

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070622\
 Data File : VX029943.D
 Acq On : 06 Jul 2022 14:54
 Operator : JC/MD
 Sample : N3599-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 INF0722

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\82X062822W.M
 Title : SW846 8260

Signal : TIC: VX029943.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	43	46	52	rBV	383995	370242	2.30%	0.385%
2	1.745	103	108	123	rBV	2372895	3247690	20.14%	3.375%
3	1.952	137	142	156	rVB2	947586	1387905	8.61%	1.442%
4	2.068	156	161	167	rBV	120004	162799	1.01%	0.169%
5	2.215	180	185	194	rVB	345104	515777	3.20%	0.536%
6	2.337	199	205	211	rBV	92790	180151	1.12%	0.187%
7	2.782	258	278	281	rBV2	372360	1023539	6.35%	1.064%
8	2.824	281	285	289	rVV	616199	1294744	8.03%	1.346%
9	2.867	289	292	305	rVB2	558762	1213532	7.53%	1.261%
10	3.105	319	331	345	rVB	439921	1003354	6.22%	1.043%
11	3.318	355	366	377	rBV	86818	198631	1.23%	0.206%
12	3.446	377	387	400	rBV	161735	364243	2.26%	0.379%
13	3.733	427	434	444	rVB	213047	499721	3.10%	0.519%
14	3.842	444	452	458	rBV	152673	384063	2.38%	0.399%
15	4.104	486	495	504	rVV2	150848	388610	2.41%	0.404%
16	4.214	504	513	519	rVV3	58041	163406	1.01%	0.170%
17	4.306	519	528	540	rVV	903564	2576968	15.98%	2.678%
18	4.428	540	548	563	rVB3	74176	224790	1.39%	0.234%
19	5.196	651	674	691	rVB2	220761	740137	4.59%	0.769%
20	5.391	691	706	712	rBV	125035	381632	2.37%	0.397%
21	5.476	712	720	728	rVV2	250782	772608	4.79%	0.803%
22	5.562	728	734	739	rVV2	160701	430800	2.67%	0.448%
23	5.629	739	745	762	rVB3	164070	564245	3.50%	0.586%
24	5.830	766	778	790	rBV3	83904	264230	1.64%	0.275%
25	5.964	790	800	804	rBV3	123638	310036	1.92%	0.322%
26	6.043	804	813	825	rVB	2628019	6886395	42.71%	7.157%
27	6.208	825	840	843	rBV5	115484	439338	2.72%	0.457%
28	6.366	857	866	877	rVB2	83159	246634	1.53%	0.256%
29	6.769	923	932	941	rBV	339267	960211	5.96%	0.998%
30	6.854	943	946	958	rVB4	123939	274863	1.70%	0.286%
31	7.177	990	999	1008	rVB3	111384	261312	1.62%	0.272%
32	7.384	1020	1033	1045	rBV4	244911	680743	4.22%	0.707%
33	8.110	1143	1152	1154	rBV2	106691	196688	1.22%	0.204%
34	8.146	1154	1158	1163	rVB	200176	318955	1.98%	0.331%
35	8.506	1210	1217	1225	rVB	223054	375026	2.33%	0.390%
36	8.652	1235	1241	1247	rVB	668964	1043349	6.47%	1.084%

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37	8.720	1247	1252	1259	rVB	1016232	1546594	9.59%	1.607%
38	10.055	1461	1471	1476	rBV	660170	934171	5.79%	0.971%
39	10.195	1489	1494	1500	rBV	5348915	7116096	44.13%	7.395%
40	10.305	1506	1512	1518	rVB	11389265	16123854	100.00%	16.756%
41	10.646	1562	1568	1577	rVB	1829978	2394254	14.85%	2.488%
42	10.963	1614	1620	1627	rVB	706832	876453	5.44%	0.911%
43	11.085	1635	1640	1645	rBV	505181	651088	4.04%	0.677%
44	11.304	1667	1676	1682	rBV	1388642	1700644	10.55%	1.767%
45	11.402	1689	1692	1696	rVB	1749176	2184440	13.55%	2.270%
46	11.451	1696	1700	1706	rVB	1282913	1580996	9.81%	1.643%
47	11.615	1721	1727	1735	rVB	1826970	2230050	13.83%	2.318%
48	11.756	1744	1750	1755	rBV	6509830	7732841	47.96%	8.036%
49	12.024	1789	1794	1799	rVB	748939	942304	5.84%	0.979%
50	12.091	1799	1805	1810	rBV	3178086	3776000	23.42%	3.924%
51	12.243	1824	1830	1838	rBV	4122067	5227107	32.42%	5.432%
52	12.316	1838	1842	1852	rVB3	392574	616895	3.83%	0.641%
53	12.414	1852	1858	1862	rBV2	160899	227714	1.41%	0.237%
54	12.463	1862	1866	1872	rVB	234598	287486	1.78%	0.299%
55	12.530	1872	1877	1880	rBV	325657	455090	2.82%	0.473%
56	12.615	1886	1891	1894	rBV	724993	886062	5.50%	0.921%
57	12.646	1894	1896	1900	rVV	234631	246593	1.53%	0.256%
58	12.701	1900	1905	1913	rVB	798062	1029358	6.38%	1.070%
59	12.847	1925	1929	1934	rVB	189538	242705	1.51%	0.252%
60	12.926	1934	1942	1945	rBV	529777	669122	4.15%	0.695%
61	12.963	1945	1948	1954	rVB	498949	573085	3.55%	0.596%
62	13.170	1978	1982	1992	rVB	587149	724126	4.49%	0.753%
63	13.292	1997	2002	2007	rVB2	1085615	1442913	8.95%	1.500%
64	13.426	2019	2024	2032	rVB	194059	251961	1.56%	0.262%
65	13.780	2076	2082	2088	rBV	2057860	2613331	16.21%	2.716%
66	14.639	2219	2223	2229	rVB	238908	290230	1.80%	0.302%
67	14.779	2241	2246	2254	rVB	243550	304451	1.89%	0.316%

