

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
 Data File : VX031582.D
 Acq On : 22 Sep 2022 19:51
 Operator : JC/MD
 Sample : N4614-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-42

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\82X091922W.M
 Title : SW846 8260

Signal : TIC: VX031582.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	41	46	52	rBV	1152922	1164818	2.91%	0.489%
2	1.745	103	108	123	rVB	4251096	5398767	13.51%	2.267%
3	1.953	138	142	155	rVB	956742	1258648	3.15%	0.529%
4	2.069	155	161	167	rBV	450543	607388	1.52%	0.255%
5	2.776	257	277	281	rBV3	168500	642943	1.61%	0.270%
6	2.824	281	285	289	rVV	283147	545978	1.37%	0.229%
7	3.105	322	331	351	rVB2	323001	775895	1.94%	0.326%
8	4.306	517	528	541	rVB	644155	1804602	4.52%	0.758%
9	5.476	711	720	728	rBV3	188476	574744	1.44%	0.241%
10	6.043	804	813	823	rVB	784903	2005638	5.02%	0.842%
11	6.257	841	848	858	rVB3	207650	620764	1.55%	0.261%
12	7.379	1019	1032	1044	rBV5	319028	847908	2.12%	0.356%
13	8.506	1211	1217	1227	rVB	253418	429832	1.08%	0.181%
14	8.647	1235	1240	1246	rVB	470375	739415	1.85%	0.311%
15	8.720	1246	1252	1258	rBV	1977598	2760959	6.91%	1.160%
16	8.842	1265	1272	1280	rBV	276704	455292	1.14%	0.191%
17	10.055	1461	1471	1476	rBV2	296581	554085	1.39%	0.233%
18	10.201	1489	1495	1500	rVB	11295314	14405550	36.04%	6.050%
19	10.311	1506	1513	1518	rBV	28438440	39966978	100.00%	16.786%
20	10.646	1562	1568	1574	rVB	14234884	18215758	45.58%	7.651%
21	10.963	1614	1620	1631	rVB	992025	1240825	3.10%	0.521%
22	11.085	1635	1640	1644	rVB	667651	836682	2.09%	0.351%
23	11.305	1667	1676	1683	rVB	3018697	3729031	9.33%	1.566%
24	11.384	1683	1689	1696	rBV	12840618	23945438	59.91%	10.057%
25	11.457	1696	1701	1706	rVB	7678269	9360447	23.42%	3.931%
26	11.616	1721	1727	1736	rBV	7010154	8454365	21.15%	3.551%
27	11.762	1744	1751	1756	rBV	26945034	32620370	81.62%	13.700%
28	11.975	1779	1786	1789	rBV	404805	532460	1.33%	0.224%
29	12.024	1789	1794	1799	rVB2	644500	904065	2.26%	0.380%
30	12.091	1799	1805	1810	rBV	7722308	9000272	22.52%	3.780%
31	12.244	1825	1830	1833	rBV	5589988	7360151	18.42%	3.091%
32	12.317	1838	1842	1849	rVV2	2725584	3907612	9.78%	1.641%
33	12.408	1852	1857	1862	rBV2	394749	536259	1.34%	0.225%
34	12.463	1862	1866	1872	rVB	695795	815363	2.04%	0.342%
35	12.530	1872	1877	1879	rBV	1676837	2076189	5.19%	0.872%
36	12.554	1879	1881	1886	rVB	1503944	1732722	4.34%	0.728%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

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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37	12.615	1886	1891	1894	rBV	2790167	3231179	8.08%	1.357%
38	12.646	1894	1896	1900	rVB	607721	632864	1.58%	0.266%
39	12.701	1900	1905	1913	rBV2	1800325	2462680	6.16%	1.034%
40	12.847	1924	1929	1934	rBV	766575	930070	2.33%	0.391%
41	12.920	1934	1941	1945	rVV	1548661	2000736	5.01%	0.840%
42	12.963	1945	1948	1954	rVB	2377004	2675671	6.69%	1.124%
43	13.170	1978	1982	1986	rVB	1857893	2076568	5.20%	0.872%
44	13.292	1998	2002	2007	rVB2	3429908	4450597	11.14%	1.869%
45	13.426	2019	2024	2029	rVB	532422	688918	1.72%	0.289%
46	13.585	2047	2050	2056	rVB3	300413	459581	1.15%	0.193%
47	13.664	2061	2063	2069	rVB2	326016	441704	1.11%	0.186%
48	13.780	2076	2082	2088	rBV	7830240	10021422	25.07%	4.209%
49	13.871	2091	2097	2101	rVB	311251	453896	1.14%	0.191%
50	14.219	2149	2154	2160	rBV2	228023	419585	1.05%	0.176%
51	14.639	2218	2223	2234	rVB	3407221	4112574	10.29%	1.727%
52	14.780	2241	2246	2255	rBV	1779336	2211681	5.53%	0.929%

