
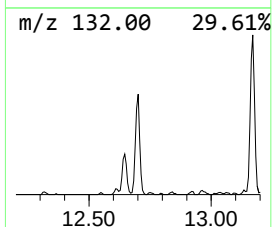
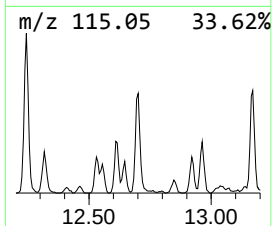
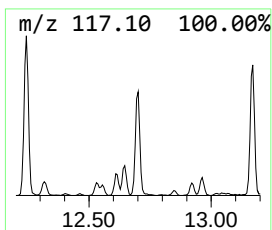
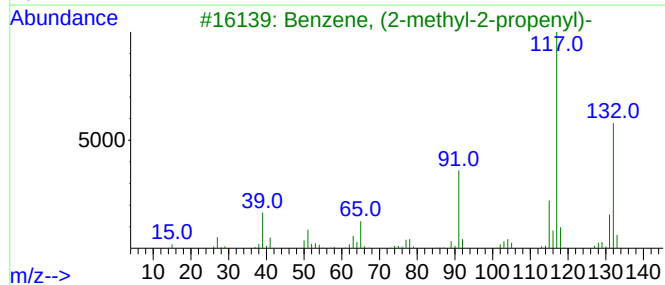
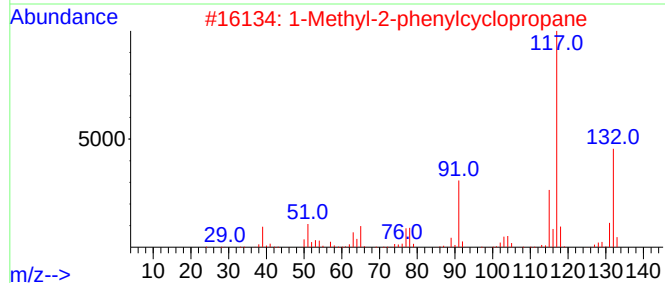
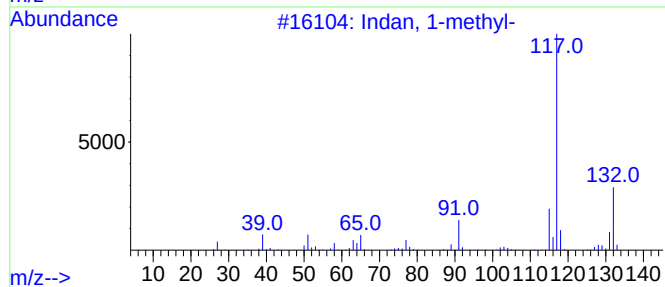
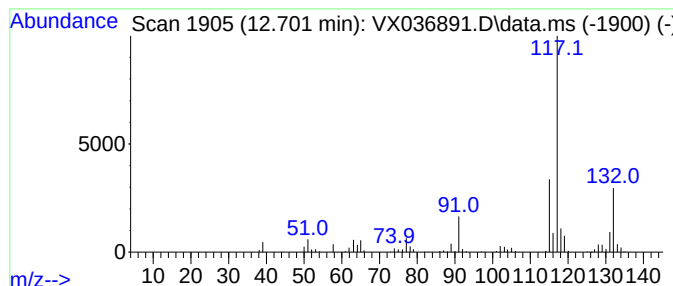
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Quant Title : SW846 8260

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

Peak Number 5 Indan, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	9.04 ug/l	120193	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	94
2			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	91
3			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	91
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	90
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080923\
Data File : VX036891.D
Acq On : 09 Aug 2023 16:44
Operator : JC/MD
Sample : 03903-11 20X
