

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
 Data File : VX021516.D
 Acq On : 26 Mar 2021 03:38
 Operator : JC/MD
 Sample : M1806-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW5

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\82X032421W.M
 Title : SW846 8260

Signal : TIC: VX021516.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.287	28	34	48	rBV	1344136	1650863	4.75%	1.147%
2	1.393	48	52	59	rBV	4036731	4453363	12.80%	3.095%
3	1.769	111	116	133	rVB	7536204	10303477	29.62%	7.162%
4	1.981	147	152	166	rVB2	2283483	3605039	10.37%	2.506%
5	2.099	166	172	180	rBV	1294782	1798112	5.17%	1.250%
6	2.193	183	188	192	rVV	626160	913939	2.63%	0.635%
7	2.246	192	197	209	rVB	1519550	2310707	6.64%	1.606%
8	2.822	275	295	298	rBV3	360219	1268311	3.65%	0.882%
9	2.869	298	303	306	rVV	576564	1191775	3.43%	0.828%
10	2.911	306	310	326	rVB2	668390	1646256	4.73%	1.144%
11	3.146	340	350	363	rVB	396991	908480	2.61%	0.631%
12	3.722	441	448	454	rBV	150733	357394	1.03%	0.248%
13	3.787	454	459	469	rVB	237284	558694	1.61%	0.388%
14	3.899	469	478	484	rBV	156992	406264	1.17%	0.282%
15	4.170	514	524	536	rBV	201384	529053	1.52%	0.368%
16	4.375	548	559	571	rVV	805785	2304837	6.63%	1.602%
17	5.546	750	758	767	rBV2	161974	498048	1.43%	0.346%
18	6.111	846	854	865	rVB	403507	1024146	2.94%	0.712%
19	6.311	865	888	900	rVB4	191454	890971	2.56%	0.619%
20	7.435	1067	1079	1089	rBV5	168861	460925	1.33%	0.320%
21	8.694	1287	1293	1299	rVB	275394	416296	1.20%	0.289%
22	8.764	1299	1305	1313	rBV	3392311	5296901	15.23%	3.682%
23	10.094	1520	1531	1537	rBV	304542	434822	1.25%	0.302%
24	10.241	1550	1556	1562	rBV	7524124	9840873	28.29%	6.840%
25	10.359	1567	1576	1581	rBV	21911173	34779883	100.00%	24.175%
26	10.688	1625	1632	1638	rBV	9983404	12883567	37.04%	8.955%
27	11.000	1678	1685	1691	rVB	339123	431917	1.24%	0.300%
28	11.341	1734	1743	1750	rBV	999465	1255665	3.61%	0.873%
29	11.423	1750	1757	1764	rVV	5109807	8877386	25.52%	6.171%
30	11.494	1764	1769	1781	rVB	2540028	3165839	9.10%	2.201%
31	11.653	1790	1796	1803	rBV	2276226	2732367	7.86%	1.899%
32	11.794	1814	1820	1825	rBV	9691866	11824046	34.00%	8.219%
33	12.059	1860	1865	1871	rVB	326374	432449	1.24%	0.301%
34	12.129	1871	1877	1882	rBV	2567096	3095224	8.90%	2.151%
35	12.282	1897	1903	1911	rBV2	1818685	2517448	7.24%	1.750%
36	12.359	1911	1916	1923	rVB2	507940	715617	2.06%	0.497%

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 Title : SW846 8260

37	12.571	1946	1952	1954	rBV	342680	428596	1.23%	0.298%
38	12.653	1961	1966	1969	rBV	499559	600728	1.73%	0.418%
39	12.735	1976	1980	1988	rBV2	350812	501416	1.44%	0.349%
40	12.959	2011	2018	2022	rBV	333864	407367	1.17%	0.283%
41	13.000	2022	2025	2031	rVB	482945	569651	1.64%	0.396%
42	13.206	2052	2060	2065	rBV	392554	492996	1.42%	0.343%
43	13.330	2076	2081	2086	rVB2	736494	977585	2.81%	0.680%
44	13.818	2156	2164	2170	rBV	2124391	2637986	7.58%	1.834%
45	14.677	2305	2310	2320	rVB	852634	993163	2.86%	0.690%
46	14.818	2329	2334	2347	rVB	373079	477318	1.37%	0.332%

