

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020222\
 Data File : VX026739.D
 Acq On : 02 Feb 2022 16:10
 Operator : JC/MD
 Sample : N1380-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 INF0222

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\82X011122W.M
 Title : SW846 8260

Signal : TIC: VX026739.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	52	rBV	189170	185265	3.16%	0.481%
2	1.752	104	109	124	rVB	1004496	1365950	23.32%	3.546%
3	1.959	138	143	156	rVB2	375836	580096	9.90%	1.506%
4	2.075	156	162	168	rBV	49927	69272	1.18%	0.180%
5	2.221	181	186	197	rVB	198576	307516	5.25%	0.798%
6	2.343	199	206	219	rVB	45220	89099	1.52%	0.231%
7	2.788	260	279	282	rBV2	168976	468492	8.00%	1.216%
8	2.831	282	286	289	rVV	261779	508450	8.68%	1.320%
9	2.873	289	293	306	rVB2	269750	629041	10.74%	1.633%
10	3.105	320	331	345	rBV	192004	434405	7.42%	1.128%
11	3.325	358	367	378	rBV	47836	107243	1.83%	0.278%
12	3.453	378	388	400	rBV	67958	151749	2.59%	0.394%
13	3.587	400	410	417	rBV	26631	69131	1.18%	0.179%
14	3.739	427	435	444	rVB	123816	297044	5.07%	0.771%
15	3.843	444	452	459	rVV	91872	236792	4.04%	0.615%
16	3.910	459	463	472	rVV	40328	114425	1.95%	0.297%
17	4.105	485	495	505	rVV	89519	242070	4.13%	0.628%
18	4.221	505	514	519	rVV2	28187	79338	1.35%	0.206%
19	4.312	519	529	540	rVV	393411	1130434	19.30%	2.935%
20	4.434	540	549	563	rVB	62413	181096	3.09%	0.470%
21	5.202	649	675	693	rBV	167302	541780	9.25%	1.406%
22	5.391	693	706	713	rVV	77163	235856	4.03%	0.612%
23	5.483	713	721	727	rVV2	125200	415825	7.10%	1.079%
24	5.556	727	733	740	rVV	131875	415144	7.09%	1.078%
25	5.629	740	745	763	rVB2	78895	258904	4.42%	0.672%
26	5.836	767	779	790	rBV3	38472	122340	2.09%	0.318%
27	5.964	790	800	804	rVV	77999	198532	3.39%	0.515%
28	6.044	804	813	826	rVV	1106138	2964135	50.60%	7.695%
29	6.202	826	839	844	rVV3	62904	263597	4.50%	0.684%
30	6.257	845	848	858	rVV4	60978	152540	2.60%	0.396%
31	6.367	858	866	878	rVB2	38239	112129	1.91%	0.291%
32	6.769	923	932	942	rBV2	201356	608046	10.38%	1.578%
33	7.178	989	999	1008	rVB	83340	188115	3.21%	0.488%
34	7.379	1021	1032	1045	rBV5	105026	295170	5.04%	0.766%
35	7.885	1112	1115	1122	rVV3	31876	63355	1.08%	0.164%
36	7.988	1122	1132	1144	rVB3	30630	84867	1.45%	0.220%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

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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

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37	8.110	1144	1152	1154	rBV	54940	102665	1.75%	0.267%
38	8.147	1154	1158	1163	rVV	151469	261158	4.46%	0.678%
39	8.507	1210	1217	1226	rVB	109890	185553	3.17%	0.482%
40	8.653	1226	1241	1247	rBV	405728	666345	11.37%	1.730%
41	8.720	1247	1252	1259	rVB	464208	714977	12.20%	1.856%
42	8.958	1288	1291	1298	rVB	40773	66347	1.13%	0.172%
43	9.049	1298	1306	1312	rBV2	42150	71201	1.22%	0.185%
44	9.165	1320	1325	1330	rBV	45083	68081	1.16%	0.177%
45	9.458	1365	1373	1377	rBV2	29350	62203	1.06%	0.161%
46	10.055	1460	1471	1476	rBV	386483	542616	9.26%	1.409%
47	10.195	1489	1494	1500	rVB	1813551	2328493	39.75%	6.045%
48	10.305	1505	1512	1518	rVB	4305901	5858081	100.00%	15.208%
49	10.640	1562	1567	1575	rVB	665061	864505	14.76%	2.244%
50	10.963	1613	1620	1625	rBV	232087	283419	4.84%	0.736%
51	11.085	1634	1640	1645	rBV	293385	388595	6.63%	1.009%
52	11.305	1667	1676	1683	rBV	405548	489319	8.35%	1.270%
53	11.402	1683	1692	1696	rVV	539479	1003300	17.13%	2.605%
54	11.451	1696	1700	1707	rVB	418566	501682	8.56%	1.302%
55	11.616	1721	1727	1737	rBV	616556	763878	13.04%	1.983%
56	11.756	1744	1750	1755	rBV	1891334	2277747	38.88%	5.913%
57	12.024	1789	1794	1799	rVB	398150	485457	8.29%	1.260%
58	12.091	1799	1805	1810	rBV	973922	1240378	21.17%	3.220%
59	12.244	1823	1830	1838	rBV	1400614	1705436	29.11%	4.427%
60	12.317	1838	1842	1849	rVB4	122675	185616	3.17%	0.482%
61	12.408	1852	1857	1862	rBV2	50978	70537	1.20%	0.183%
62	12.463	1862	1866	1871	rVB	79684	94550	1.61%	0.245%
63	12.530	1871	1877	1880	rBV	105241	141431	2.41%	0.367%
64	12.616	1886	1891	1894	rBV	251532	302825	5.17%	0.786%
65	12.646	1894	1896	1900	rVV	75757	77548	1.32%	0.201%
66	12.701	1900	1905	1913	rVV	253835	337308	5.76%	0.876%
67	12.847	1924	1929	1934	rVB	63848	81571	1.39%	0.212%
68	12.920	1934	1941	1945	rBV	180638	227028	3.88%	0.589%
69	12.963	1945	1948	1954	rVB	156821	182150	3.11%	0.473%
70	13.170	1978	1982	1992	rVB	204588	246459	4.21%	0.640%
71	13.292	1997	2002	2007	rVB2	366237	487865	8.33%	1.266%
72	13.426	2019	2024	2032	rVB	61573	81285	1.39%	0.211%
73	13.774	2074	2081	2091	rBV	578701	730623	12.47%	1.897%
74	14.640	2219	2223	2232	rVB	66382	85302	1.46%	0.221%
75	14.780	2241	2246	2255	rVB	69504	90024	1.54%	0.234%

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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\82X011122W.M
Title : SW846 8260

