

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
 Data File : VX021515.D
 Acq On : 26 Mar 2021 03:15
 Operator : JC/MD
 Sample : M1806-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW2R

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: VX021515.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	30	34	48	rBV	480154	579314	4.66%	0.756%
2	1.393	48	52	59	rBV	1291585	1339027	10.77%	1.748%
3	1.775	111	117	132	rVB	2000138	2812166	22.62%	3.671%
4	1.981	147	152	166	rVB2	503732	786505	6.33%	1.027%
5	2.099	166	172	180	rVV	262734	363609	2.93%	0.475%
6	2.193	183	188	193	rVV	123626	193635	1.56%	0.253%
7	2.246	193	197	208	rVB	224074	342421	2.75%	0.447%
8	2.823	274	295	298	rBV2	79926	245117	1.97%	0.320%
9	2.870	298	303	306	rVV	118054	247553	1.99%	0.323%
10	2.911	306	310	324	rVB2	171662	399502	3.21%	0.521%
11	3.146	339	350	367	rVB	82126	189290	1.52%	0.247%
12	4.370	548	558	571	rVB	183961	526865	4.24%	0.688%
13	5.464	731	744	751	rBV	48529	144676	1.16%	0.189%
14	5.552	751	759	765	rVV4	42203	146336	1.18%	0.191%
15	5.629	766	772	801	rVB2	75257	268246	2.16%	0.350%
16	6.035	830	841	848	rBV	51032	135242	1.09%	0.177%
17	6.317	865	889	901	rVB4	58403	263262	2.12%	0.344%
18	6.829	968	976	985	rBV	116268	293782	2.36%	0.383%
19	7.435	1067	1079	1090	rBV5	56385	156378	1.26%	0.204%
20	8.159	1192	1202	1205	rBV	69420	139008	1.12%	0.181%
21	8.694	1287	1293	1299	rVB	251086	393156	3.16%	0.513%
22	8.765	1299	1305	1311	rBV	274586	403073	3.24%	0.526%
23	10.094	1526	1531	1537	rVB	276080	359014	2.89%	0.469%
24	10.235	1549	1555	1566	rVV	1863888	2380420	19.15%	3.107%
25	10.347	1566	1574	1587	rVB	9366087	12429495	100.00%	16.224%
26	10.682	1625	1631	1641	rVB	4964632	6410017	51.57%	8.367%
27	11.000	1679	1685	1691	rBV	144386	185786	1.49%	0.242%
28	11.118	1700	1705	1712	rBV	229987	304754	2.45%	0.398%
29	11.341	1734	1743	1750	rBV	378535	466022	3.75%	0.608%
30	11.418	1750	1756	1764	rVV	3728839	6689195	53.82%	8.731%
31	11.494	1764	1769	1780	rVB	2624120	3277120	26.37%	4.277%
32	11.653	1790	1796	1805	rBV	2326921	2776247	22.34%	3.624%
33	11.794	1814	1820	1825	rBV	8723995	10342251	83.21%	13.499%
34	12.012	1852	1857	1860	rBV	123942	149065	1.20%	0.195%
35	12.059	1860	1865	1871	rVB2	320017	425405	3.42%	0.555%
36	12.130	1871	1877	1882	rBV	2763375	3353975	26.98%	4.378%

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37	12.283	1897	1903	1911	rBV2	1370993	2209592	17.78%	2.884%
38	12.359	1911	1916	1922	rVB2	1098099	1483085	11.93%	1.936%
39	12.447	1926	1931	1936	rBV2	109638	149105	1.20%	0.195%
40	12.500	1936	1940	1946	rVB	250812	290056	2.33%	0.379%
41	12.571	1946	1952	1954	rBV	651603	816672	6.57%	1.066%
42	12.594	1954	1956	1961	rVB	570333	567121	4.56%	0.740%
43	12.653	1961	1966	1969	rBV	970950	1154070	9.28%	1.506%
44	12.683	1969	1971	1976	rVB	156860	172226	1.39%	0.225%
45	12.742	1976	1981	1989	rBV2	531533	792624	6.38%	1.035%
46	12.889	2000	2006	2011	rVB	325489	399811	3.22%	0.522%
47	12.959	2011	2018	2022	rBV	684831	850987	6.85%	1.111%
48	13.000	2022	2025	2031	rVB	1110936	1258540	10.13%	1.643%
49	13.083	2031	2039	2042	rBV2	98197	200205	1.61%	0.261%
50	13.206	2056	2060	2064	rVB	492856	580390	4.67%	0.758%
51	13.330	2077	2081	2087	rVB2	1303665	1758369	14.15%	2.295%
52	13.465	2099	2104	2112	rVB	164570	214221	1.72%	0.280%
53	13.583	2120	2124	2127	rVV	147050	191453	1.54%	0.250%
54	13.624	2127	2131	2137	rVB4	180834	336884	2.71%	0.440%
55	13.706	2142	2145	2150	rVB2	172932	254509	2.05%	0.332%
56	13.818	2156	2164	2173	rBV	985478	1280013	10.30%	1.671%
57	14.112	2210	2214	2220	rBV	149959	187986	1.51%	0.245%
58	14.254	2234	2238	2244	rBV	140014	211424	1.70%	0.276%
59	14.677	2305	2310	2321	rVB	681666	834955	6.72%	1.090%
60	14.818	2329	2334	2344	rBV	406786	502509	4.04%	0.656%

