

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
 Data File : VX033137.D
 Acq On : 30 Nov 2022 17:14
 Operator : JC/MD
 Sample : N5815-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-01

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\82X112222W.M
 Title : SW846 8260

Signal : TIC: VX033137.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	43	rBV	125015	132244	6.71%	1.410%
2	1.374	43	47	52	rVV	419308	443149	22.49%	4.725%
3	1.416	52	54	63	rVB	27337	33288	1.69%	0.355%
4	1.752	103	109	121	rBV	1517149	1970699	100.00%	21.012%
5	1.959	137	143	152	rVB2	19988	30739	1.56%	0.328%
6	2.215	179	185	195	rVB	37394	58780	2.98%	0.627%
7	2.343	199	206	217	rBV	54613	104861	5.32%	1.118%
8	2.782	266	278	283	rBV	111216	250823	12.73%	2.674%
9	2.831	283	286	288	rVV	56956	92713	4.70%	0.989%
10	2.867	288	292	303	rVV	118675	244707	12.42%	2.609%
11	2.983	303	311	323	rVV3	30876	117639	5.97%	1.254%
12	3.111	323	332	348	rVB2	387974	905685	45.96%	9.657%
13	3.757	427	438	446	rBV4	12646	41767	2.12%	0.445%
14	4.105	479	495	503	rBV4	7996	22822	1.16%	0.243%
15	4.306	519	528	539	rVV	95536	272758	13.84%	2.908%
16	4.428	539	548	561	rVB2	14862	44468	2.26%	0.474%
17	5.196	665	674	687	rVB3	14716	45049	2.29%	0.480%
18	5.385	693	705	714	rBV	59949	180372	9.15%	1.923%
19	5.477	714	720	724	rVV2	16280	38836	1.97%	0.414%
20	5.556	724	733	742	rVV	126583	343502	17.43%	3.662%
21	5.958	789	799	806	rBV	69632	182201	9.25%	1.943%
22	6.037	806	812	825	rVB2	54300	143655	7.29%	1.532%
23	6.172	825	834	838	rBV4	7252	23064	1.17%	0.246%
24	6.251	840	847	859	rVB3	24839	77189	3.92%	0.823%
25	6.763	922	931	942	rBV	204433	493383	25.04%	5.261%
26	7.373	1021	1031	1041	rVB5	10085	29640	1.50%	0.316%
27	8.507	1211	1217	1226	rVB2	19479	33344	1.69%	0.356%
28	8.647	1234	1240	1248	rVB	311119	491121	24.92%	5.236%
29	8.848	1265	1273	1280	rBV	11706	21437	1.09%	0.229%
30	10.055	1460	1471	1477	rBV	419146	573103	29.08%	6.111%
31	10.195	1489	1494	1500	rBV	184997	233441	11.85%	2.489%
32	10.305	1507	1512	1517	rVB	18214	25135	1.28%	0.268%
33	10.963	1613	1620	1625	rVB	27489	35054	1.78%	0.374%
34	11.079	1634	1639	1649	rBV	273054	347791	17.65%	3.708%
35	11.305	1672	1676	1684	rVB	23948	30500	1.55%	0.325%
36	11.616	1718	1727	1734	rVB	46918	61868	3.14%	0.660%

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37	11.756	1745	1750	1755	rBV	26479	33226	1.69%	0.354%
38	12.024	1788	1794	1801	rBV	427976	532011	27.00%	5.672%
39	12.244	1824	1830	1838	rBV	391512	469071	23.80%	5.001%
40	12.616	1886	1891	1894	rBV	41175	49170	2.50%	0.524%
41	12.701	1900	1905	1911	rBV	25942	34147	1.73%	0.364%
42	12.920	1934	1941	1945	rBV	16842	20066	1.02%	0.214%
43	13.292	1997	2002	2008	rVB2	48286	64457	3.27%	0.687%

