

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
 Data File : VX028979.D
 Acq On : 26 May 2022 03:28
 Operator : JC/MD
 Sample : N3002-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-12

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\82X051222W.M
 Title : SW846 8260

Signal : TIC: VX028979.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	27	29	38	rVB	98892	98604	1.43%	0.161%
2	1.373	41	47	52	rBV	366352	378054	5.48%	0.619%
3	1.751	103	109	120	rVB	522654	729053	10.57%	1.193%
4	1.953	138	142	151	rVV	180548	272291	3.95%	0.446%
5	2.068	155	161	170	rVV	116830	167841	2.43%	0.275%
6	2.166	171	177	181	rVV	84165	128031	1.86%	0.210%
7	2.215	181	185	194	rVB	57827	91103	1.32%	0.149%
8	2.751	259	273	276	rBV	57601	143935	2.09%	0.236%
9	2.824	281	285	288	rVV	108236	211112	3.06%	0.346%
10	2.867	288	292	303	rVB	170232	362309	5.25%	0.593%
11	3.105	321	331	346	rVB3	113628	269625	3.91%	0.441%
12	3.446	378	387	401	rVB2	33248	77417	1.12%	0.127%
13	3.910	456	463	471	rBV	24478	70118	1.02%	0.115%
14	4.306	518	528	542	rVB	178552	507345	7.35%	0.831%
15	5.391	694	706	714	rBV	223646	662301	9.60%	1.084%
16	5.476	714	720	725	rVV	91599	273552	3.96%	0.448%
17	5.556	725	733	757	rVB	353935	1113961	16.14%	1.824%
18	5.964	789	800	804	rBV	222143	581405	8.43%	0.952%
19	6.043	804	813	827	rVB	2282311	5987563	86.78%	9.802%
20	6.208	827	840	845	rBV3	48678	174982	2.54%	0.286%
21	6.360	857	865	879	rVB6	23631	89410	1.30%	0.146%
22	6.763	922	931	942	rBV	561044	1347758	19.53%	2.206%
23	7.385	1020	1033	1043	rBV3	94329	255197	3.70%	0.418%
24	8.147	1154	1158	1170	rVB2	36491	82949	1.20%	0.136%
25	8.506	1209	1217	1225	rVB4	37281	70015	1.01%	0.115%
26	8.653	1235	1241	1247	rBV	1176418	1810575	26.24%	2.964%
27	8.720	1247	1252	1259	rVB	686153	1042063	15.10%	1.706%
28	8.957	1281	1291	1297	rBV	154315	256885	3.72%	0.421%
29	9.049	1297	1306	1312	rVB2	174487	279685	4.05%	0.458%
30	10.055	1461	1471	1476	rBV	1284877	1716838	24.88%	2.810%
31	10.195	1489	1494	1500	rBV	5351577	6899785	100.00%	11.295%
32	10.305	1505	1512	1518	rVB	2075929	2595218	37.61%	4.248%
33	10.646	1563	1568	1578	rVB	973762	1328006	19.25%	2.174%
34	10.963	1614	1620	1625	rBV	254281	326330	4.73%	0.534%
35	11.085	1634	1640	1645	rBV	1047849	1336384	19.37%	2.188%
36	11.305	1668	1676	1682	rBV	418973	526985	7.64%	0.863%

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37	11.402	1684	1692	1696	rVV	450443	604291	8.76%	0.989%
38	11.451	1696	1700	1711	rVB	1779240	2175457	31.53%	3.561%
39	11.615	1721	1727	1735	rBV	2529693	3148596	45.63%	5.154%
40	11.756	1744	1750	1756	rVB	4095299	5004403	72.53%	8.192%
41	12.024	1789	1794	1798	rVV	1417553	1710169	24.79%	2.800%
42	12.085	1798	1804	1810	rVB	2850672	3637281	52.72%	5.954%
43	12.243	1824	1830	1838	rBV	3533504	4492902	65.12%	7.355%
44	12.317	1838	1842	1850	rVB2	537236	740253	10.73%	1.212%
45	12.414	1852	1858	1862	rBV	392040	498901	7.23%	0.817%
46	12.463	1862	1866	1872	rVB	148939	192523	2.79%	0.315%
47	12.530	1872	1877	1880	rBV	340837	443703	6.43%	0.726%
48	12.615	1886	1891	1894	rBV	604597	726219	10.53%	1.189%
49	12.646	1894	1896	1900	rVB	149261	150721	2.18%	0.247%
50	12.701	1900	1905	1912	rBV2	585118	786812	11.40%	1.288%
51	12.847	1924	1929	1935	rVB	217857	275514	3.99%	0.451%
52	12.920	1935	1941	1945	rBV	311482	402578	5.83%	0.659%
53	12.963	1945	1948	1954	rVB	340628	385228	5.58%	0.631%
54	13.170	1978	1982	1987	rVB	335230	386344	5.60%	0.632%
55	13.292	1997	2002	2007	rVV2	1056981	1317246	19.09%	2.156%
56	13.347	2007	2011	2019	rVB3	100513	151729	2.20%	0.248%
57	13.426	2019	2024	2030	rVB	153811	209395	3.03%	0.343%
58	13.542	2040	2043	2047	rBV	57082	75128	1.09%	0.123%
59	13.585	2047	2050	2055	rVB4	53936	87036	1.26%	0.142%
60	13.664	2060	2063	2069	rVB2	77885	116845	1.69%	0.191%
61	13.774	2075	2081	2087	rBV	447838	571484	8.28%	0.936%
62	13.871	2092	2097	2102	rVB	239806	305418	4.43%	0.500%
63	14.780	2241	2246	2253	rBV	172236	226787	3.29%	0.371%