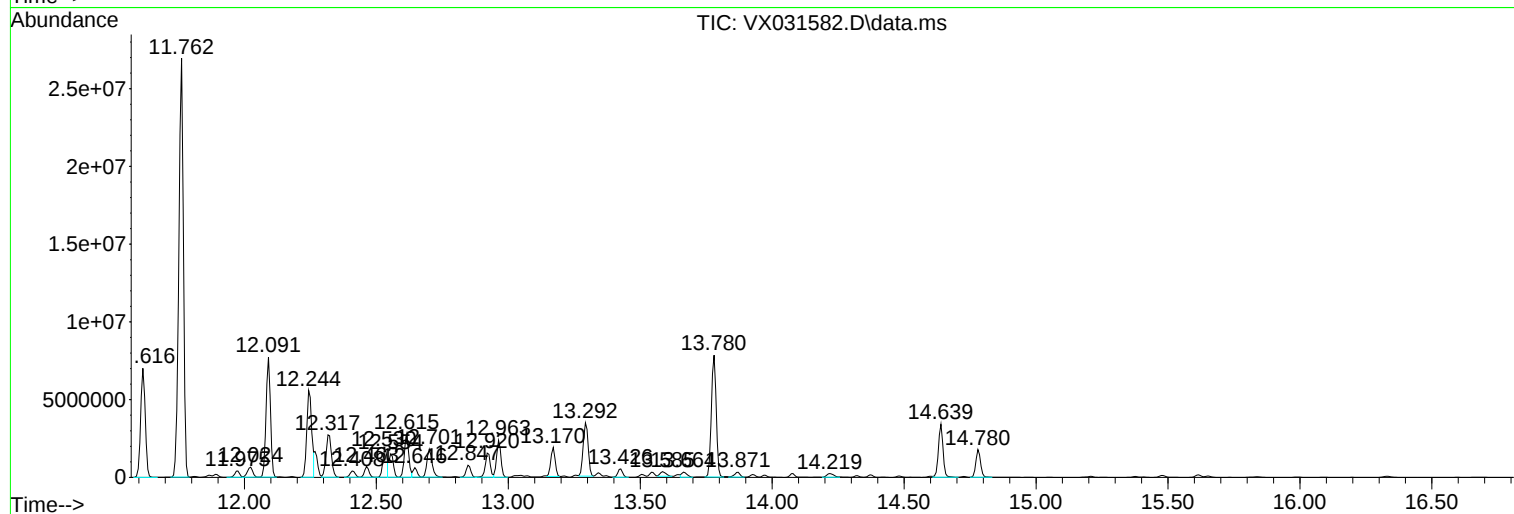
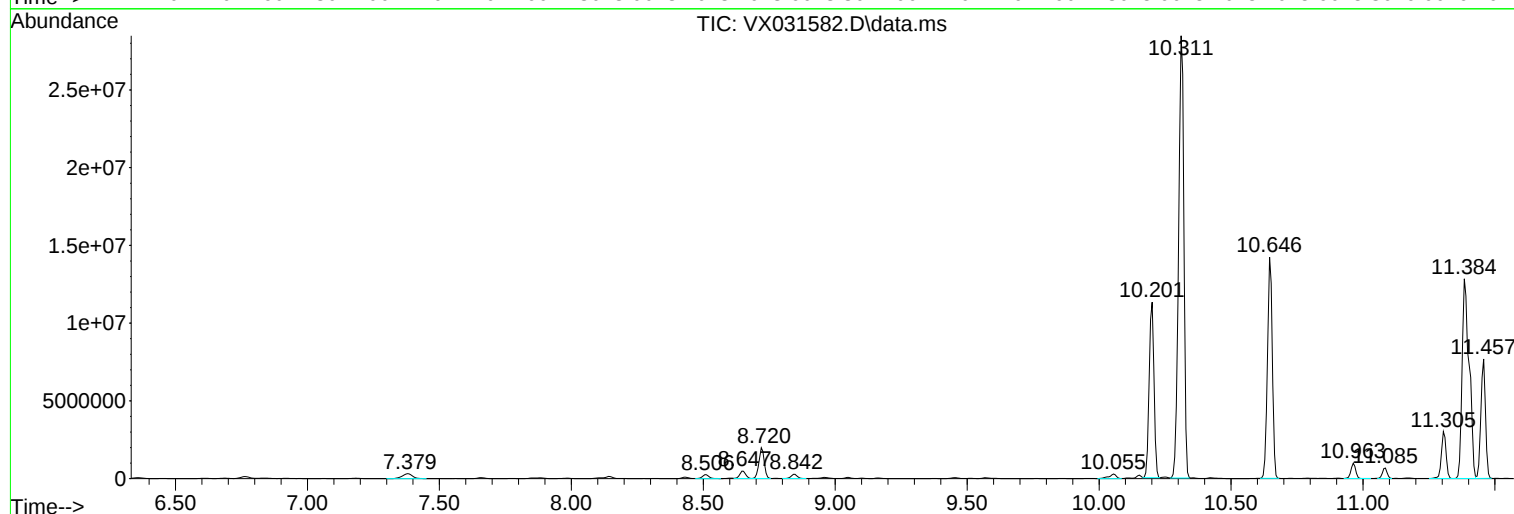
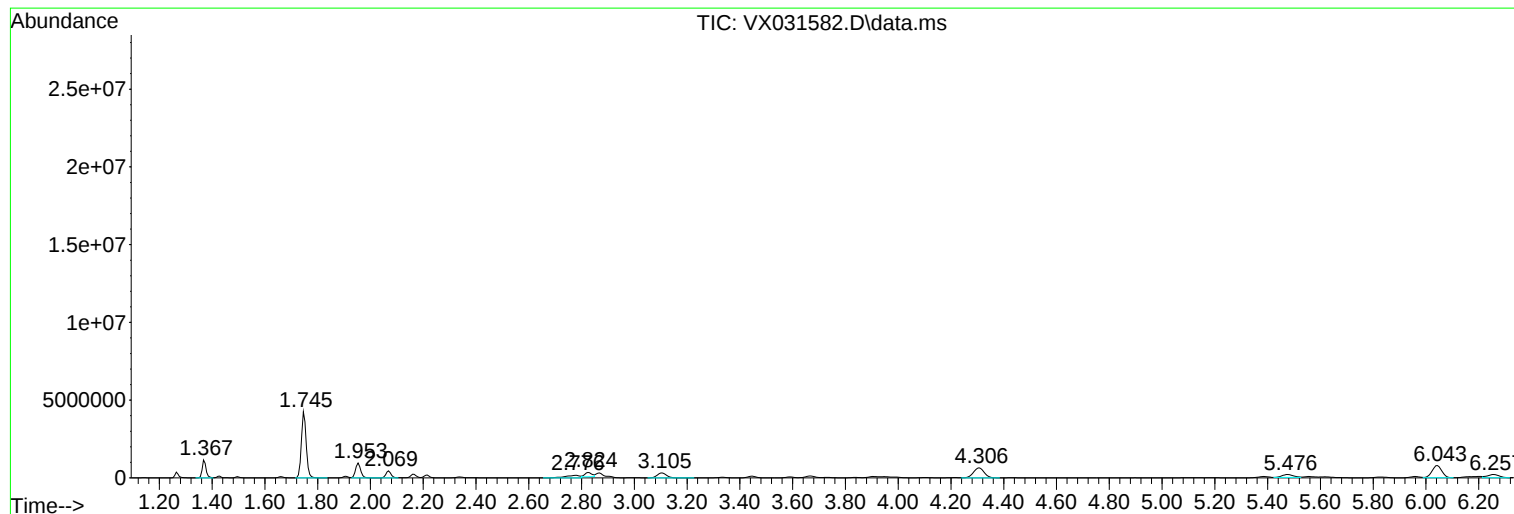
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Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
MW-42