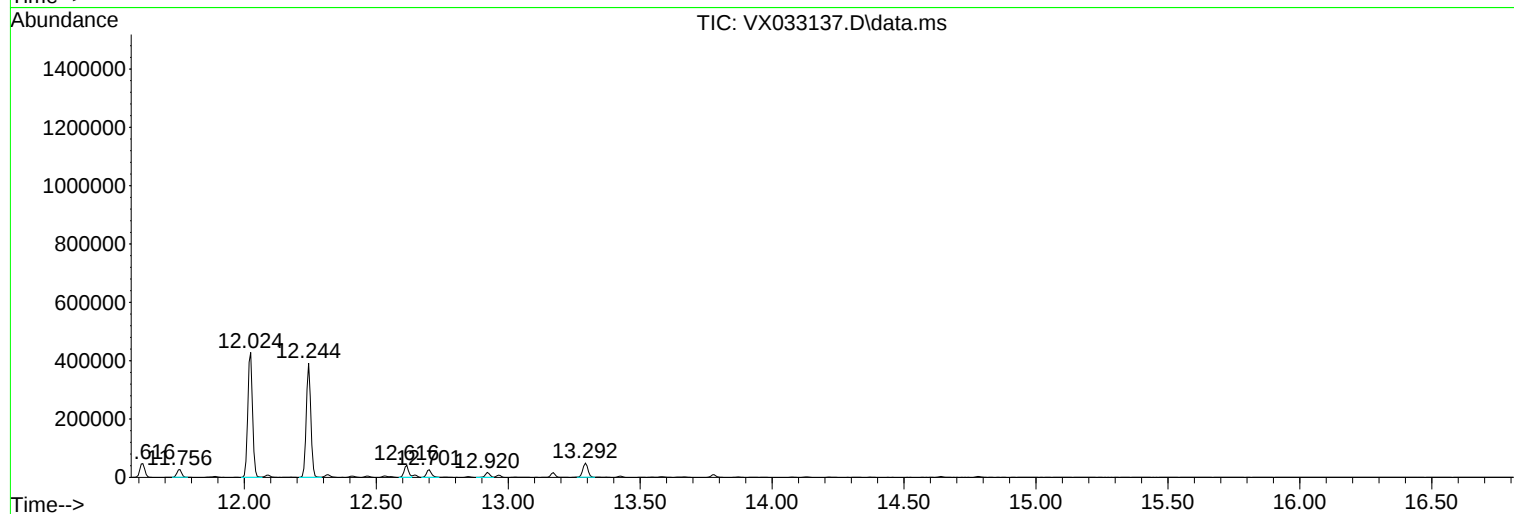
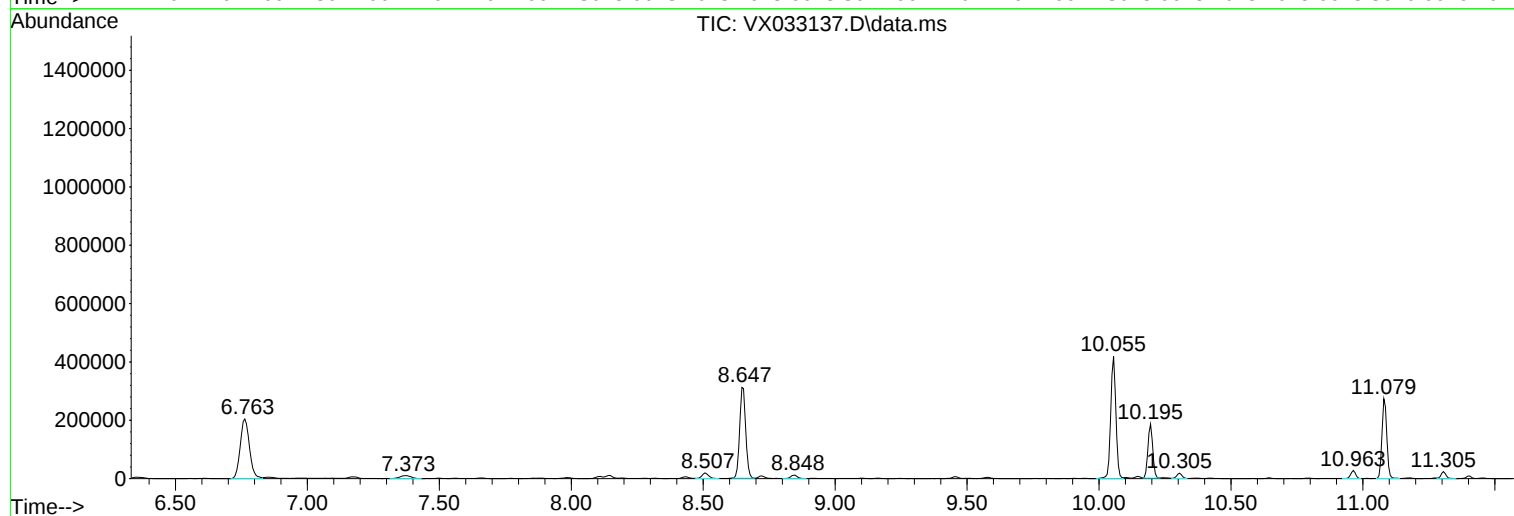