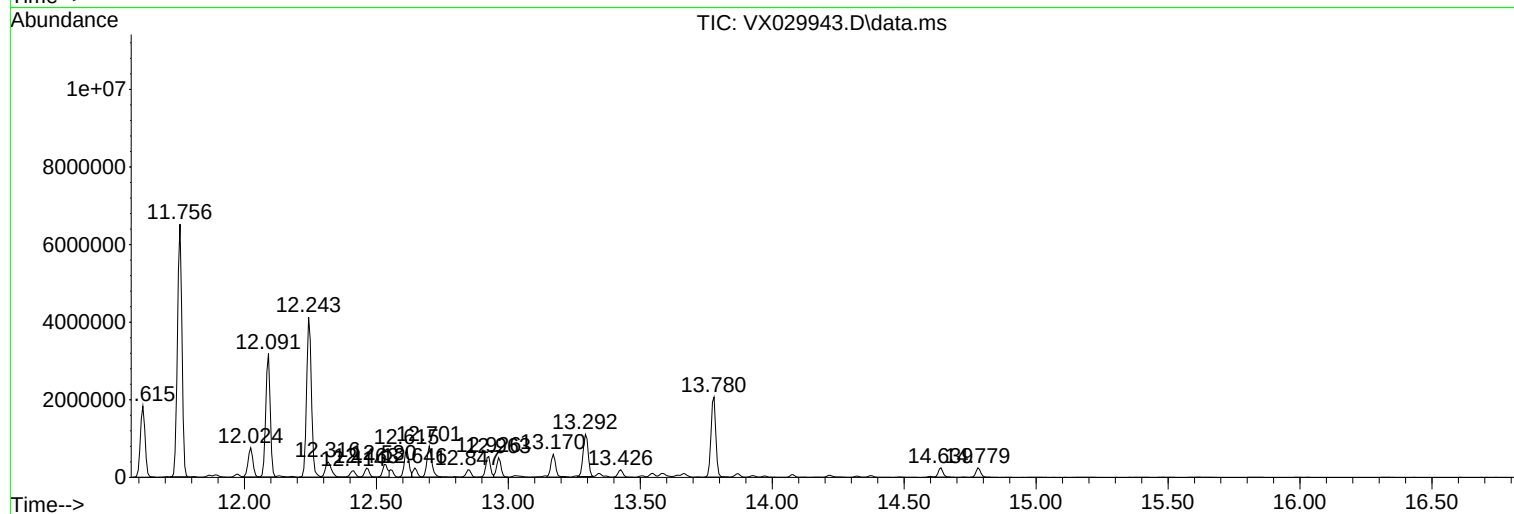
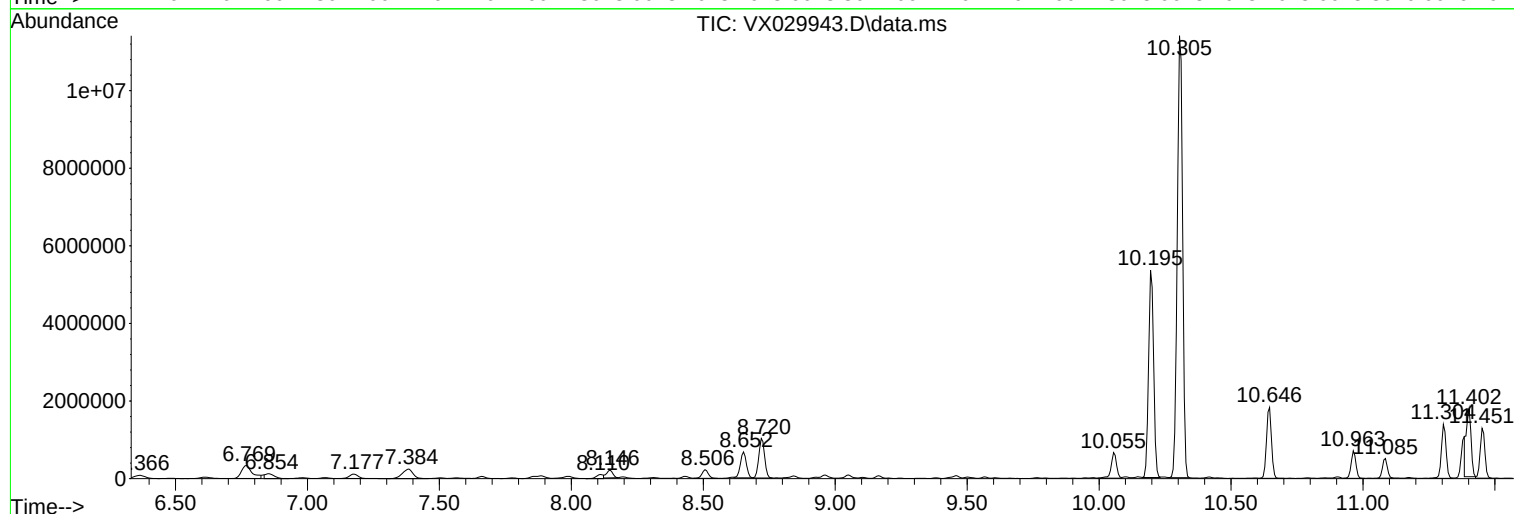
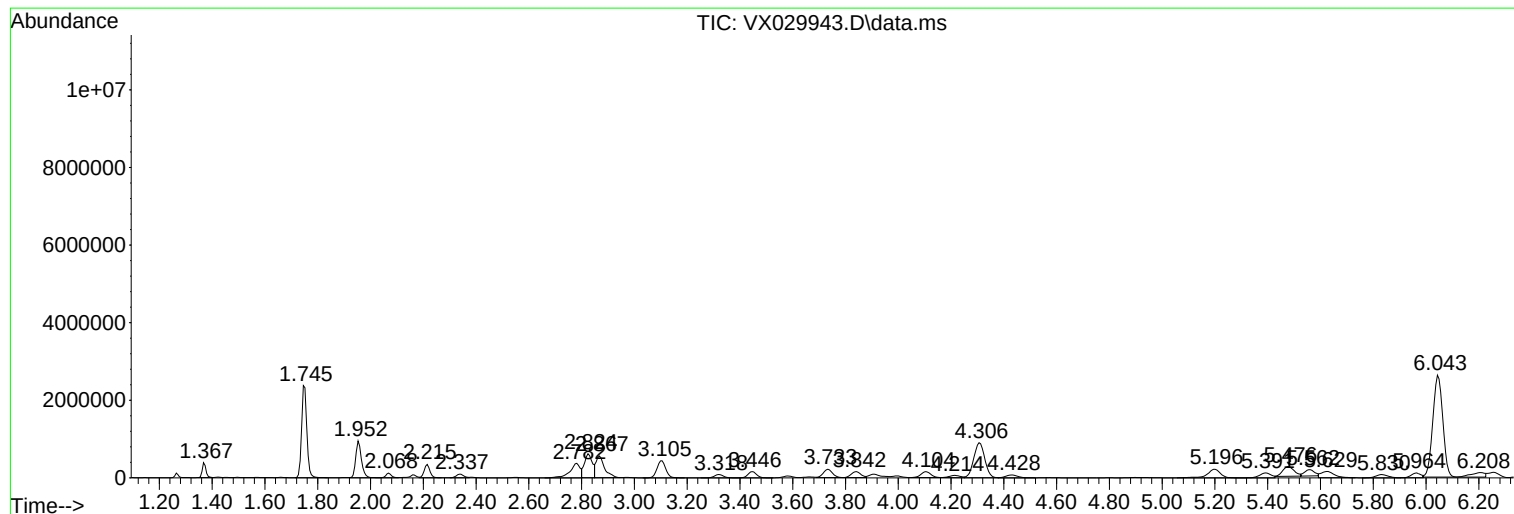
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ClientSampleId :
INF0722