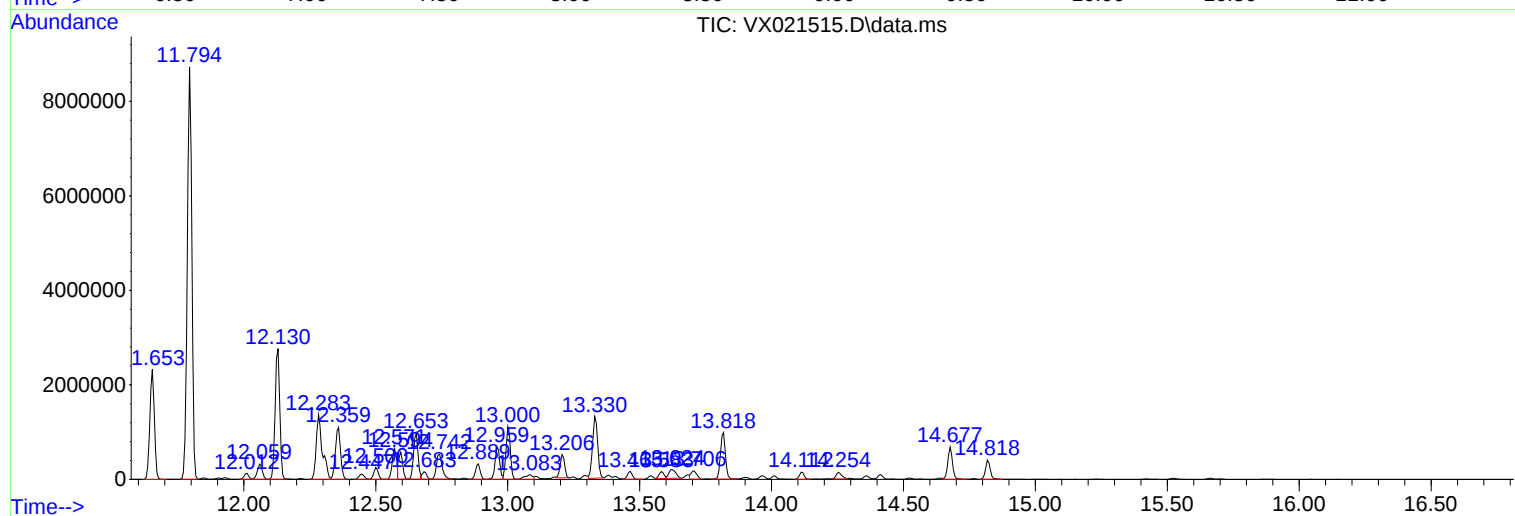
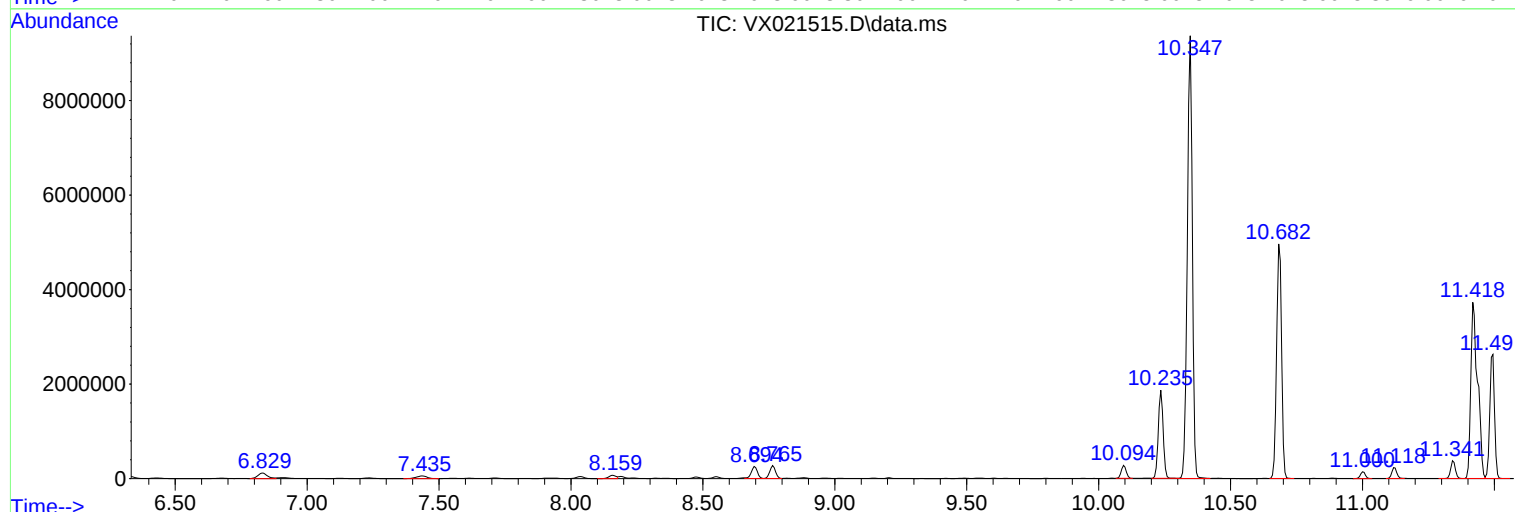
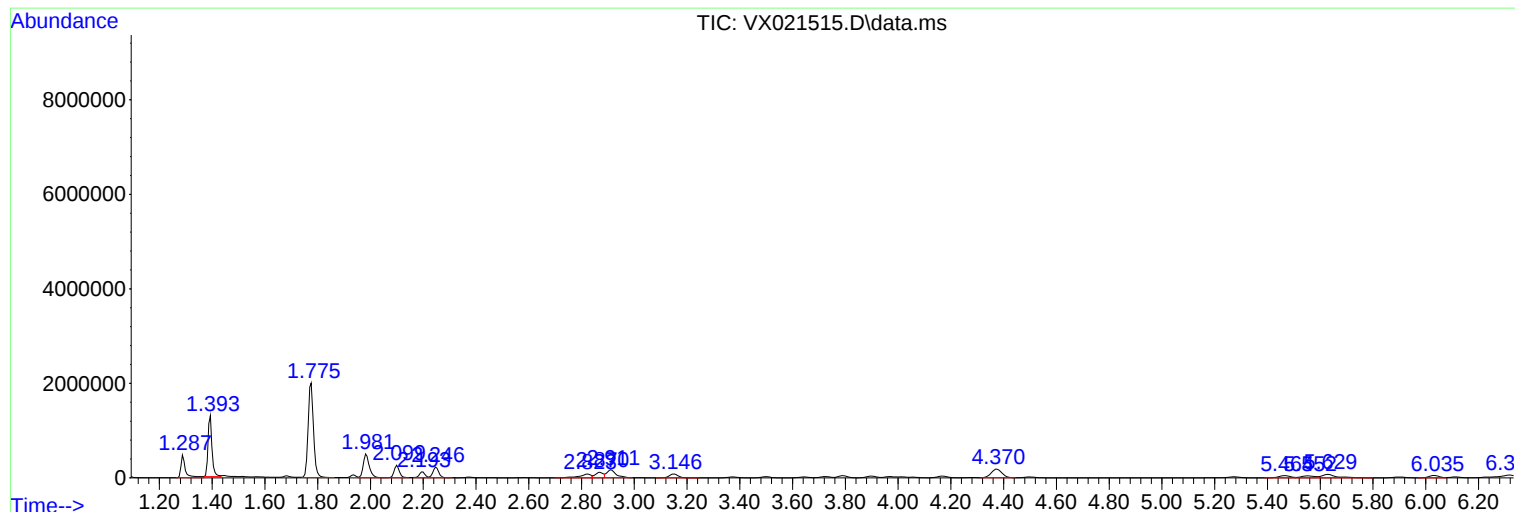
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Quant Title : SW846 8260

