

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
 Data File : VX029236.D
 Acq On : 06 Jun 2022 14:00
 Operator : JC/MD
 Sample : N3174-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 INF0622

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\82X053122W.M
 Title : SW846 8260

Signal : TIC: VX029236.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	417129	412875	1.50%	0.286%
2	1.751	103	109	123	rBV	2478344	3395092	12.31%	2.350%
3	1.953	137	142	154	rVB2	997892	1512634	5.48%	1.047%
4	2.215	180	185	196	rVB	548901	820627	2.97%	0.568%
5	2.782	256	278	281	rBV2	432518	1241733	4.50%	0.860%
6	2.824	281	285	289	rVV	706941	1488042	5.39%	1.030%
7	2.867	289	292	305	rVB2	643020	1419626	5.15%	0.983%
8	3.105	320	331	346	rVB	537146	1212180	4.39%	0.839%
9	3.446	377	387	400	rVV	189953	420111	1.52%	0.291%
10	3.733	427	434	443	rVB	296156	703134	2.55%	0.487%
11	3.843	443	452	457	rBV	201724	515435	1.87%	0.357%
12	4.105	485	495	505	rBV	206003	532591	1.93%	0.369%
13	4.306	519	528	539	rVB	1087672	3067209	11.12%	2.123%
14	4.428	539	548	562	rVB	124258	370670	1.34%	0.257%
15	5.196	646	674	691	rBV	279502	941886	3.41%	0.652%
16	5.391	691	706	712	rBV2	235508	704593	2.55%	0.488%
17	5.476	712	720	727	rVV2	308348	903937	3.28%	0.626%
18	5.556	727	733	739	rVV	290152	787154	2.85%	0.545%
19	5.623	740	744	765	rVB3	203421	640807	2.32%	0.444%
20	5.830	765	778	790	rBV4	95860	311873	1.13%	0.216%
21	5.958	790	799	804	rBV	218584	564752	2.05%	0.391%
22	6.043	804	813	825	rVB	3622102	9486108	34.39%	6.567%
23	6.202	825	839	844	rBV3	168071	645676	2.34%	0.447%
24	6.360	857	865	877	rVB2	102669	305414	1.11%	0.211%
25	6.763	922	931	940	rBV	574052	1529136	5.54%	1.059%
26	6.854	942	946	958	rVB4	159585	394162	1.43%	0.273%
27	7.177	990	999	1009	rVB	152633	338478	1.23%	0.234%
28	7.378	1017	1032	1045	rBV4	309940	872394	3.16%	0.604%
29	8.147	1153	1158	1163	rVB	364668	641567	2.33%	0.444%
30	8.506	1210	1217	1226	rVB	329545	552037	2.00%	0.382%
31	8.653	1235	1241	1247	rVB	1176132	1807696	6.55%	1.251%
32	8.720	1247	1252	1259	rVB	2102646	3096052	11.22%	2.143%
33	10.055	1461	1471	1476	rBV	1287545	1775399	6.44%	1.229%
34	10.195	1489	1494	1500	rBV	8949685	11883678	43.08%	8.226%
35	10.305	1506	1512	1518	rBV	19134811	27587189	100.00%	19.097%
36	10.646	1562	1568	1578	rVB	3038146	4046995	14.67%	2.801%

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Integrator: RTE

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Peak Location: TOP

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37	10.963	1614	1620	1627	rVB	1095005	1324852	4.80%	0.917%
38	11.085	1635	1640	1646	rBV	1057867	1341789	4.86%	0.929%
39	11.305	1671	1676	1683	rVB	2058719	2464282	8.93%	1.706%
40	11.384	1683	1689	1690	rVV	1875750	2505761	9.08%	1.735%
41	11.402	1690	1692	1696	rVV	2749526	2851191	10.34%	1.974%
42	11.451	1696	1700	1706	rVB	2055323	2567050	9.31%	1.777%
43	11.616	1721	1727	1737	rBV	3062720	3721160	13.49%	2.576%
44	11.756	1744	1750	1755	rBV	9967553	11742663	42.57%	8.129%
45	12.024	1789	1794	1799	rVB	1472383	1811243	6.57%	1.254%
46	12.091	1799	1805	1810	rBV	4284163	5304164	19.23%	3.672%
47	12.243	1824	1830	1838	rBV	5287609	6772560	24.55%	4.688%
48	12.317	1838	1842	1852	rVB4	590131	901921	3.27%	0.624%
49	12.408	1852	1857	1862	rBV2	221342	300540	1.09%	0.208%
50	12.463	1862	1866	1872	rVB	340477	402268	1.46%	0.278%
51	12.530	1872	1877	1880	rBV	493838	670948	2.43%	0.464%
52	12.615	1886	1891	1894	rBV	1149181	1380986	5.01%	0.956%
53	12.646	1894	1896	1900	rVV	326880	354129	1.28%	0.245%
54	12.701	1900	1905	1913	rVB	1132476	1468025	5.32%	1.016%
55	12.847	1924	1929	1935	rVB	276139	355409	1.29%	0.246%
56	12.920	1935	1941	1945	rBV	808015	1014100	3.68%	0.702%
57	12.963	1945	1948	1954	rVB	732142	844859	3.06%	0.585%
58	13.170	1978	1982	1992	rVB	875242	1084479	3.93%	0.751%
59	13.292	1997	2002	2007	rVB2	1649228	2127524	7.71%	1.473%
60	13.426	2019	2024	2030	rVB	276417	348171	1.26%	0.241%
61	13.774	2075	2081	2091	rBV	2488580	3170258	11.49%	2.195%
62	14.639	2219	2223	2234	rVB	281394	360374	1.31%	0.249%
63	14.780	2241	2246	2257	rBV	265985	339839	1.23%	0.235%

