

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
 Data File : VX028207.D
 Acq On : 20 Apr 2022 18:54
 Operator : JC/MD
 Sample : N2459-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31574

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\82X041922W.M
 Title : SW846 8260

Signal : TIC: VX028207.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	17	rVB	206477	171750	1.90%	0.205%
2	1.264	26	29	40	rVB	1049097	1066346	11.77%	1.276%
3	1.374	41	47	53	rBV	6987937	7572250	83.56%	9.058%
4	1.429	53	56	63	rVB	567217	560268	6.18%	0.670%
5	1.496	63	67	72	rBV	494134	468832	5.17%	0.561%
6	1.752	103	109	121	rBV	2252374	3071562	33.89%	3.674%
7	1.910	130	135	138	rBV	129916	175665	1.94%	0.210%
8	1.959	138	143	153	rVV2	1094307	1955669	21.58%	2.339%
9	2.069	153	161	170	rVV2	646123	1129762	12.47%	1.351%
10	2.166	170	177	181	rVV	299843	471666	5.20%	0.564%
11	2.215	181	185	196	rVB	990607	1447580	15.97%	1.732%
12	2.374	208	211	223	rVB	53215	92284	1.02%	0.110%
13	2.752	261	273	281	rBV	213892	528541	5.83%	0.632%
14	2.825	281	285	288	rVV	151564	297248	3.28%	0.356%
15	2.867	288	292	303	rVB	296583	618145	6.82%	0.739%
16	3.105	321	331	345	rVB2	107572	246609	2.72%	0.295%
17	3.447	377	387	397	rBV	72249	163095	1.80%	0.195%
18	3.733	428	434	445	rVB3	41230	111505	1.23%	0.133%
19	4.105	486	495	506	rVB2	37095	99129	1.09%	0.119%
20	4.306	518	528	541	rVB	194119	557014	6.15%	0.666%
21	5.196	664	674	688	rVB	49341	149765	1.65%	0.179%
22	5.391	691	706	714	rBV	277990	828223	9.14%	0.991%
23	5.477	714	720	725	rVV2	104670	306140	3.38%	0.366%
24	5.556	725	733	763	rVB	397223	1166507	12.87%	1.395%
25	5.958	789	799	805	rBV	273739	730312	8.06%	0.874%
26	6.044	805	813	826	rVB	1588436	4152272	45.82%	4.967%
27	6.239	837	845	857	rVB6	35479	137801	1.52%	0.165%
28	6.763	922	931	943	rBV	616907	1465597	16.17%	1.753%
29	7.385	1021	1033	1041	rBV2	56072	137377	1.52%	0.164%
30	8.653	1234	1241	1246	rBV	1456062	2251543	24.84%	2.693%
31	8.720	1246	1252	1264	rVB	5987918	9062592	100.00%	10.841%
32	10.055	1459	1471	1481	rBV	1392866	1847305	20.38%	2.210%
33	10.195	1489	1494	1500	rBV	202222	256128	2.83%	0.306%
34	10.299	1505	1511	1523	rBV	6302337	8668459	95.65%	10.370%
35	10.640	1562	1567	1579	rVB	3762244	4947614	54.59%	5.919%
36	11.079	1634	1639	1654	rBV	1308469	1734170	19.14%	2.074%

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37	11.378	1683	1688	1696	rBV	2460828	3930371	43.37%	4.702%
38	11.451	1696	1700	1710	rVB	1143113	1388620	15.32%	1.661%
39	11.616	1721	1727	1738	rVB	1083927	1339044	14.78%	1.602%
40	11.756	1744	1750	1756	rBV	3906843	4932364	54.43%	5.900%
41	11.969	1780	1785	1789	rBV	92350	114567	1.26%	0.137%
42	12.024	1789	1794	1799	rVV	1635547	2015382	22.24%	2.411%
43	12.085	1799	1804	1810	rVB	1205239	1512014	16.68%	1.809%
44	12.244	1822	1830	1838	rBV2	1188660	1931750	21.32%	2.311%
45	12.317	1838	1842	1852	rVB2	571992	759851	8.38%	0.909%
46	12.463	1862	1866	1872	rVB	134342	166229	1.83%	0.199%
47	12.530	1872	1877	1879	rBV	330501	404280	4.46%	0.484%
48	12.555	1879	1881	1886	rVB	308084	331681	3.66%	0.397%
49	12.616	1886	1891	1894	rBV	541303	651843	7.19%	0.780%
50	12.646	1894	1896	1900	rVB	128278	131655	1.45%	0.157%
51	12.701	1900	1905	1913	rBV2	363330	508754	5.61%	0.609%
52	12.847	1925	1929	1934	rVB	145010	183372	2.02%	0.219%
53	12.920	1934	1941	1945	rVV	292633	385472	4.25%	0.461%
54	12.963	1945	1948	1953	rVB	475757	535306	5.91%	0.640%
55	13.170	1978	1982	1986	rVB	397209	478054	5.28%	0.572%
56	13.292	1998	2002	2008	rVB2	723479	943551	10.41%	1.129%
57	13.420	2018	2023	2032	rVB	223725	287461	3.17%	0.344%
58	13.542	2040	2043	2046	rVV	114407	153676	1.70%	0.184%
59	13.585	2046	2050	2056	rVV3	129596	250126	2.76%	0.299%
60	13.664	2060	2063	2069	rVB2	102302	153753	1.70%	0.184%
61	13.774	2075	2081	2087	rBV	445015	569798	6.29%	0.682%
62	13.926	2100	2106	2110	rBV2	66885	97603	1.08%	0.117%
63	14.079	2125	2131	2135	rBV	87667	108497	1.20%	0.130%
64	14.219	2149	2154	2159	rBV3	82302	156720	1.73%	0.187%
65	14.640	2213	2223	2228	rBV	261742	357123	3.94%	0.427%
66	14.780	2241	2246	2250	rBV	136684	169931	1.88%	0.203%