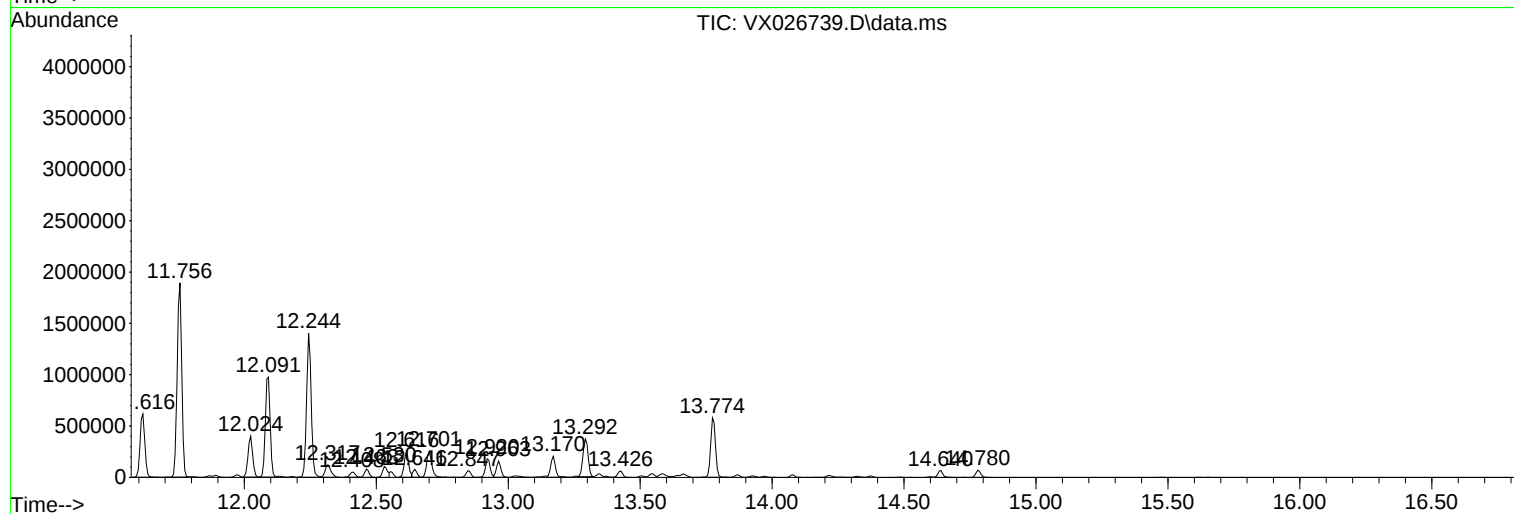
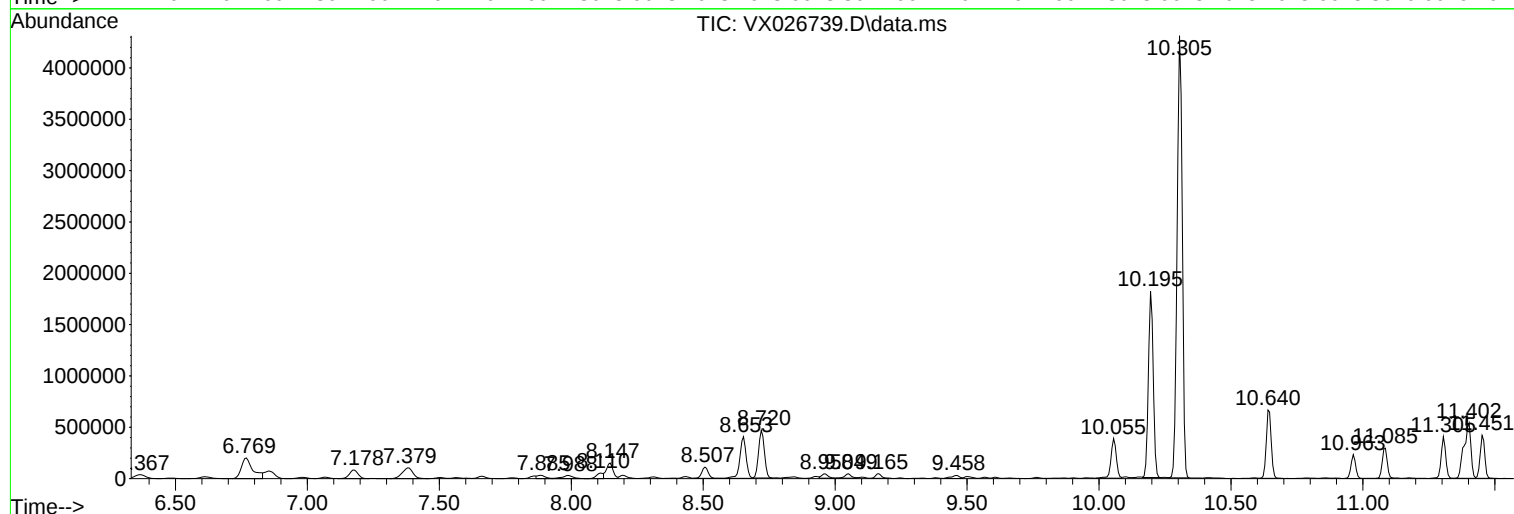
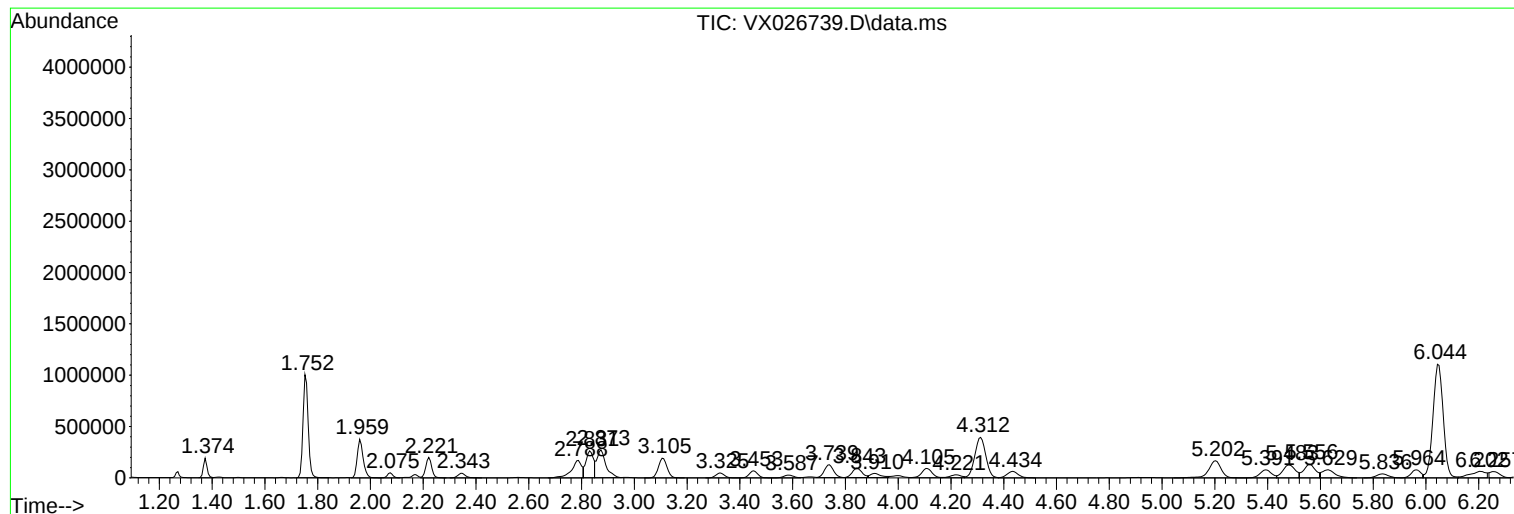
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020222\
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Instrument :
MSVOA_X
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INF0222