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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



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Sample : N3599-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0722

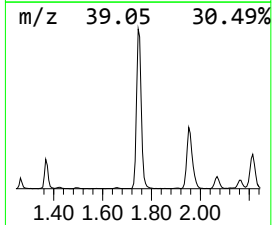
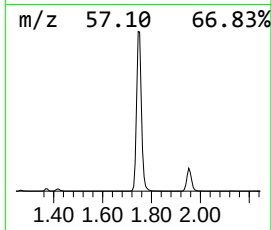
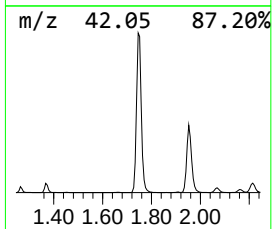
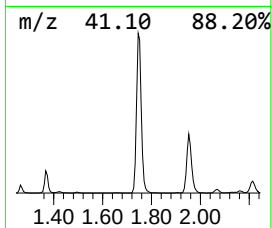
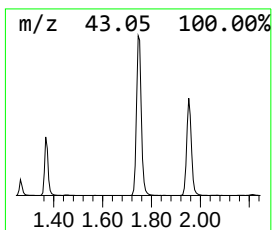
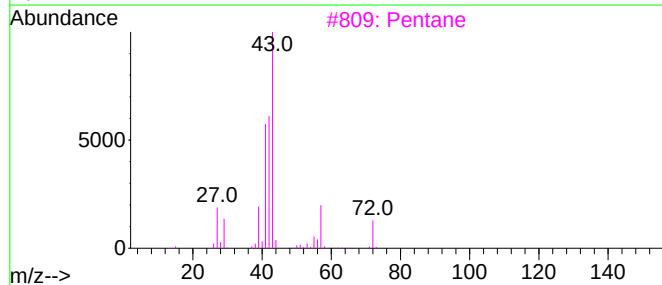
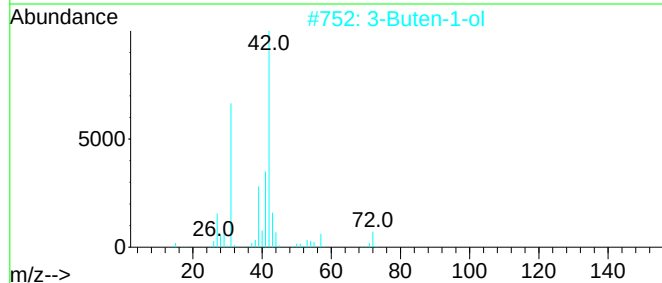
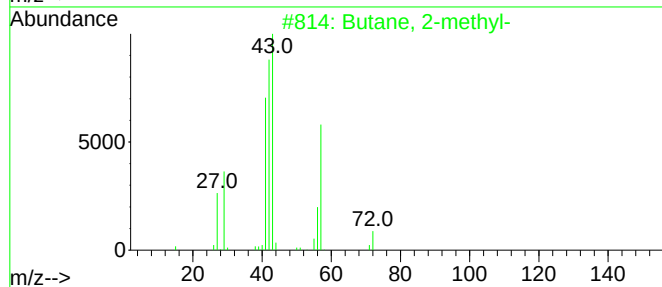
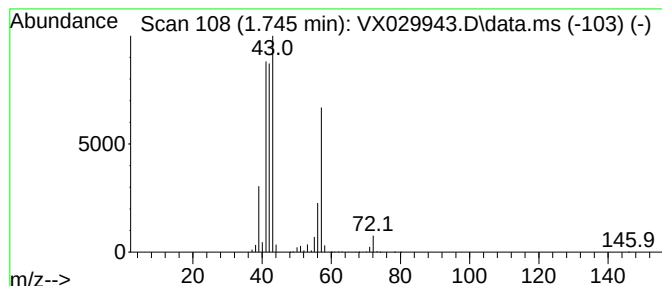
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.745	376.94 ug/l	3247690	Pentafluorobenzene	5.555

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



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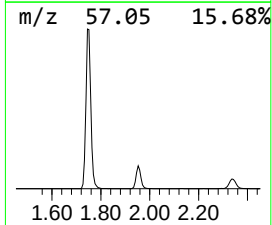
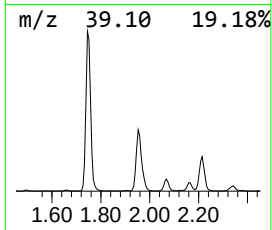
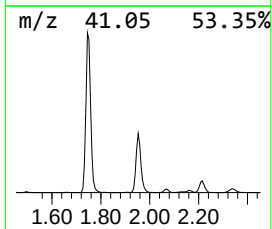
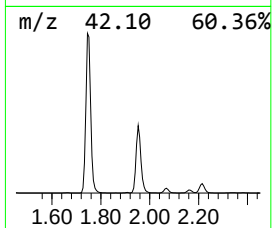
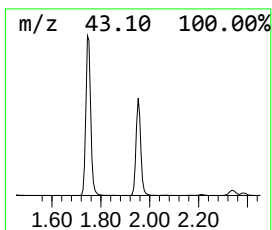
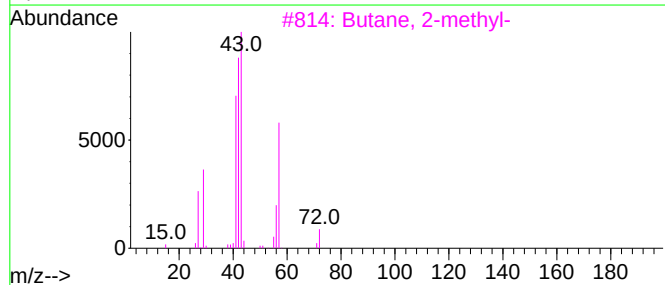
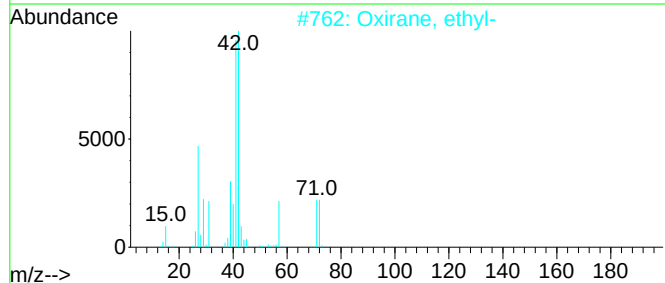
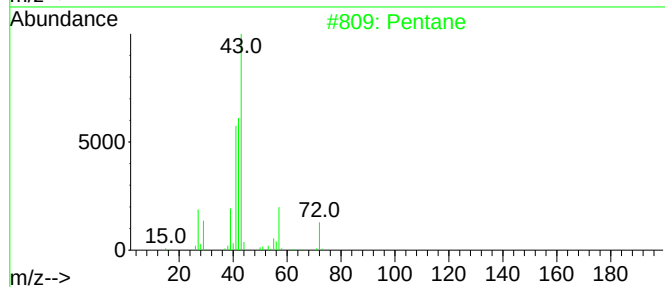
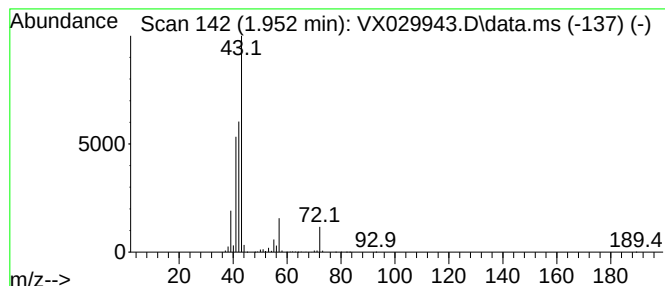
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.952	161.09 ug/l	1387910	Pentafluorobenzene	5.555