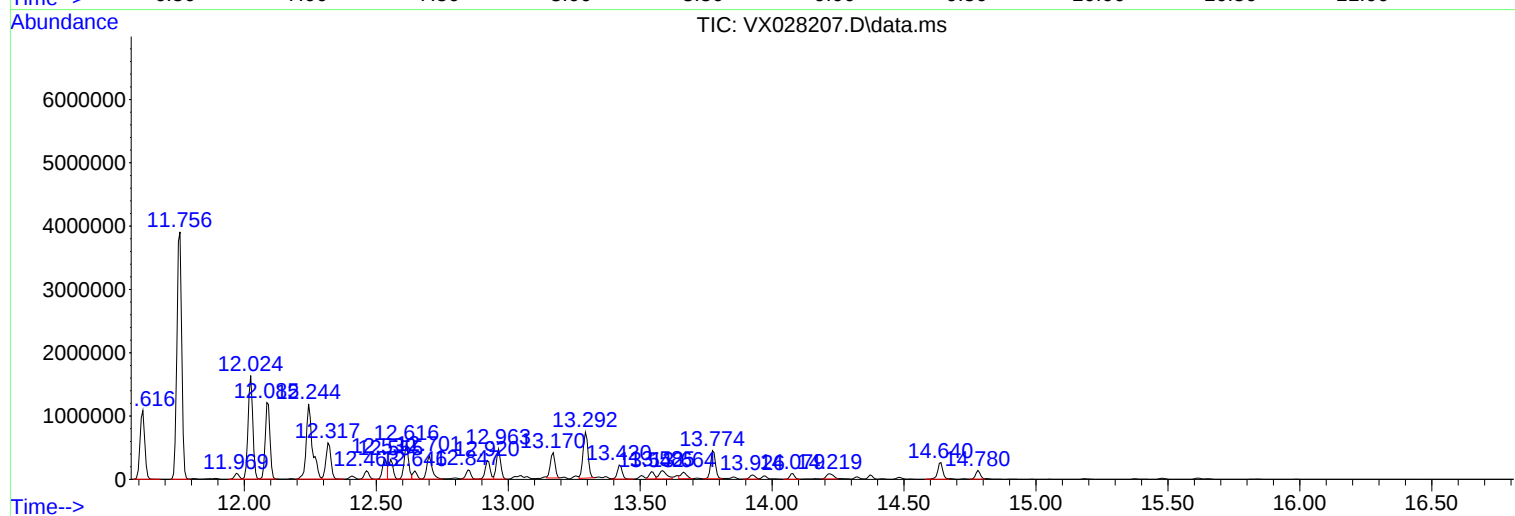
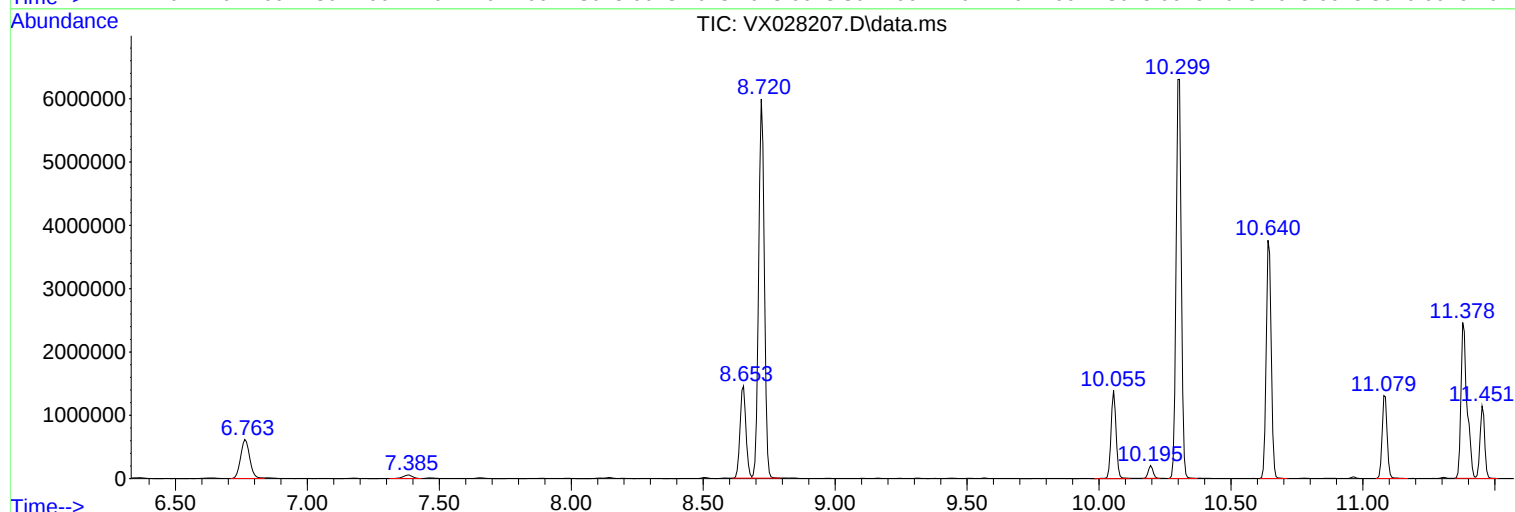
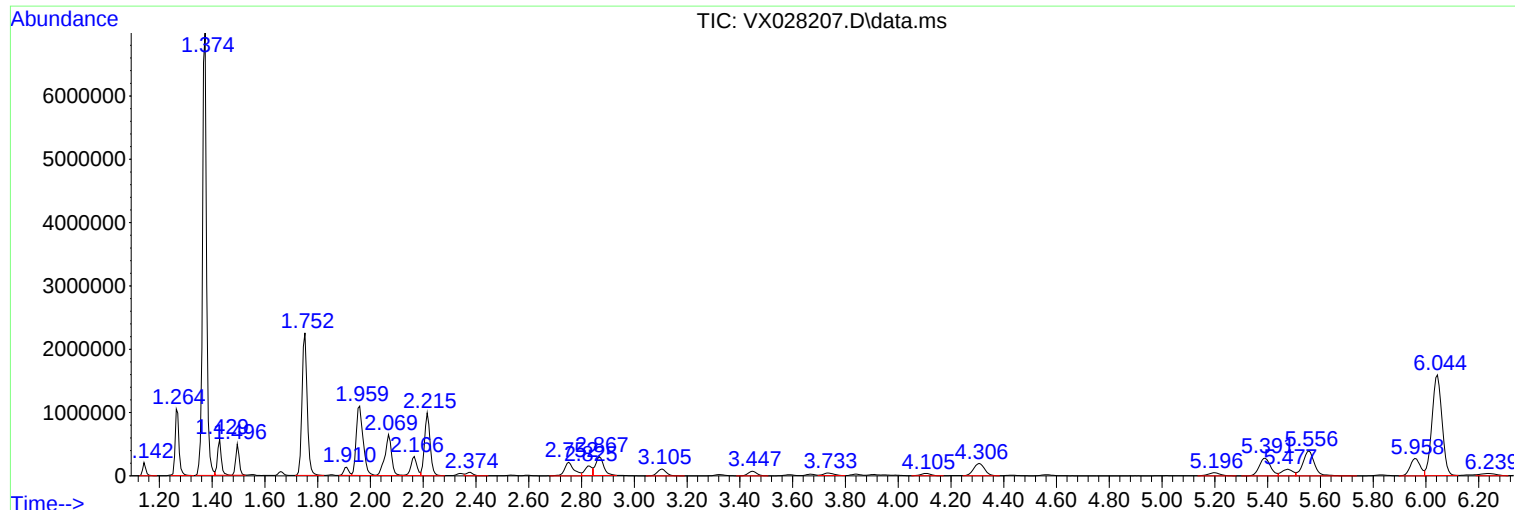
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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