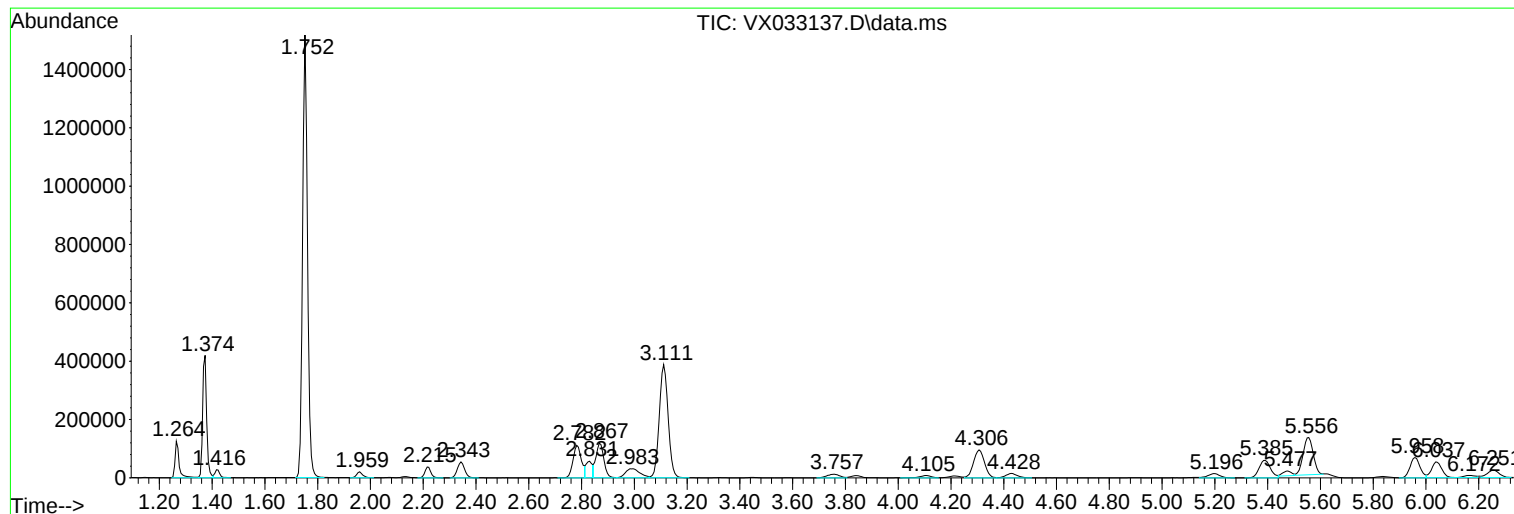
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Quant Title : SW846 8260

