

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
 Data File : VX034351.D
 Acq On : 06 Mar 2023 15:47
 Operator : JC/MD
 Sample : 01816-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 2325

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\82X021723W.M
 Title : SW846 8260

Signal : TIC: VX034351.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	73	rBV	1059481	1304584	1.81%	0.586%
2	2.154	151	175	178	rBV	14919237	71930786	100.00%	32.298%
3	2.386	208	213	227	rVB	774591	1262488	1.76%	0.567%
4	3.117	322	333	344	rBV	316538	731335	1.02%	0.328%
5	5.550	722	732	750	rVB	268075	765673	1.06%	0.344%
6	6.763	921	931	949	rVB	427373	1038209	1.44%	0.466%
7	8.647	1234	1240	1246	rBV	935961	1433574	1.99%	0.644%
8	8.720	1246	1252	1257	rVV	2088150	3336555	4.64%	1.498%
9	10.055	1466	1471	1477	rVB	913655	1219745	1.70%	0.548%
10	10.195	1488	1494	1502	rBV	2117229	2840890	3.95%	1.276%
11	10.299	1503	1511	1517	rVV	7597367	10206836	14.19%	4.583%
12	10.640	1562	1567	1573	rVV	5623989	7148685	9.94%	3.210%
13	10.963	1613	1620	1624	rBV	543073	746301	1.04%	0.335%
14	11.079	1634	1639	1650	rBV2	899040	1343566	1.87%	0.603%
15	11.305	1668	1676	1680	rBV	1413345	1780333	2.48%	0.799%
16	11.378	1683	1688	1695	rBV	5323630	8839948	12.29%	3.969%
17	11.451	1695	1700	1703	rBV	2348938	2843595	3.95%	1.277%
18	11.610	1721	1726	1732	rBV	3144587	4074688	5.66%	1.830%
19	11.750	1745	1749	1759	rVB	9575337	12435064	17.29%	5.583%
20	11.890	1765	1772	1777	rBV2	545147	757668	1.05%	0.340%
21	12.018	1789	1793	1799	rVB2	1124655	1669808	2.32%	0.750%
22	12.085	1799	1804	1810	rBV	4421287	5647582	7.85%	2.536%
23	12.244	1826	1830	1833	rBV	4145732	4673068	6.50%	2.098%
24	12.317	1838	1842	1848	rVB3	2142224	3492313	4.86%	1.568%
25	12.421	1848	1859	1863	rBV2	845330	1364841	1.90%	0.613%
26	12.463	1863	1866	1872	rVB	1023118	1233005	1.71%	0.554%
27	12.530	1872	1877	1879	rBV	1343857	1716900	2.39%	0.771%
28	12.555	1879	1881	1885	rVV	1243976	1310960	1.82%	0.589%
29	12.616	1885	1891	1893	rVV	1667494	2096455	2.91%	0.941%
30	12.646	1893	1896	1900	rVB	743896	839075	1.17%	0.377%
31	12.701	1900	1905	1913	rBV2	1781400	3032875	4.22%	1.362%
32	12.847	1926	1929	1933	rVB2	713236	829025	1.15%	0.372%
33	12.920	1933	1941	1944	rBV	1129170	1597097	2.22%	0.717%
34	12.963	1944	1948	1954	rVB	1933726	2510020	3.49%	1.127%
35	13.042	1954	1961	1964	rBV5	420638	844261	1.17%	0.379%
36	13.170	1977	1982	1986	rVB	2698897	3474543	4.83%	1.560%

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Min Area: 3 % of largest Peak

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Peak Location: TOP

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

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37	13.292	1992	2002	2007	rBV3	6002305	9423893	13.10%	4.231%
38	13.420	2019	2023	2032	rVB	5474431	7183831	9.99%	3.226%
39	13.542	2040	2043	2046	rBV	689083	855250	1.19%	0.384%
40	13.585	2046	2050	2054	rVV3	863130	1320985	1.84%	0.593%
41	13.664	2060	2063	2068	rVB2	845612	1166401	1.62%	0.524%
42	13.774	2077	2081	2088	rVB	2535128	3259465	4.53%	1.464%
43	13.853	2088	2094	2099	rVB2	1339107	2011822	2.80%	0.903%
44	13.926	2099	2106	2110	rBV2	1342805	1999935	2.78%	0.898%
45	14.036	2121	2124	2127	rBV	861590	893957	1.24%	0.401%
46	14.073	2127	2130	2134	rBV	960939	1124848	1.56%	0.505%
47	14.231	2149	2156	2163	rVB	3267059	5123314	7.12%	2.300%
48	14.371	2175	2179	2183	rVV2	895279	1092948	1.52%	0.491%
49	14.481	2192	2197	2206	rBV2	2169701	3137481	4.36%	1.409%
50	14.640	2215	2223	2226	rBV2	2202559	4055912	5.64%	1.821%
51	14.755	2239	2242	2244	rVV	1034804	1203911	1.67%	0.541%
52	14.780	2244	2246	2250	rVV	1211057	1440303	2.00%	0.647%
53	15.182	2308	2312	2314	rVV	705288	966545	1.34%	0.434%
54	15.207	2314	2316	2320	rVB2	678690	817787	1.14%	0.367%
55	15.487	2356	2362	2367	rBV2	1006861	1743117	2.42%	0.783%
56	15.615	2378	2383	2386	rBV	453008	748142	1.04%	0.336%
57	16.377	2502	2508	2516	rVB	445033	769059	1.07%	0.345%