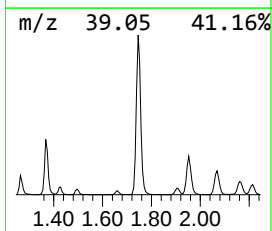
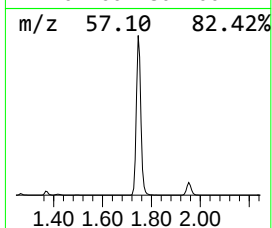
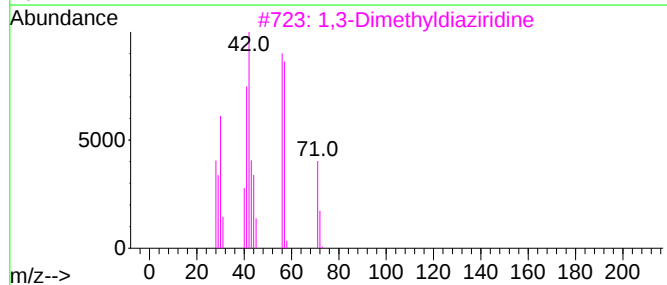
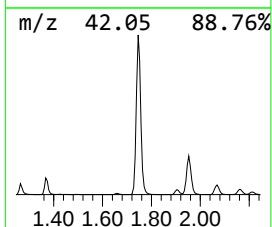
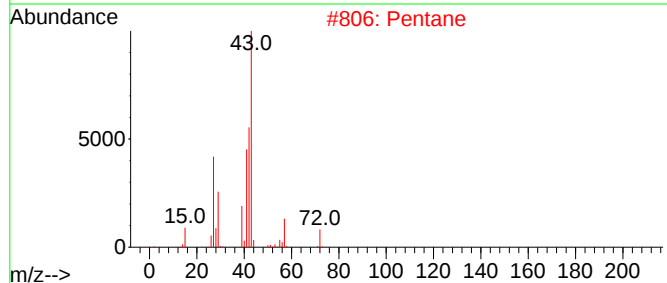
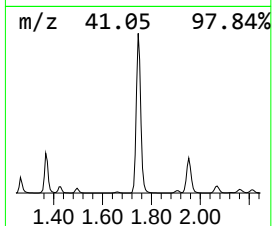
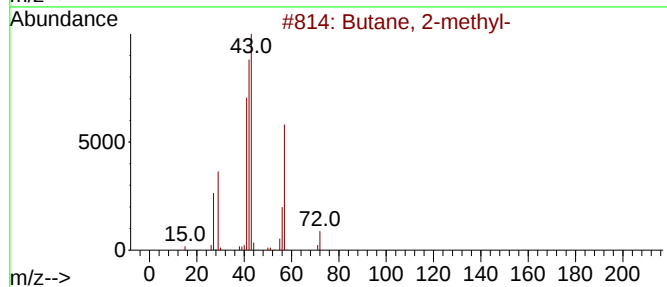
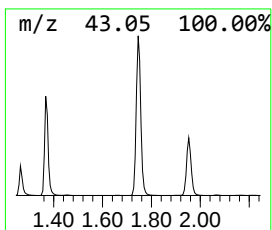
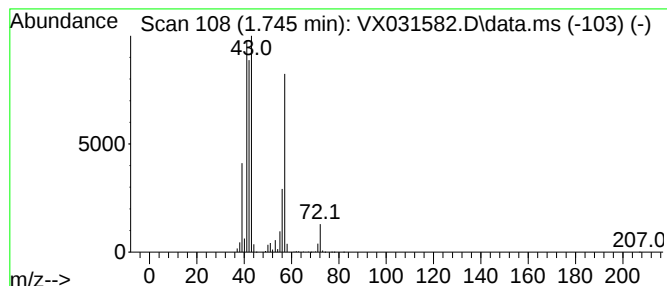
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.745	469.67 ug/l	5398770	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	64
2			Pentane	72	C5H12	000109-66-0	36
3			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	25
4			Oxirane, trimethyl-	86	C5H10O	005076-19-7	25
5			3-Buten-1-ol	72	C4H8O	000627-27-0	23



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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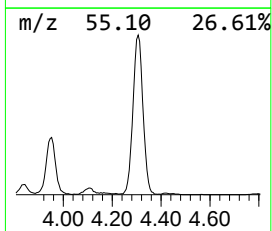
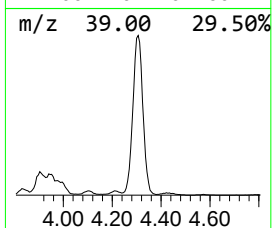
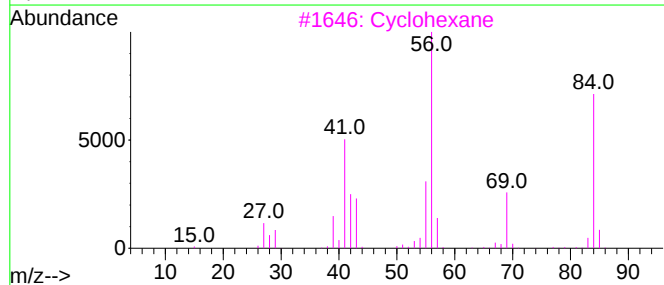
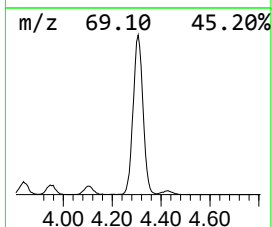
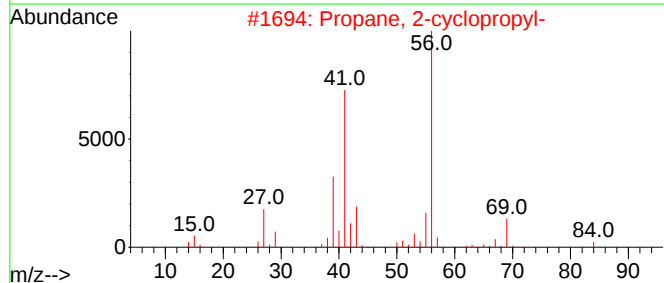
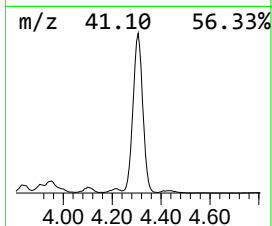
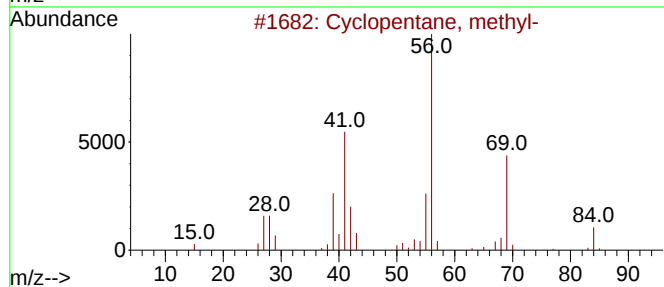
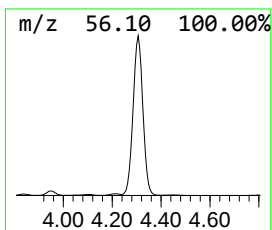
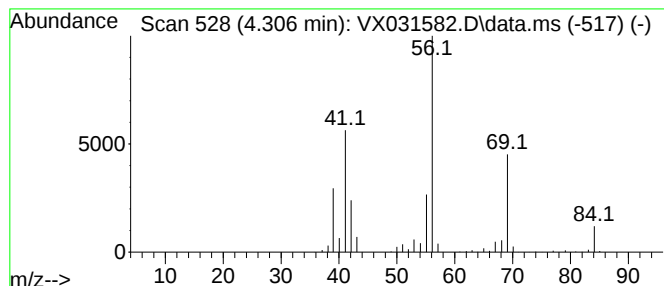
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopentane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	156.99 ug/l	1804600	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
3			Cyclohexane	84	C6H12	000110-82-7	78
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

