

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031122\
 Data File : VX027399.D
 Acq On : 11 Mar 2022 14:08
 Operator : JC/MD
 Sample : N1895-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-4

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\82X030822W.M
 Title : SW846 8260

Signal : TIC: VX027399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	23	30	45	rBV	624073	2172012	4.59%	0.868%
2	1.746	104	108	131	rVB2	439649	795092	1.68%	0.318%
3	2.825	280	285	297	rVB	250924	542415	1.15%	0.217%
4	3.099	322	330	344	rVB	216180	490663	1.04%	0.196%
5	4.306	519	528	540	rVB	253955	729527	1.54%	0.291%
6	5.391	691	706	714	rBV	230071	696201	1.47%	0.278%
7	5.556	726	733	741	rVB	301045	746575	1.58%	0.298%
8	5.958	790	799	808	rBV	206614	552265	1.17%	0.221%
9	6.763	923	931	939	rBV	570632	1424739	3.01%	0.569%
10	7.379	1020	1032	1044	rBV3	262660	712892	1.50%	0.285%
11	8.653	1227	1241	1246	rBV	1212139	2002672	4.23%	0.800%
12	8.720	1246	1252	1259	rVB	1965675	2961596	6.25%	1.183%
13	10.055	1466	1471	1476	rBV	1181061	1556661	3.29%	0.622%
14	10.201	1489	1495	1501	rVB	15078406	21023863	44.38%	8.400%
15	10.311	1506	1513	1518	rBV	31377173	47370946	100.00%	18.927%
16	10.646	1562	1568	1582	rVB	13307332	17163244	36.23%	6.857%
17	10.963	1614	1620	1629	rBV	2026229	2480172	5.24%	0.991%
18	11.085	1634	1640	1645	rBV	987479	1231008	2.60%	0.492%
19	11.305	1669	1676	1683	rVB	3968536	4881870	10.31%	1.951%
20	11.384	1683	1689	1696	rBV	12451352	23287023	49.16%	9.304%
21	11.457	1696	1701	1706	rVB	8146915	10119338	21.36%	4.043%
22	11.616	1721	1727	1738	rBV	8429077	10605553	22.39%	4.237%
23	11.756	1744	1750	1755	rBV	24474107	32809563	69.26%	13.109%
24	12.024	1789	1794	1799	rVB	1352632	1714787	3.62%	0.685%
25	12.091	1799	1805	1810	rBV	8103253	9628002	20.32%	3.847%
26	12.244	1825	1830	1838	rBV2	8647226	12833371	27.09%	5.127%
27	12.317	1838	1842	1850	rVB2	2209015	3262460	6.89%	1.303%
28	12.414	1852	1858	1862	rBV2	432027	601318	1.27%	0.240%
29	12.463	1862	1866	1873	rVB2	609337	828410	1.75%	0.331%
30	12.536	1873	1878	1880	rBV	1388552	1976102	4.17%	0.790%
31	12.555	1880	1881	1886	rVB	1062155	992336	2.09%	0.396%
32	12.616	1886	1891	1894	rBV	2811256	3302126	6.97%	1.319%
33	12.646	1894	1896	1900	rVB	436977	482274	1.02%	0.193%
34	12.701	1900	1905	1913	rBV2	1429638	2057171	4.34%	0.822%
35	12.853	1925	1930	1934	rVB	468115	609883	1.29%	0.244%
36	12.927	1934	1942	1945	rBV	1447816	1856788	3.92%	0.742%

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Integrator: RTE

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Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

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Title : SW846 8260

37	12.963	1945	1948	1954	rVB	2173237	2544718	5.37%	1.017%
38	13.170	1974	1982	1987	rBV	1666656	2045380	4.32%	0.817%
39	13.292	1998	2002	2007	rVB2	3150112	4084634	8.62%	1.632%
40	13.426	2019	2024	2032	rVB	747925	943784	1.99%	0.377%
41	13.585	2047	2050	2056	rVB3	372137	615828	1.30%	0.246%
42	13.664	2061	2063	2069	rVB2	329772	503328	1.06%	0.201%
43	13.780	2075	2082	2088	rBV	7107067	8755092	18.48%	3.498%
44	14.640	2219	2223	2233	rVB	2151576	2637800	5.57%	1.054%
45	14.780	2241	2246	2257	rBV	1299245	1656561	3.50%	0.662%

