

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
 Data File : VX027959.D
 Acq On : 04 Apr 2022 15:48
 Operator : JC/MD
 Sample : N2249-08 40X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-101R

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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\82X032922W.M
 Title : SW846 8260

Signal : TIC: VX027959.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	20	25	27	rBV	15754	19647	1.61%	0.282%
2	1.264	27	29	37	rVB	35821	35670	2.93%	0.513%
3	1.368	43	46	53	rVB	124900	129302	10.63%	1.858%
4	1.746	103	108	120	rBV	192569	268434	22.06%	3.858%
5	1.904	130	134	138	rBV	9913	13444	1.11%	0.193%
6	1.953	138	142	153	rVV3	61800	117956	9.70%	1.695%
7	2.069	156	161	170	rBV	61889	85844	7.06%	1.234%
8	2.166	170	177	181	rVV	29857	46892	3.85%	0.674%
9	2.215	181	185	196	rVB	76943	121123	9.96%	1.741%
10	2.752	260	273	274	rBV4	7804	17031	1.40%	0.245%
11	2.825	281	285	289	rBV	13703	26106	2.15%	0.375%
12	2.867	289	292	308	rVB2	21021	48568	3.99%	0.698%
13	3.099	322	330	342	rVB2	13260	30787	2.53%	0.442%
14	3.325	360	367	375	rBV4	5610	12948	1.06%	0.186%
15	3.666	416	423	428	rBV3	6615	14280	1.17%	0.205%
16	3.733	428	434	443	rVB2	8895	21546	1.77%	0.310%
17	3.837	443	451	457	rBV	6070	15576	1.28%	0.224%
18	4.099	487	494	505	rBV2	8984	23316	1.92%	0.335%
19	4.306	518	528	540	rVB2	21856	63358	5.21%	0.911%
20	5.202	664	675	683	rBV2	10419	30619	2.52%	0.440%
21	5.391	694	706	716	rBV2	55278	159089	13.08%	2.287%
22	5.556	723	733	757	rVB	97933	295261	24.27%	4.244%
23	5.958	789	799	812	rBV	60153	162500	13.36%	2.336%
24	6.208	827	840	843	rBV4	5328	17538	1.44%	0.252%
25	6.239	843	845	856	rVB5	5861	15029	1.24%	0.216%
26	6.763	922	931	941	rBV	143862	346783	28.50%	4.984%
27	8.653	1234	1241	1247	rBV	283709	448280	36.85%	6.443%
28	8.720	1247	1252	1263	rVB	134894	204287	16.79%	2.936%
29	10.055	1465	1471	1482	rVB	294068	392758	32.28%	5.645%
30	10.195	1488	1494	1505	rBV	310055	400675	32.93%	5.759%
31	10.305	1505	1512	1524	rVV	873556	1216580	100.00%	17.485%
32	10.640	1562	1567	1579	rVB	367205	485388	39.90%	6.976%
33	11.085	1634	1640	1648	rBV	260985	336278	27.64%	4.833%
34	11.305	1671	1676	1683	rBV	26938	31847	2.62%	0.458%
35	11.378	1683	1688	1696	rVV	117721	205284	16.87%	2.950%
36	11.451	1696	1700	1710	rVB	65728	79707	6.55%	1.146%

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37	11.616	1722	1727	1732	rBV	52705	66432	5.46%	0.955%
38	11.756	1744	1750	1756	rBV	245914	306256	25.17%	4.402%
39	12.024	1789	1794	1800	rBV	292790	356312	29.29%	5.121%
40	12.091	1800	1805	1810	rVB	61668	78338	6.44%	1.126%
41	12.244	1825	1830	1838	rBV2	57540	79202	6.51%	1.138%
42	12.317	1838	1842	1850	rVB2	11594	16940	1.39%	0.243%
43	12.616	1887	1891	1894	rBV	10722	12621	1.04%	0.181%
44	13.292	1993	2002	2007	rBV2	16982	21885	1.80%	0.315%
45	13.780	2076	2082	2088	rBV	60981	80034	6.58%	1.150%