Sum of corrected areas: 61087648

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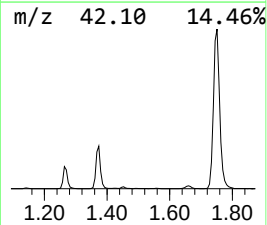
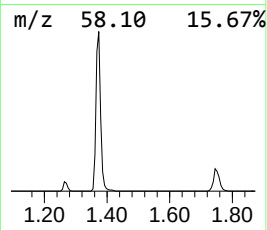
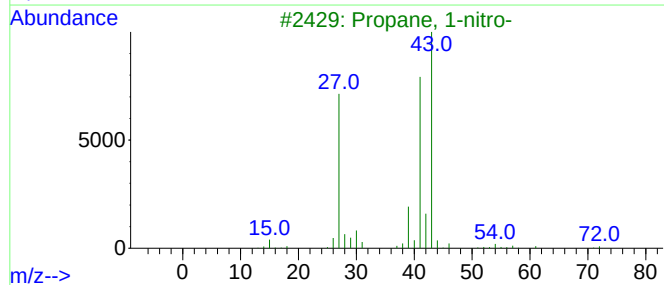
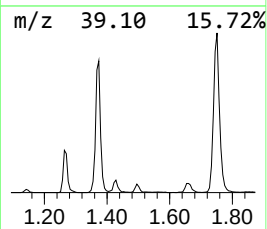
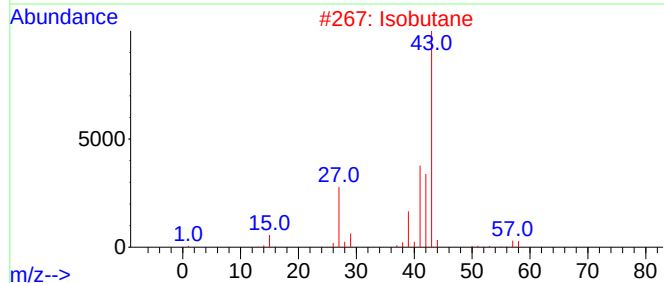
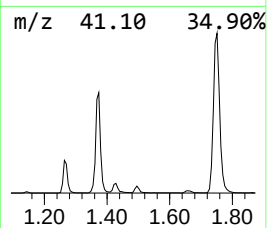
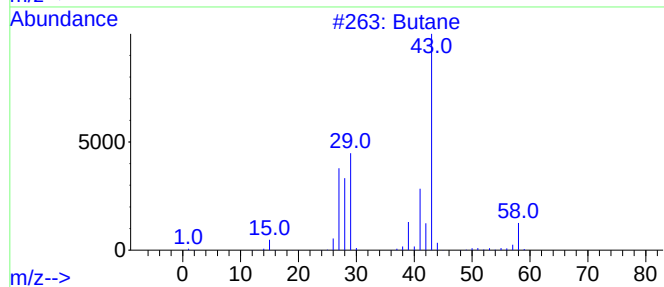
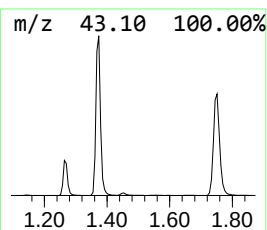
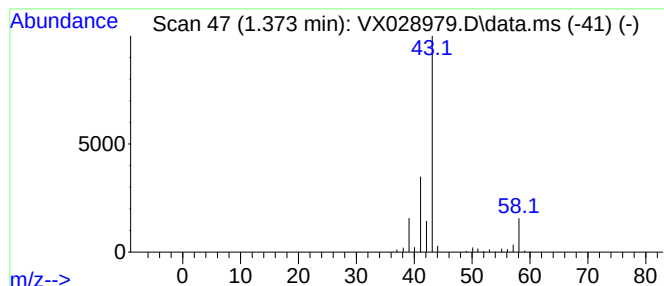
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.373	16.97 ug/l	378054	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Isobutane	58	C4H10	000075-28-5	9
3			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
4			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5			Acetone	58	C3H6O	000067-64-1	7



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ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-12