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



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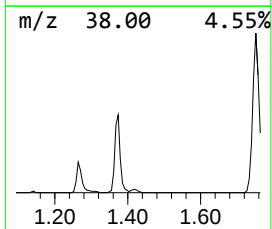
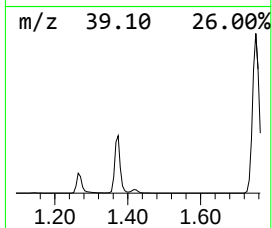
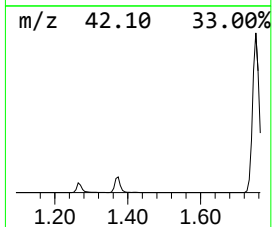
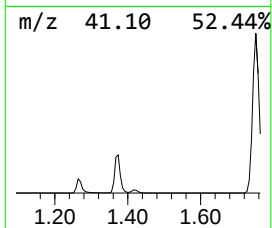
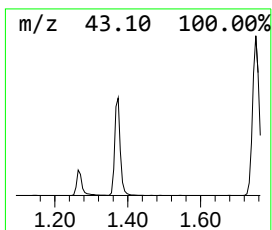
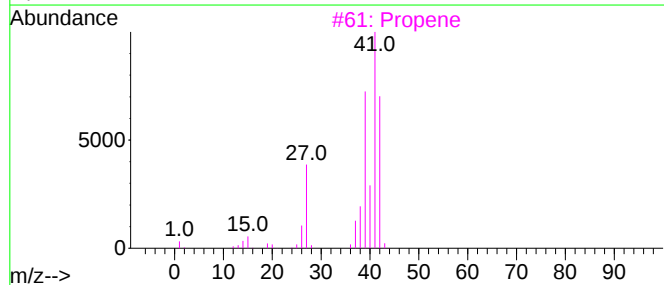
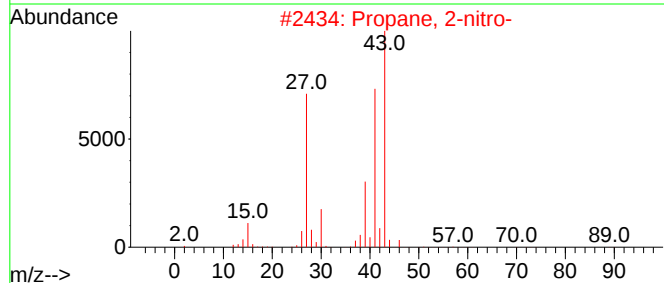
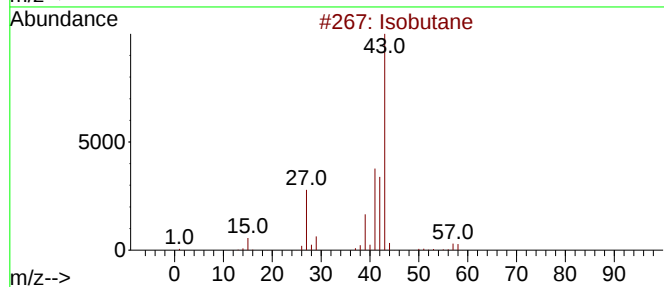
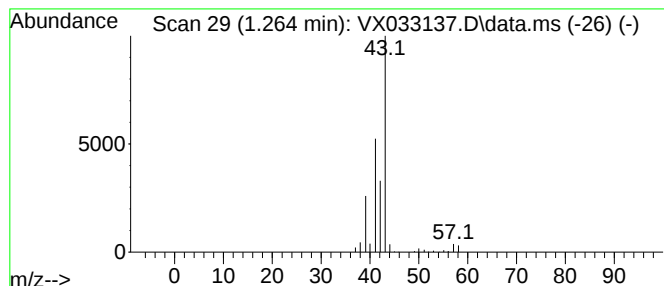
Instrument :
MSVOA_X
ClientSampleId :
MW-01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.264	19.25 ug/l	132244	Pentafluorobenzene	5.550	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	64
2	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3	Propene	42	C3H6	000115-07-1	5
4	Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	4



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Instrument :
MSVOA_X
ClientSampleId :
MW-01