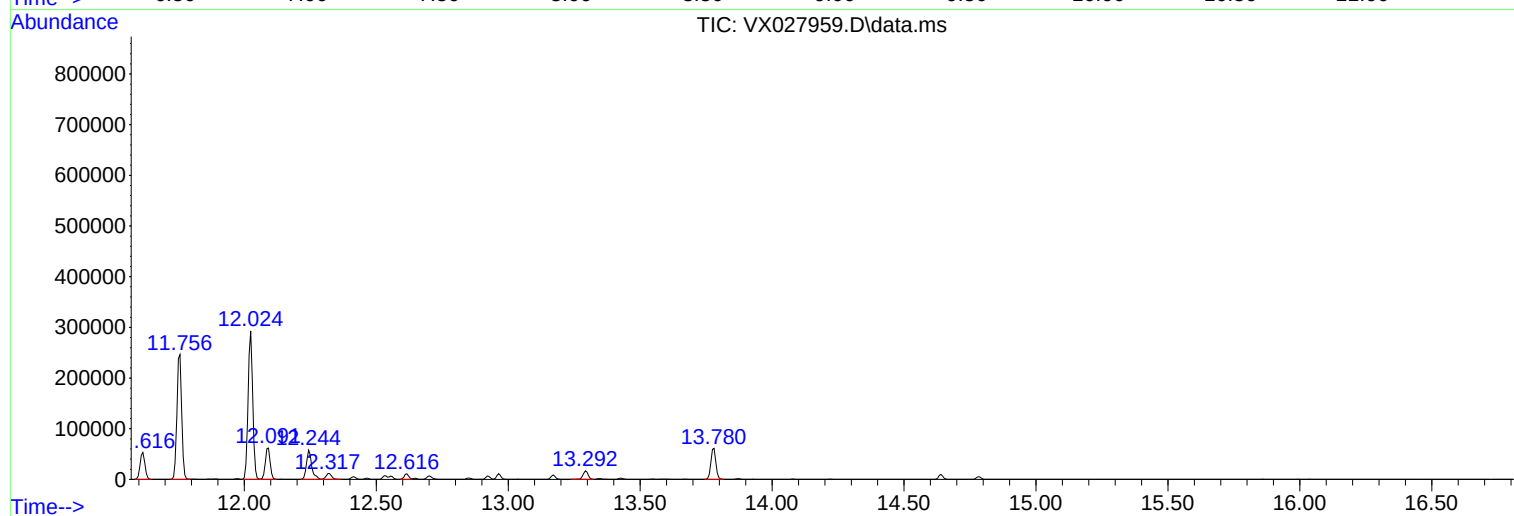
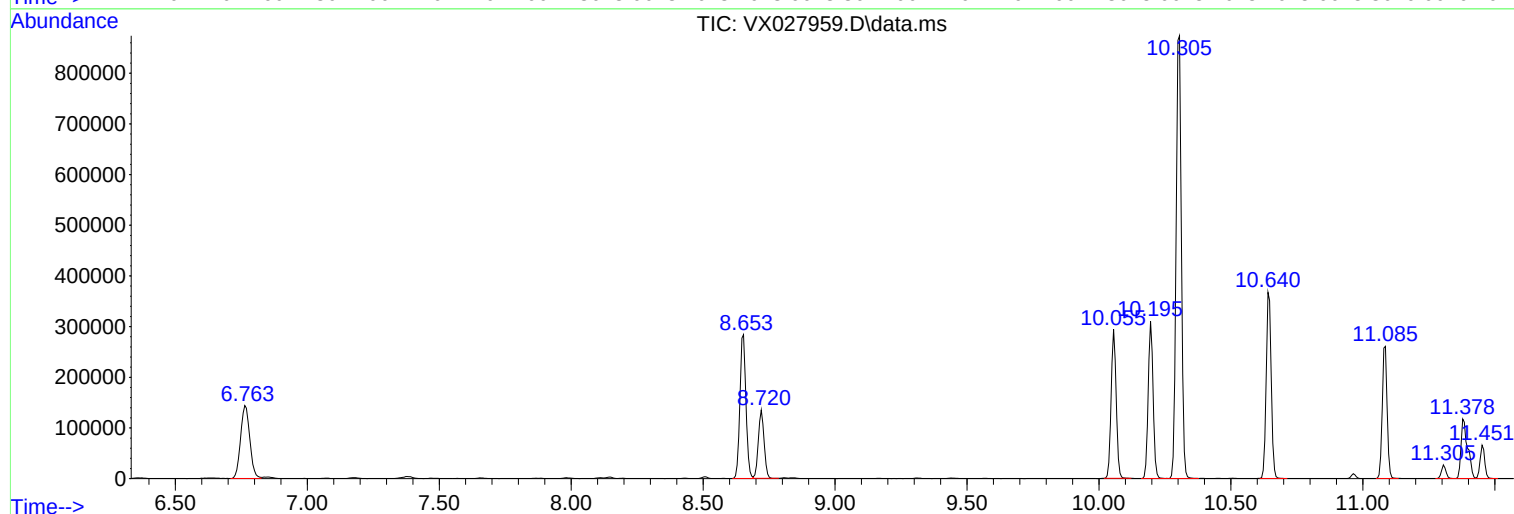
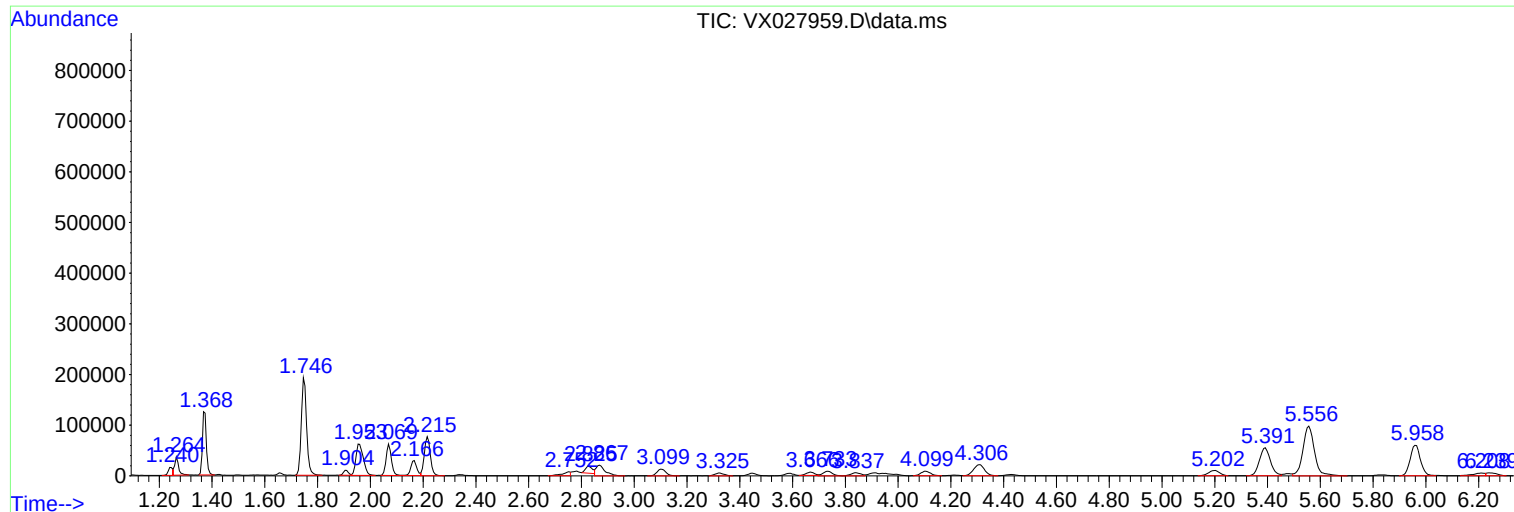
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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



