

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
 Data File : VX028208.D
 Acq On : 20 Apr 2022 19:17
 Operator : JC/MD
 Sample : N2459-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31575

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: VX028208.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	rBV	77488	68472	1.62%	0.167%
2	1.264	26	29	40	rVB	460151	441493	10.42%	1.074%
3	1.374	41	47	53	rBV	2766204	3023142	71.32%	7.354%
4	1.429	53	56	63	rVB	210950	212353	5.01%	0.517%
5	1.496	63	67	71	rBV	189287	177652	4.19%	0.432%
6	1.752	103	109	120	rBV	911599	1241965	29.30%	3.021%
7	1.910	130	135	138	rBV	50879	70963	1.67%	0.173%
8	1.959	138	143	155	rVV2	430166	768376	18.13%	1.869%
9	2.069	156	161	169	rVV	225759	320600	7.56%	0.780%
10	2.166	170	177	181	rVV	113714	184839	4.36%	0.450%
11	2.215	181	185	195	rVB	353839	515746	12.17%	1.255%
12	2.752	258	273	281	rBV2	80774	207924	4.91%	0.506%
13	2.825	281	285	288	rVV	59860	119568	2.82%	0.291%
14	2.867	288	292	305	rVB	116742	245312	5.79%	0.597%
15	3.105	323	331	343	rBV2	44098	103044	2.43%	0.251%
16	3.447	379	387	398	rVB2	26717	59575	1.41%	0.145%
17	4.306	517	528	539	rVB2	77311	219268	5.17%	0.533%
18	5.202	665	675	686	rVB2	18098	56198	1.33%	0.137%
19	5.391	694	706	715	rBV2	288549	851721	20.09%	2.072%
20	5.477	715	720	724	rVV2	41543	112425	2.65%	0.273%
21	5.556	724	733	755	rVB	400273	1161806	27.41%	2.826%
22	5.958	788	799	805	rBV	279355	744623	17.57%	1.811%
23	6.044	805	813	828	rVB	662550	1744646	41.16%	4.244%
24	6.763	921	931	944	rBV	617353	1486042	35.06%	3.615%
25	7.385	1023	1033	1042	rVB4	22772	57534	1.36%	0.140%
26	8.653	1234	1241	1246	rBV	1465435	2322270	54.79%	5.649%
27	8.720	1246	1252	1265	rVB	2860639	4238680	100.00%	10.310%