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	50
3			Butane, 2-methyl-	72	C5H12	000078-78-4	50
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5			Butanenitrile, 2-hydroxy-3-methyl-	99	C5H9NO	010021-64-4	9



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ALS Vial : 13 Sample Multiplier: 1

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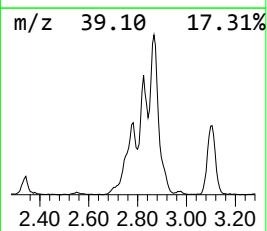
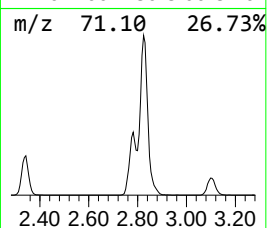
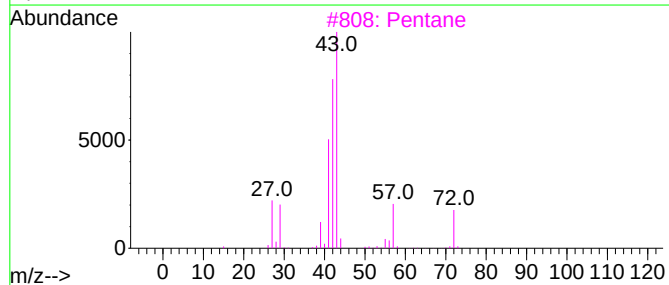
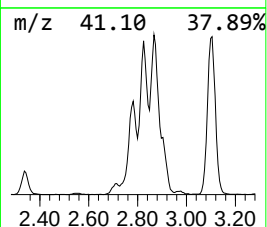
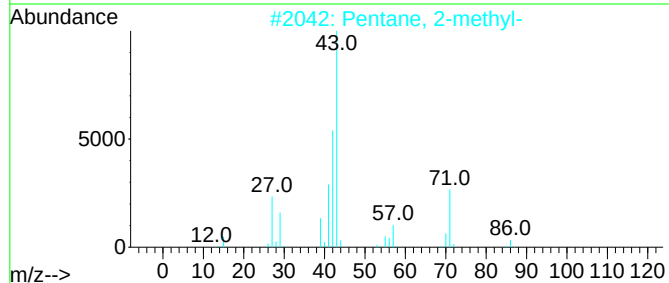
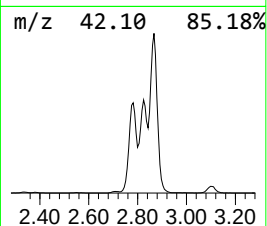
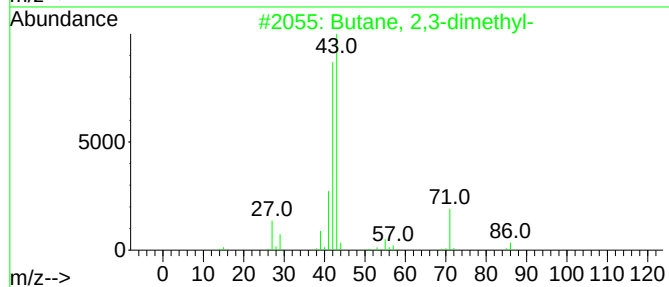
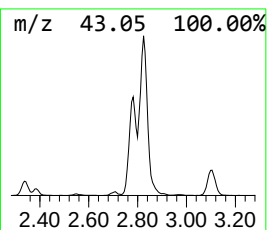
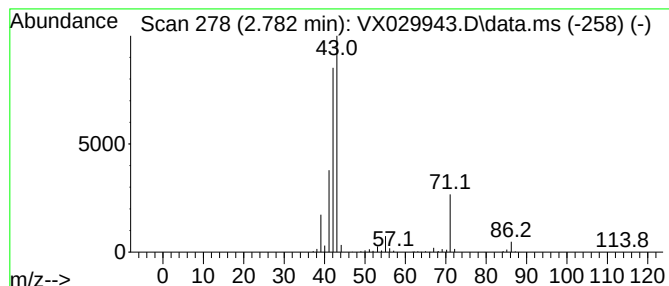
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	118.80 ug/l	1023540	Pentafluorobenzene	5.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3			Pentane	72	C5H12	000109-66-0	36
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	28
5			C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	12