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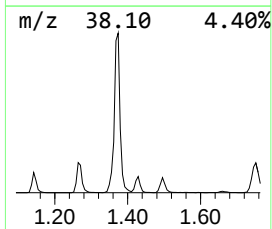
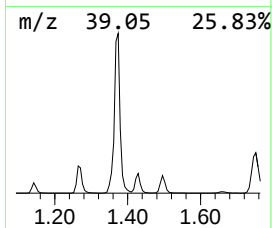
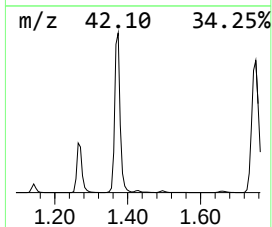
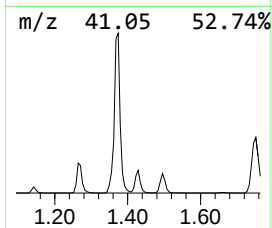
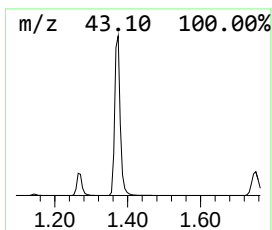
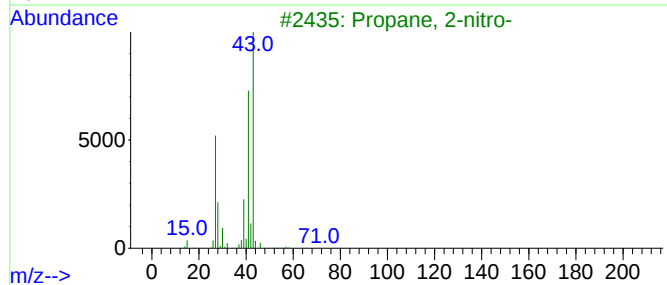
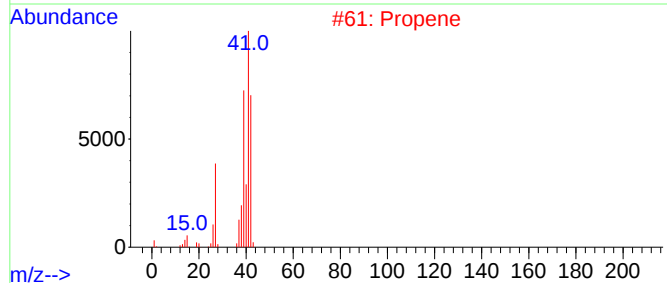
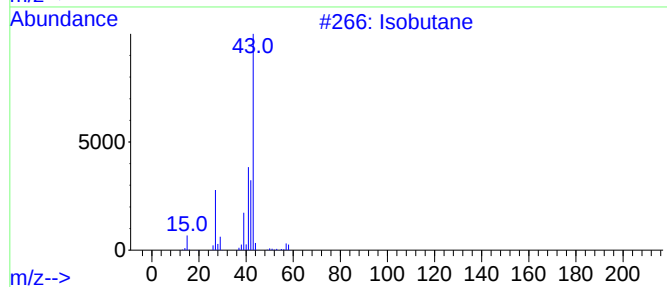
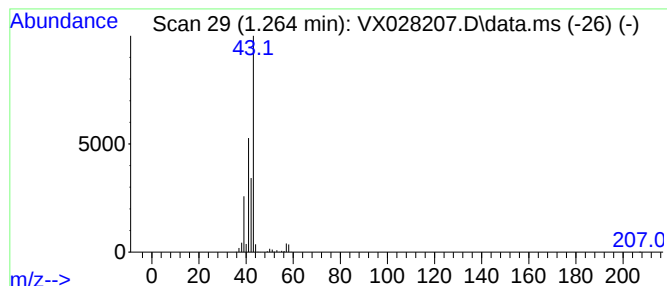
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	45.71 ug/l	1066350	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	72
2			Propene	42	C3H6	000115-07-1	5
3			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4
4			5-Methyloxazolidine	87	C4H9NO	058328-22-6	4
5			Cyclobutylamine	71	C4H9N	002516-34-9	4



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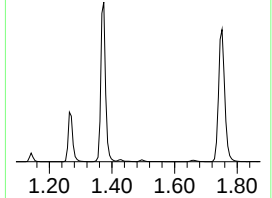
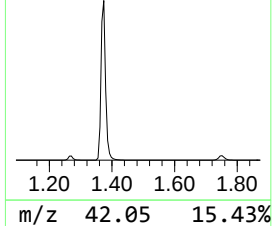
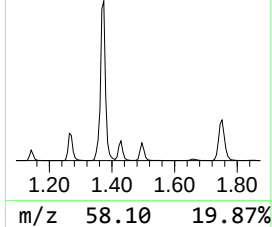
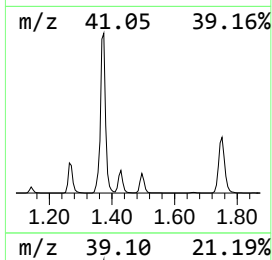
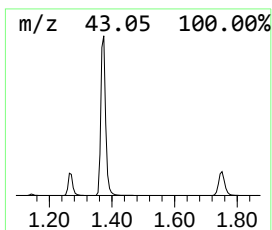
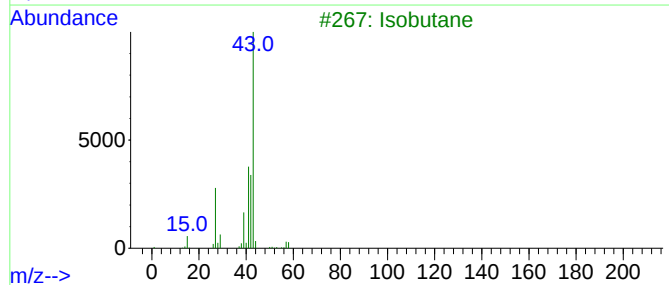
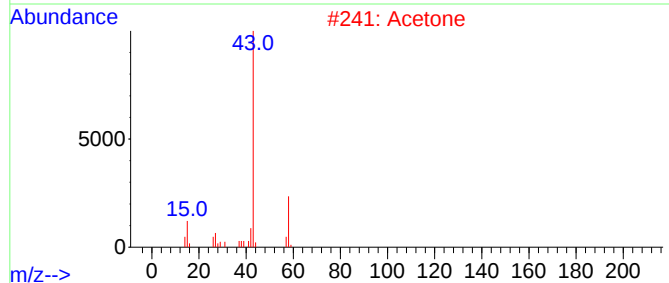
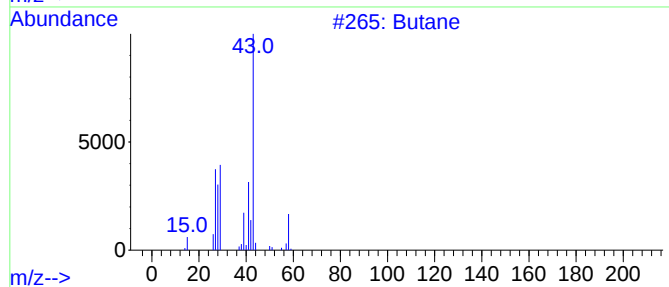
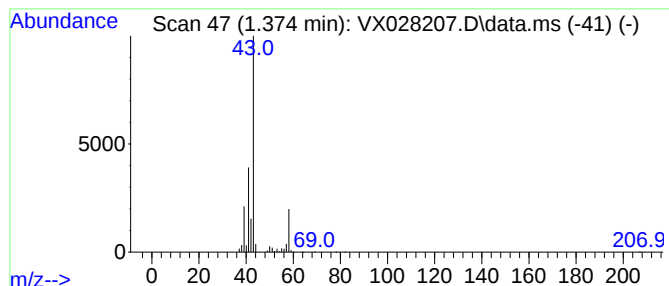
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	324.57 ug/l	7572250	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	86
2			Acetone	58	C3H6O	000067-64-1	50
3			Isobutane	58	C4H10	000075-28-5	9
4			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9