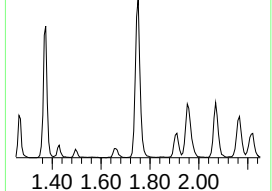
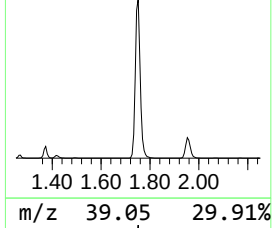
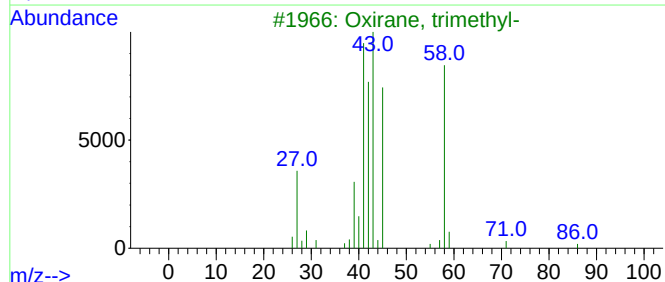
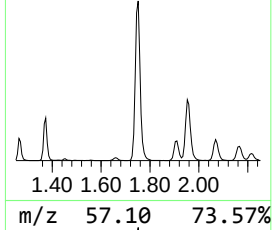
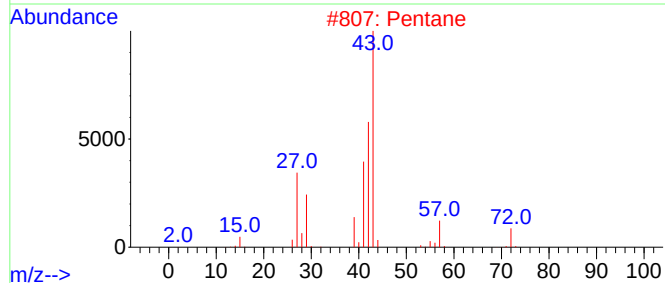
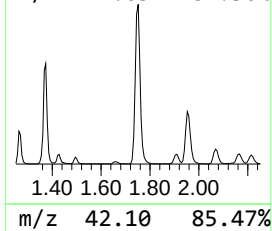
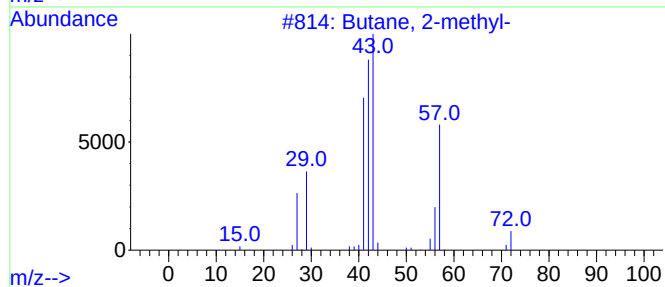
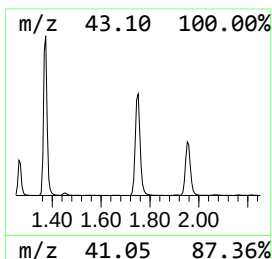
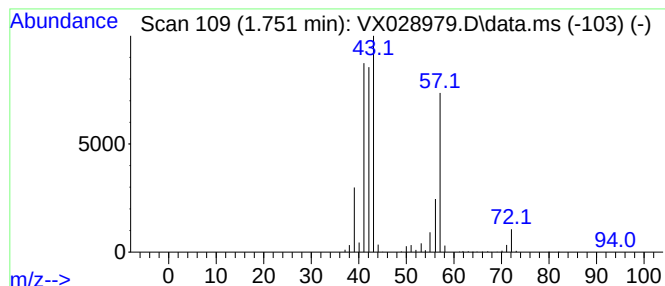
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.751	32.72 ug/l	729053	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			Pentane	72	C5H12	000109-66-0	45
3			Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
4			3-Buten-1-ol	72	C4H8O	000627-27-0	25
5			1-Butene	56	C4H8	000106-98-9	10



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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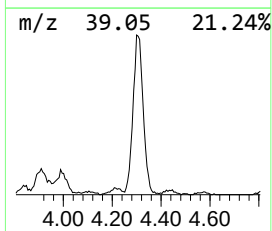
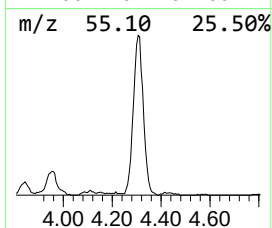
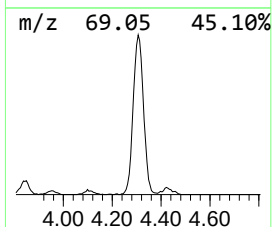
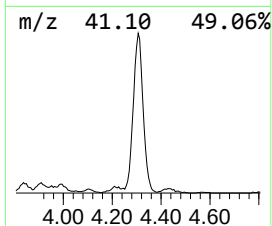
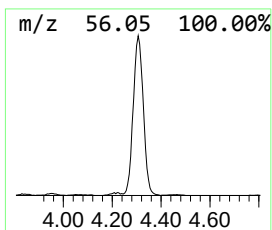
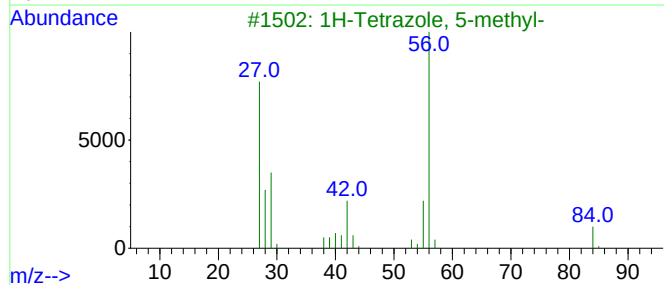
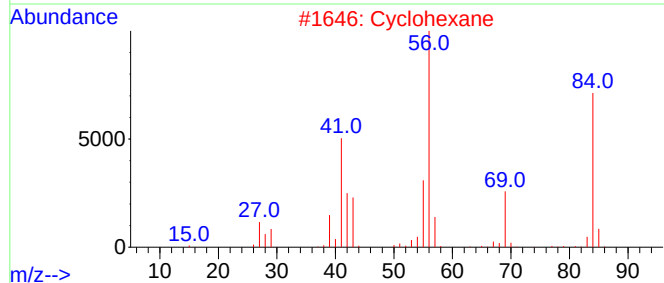
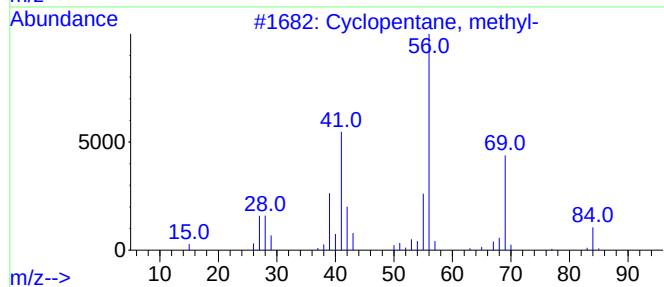
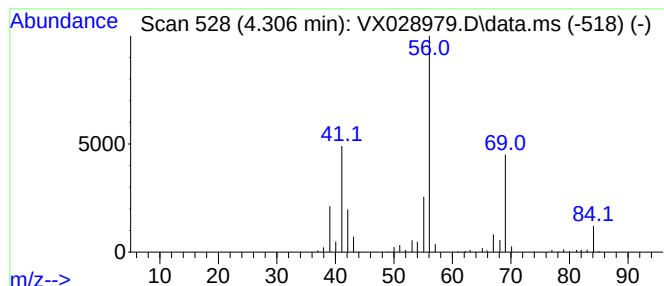
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	22.77 ug/l	507345	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclohexane	84	C6H12	000110-82-7	78
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50