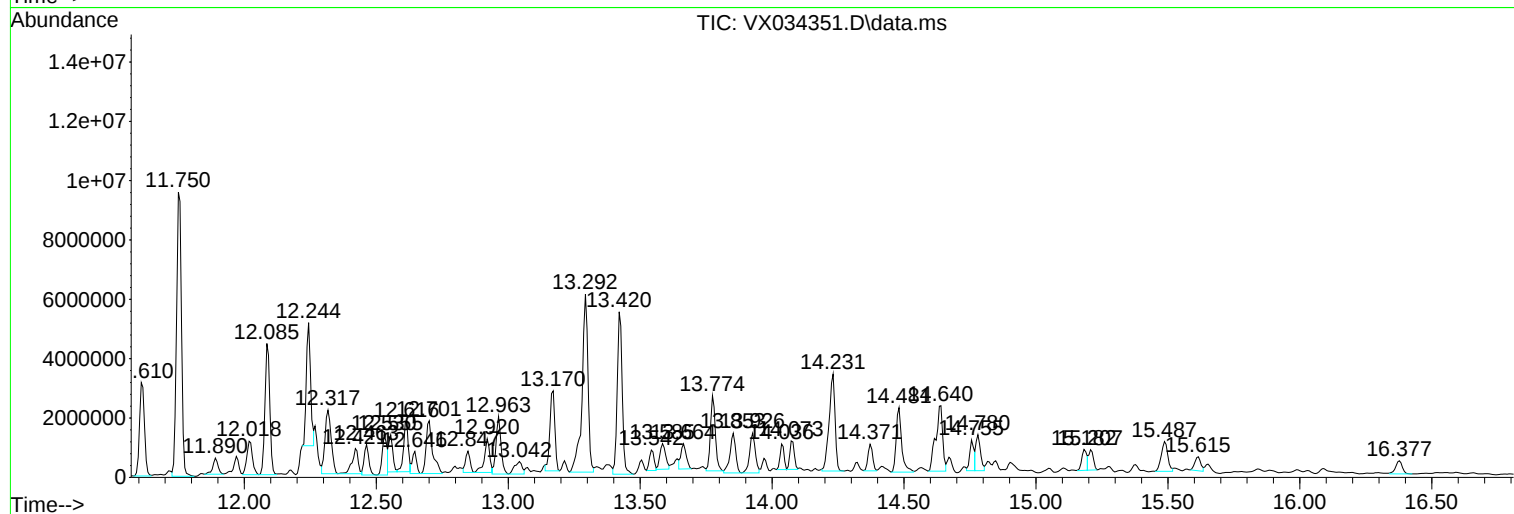
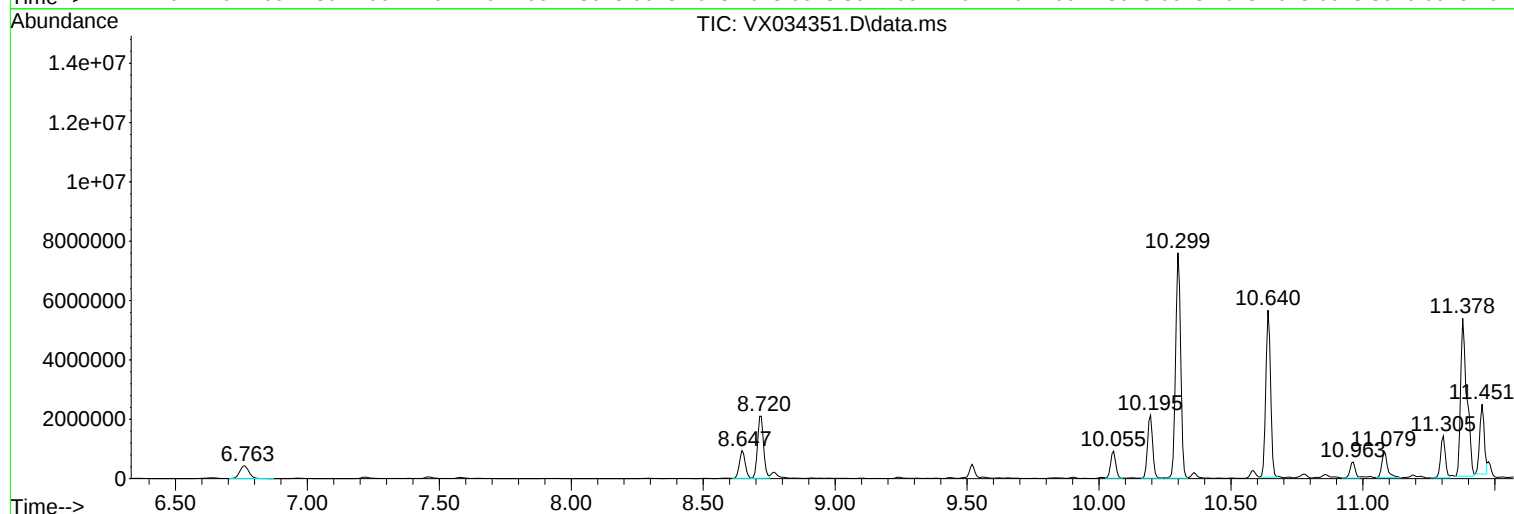
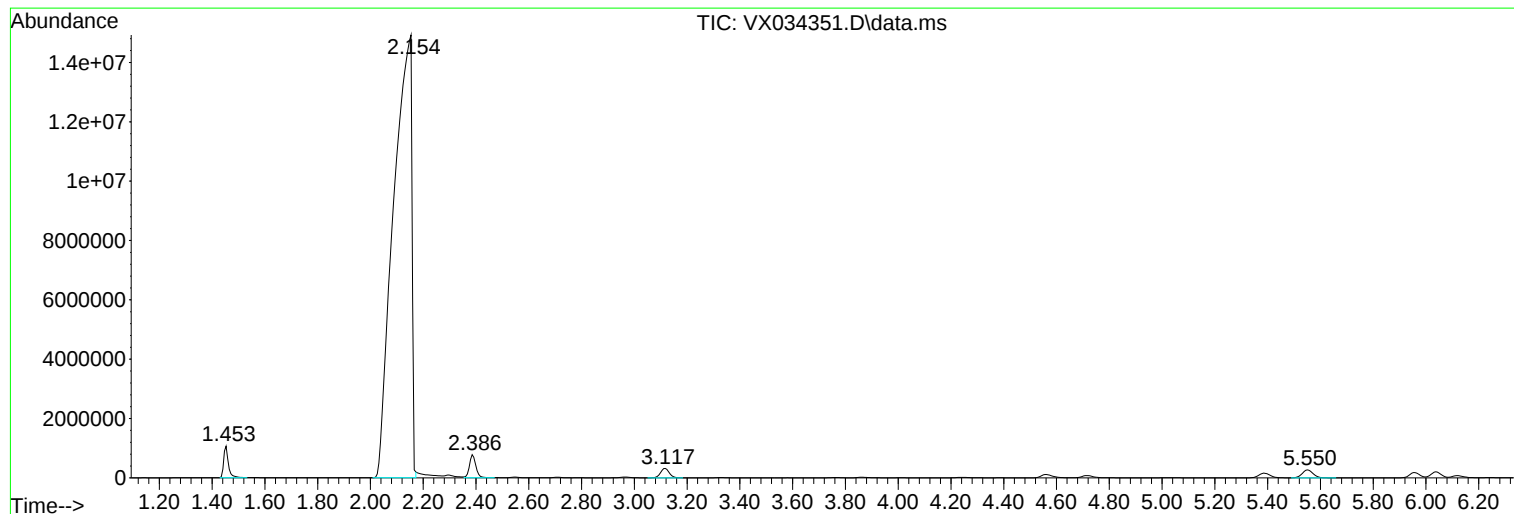
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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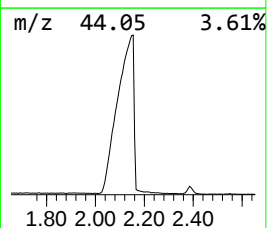
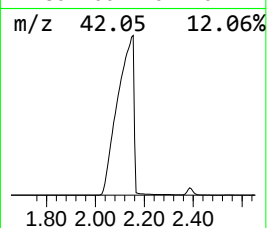
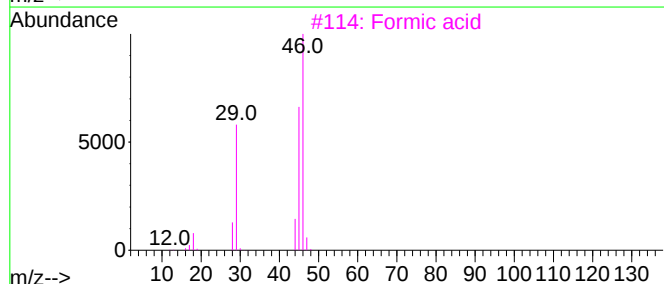
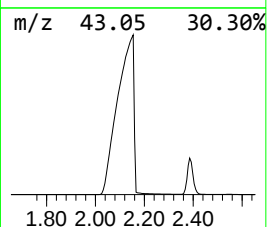
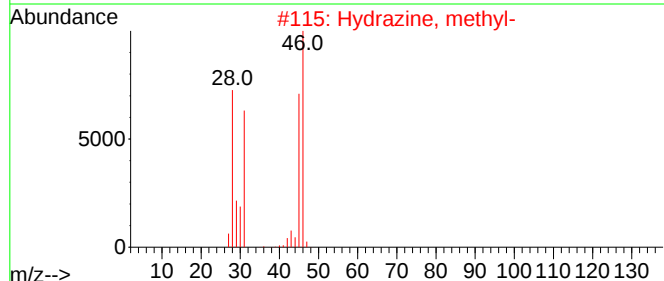
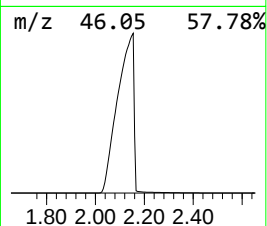
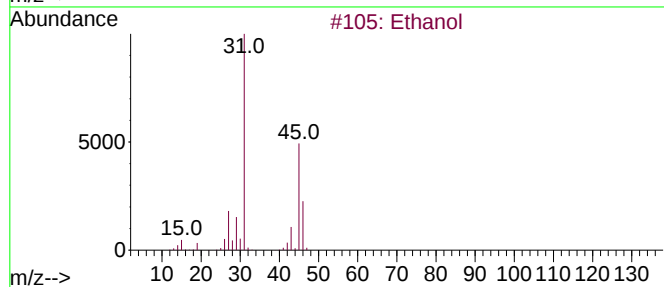
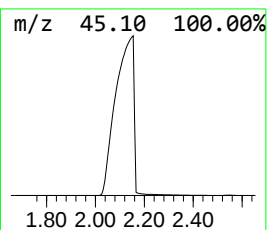
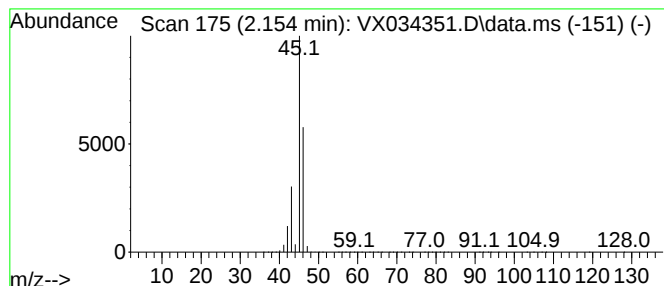
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.154	4697.23 ug/l	71930800	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	83
2	Hydrazine, methyl-			46	CH6N2	000060-34-4	9
3	Formic acid			46	CH2O2	000064-18-6	5
4	Dimethyl ether			46	C2H6O	000115-10-6	5
5	Methane, nitroso-			45	CH3NO	000865-40-7	4