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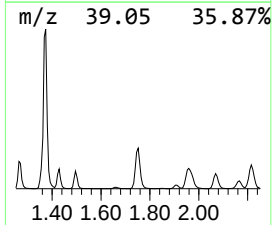
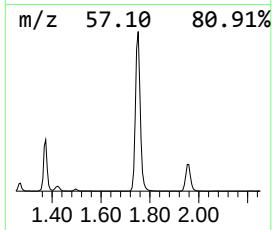
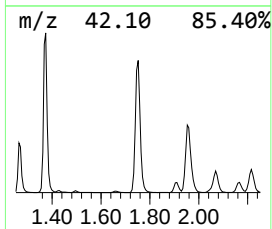
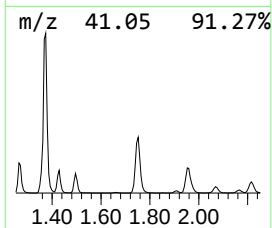
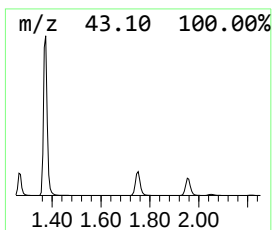
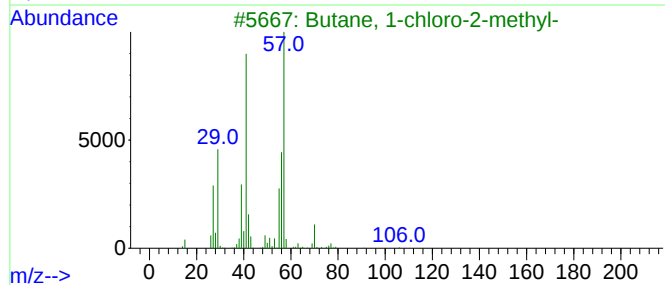
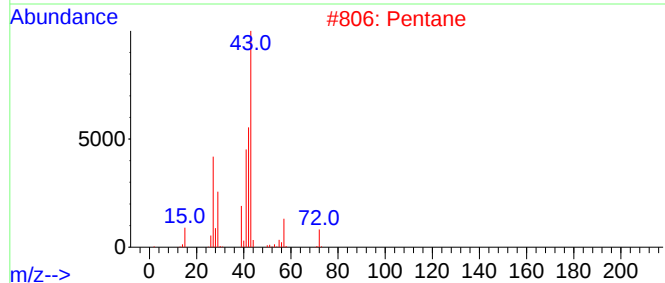
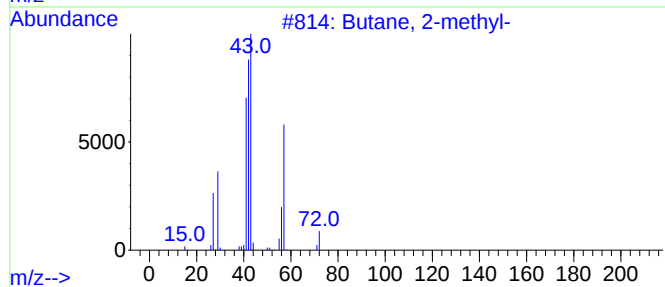
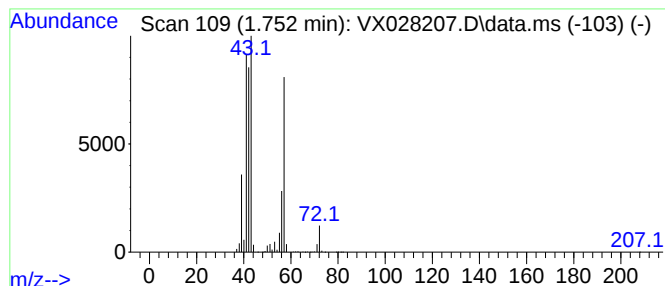
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	131.66 ug/l	3071560	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	33
3			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	27
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10
5			1-Butene	56	C4H8	000106-98-9	10