Misc : 5.63g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11

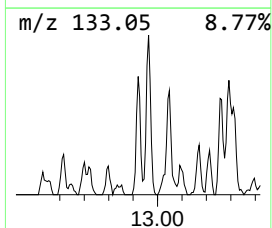
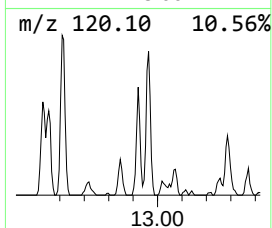
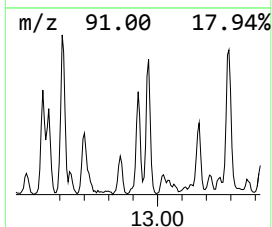
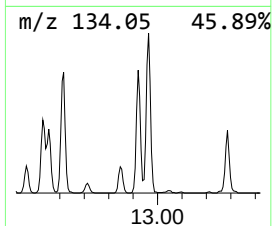
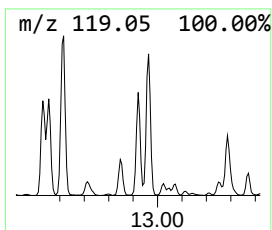
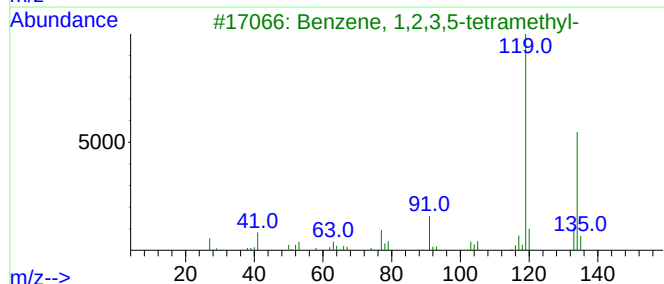
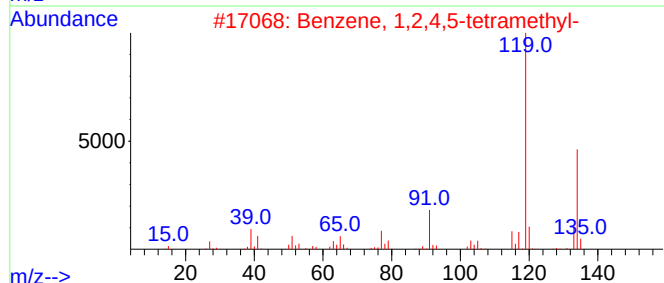
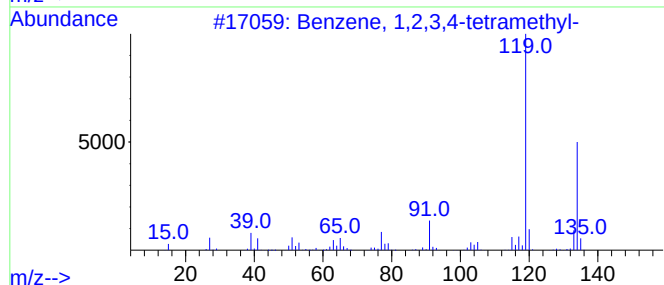
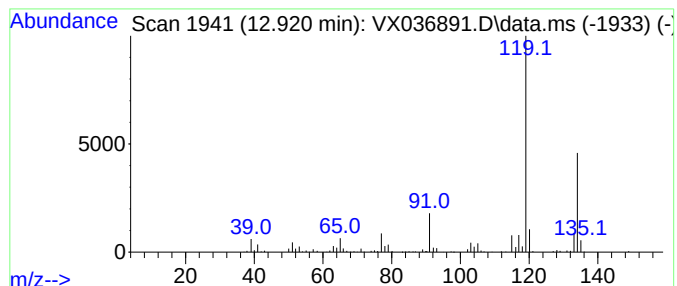
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	10.46 ug/l	139002	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080923\
Data File : VX036891.D
Acq On : 09 Aug 2023 16:44
Operator : JC/MD
Sample : 03903-11 20X
Misc : 5.63g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11

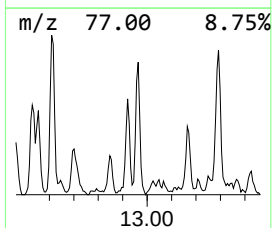
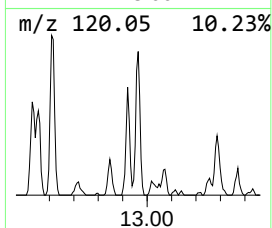
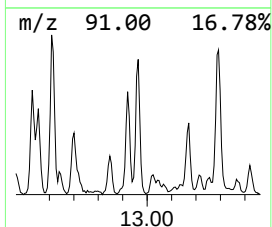
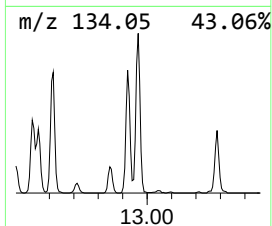
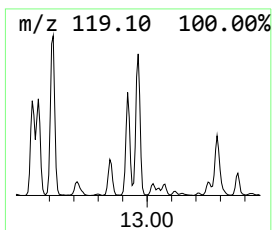
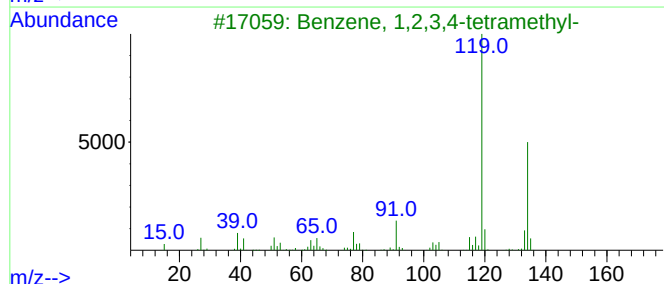