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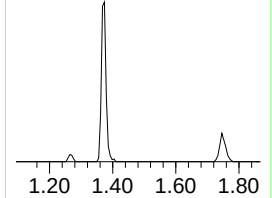
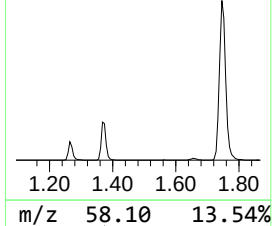
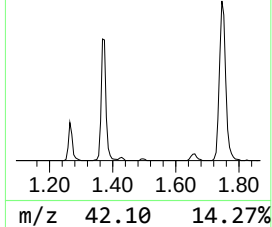
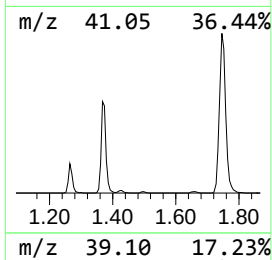
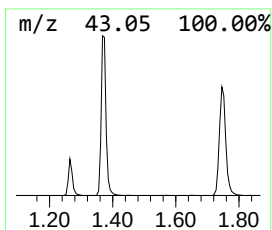
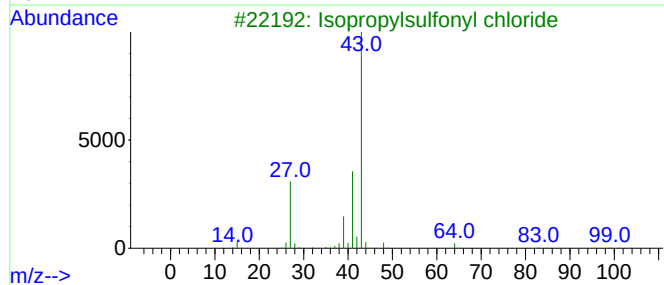
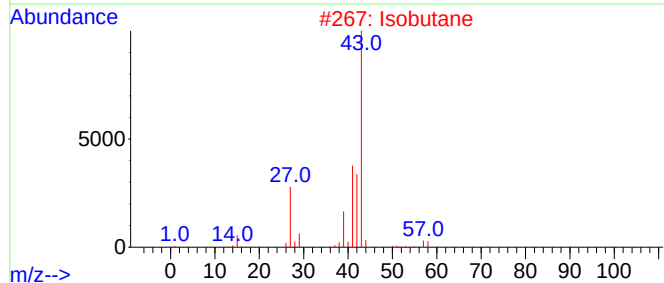
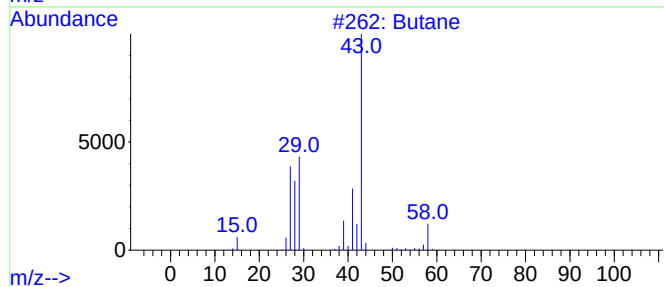
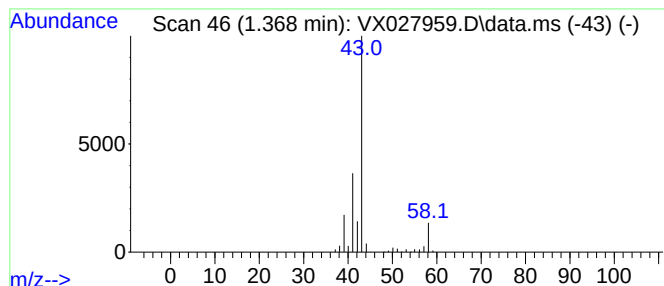
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	21.90 ug/l	129302	Pentafluorobenzene	5.556

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



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Instrument :
MSVOA_X
ClientSampleId :
MW-101R

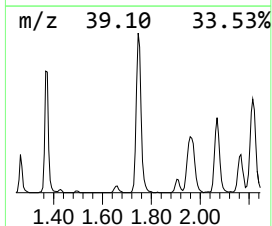
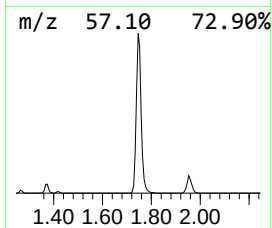
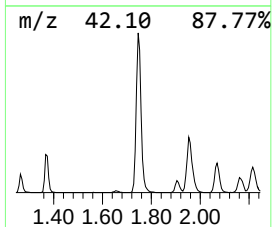
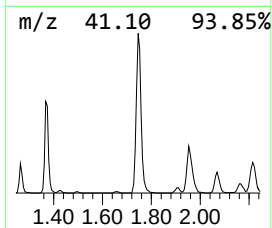
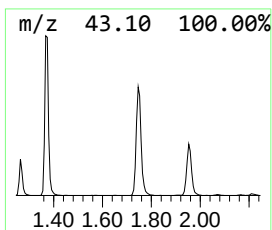
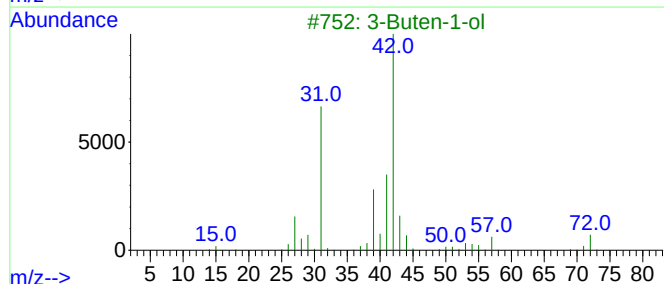
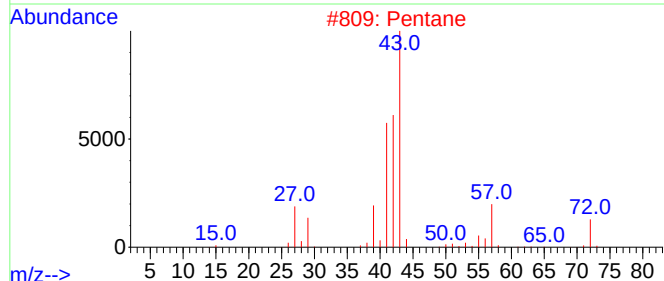
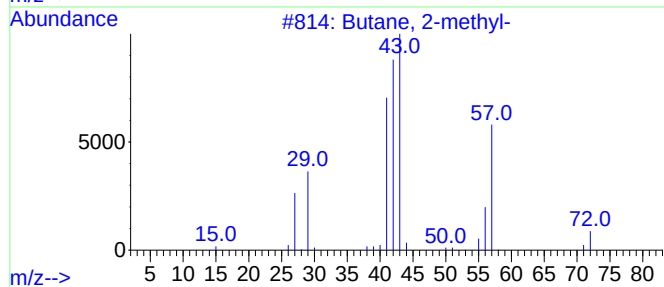
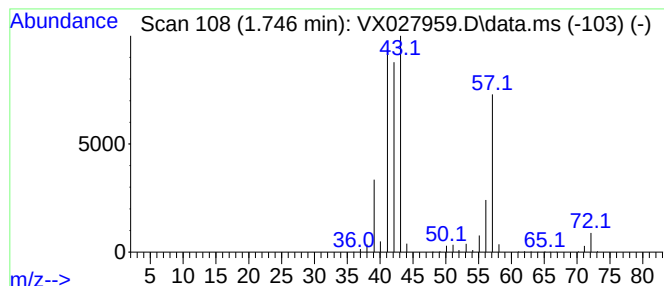
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	45.46 ug/l	268434	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	87
2			Pentane	72	C5H12	000109-66-0	38
3			3-Buten-1-ol	72	C4H8O	000627-27-0	25
4			2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	23
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10