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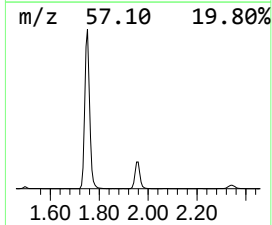
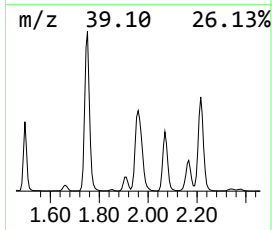
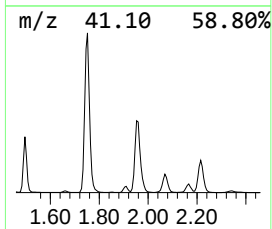
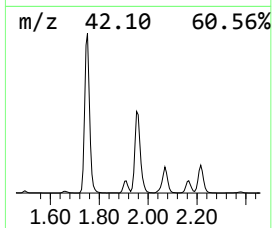
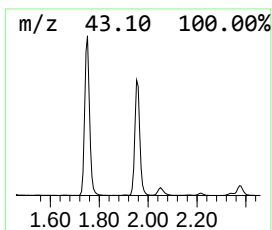
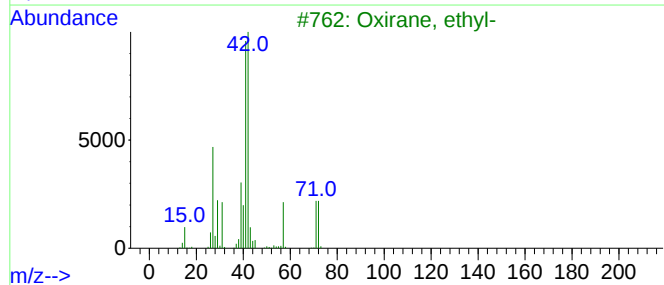
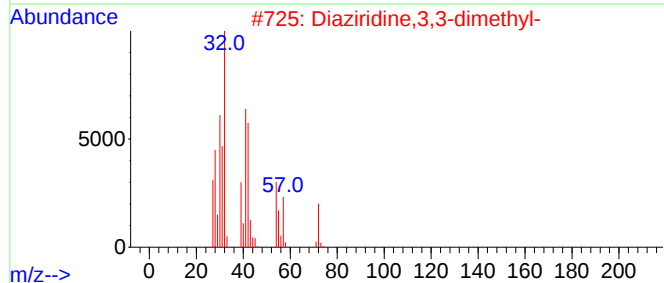
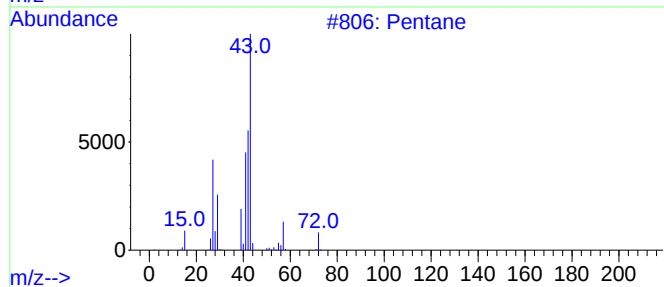
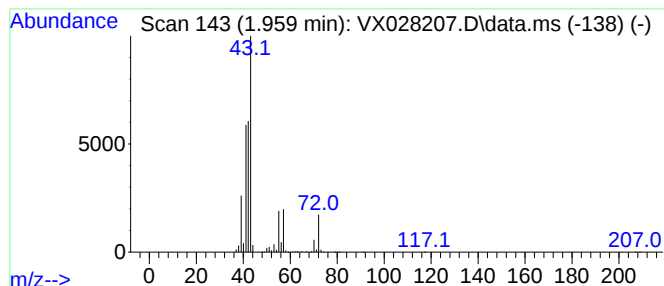
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	83.83 ug/l	1955670	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	78
2			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	52
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	47
4			1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	25
5			2-Butanone	72	C4H8O	000078-93-3	25



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Sample : N2459-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31574

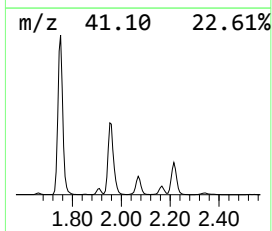
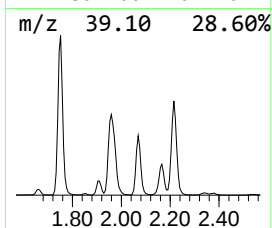
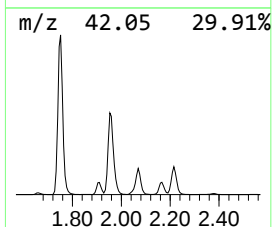
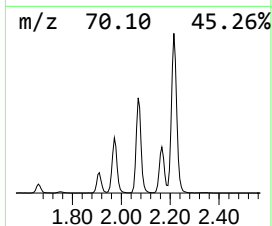
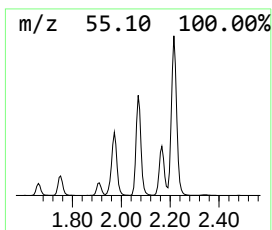
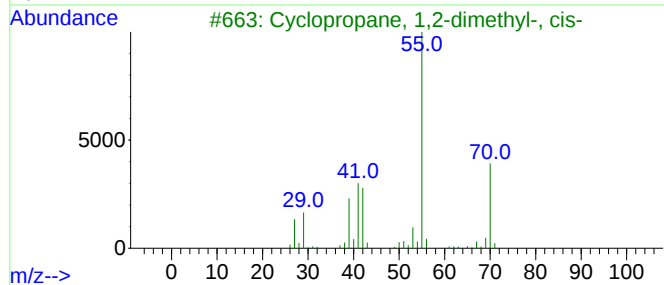
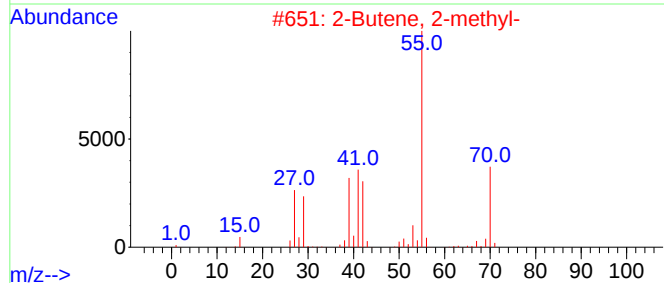
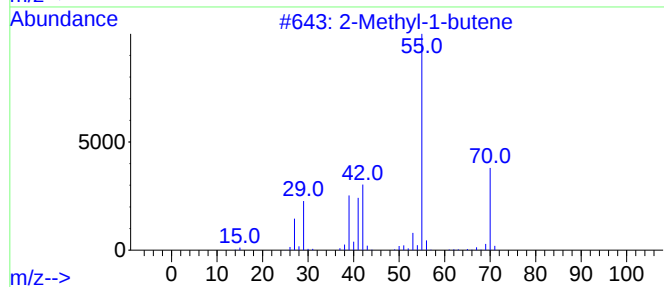
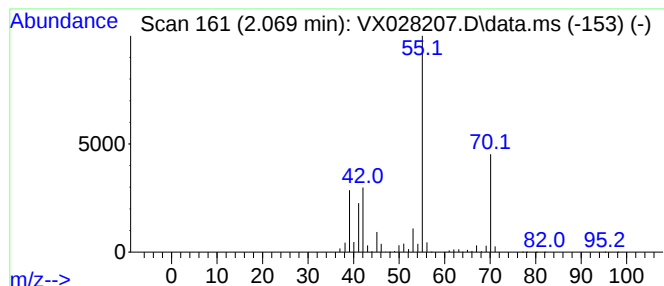
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Quant Title : SW846 8260

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

Peak Number 5 2-Methyl-1-butene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	48.42 ug/l	1129760	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-1-butene	70	C5H10	000563-46-2	87
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	83
3			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	83
4			2-Pentene, (E)-	70	C5H10	000646-04-8	74
5			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028207.D
Acq On : 20 Apr 2022 18:54
Operator : JC/MD
Sample : N2459-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31574