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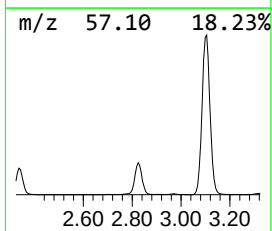
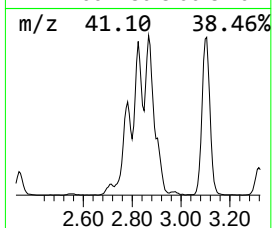
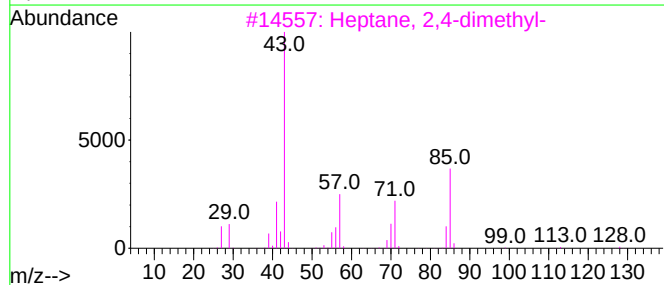
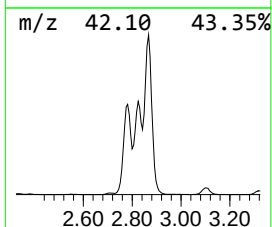
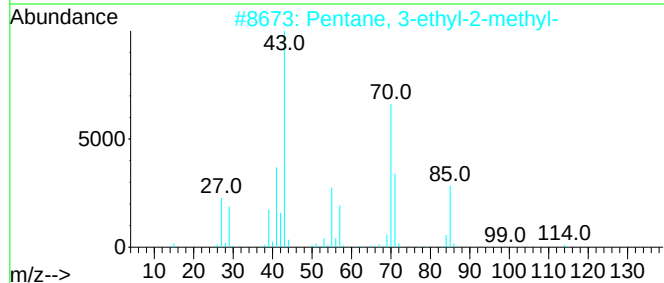
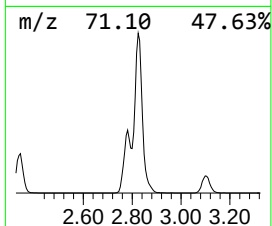
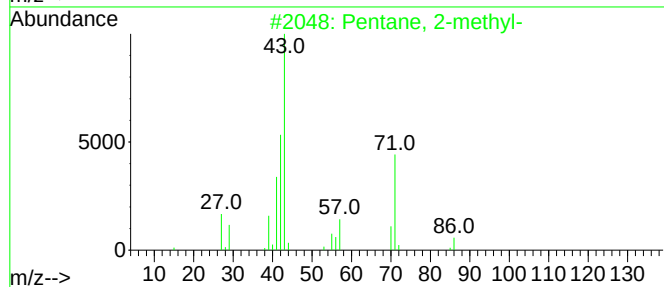
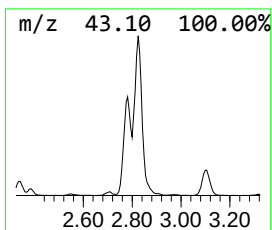
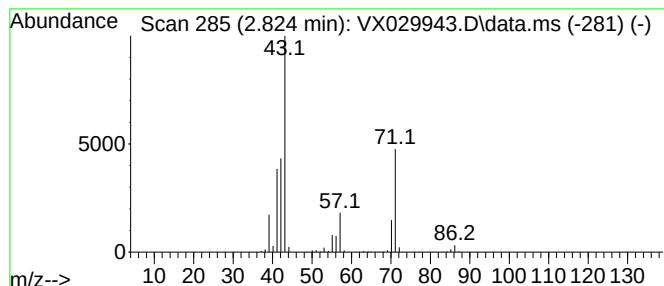
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.824	150.27 ug/l	1294740	Pentafluorobenzene	5.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	33
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	32
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	28
5			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	23



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Data File : VX029943.D
Acq On : 06 Jul 2022 14:54
Operator : JC/MD
Sample : N3599-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0722

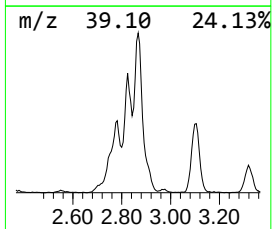
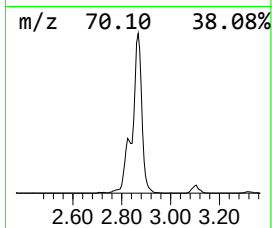
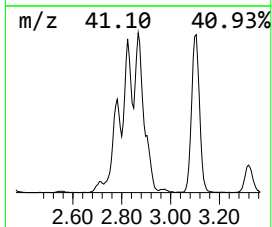
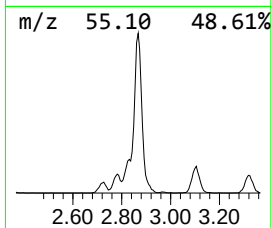
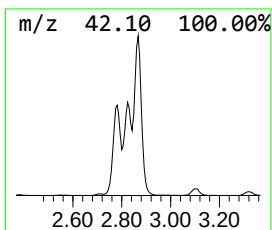
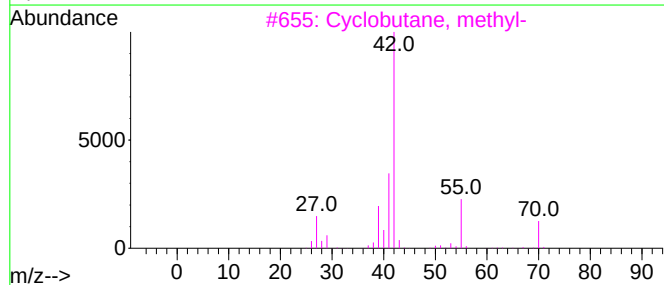
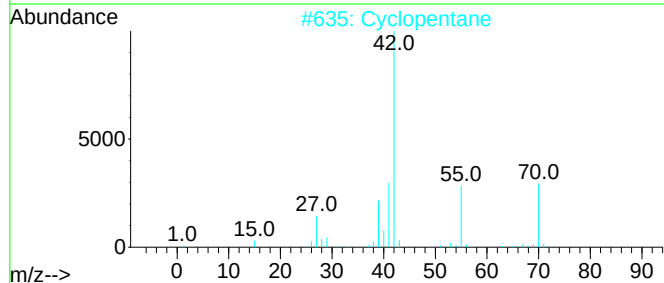
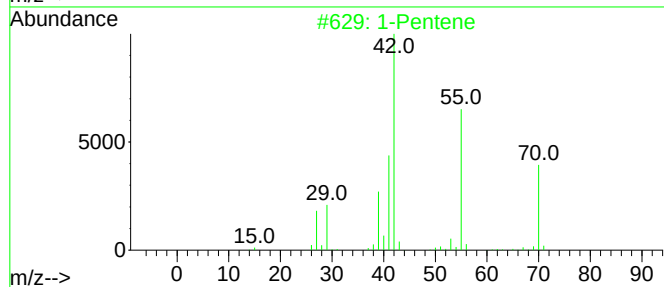
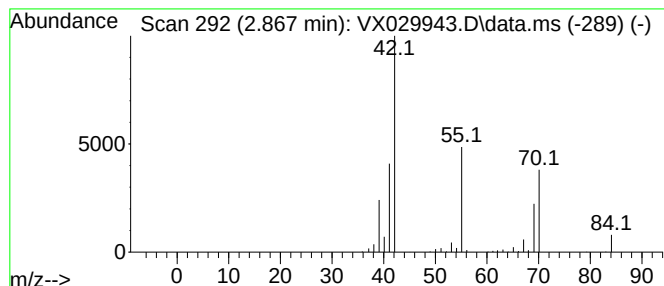
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Quant Title : SW846 8260

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

Peak Number 5 1-Pentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	140.85 ug/l	1213530	Pentafluorobenzene	5.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene	70	C5H10	000109-67-1	86
2			Cyclopentane	70	C5H10	000287-92-3	78
3			Cyclobutane, methyl-	70	C5H10	000598-61-8	72
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	45
5			1-Pentanol	88	C5H12O	000071-41-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070622\
Data File : VX029943.D
Acq On : 06 Jul 2022 14:54
Operator : JC/MD
Sample : N3599-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0722