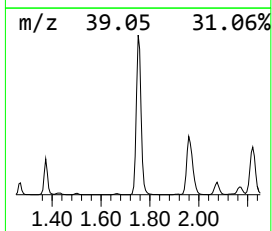
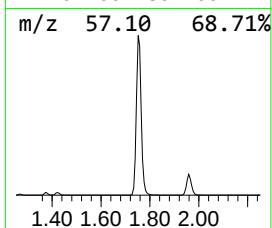
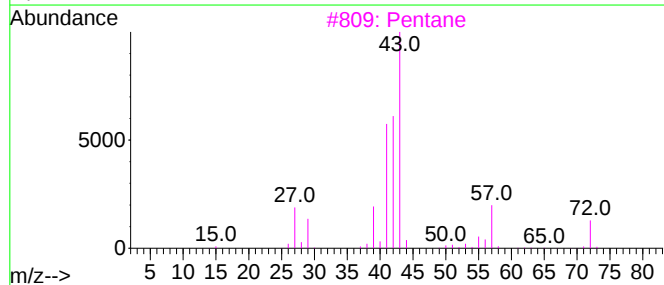
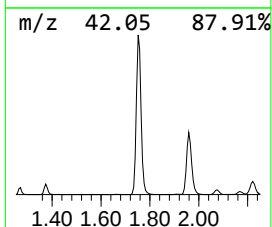
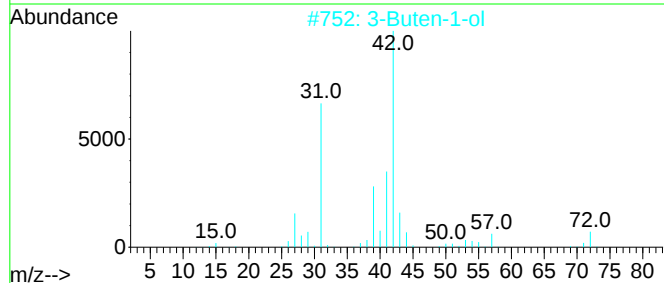
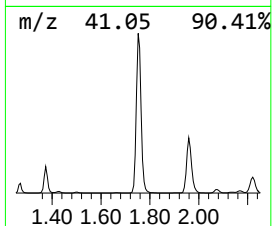
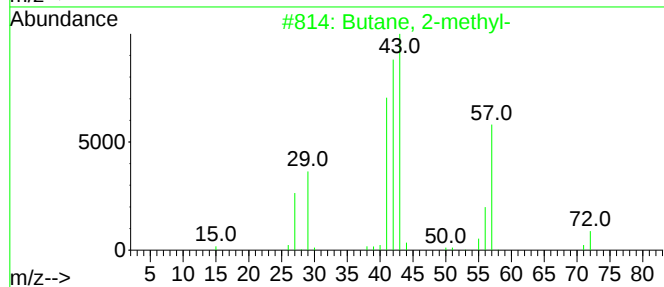
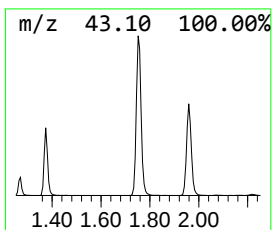
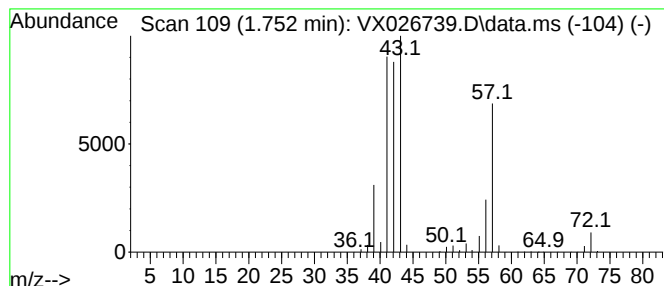
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	164.51 ug/l	1365950	Pentafluorobenzene	5.562

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	33
4			1-Butene	56	C4H8	000106-98-9	10
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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Instrument :
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ClientSampleId :
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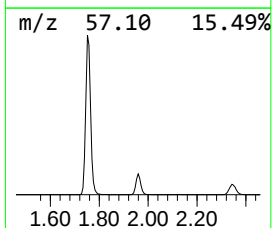
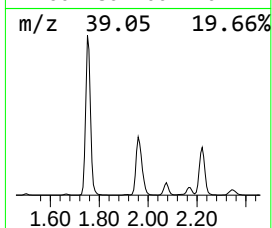
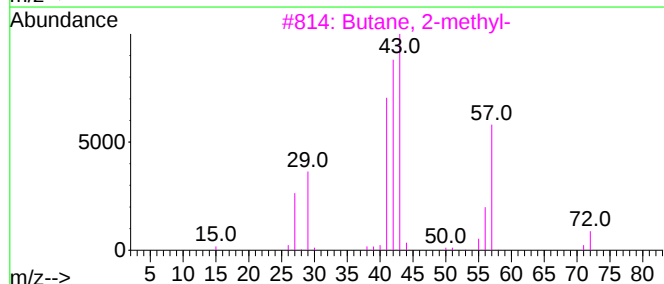
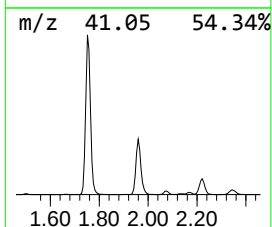
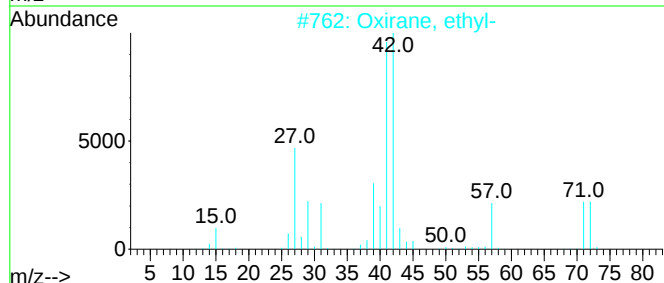
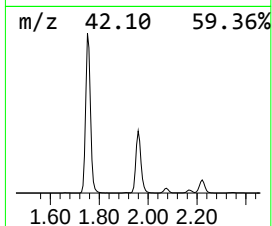
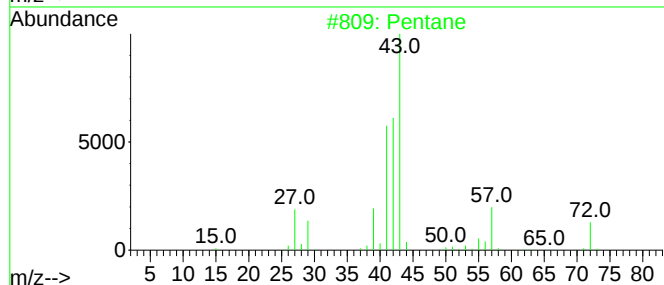
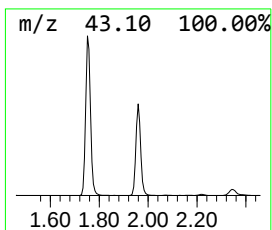
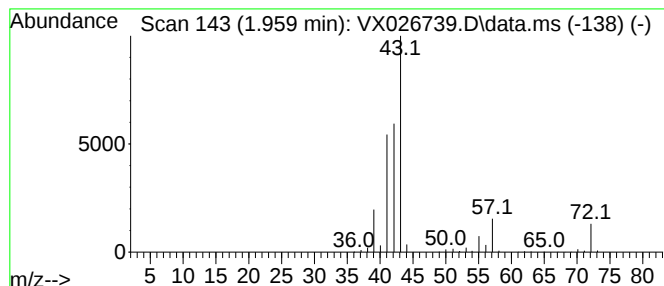
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	69.87 ug/l	580096	Pentafluorobenzene	5.562

