

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
 Data File : VX025441.D
 Acq On : 02 Dec 2021 20:14
 Operator : JC/MD
 Sample : M4917-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-27

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\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025441.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	42	rBV	151711	350614	9.88%	1.797%
2	1.971	138	145	155	rVV2	22914	41489	1.17%	0.213%
3	2.215	180	185	196	rVB	45772	70010	1.97%	0.359%
4	2.752	258	273	282	rBV	25205	49484	1.39%	0.254%
5	2.867	282	292	300	rVV2	16185	35588	1.00%	0.182%
6	2.965	300	308	323	rVV	138342	299091	8.43%	1.533%
7	3.117	324	333	348	rVB	203789	465881	13.13%	2.388%
8	3.764	428	439	446	rBV2	13758	46565	1.31%	0.239%
9	4.318	517	530	540	rBV3	15989	50842	1.43%	0.261%
10	5.196	663	674	687	rBV2	11851	35867	1.01%	0.184%
11	5.391	694	706	715	rBV	64987	185999	5.24%	0.954%
12	5.556	724	733	749	rVB	104266	295730	8.34%	1.516%
13	5.964	789	800	804	rBV	66805	170788	4.81%	0.876%
14	6.044	804	813	830	rVB	1339639	3547974	100.00%	18.189%
15	6.769	921	932	942	rBV	164639	401802	11.32%	2.060%
16	8.427	1198	1204	1211	rBV	21238	36320	1.02%	0.186%
17	8.653	1234	1241	1247	rBV	345567	542375	15.29%	2.781%
18	8.720	1247	1252	1261	rVB	155773	238454	6.72%	1.222%
19	9.458	1364	1373	1387	rBV2	34550	61843	1.74%	0.317%
20	10.055	1460	1471	1484	rBV	348455	491030	13.84%	2.517%
21	10.195	1488	1494	1505	rVV	1487721	1930847	54.42%	9.899%
22	10.305	1506	1512	1520	rVB	1086372	1396930	39.37%	7.162%
23	10.646	1562	1568	1578	rVB	875436	1118546	31.53%	5.734%
24	10.963	1614	1620	1625	rVB	92726	115262	3.25%	0.591%
25	11.085	1634	1640	1649	rBV	287790	369986	10.43%	1.897%
26	11.305	1671	1676	1683	rBV	174829	215867	6.08%	1.107%
27	11.384	1683	1689	1690	rVV	131551	174172	4.91%	0.893%
28	11.402	1690	1692	1696	rVV	174426	186568	5.26%	0.956%
29	11.451	1696	1700	1705	rVB	58933	75684	2.13%	0.388%
30	11.616	1721	1727	1736	rBV	390253	471071	13.28%	2.415%
31	11.756	1744	1750	1756	rVB	1076005	1330612	37.50%	6.822%
32	12.024	1789	1794	1799	rBV	385931	464795	13.10%	2.383%
33	12.091	1799	1805	1810	rVB	467441	574857	16.20%	2.947%
34	12.244	1823	1830	1838	rBV	576311	721791	20.34%	3.700%
35	12.317	1838	1842	1850	rVB3	36318	56160	1.58%	0.288%
36	12.414	1852	1858	1862	rBV2	50348	64676	1.82%	0.332%

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Stop Thrs : 0

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

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37	12.463	1862	1866	1873	rVB	33328	41269	1.16%	0.212%
38	12.530	1873	1877	1880	rBV	53726	77102	2.17%	0.395%
39	12.616	1886	1891	1894	rVV	119518	141820	4.00%	0.727%
40	12.646	1894	1896	1900	rVV	34534	37333	1.05%	0.191%
41	12.701	1900	1905	1913	rVB2	112810	157876	4.45%	0.809%
42	12.847	1924	1929	1934	rVB2	40042	51710	1.46%	0.265%
43	12.920	1934	1941	1945	rBV	87245	112654	3.18%	0.578%
44	12.963	1945	1948	1954	rVB	117738	138659	3.91%	0.711%
45	13.170	1978	1982	1992	rVB	82549	105631	2.98%	0.542%
46	13.292	1997	2002	2007	rVB2	239278	321246	9.05%	1.647%
47	13.426	2019	2024	2032	rVB	74129	96188	2.71%	0.493%
48	13.585	2047	2050	2055	rVB4	24670	38215	1.08%	0.196%
49	13.664	2061	2063	2071	rVB2	29052	47744	1.35%	0.245%
50	13.780	2073	2082	2089	rBV	424425	551624	15.55%	2.828%
51	14.219	2150	2154	2160	rBV2	26767	52395	1.48%	0.269%
52	14.481	2192	2197	2203	rBV2	25320	40623	1.14%	0.208%
53	14.640	2209	2223	2227	rBV	148858	201666	5.68%	1.034%
54	14.780	2240	2246	2255	rBV	227347	301286	8.49%	1.545%
55	15.481	2355	2361	2375	rVB	51027	88176	2.49%	0.452%
56	15.615	2375	2383	2387	rBV	72637	121794	3.43%	0.624%
57	15.652	2387	2389	2396	rVB	29702	38761	1.09%	0.199%
58	15.841	2411	2420	2431	rVB2	19301	56584	1.59%	0.290%