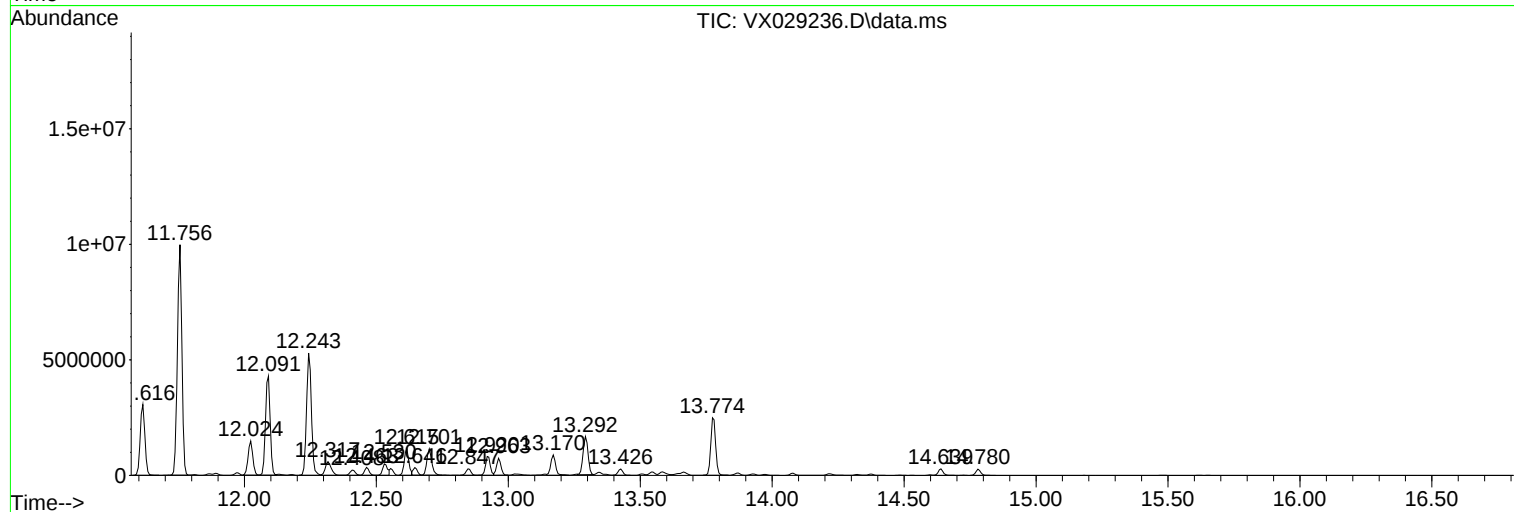
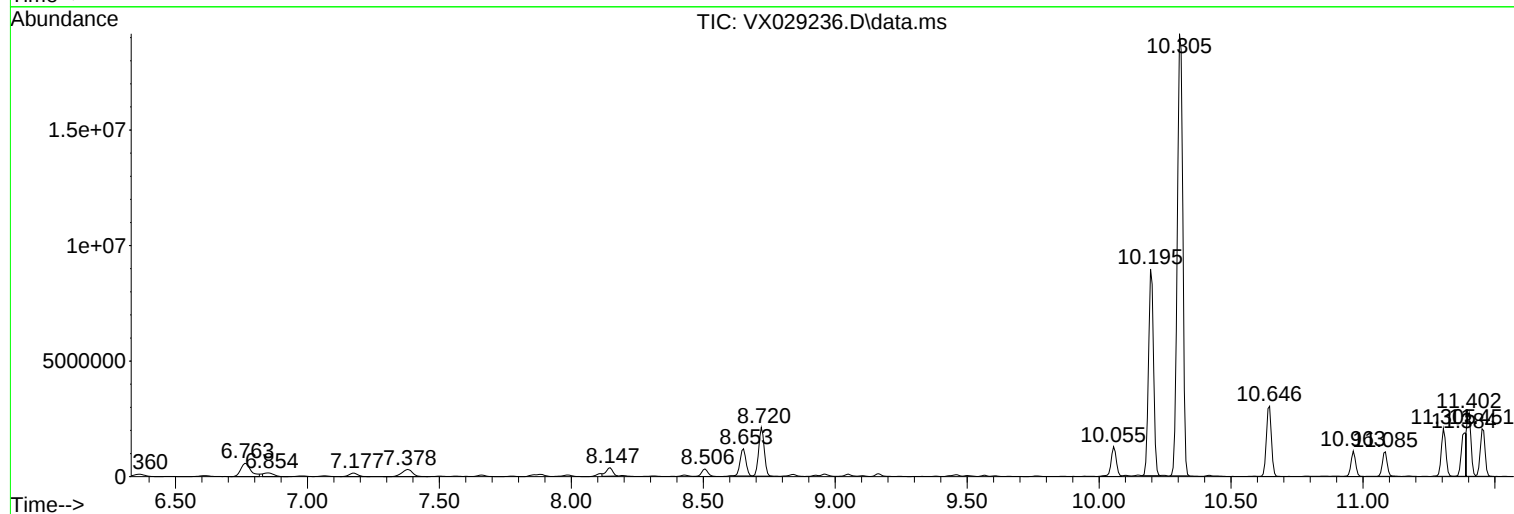
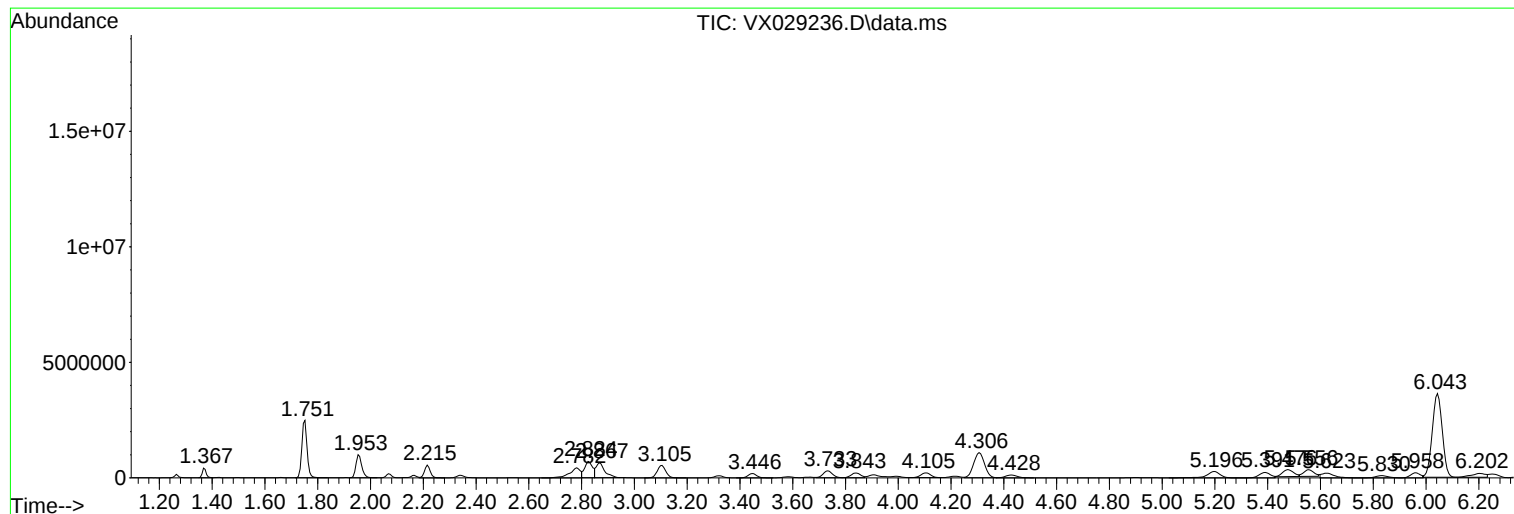
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0622