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	39
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	9



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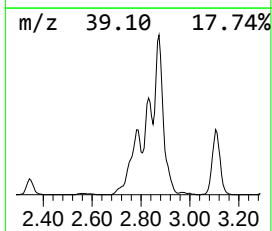
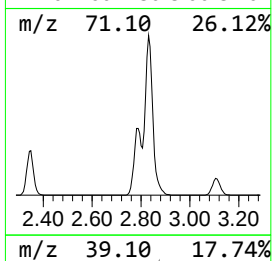
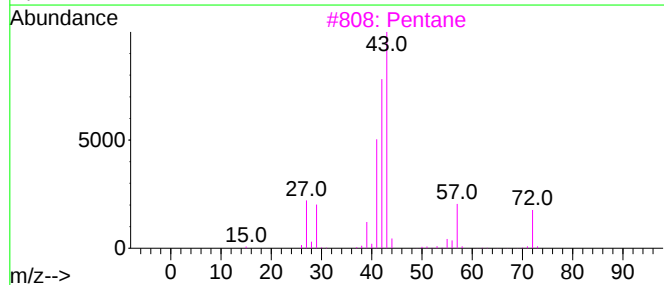
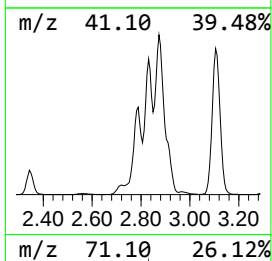
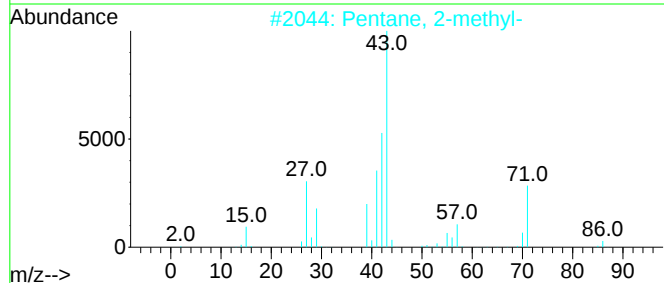
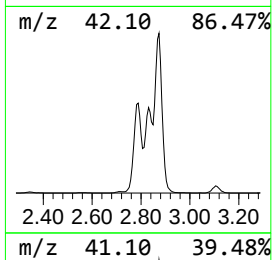
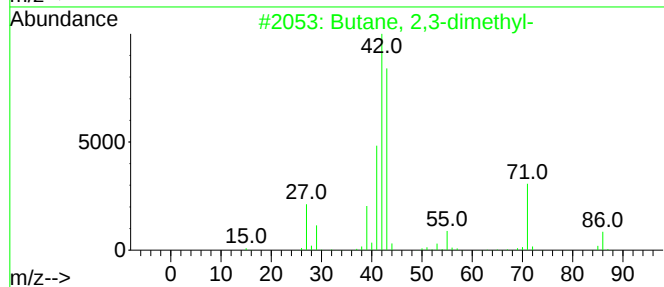
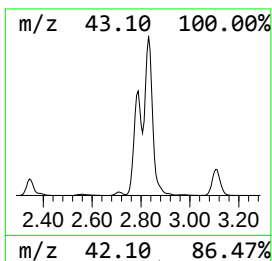
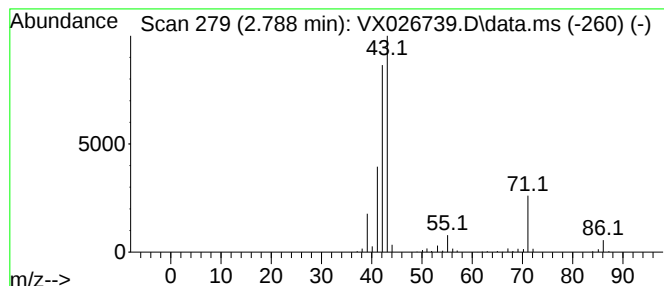
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.788	56.43 ug/l	468492	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3			Pentane	72	C5H12	000109-66-0	38
4			Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	12
5			Pyrrolidine	71	C4H9N	000123-75-1	10