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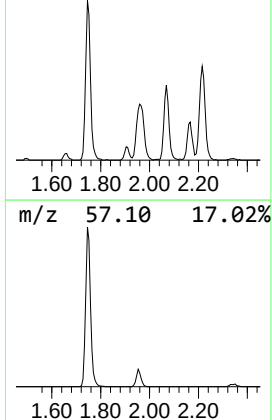
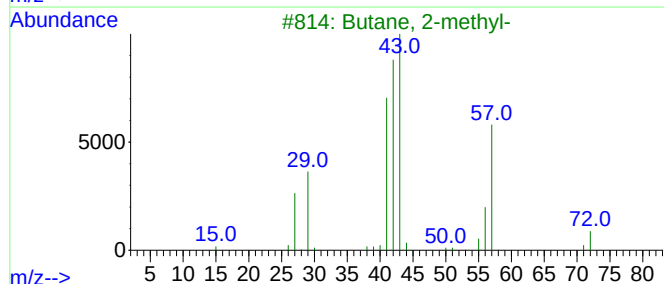
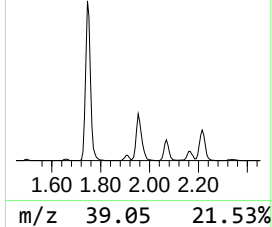
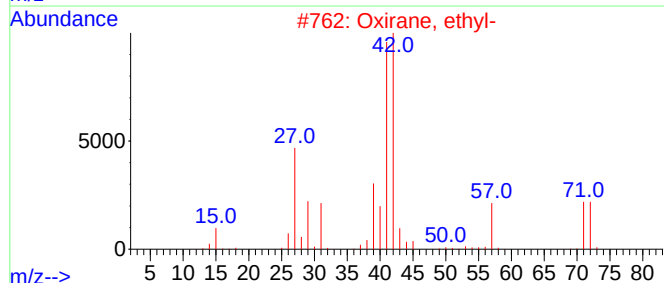
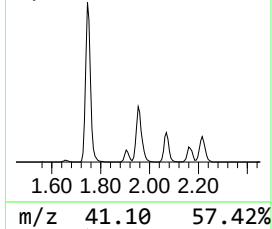
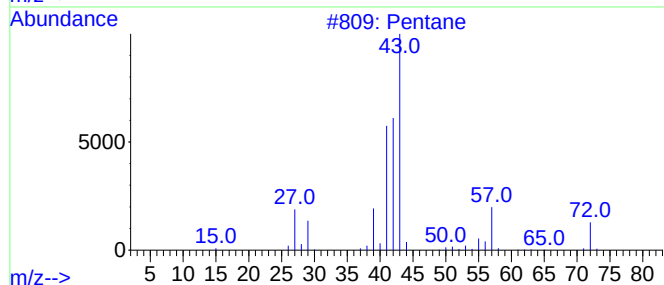
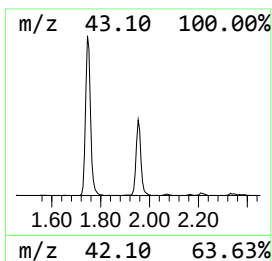
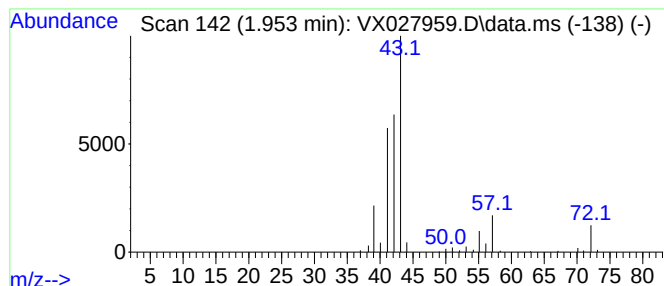
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	19.97 ug/l	117956	Pentafluorobenzene	5.556

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	38
5			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	12



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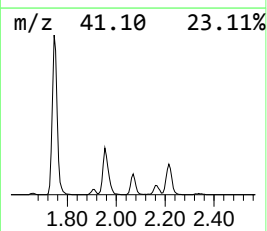
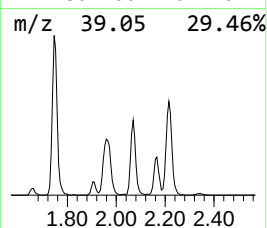
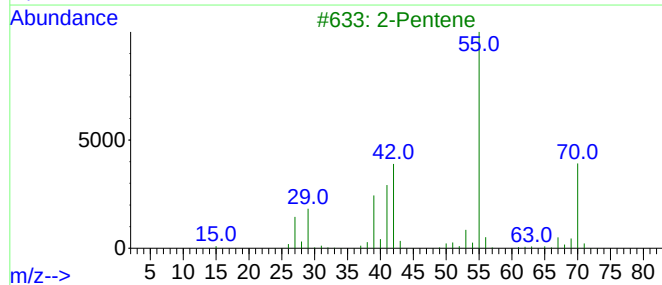
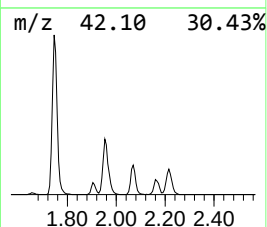
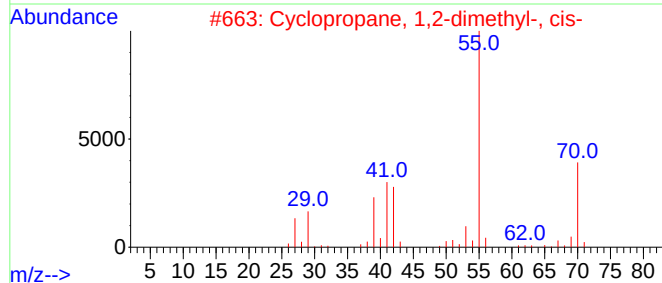
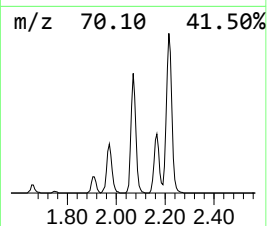
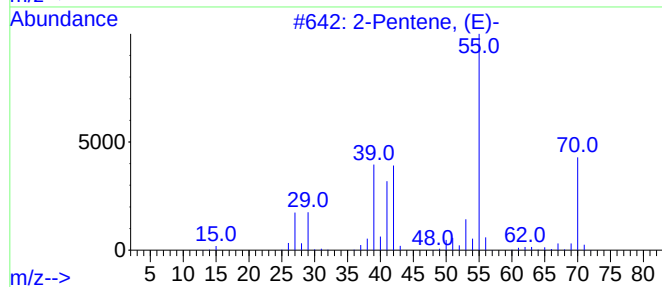
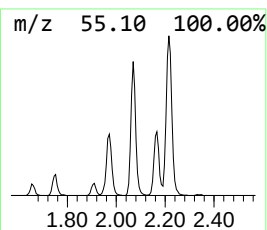
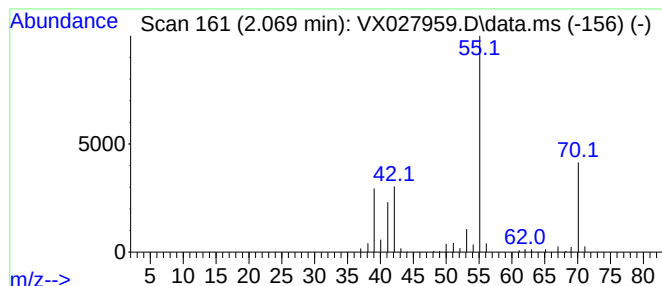
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	14.54 ug/l	85844	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentene, (E)-	70	C5H10	000646-04-8	93
2		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
3		2-Pentene	70	C5H10	000109-68-2	87
4		2-Pentene, (Z)-	70	C5H10	000627-20-3	87
5		2-Methyl-1-butene	70	C5H10	000563-46-2	87