28	10.055	1465	1471	1485	rBV	1404229	1844647	43.52%	4.487%
29	10.195	1489	1494	1505	rVB	240139	308928	7.29%	0.751%
30	10.299	1505	1511	1525	rBV	1997461	2767079	65.28%	6.731%
31	10.640	1562	1567	1579	rVB	1501243	1984728	46.82%	4.828%
32	11.079	1634	1639	1652	rBV	1292617	1694627	39.98%	4.122%
33	11.378	1683	1688	1696	rVV	825538	1396835	32.95%	3.398%
34	11.451	1696	1700	1713	rVB	444716	542352	12.80%	1.319%
35	11.616	1721	1727	1733	rBV	414219	522421	12.33%	1.271%
36	11.750	1744	1749	1756	rBV	897117	1122055	26.47%	2.729%

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37	11.969	1778	1785	1789	rBV	48253	61884	1.46%	0.151%
38	12.024	1789	1794	1800	rVV	1572795	1907502	45.00%	4.640%
39	12.091	1800	1805	1811	rVB	510221	635903	15.00%	1.547%
40	12.244	1822	1830	1833	rBV	472356	663713	15.66%	1.614%
41	12.317	1838	1842	1851	rVB2	251551	342791	8.09%	0.834%
42	12.463	1862	1866	1871	rVB	78188	92237	2.18%	0.224%
43	12.530	1871	1877	1879	rBV	111628	140109	3.31%	0.341%
44	12.555	1879	1881	1886	rVB	113091	128980	3.04%	0.314%
45	12.616	1886	1891	1894	rBV	232151	282526	6.67%	0.687%
46	12.646	1894	1896	1900	rVB	61933	64892	1.53%	0.158%
47	12.701	1900	1905	1913	rBV2	166882	262199	6.19%	0.638%
48	12.847	1925	1929	1934	rVB2	76875	100742	2.38%	0.245%
49	12.920	1934	1941	1945	rBV	137505	176598	4.17%	0.430%
50	12.963	1945	1948	1954	rVB	219177	247128	5.83%	0.601%
51	13.170	1978	1982	1986	rVB	164342	196615	4.64%	0.478%
52	13.256	1992	1996	1998	rBV3	29579	44450	1.05%	0.108%
53	13.292	1998	2002	2007	rVB2	396531	523370	12.35%	1.273%
54	13.420	2018	2023	2031	rVB	192140	258781	6.11%	0.629%
55	13.506	2032	2037	2040	rBV2	35071	49043	1.16%	0.119%
56	13.542	2040	2043	2046	rBV	58244	76637	1.81%	0.186%