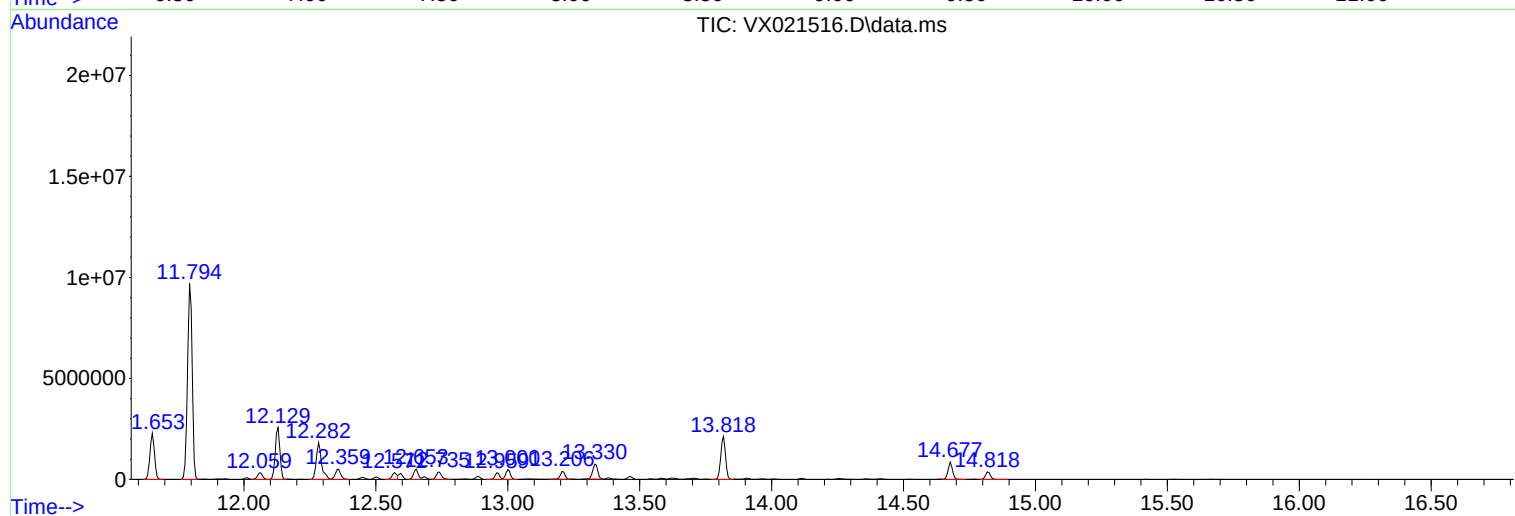
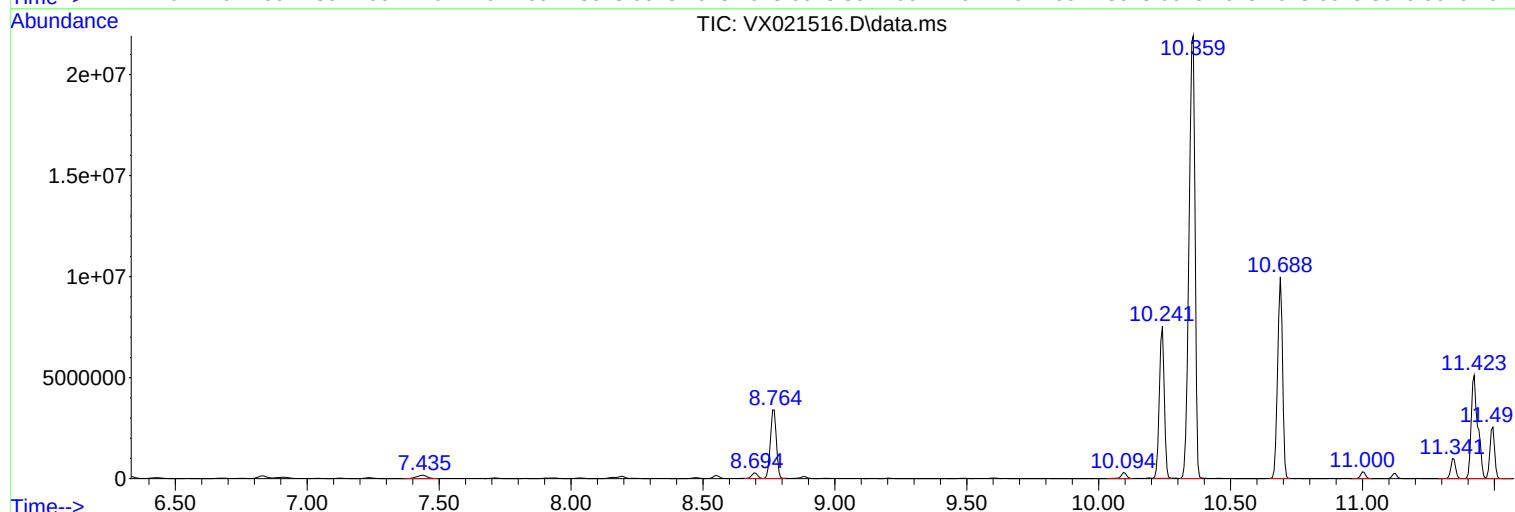
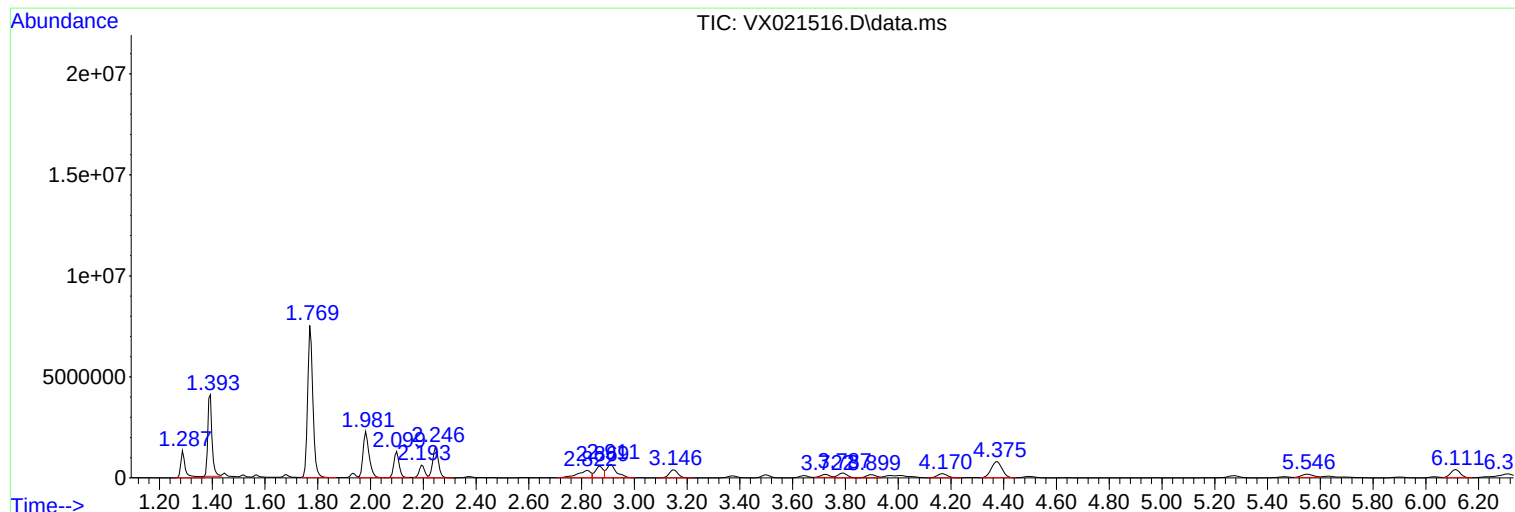
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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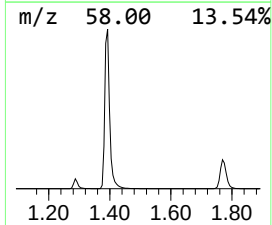
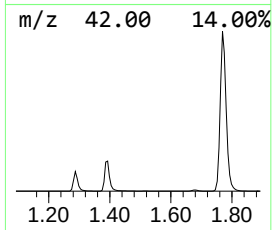
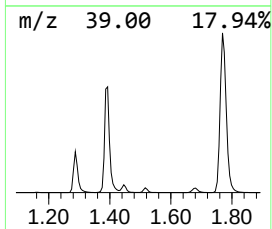
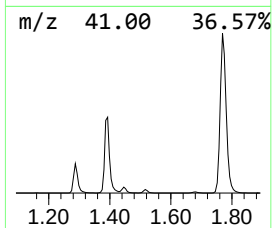
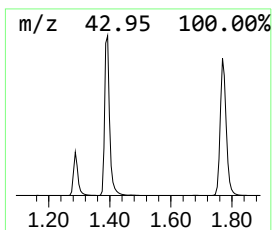
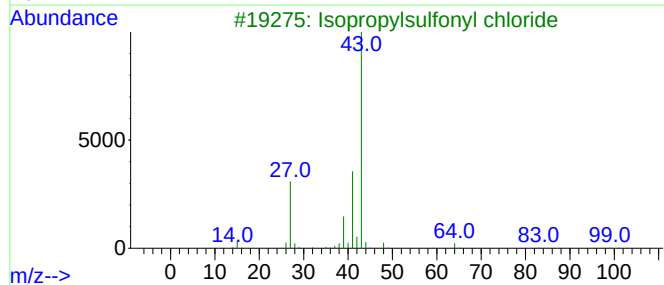
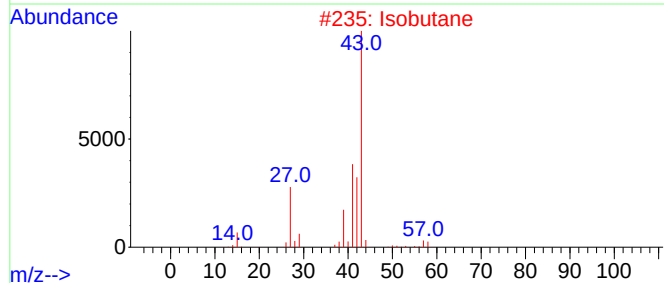
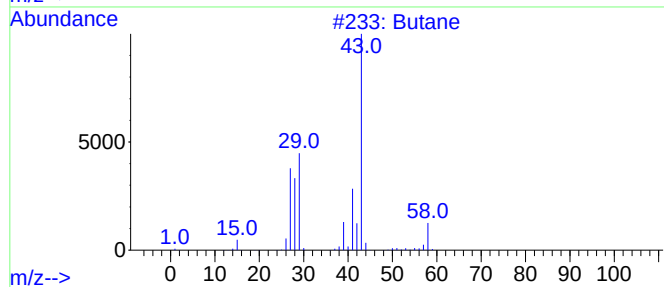
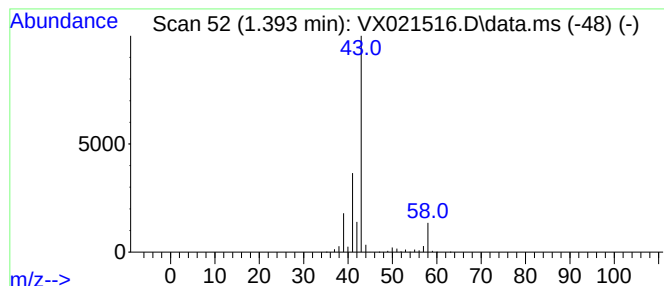
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.393	447.08 ug/l	4453360	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Isobutane	58	C4H10	000075-28-5	9
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Diazene, dimethyl-	58	C2H6N2	000503-28-6	5