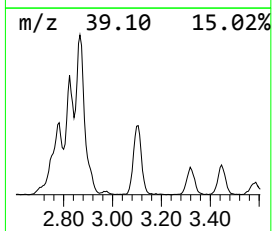
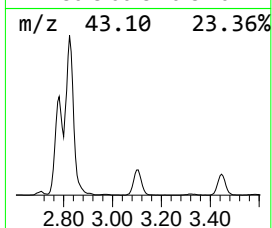
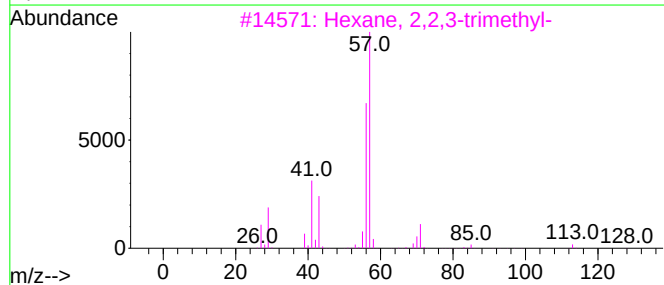
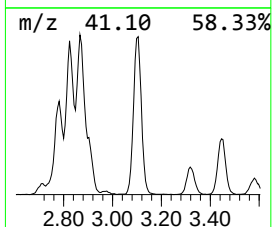
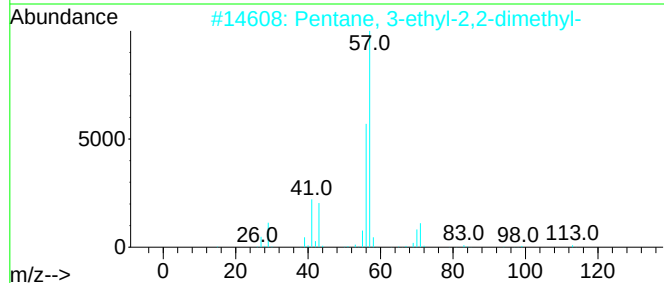
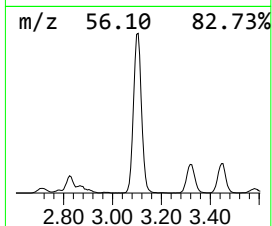
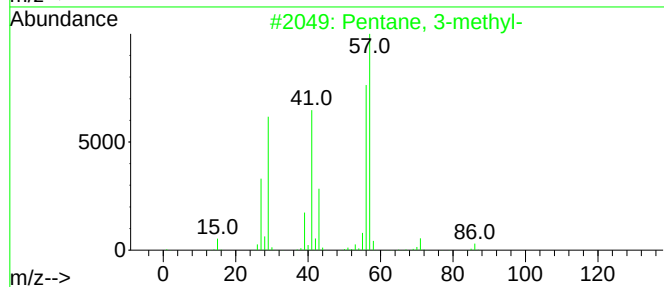
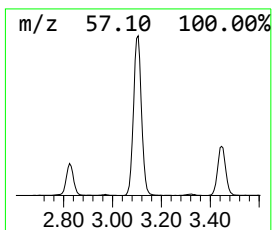
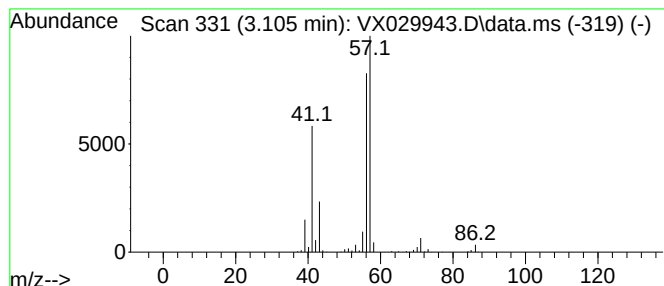
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	116.45 ug/l	1003350	Pentafluorobenzene	5.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	78
3			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
4			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	56
5			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070622\
Data File : VX029943.D
Acq On : 06 Jul 2022 14:54
Operator : JC/MD
Sample : N3599-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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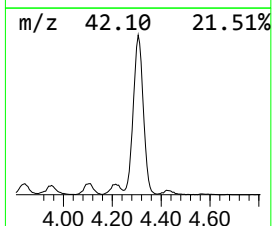
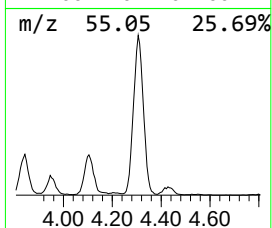
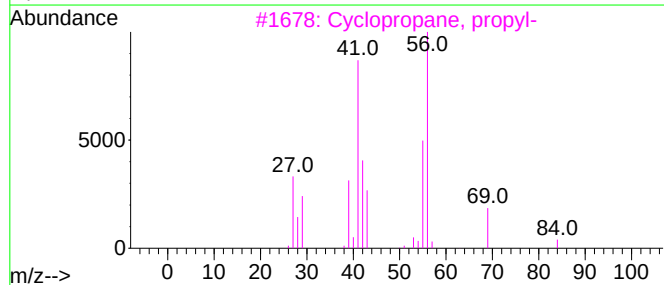
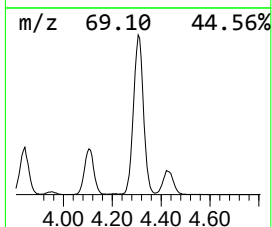
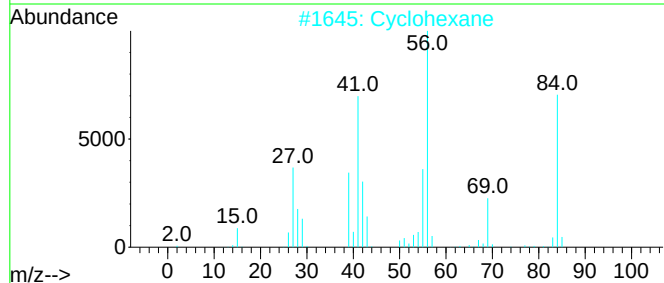
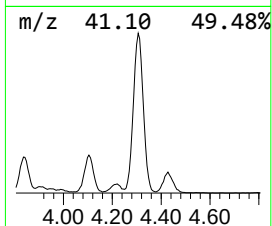
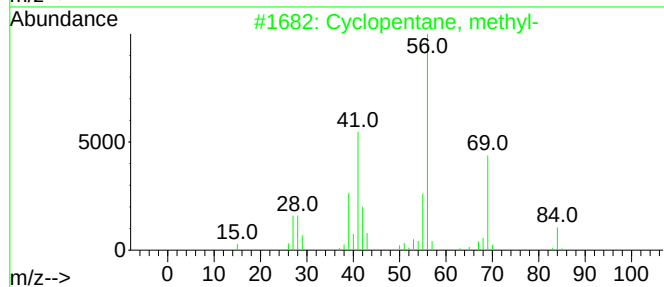
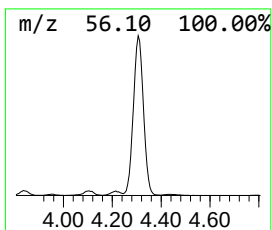
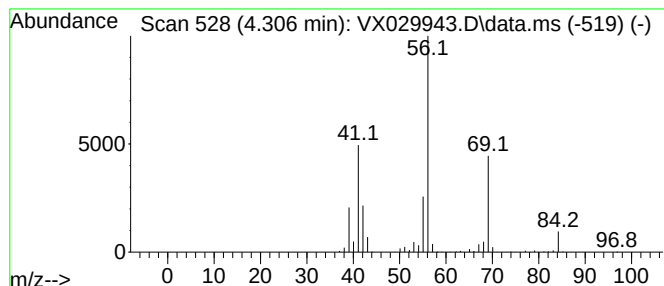
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	299.09 ug/l	2576970	Pentafluorobenzene	5.555