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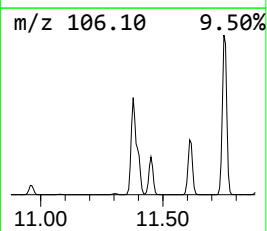
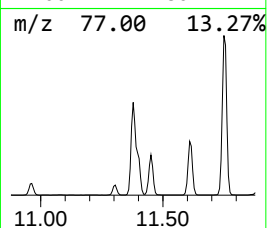
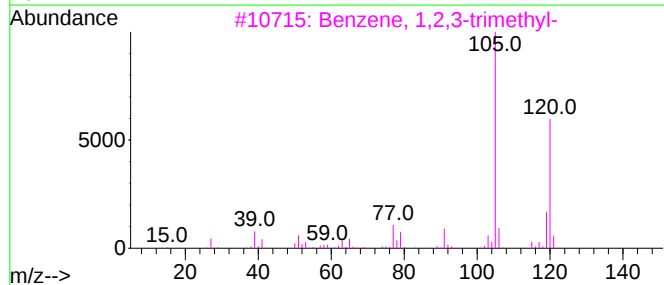
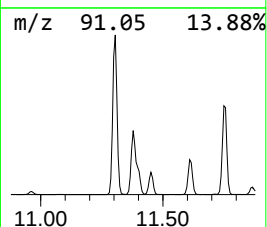
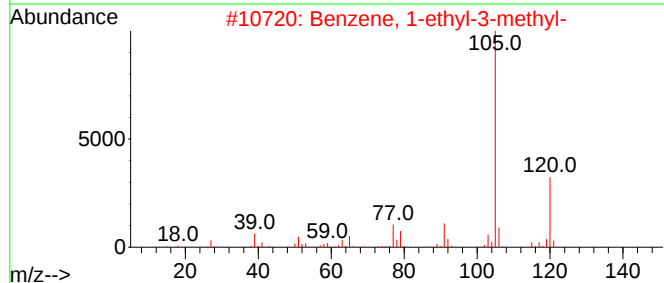
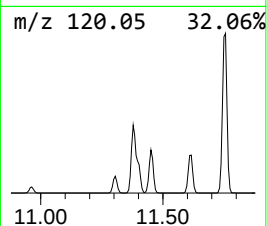
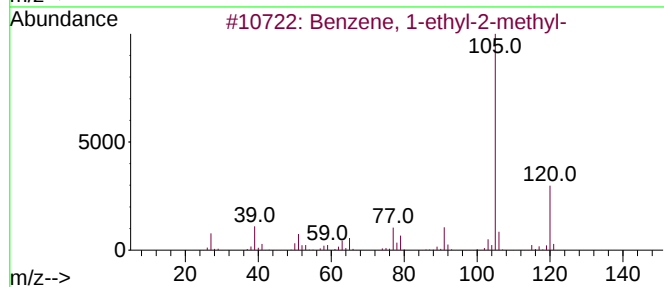
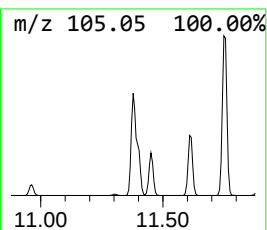
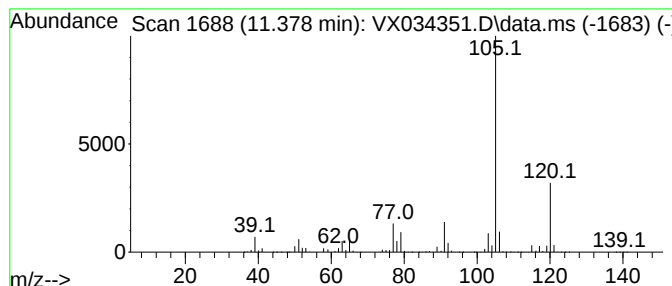
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	264.70 ug/l	8839950	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	91