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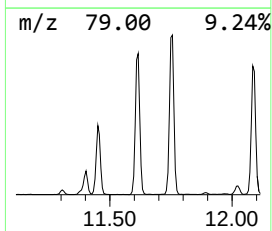
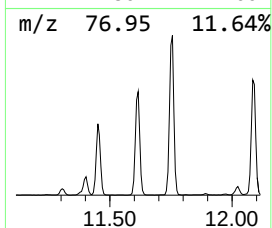
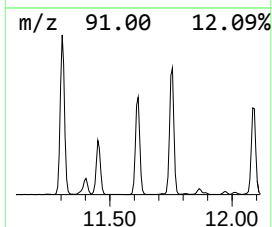
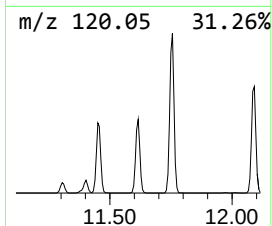
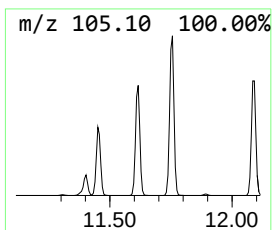
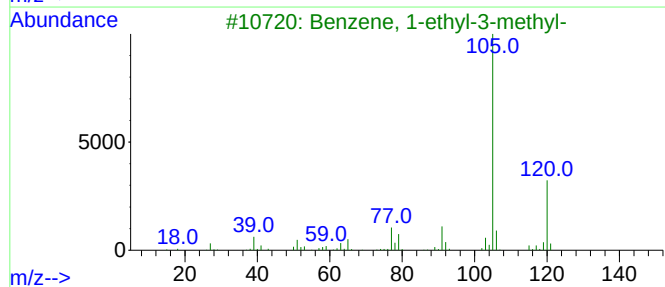
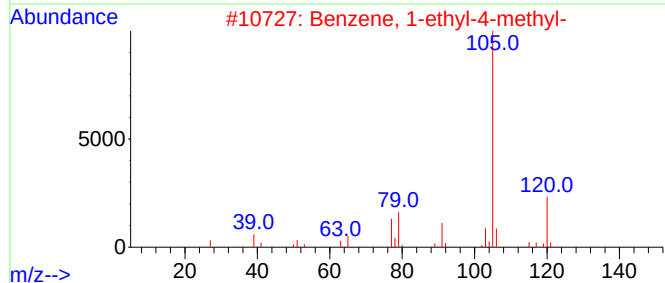
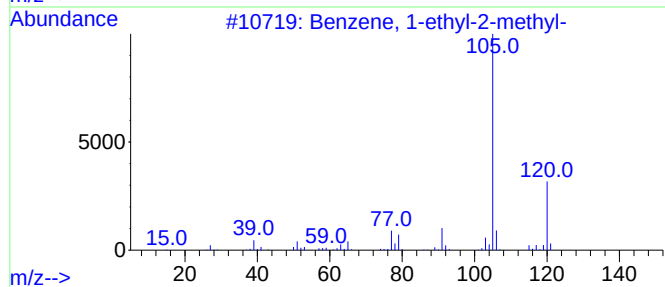
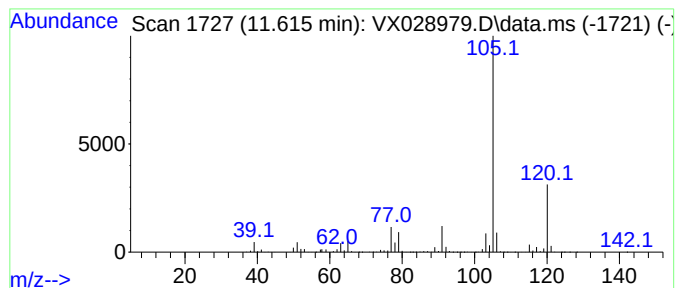
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	92.06 ug/l	3148600	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	94
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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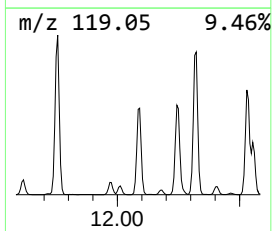
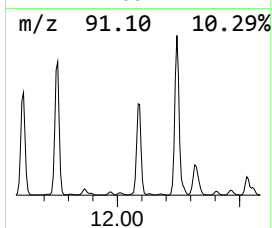
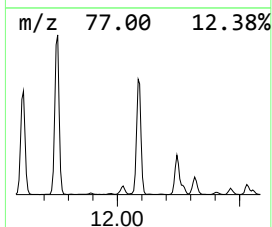
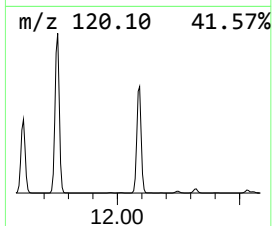
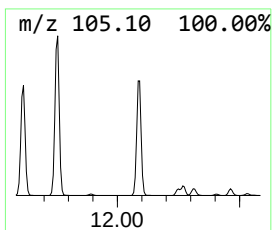
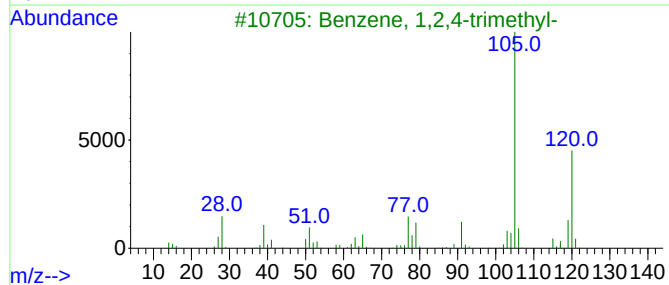
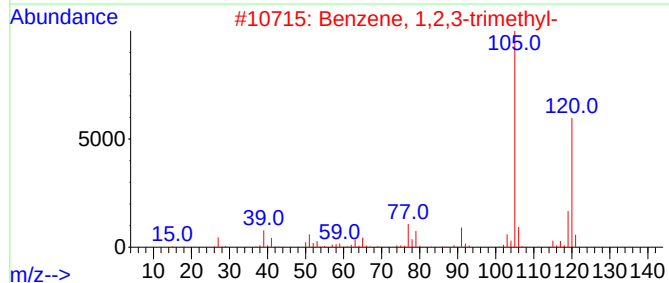
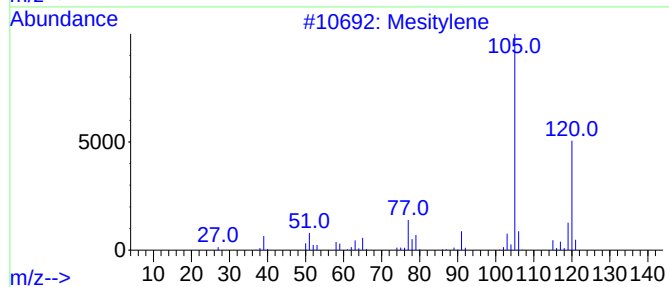
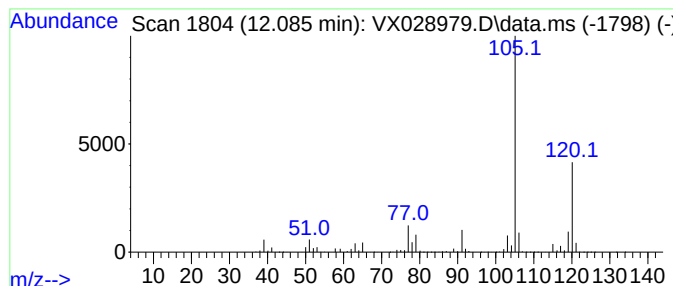
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	106.34 ug/l	3637280	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-2-methyl-	120	C9H12	000611-14-3	93
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028979.D
Acq On : 26 May 2022 03:28
Operator : JC/MD
Sample : N3002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