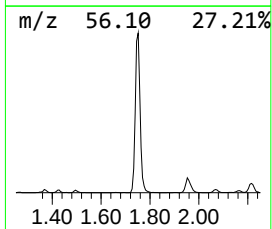
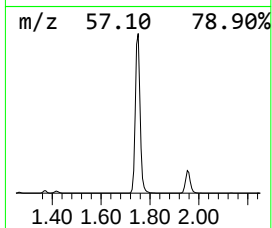
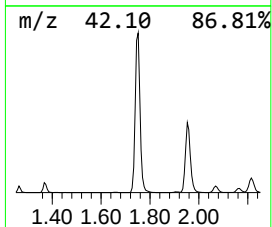
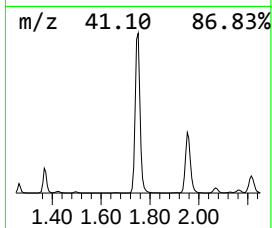
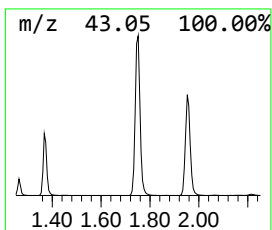
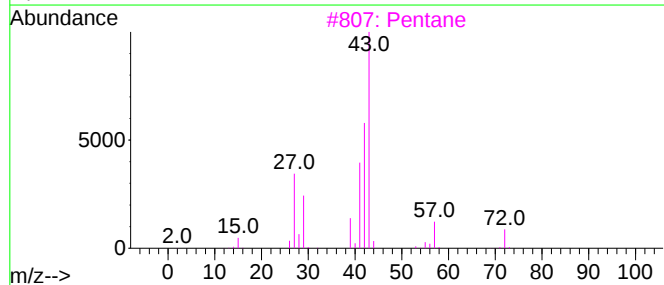
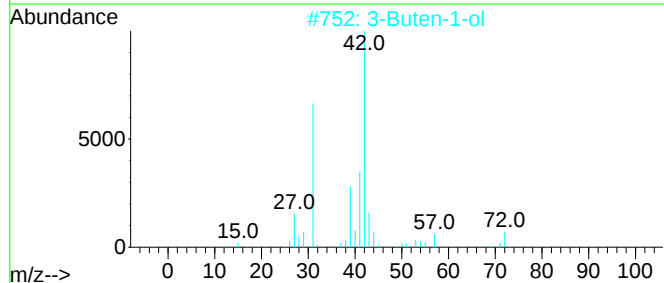
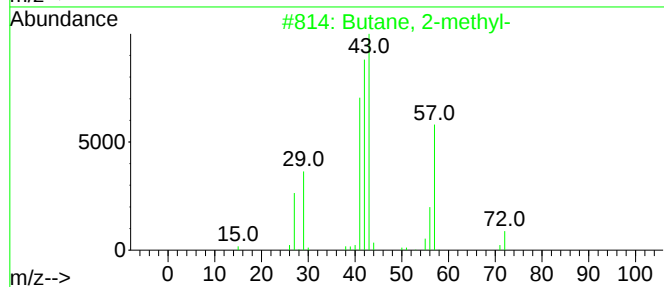
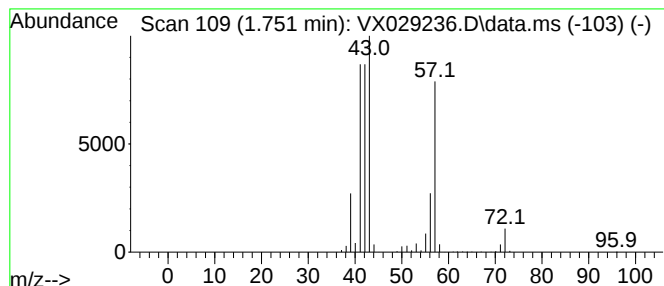
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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.
1.751	215.66 ug/l	3395090	Pentafluorobenzene	5.556

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	42
4			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33
5			Butane, 2-nitro-	103	C4H9NO2	000600-24-8	10