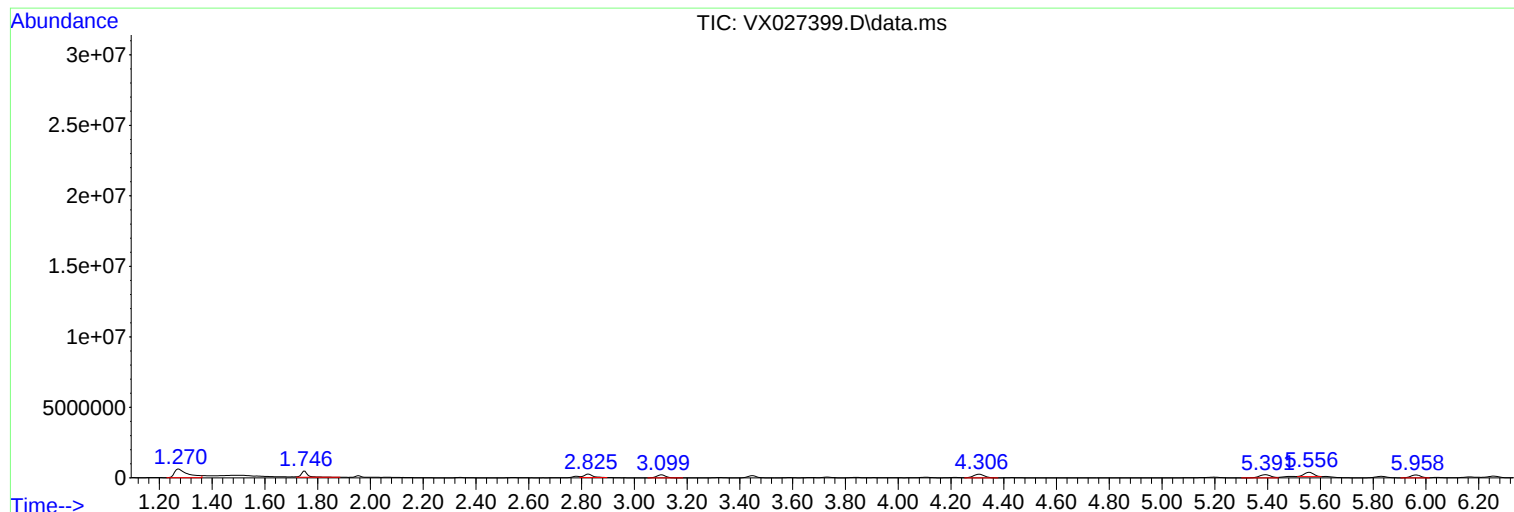
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
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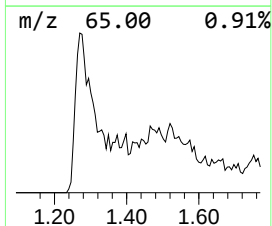
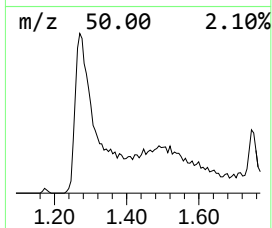
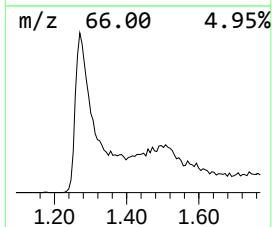
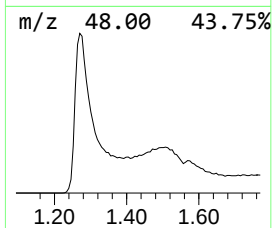
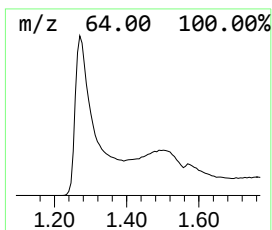
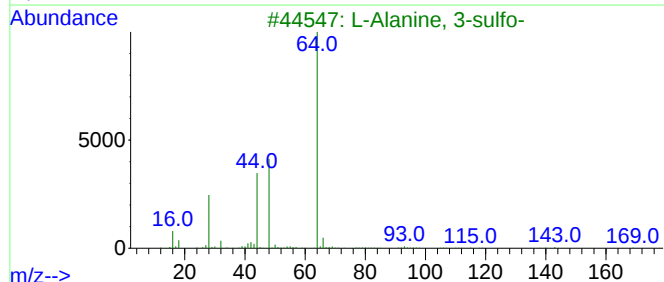
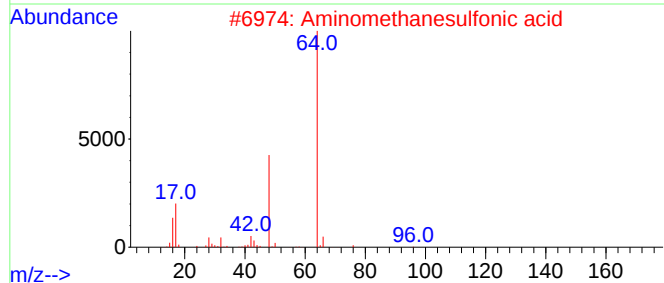
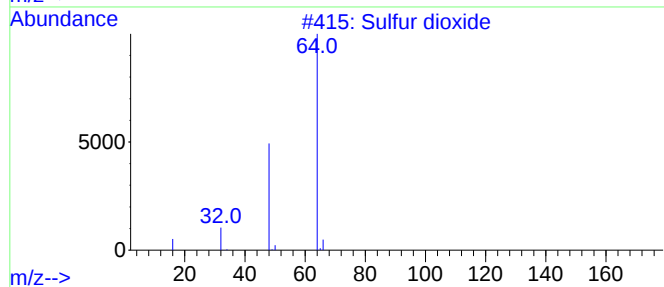
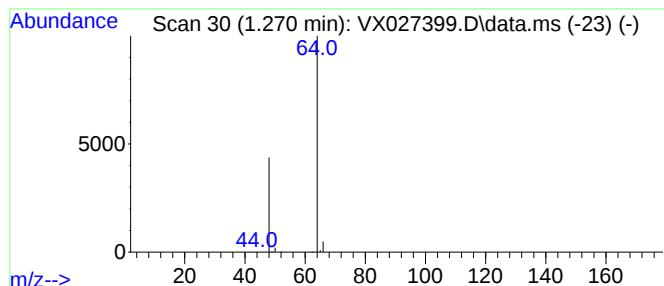
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	145.47 ug/l	2172010	Pentafluorobenzene	5.556

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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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