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ALS Vial : 17 Sample Multiplier: 1

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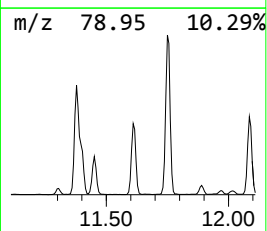
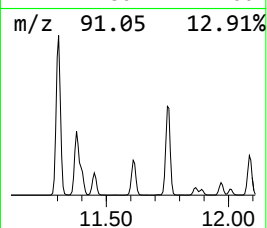
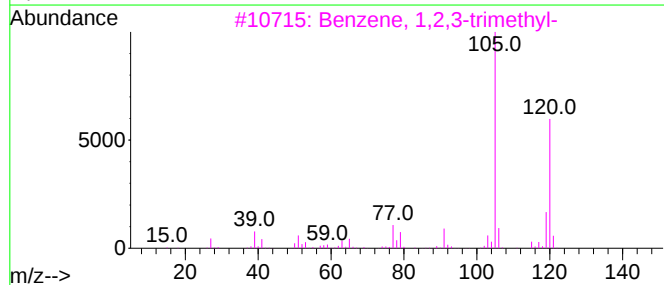
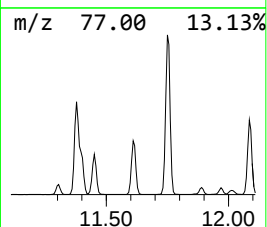
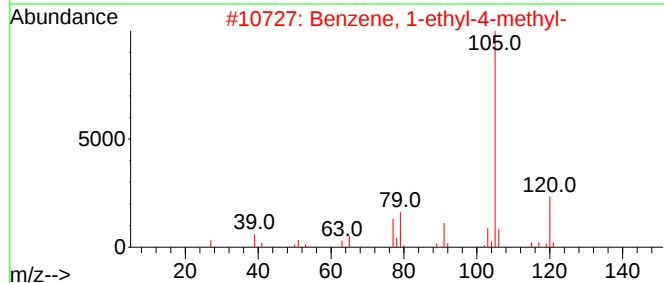
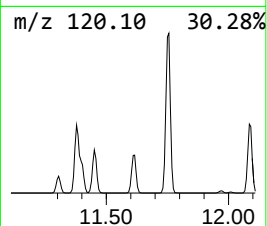
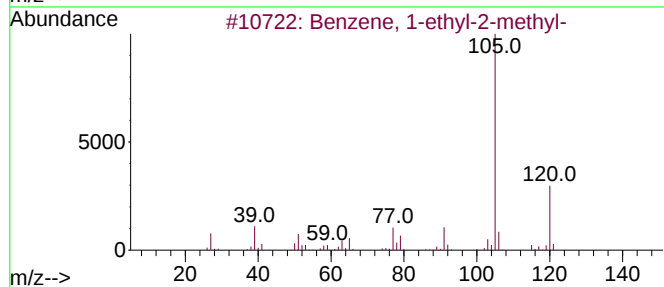
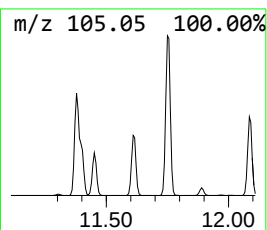
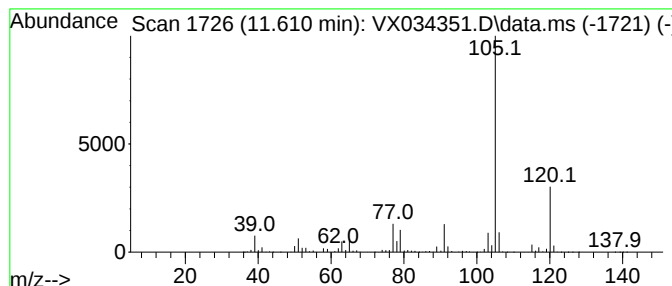
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	122.01 ug/l	4074690	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Mesitylene	120	C9H12	000108-67-8	91