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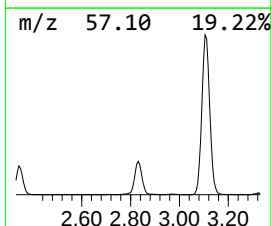
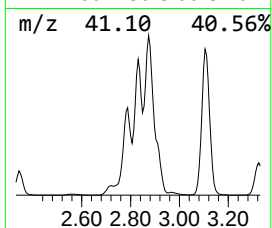
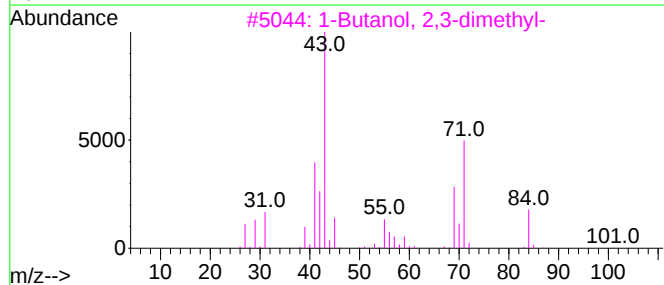
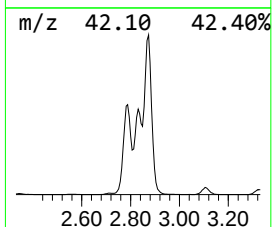
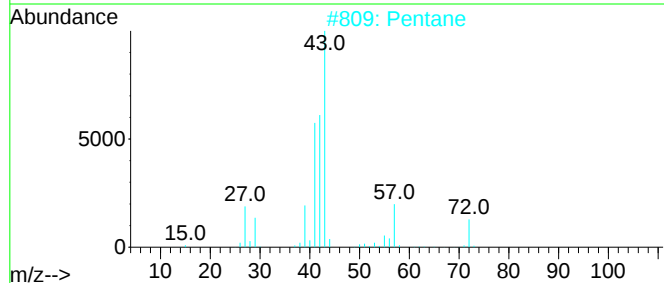
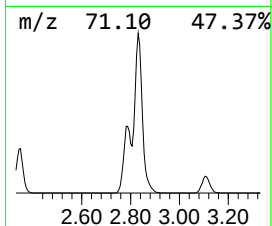
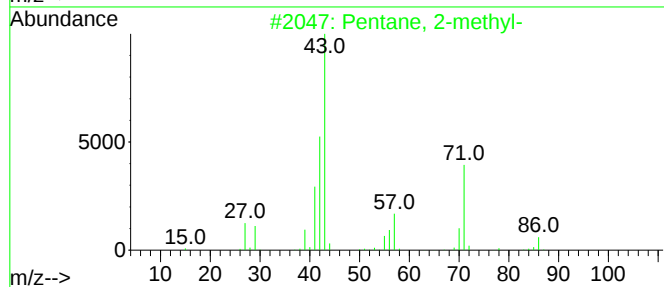
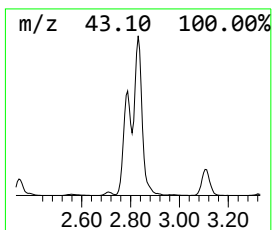
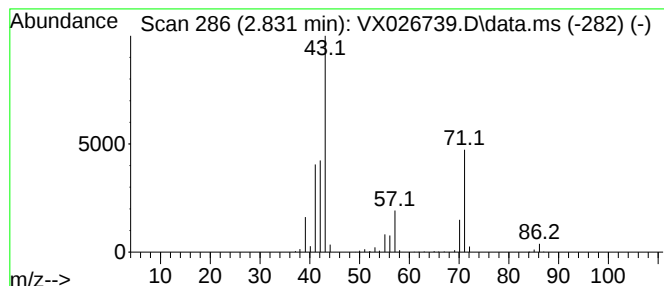
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.831	61.24 ug/l	508450	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Pentane	72	C5H12	000109-66-0	46
3			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	43
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020222\
Data File : VX026739.D
Acq On : 02 Feb 2022 16:10
Operator : JC/MD
Sample : N1380-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0222

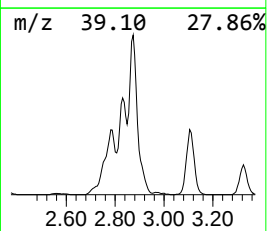
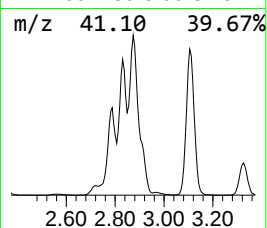
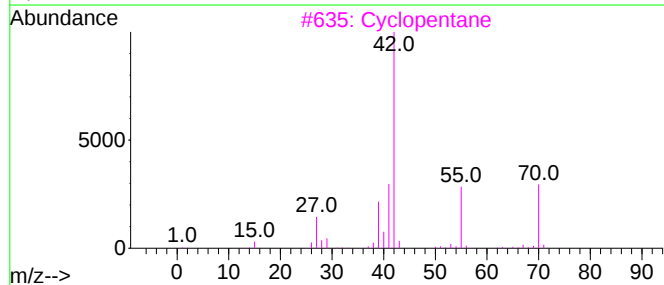
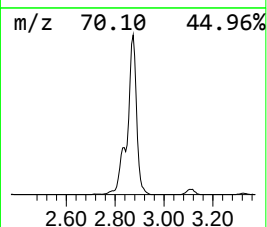
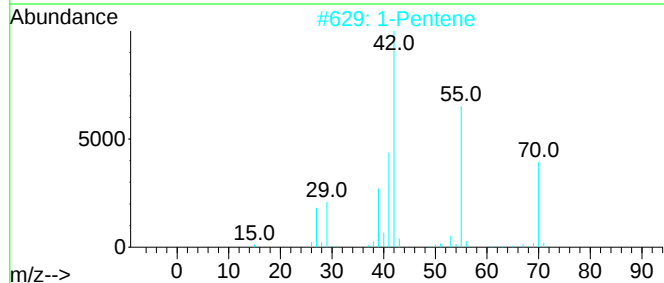
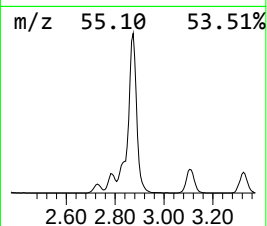
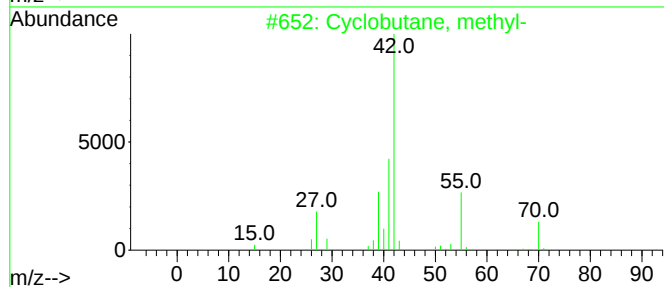
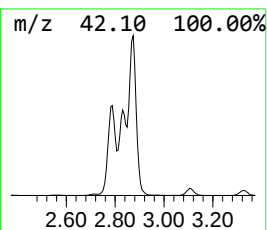
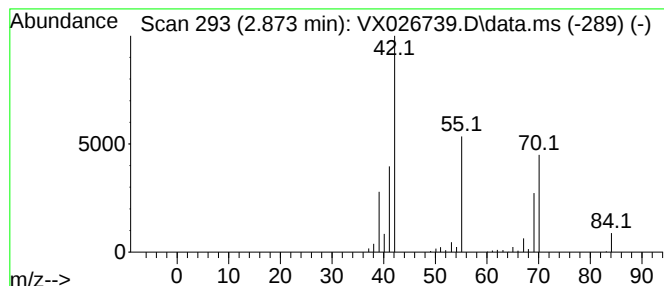
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Quant Title : SW846 8260

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

Peak Number 5 Cyclobutane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.873	75.76 ug/l	629041	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	86
2			1-Pentene	70	C5H10	000109-67-1	86
3			Cyclopentane	70	C5H10	000287-92-3	86
4			3-Buten-1-ol	72	C4H8O	000627-27-0	38
5			2-Pentene, (E)-	70	C5H10	000646-04-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020222\
Data File : VX026739.D
Acq On : 02 Feb 2022 16:10
Operator : JC/MD
Sample : N1380-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0222