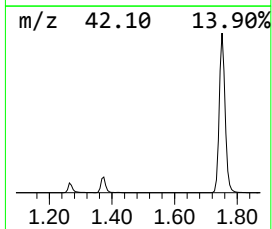
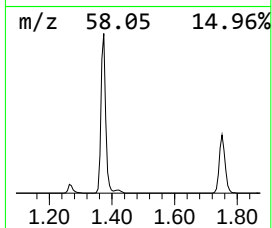
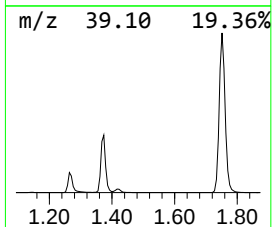
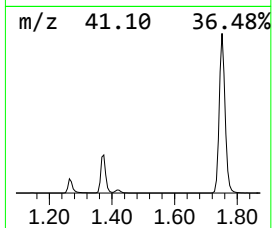
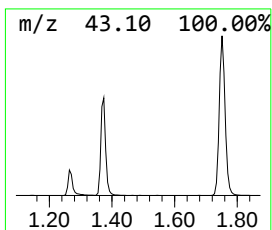
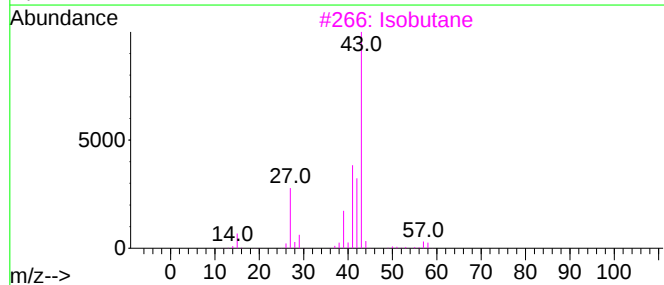
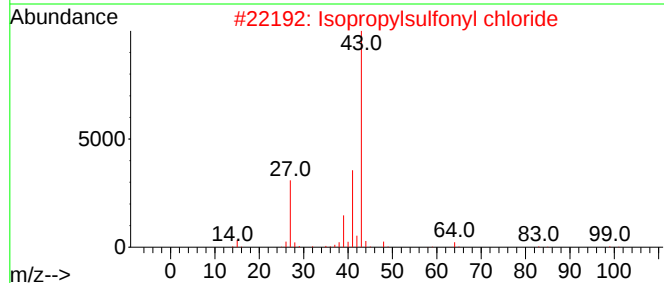
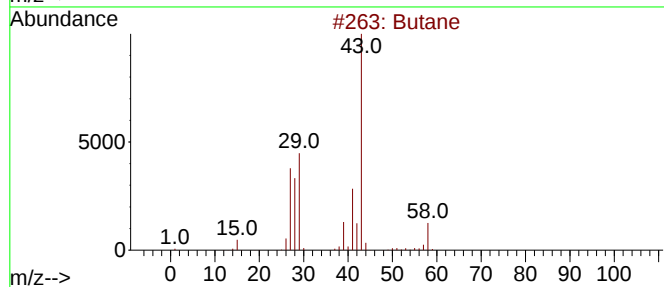
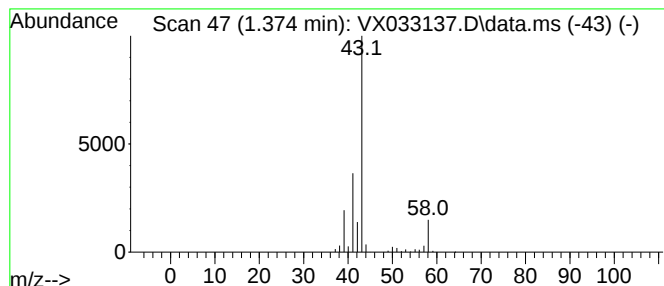
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	64.50 ug/l	443149	Pentafluorobenzene	5.550