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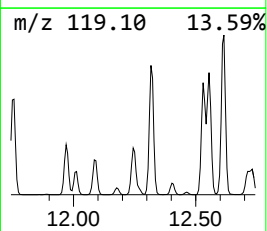
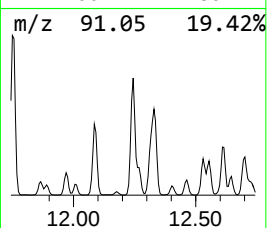
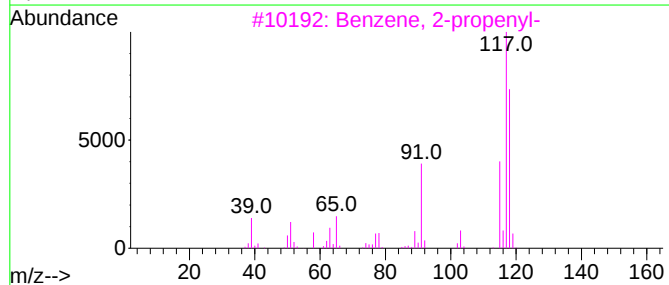
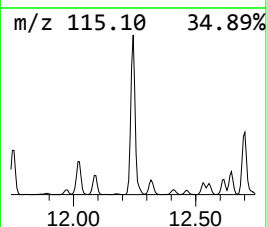
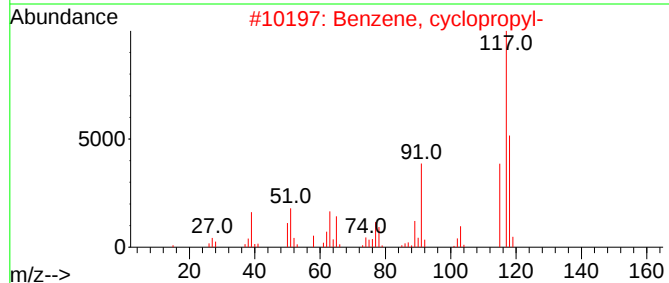
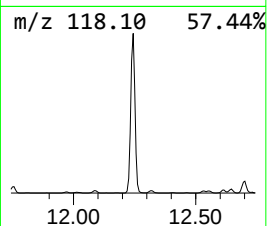
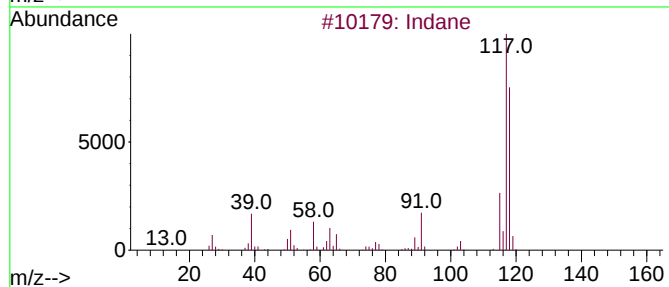
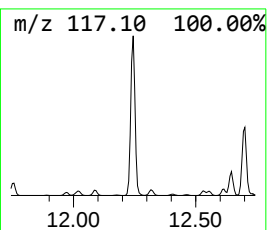
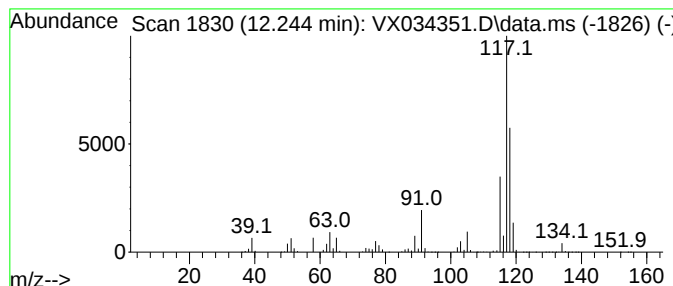
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Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	139.93 ug/l	4673070	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	76
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4			Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	64
5			Deltacyclene	118	C9H10	007785-10-6	52



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2325

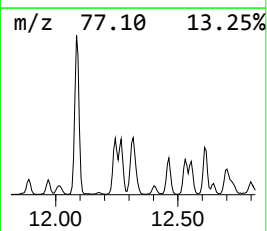
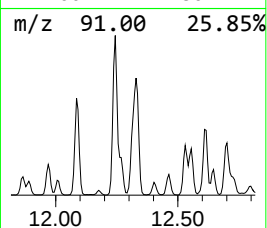
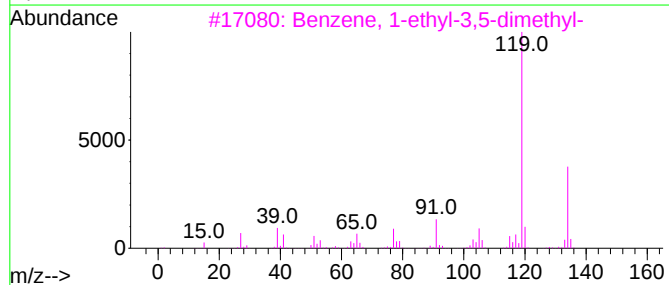
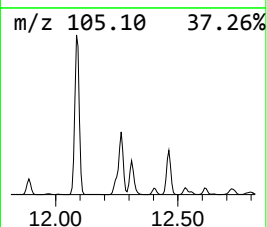
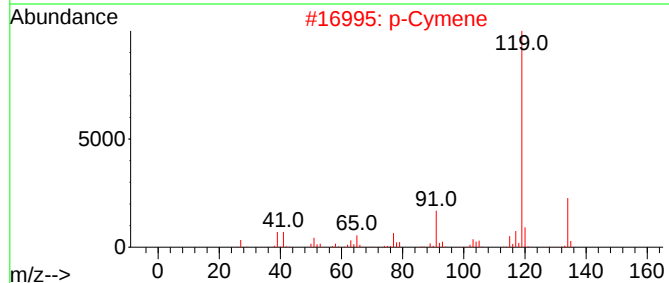
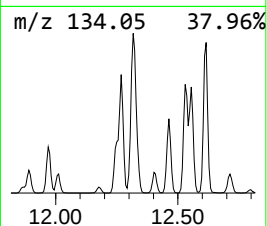
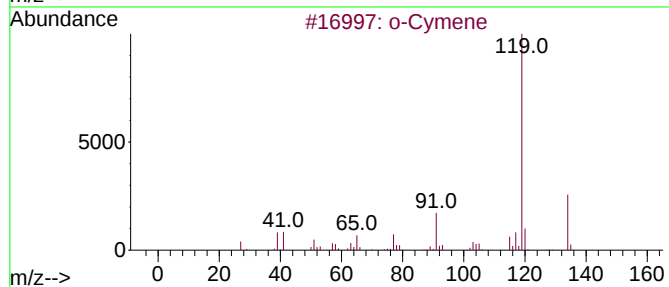
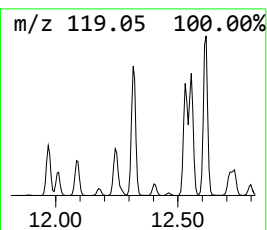
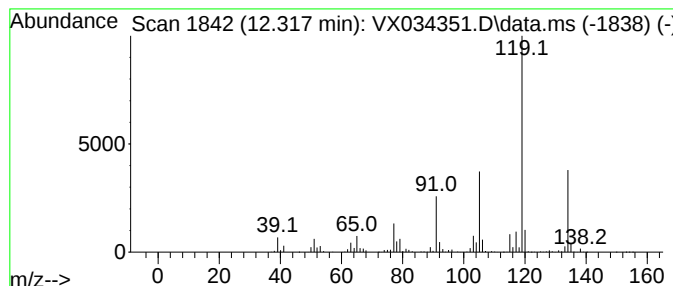
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Quant Title : SW846 8260