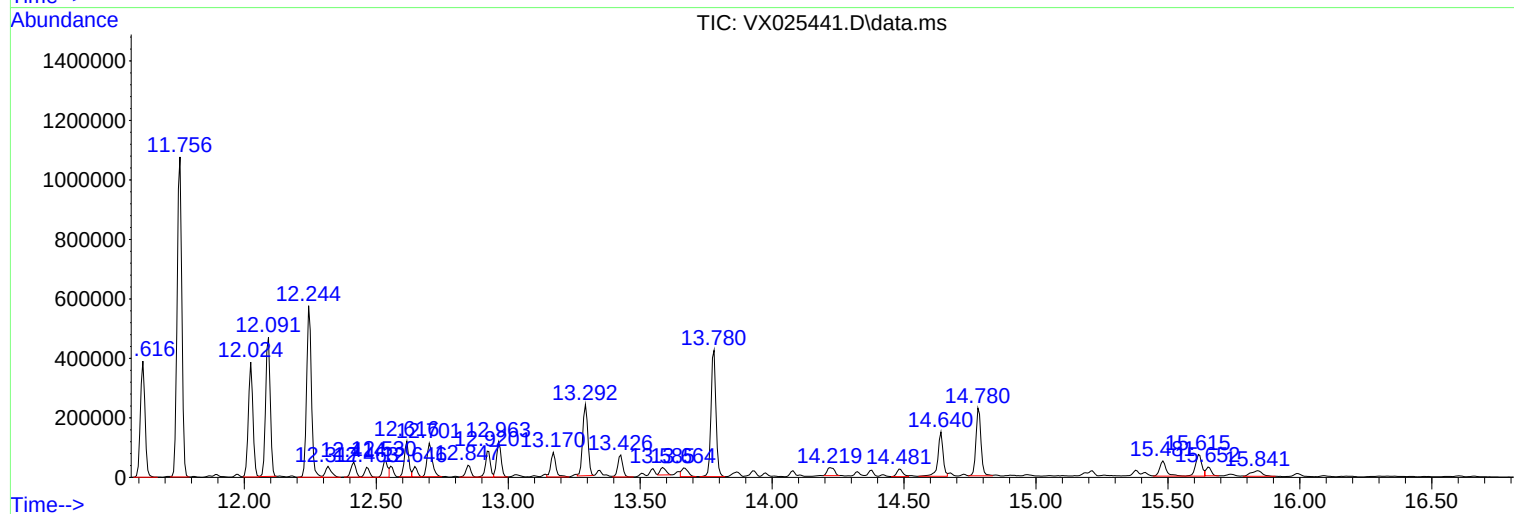
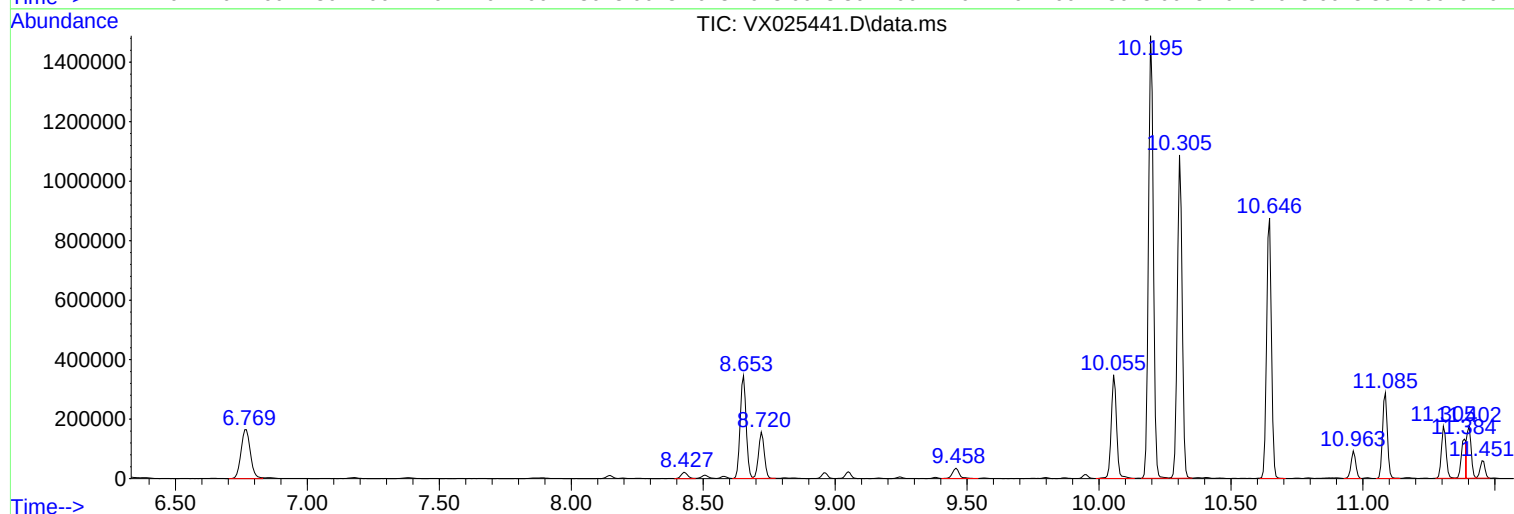
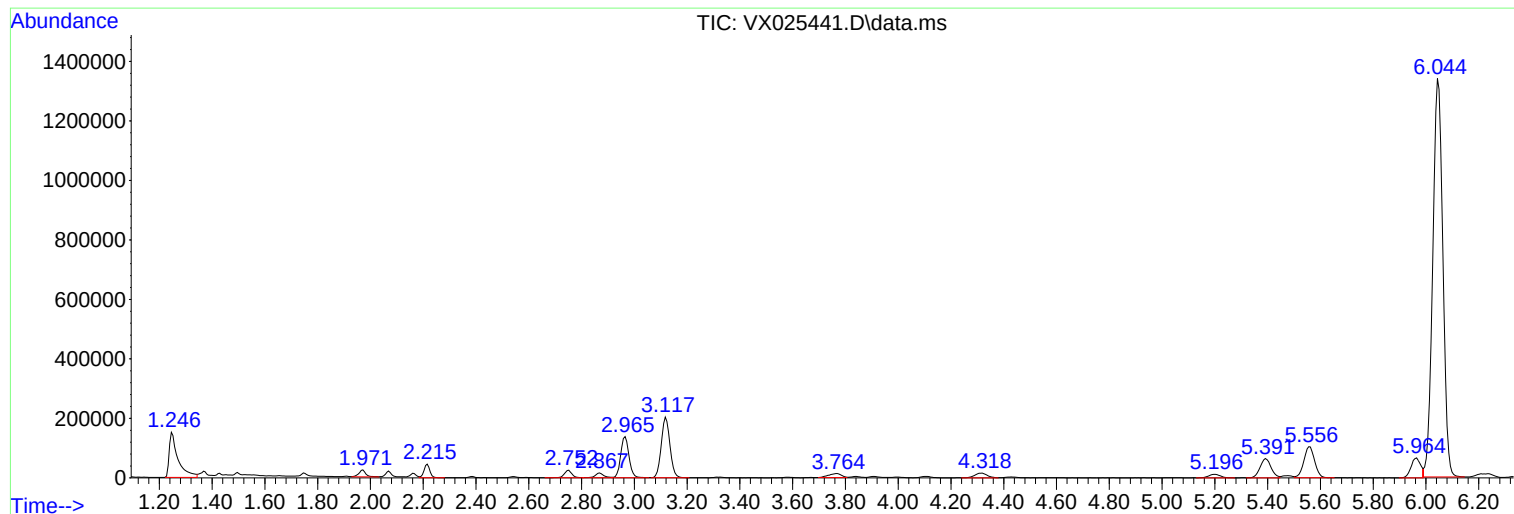
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Quant Title : SW846 8260