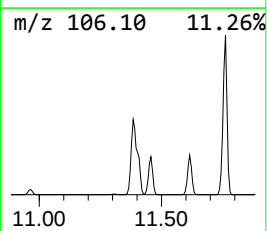
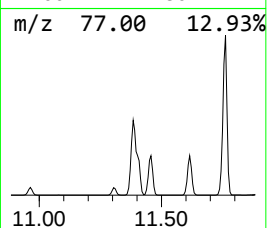
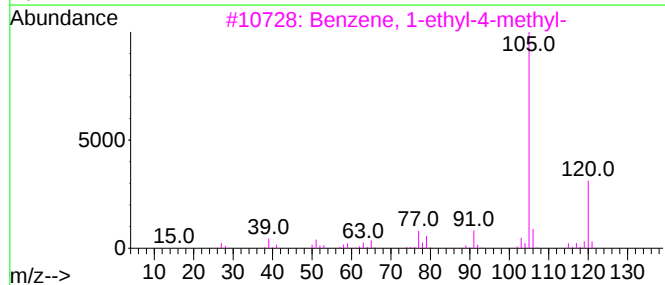
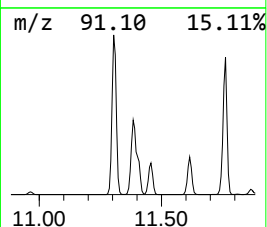
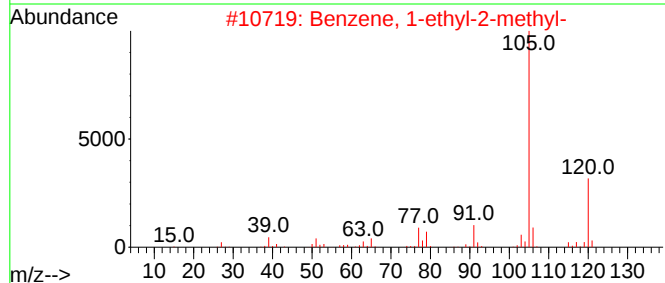
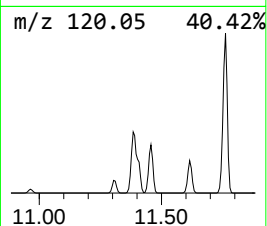
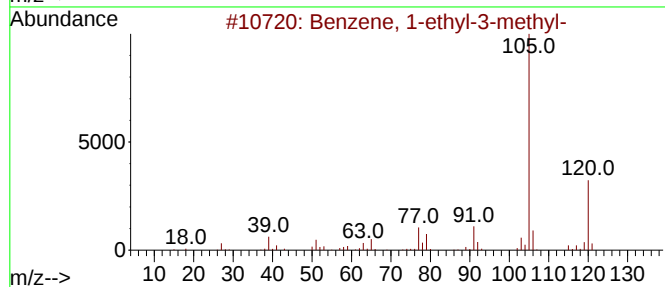
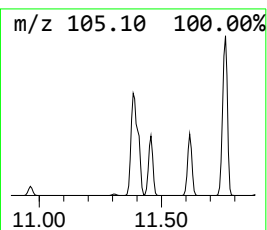
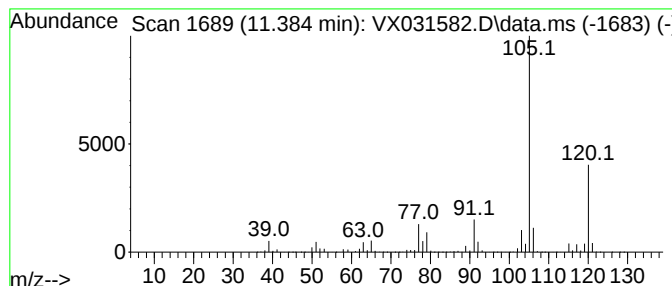
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	1324.32 ug/l	23945400	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	94
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	90