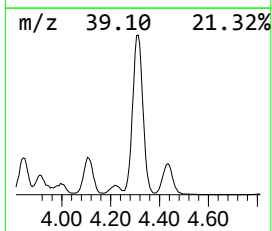
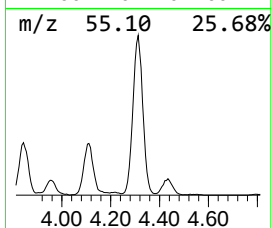
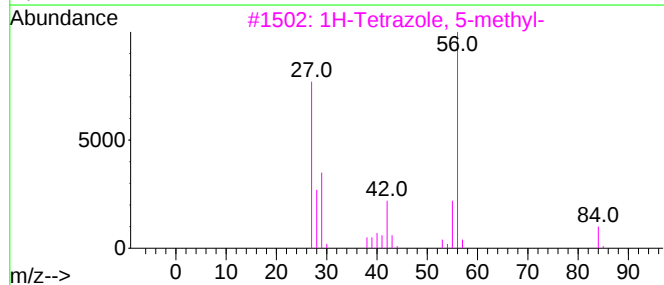
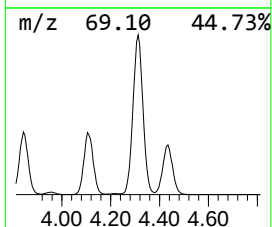
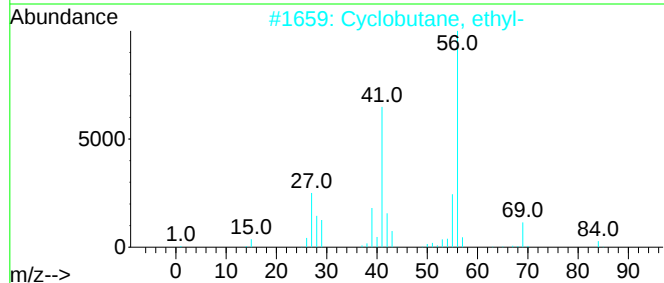
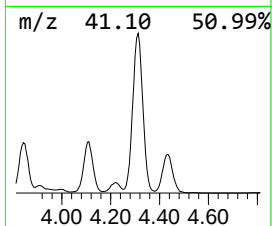
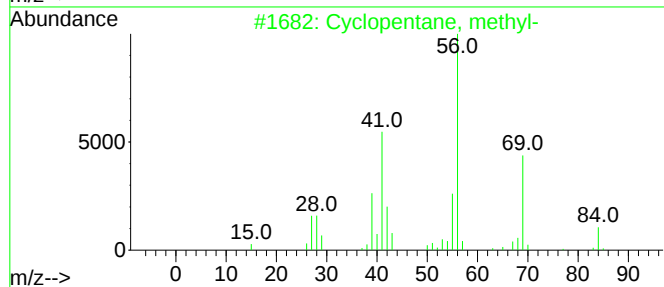
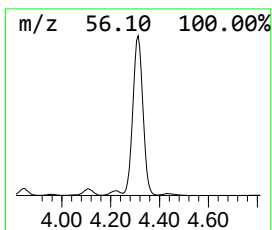
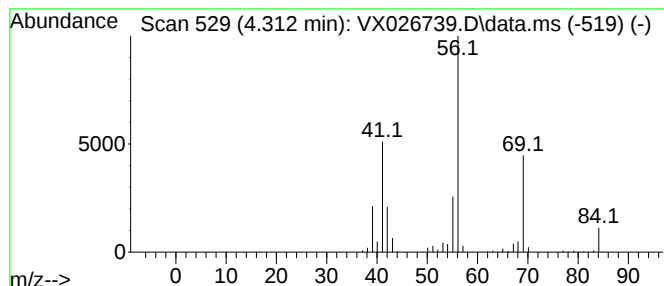
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	136.15 ug/l	1130430	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4			Cyclopropane, propyl-	84	C6H12	002415-72-7	56
5			1-Hexene	84	C6H12	000592-41-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020222\
Data File : VX026739.D
Acq On : 02 Feb 2022 16:10
Operator : JC/MD
Sample : N1380-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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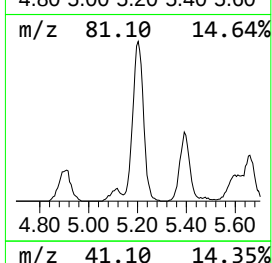
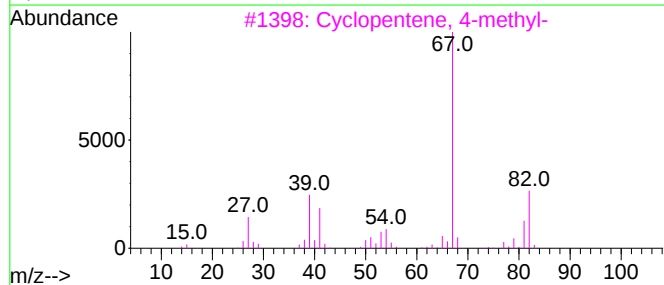
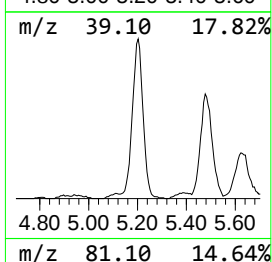
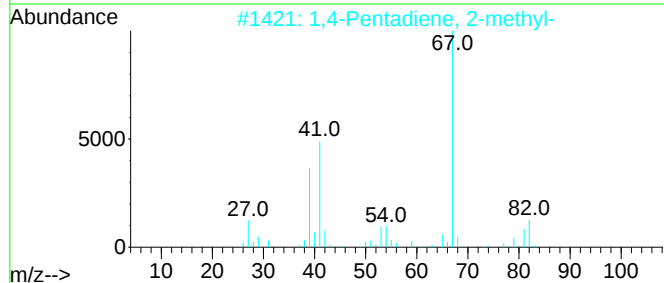
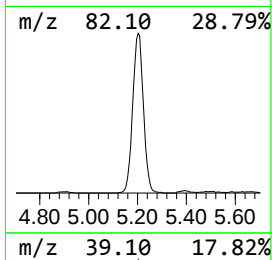
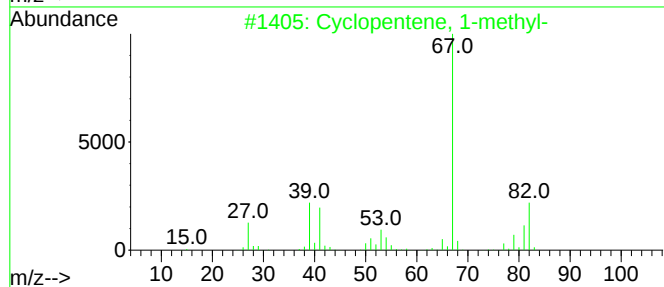
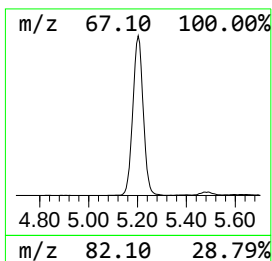
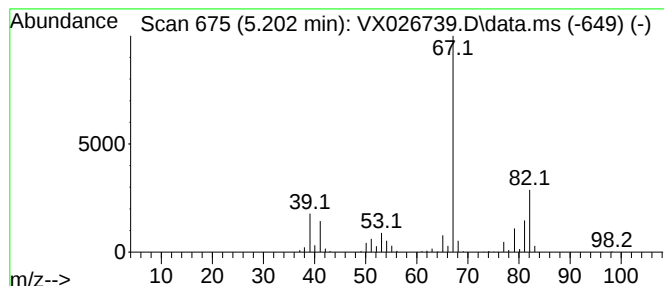
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.202	65.25 ug/l	541780	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	90