57	13.585	2046	2050	2055	rVV3	77673	120044	2.83%	0.292%
58	13.664	2060	2063	2070	rVB2	80371	116622	2.75%	0.284%
59	13.774	2075	2081	2088	rVV	143063	211371	4.99%	0.514%
60	13.853	2089	2094	2100	rVB	69714	96969	2.29%	0.236%
61	13.926	2100	2106	2110	rBV2	89179	125726	2.97%	0.306%
62	14.079	2126	2131	2135	rBV	70351	91856	2.17%	0.223%
63	14.225	2149	2155	2163	rBV3	157540	287311	6.78%	0.699%
64	14.323	2167	2171	2175	rBV	36490	45782	1.08%	0.111%
65	14.371	2175	2179	2184	rVB	74257	94879	2.24%	0.231%
66	14.481	2192	2197	2202	rBV2	134038	178953	4.22%	0.435%
67	14.615	2215	2219	2220	rBV	63829	69375	1.64%	0.169%
68	14.640	2220	2223	2226	rVV	106538	143747	3.39%	0.350%
69	14.670	2226	2228	2234	rVB	43136	53910	1.27%	0.131%
70	14.780	2241	2246	2249	rBV	49902	63440	1.50%	0.154%
71	14.902	2262	2266	2272	rVV3	30193	53548	1.26%	0.130%
72	15.182	2308	2312	2319	rVB	66075	114566	2.70%	0.279%
73	15.615	2377	2383	2386	rBV3	29473	46273	1.09%	0.113%

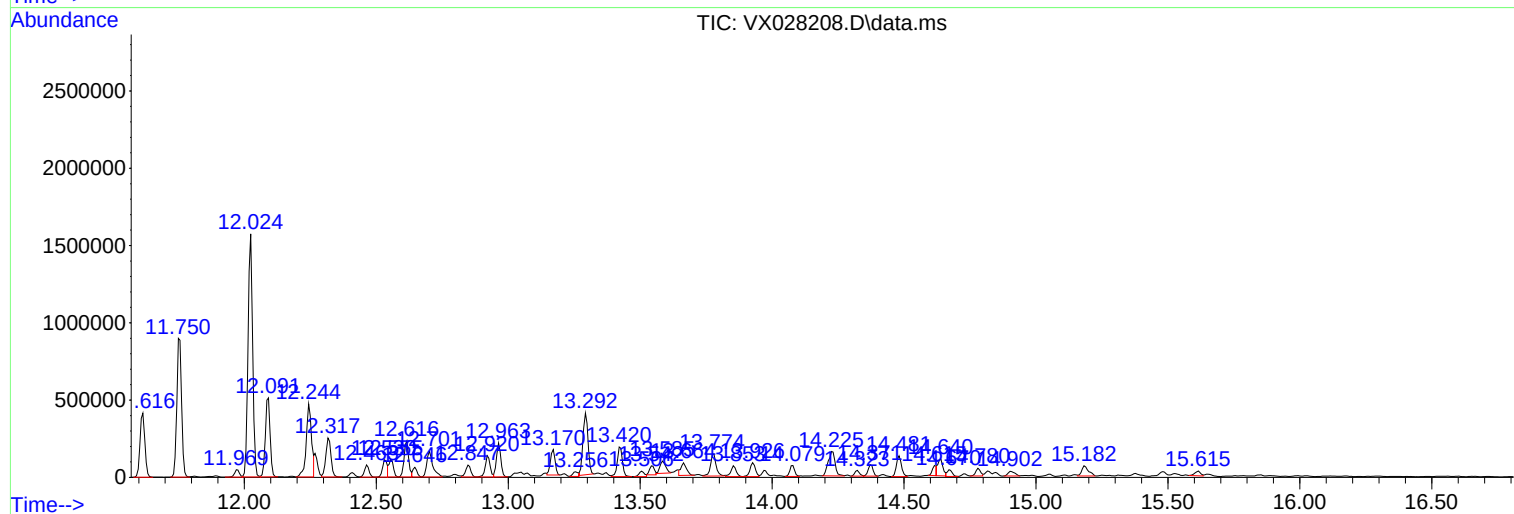
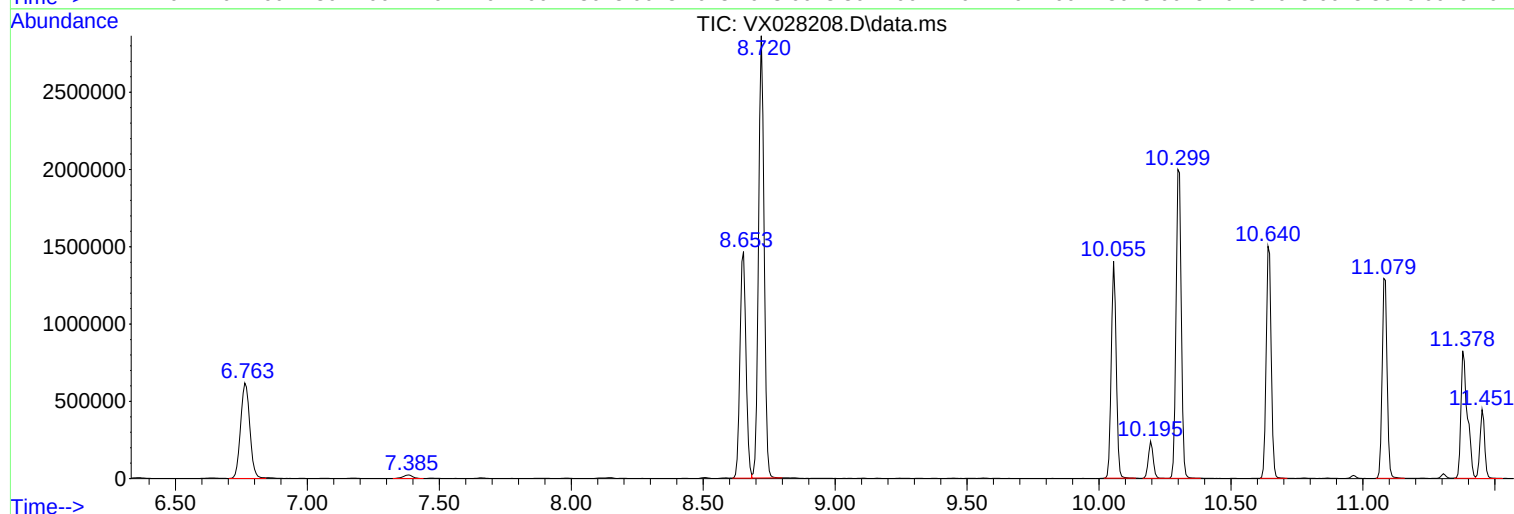
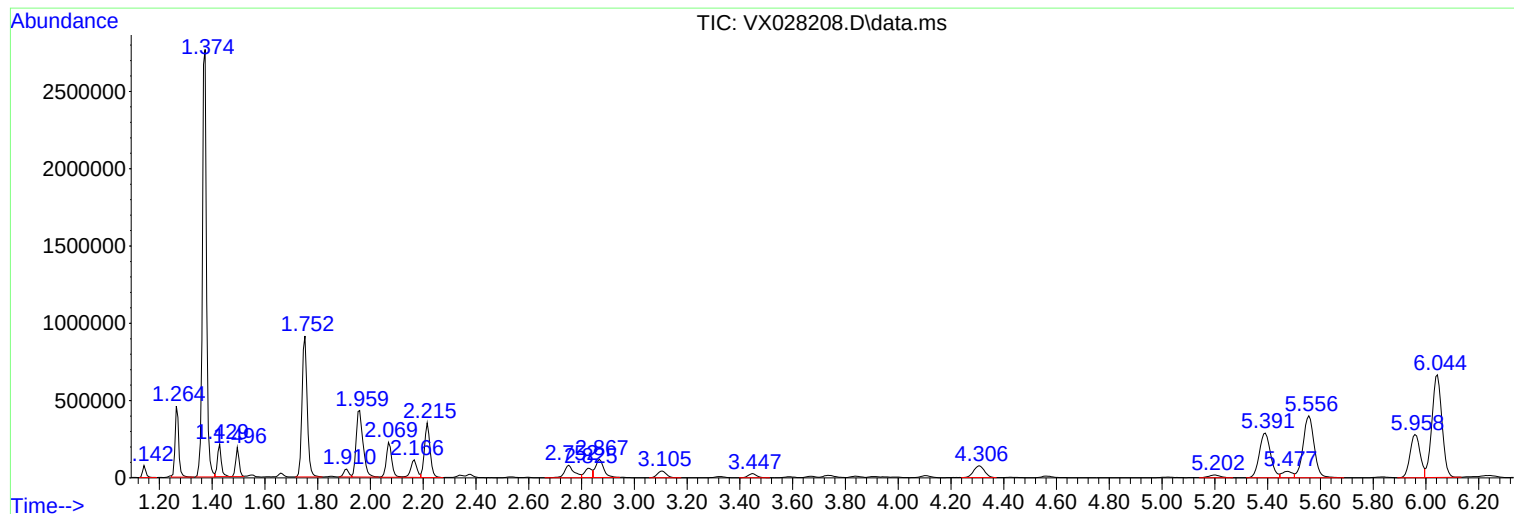
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX042022\
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Acq On : 20 Apr 2022 19:17
Operator : JC/MD
Sample : N2459-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31575

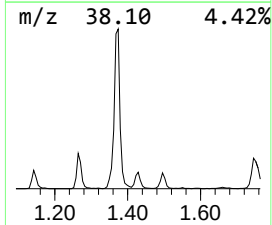
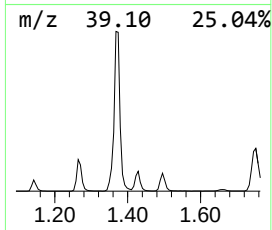
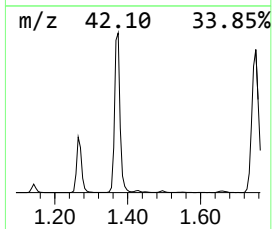
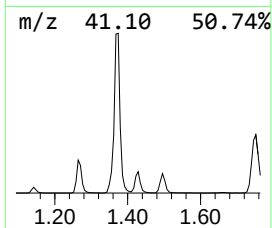
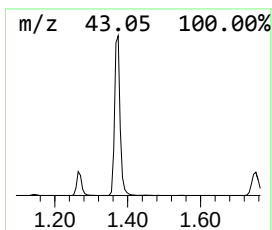
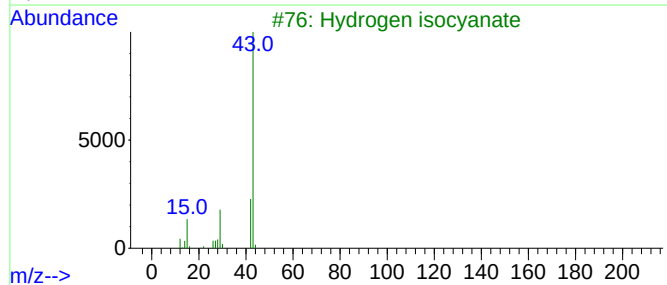
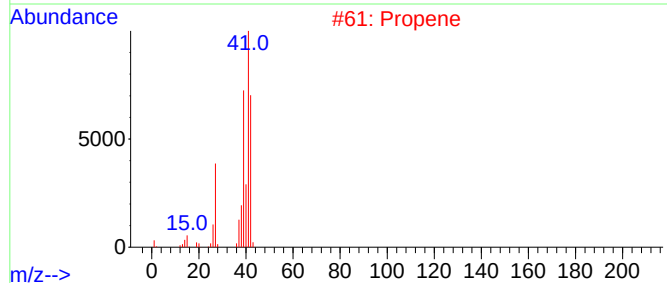
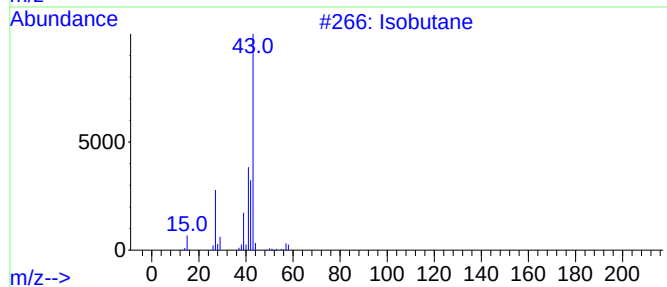
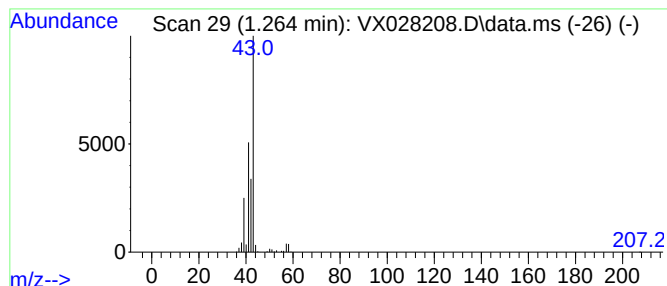