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

Peak Number 6 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	104.57 ug/l	3492310	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	95
2			p-Cymene	134	C10H14	000099-87-6	94
3			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034351.D
Acq On : 06 Mar 2023 15:47
Operator : JC/MD
Sample : 01816-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2325

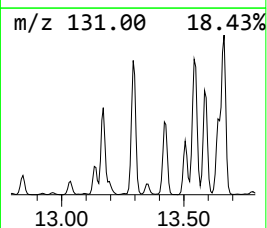
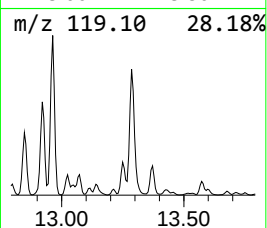
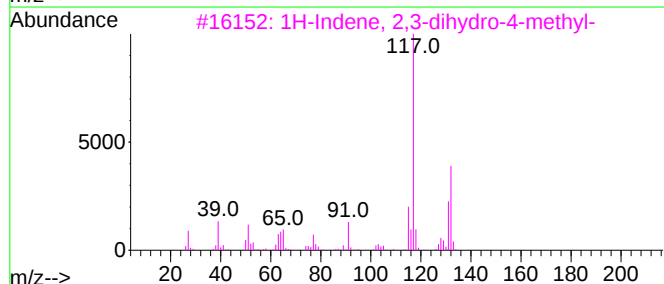
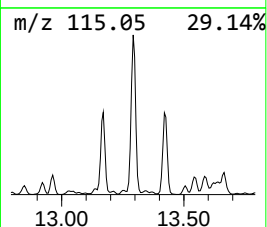
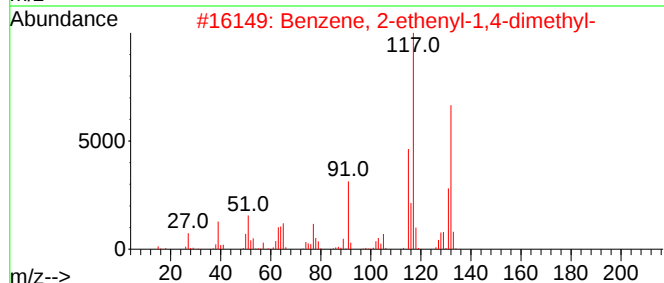
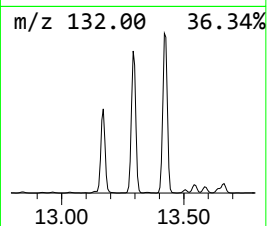
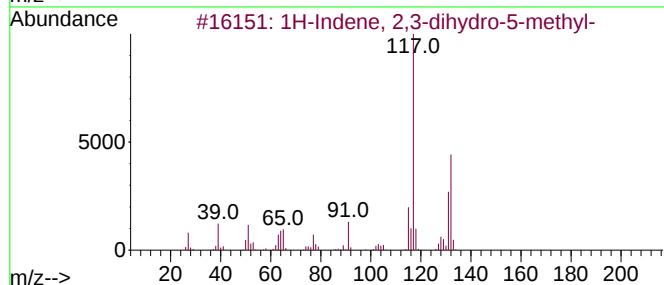
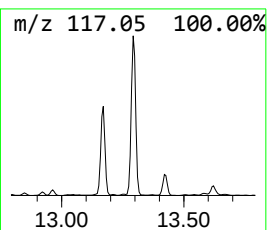
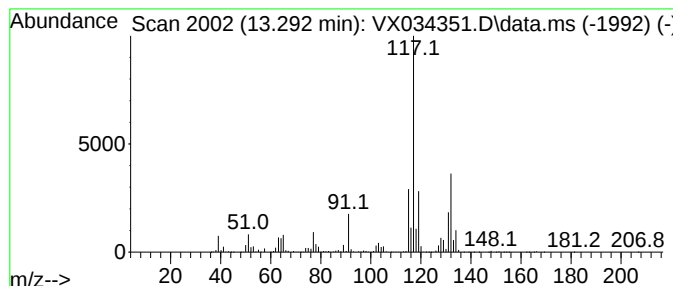
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Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	282.19 ug/l	9423890	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	95	
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95	
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93	
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	90	
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034351.D
Acq On : 06 Mar 2023 15:47
Operator : JC/MD
Sample : 01816-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2325