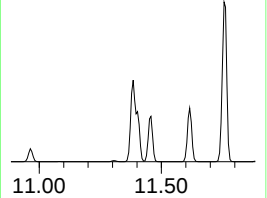
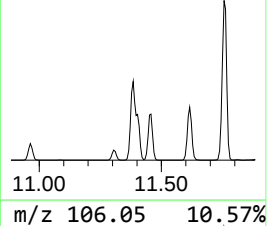
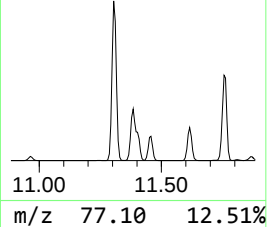
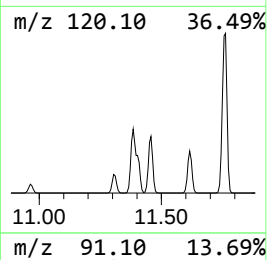
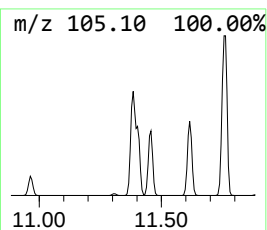
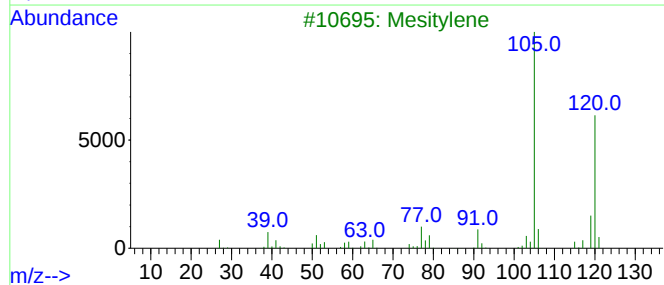
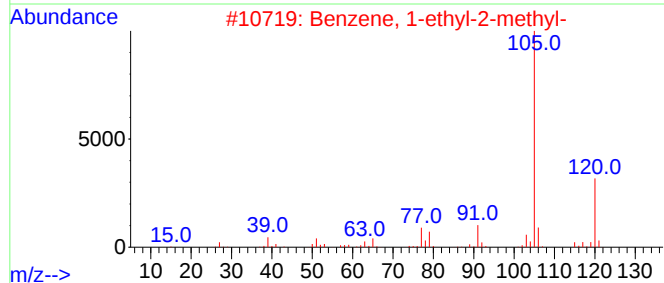
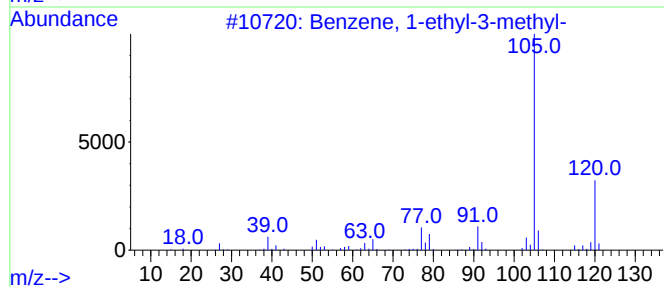
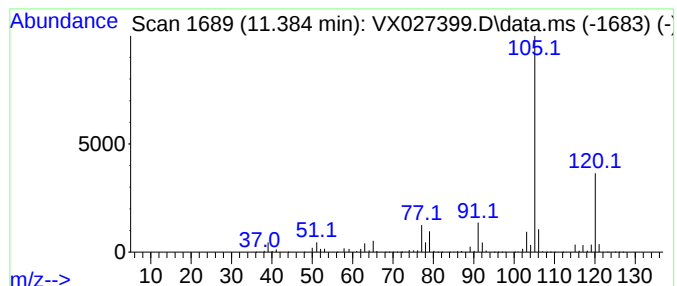
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	679.01 ug/l	23287000	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	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