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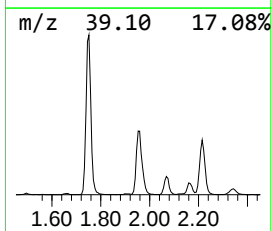
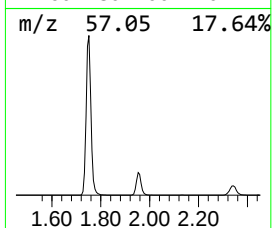
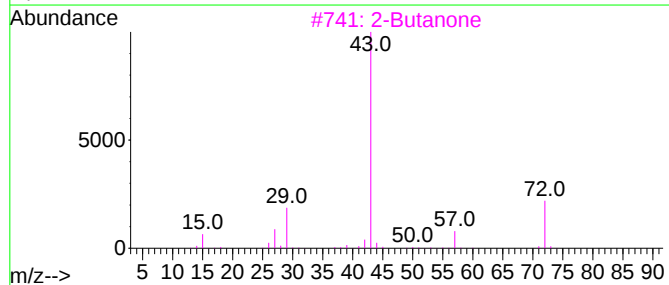
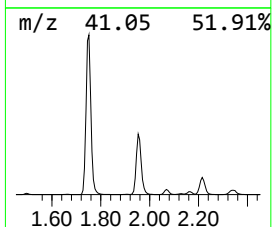
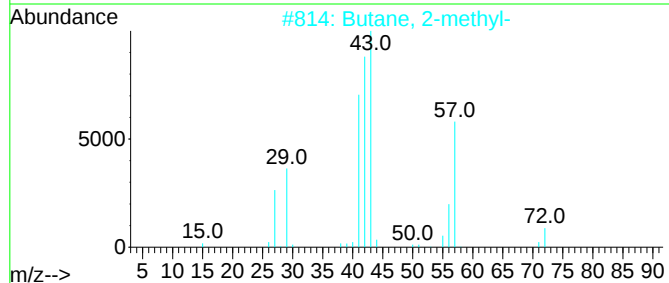
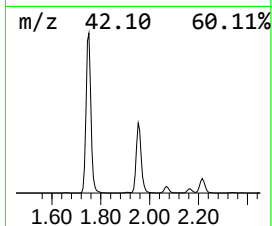
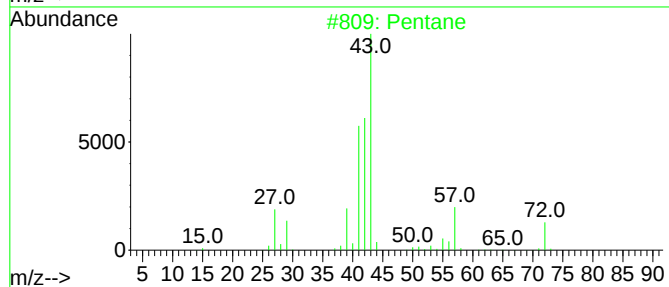
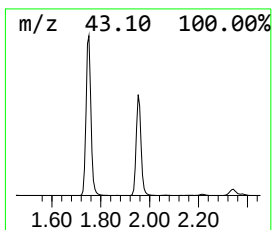
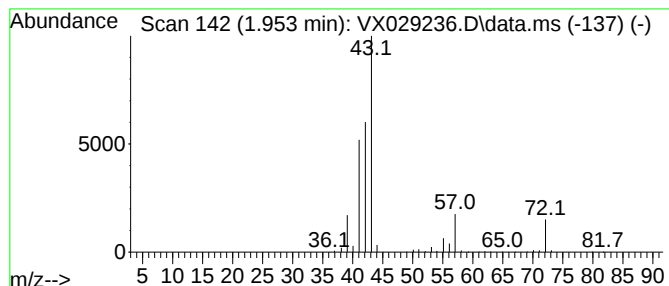
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	96.08 ug/l	1512630	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Butane, 2-methyl-	72	C5H12	000078-78-4	38
3			2-Butanone	72	C4H8O	000078-93-3	35
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	17
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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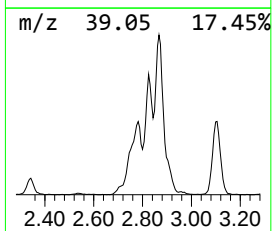
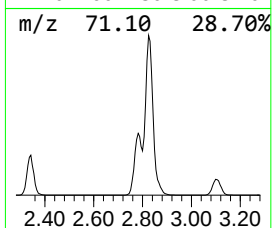
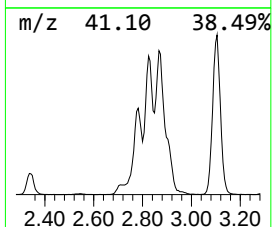
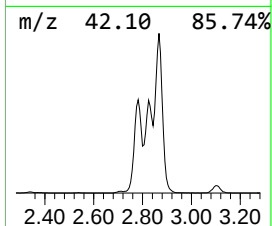
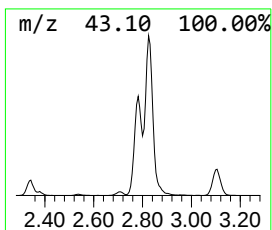
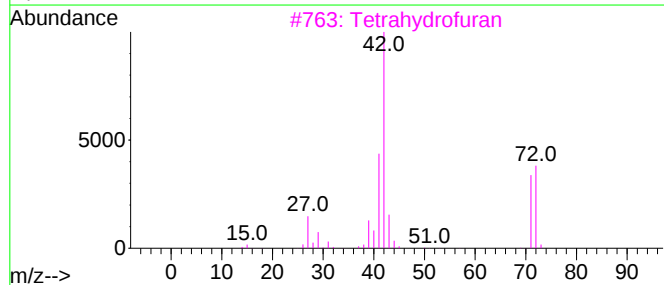
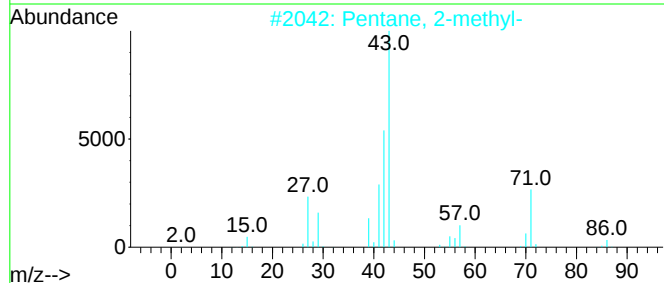
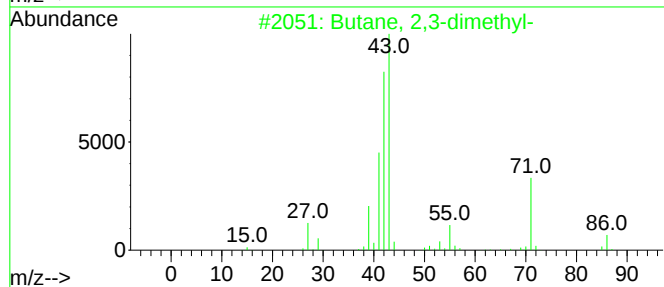
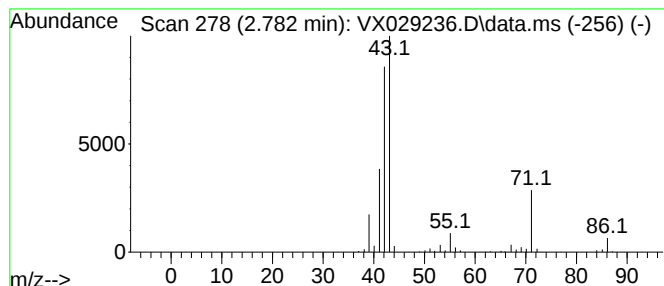
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	78.87 ug/l	1241730	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	64
3			Tetrahydrofuran	72	C4H8O	000109-99-9	36
4			Pyrrolidine	71	C4H9N	000123-75-1	12
5			Oxalic acid, pentyl propyl ester	202	C10H18O4	1000309-25-7	10