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Misc : 5.0mL/MSVOA_X/WATER
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Instrument :
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ClientSampleId :
MW5

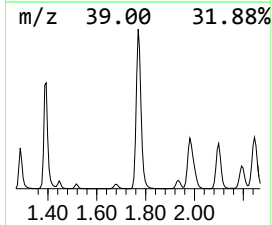
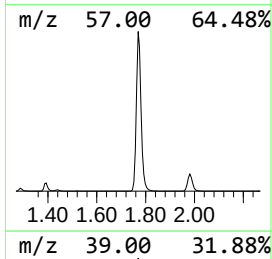
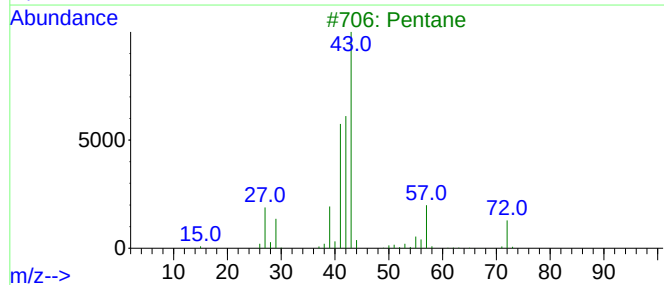
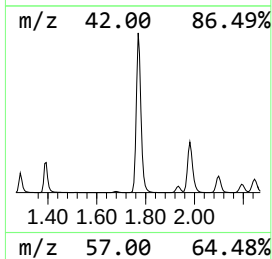
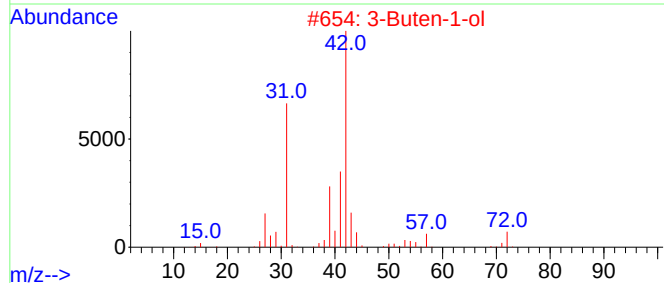
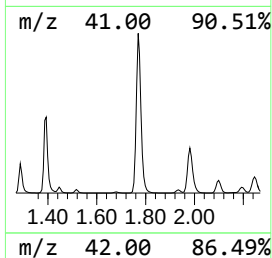
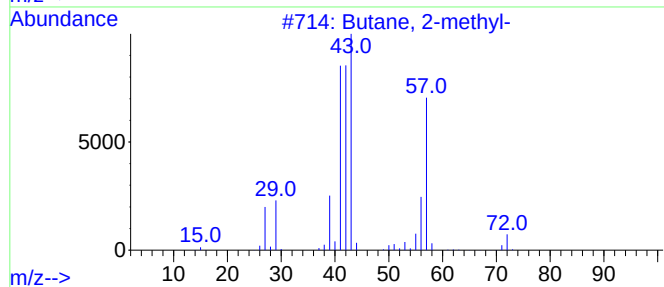
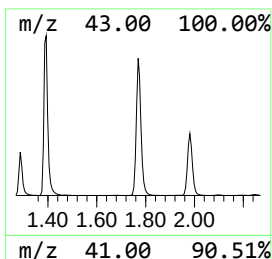
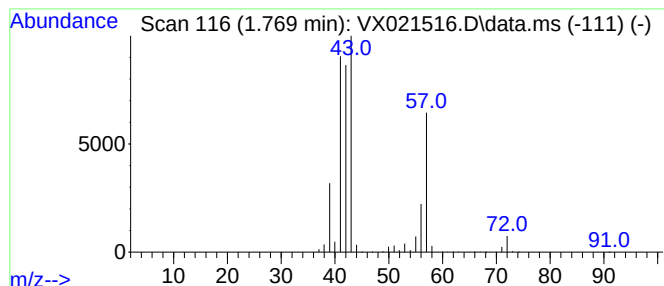
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.769	1034.39 ug/l	10303500	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	94
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	45
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	10
5			Methane, isocyanato-	57	C2H3NO	000624-83-9	9