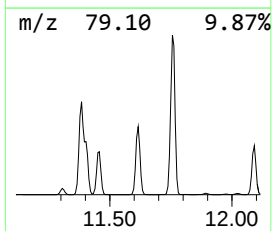
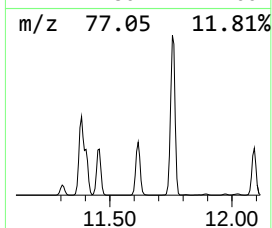
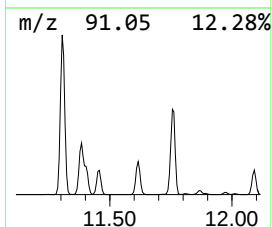
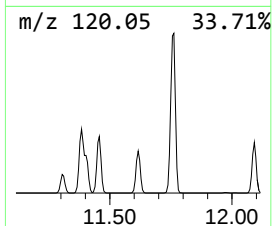
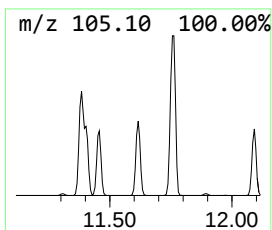
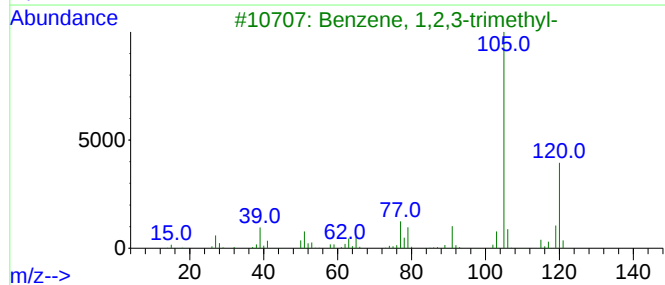
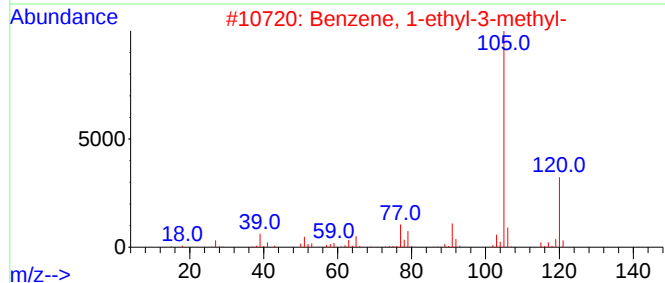
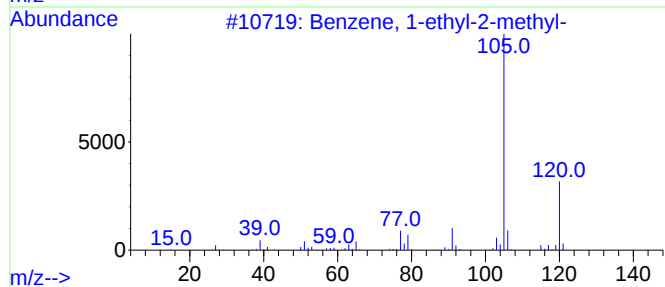
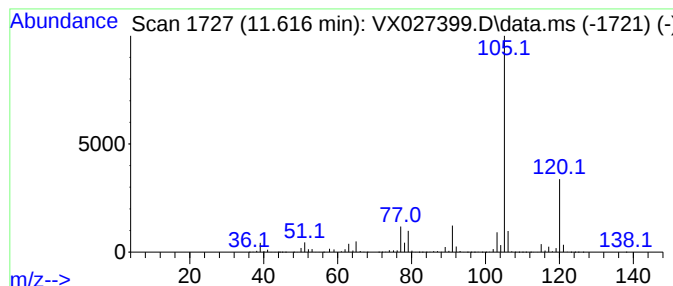
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	309.24 ug/l	10605600	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-3-methyl-	120	C9H12	000620-14-4	91
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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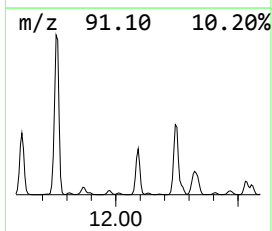
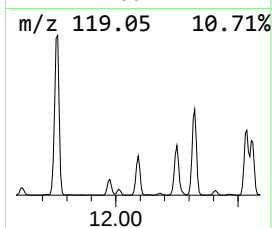
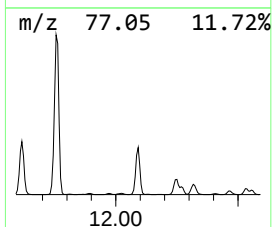
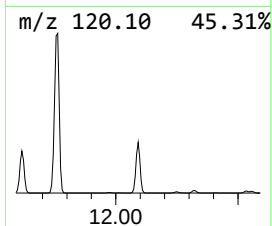
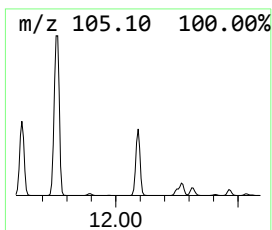
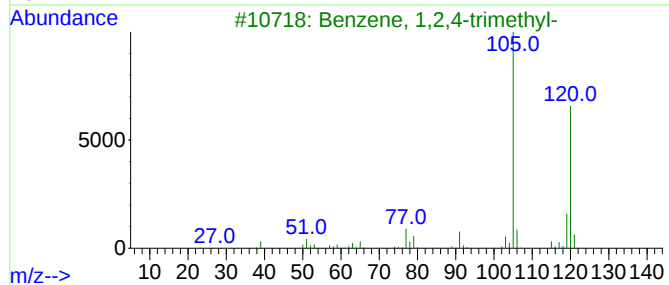
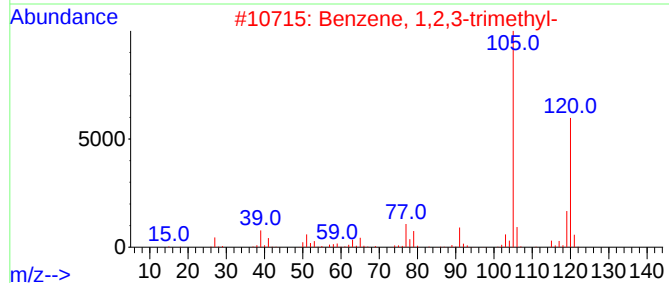
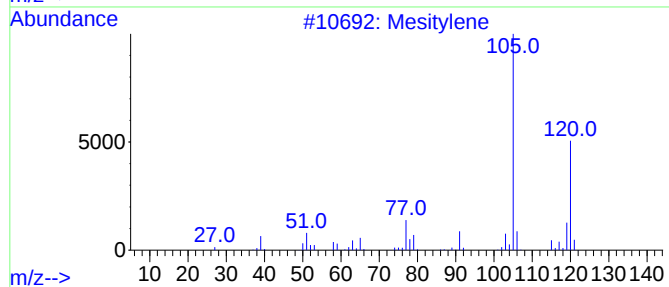
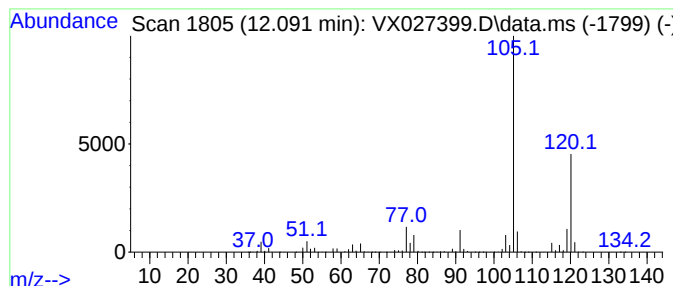
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	280.74 ug/l	9628000	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	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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ClientSampleId :
MW-4