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



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Instrument :
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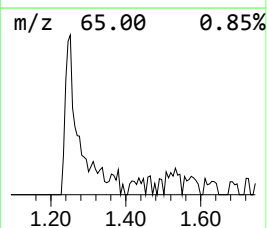
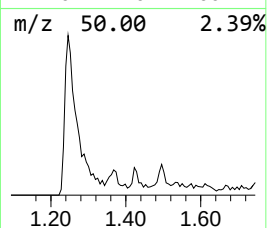
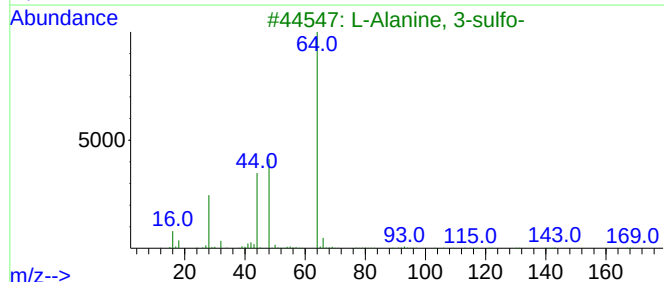
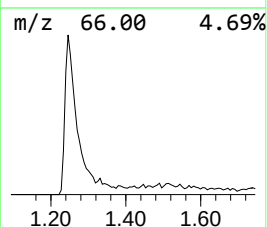
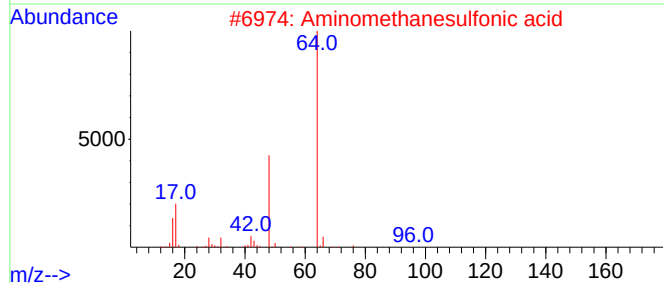
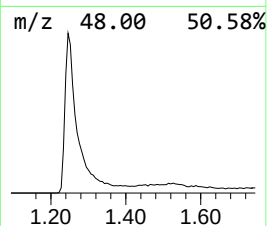
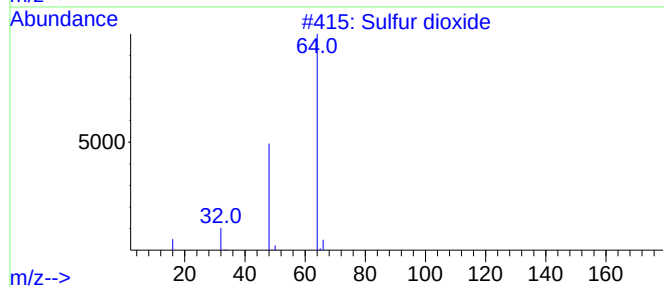
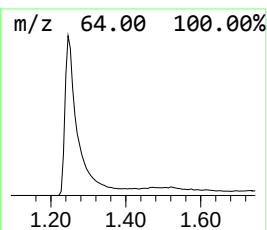
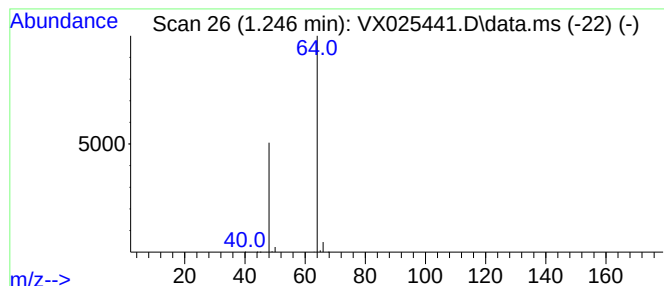
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	59.28 ug/l	350614	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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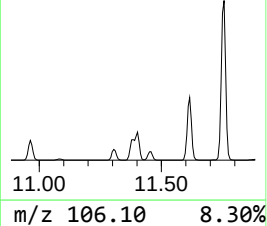
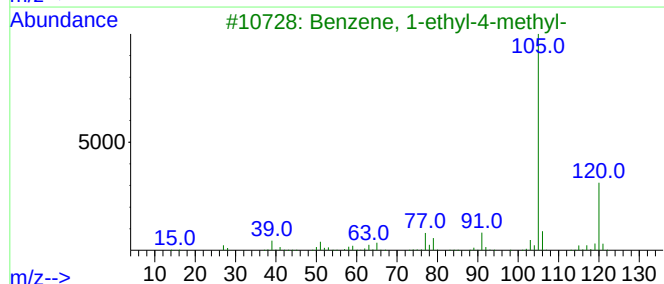
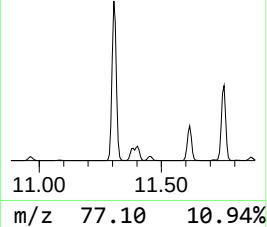
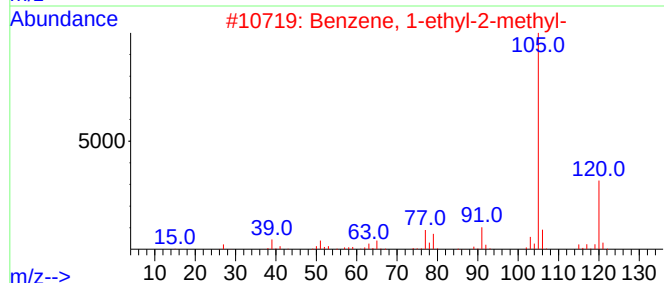
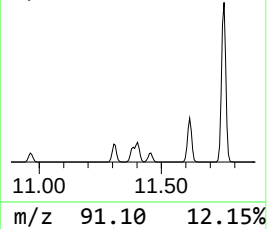
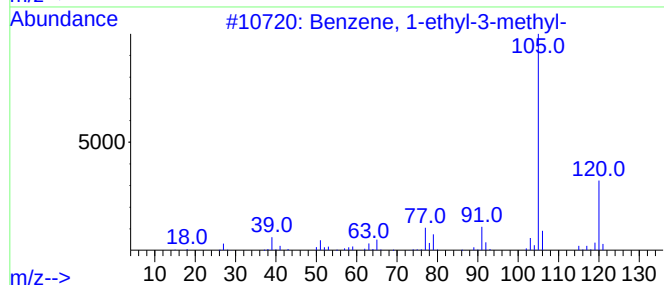
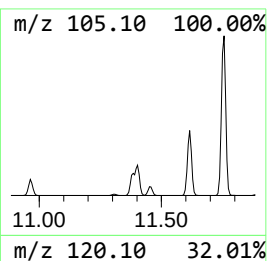
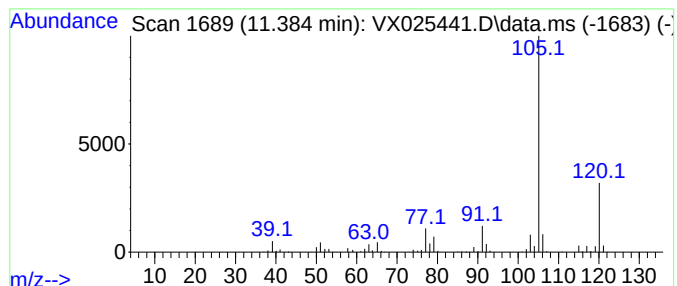
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	18.74 ug/l	174172	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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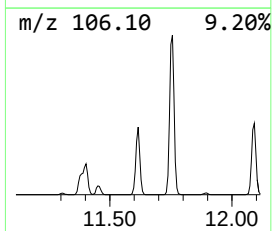
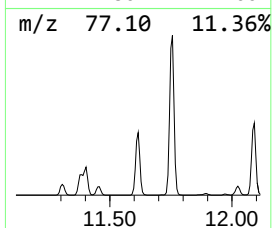
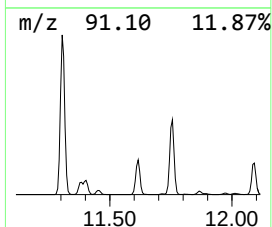
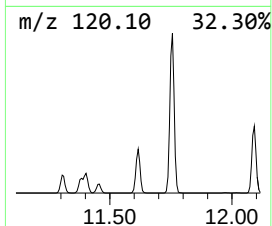
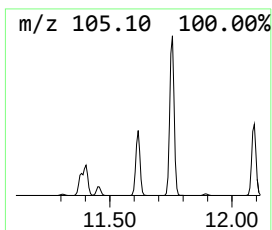
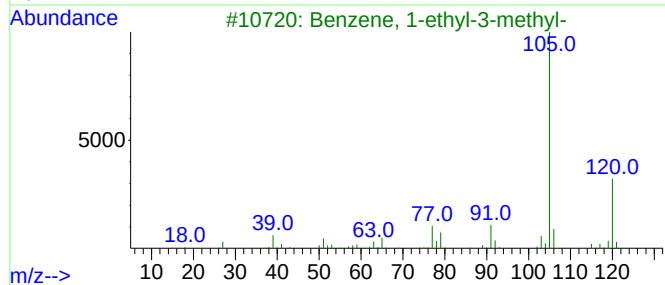
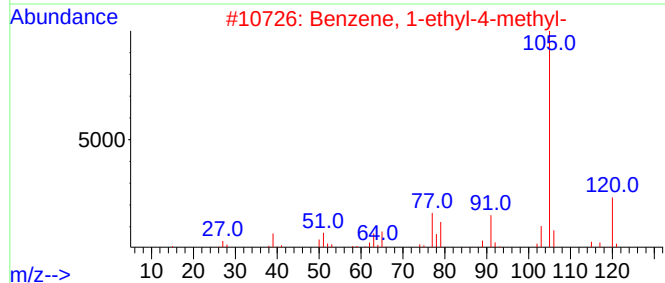
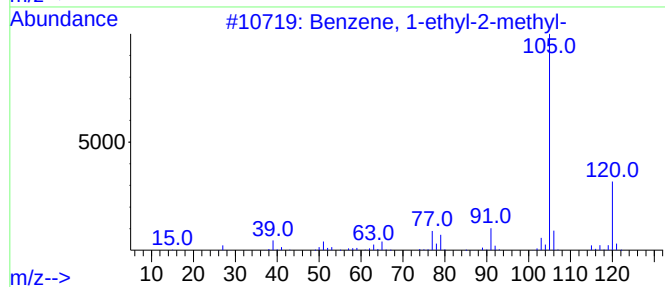
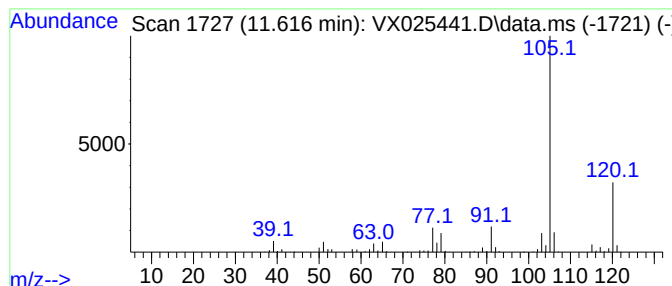
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	50.68 ug/l	471071	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	93
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
4			Mesitylene	120	C9H12	000108-67-8	90
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90