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MSVOA_X
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MW-101R

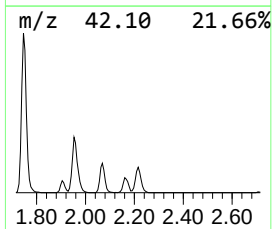
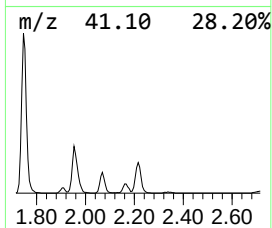
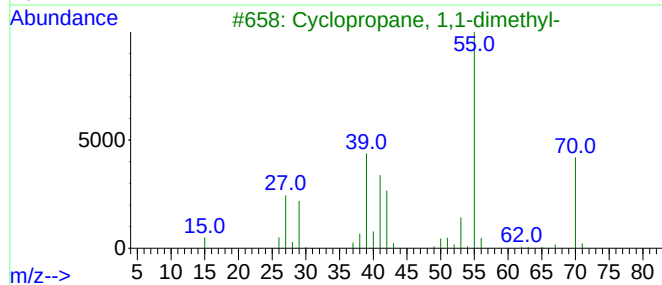
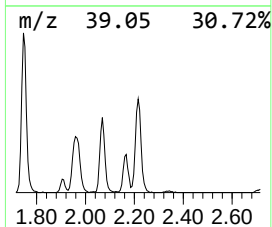
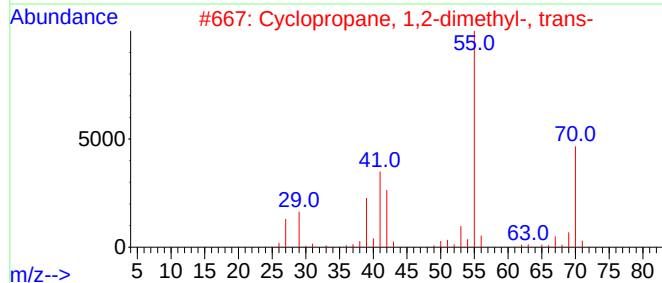
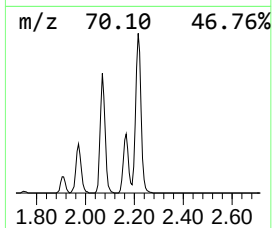
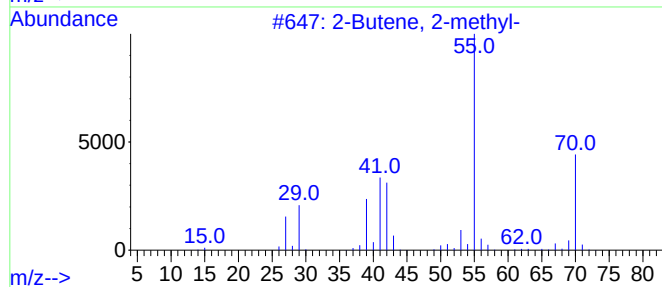
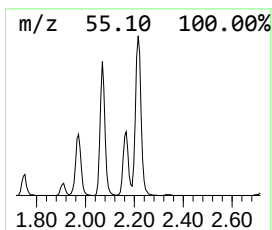
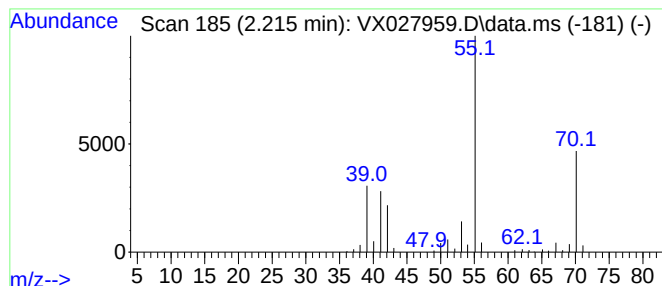
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

Peak Number 5 2-Butene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	20.51 ug/l	121123	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
2			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
3			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
4			2-Methyl-1-butene	70	C5H10	000563-46-2	78
5			1-Butene, 3-methyl-	70	C5H10	000563-45-1	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX040422\
Data File : VX027959.D
Acq On : 04 Apr 2022 15:48
Operator : JC/MD
Sample : N2249-08 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-101R