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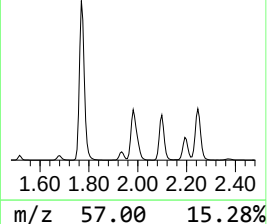
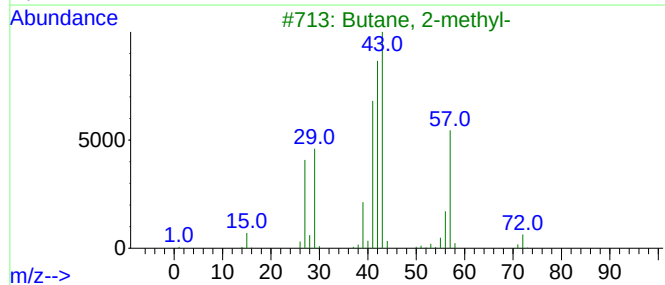
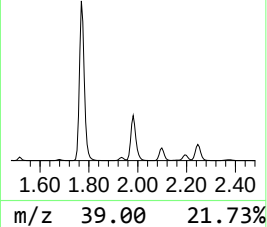
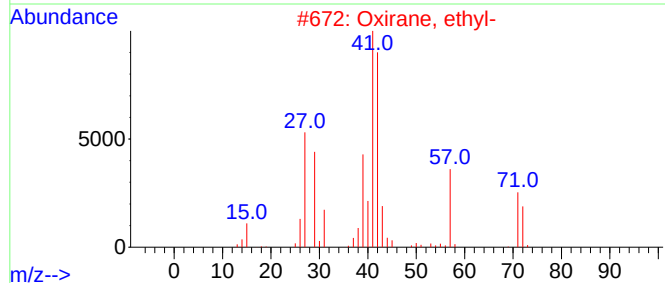
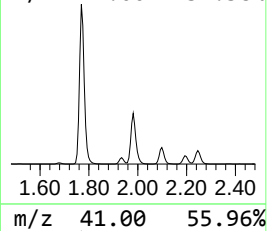
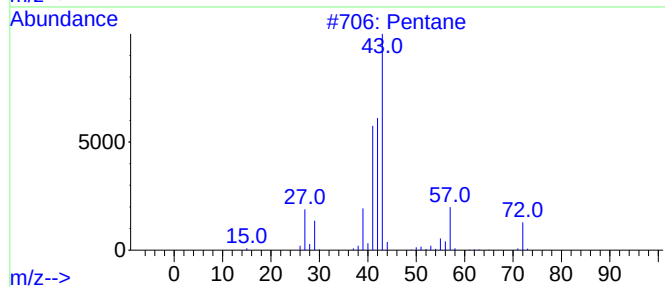
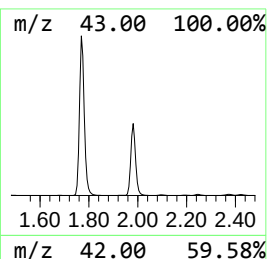
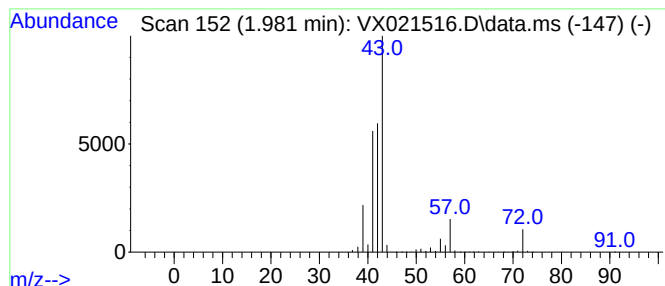
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.981	361.92 ug/l	3605040	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	43
3			Butane, 2-methyl-	72	C5H12	000078-78-4	38
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9



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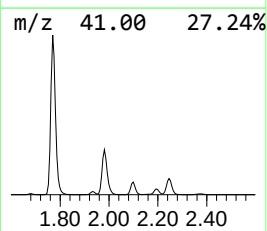
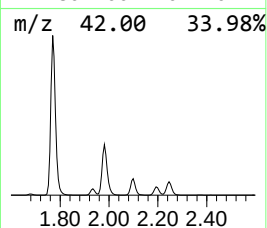
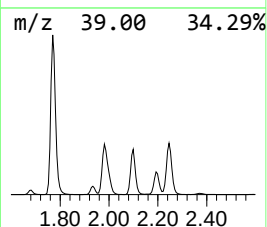
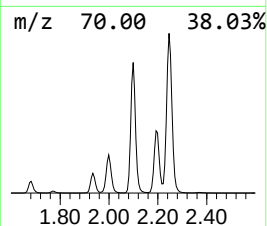
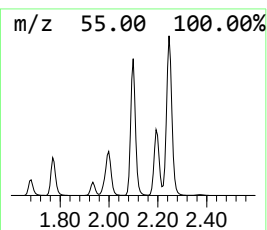
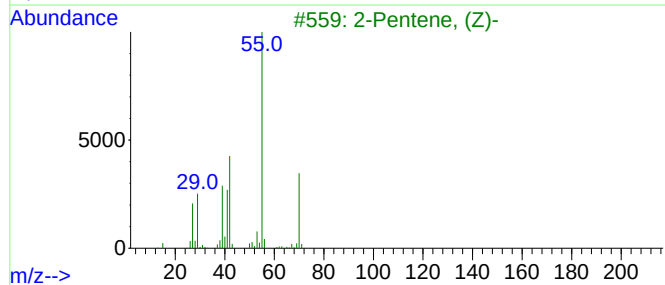
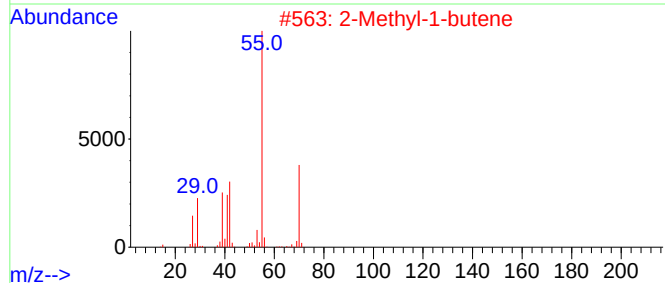
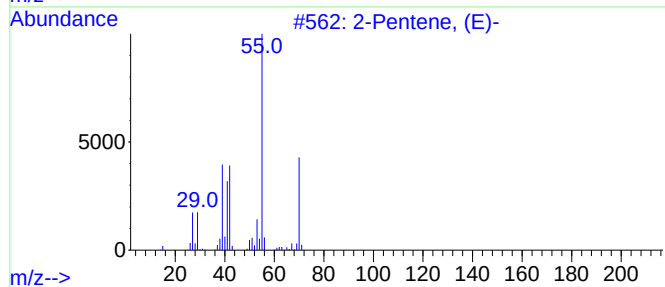
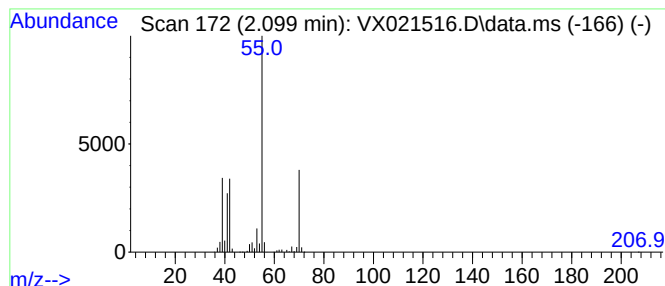
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentene, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	180.52 ug/l	1798110	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentene, (E)-	70	C5H10	000646-04-8	93
2			2-Methyl-1-butene	70	C5H10	000563-46-2	90
3			2-Pentene, (Z)-	70	C5H10	000627-20-3	90
4			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
5			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87