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Instrument :
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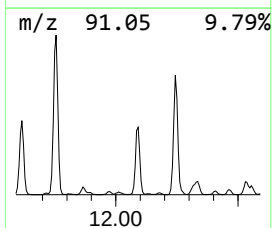
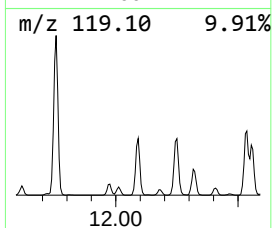
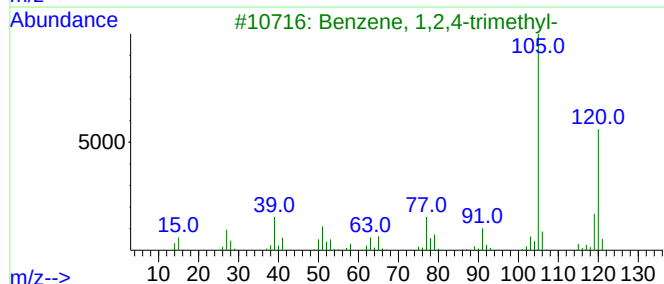
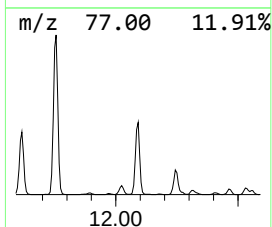
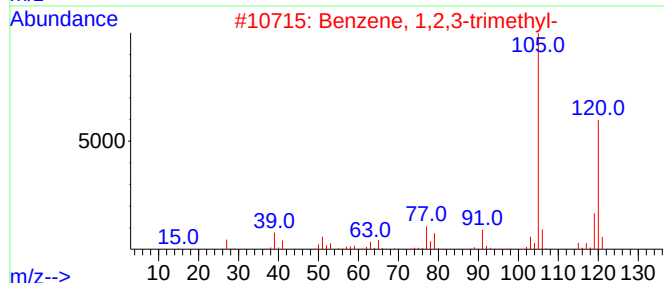
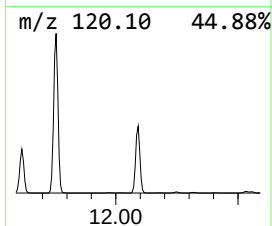
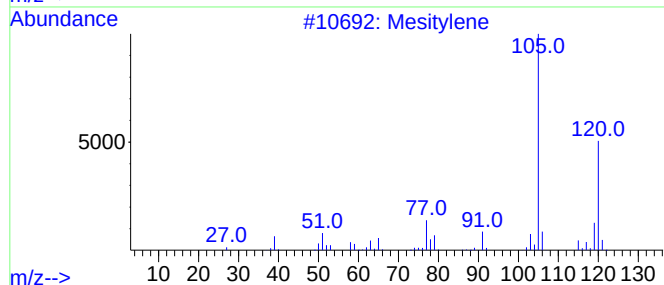
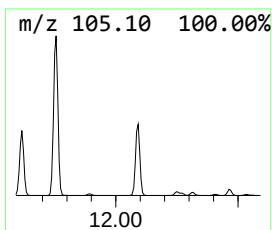
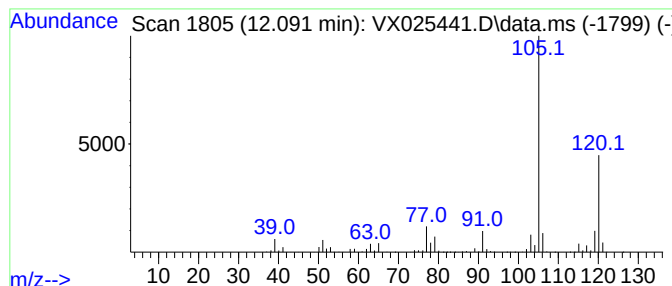
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	61.84 ug/l	574857	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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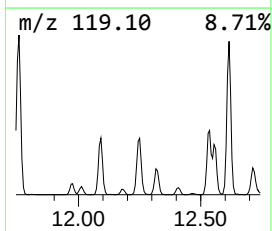
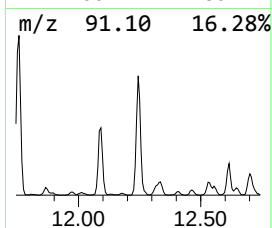
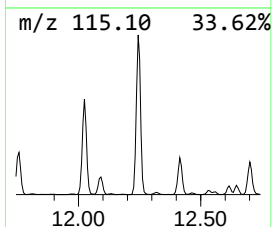
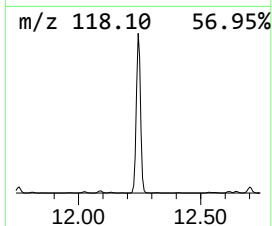
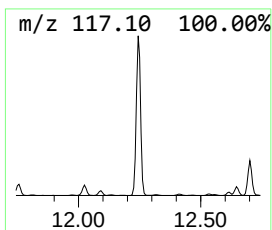
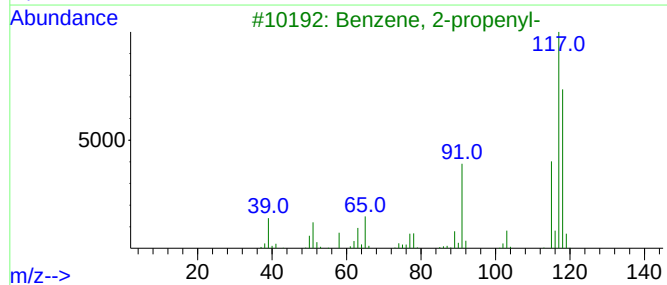
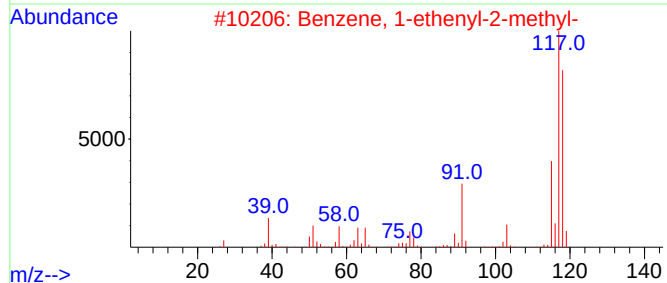
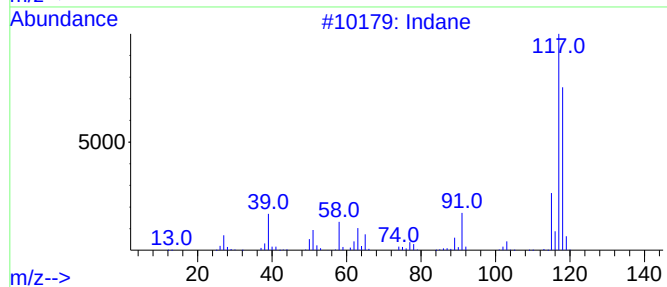
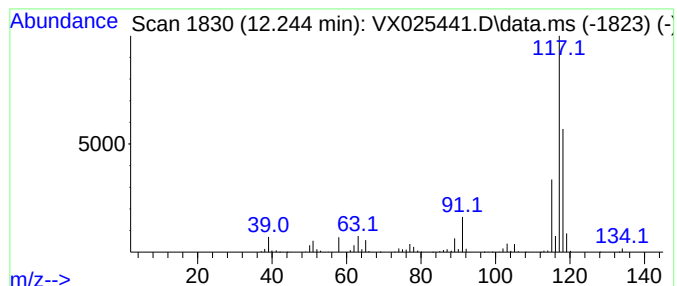
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Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	77.65 ug/l	721791	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, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025441.D
Acq On : 02 Dec 2021 20:14
Operator : JC/MD
Sample : M4917-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-27