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			Cyclopropane, propyl-	84	C6H12	002415-72-7	72
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070622\
Data File : VX029943.D
Acq On : 06 Jul 2022 14:54
Operator : JC/MD
Sample : N3599-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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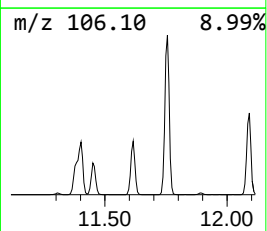
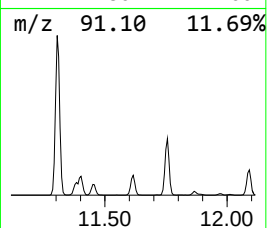
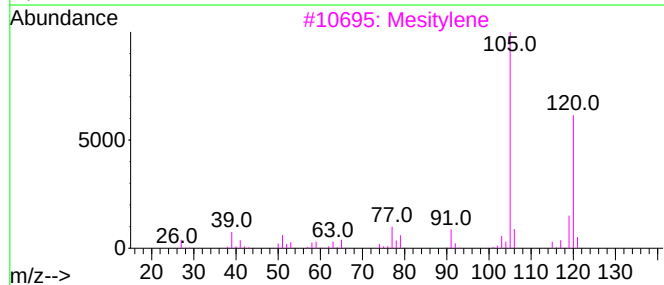
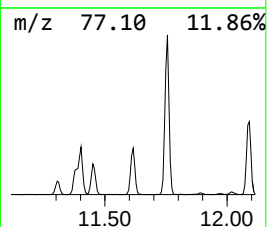
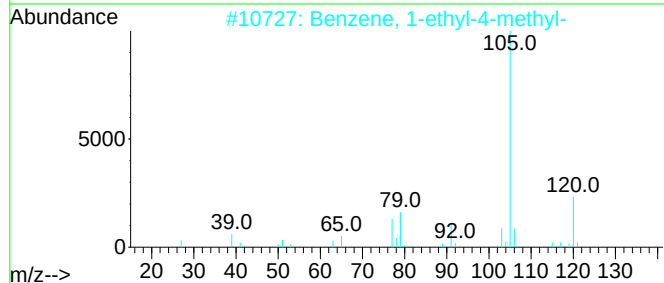
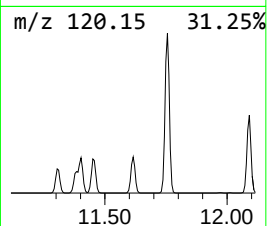
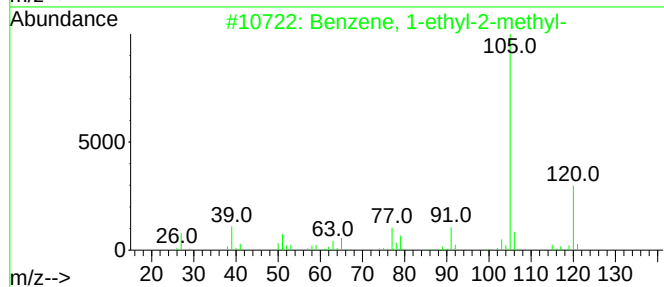
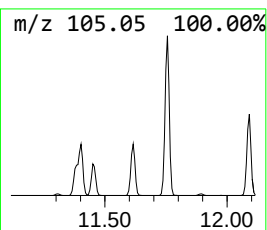
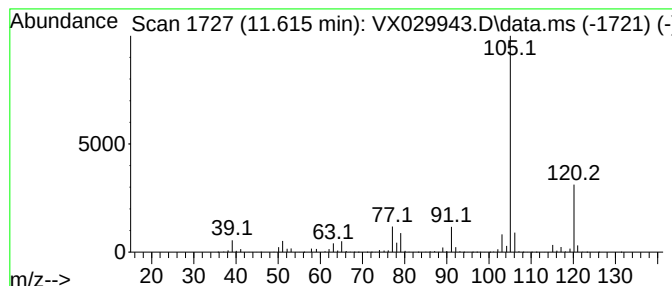
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.615	118.33 ug/l	2230050	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	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070622\
Data File : VX029943.D
Acq On : 06 Jul 2022 14:54
Operator : JC/MD
Sample : N3599-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0722

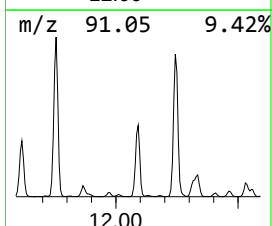
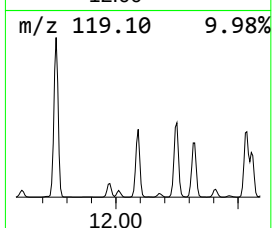
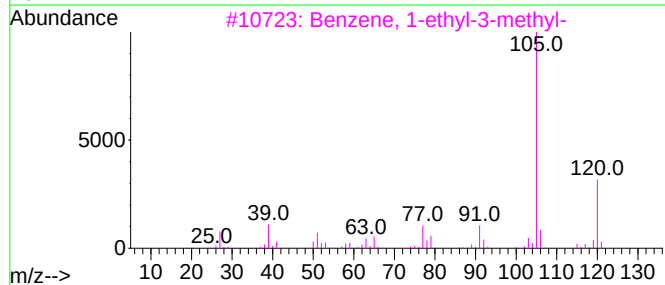
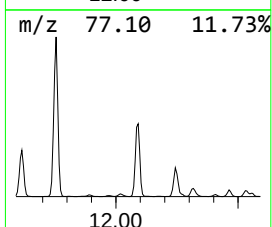
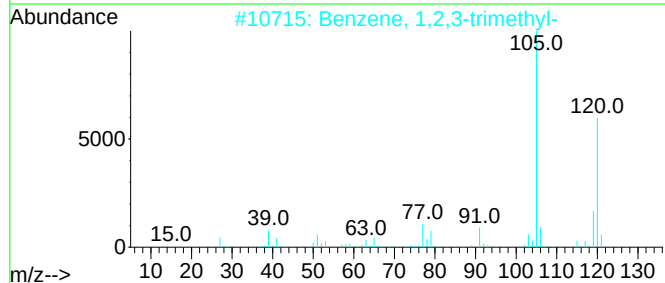
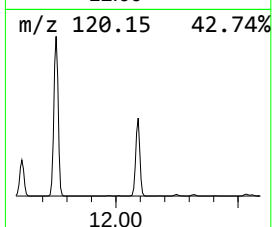
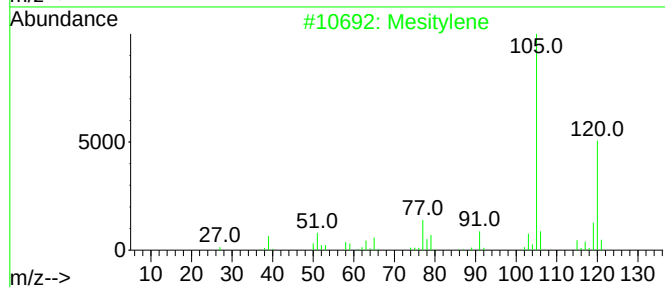
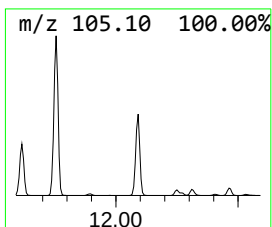
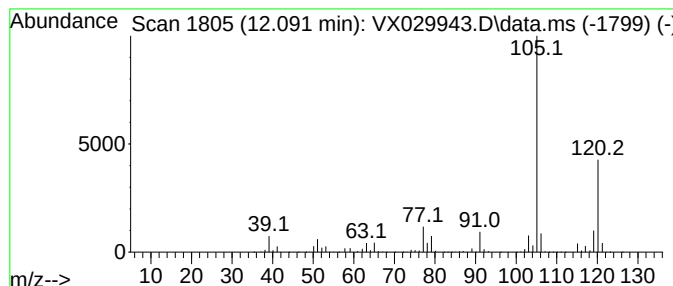
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Quant Title : SW846 8260