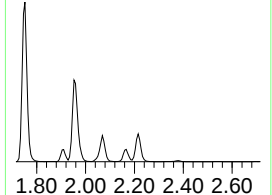
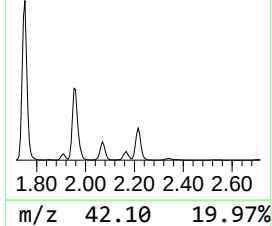
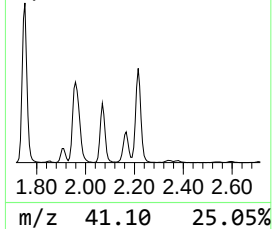
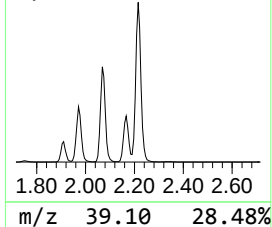
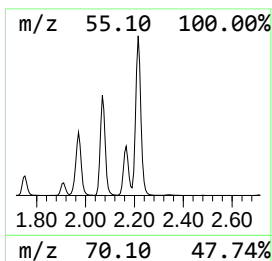
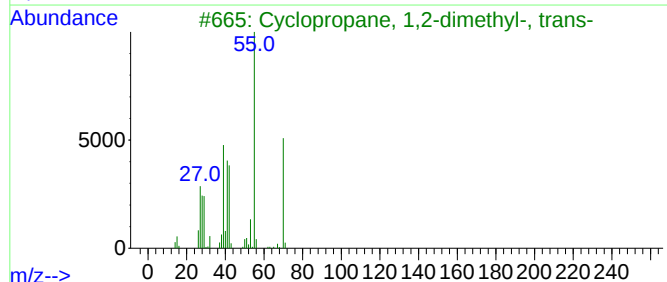
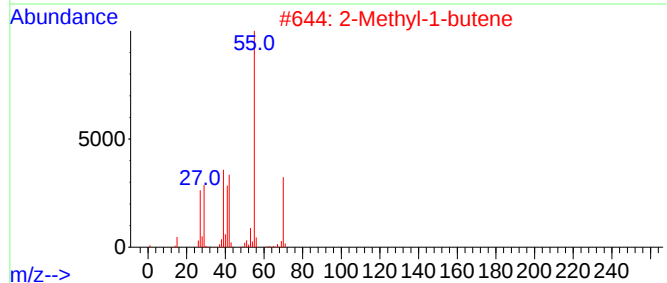
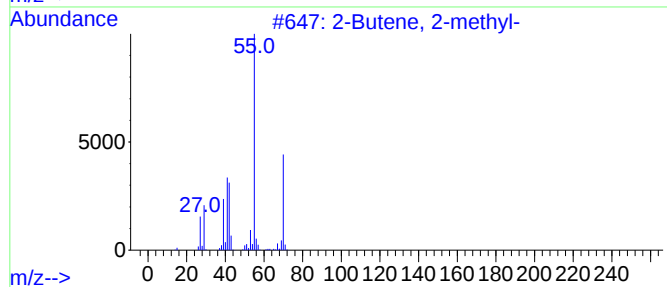
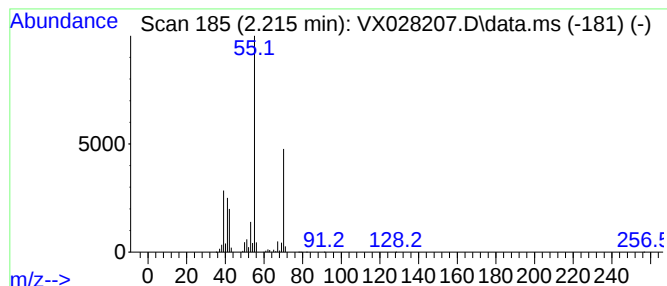
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Quant Title : SW846 8260

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

Peak Number 6 2-Butene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	62.05 ug/l	1447580	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-			70	C5H10	000513-35-9	90
2	2-Methyl-1-butene			70	C5H10	000563-46-2	83
3	Cyclopropane, 1,2-dimethyl-, trans-			70	C5H10	002402-06-4	83
4	Cyclopropane, 1,1-dimethyl-			70	C5H10	001630-94-0	80
5	2-Pentene, (Z)-			70	C5H10	000627-20-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028207.D
Acq On : 20 Apr 2022 18:54
Operator : JC/MD
Sample : N2459-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31574