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	19.00 ug/l	441493	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			Hydrogen isocyanate	43	CHNO	000075-13-8	4
4			Cyclobutylamine	71	C4H9N	002516-34-9	4
5			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4



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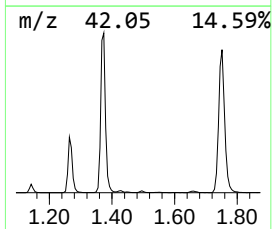
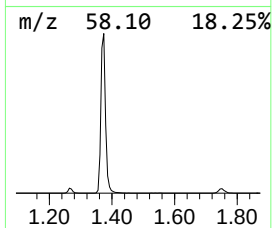
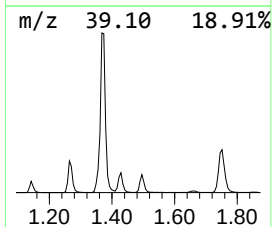
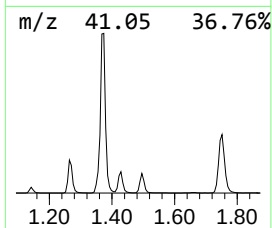
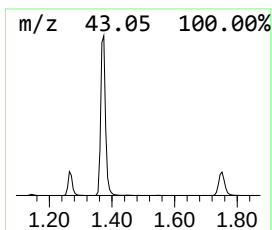
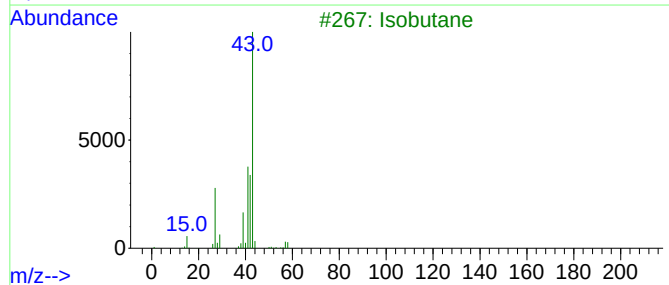
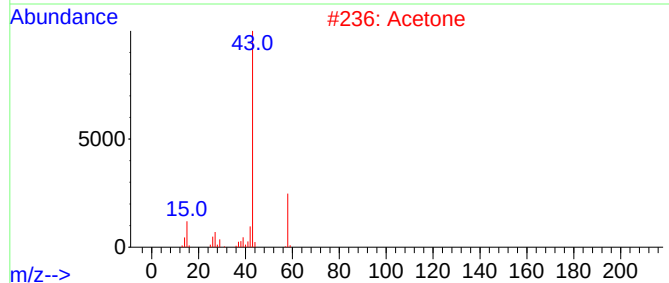
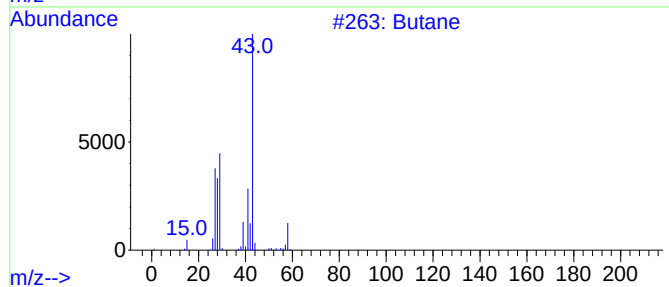
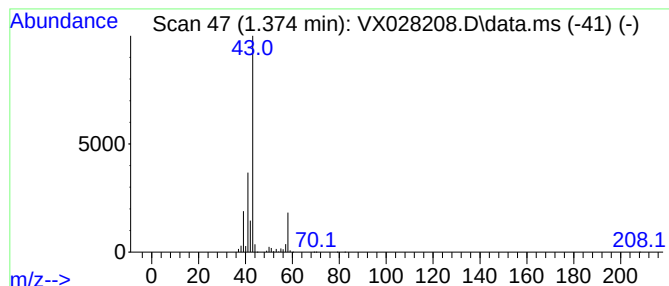
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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	130.10 ug/l	3023140	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Acetone	58	C3H6O	000067-64-1	9
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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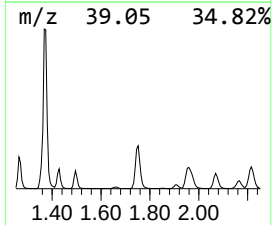
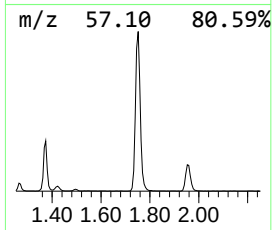
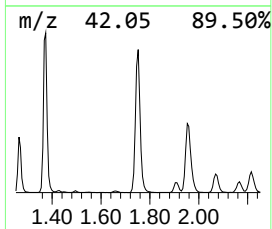
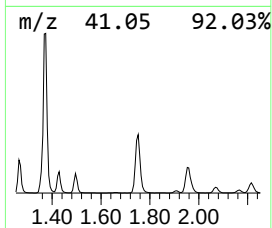
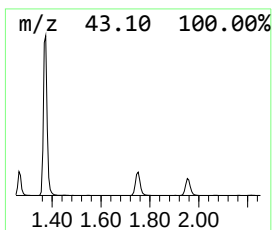
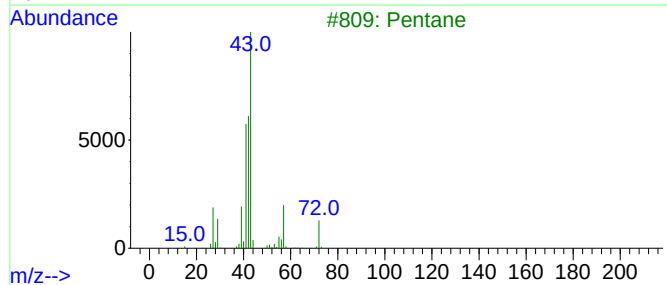
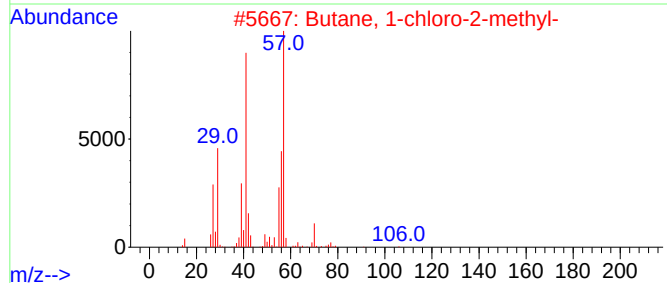
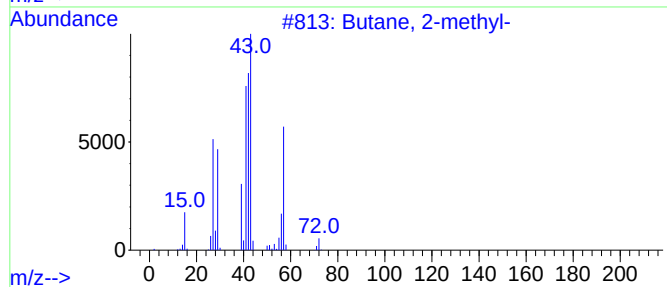
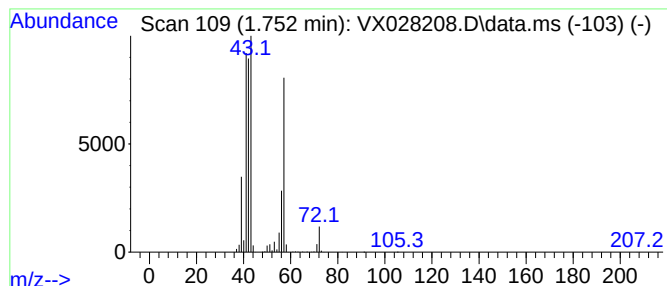
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	53.45 ug/l	1241970	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	35
3			Pentane	72	C5H12	000109-66-0	32
4			3-Buten-1-ol	72	C4H8O	000627-27-0	25
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10



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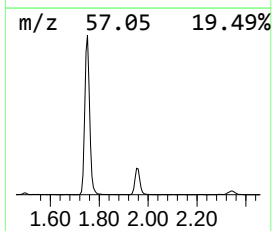