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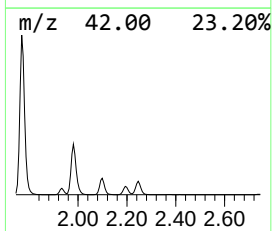
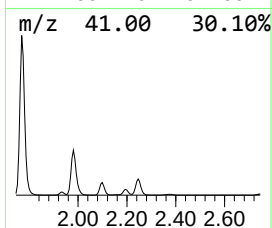
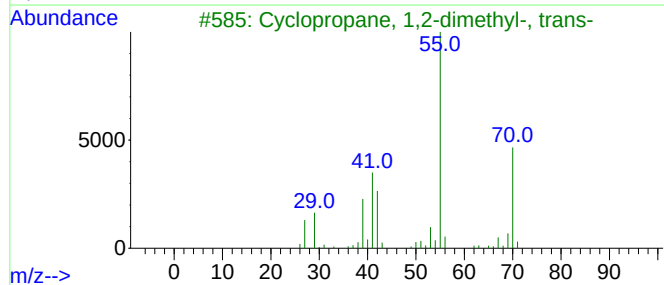
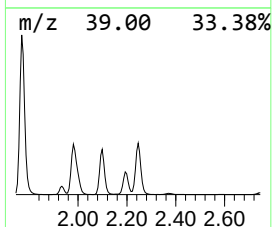
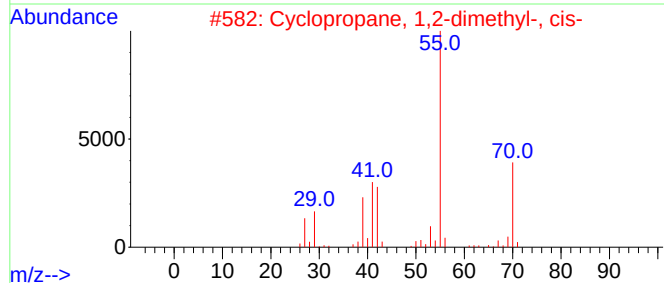
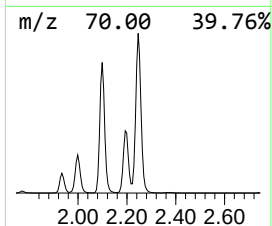
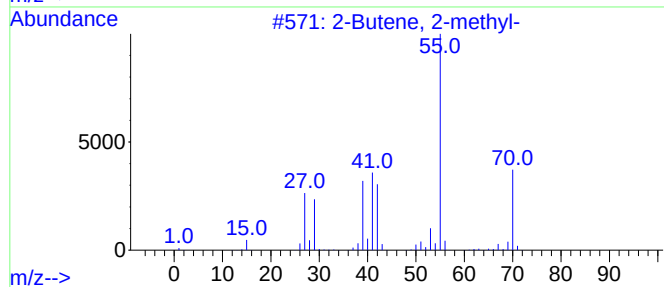
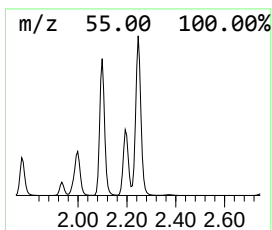
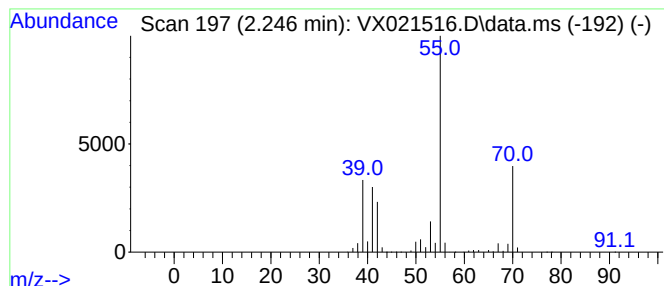
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Butene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.246	231.98 ug/l	2310710	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-			70	C5H10	000513-35-9	91
2	Cyclopropane, 1,2-dimethyl-, cis-			70	C5H10	000930-18-7	90
3	Cyclopropane, 1,2-dimethyl-, trans-			70	C5H10	002402-06-4	83
4	2-Pentene, (Z)-			70	C5H10	000627-20-3	81
5	Cyclopropane, 1,1-dimethyl-			70	C5H10	001630-94-0	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021516.D
Acq On : 26 Mar 2021 03:38
Operator : JC/MD
Sample : M1806-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW5