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



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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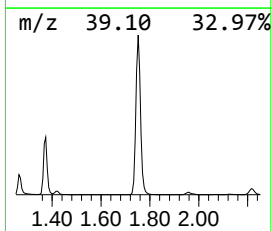
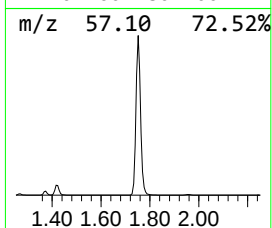
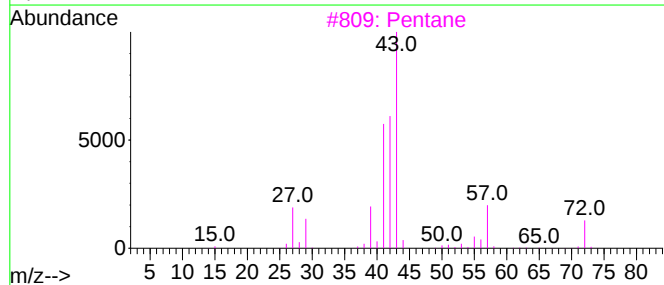
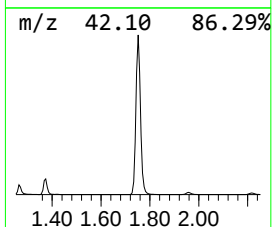
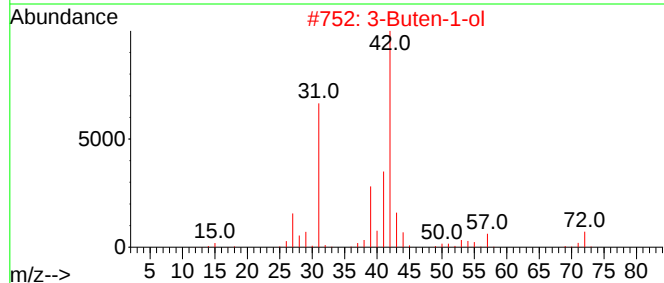
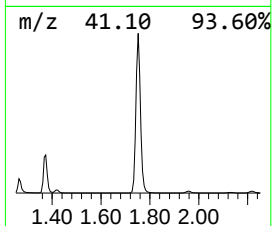
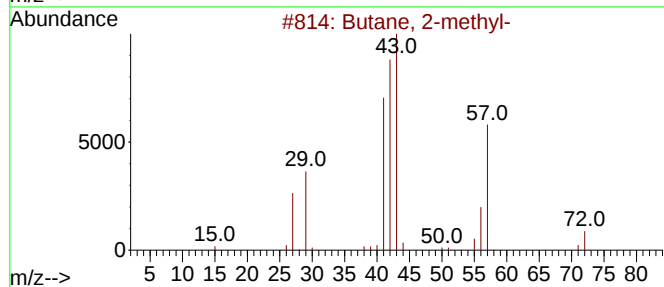
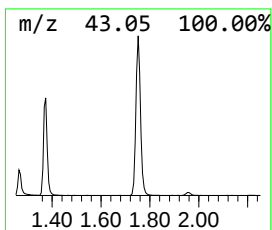
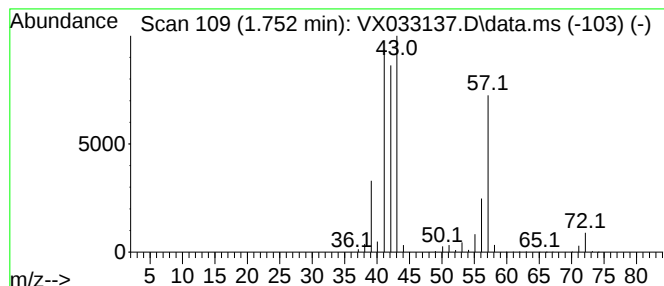
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	286.85 ug/l	1970700	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	90
2	3-Buten-1-ol			72	C4H8O	000627-27-0	47
3	Pentane			72	C5H12	000109-66-0	36
4	1-Butene			56	C4H8	000106-98-9	10
5	3-Buten-2-ol			72	C4H8O	000598-32-3	9