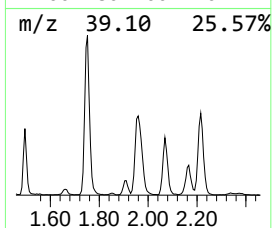
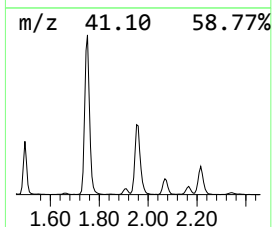
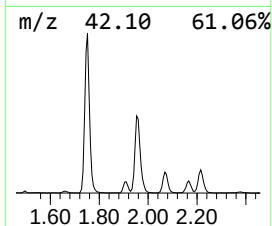
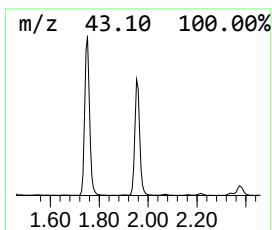
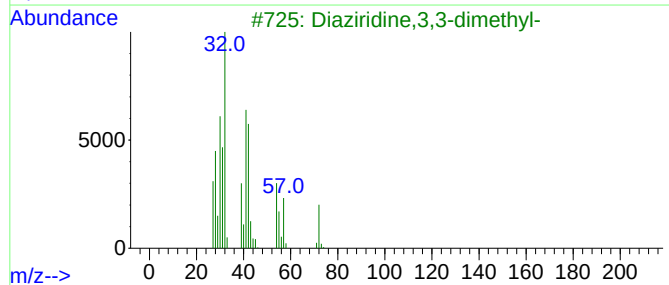
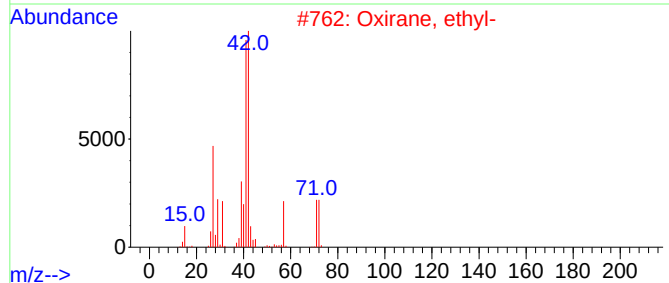
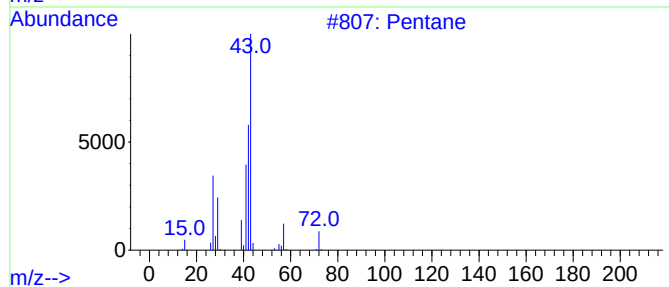
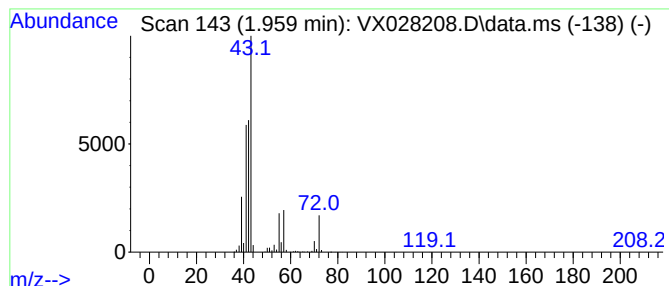
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Quant Title : SW846 8260

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

Peak Number 4 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	33.07 ug/l	768376	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	72
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	53
3			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	52
4			Isobutylene epoxide	72	C4H8O	000558-30-5	47
5			1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028208.D
Acq On : 20 Apr 2022 19:17
Operator : JC/MD
Sample : N2459-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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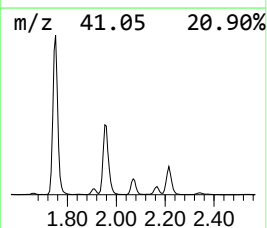
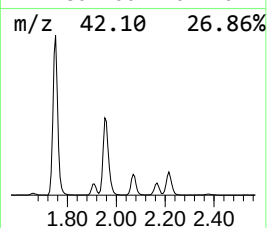
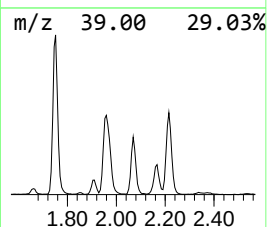
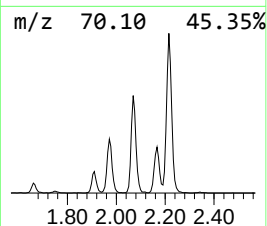
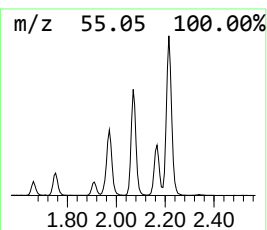
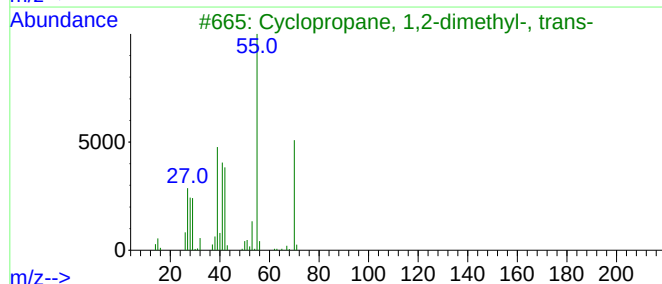
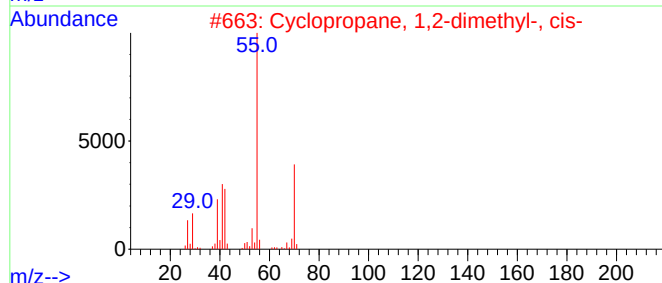
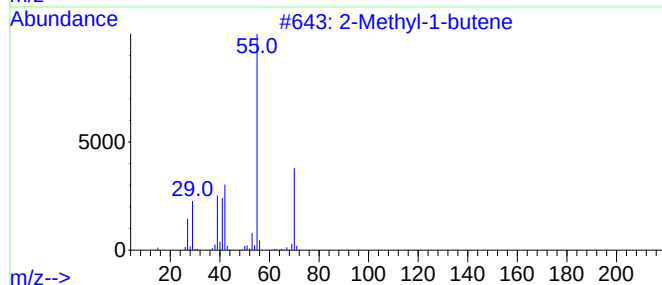
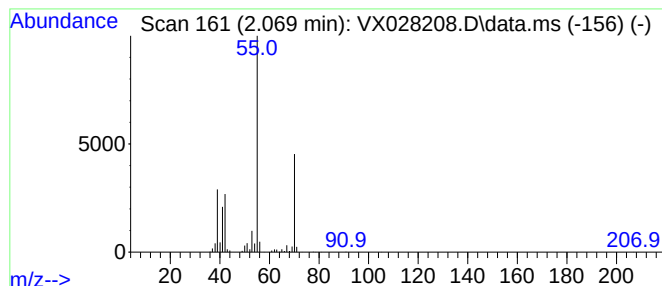
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Quant Title : SW846 8260

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

Peak Number 5 2-Methyl-1-butene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	13.80 ug/l	320600	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-1-butene	70	C5H10	000563-46-2	91