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

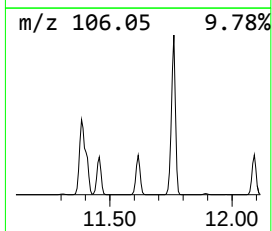
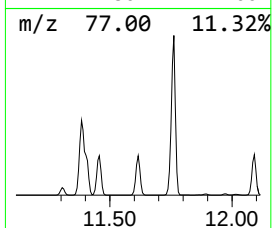
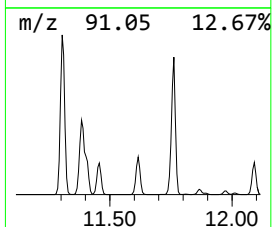
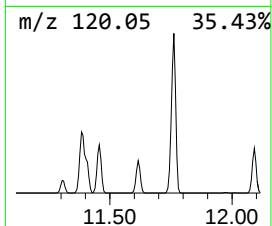
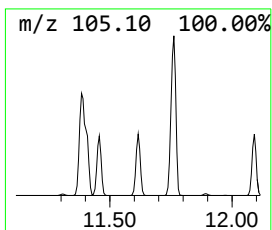
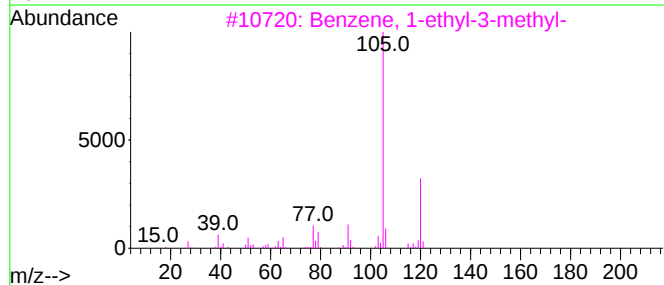
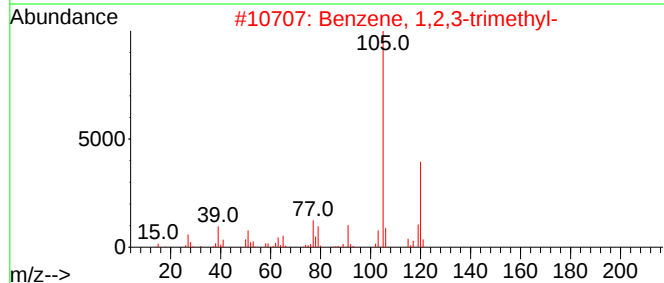
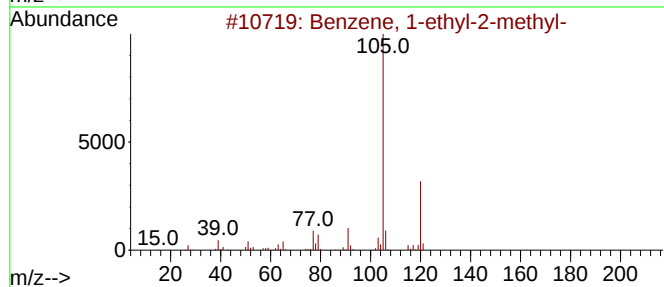
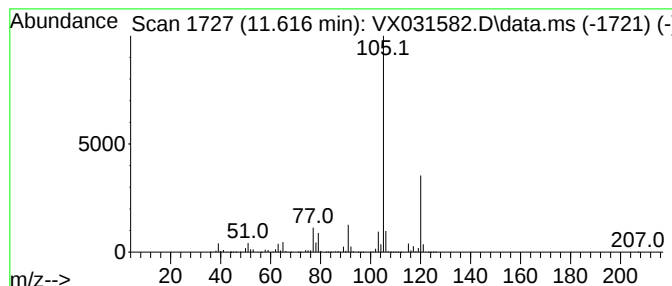
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	467.57 ug/l	8454370	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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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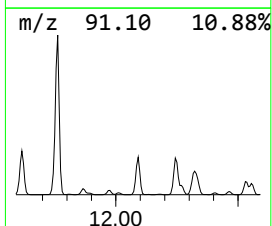
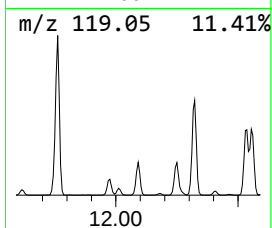
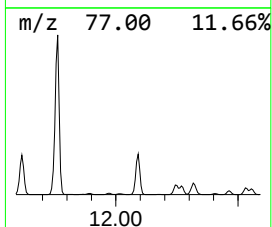
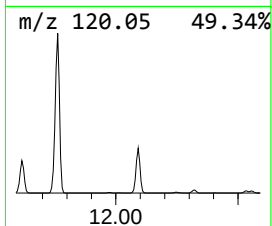
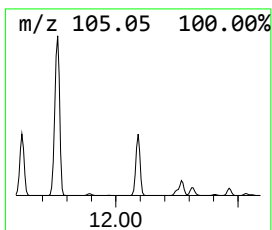
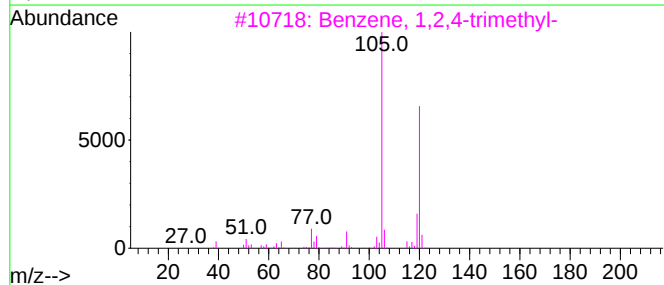
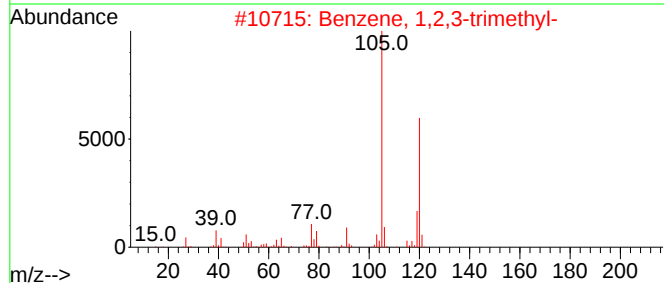
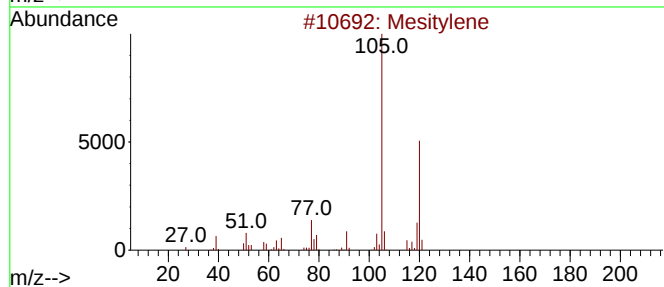
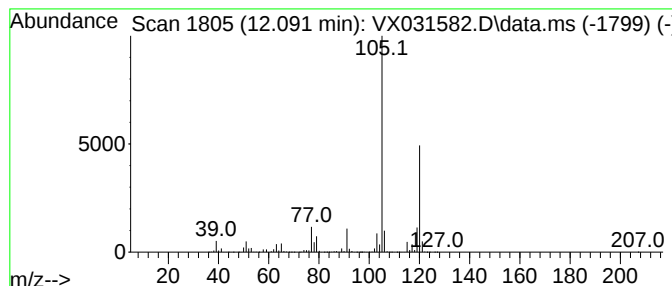
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	497.77 ug/l	9000270	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	94
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031582.D
Acq On : 22 Sep 2022 19:51
Operator : JC/MD
Sample : N4614-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