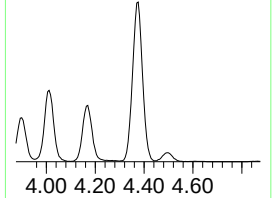
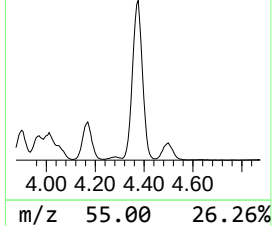
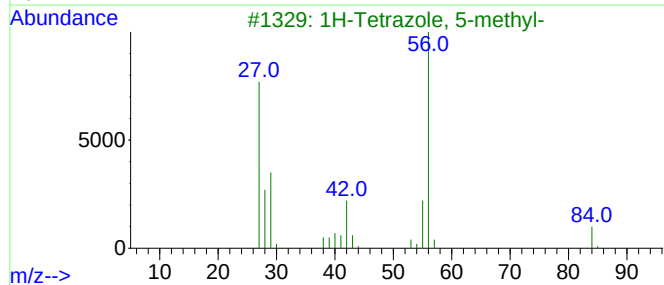
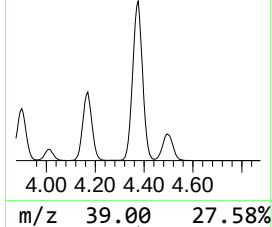
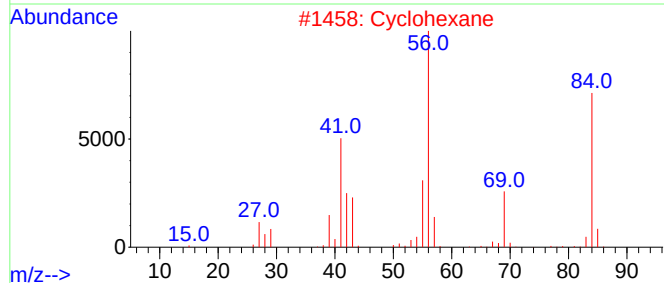
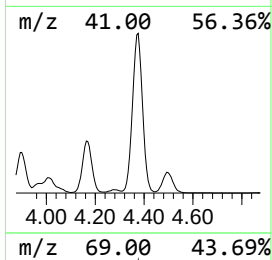
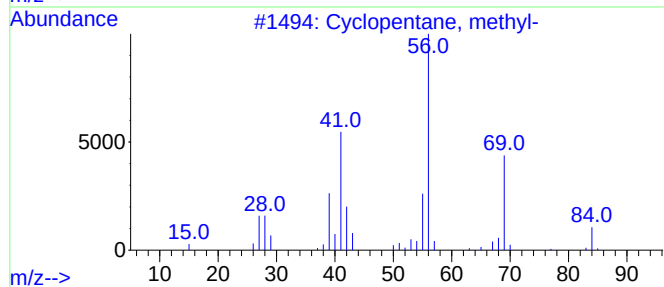
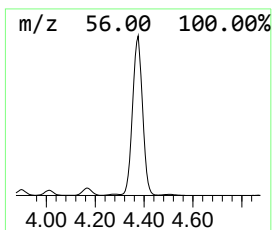
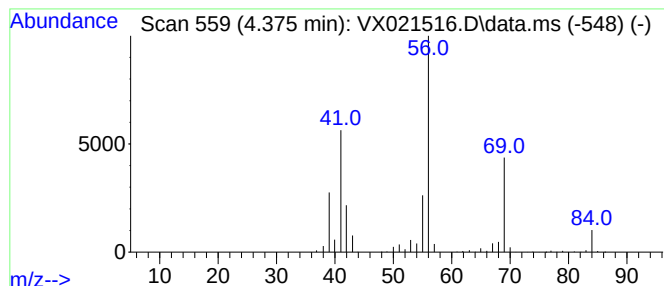
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.375	231.39 ug/l	2304840	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclohexane	84	C6H12	000110-82-7	78
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	72
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021516.D
Acq On : 26 Mar 2021 03:38
Operator : JC/MD
Sample : M1806-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW5

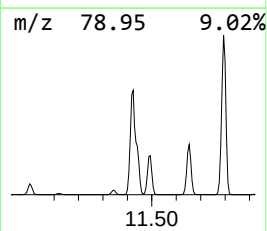
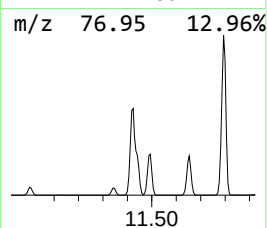
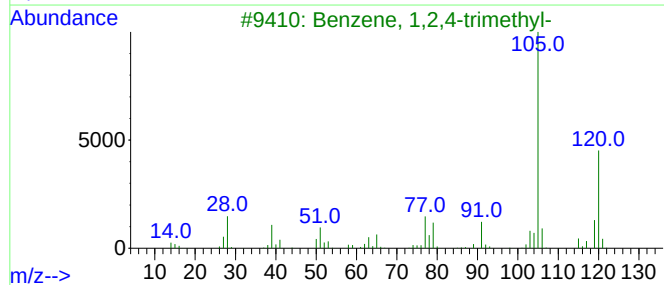
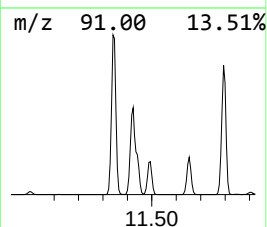
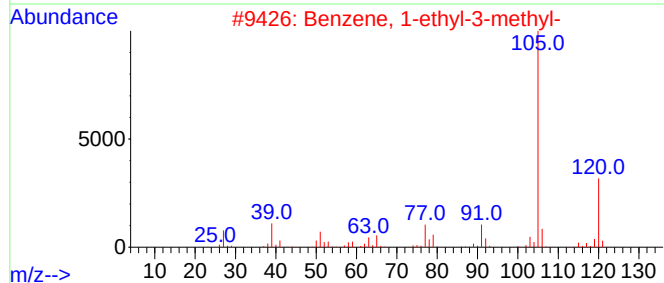
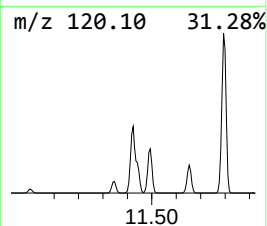
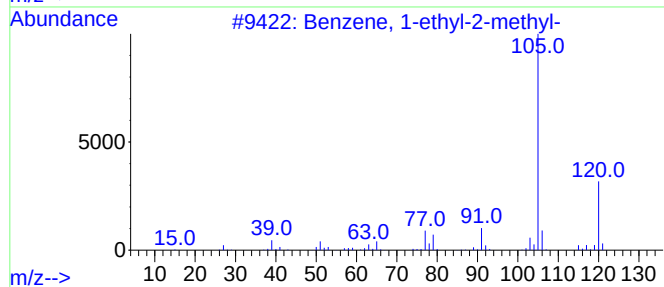
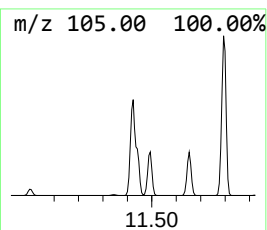
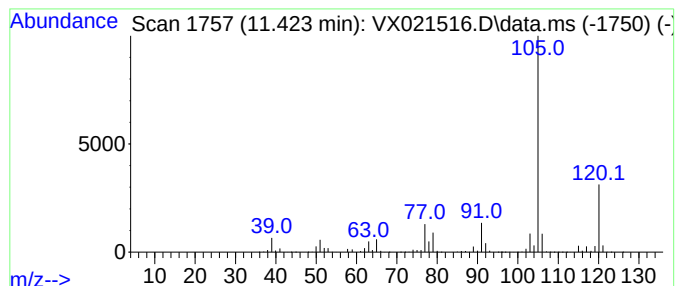
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.423	1026.41 ug/l	8877390	1,4-Dichlorobenzene-d4	12.065