2			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
3			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
4			2-Butene, 2-methyl-	70	C5H10	000513-35-9	87
5			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028208.D
Acq On : 20 Apr 2022 19:17
Operator : JC/MD
Sample : N2459-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

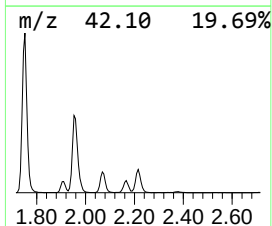
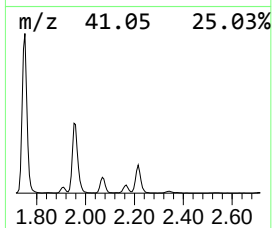
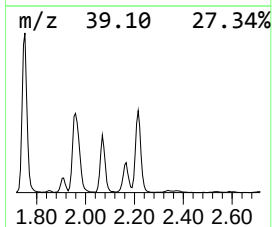
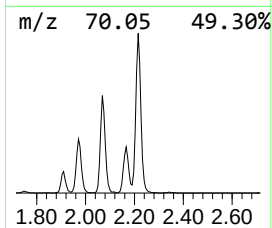
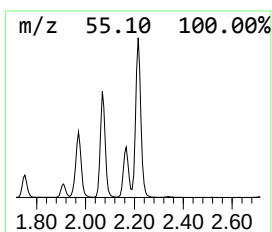
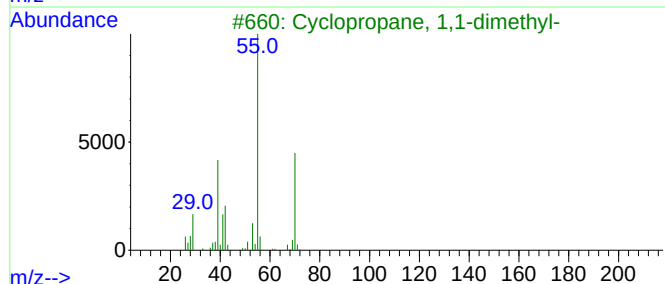
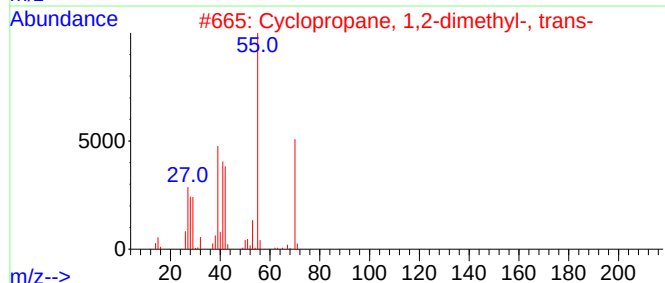
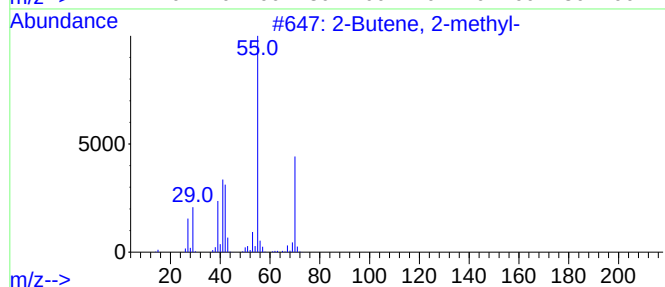
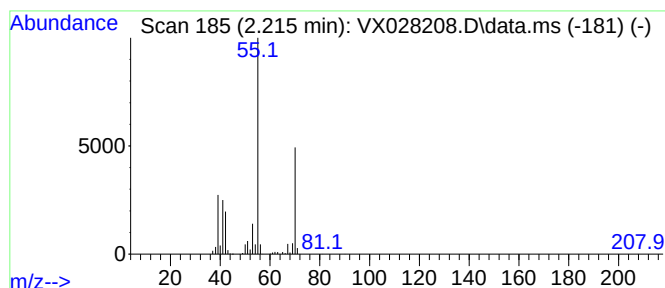
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MSVOA_X
ClientSampleId :
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Quant Title : SW846 8260

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	22.20 ug/l	515746	Pentafluorobenzene	5.556	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
2	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83
3	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
4	2-Methyl-1-butene	70	C5H10	000563-46-2	78
5	1-Butene, 3-methyl-	70	C5H10	000563-45-1	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028208.D
Acq On : 20 Apr 2022 19:17
Operator : JC/MD
Sample : N2459-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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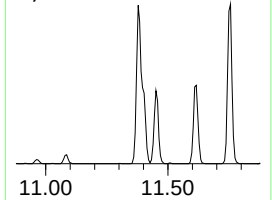
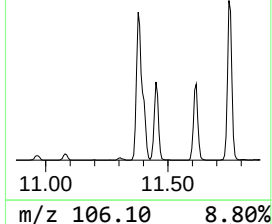
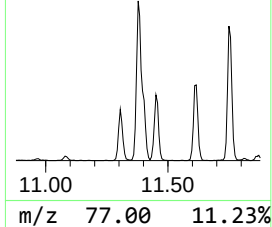
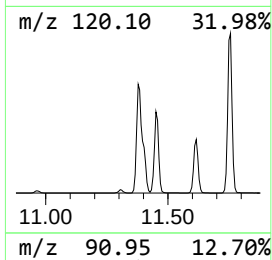
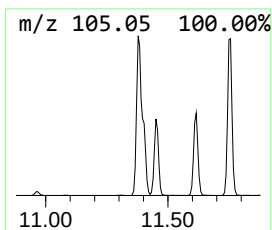
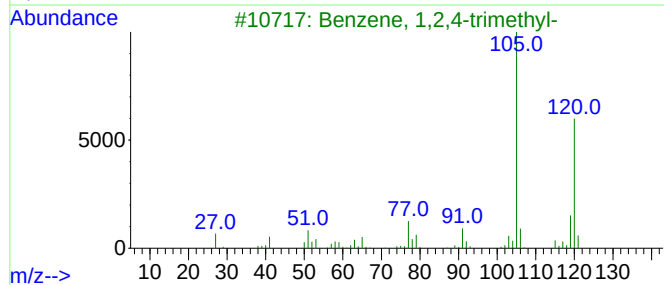