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



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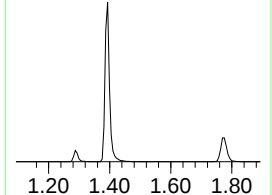
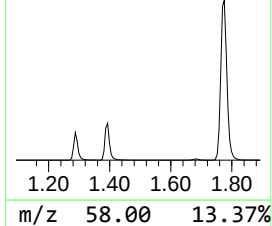
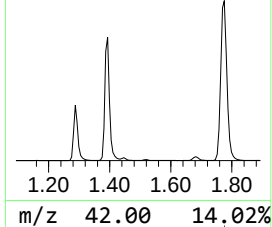
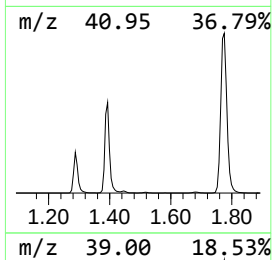
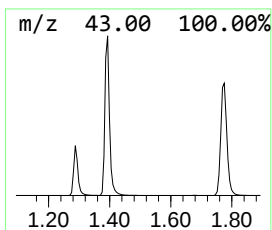
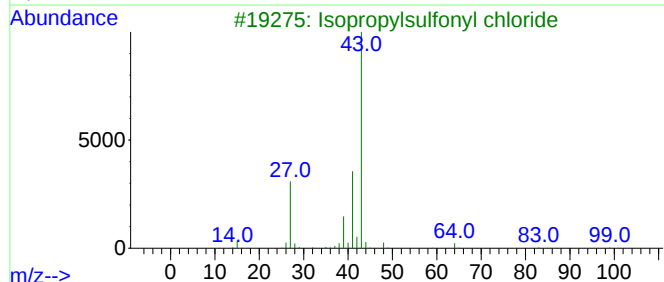
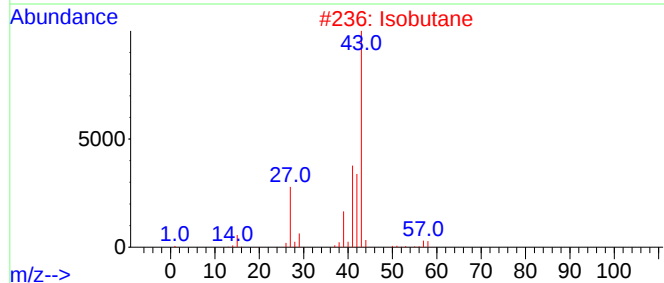
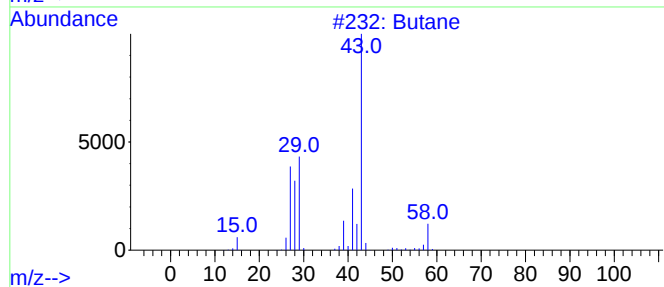
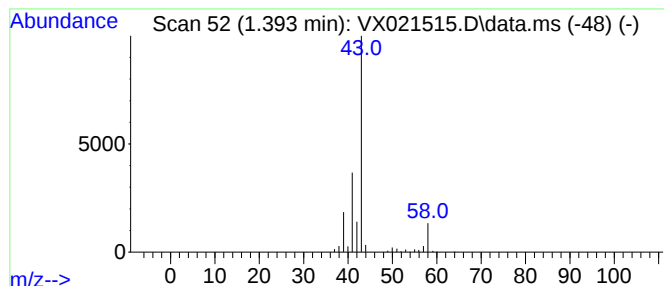
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.393	249.59 ug/l	1339030	Pentafluorobenzene	5.629

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			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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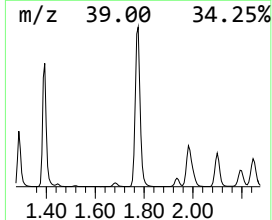
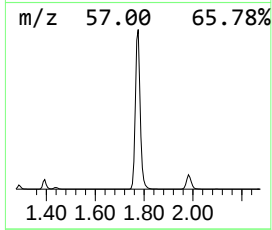
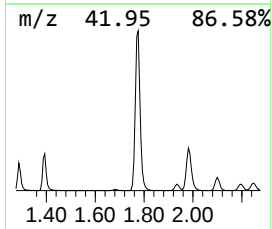
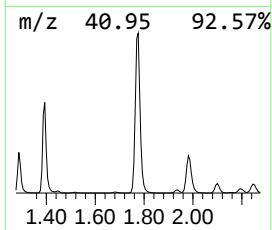
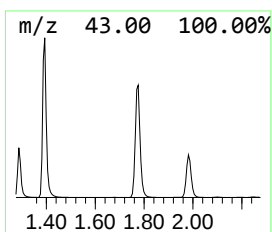
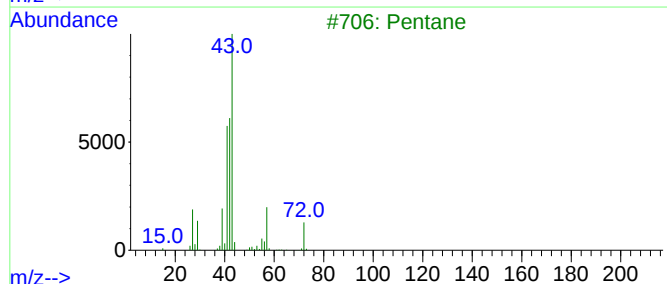
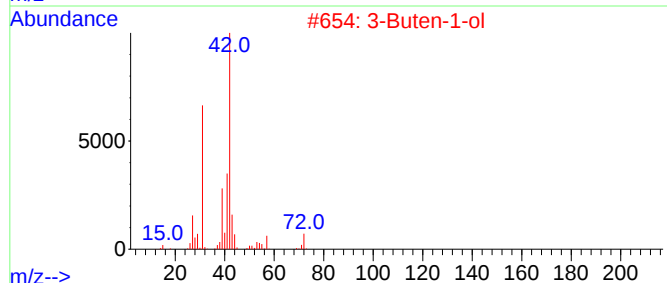
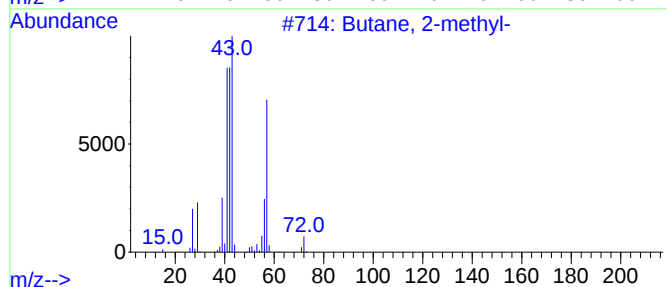
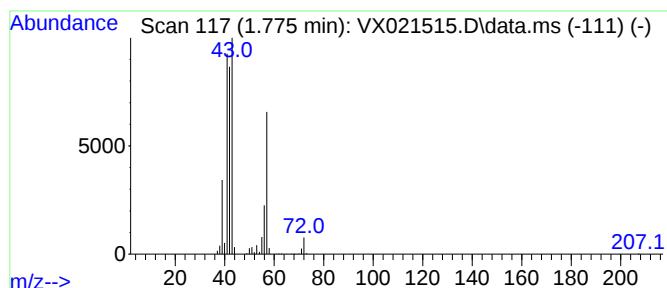
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.775	524.18 ug/l	2812170	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			1-Butene	56	C4H8	000106-98-9	10
5			Azetidine	57	C3H7N	000503-29-7	9