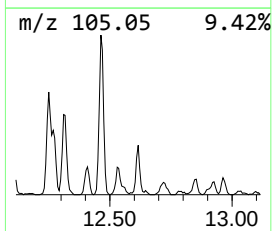
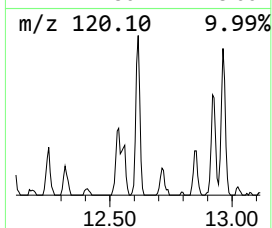
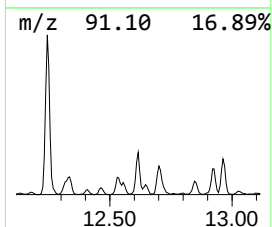
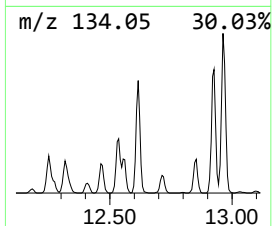
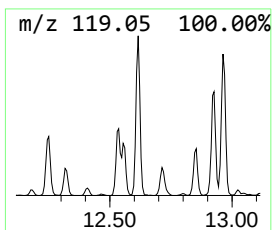
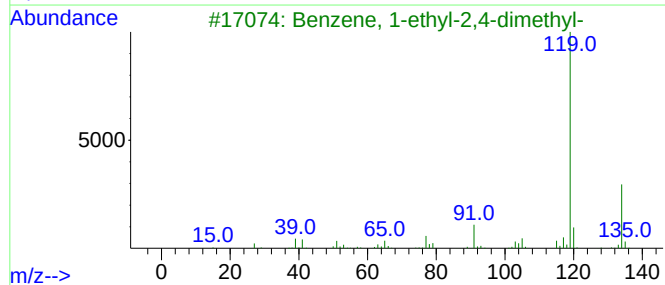
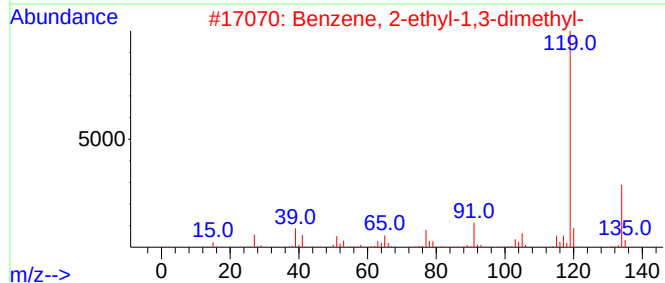
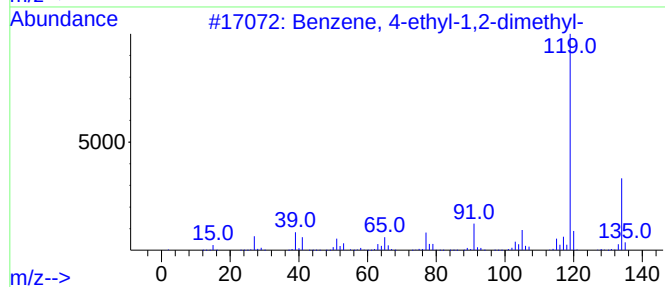
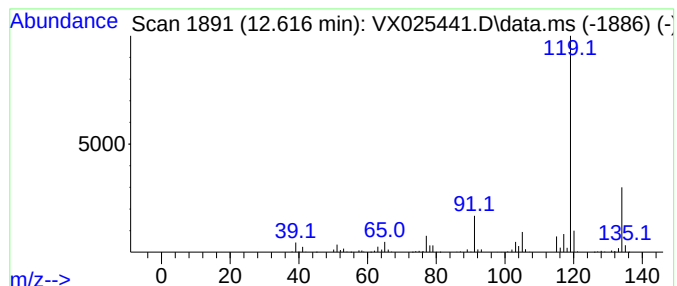
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	15.26 ug/l	141820	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
5			o-Cymene	134	C10H14	000527-84-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025441.D
Acq On : 02 Dec 2021 20:14
Operator : JC/MD
Sample : M4917-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-27