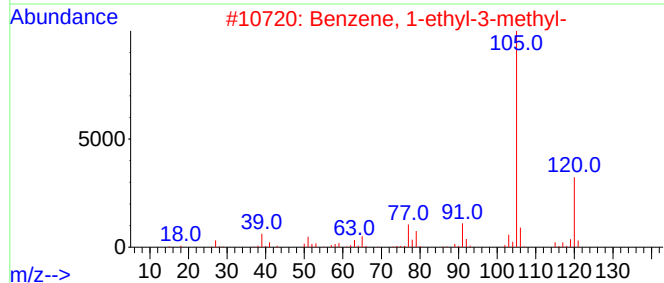
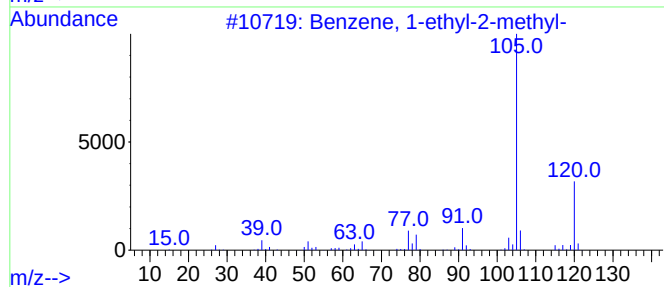
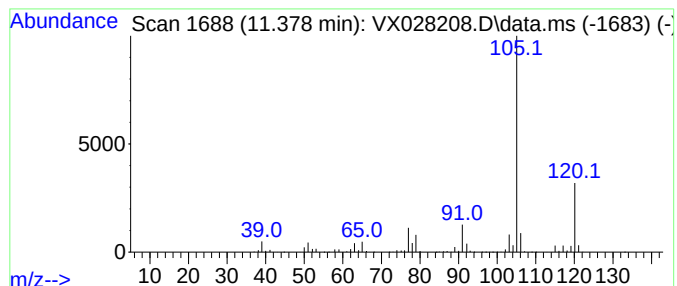
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	36.61 ug/l	1396840	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028208.D
Acq On : 20 Apr 2022 19:17
Operator : JC/MD
Sample : N2459-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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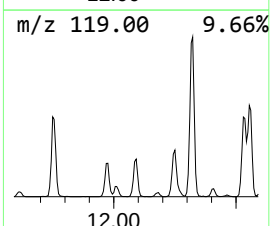
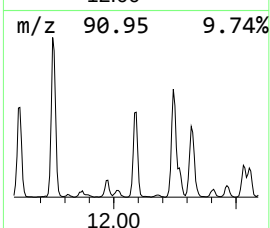
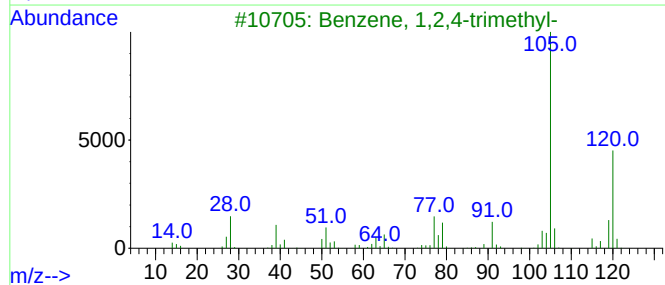
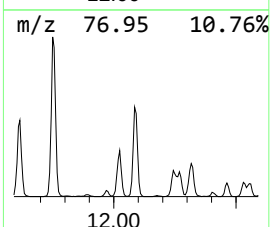
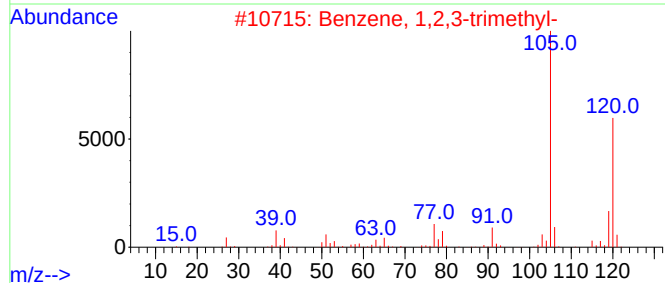
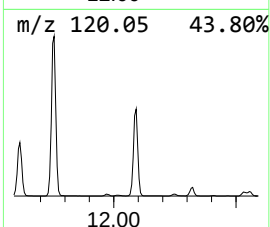
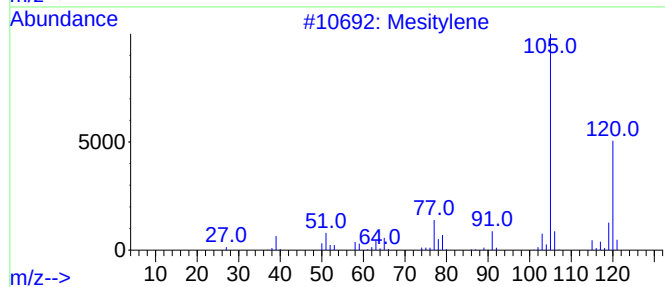
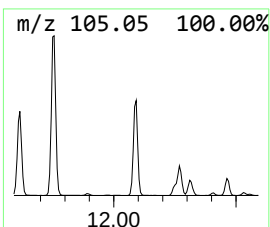
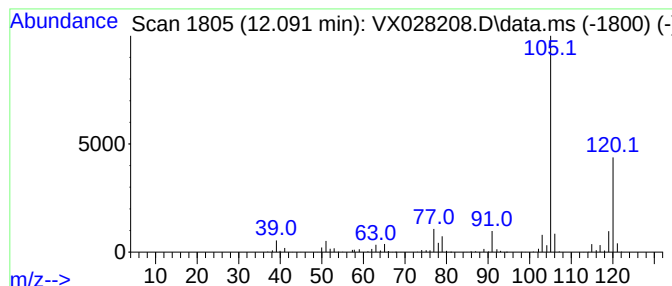
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	16.67 ug/l	635903	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 : VX028208.D
Acq On : 20 Apr 2022 19:17
Operator : JC/MD
Sample : N2459-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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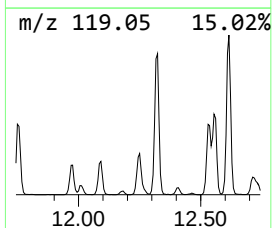
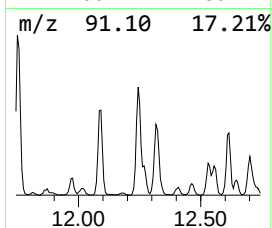
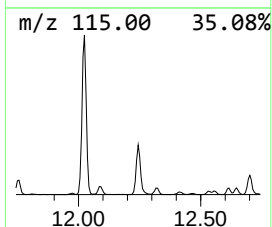
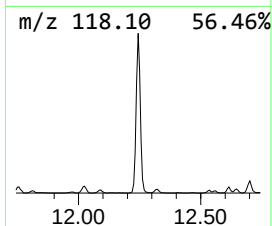
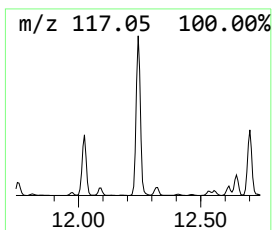
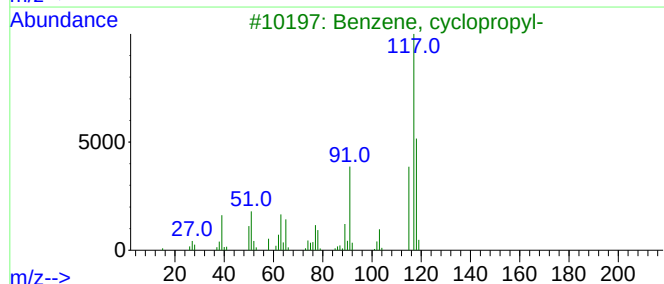
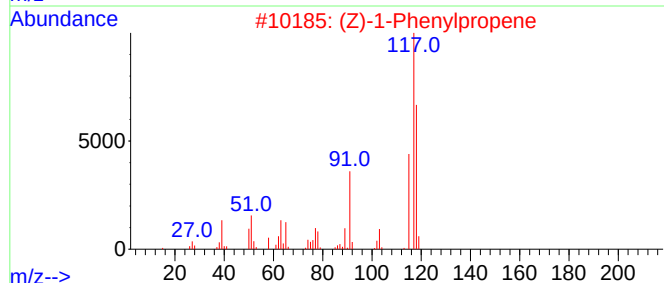
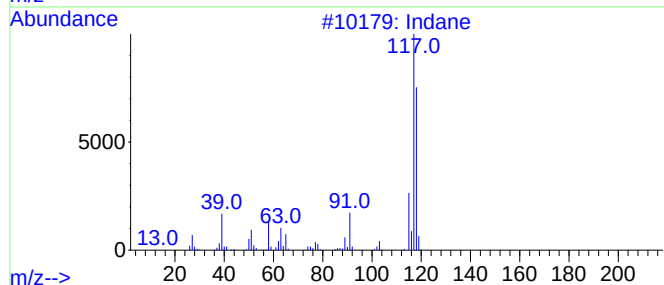
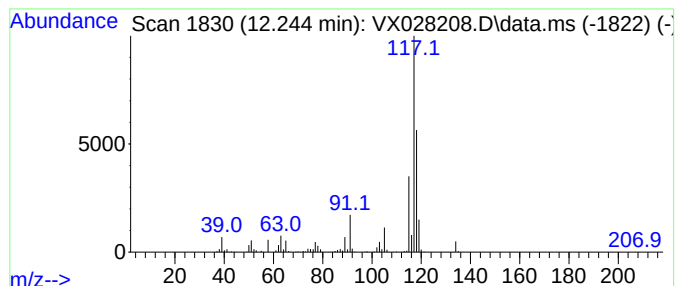
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Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	17.40 ug/l	663713	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	76
2			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	76