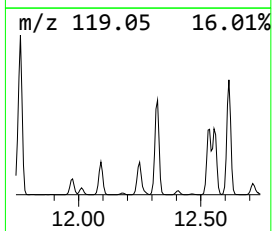
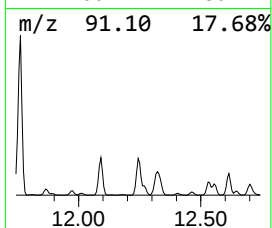
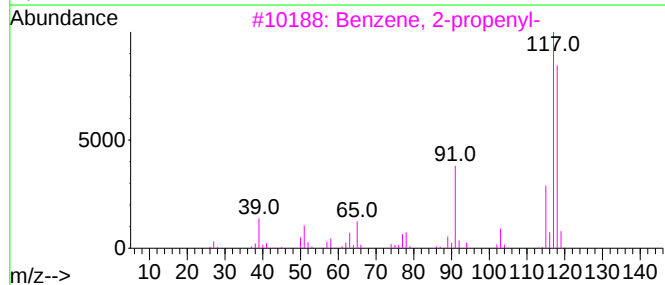
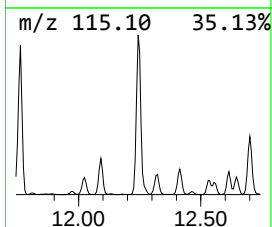
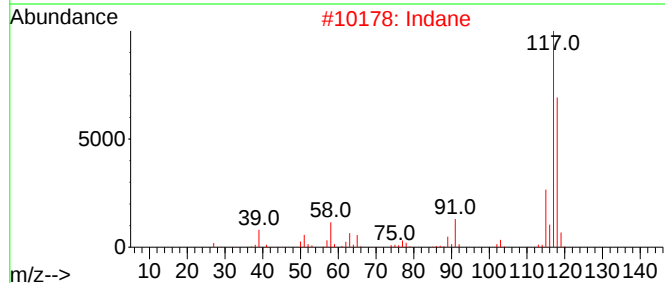
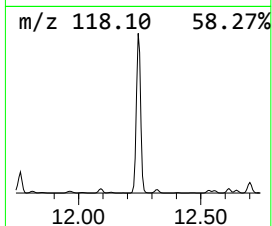
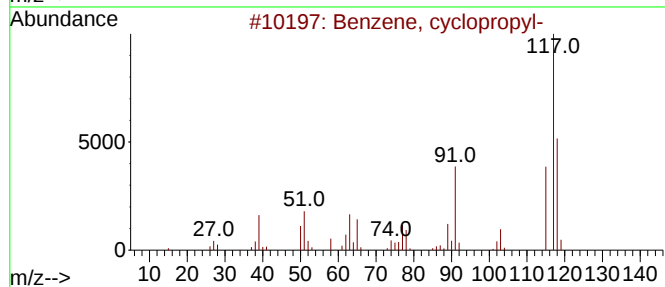
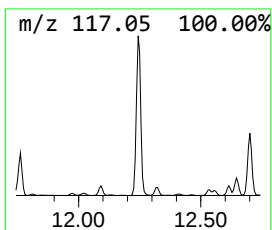
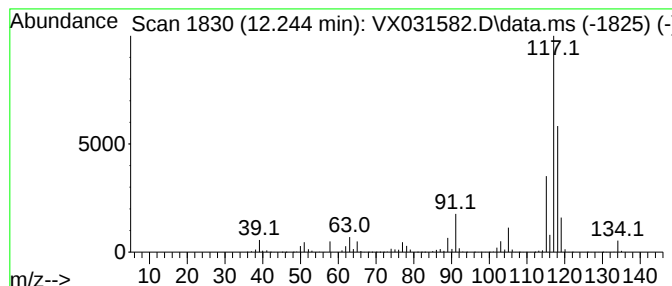
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, cyclopropyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	407.06 ug/l	7360150	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
2			Indane	118	C9H10	000496-11-7	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	49
5			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031582.D
Acq On : 22 Sep 2022 19:51
Operator : JC/MD
Sample : N4614-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

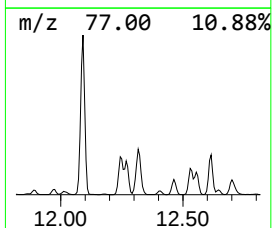
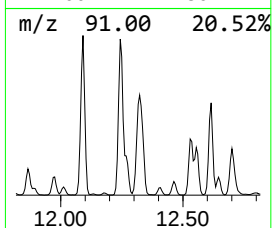
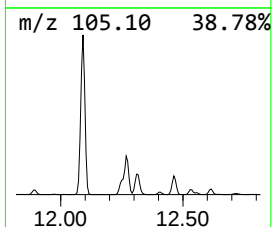
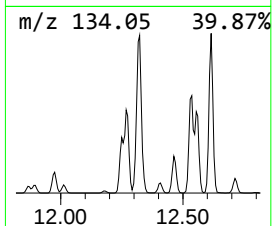
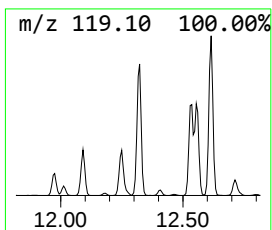
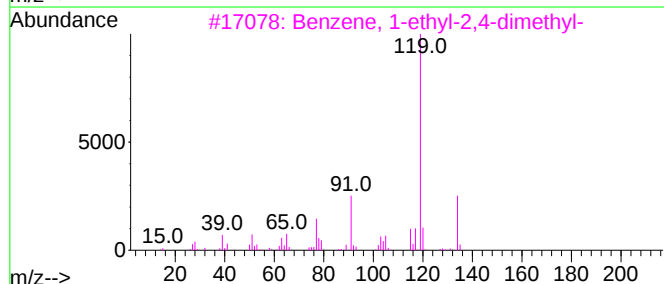
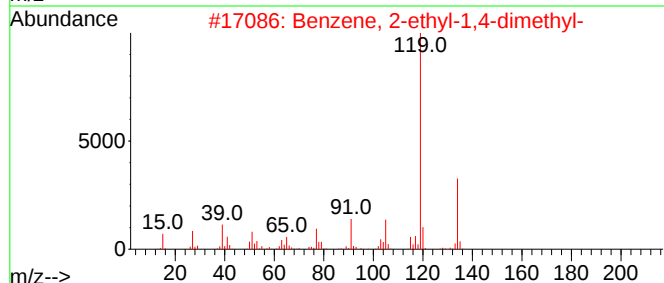
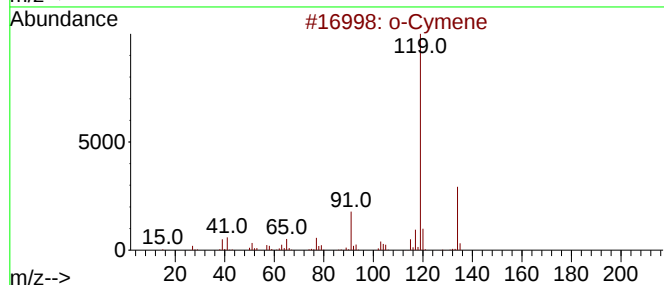
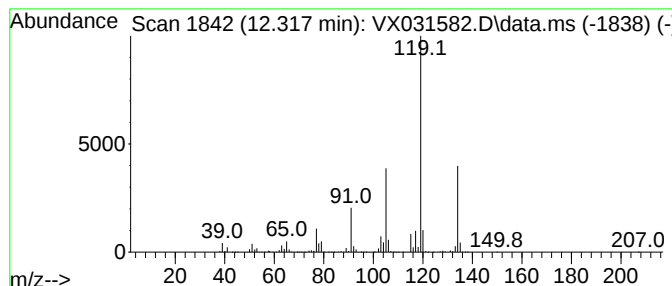
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Quant Title : SW846 8260