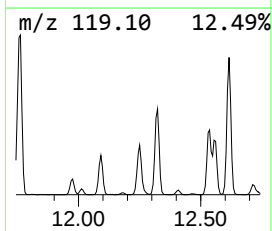
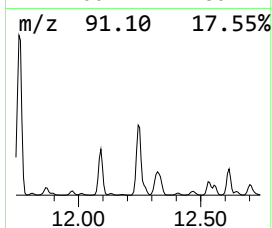
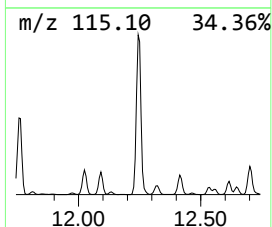
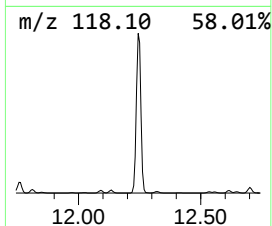
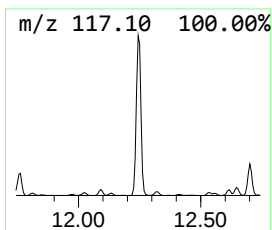
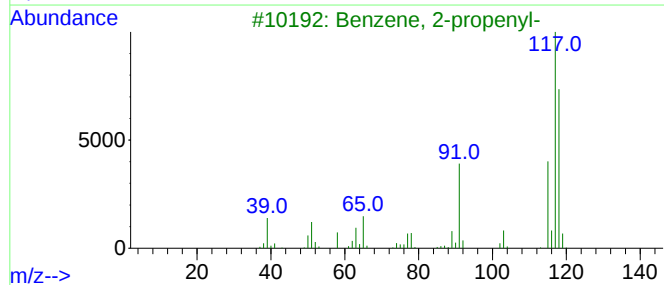
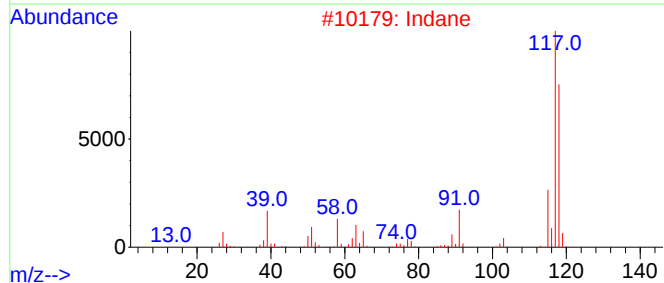
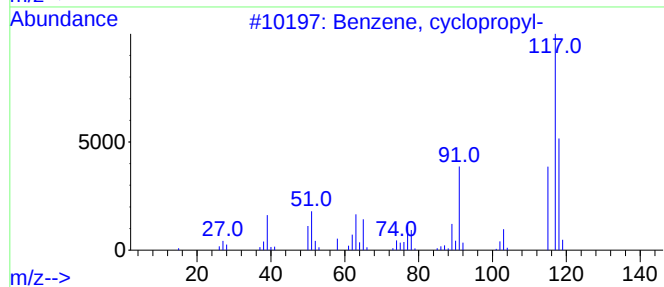
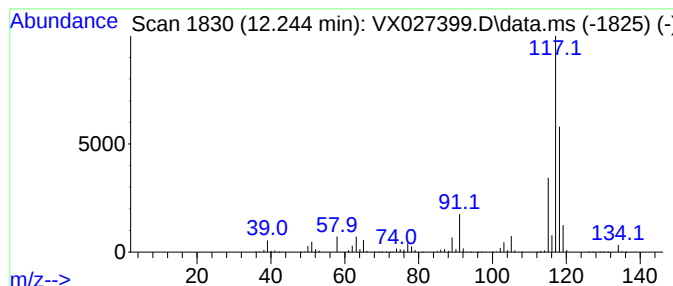
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, cyclopropyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	374.20 ug/l	12833400	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
2			Indane	118	C9H10	000496-11-7	81
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4			Δ-tetralene	118	C9H10	007785-10-6	64
5			Benzeneethanol, .beta.-ethenyl-....	162	C11H14O	040596-14-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031122\
Data File : VX027399.D
Acq On : 11 Mar 2022 14:08
Operator : JC/MD
Sample : N1895-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

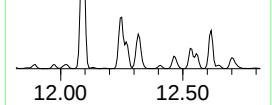
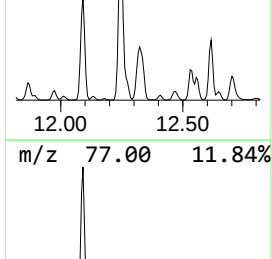
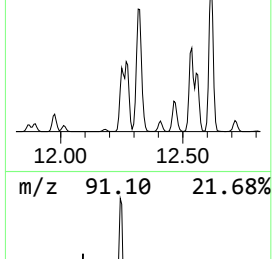
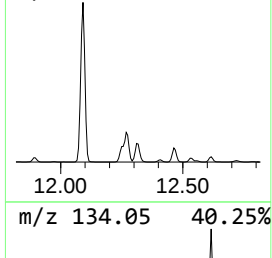
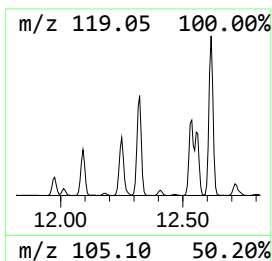
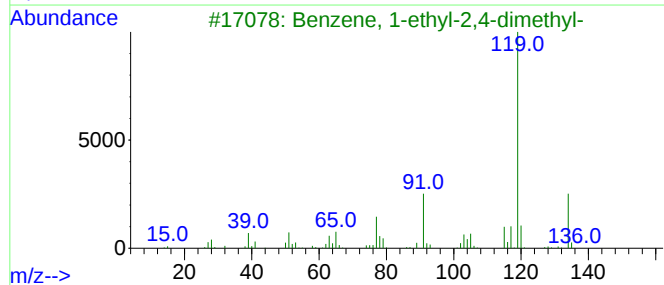
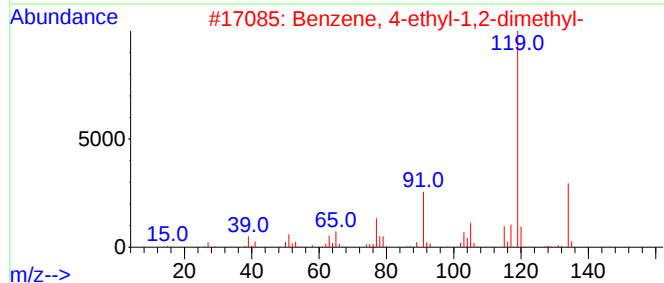
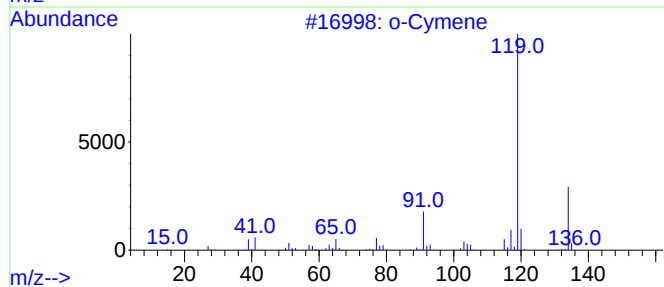
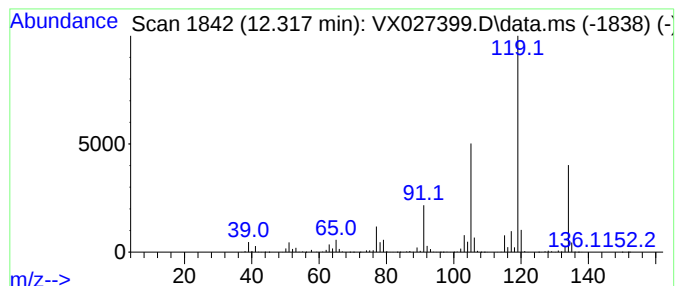
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Quant Title : SW846 8260