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028208.D
Acq On : 20 Apr 2022 19:17
Operator : JC/MD
Sample : N2459-05
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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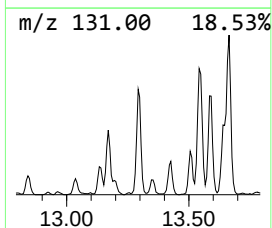
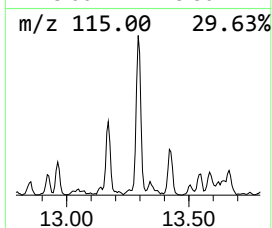
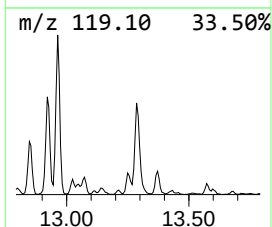
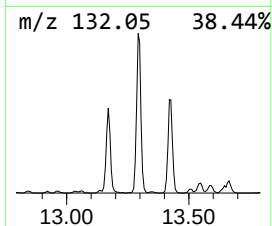
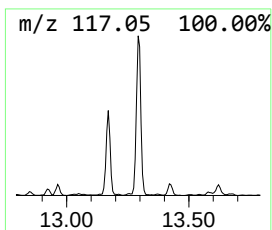
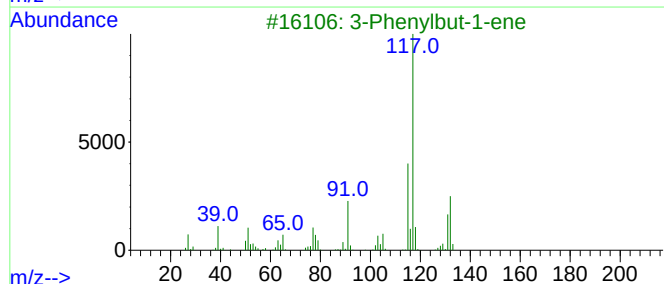
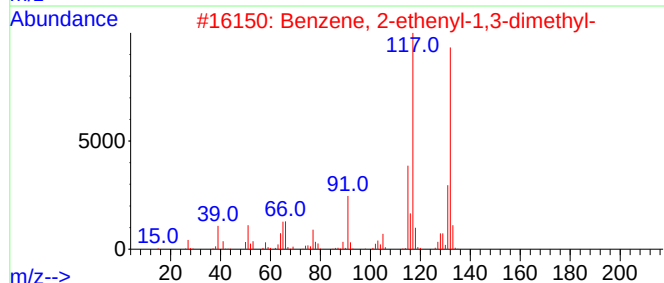
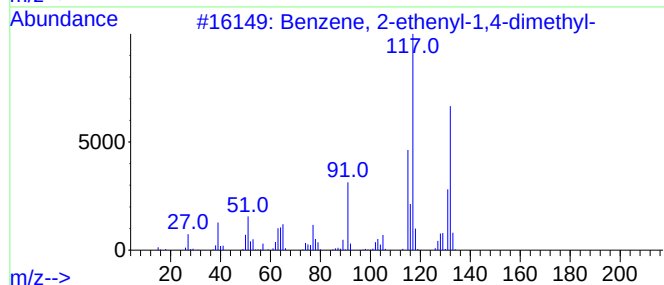
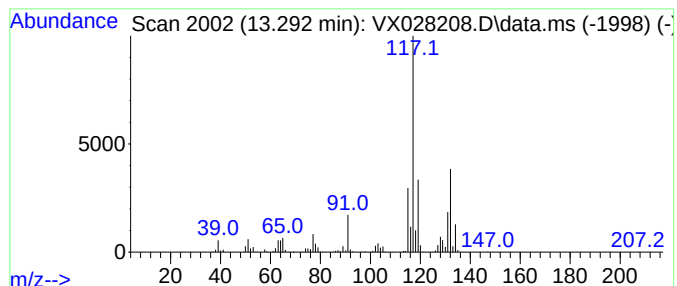
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	13.72 ug/l	523370	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	83
2		Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	81
3		3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
4		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	76
5		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028208.D
Acq On : 20 Apr 2022 19:17
Operator : JC/MD
Sample : N2459-05
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\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	130.1	ug/l	3023140	1	5.556	1161810	50.0
Butane, 2-methyl-	1.752	53.5	ug/l	1241970	1	5.556	1161810	50.0
Pentane	1.959	33.1	ug/l	768376	1	5.556	1161810	50.0
2-Methyl-1-butene	2.069	13.8	ug/l	320600	1	5.556	1161810	50.0
2-Butene, 2-met...	2.215	22.2	ug/l	515746	1	5.556	1161810	50.0
Benzene, 1-ethy...	11.378	36.6	ug/l	1396840	4	12.024	1907500	50.0
Benzene, 1,2,3-...	12.091	16.7	ug/l	635903	4	12.024	1907500	50.0
Indane	12.244	17.4	ug/l	663713	4	12.024	1907500	50.0
Benzene, 2-ethe...	13.292	13.7	ug/l	523370	4	12.024	1907500	50.0