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

Peak Number 7 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	216.11 ug/l	3907610	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, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
5			p-Cymene	134	C10H14	000099-87-6	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031582.D
Acq On : 22 Sep 2022 19:51
Operator : JC/MD
Sample : N4614-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

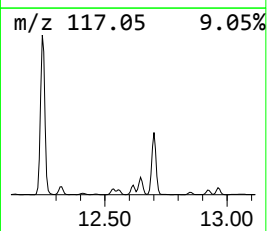
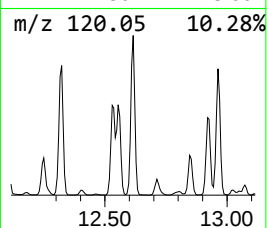
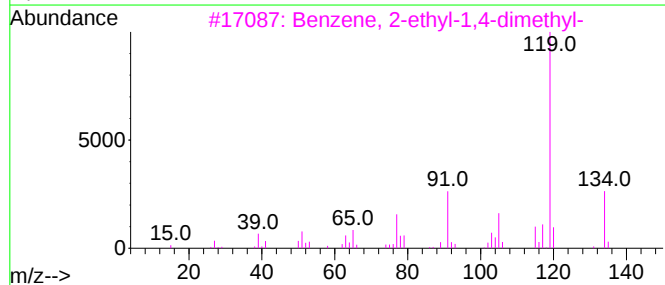
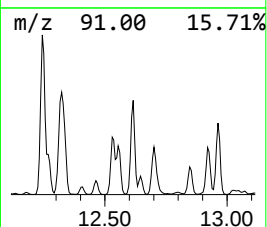
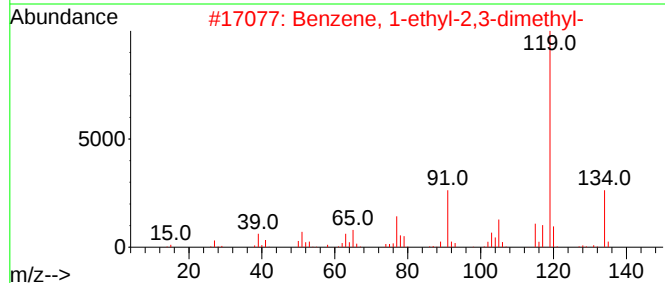
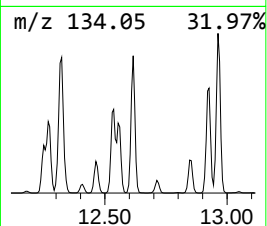
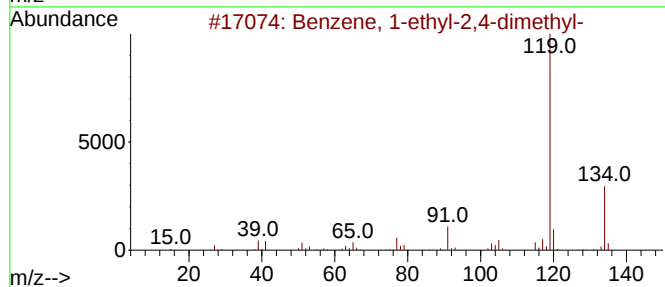
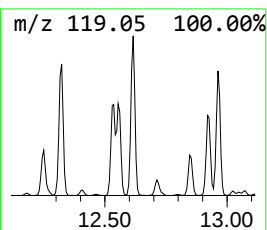
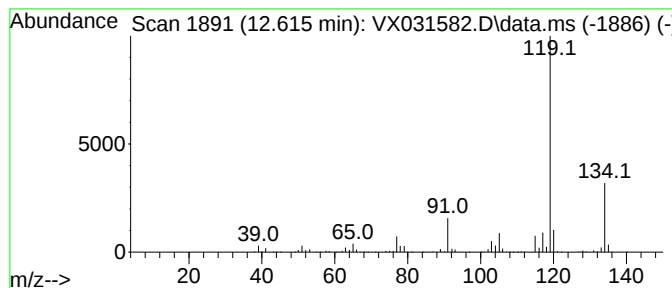
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.615	178.70 ug/l	3231180	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031582.D
Acq On : 22 Sep 2022 19:51
Operator : JC/MD
Sample : N4614-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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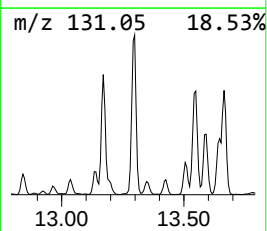
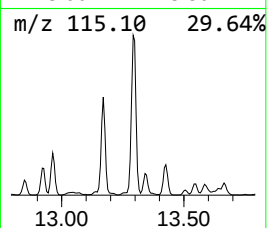
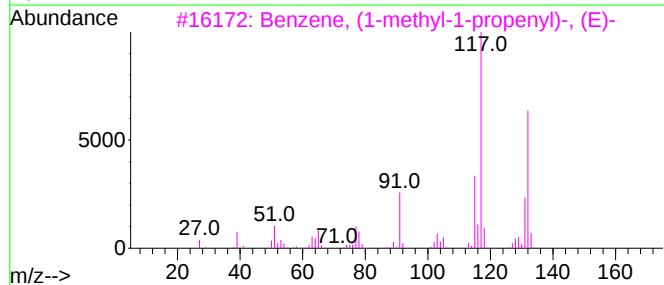
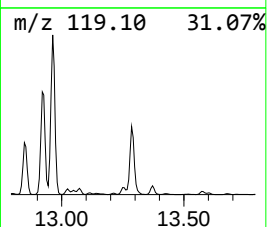
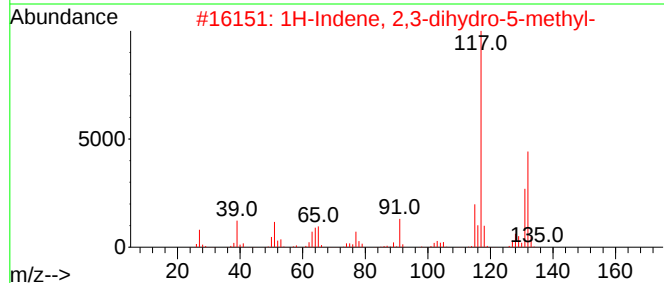
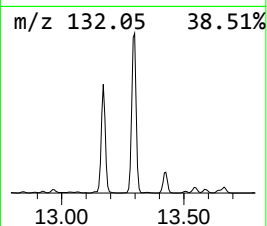
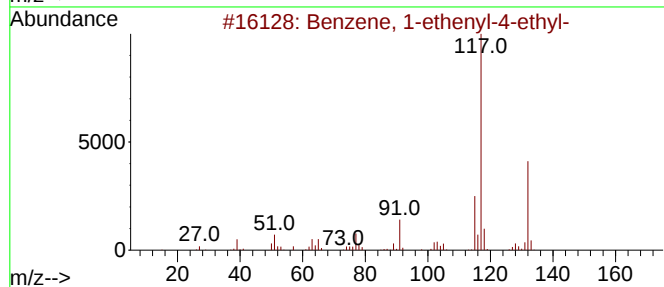
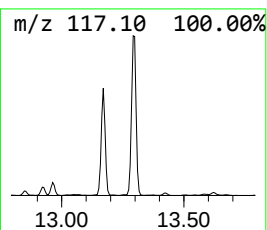
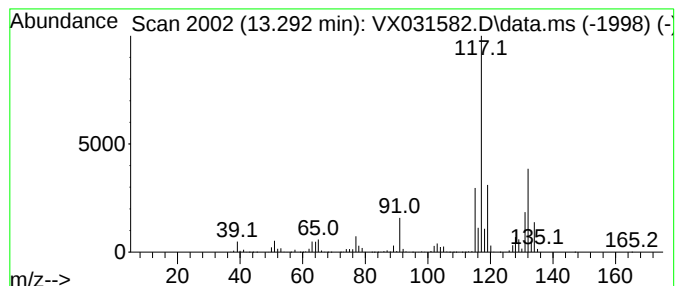
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	246.14 ug/l	4450600	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			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031582.D
Acq On : 22 Sep 2022 19:51
Operator : JC/MD
Sample : N4614-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