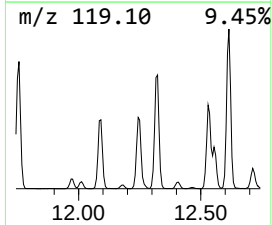
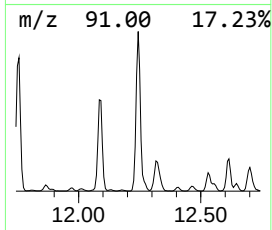
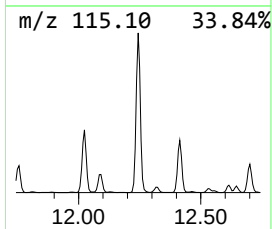
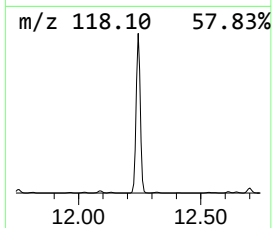
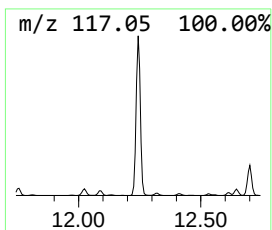
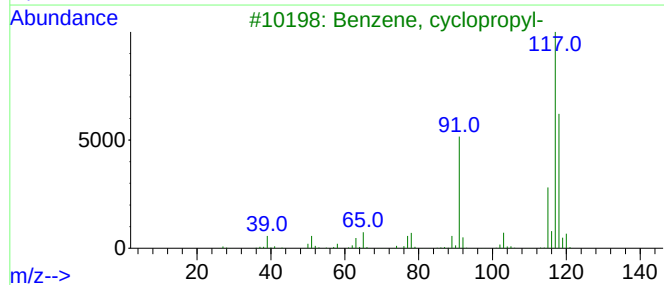
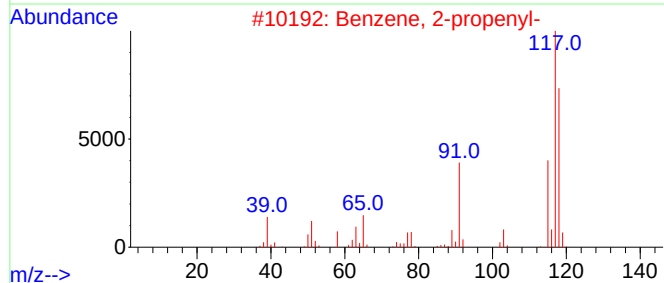
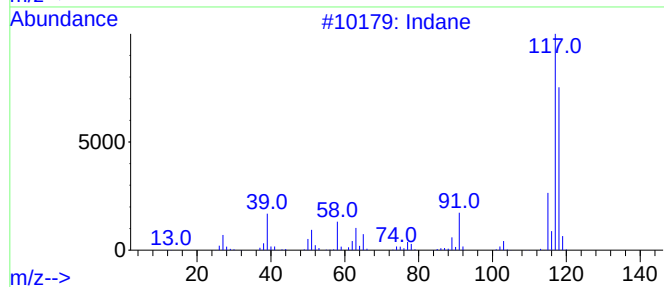
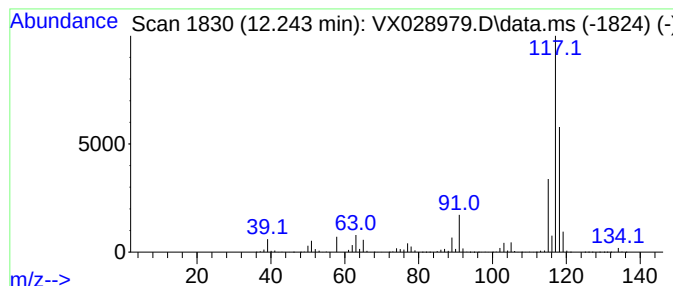
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Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	131.36 ug/l	4492900	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, 2-propenyl-	118	C9H10	000300-57-2	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	80
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028979.D
Acq On : 26 May 2022 03:28
Operator : JC/MD
Sample : N3002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