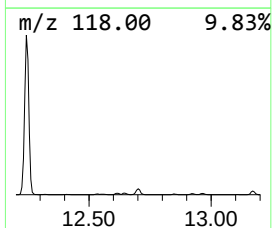
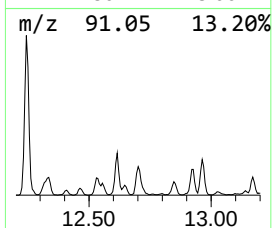
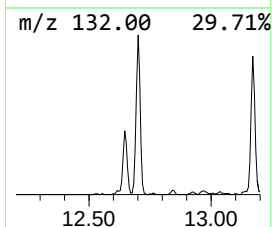
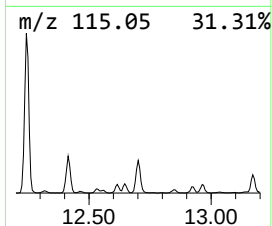
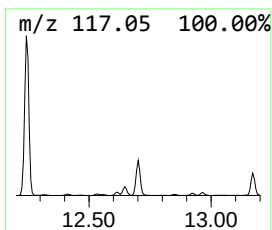
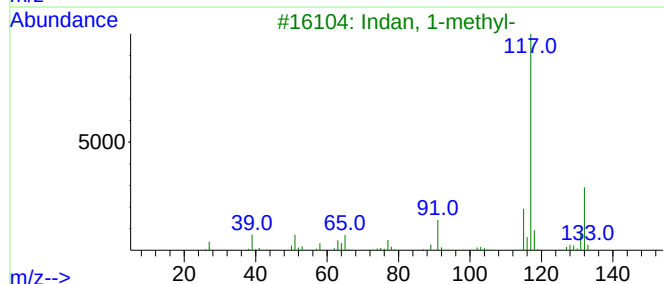
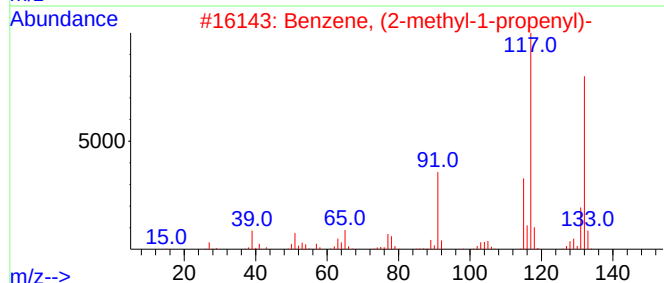
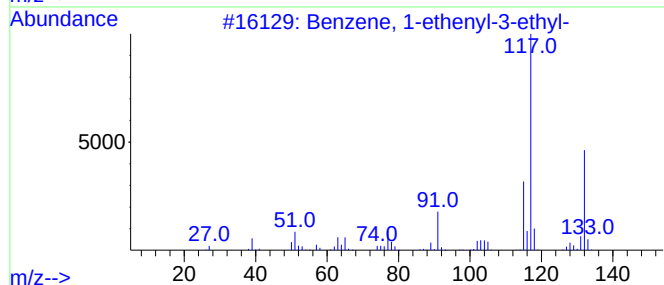
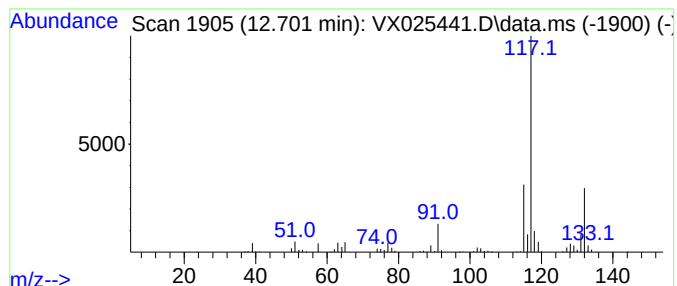
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	16.98 ug/l	157876	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
3			Indan, 1-methyl-	132	C10H12	000767-58-8	87
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025441.D
Acq On : 02 Dec 2021 20:14
Operator : JC/MD
Sample : M4917-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-27