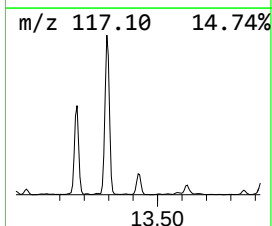
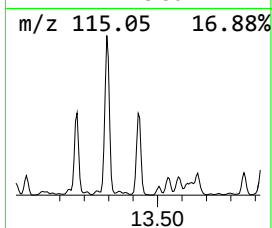
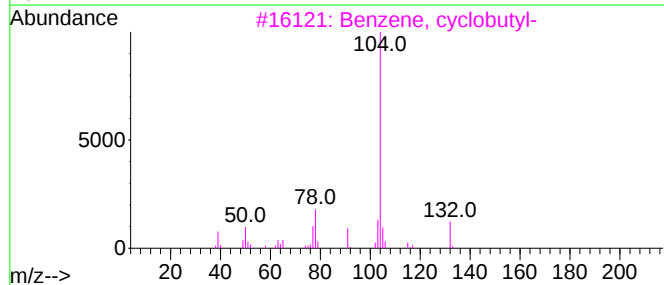
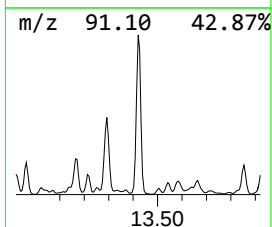
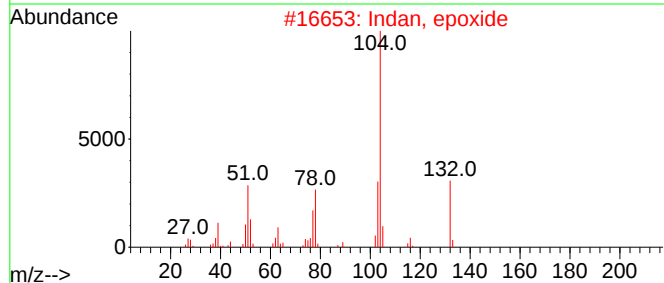
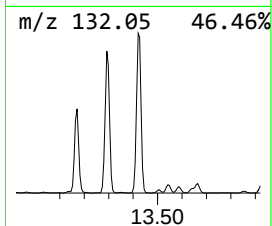
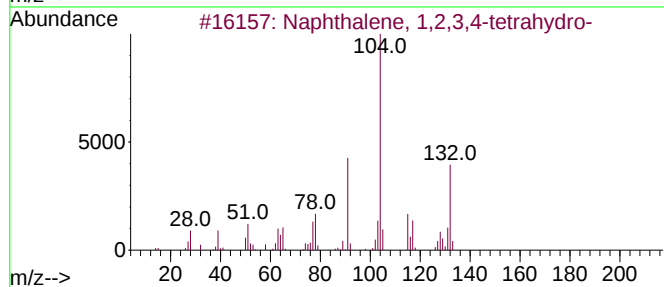
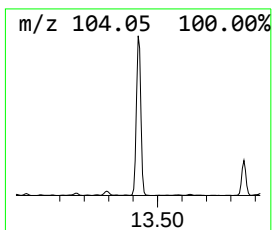
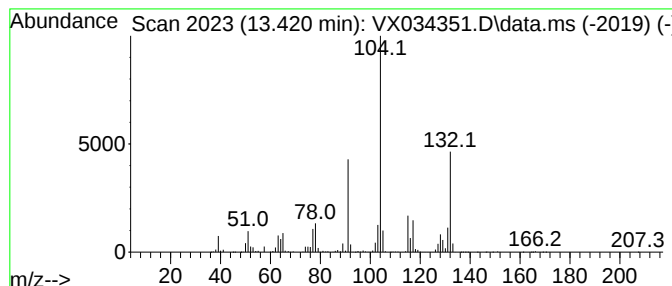
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetrahydro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	215.11 ug/l	7183830	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2			Indan, epoxide	132	C9H8O	000768-22-9	62
3			Benzene, cyclobutyl-	132	C10H12	004392-30-7	59
4			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	50
5			Benzene, 3-cyclohexen-1-yl-	158	C12H14	004994-16-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034351.D
Acq On : 06 Mar 2023 15:47
Operator : JC/MD
Sample : 01816-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2325