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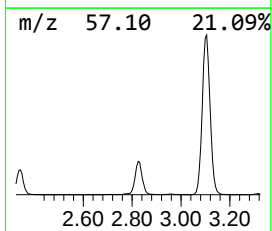
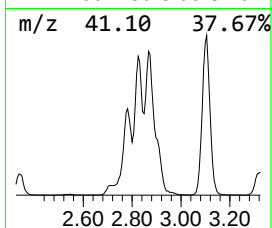
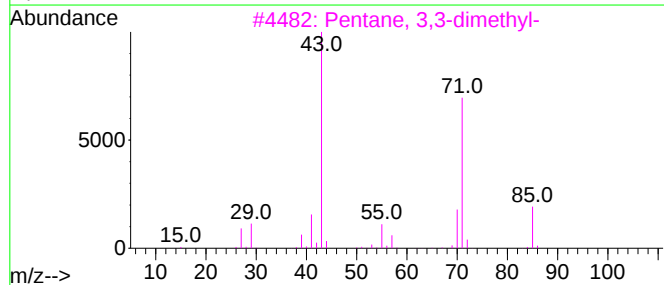
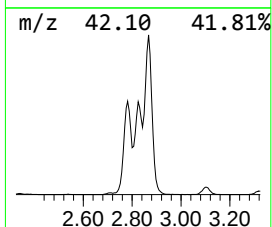
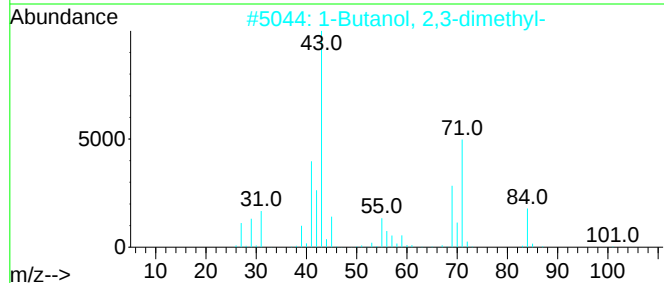
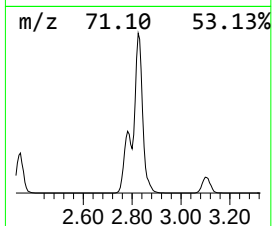
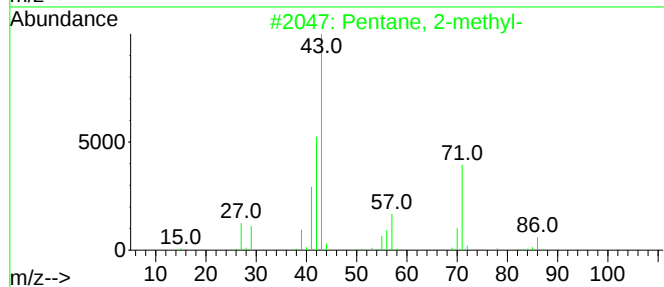
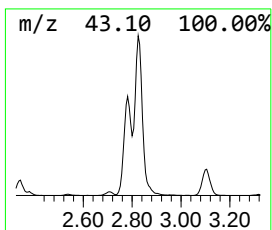
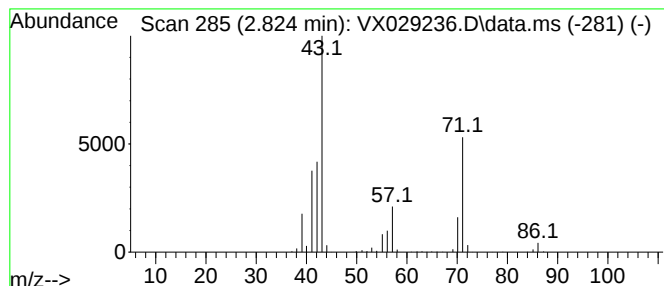
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.824	94.52 ug/l	1488040	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
3			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38
4			Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	36
5			Butane, 2-methyl-	72	C5H12	000078-78-4	35



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MSVOA_X
ClientSampleId :
INF0622

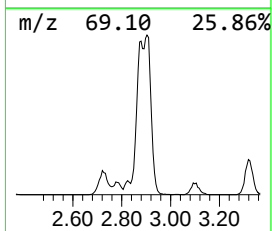
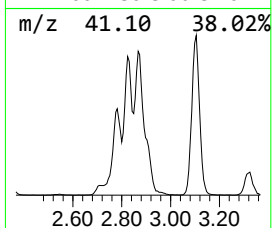
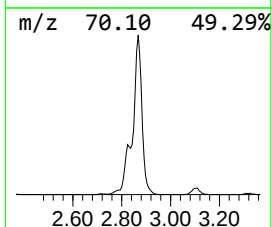
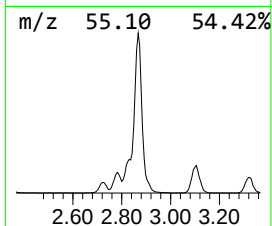
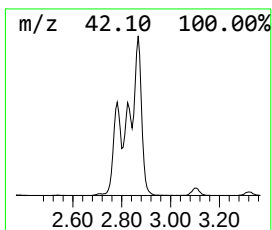
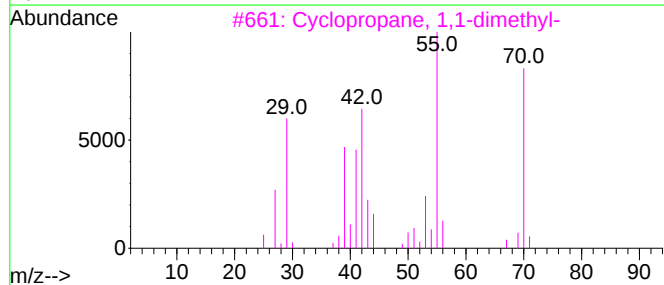
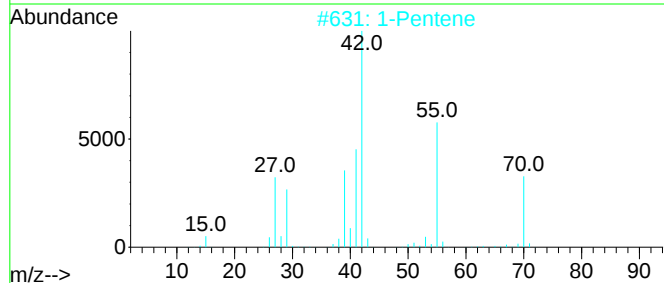
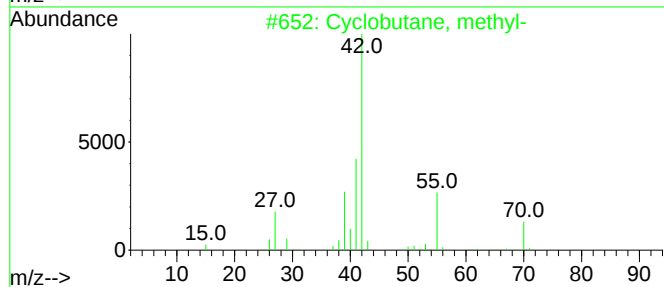
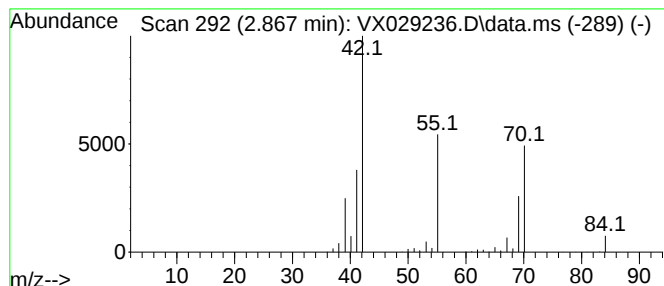
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Quant Title : SW846 8260

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

Peak Number 5 Cyclobutane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	90.17 ug/l	1419630	Pentafluorobenzene	5.556

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			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	23
4			2-Pentene, (E)-	70	C5H10	000646-04-8	12
5			Cyclopentane	70	C5H10	000287-92-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029236.D
Acq On : 06 Jun 2022 14:00
Operator : JC/MD
Sample : N3174-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0622