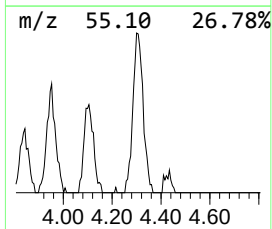
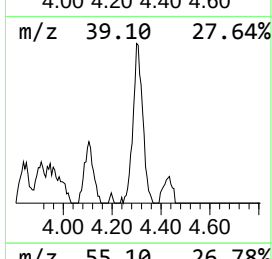
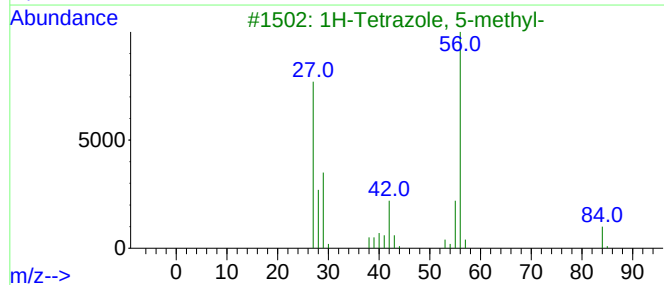
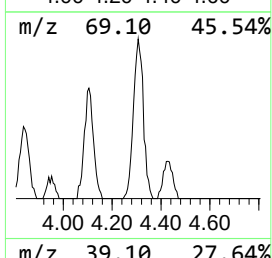
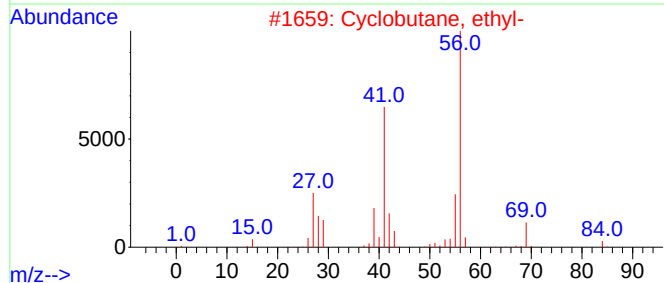
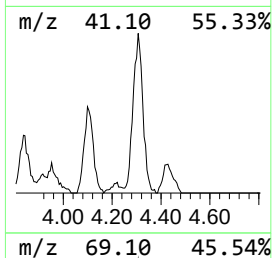
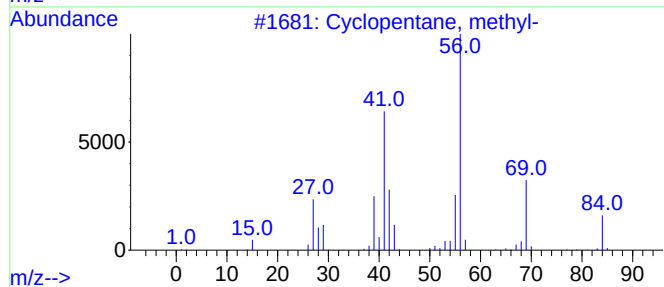
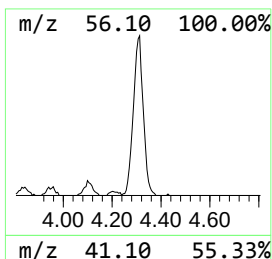
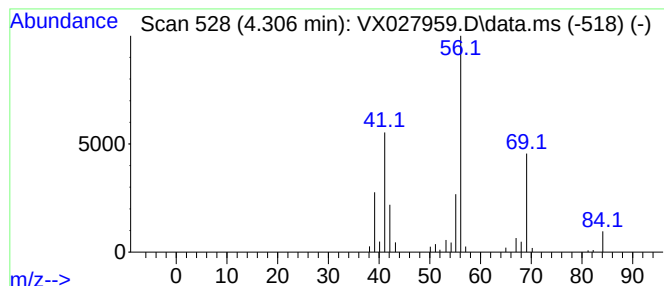
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	10.73 ug/l	63358	Pentafluorobenzene	5.556

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			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56
5			Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO040422\
Data File : VX027959.D
Acq On : 04 Apr 2022 15:48
Operator : JC/MD
Sample : N2249-08 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-101R

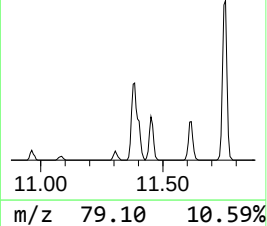
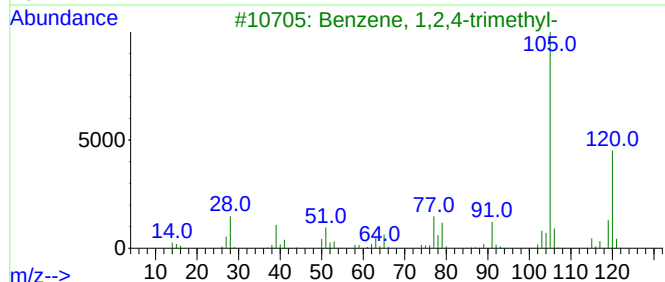
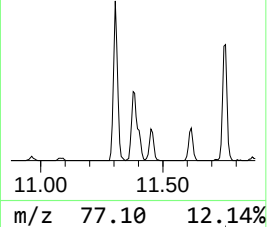
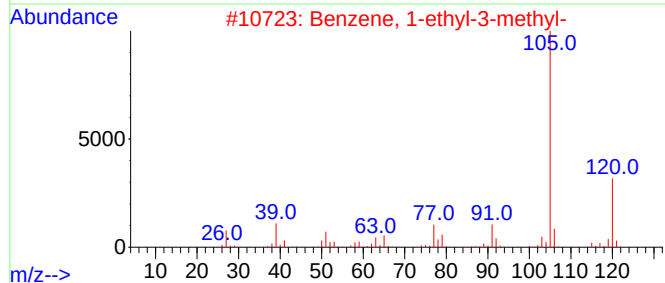
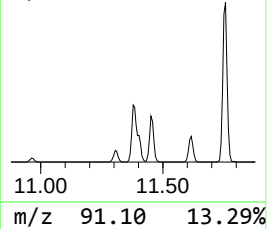
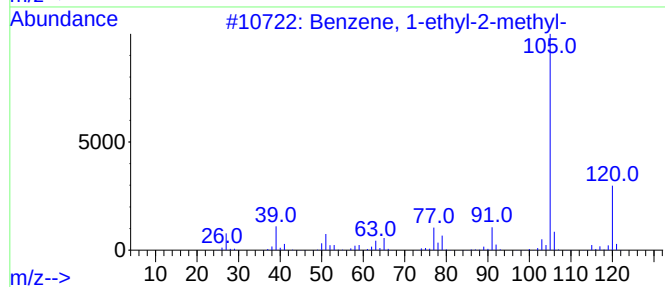
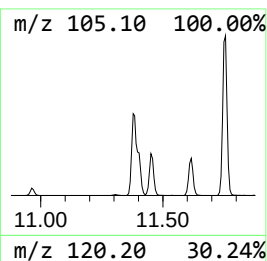
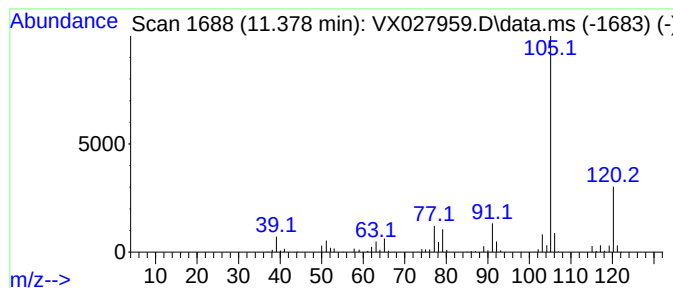
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	28.81 ug/l	205284	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-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO040422\
Data File : VX027959.D
Acq On : 04 Apr 2022 15:48
Operator : JC/MD
Sample : N2249-08 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-101R