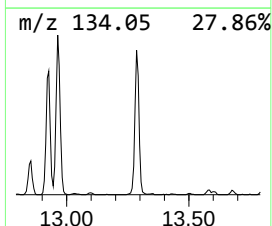
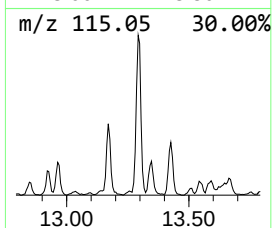
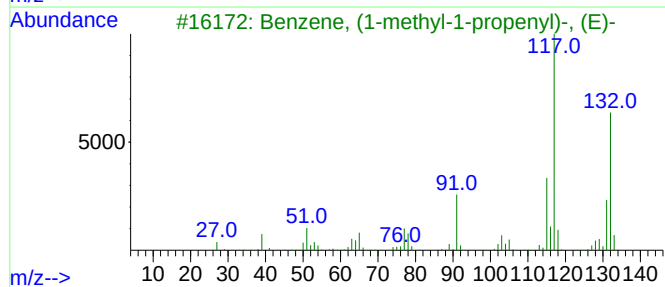
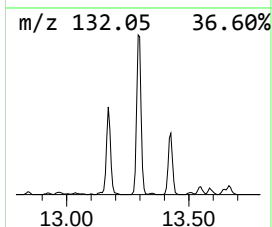
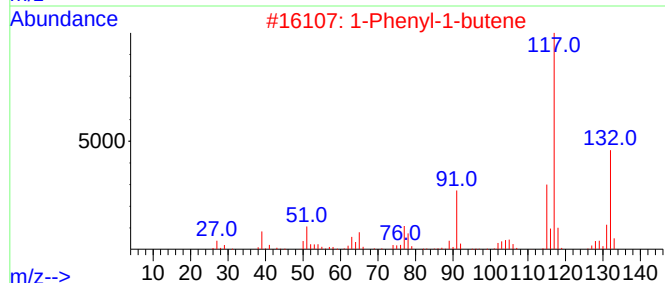
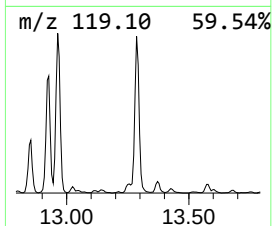
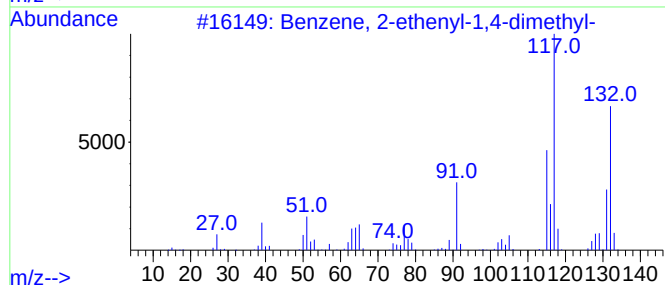
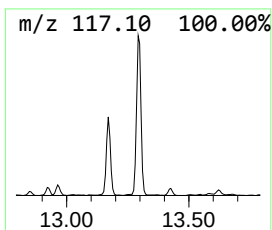
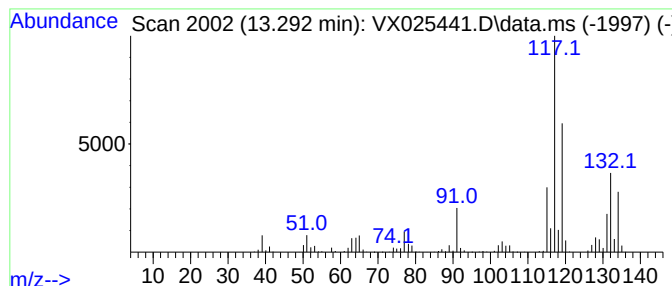
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	34.56 ug/l	321246	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	93
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	86
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025441.D
Acq On : 02 Dec 2021 20:14
Operator : JC/MD
Sample : M4917-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-27

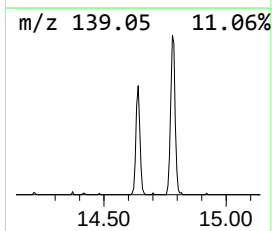
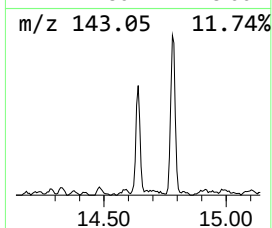
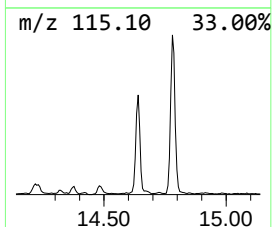
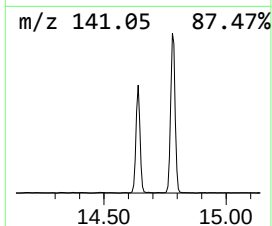
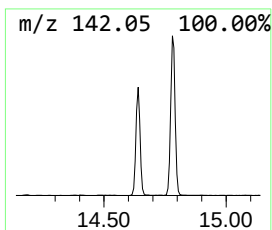
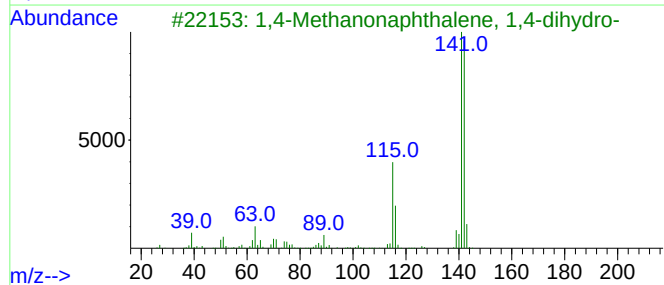
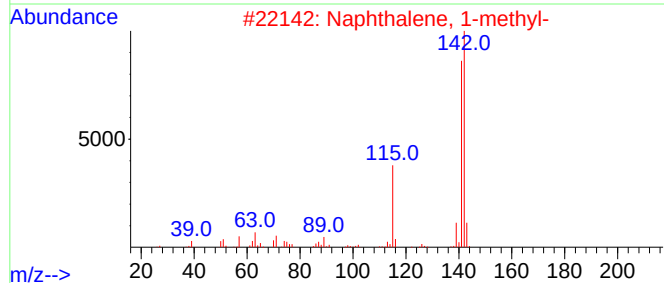
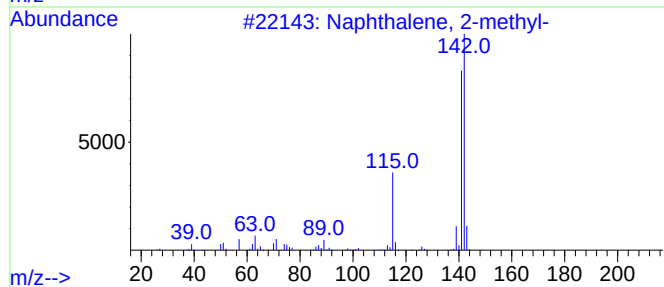
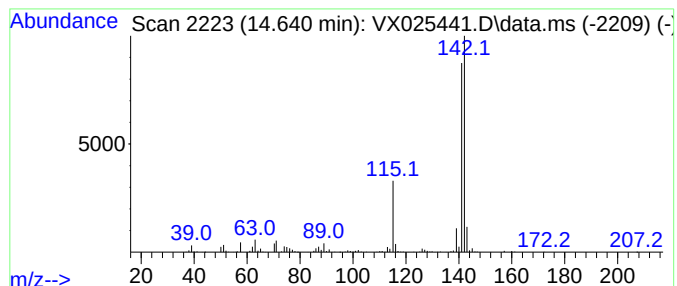
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	21.69 ug/l	201666	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			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025441.D
Acq On : 02 Dec 2021 20:14
Operator : JC/MD
Sample : M4917-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-27