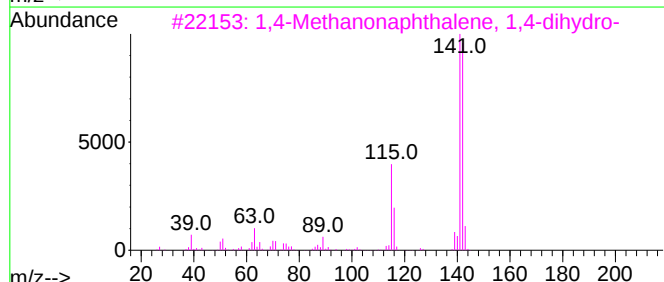
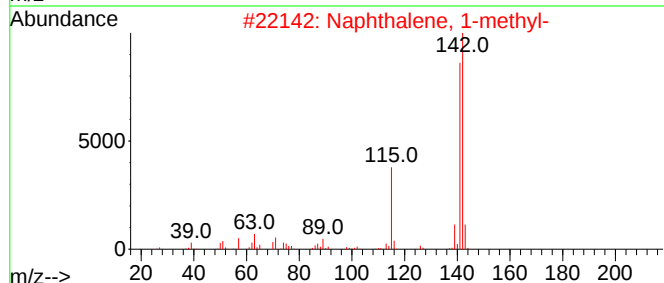
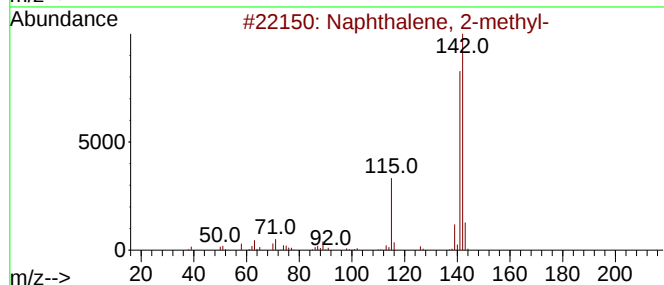
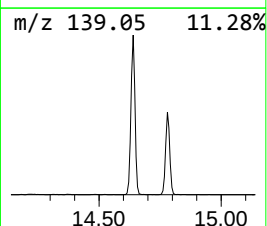
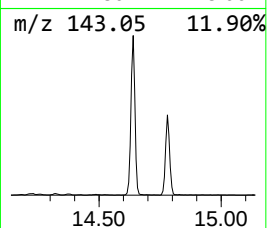
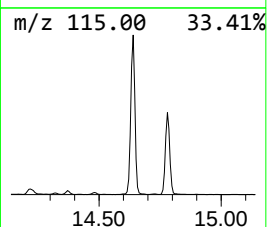
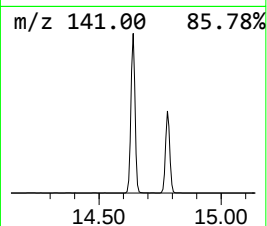
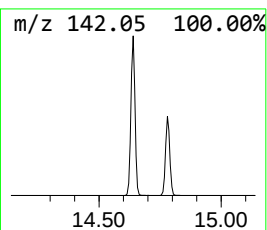
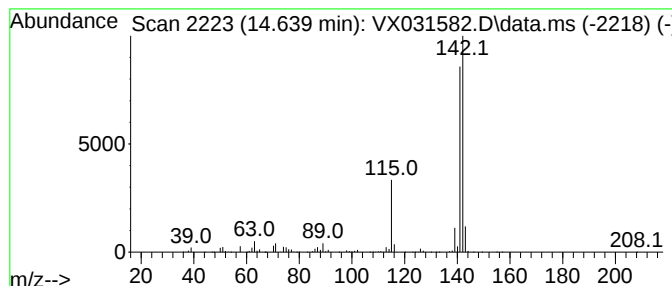
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.639	227.45 ug/l	4112570	1,4-Dichlorobenzene-d4	12.024

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031582.D
Acq On : 22 Sep 2022 19:51
Operator : JC/MD
Sample : N4614-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.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
Butane, 2-methyl-	1.745	469.7	ug/l	5398770	1	5.556	574744	50.0
Cyclopentane, m...	4.306	157.0	ug/l	1804600	1	5.556	574744	50.0
Benzene, 1-ethy...	11.384	1324.3	ug/l	23945400	4	12.024	904065	50.0
Benzene, 1-ethy...	11.616	467.6	ug/l	8454370	4	12.024	904065	50.0
Benzene, 1,2,3-...	12.091	497.8	ug/l	9000270	4	12.024	904065	50.0
Benzene, cyclop...	12.243	407.1	ug/l	7360150	4	12.024	904065	50.0
o-Cymene	12.317	216.1	ug/l	3907610	4	12.024	904065	50.0
Benzene, 1-ethy...	12.615	178.7	ug/l	3231180	4	12.024	904065	50.0
Benzene, 1-ethe...	13.292	246.1	ug/l	4450600	4	12.024	904065	50.0
Naphthalene, 2-...	14.639	227.4	ug/l	4112570	4	12.024	904065	50.0