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	94
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			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021516.D
Acq On : 26 Mar 2021 03:38
Operator : JC/MD
Sample : M1806-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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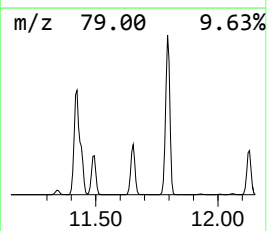
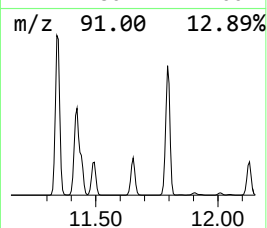
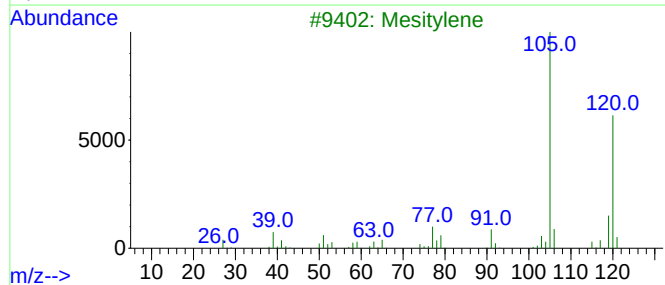
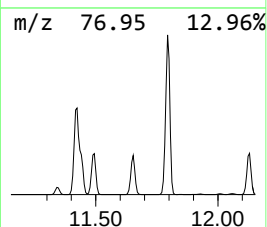
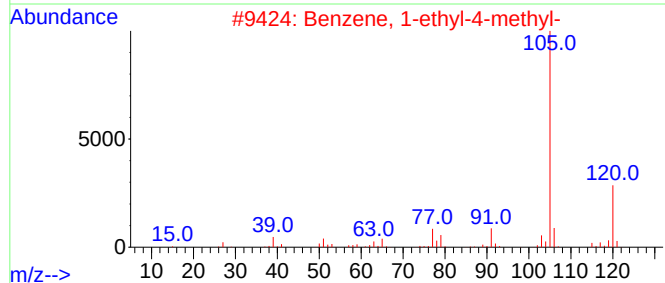
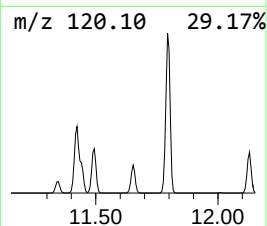
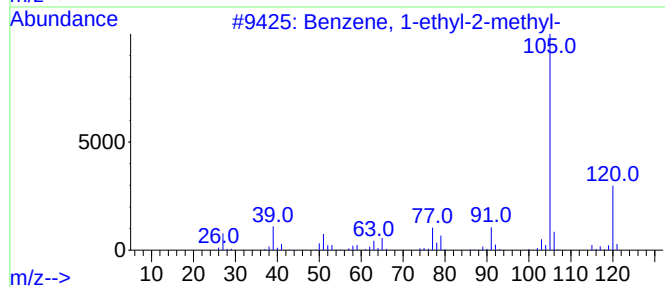
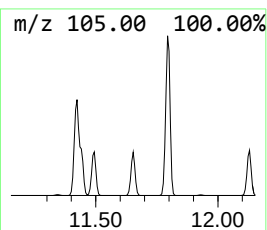
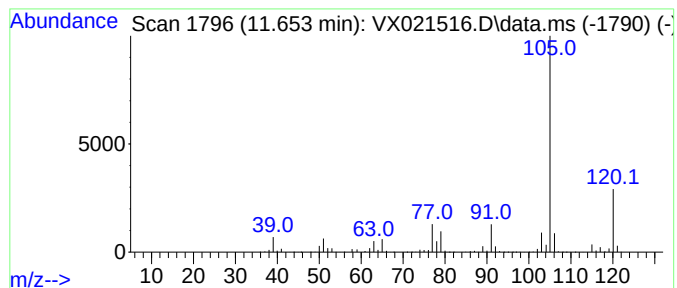
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.653	315.92 ug/l	2732370	1,4-Dichlorobenzene-d4	12.065

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	91
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021516.D
Acq On : 26 Mar 2021 03:38
Operator : JC/MD
Sample : M1806-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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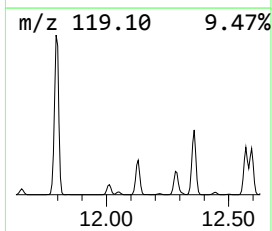
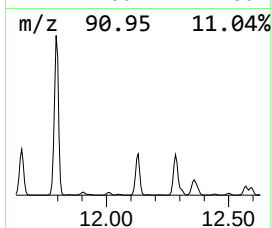
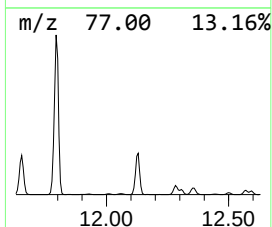
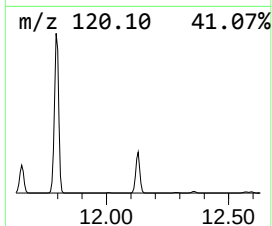
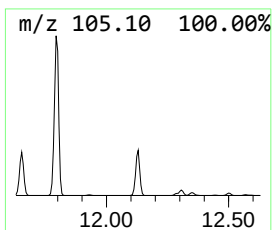
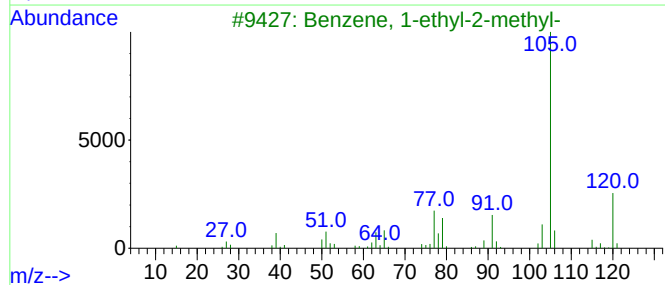
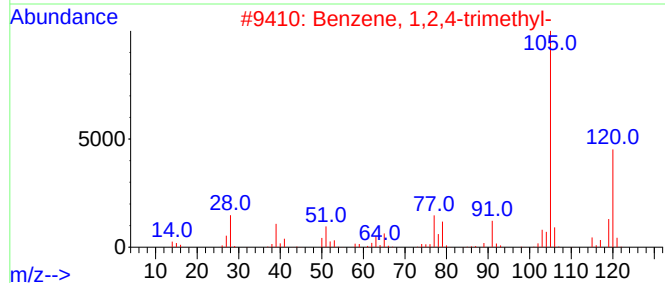
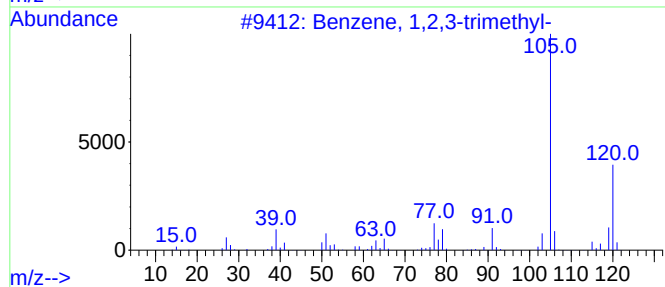
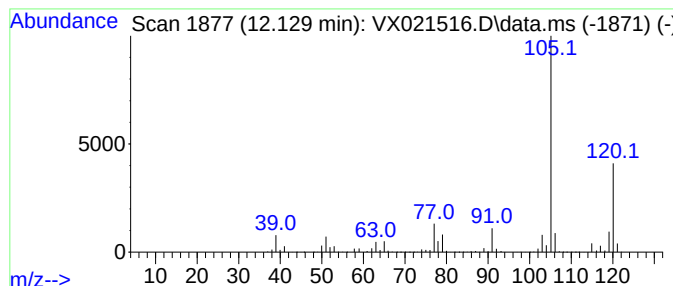
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.129	357.87 ug/l	3095220	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021516.D
Acq On : 26 Mar 2021 03:38
Operator : JC/MD
Sample : M1806-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW5