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	200.36 ug/l	3776000	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	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070622\
Data File : VX029943.D
Acq On : 06 Jul 2022 14:54
Operator : JC/MD
Sample : N3599-01
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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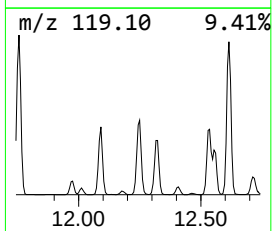
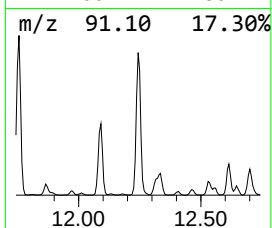
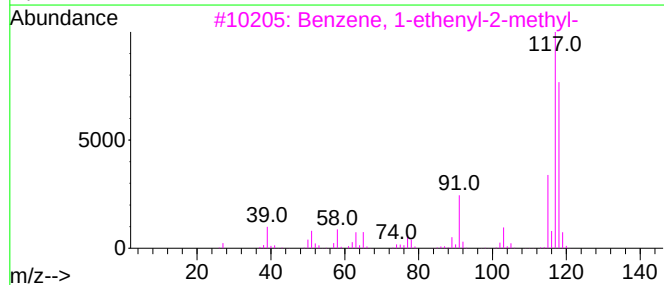
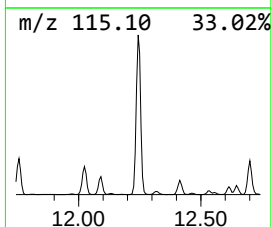
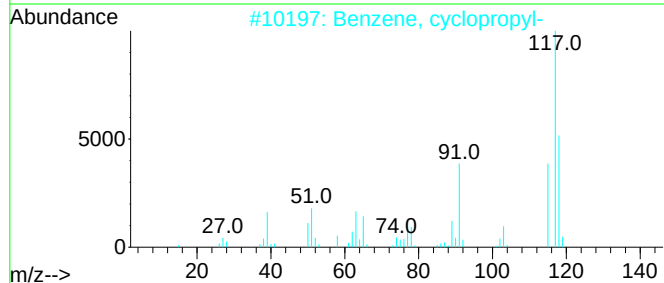
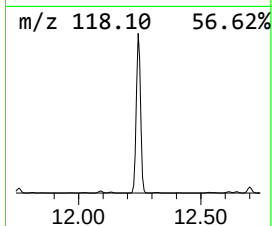
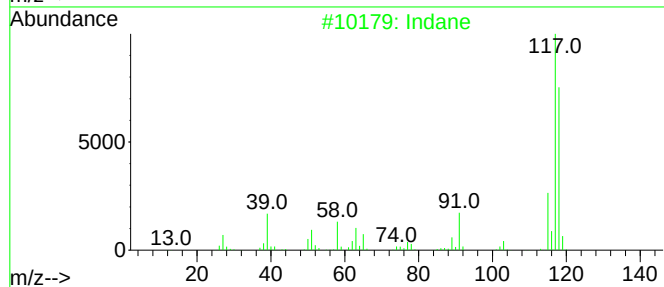
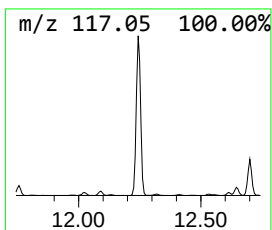
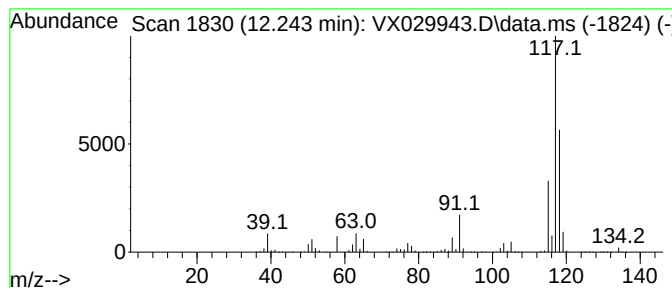
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	277.36 ug/l	5227110	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, cyclopropyl-	118	C9H10	000873-49-4	81
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5			Deltacyclene	118	C9H10	007785-10-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070622\
Data File : VX029943.D
Acq On : 06 Jul 2022 14:54
Operator : JC/MD
Sample : N3599-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0722

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.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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Pentane	1.952	161.1	ug/l	1387910	1	5.555	430800	50.0
Butane, 2,3-dim...	2.782	118.8	ug/l	1023540	1	5.555	430800	50.0
Pentane, 2-methyl-	2.824	150.3	ug/l	1294740	1	5.555	430800	50.0
1-Pentene	2.867	140.8	ug/l	1213530	1	5.555	430800	50.0
Pentane, 3-methyl-	3.105	116.5	ug/l	1003350	1	5.555	430800	50.0
Cyclopentane, m...	4.306	299.1	ug/l	2576970	1	5.555	430800	50.0
Benzene, 1-ethy...	11.615	118.3	ug/l	2230050	4	12.024	942304	50.0
Benzene, 1,2,3-...	12.091	200.4	ug/l	3776000	4	12.024	942304	50.0
Indane	12.243	277.4	ug/l	5227110	4	12.024	942304	50.0