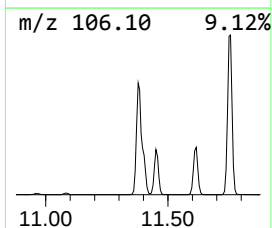
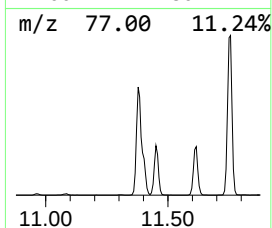
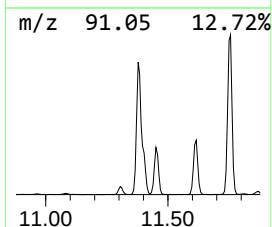
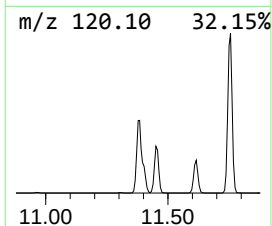
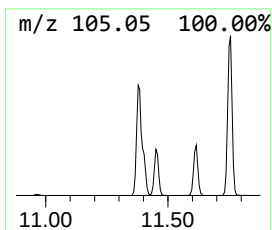
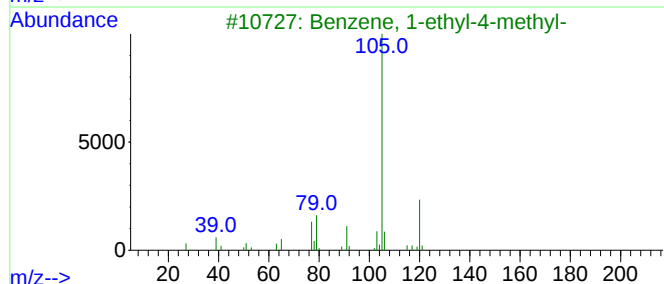
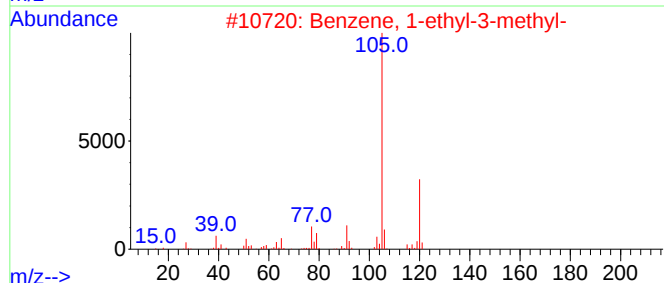
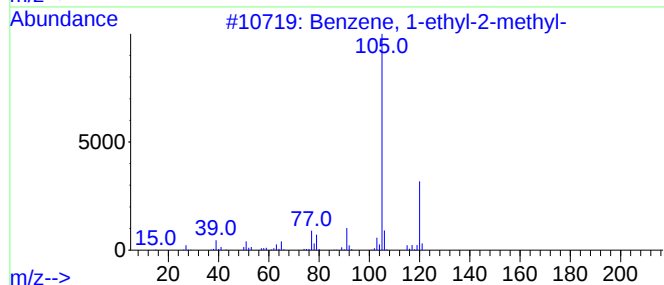
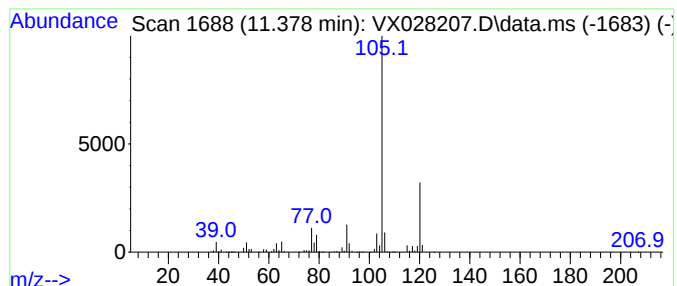
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	97.51 ug/l	3930370	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028207.D
Acq On : 20 Apr 2022 18:54
Operator : JC/MD
Sample : N2459-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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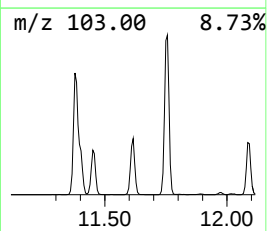
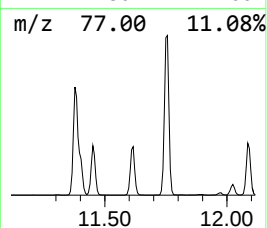
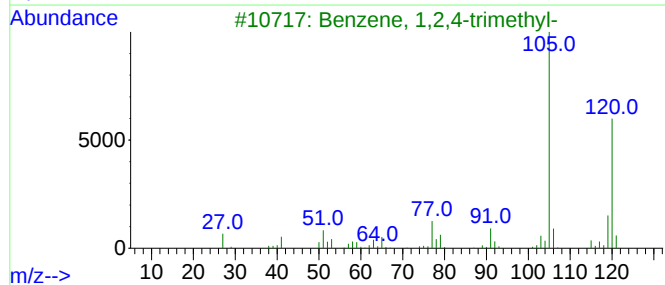
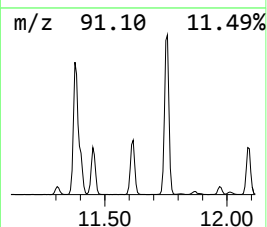
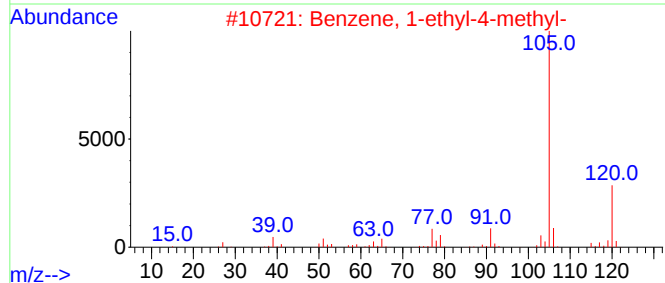
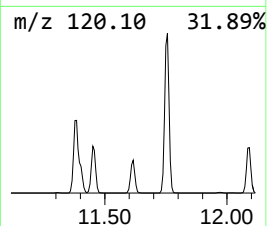
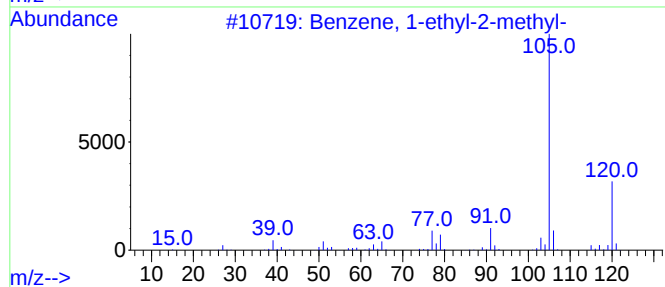
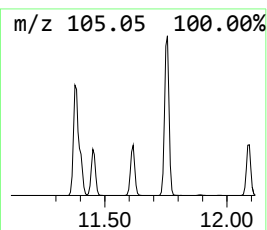
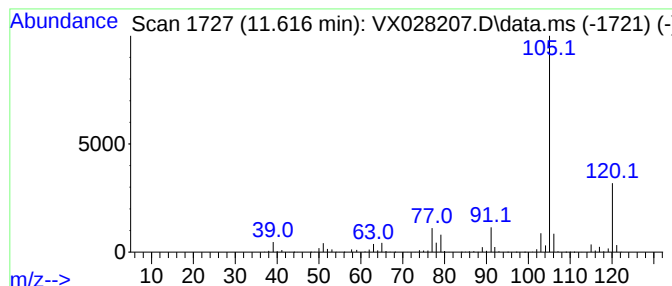
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	33.22 ug/l	1339040	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	90
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
4			Mesitylene	120	C9H12	000108-67-8	90
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028207.D
Acq On : 20 Apr 2022 18:54
Operator : JC/MD
Sample : N2459-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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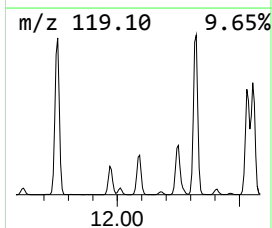
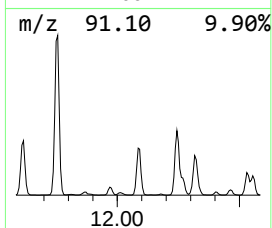
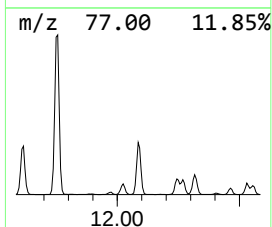
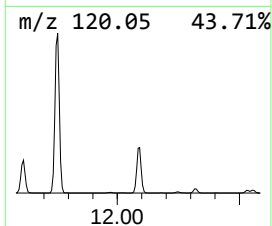
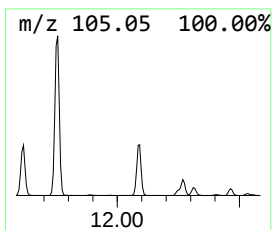
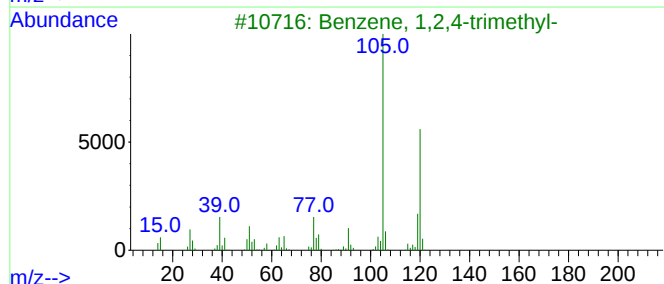
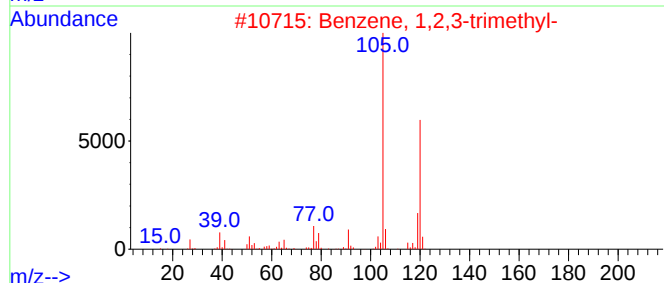
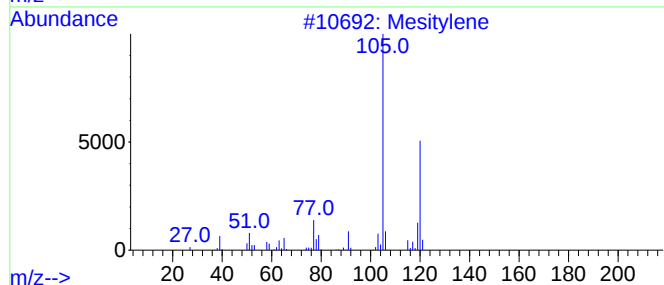