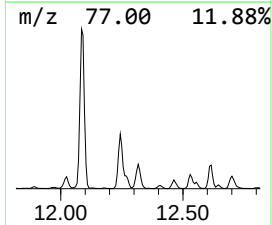
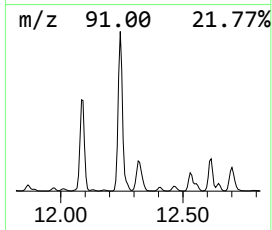
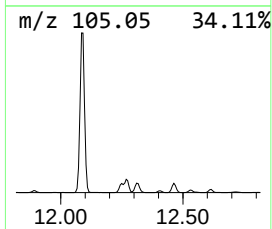
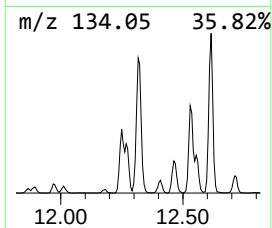
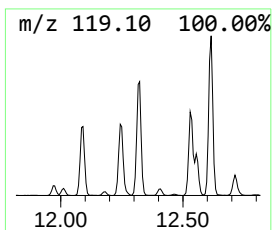
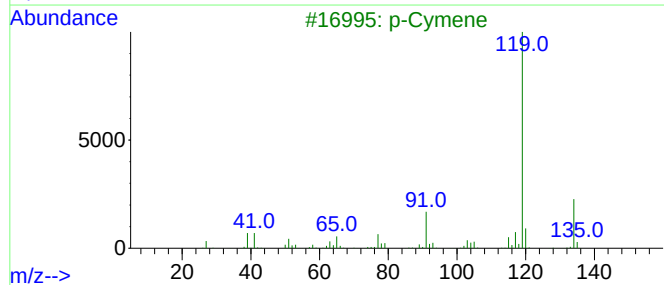
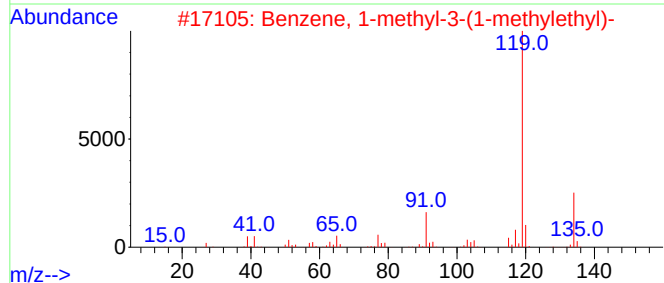
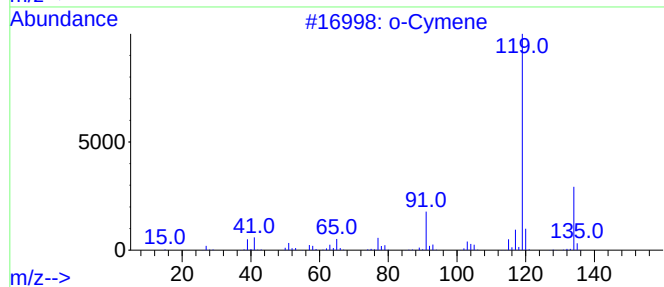
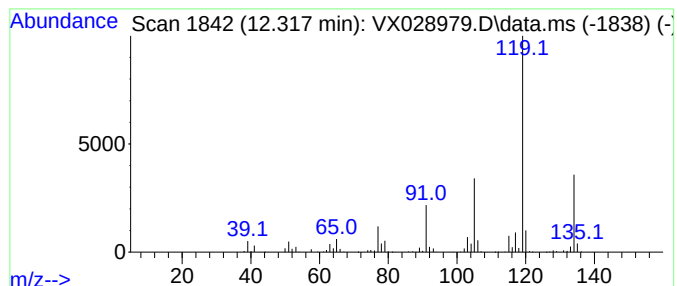
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Quant Title : SW846 8260