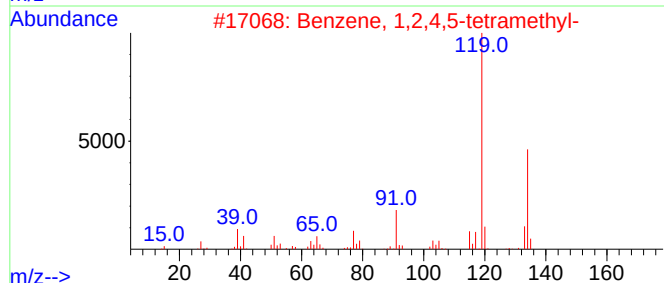
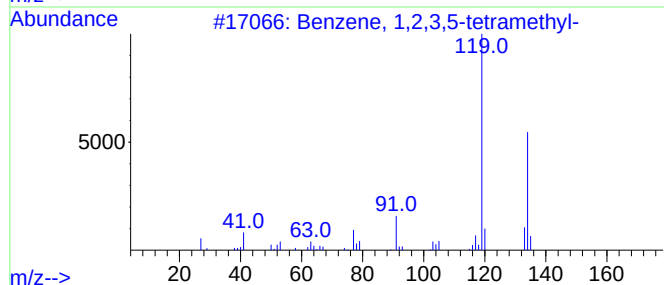
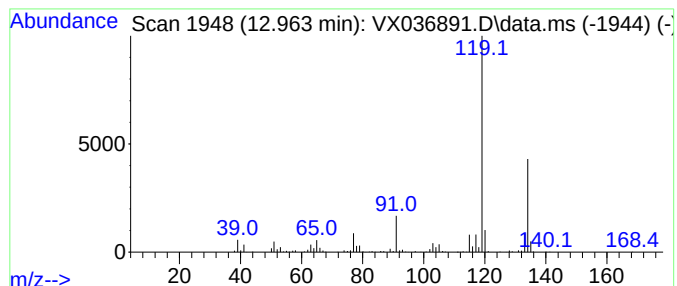
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	14.01 ug/l	186199	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4			o-Cymene	134	C10H14	000527-84-4	94
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080923\
Data File : VX036891.D
Acq On : 09 Aug 2023 16:44
Operator : JC/MD
Sample : 03903-11 20X
Misc : 5.63g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11

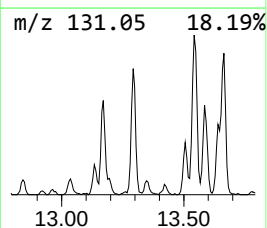
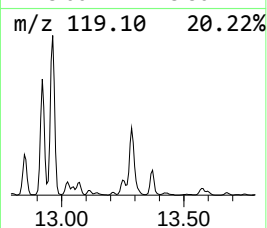
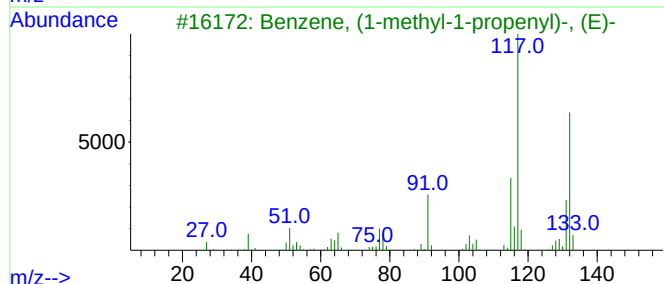
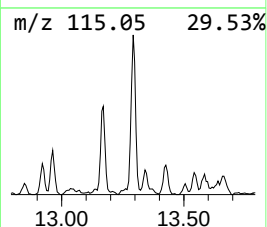
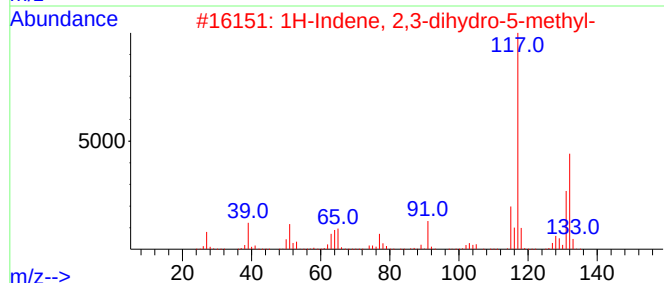
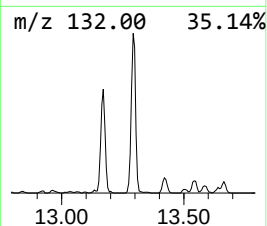
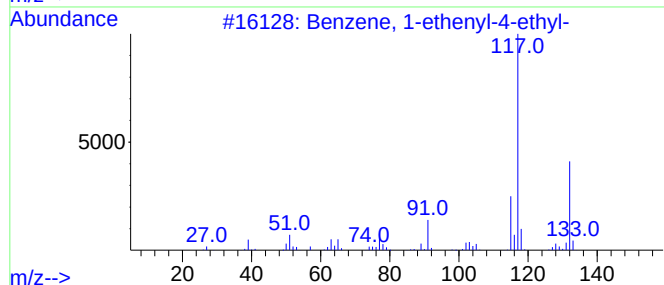
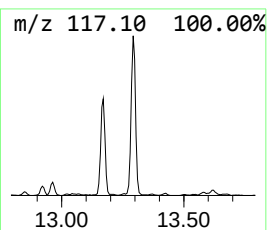
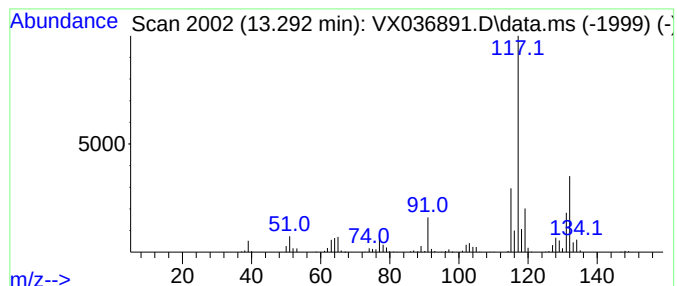