2			1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	90
3			Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	87
4			Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	86
5			Cyclopentane, methylene-	82	C6H10	001528-30-9	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX020222\
Data File : VX026739.D
Acq On : 02 Feb 2022 16:10
Operator : JC/MD
Sample : N1380-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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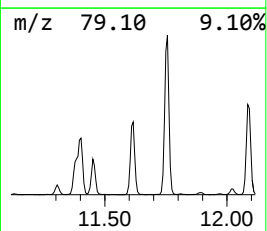
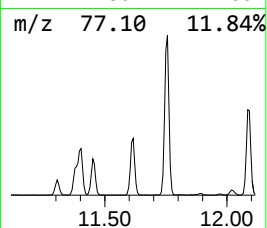
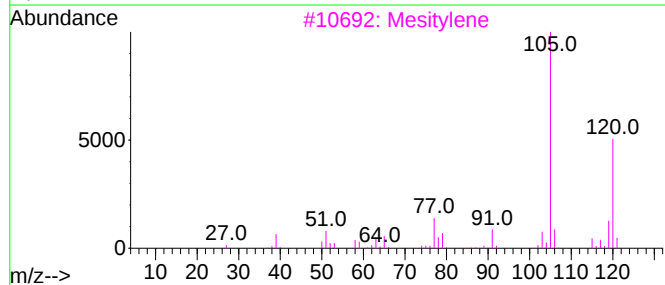
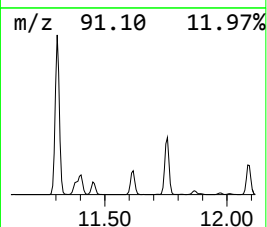
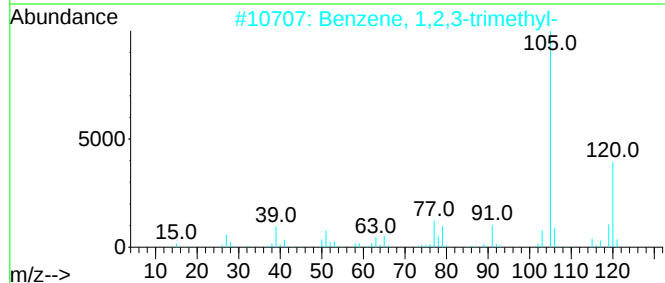
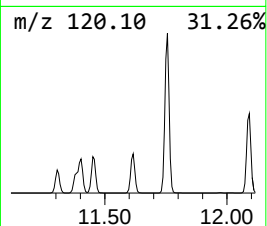
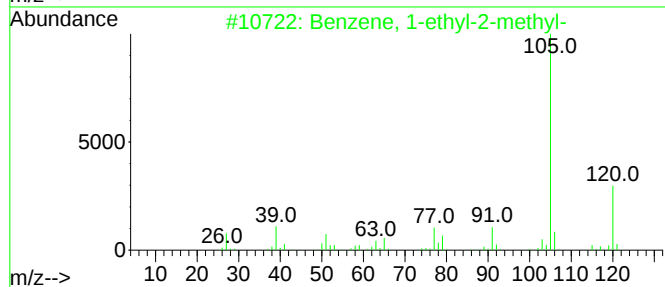
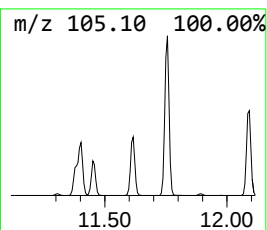
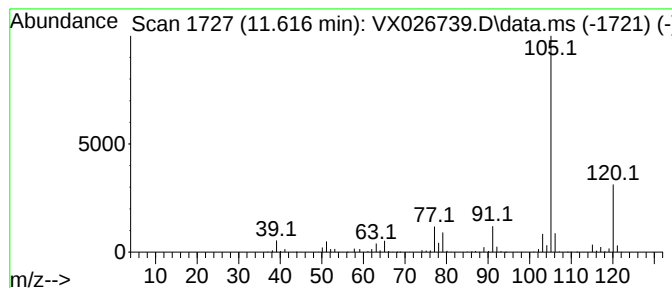
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	78.68 ug/l	763878	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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020222\
Data File : VX026739.D
Acq On : 02 Feb 2022 16:10
Operator : JC/MD
Sample : N1380-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0222