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

Peak Number 6 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	95.13 ug/l	3262460	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			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
4			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	93
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031122\
Data File : VX027399.D
Acq On : 11 Mar 2022 14:08
Operator : JC/MD
Sample : N1895-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

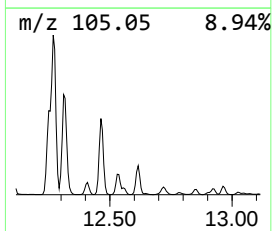
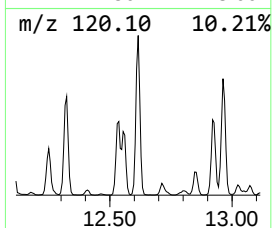
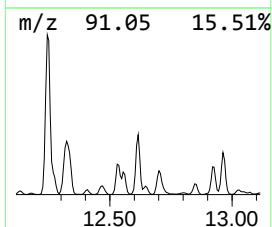
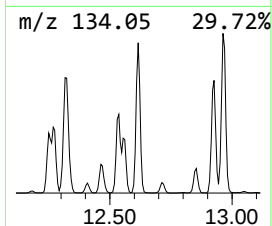
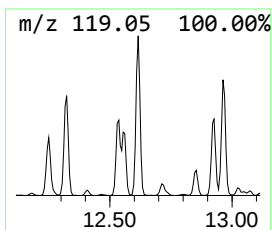
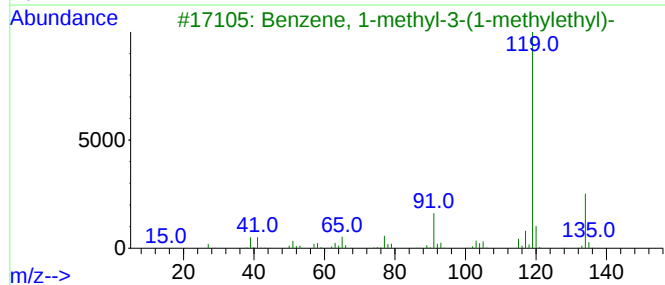
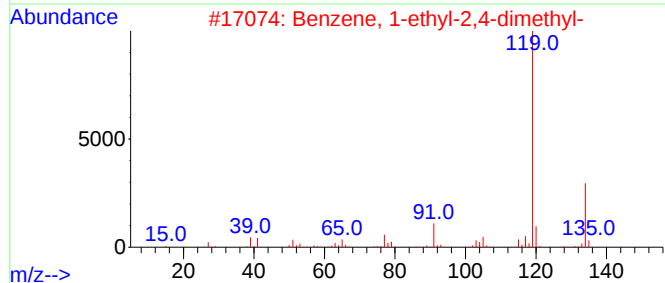
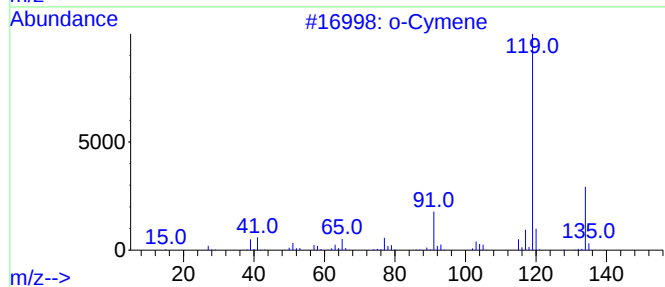
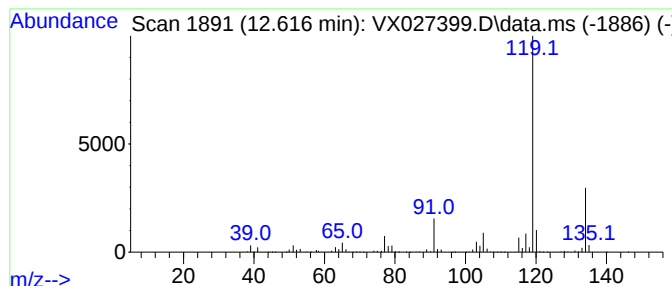
Instrument :
MSVOA_X
ClientSampleId :
MW-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.616	96.28 ug/l	3302130	1,4-Dichlorobenzene-d4			12.024
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	o-Cymene		134	C10H14	000527-84-4	97
2	Benzene, 1-ethyl-2,4-dimethyl-		134	C10H14	000874-41-9	97
3	Benzene, 1-methyl-3-(1-methyleth...		134	C10H14	000535-77-3	95
4	Benzene, 4-ethyl-1,2-dimethyl-		134	C10H14	000934-80-5	95
5	Benzene, 2-ethyl-1,3-dimethyl-		134	C10H14	002870-04-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031122\
Data File : VX027399.D
Acq On : 11 Mar 2022 14:08
Operator : JC/MD
Sample : N1895-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