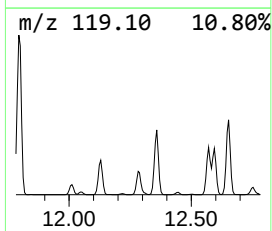
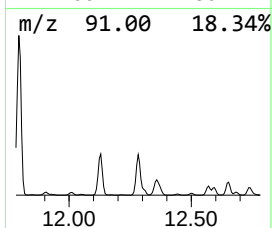
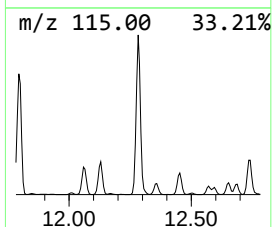
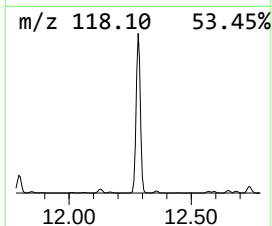
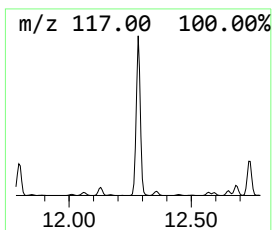
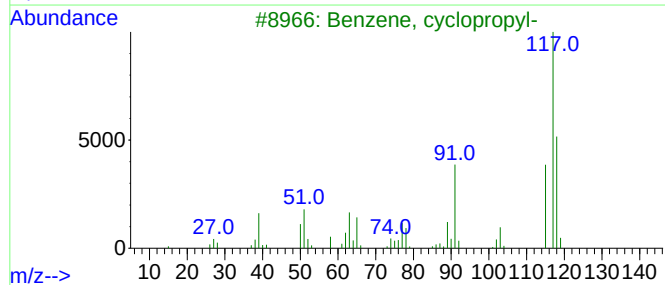
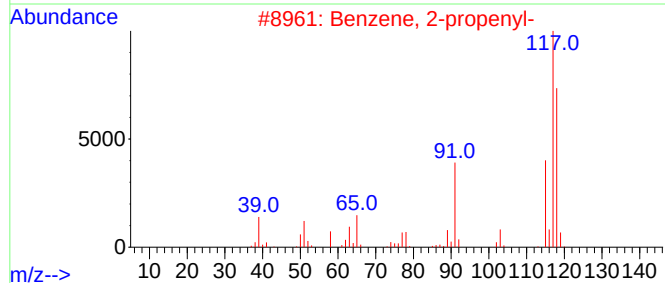
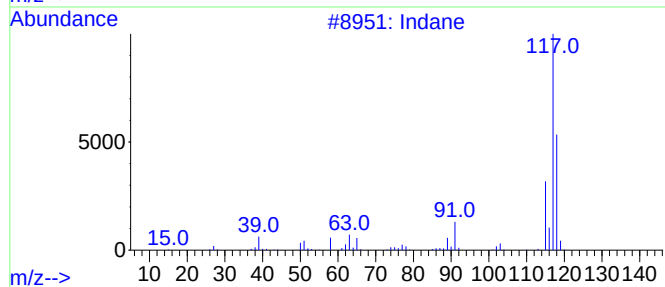
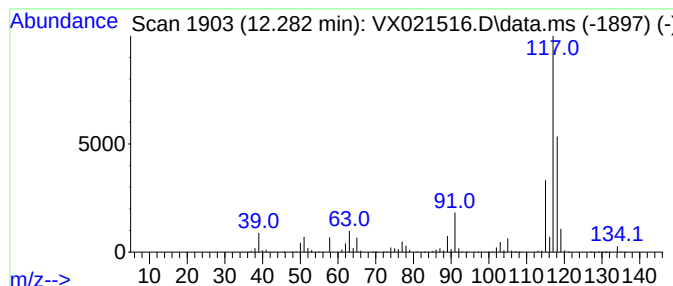
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.282	291.07 ug/l	2517450	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Deltacyclene	118	C9H10	007785-10-6	62
5			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021516.D
Acq On : 26 Mar 2021 03:38
Operator : JC/MD
Sample : M1806-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.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-	1.769	1034.4	ug/l	10303500	1	5.629	498048	50.0
Pentane	1.981	361.9	ug/l	3605040	1	5.629	498048	50.0
2-Pentene, (E)-	2.099	180.5	ug/l	1798110	1	5.629	498048	50.0
2-Butene, 2-met...	2.246	232.0	ug/l	2310710	1	5.629	498048	50.0
Cyclopentane, m...	4.375	231.4	ug/l	2304840	1	5.629	498048	50.0
Benzene, 1-ethy...	11.423	1026.4	ug/l	8877390	4	12.065	432449	50.0
Benzene, 1-ethy...	11.653	315.9	ug/l	2732370	4	12.065	432449	50.0
Benzene, 1,2,3-...	12.129	357.9	ug/l	3095220	4	12.065	432449	50.0
Indane	12.282	291.1	ug/l	2517450	4	12.065	432449	50.0