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	18.75 ug/l	249178	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
4			Indan, 1-methyl-	132	C10H12	000767-58-8	87
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080923\
Data File : VX036891.D
Acq On : 09 Aug 2023 16:44
Operator : JC/MD
Sample : 03903-11 20X
Misc : 5.63g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11

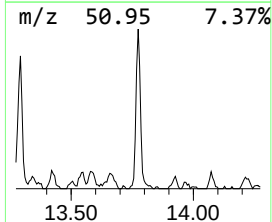
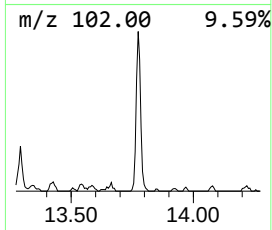
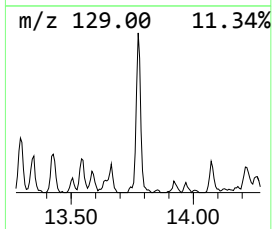
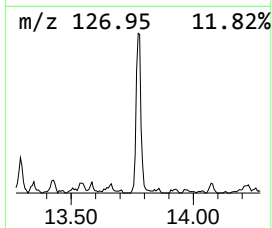
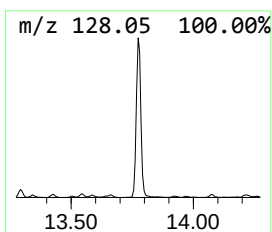
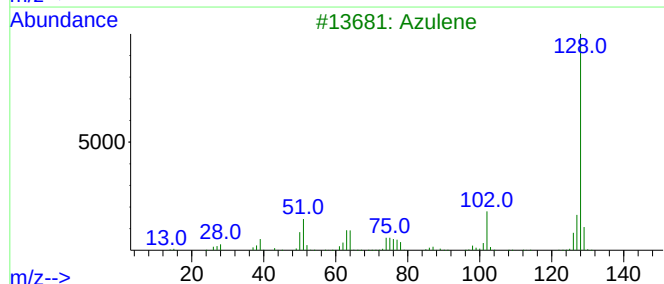
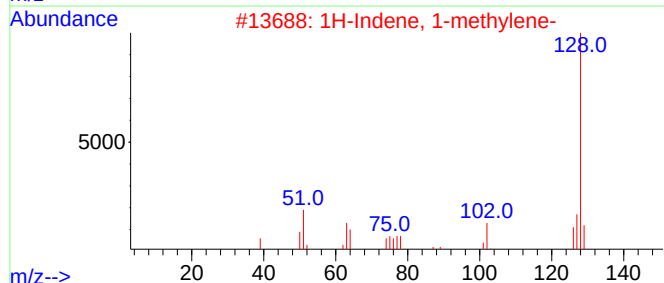
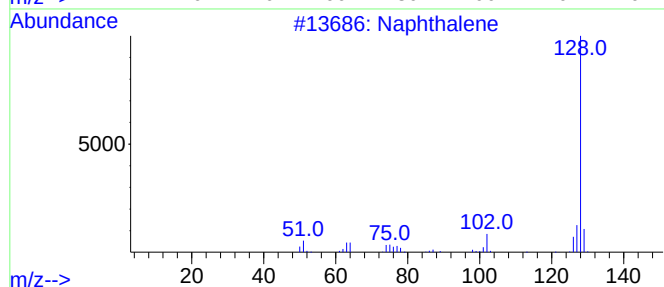
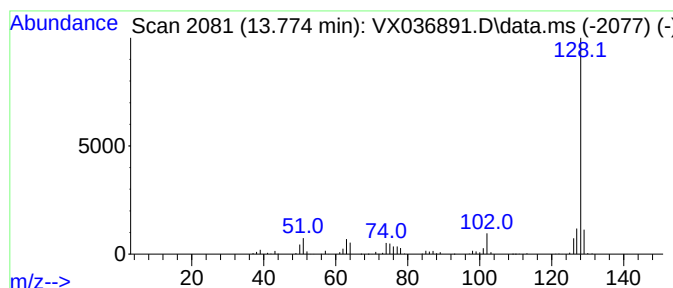
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Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, 1-methylene- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	13.57 ug/l	180313	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