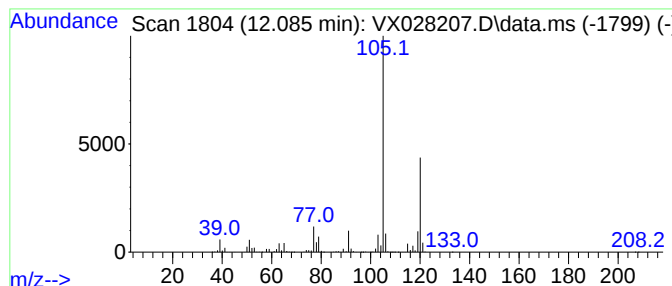
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	37.51 ug/l	1512010	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	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028207.D
Acq On : 20 Apr 2022 18:54
Operator : JC/MD
Sample : N2459-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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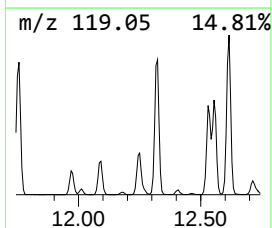
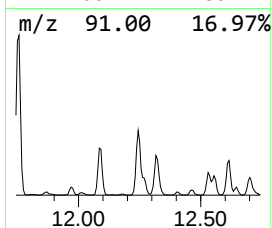
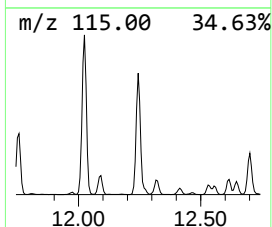
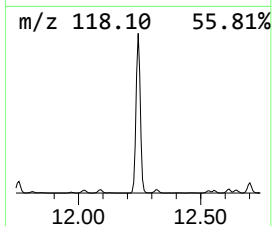
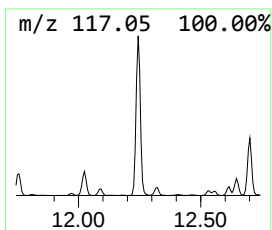
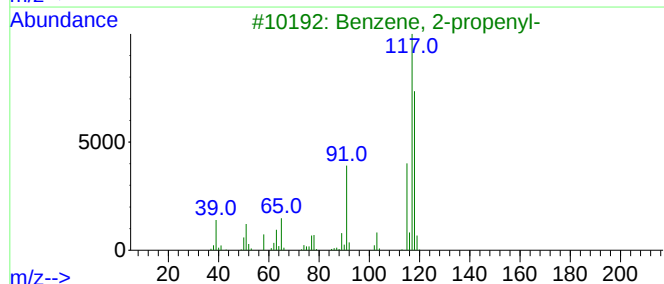
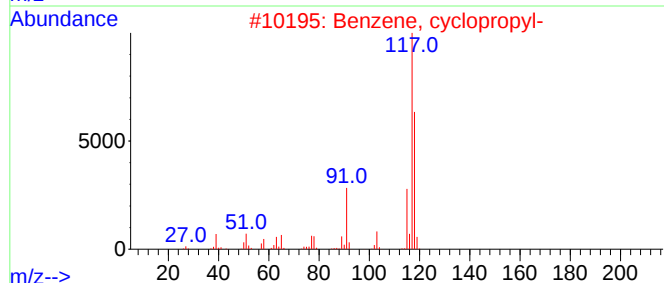
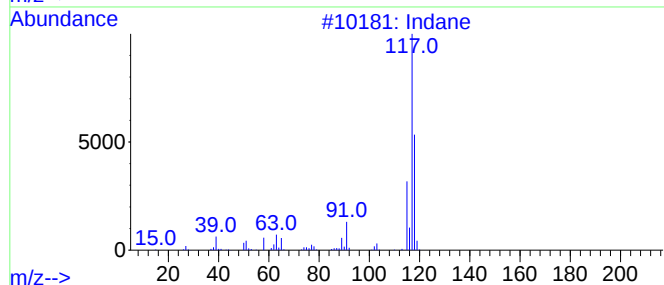
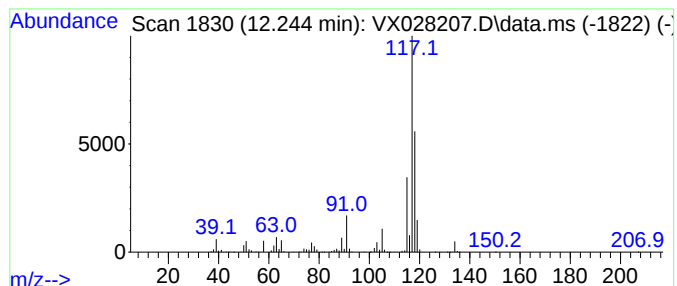
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	47.93 ug/l	1931750	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	76
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	58
5			Deltacyclene	118	C9H10	007785-10-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028207.D
Acq On : 20 Apr 2022 18:54
Operator : JC/MD
Sample : N2459-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31574

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.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	1.374	324.6	ug/l	7572250	1	5.556	1166510	50.0
Butane, 2-methyl-	1.752	131.7	ug/l	3071560	1	5.556	1166510	50.0
Pentane	1.959	83.8	ug/l	1955670	1	5.556	1166510	50.0
2-Methyl-1-butene	2.069	48.4	ug/l	1129760	1	5.556	1166510	50.0
2-Butene, 2-met...	2.215	62.0	ug/l	1447580	1	5.556	1166510	50.0
Benzene, 1-ethy...	11.378	97.5	ug/l	3930370	4	12.024	2015380	50.0
Benzene, 1-ethy...	11.616	33.2	ug/l	1339040	4	12.024	2015380	50.0
Benzene, 1,2,3-...	12.085	37.5	ug/l	1512010	4	12.024	2015380	50.0
Indane	12.244	47.9	ug/l	1931750	4	12.024	2015380	50.0