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	21.64 ug/l	740253	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, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	94
3			p-Cymene	134	C10H14	000099-87-6	94
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028979.D
Acq On : 26 May 2022 03:28
Operator : JC/MD
Sample : N3002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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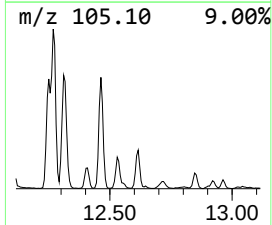
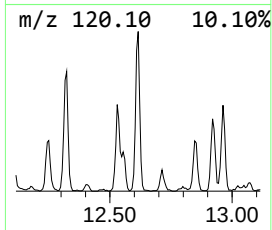
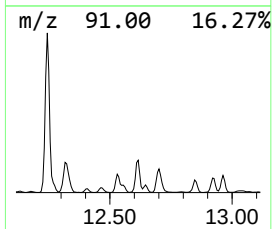
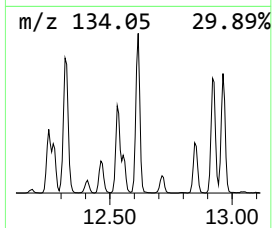
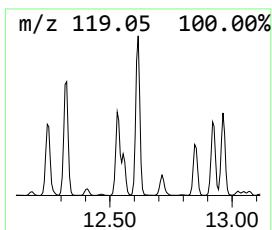
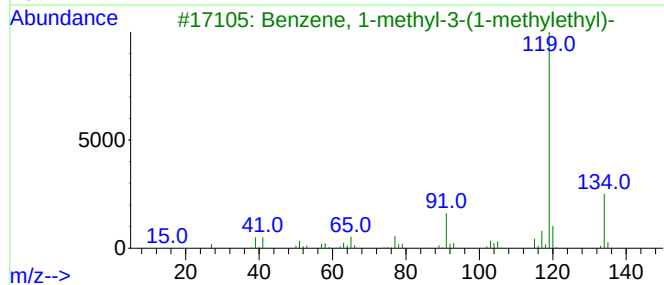
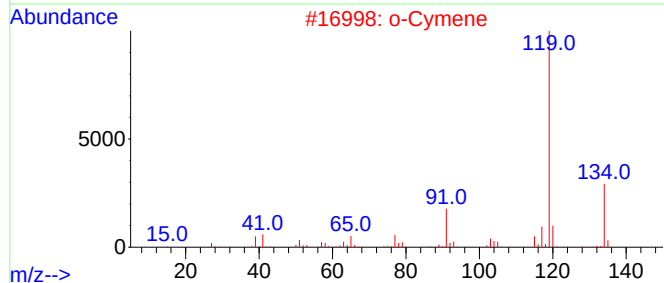
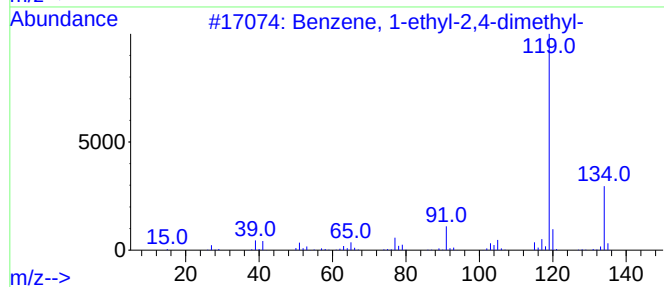
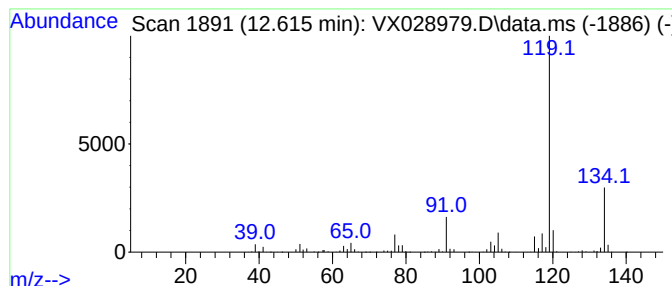
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.615	21.23 ug/l	726219	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			o-Cymene	134	C10H14	000527-84-4	97
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028979.D
Acq On : 26 May 2022 03:28
Operator : JC/MD
Sample : N3002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

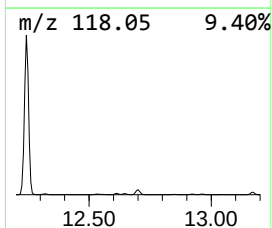
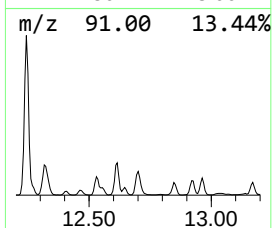
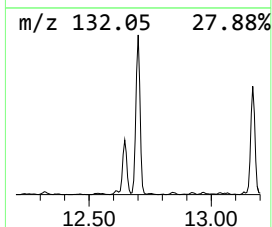
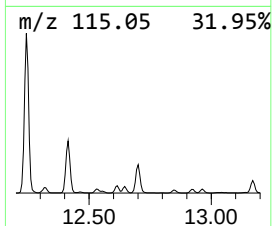
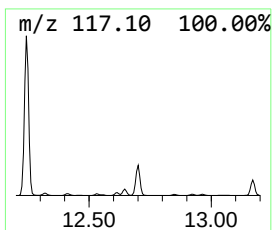
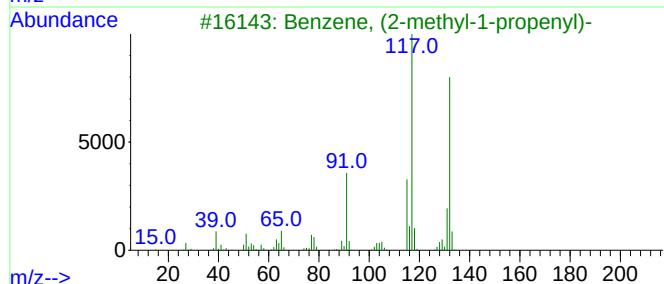
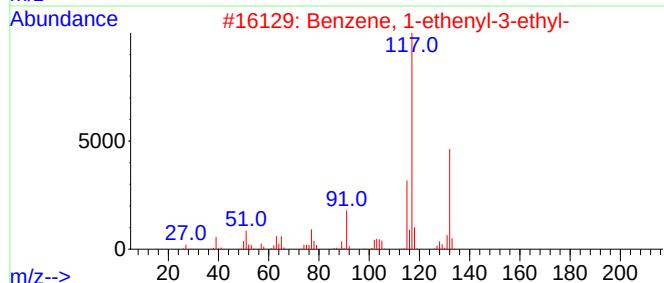
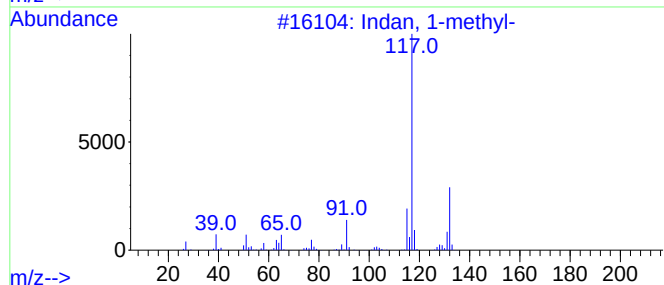
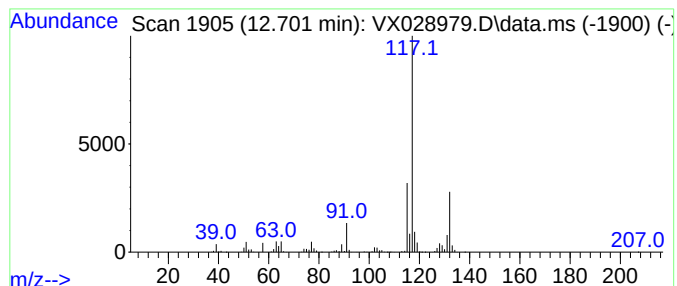
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Quant Title : SW846 8260