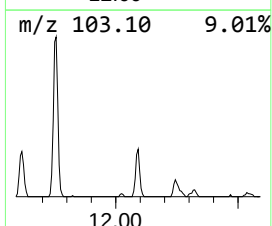
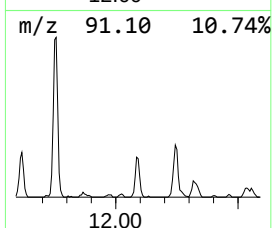
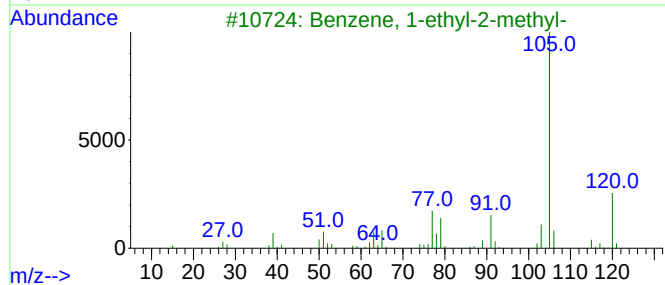
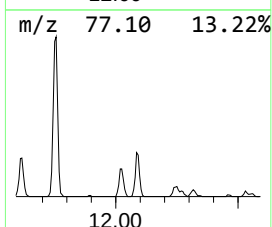
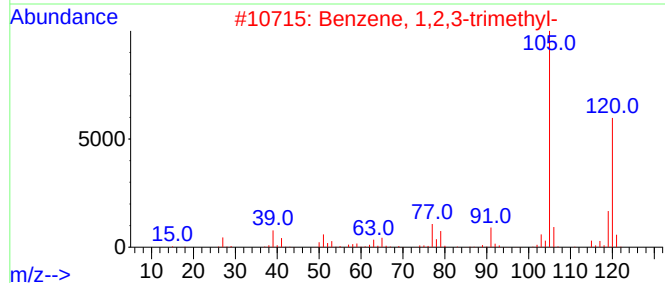
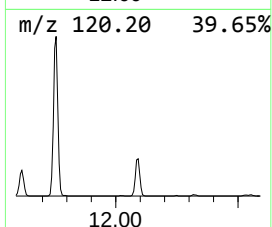
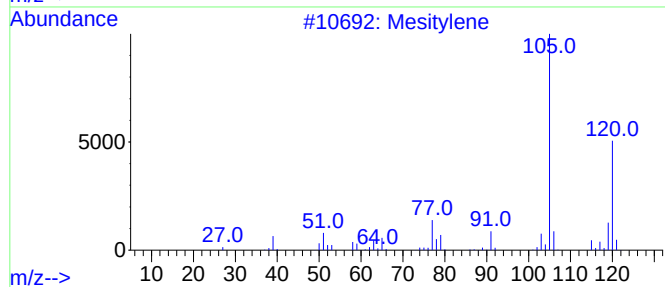
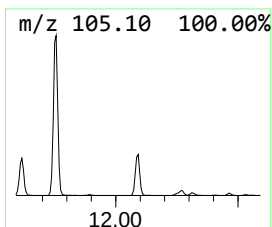
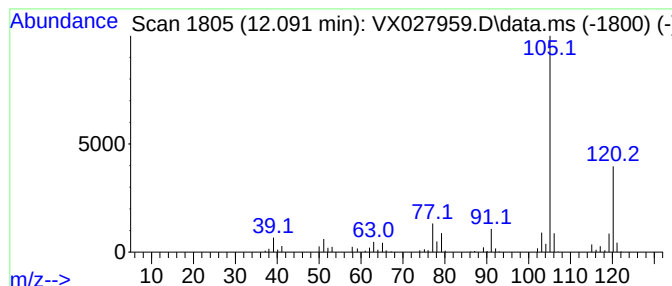
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Quant Title : SW846 8260