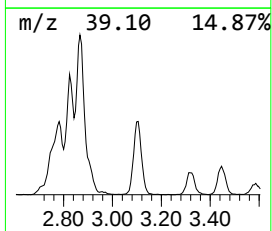
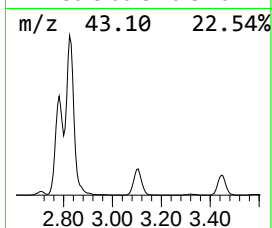
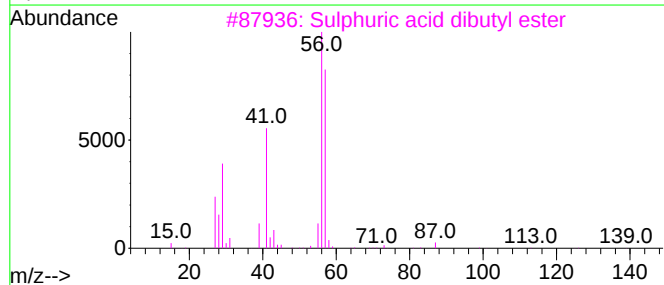
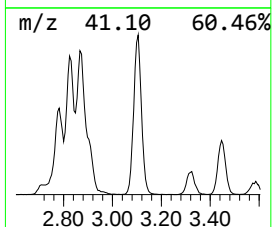
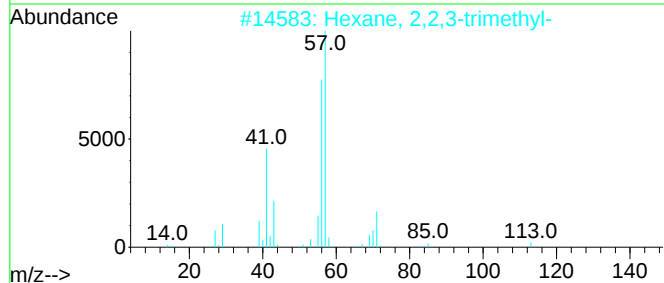
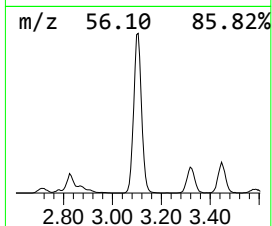
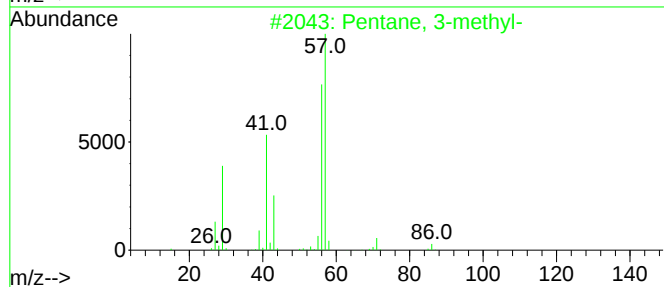
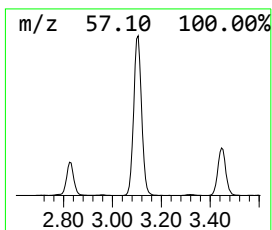
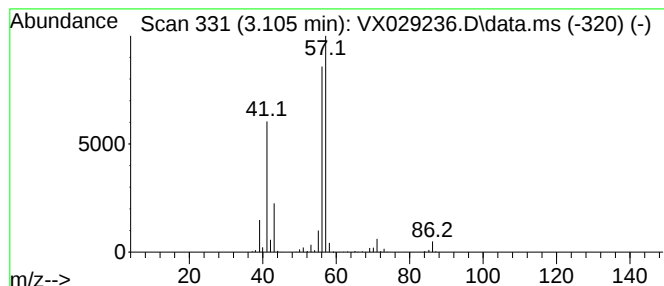
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Quant Title : SW846 8260

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	77.00 ug/l	1212180	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	64
4			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029236.D
Acq On : 06 Jun 2022 14:00
Operator : JC/MD
Sample : N3174-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0622

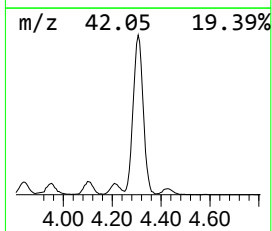
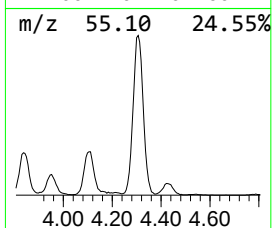
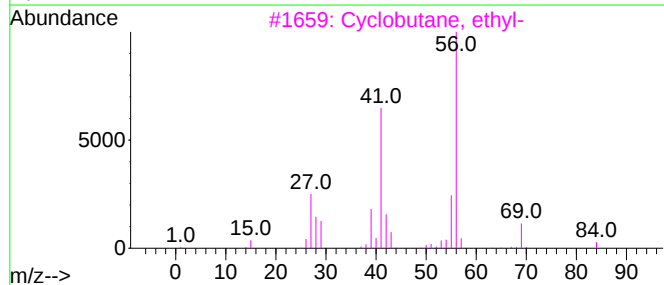
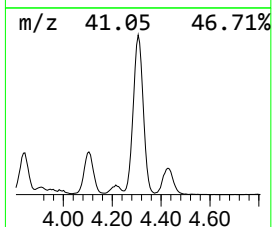
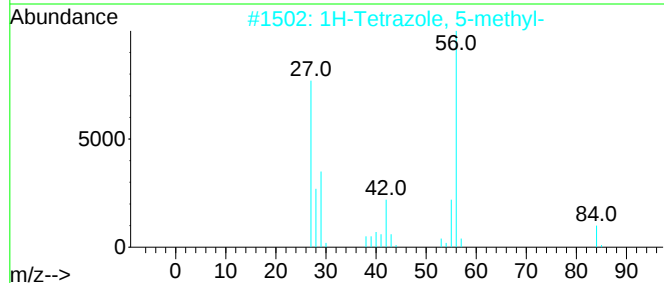
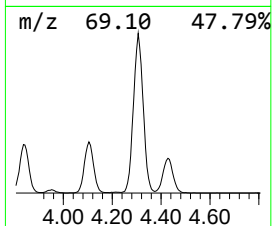
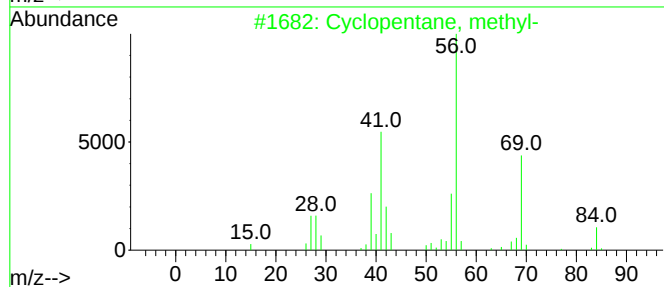
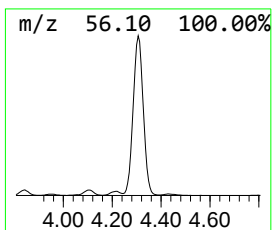
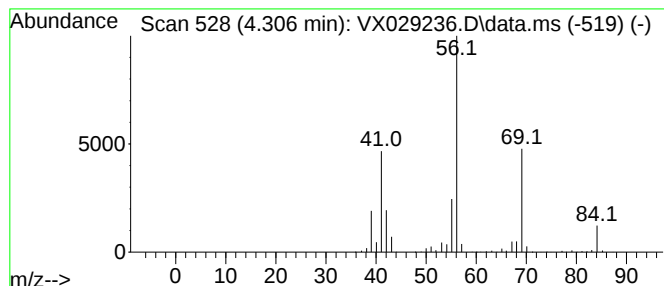
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Quant Title : SW846 8260