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.
12.701	23.00 ug/l	786812	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	87
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028979.D
Acq On : 26 May 2022 03:28
Operator : JC/MD
Sample : N3002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

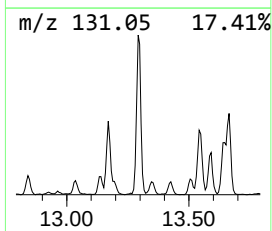
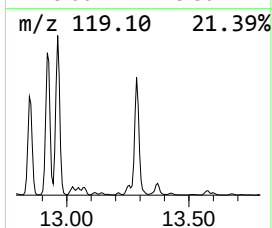
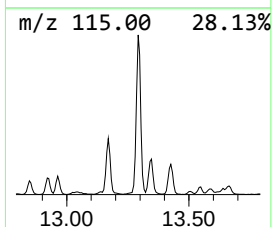
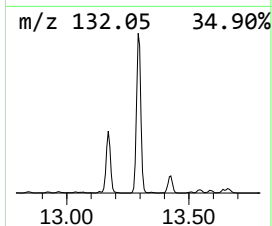
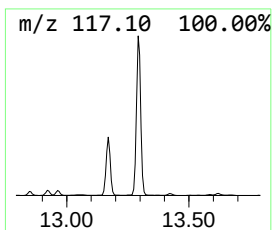
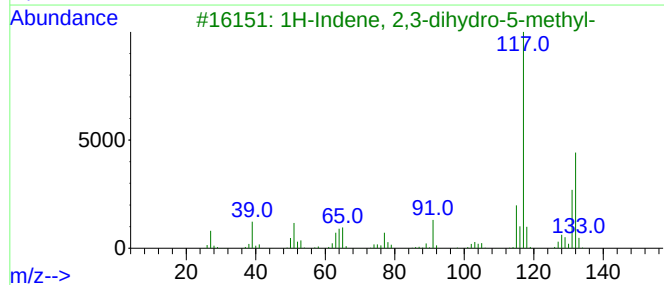
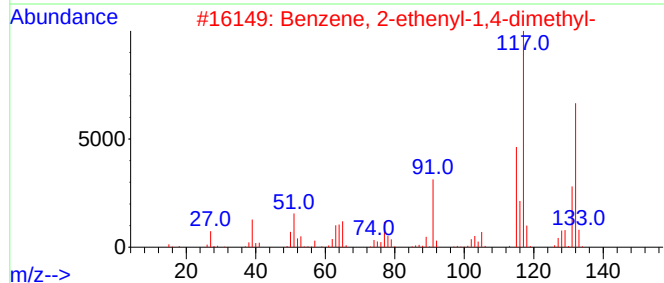
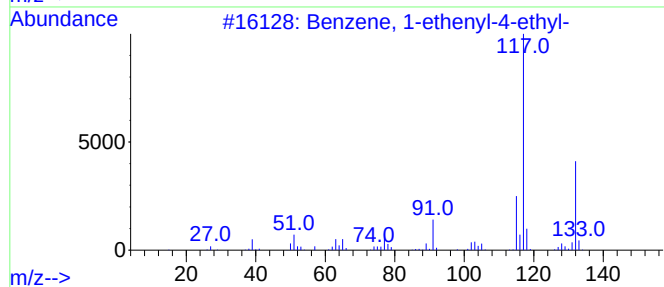
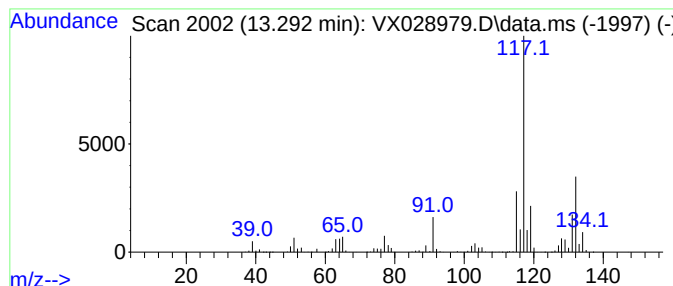
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	38.51 ug/l	1317250	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			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028979.D
Acq On : 26 May 2022 03:28
Operator : JC/MD
Sample : N3002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.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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Butane, 2-methyl-	1.751	32.7	ug/l	729053	1	5.556	1113960	50.0
Cyclopentane, m...	4.306	22.8	ug/l	507345	1	5.556	1113960	50.0
Benzene, 1-ethy...	11.616	92.1	ug/l	3148600	4	12.024	1710170	50.0
Benzene, 1,2,3-...	12.085	106.3	ug/l	3637280	4	12.024	1710170	50.0
Indane	12.243	131.4	ug/l	4492900	4	12.024	1710170	50.0
o-Cymene	12.317	21.6	ug/l	740253	4	12.024	1710170	50.0
Benzene, 1-ethy...	12.615	21.2	ug/l	726219	4	12.024	1710170	50.0
Indan, 1-methyl-	12.701	23.0	ug/l	786812	4	12.024	1710170	50.0
Benzene, 1-ethe...	13.292	38.5	ug/l	1317250	4	12.024	1710170	50.0