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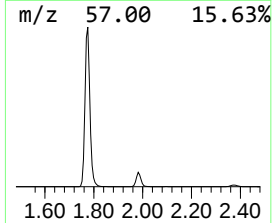
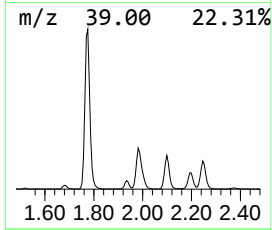
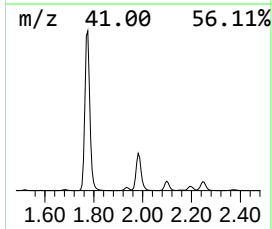
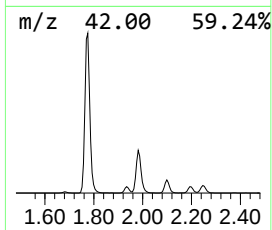
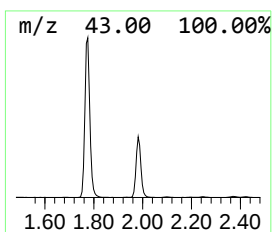
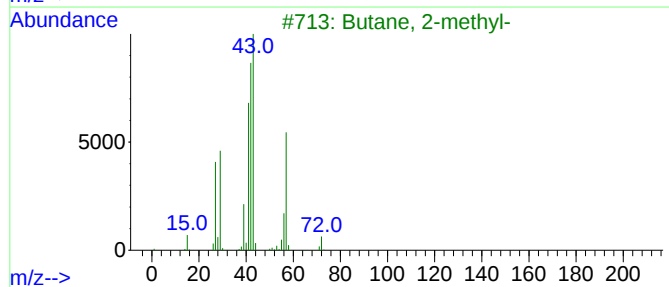
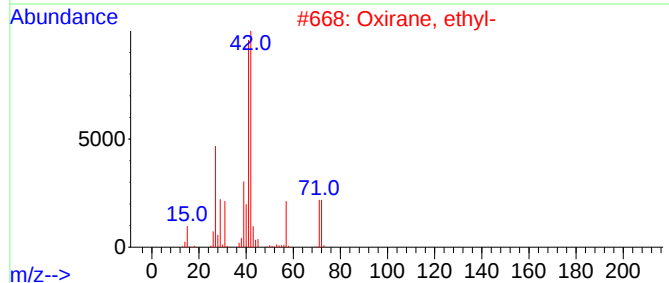
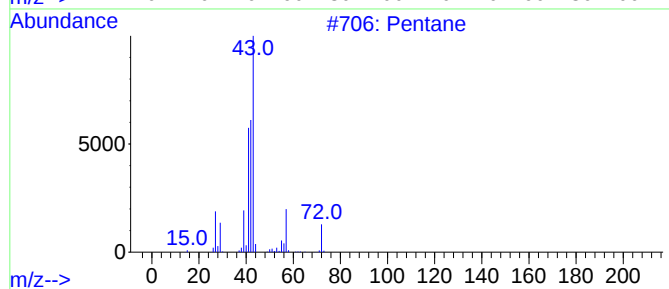
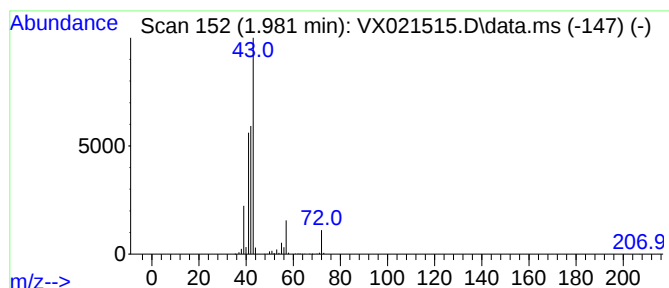
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Pentane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.981	146.60 ug/l	786505	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	40
3			Butane, 2-methyl-	72	C5H12	000078-78-4	10
4			Cyclobutylamine	71	C4H9N	002516-34-9	9
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9



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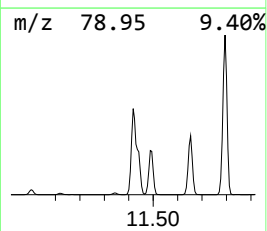
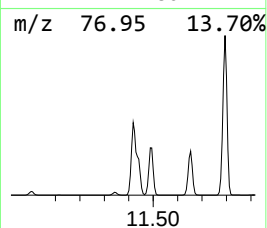
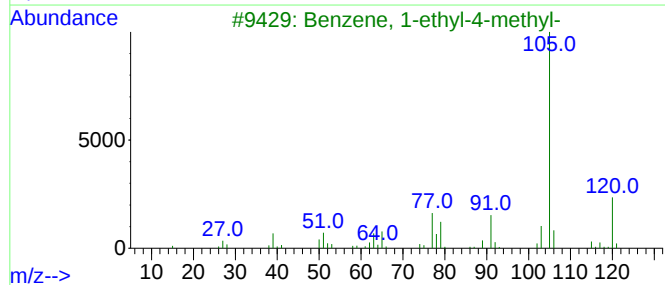
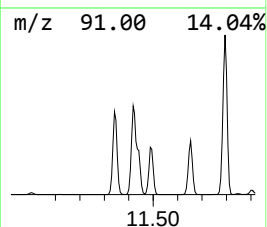
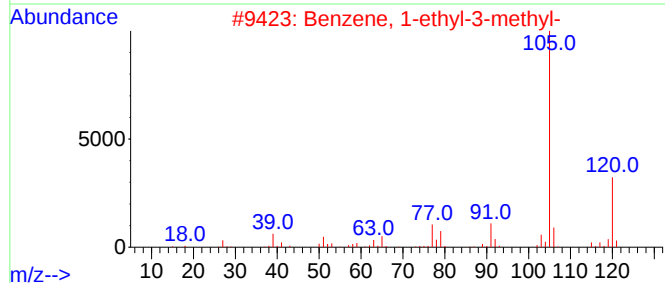
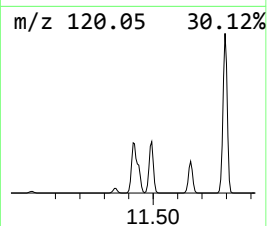
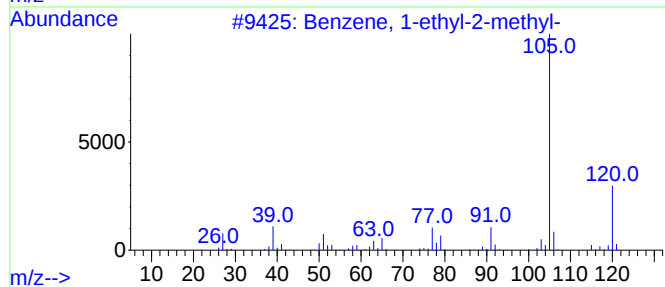
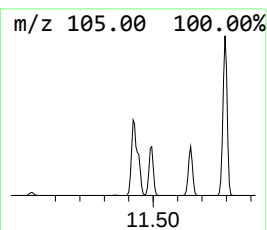
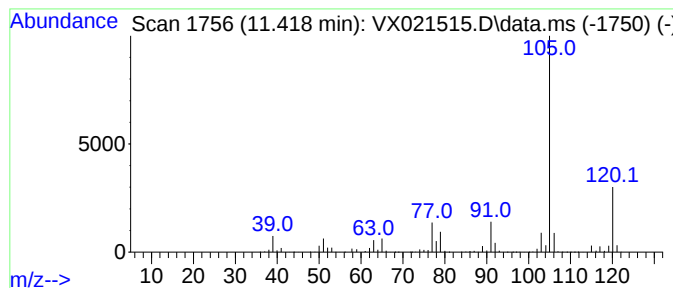
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.418	786.22 ug/l	6689200	1,4-Dichlorobenzene-d4	12.059