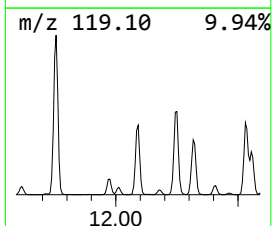
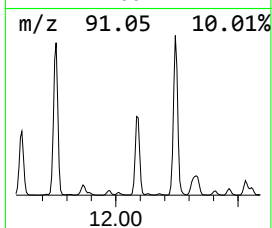
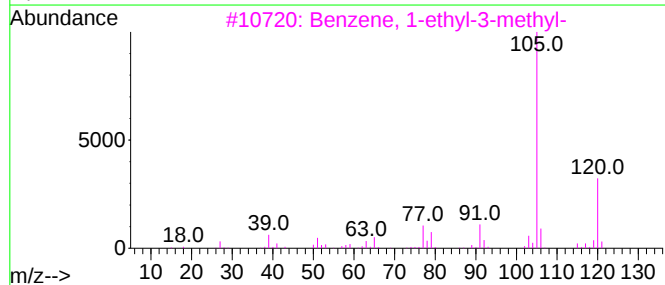
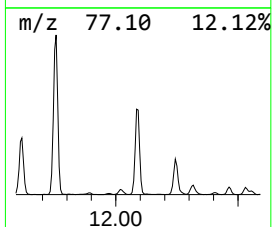
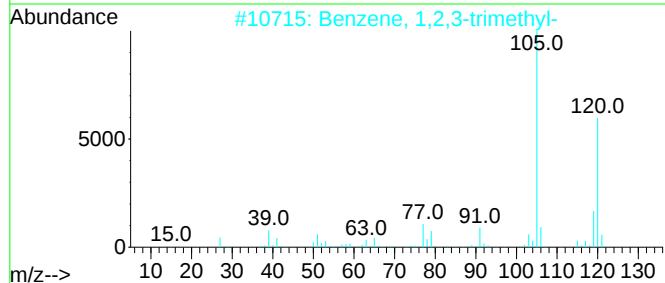
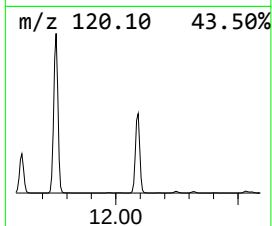
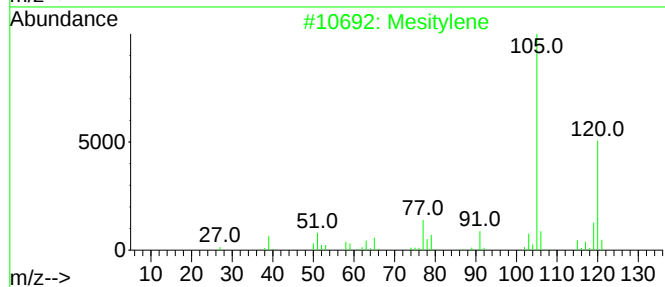
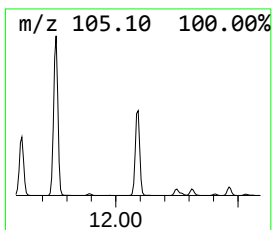
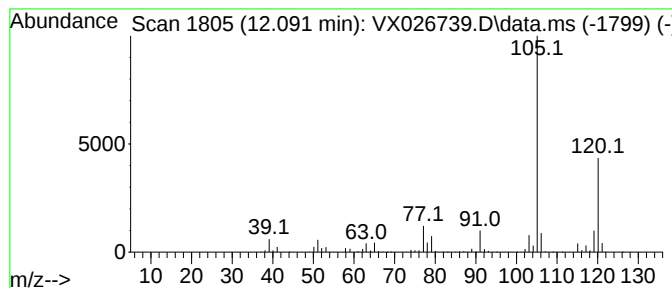
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	127.75 ug/l	1240380	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-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020222\
Data File : VX026739.D
Acq On : 02 Feb 2022 16:10
Operator : JC/MD
Sample : N1380-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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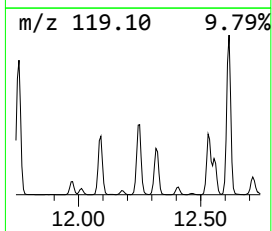
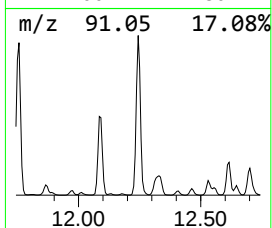
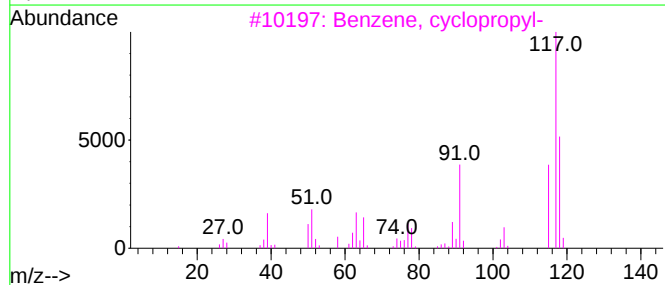
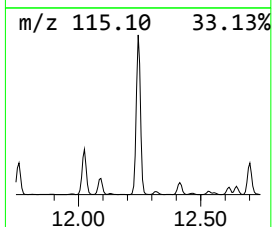
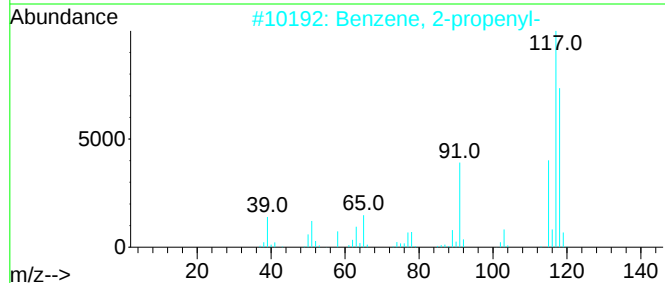
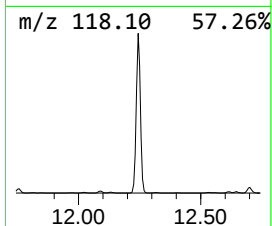
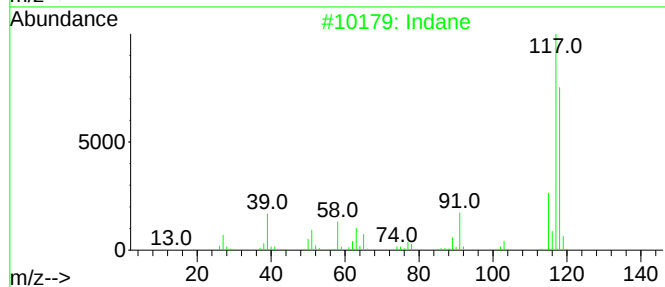
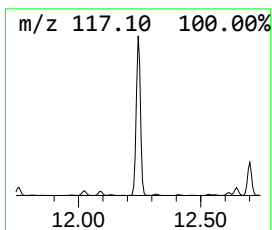
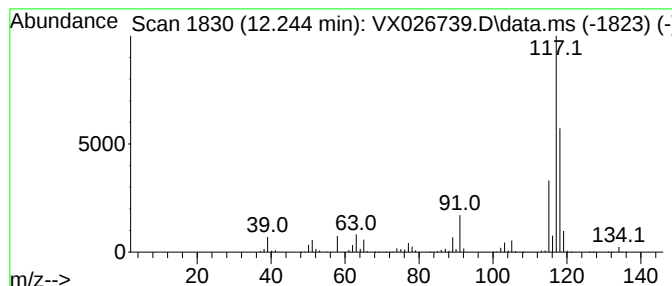
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	175.65 ug/l	1705440	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020222\
Data File : VX026739.D
Acq On : 02 Feb 2022 16:10
Operator : JC/MD
Sample : N1380-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0222

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.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
Butane, 2-methyl-	1.752	164.5	ug/l	1365950	1	5.562	415144	50.0
Pentane	1.959	69.9	ug/l	580096	1	5.562	415144	50.0
Butane, 2,3-dim...	2.788	56.4	ug/l	468492	1	5.562	415144	50.0
Pentane, 2-methyl-	2.831	61.2	ug/l	508450	1	5.562	415144	50.0
Cyclobutane, me...	2.873	75.8	ug/l	629041	1	5.562	415144	50.0
Cyclopentane, m...	4.312	136.2	ug/l	1130430	1	5.562	415144	50.0
Cyclopentene, 1...	5.202	65.3	ug/l	541780	1	5.562	415144	50.0
Benzene, 1-ethy...	11.616	78.7	ug/l	763878	4	12.024	485457	50.0
Benzene, 1,2,3-...	12.091	127.8	ug/l	1240380	4	12.024	485457	50.0
Indane	12.244	175.7	ug/l	1705440	4	12.024	485457	50.0