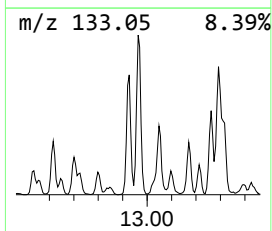
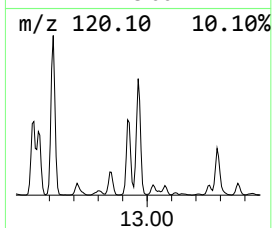
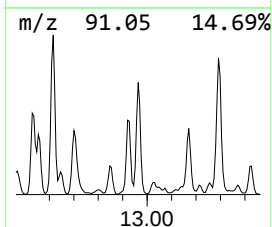
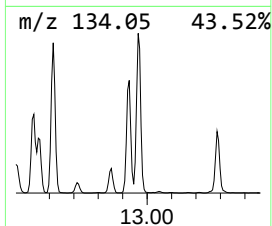
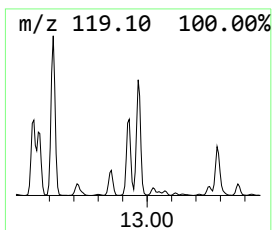
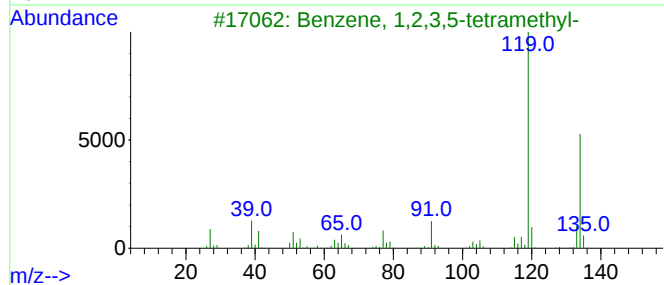
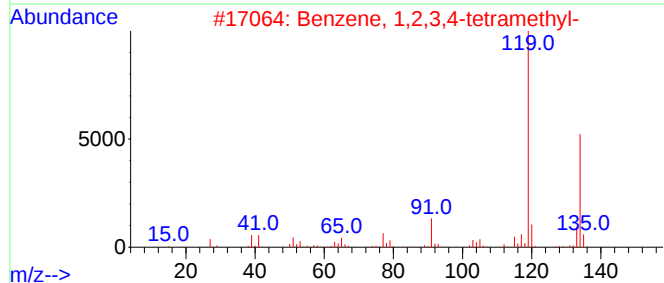
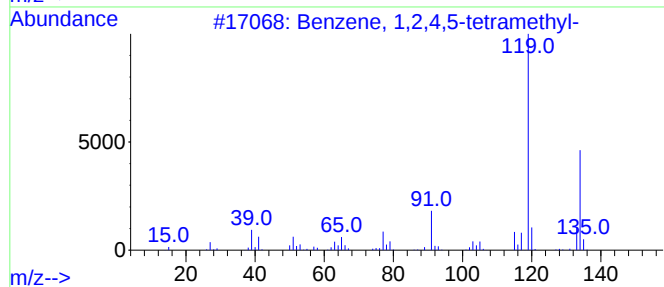
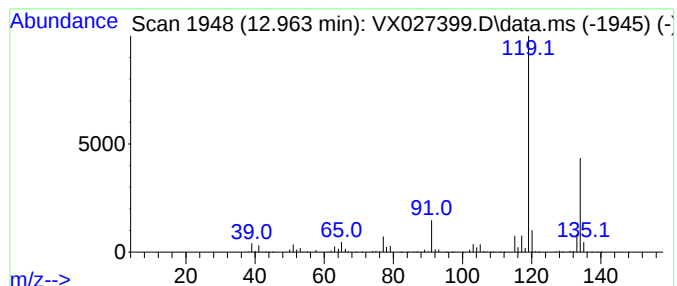
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	74.20 ug/l	2544720	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
4			o-Cymene	134	C10H14	000527-84-4	96
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031122\
Data File : VX027399.D
Acq On : 11 Mar 2022 14:08
Operator : JC/MD
Sample : N1895-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

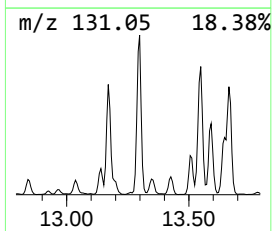
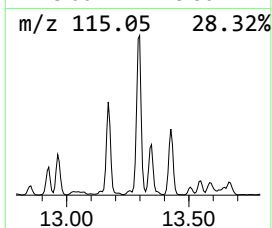
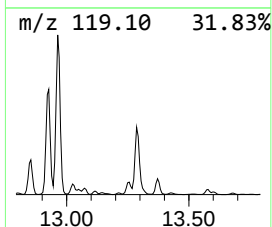
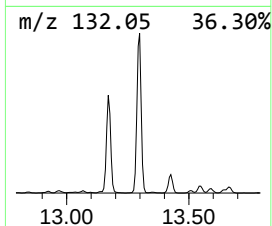
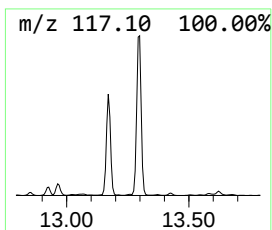
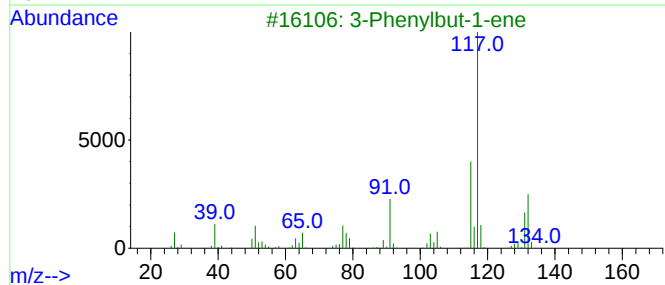
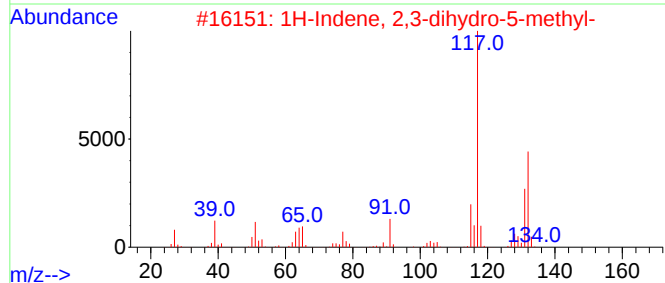
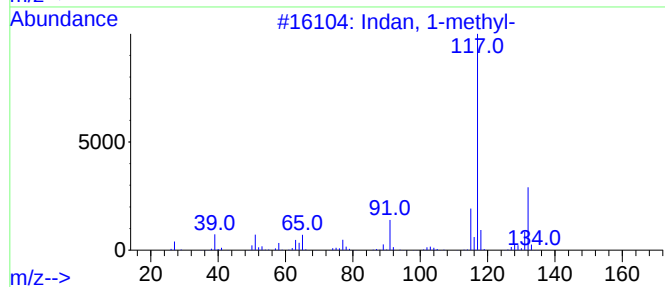
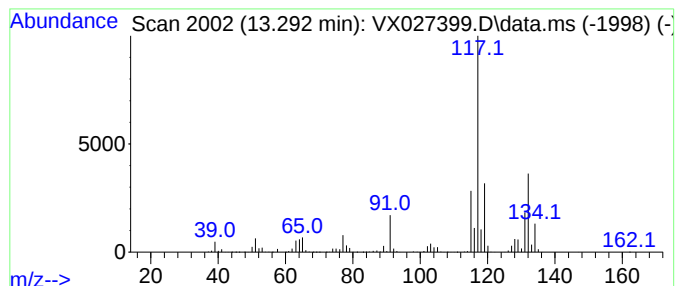
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Quant Title : SW846 8260