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-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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MW2R

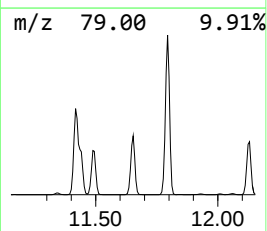
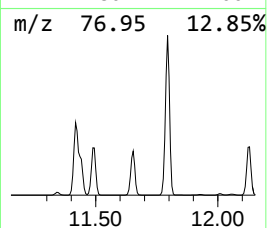
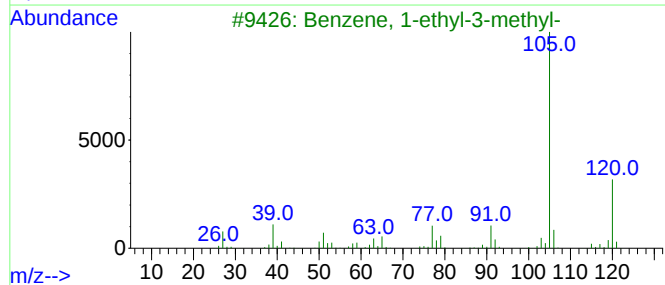
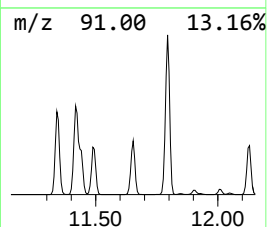
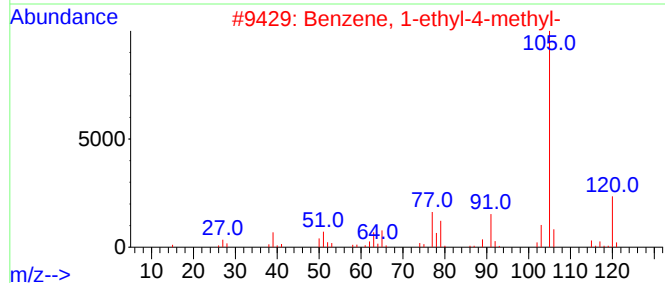
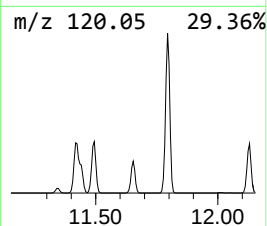
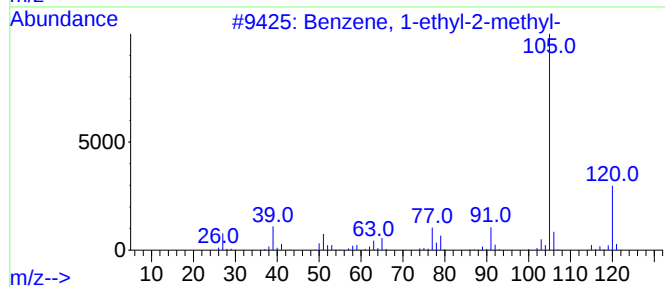
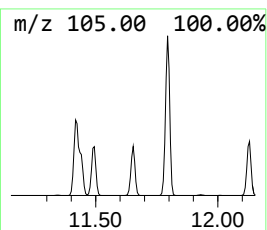
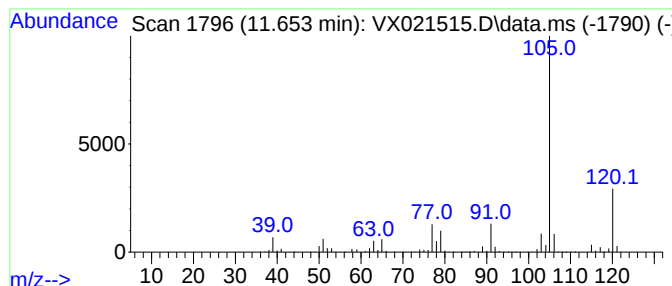
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.653	326.31 ug/l	2776250	1,4-Dichlorobenzene-d4	12.059

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			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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021515.D
Acq On : 26 Mar 2021 03:15
Operator : JC/MD
Sample : M1806-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW2R