3			Azulene	128	C10H8	000275-51-4	94
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	50
5			1H-Cyclopenta[c]thiophene, hexah...	128	C7H12S	053907-80-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080923\
Data File : VX036891.D
Acq On : 09 Aug 2023 16:44
Operator : JC/MD
Sample : 03903-11 20X
Misc : 5.63g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11

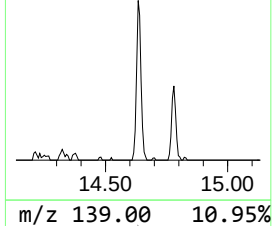
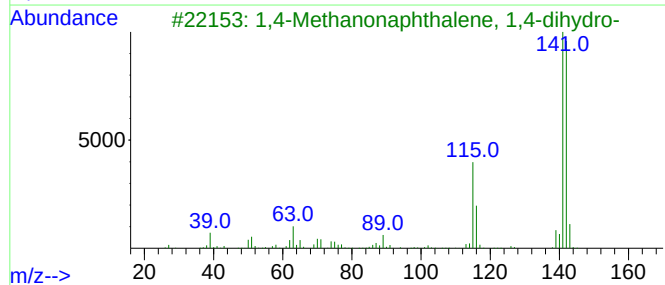
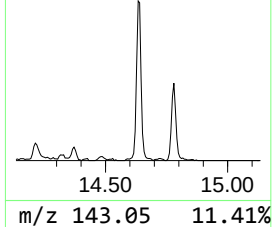
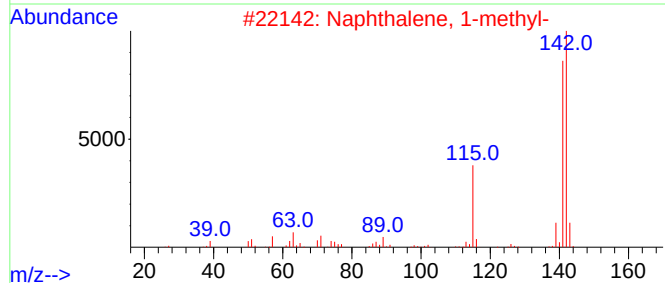
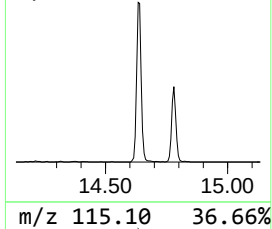
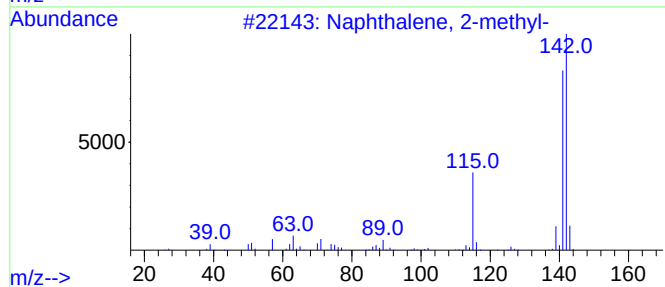
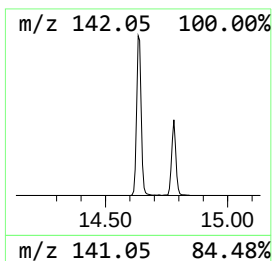
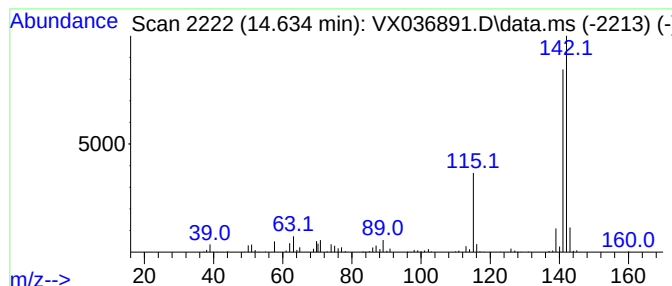
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Quant Title : SW846 8260

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

Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	13.08 ug/l	173804	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	93
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080923\
Data File : VX036891.D
Acq On : 09 Aug 2023 16:44
Operator : JC/MD
Sample : 03903-11 20X
Misc : 5.63g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11

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
Benzene, cyclop...	12.244	15.1	ug/l	200304	4	12.024	664488	50.0
Benzene, 2-ethy...	12.530	8.5	ug/l	113387	4	12.024	664488	50.0
Benzene, 4-ethy...	12.610	14.0	ug/l	186064	4	12.024	664488	50.0
Indan, 1-methyl-	12.701	9.0	ug/l	120193	4	12.024	664488	50.0
Benzene, 1,2,3,...	12.920	10.5	ug/l	139002	4	12.024	664488	50.0
Benzene, 1,2,3,...	12.963	14.0	ug/l	186199	4	12.024	664488	50.0
Benzene, 1-ethe...	13.292	18.8	ug/l	249178	4	12.024	664488	50.0
1H-Indene, 1-me...	13.774	13.6	ug/l	180313	4	12.024	664488	50.0
1,4-Methanonaph...	14.634	13.1	ug/l	173804	4	12.024	664488	50.0