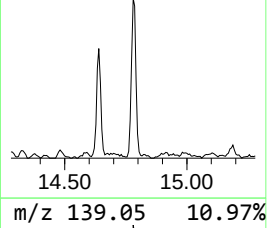
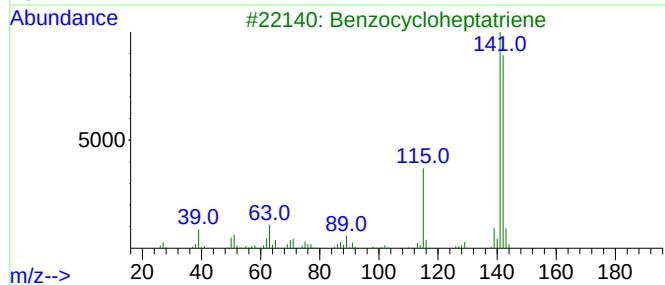
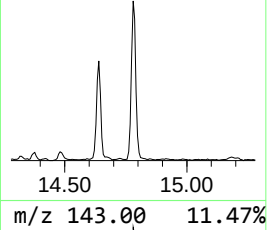
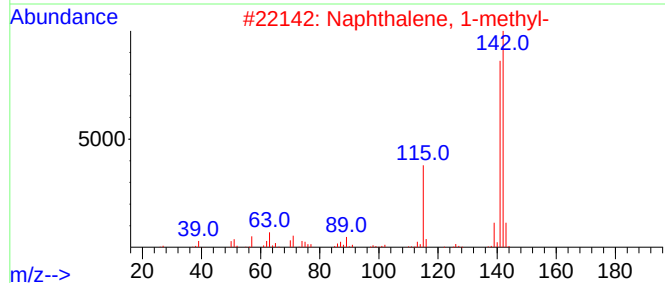
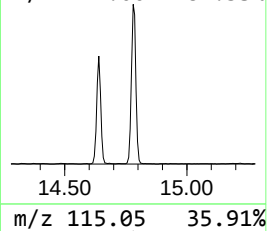
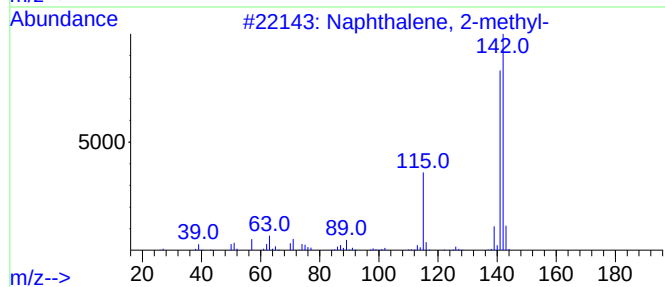
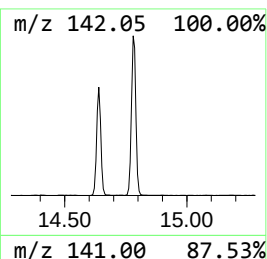
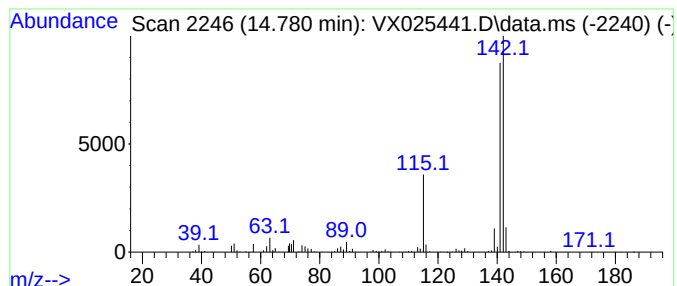
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Quant Title : SW846 8260

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

Peak Number 10 Benzocycloheptatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	32.41 ug/l	301286	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	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025441.D
Acq On : 02 Dec 2021 20:14
Operator : JC/MD
Sample : M4917-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-27

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.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, 1-ethy...	11.384	18.7	ug/l	174172	4	12.024	464795	50.0
Benzene, 1-ethy...	11.616	50.7	ug/l	471071	4	12.024	464795	50.0
Benzene, 1,2,3-...	12.091	61.8	ug/l	574857	4	12.024	464795	50.0
Indane	12.244	77.7	ug/l	721791	4	12.024	464795	50.0
Benzene, 4-ethy...	12.616	15.3	ug/l	141820	4	12.024	464795	50.0
Benzene, 1-ethe...	12.701	17.0	ug/l	157876	4	12.024	464795	50.0
Benzene, 2-ethe...	13.292	34.6	ug/l	321246	4	12.024	464795	50.0
Naphthalene, 1-...	14.640	21.7	ug/l	201666	4	12.024	464795	50.0
Benzocyclohepta...	14.780	32.4	ug/l	301286	4	12.024	464795	50.0