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

Peak Number 9 Indan, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	119.10 ug/l	4084630	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	93
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031122\
Data File : VX027399.D
Acq On : 11 Mar 2022 14:08
Operator : JC/MD
Sample : N1895-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

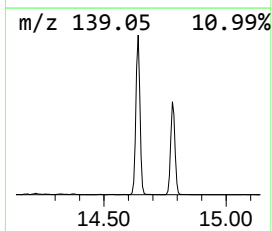
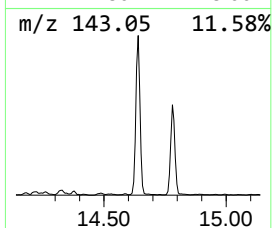
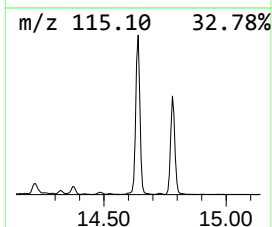
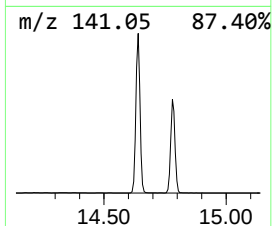
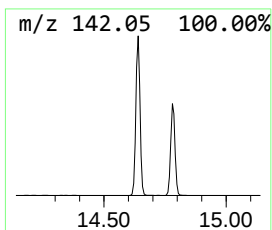
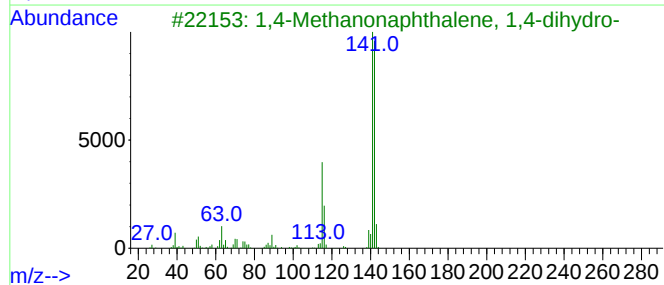
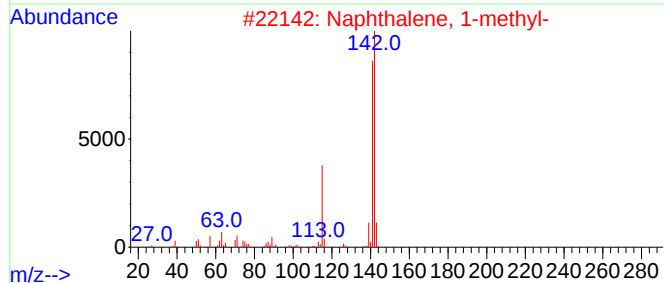
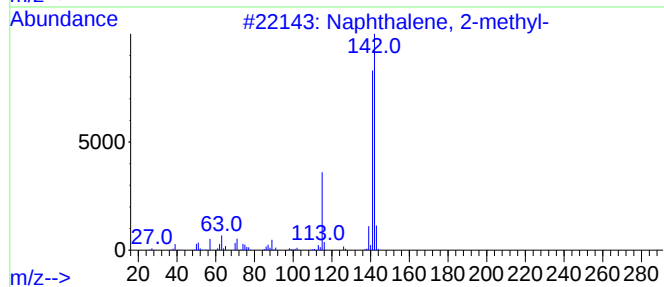
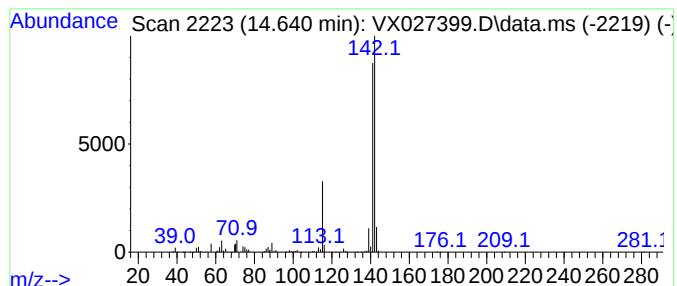
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Quant Title : SW846 8260

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

Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	76.91 ug/l	2637800	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\VX031122\
Data File : VX027399.D
Acq On : 11 Mar 2022 14:08
Operator : JC/MD
Sample : N1895-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.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	679.0	ug/l	23287000	4	12.024	1714790	50.0
Benzene, 1-ethy...	11.616	309.2	ug/l	10605600	4	12.024	1714790	50.0
Benzene, 1-ethy...	12.091	280.7	ug/l	9628000	4	12.024	1714790	50.0
Benzene, cyclop...	12.244	374.2	ug/l	12833400	4	12.024	1714790	50.0
o-Cymene	12.317	95.1	ug/l	3262460	4	12.024	1714790	50.0
Benzene, 1-ethy...	12.616	96.3	ug/l	3302130	4	12.024	1714790	50.0
Benzene, 1,2,4,...	12.963	74.2	ug/l	2544720	4	12.024	1714790	50.0
Indan, 1-methyl-	13.292	119.1	ug/l	4084630	4	12.024	1714790	50.0
1,4-Methanonaph...	14.640	76.9	ug/l	2637800	4	12.024	1714790	50.0