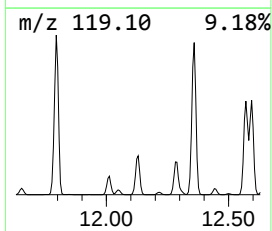
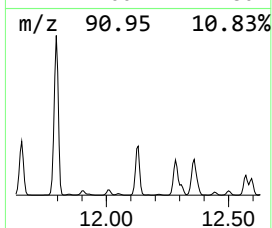
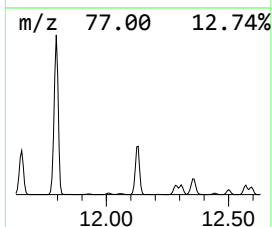
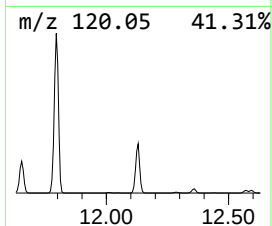
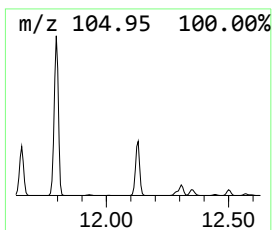
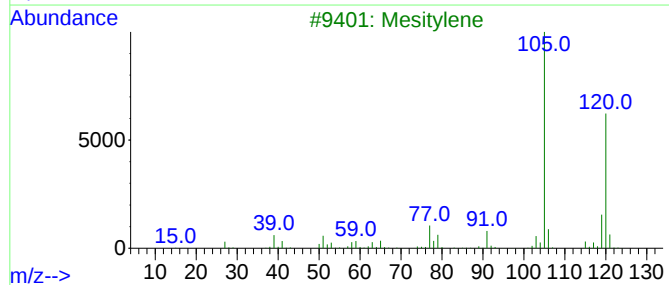
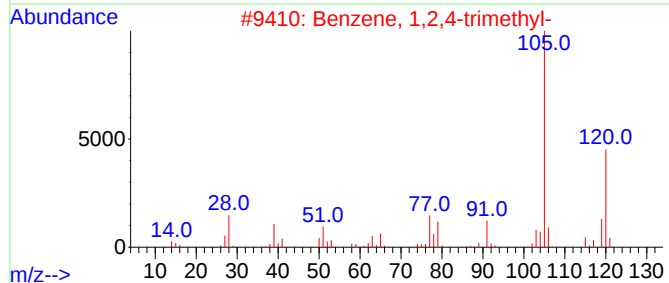
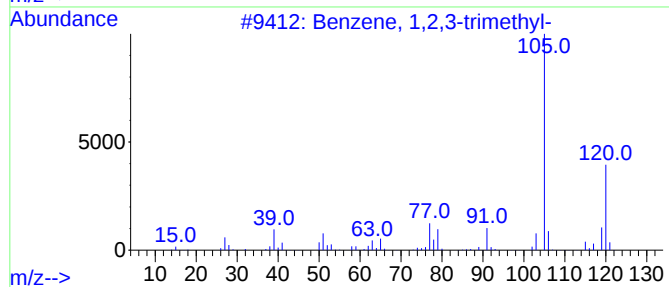
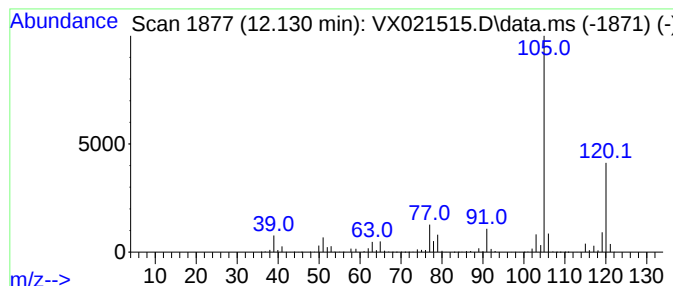
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.130	394.21 ug/l	3353980	1,4-Dichlorobenzene-d4	12.059

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			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021515.D
Acq On : 26 Mar 2021 03:15
Operator : JC/MD
Sample : M1806-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW2R

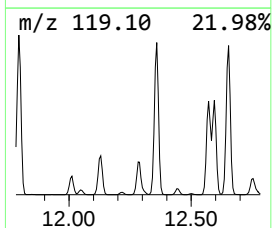
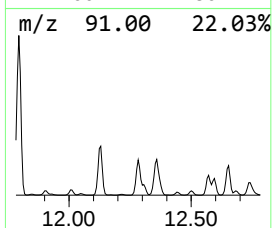
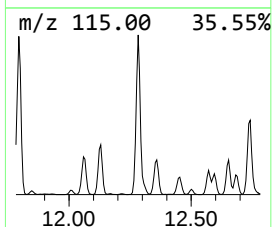
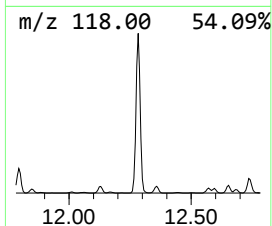
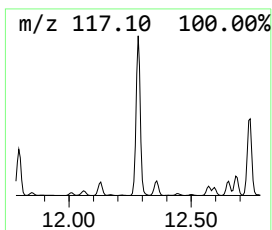
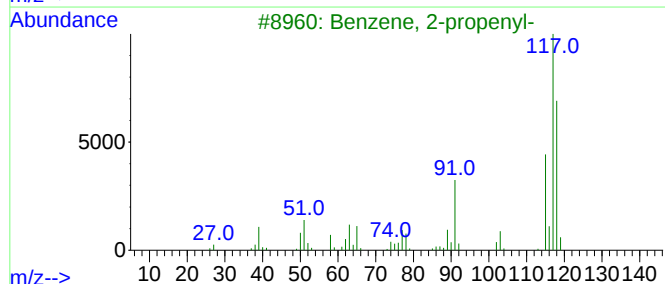
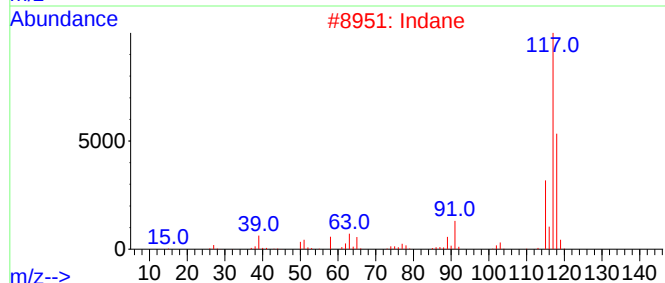
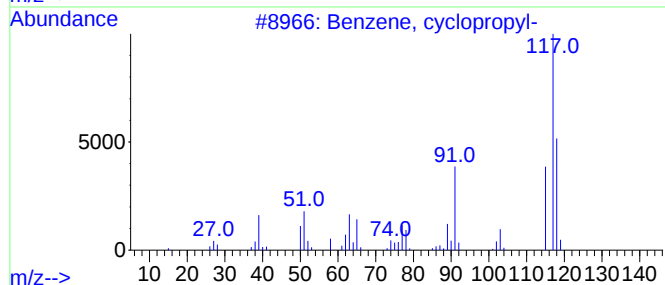
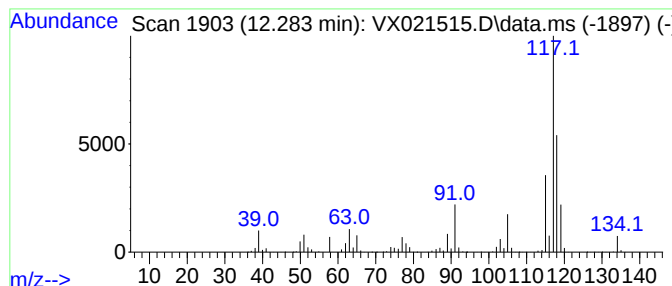
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, cyclopropyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.283	259.70 ug/l	2209590	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
2			Indane	118	C9H10	000496-11-7	70
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	55
5			Deltacyclene	118	C9H10	007785-10-6	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021515.D
Acq On : 26 Mar 2021 03:15
Operator : JC/MD
Sample : M1806-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW2R