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ClientSampleId :
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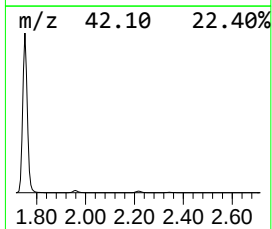
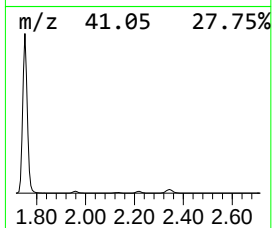
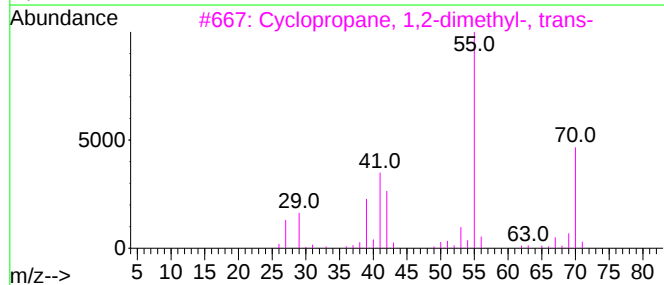
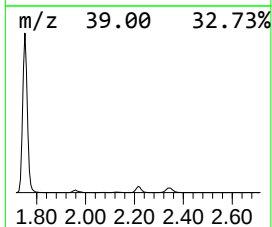
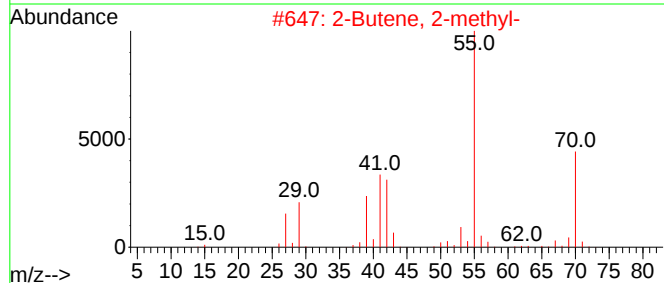
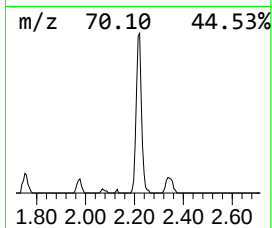
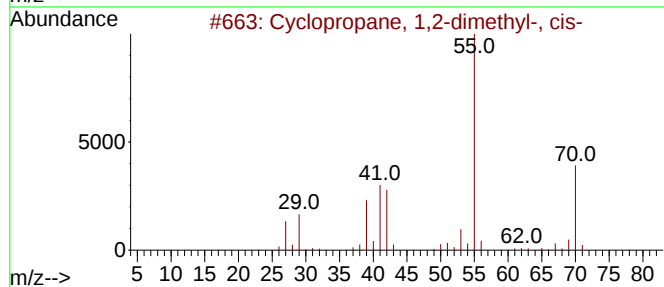
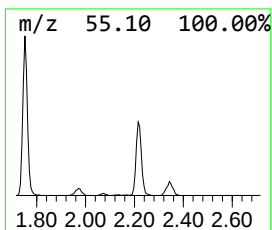
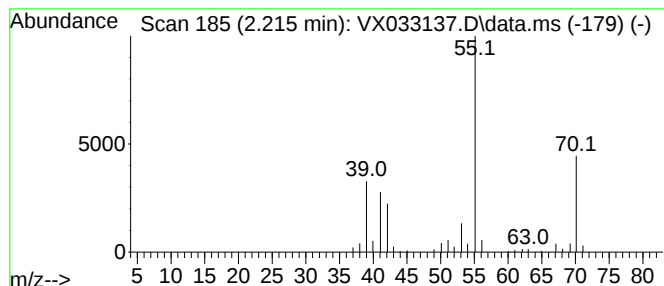
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopropane, 1,2-dimethyl-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	8.56 ug/l	58780	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	86
4			2-Pentene, (E)-	70	C5H10	000646-04-8	86
5			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80