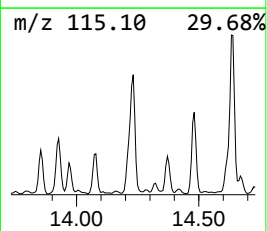
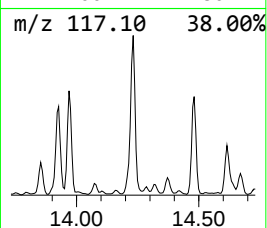
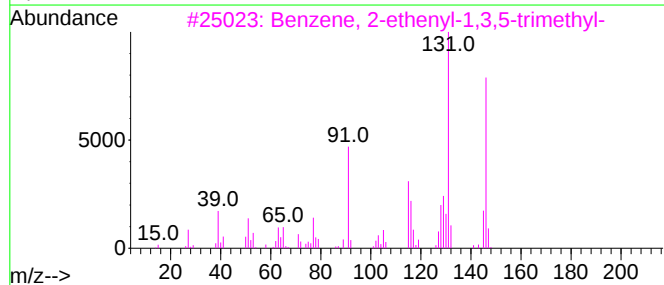
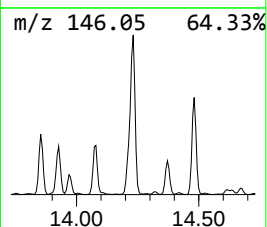
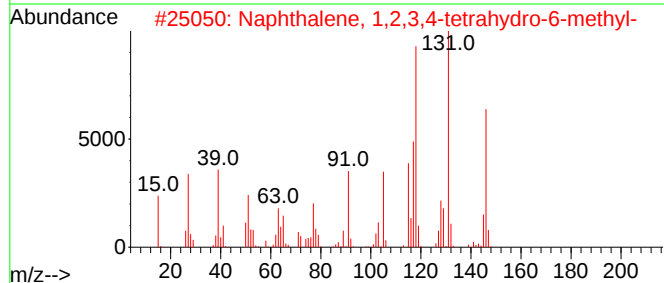
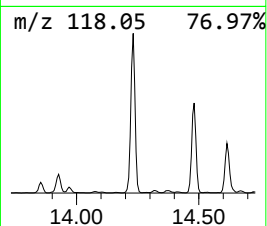
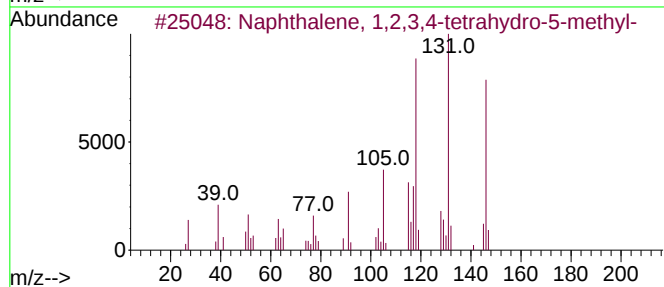
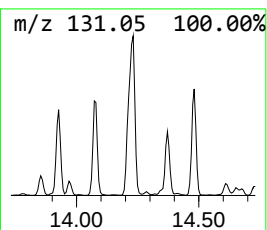
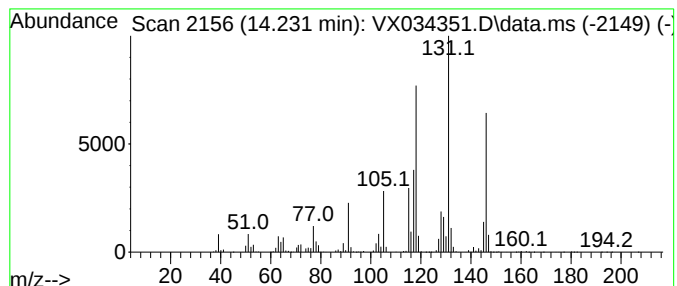
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.231	153.41 ug/l	5123310	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	97
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	96
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	78
4			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	60
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034351.D
Acq On : 06 Mar 2023 15:47
Operator : JC/MD
Sample : 01816-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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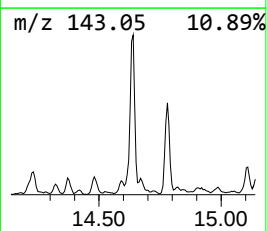
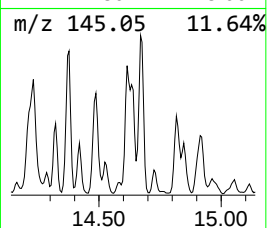
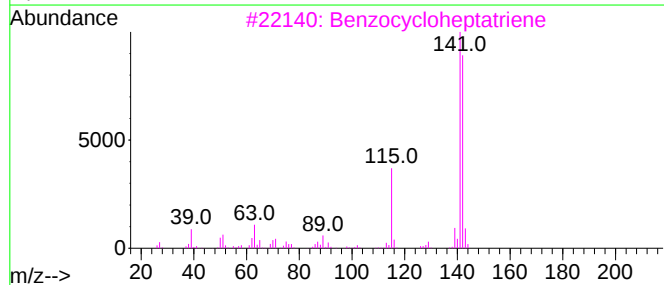
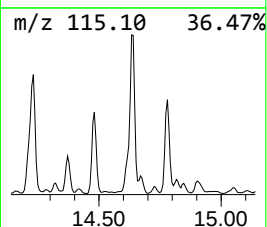
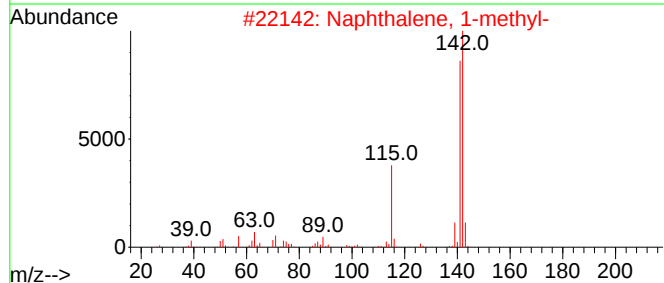
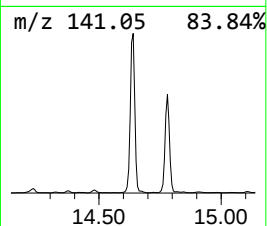
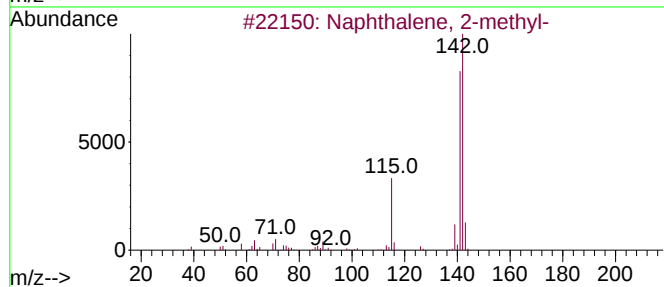
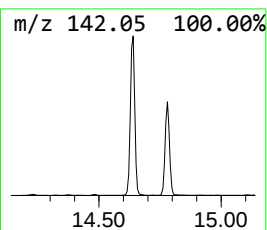
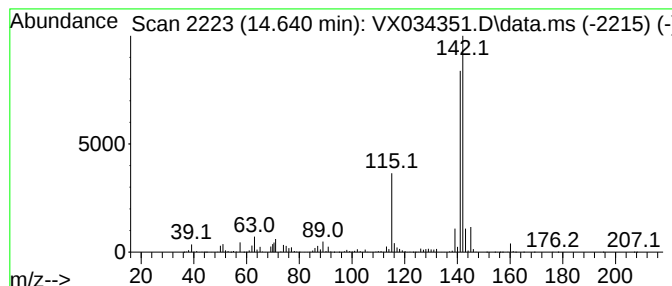
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzocycloheptatriene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	121.45 ug/l	4055910	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	90
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034351.D
Acq On : 06 Mar 2023 15:47
Operator : JC/MD
Sample : 01816-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2325

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.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
Ethanol	2.154	4697.2	ug/l	71930800	1	5.550	765673	50.0
Benzene, 1-ethy...	11.378	264.7	ug/l	8839950	4	12.024	1669810	50.0
Benzene, 1-ethy...	11.610	122.0	ug/l	4074690	4	12.024	1669810	50.0
Indane	12.244	139.9	ug/l	4673070	4	12.024	1669810	50.0
o-Cymene	12.317	104.6	ug/l	3492310	4	12.024	1669810	50.0
1H-Indene, 2,3-...	13.292	282.2	ug/l	9423890	4	12.024	1669810	50.0
Naphthalene, 1,...	13.420	215.1	ug/l	7183830	4	12.024	1669810	50.0
Naphthalene, 1,...	14.231	153.4	ug/l	5123310	4	12.024	1669810	50.0
Benzocyclohepta...	14.640	121.5	ug/l	4055910	4	12.024	1669810	50.0