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	194.83 ug/l	3067210	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	49
5			Cyclohexane	84	C6H12	000110-82-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029236.D
Acq On : 06 Jun 2022 14:00
Operator : JC/MD
Sample : N3174-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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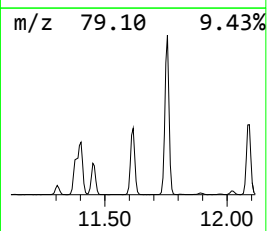
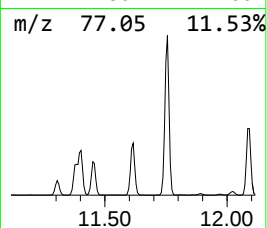
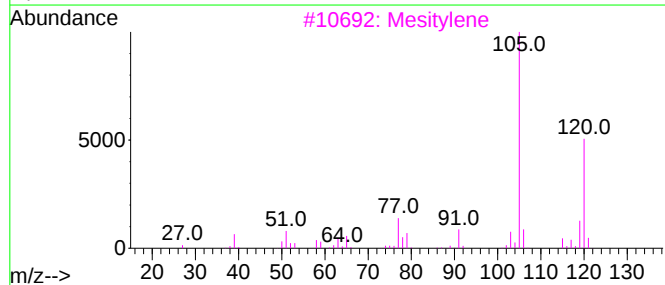
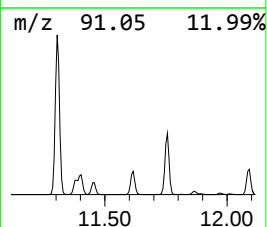
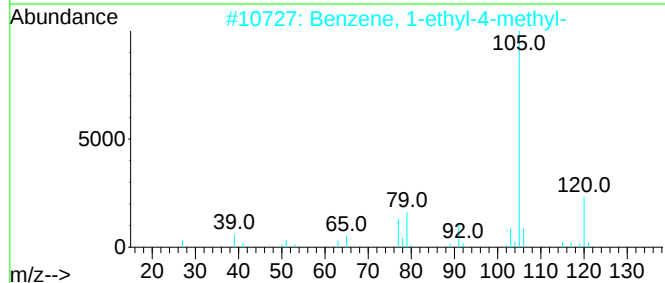
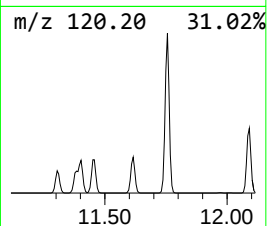
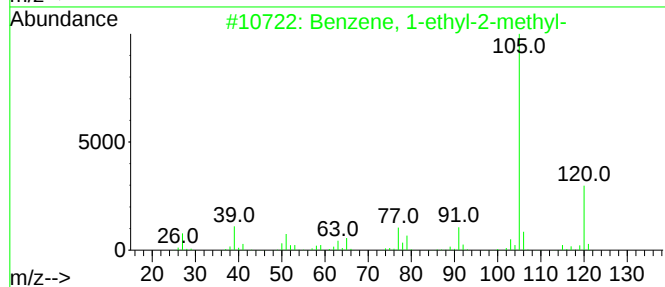
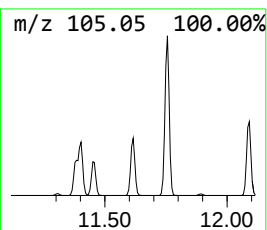
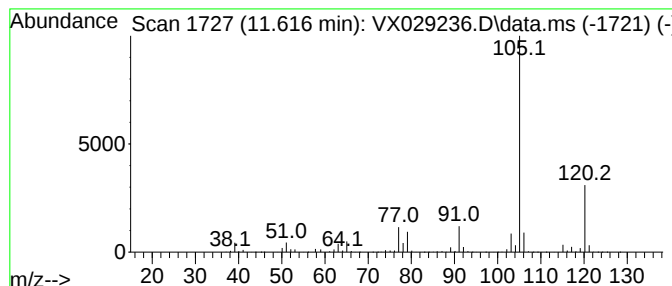
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Quant Title : SW846 8260

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	102.72 ug/l	3721160	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-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\VX060622\
Data File : VX029236.D
Acq On : 06 Jun 2022 14:00
Operator : JC/MD
Sample : N3174-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0622

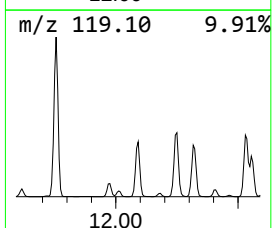
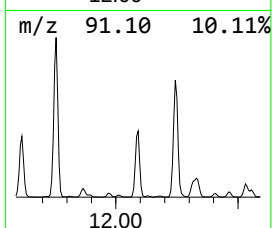
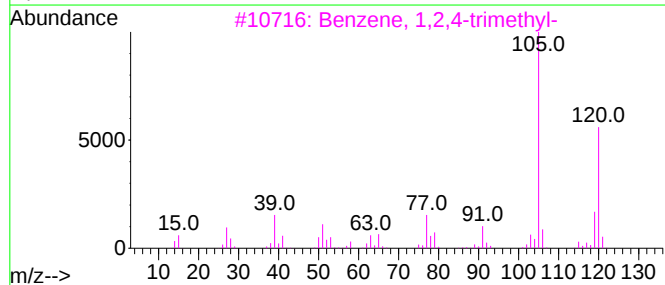
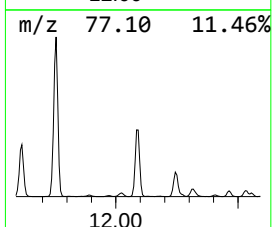
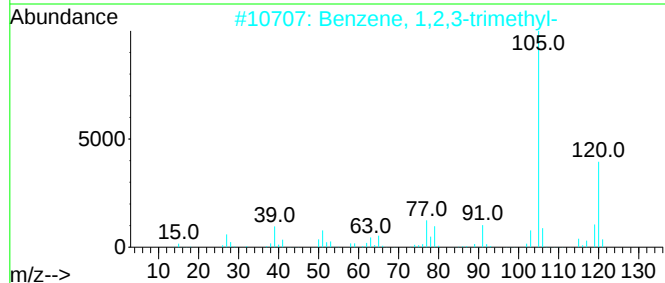
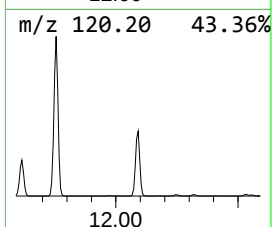
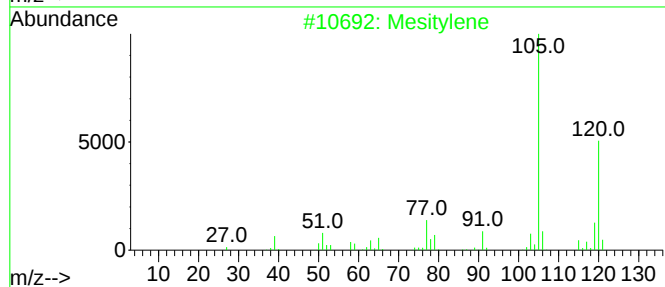
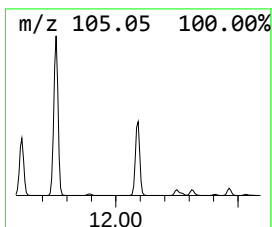
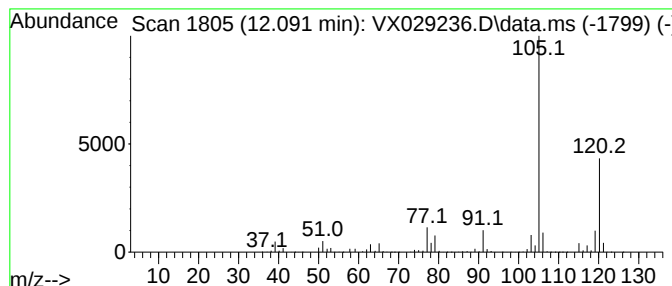
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Quant Title : SW846 8260