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

Peak Number 8 Mesitylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	10.99 ug/l	78338	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	94
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027959.D
Acq On : 04 Apr 2022 15:48
Operator : JC/MD
Sample : N2249-08 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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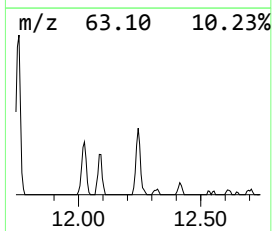
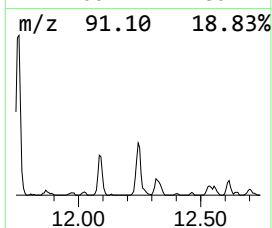
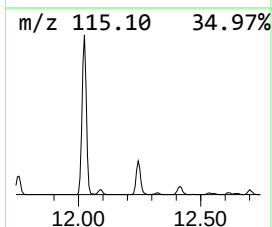
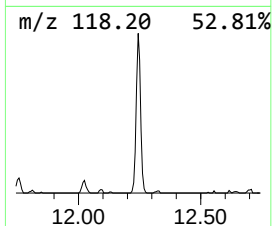
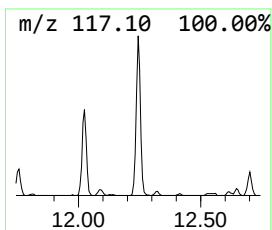
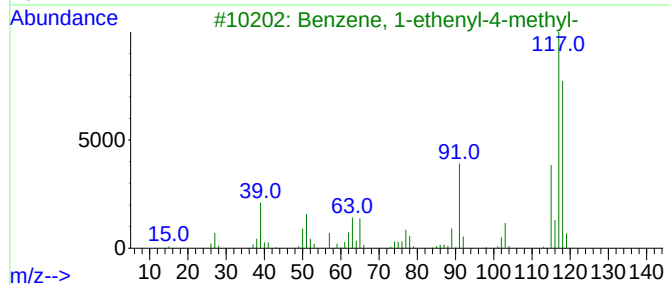
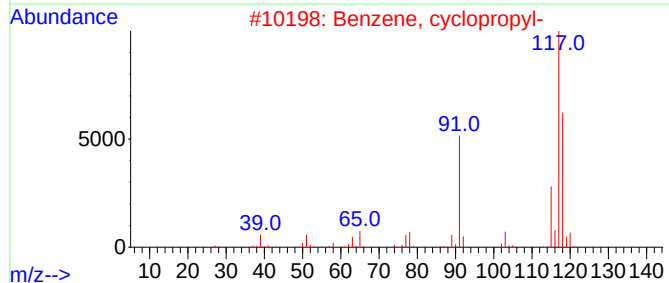
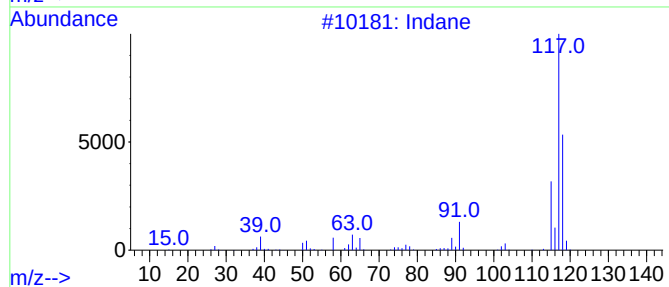
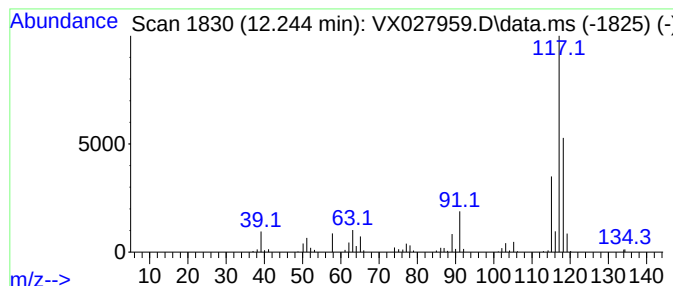
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Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	11.11 ug/l	79202	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
3			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	72
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027959.D
Acq On : 04 Apr 2022 15:48
Operator : JC/MD
Sample : N2249-08 40X
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
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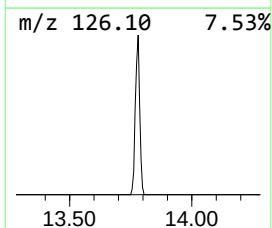
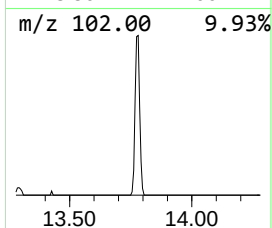
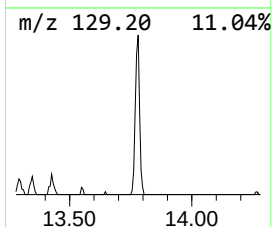
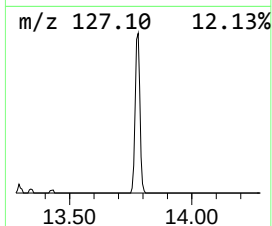
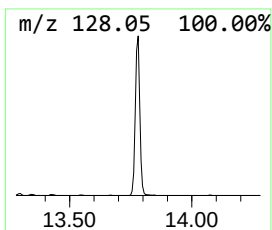
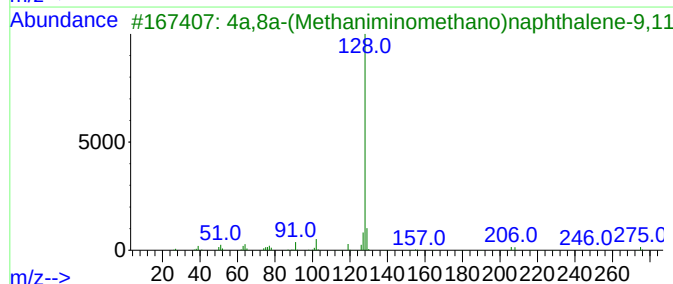
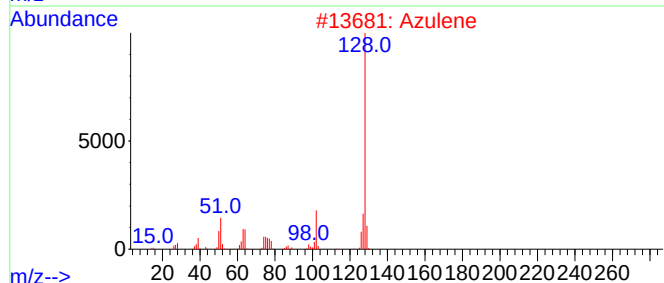
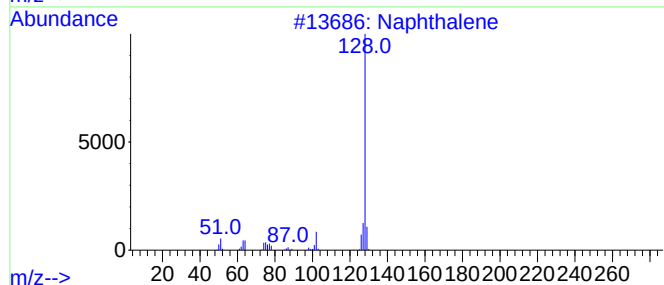
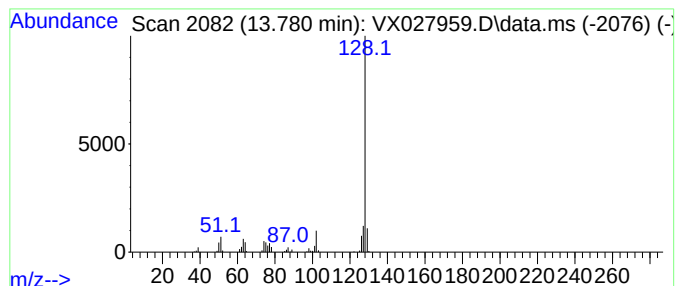
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	11.23 ug/l	80034	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	91
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
4			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	53
5			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027959.D
Acq On : 04 Apr 2022 15:48
Operator : JC/MD
Sample : N2249-08 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-101R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.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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Butane, 2-methyl-	1.746	45.5	ug/l	268434	1	5.556	295261	50.0
Pentane	1.953	20.0	ug/l	117956	1	5.556	295261	50.0
2-Pentene, (E)-	2.069	14.5	ug/l	85844	1	5.556	295261	50.0
2-Butene, 2-met...	2.215	20.5	ug/l	121123	1	5.556	295261	50.0
Cyclopentane, m...	4.306	10.7	ug/l	63358	1	5.556	295261	50.0
Benzene, 1-ethy...	11.378	28.8	ug/l	205284	4	12.024	356312	50.0
Mesitylene	12.091	11.0	ug/l	78338	4	12.024	356312	50.0
Indane	12.244	11.1	ug/l	79202	4	12.024	356312	50.0
Naphthalene	13.780	11.2	ug/l	80034	4	12.024	356312	50.0