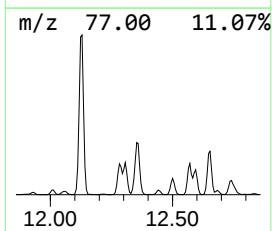
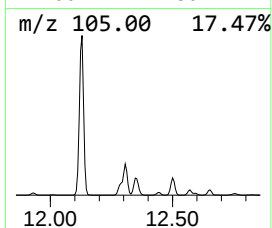
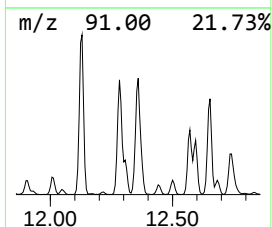
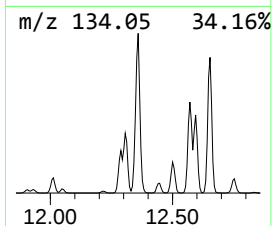
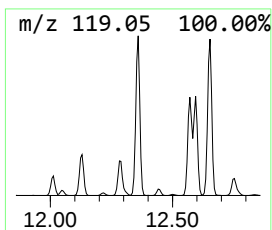
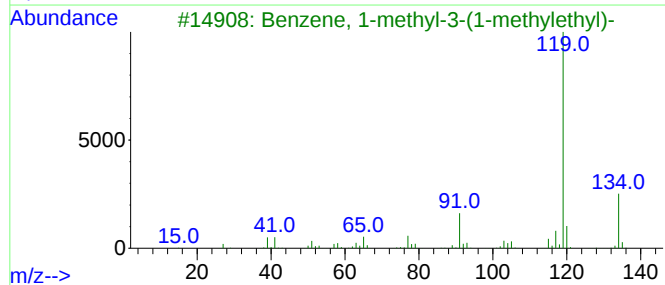
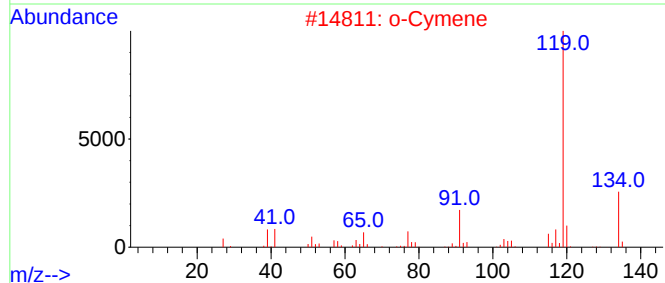
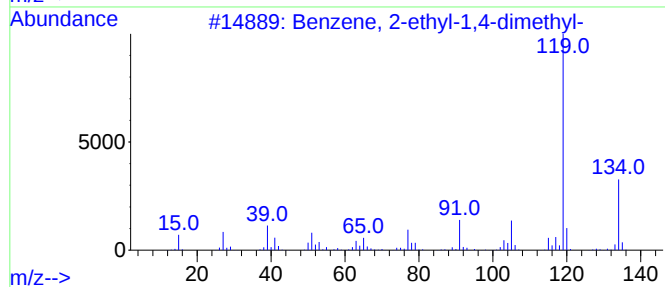
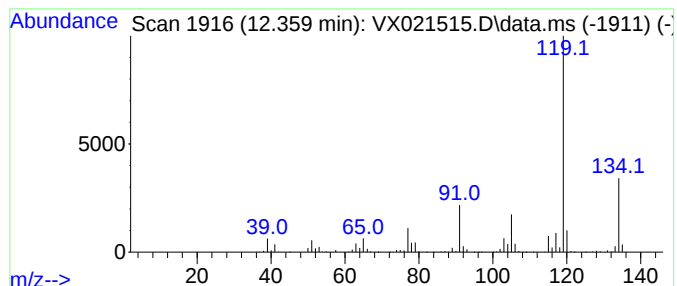
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.359	174.31 ug/l	1483090	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
2			o-Cymene	134	C10H14	000527-84-4	95
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			p-Cymene	134	C10H14	000099-87-6	94
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021515.D
Acq On : 26 Mar 2021 03:15
Operator : JC/MD
Sample : M1806-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW2R

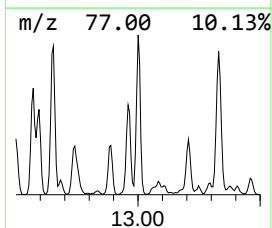
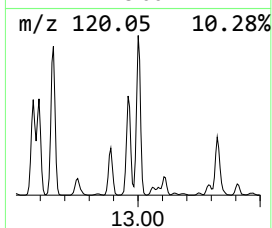
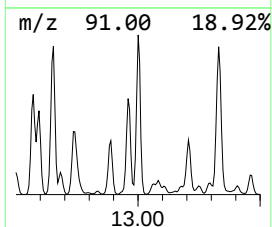
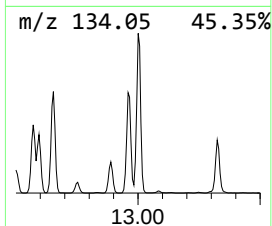
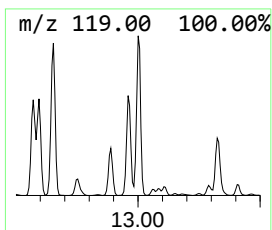
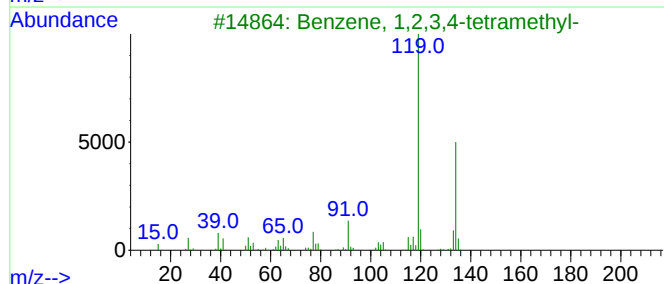
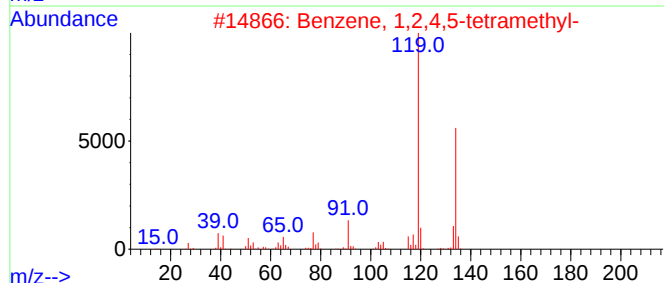
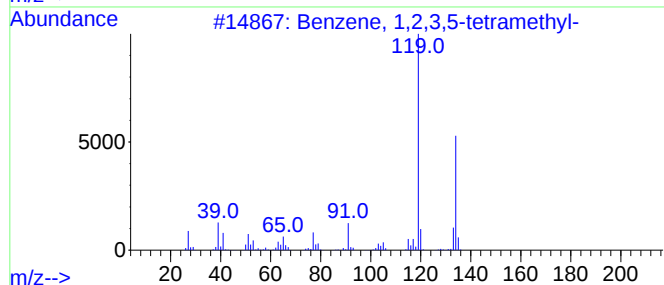
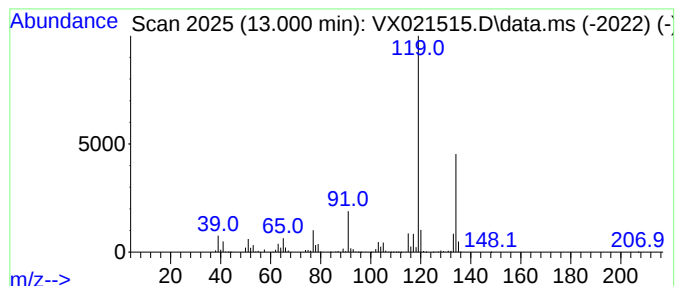
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.000	147.92 ug/l	1258540	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
5			o-Cymene	134	C10H14	000527-84-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021515.D
Acq On : 26 Mar 2021 03:15
Operator : JC/MD
Sample : M1806-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW2R