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	146.42 ug/l	5304160	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029236.D
Acq On : 06 Jun 2022 14:00
Operator : JC/MD
Sample : N3174-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0622

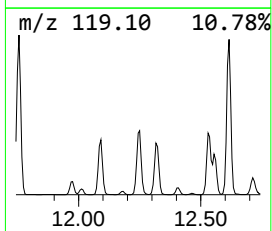
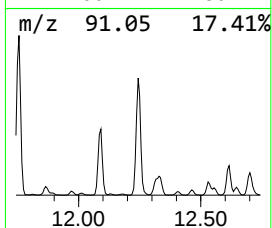
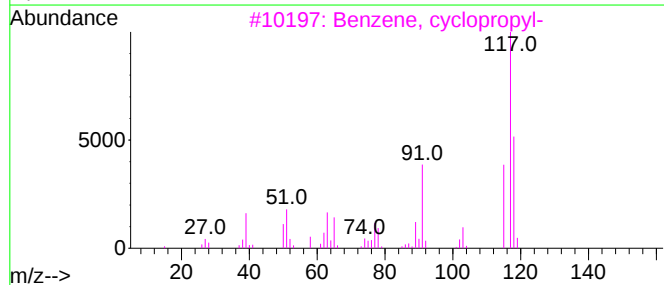
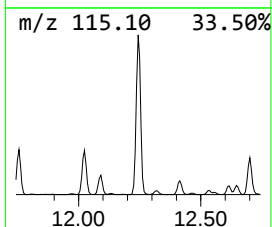
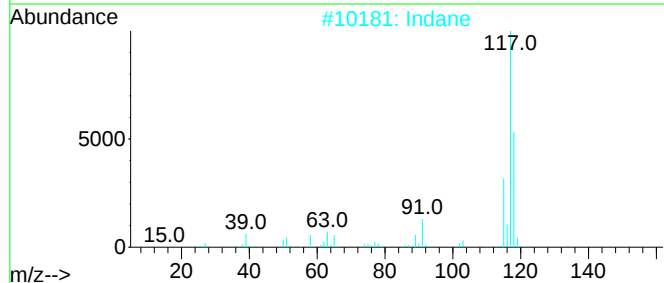
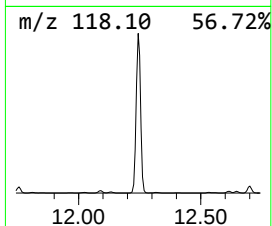
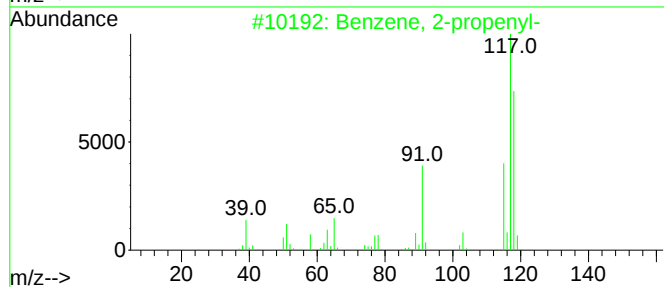
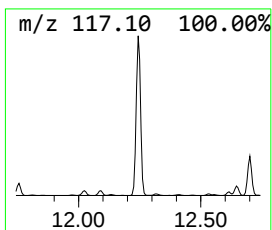
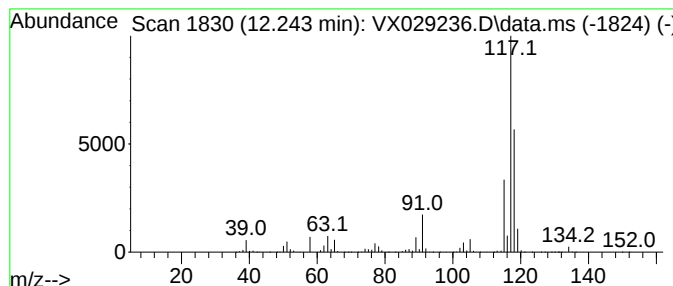
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-propenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	186.96 ug/l	6772560	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
2		Indane	118	C9H10	000496-11-7	81
3		Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4		Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5		Deltacyclene	118	C9H10	007785-10-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029236.D
Acq On : 06 Jun 2022 14:00
Operator : JC/MD
Sample : N3174-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF0622

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.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	1.953	96.1	ug/l	1512630	1	5.556	787154	50.0
Butane, 2,3-dim...	2.782	78.9	ug/l	1241730	1	5.556	787154	50.0
Pentane, 2-methyl-	2.824	94.5	ug/l	1488040	1	5.556	787154	50.0
Cyclobutane, me...	2.867	90.2	ug/l	1419630	1	5.556	787154	50.0
Pentane, 3-methyl-	3.105	77.0	ug/l	1212180	1	5.556	787154	50.0
Cyclopentane, m...	4.306	194.8	ug/l	3067210	1	5.556	787154	50.0
Benzene, 1-ethy...	11.616	102.7	ug/l	3721160	4	12.024	1811240	50.0
Benzene, 1,2,3-...	12.091	146.4	ug/l	5304160	4	12.024	1811240	50.0
Benzene, 2-prop...	12.243	187.0	ug/l	6772560	4	12.024	1811240	50.0