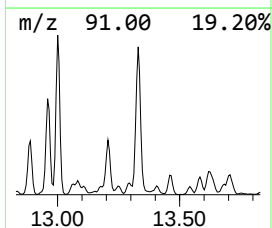
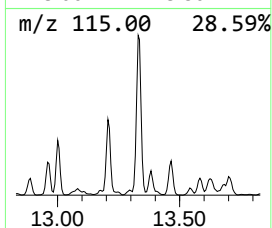
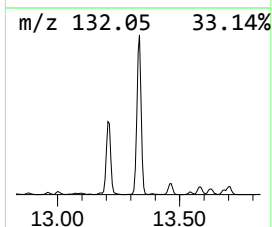
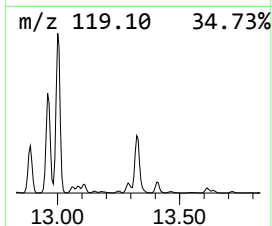
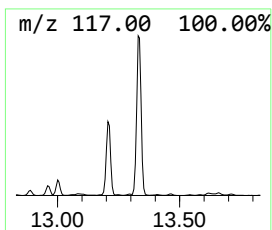
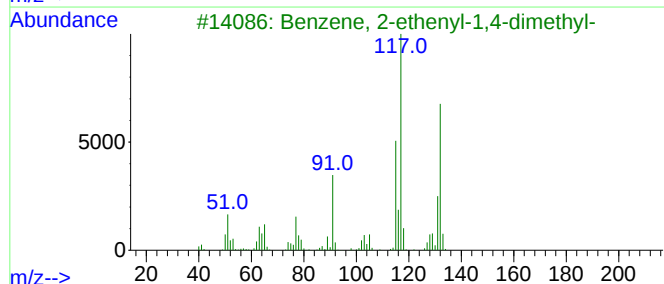
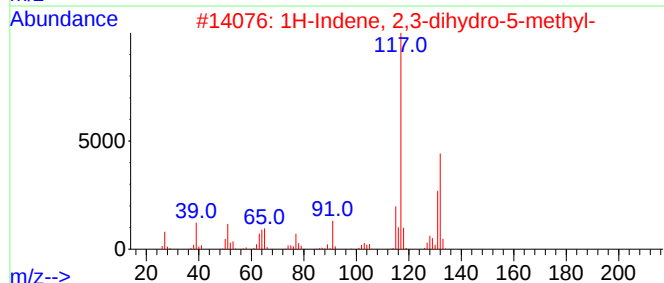
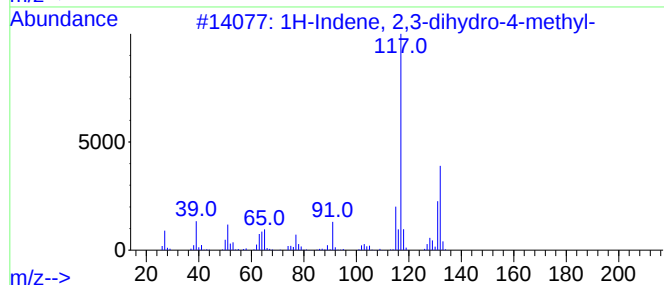
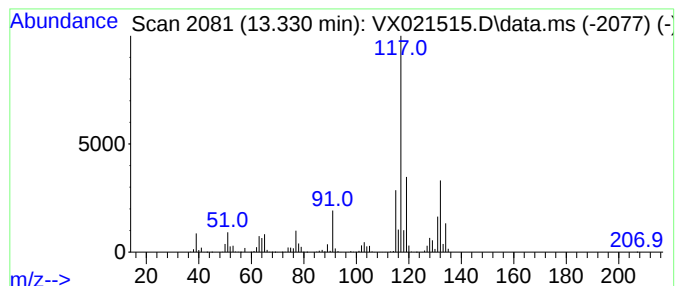
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.330	206.67 ug/l	1758370	1,4-Dichlorobenzene-d4	12.059

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
4		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
5		Benzene, 2-butenyl-	132	C10H12	001560-06-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021515.D
Acq On : 26 Mar 2021 03:15
Operator : JC/MD
Sample : M1806-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW2R

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-	1.775	524.2	ug/l	2812170	1	5.629	268246	50.0
Pentane	1.981	146.6	ug/l	786505	1	5.629	268246	50.0
Benzene, 1-ethy...	11.418	786.2	ug/l	6689200	4	12.059	425405	50.0
Benzene, 1-ethy...	11.653	326.3	ug/l	2776250	4	12.059	425405	50.0
Benzene, 1,2,3-...	12.130	394.2	ug/l	3353980	4	12.059	425405	50.0
Benzene, cyclop...	12.283	259.7	ug/l	2209590	4	12.059	425405	50.0
Benzene, 2-ethy...	12.359	174.3	ug/l	1483090	4	12.059	425405	50.0
Benzene, 1,2,3,...	13.000	147.9	ug/l	1258540	4	12.059	425405	50.0
1H-Indene, 2,3-...	13.330	206.7	ug/l	1758370	4	12.059	425405	50.0