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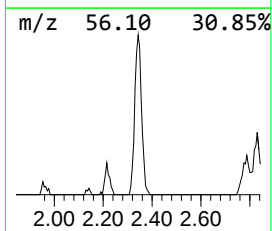
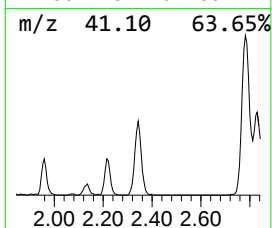
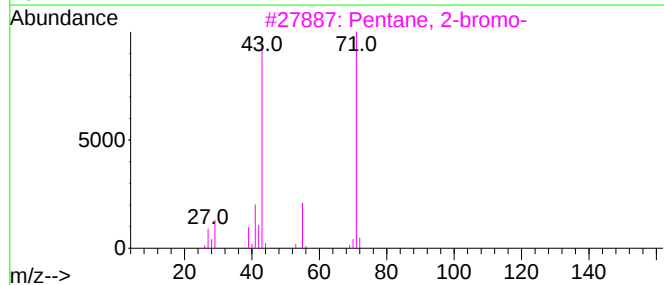
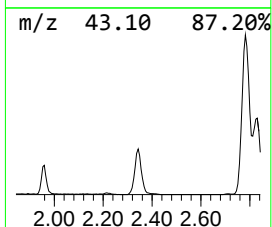
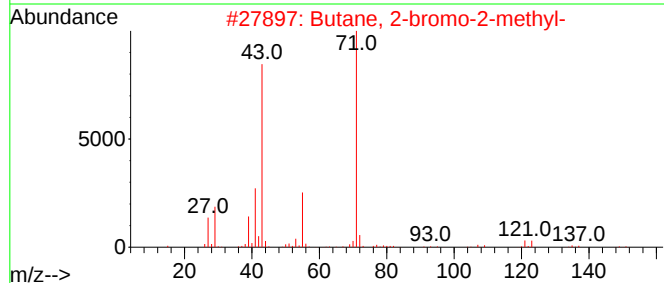
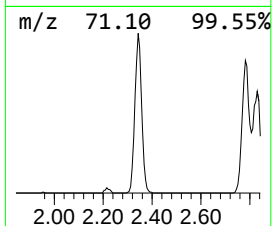
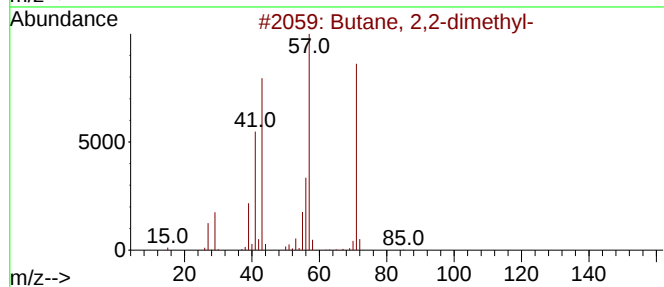
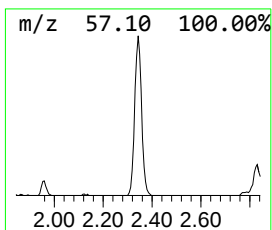
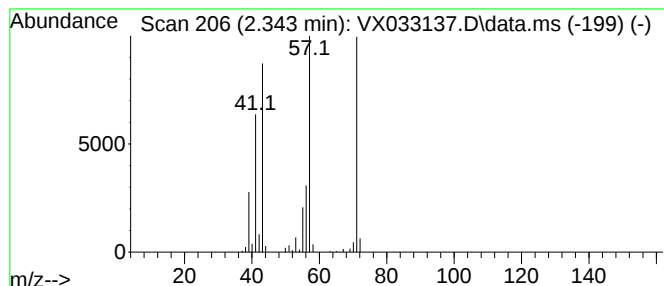
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Quant Title : SW846 8260

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

Peak Number 5 Butane, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.343	15.26 ug/l	104861	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	90
2			Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	59
3			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	53
4			Sulfurous acid, isobutyl pentyl ...	208	C9H20O3S	1000309-13-8	50
5			Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033137.D
Acq On : 30 Nov 2022 17:14
Operator : JC/MD
Sample : N5815-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-01

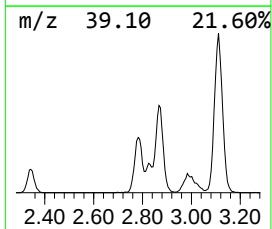
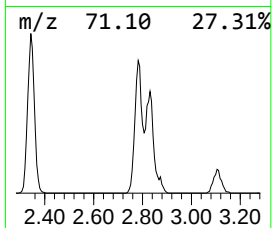
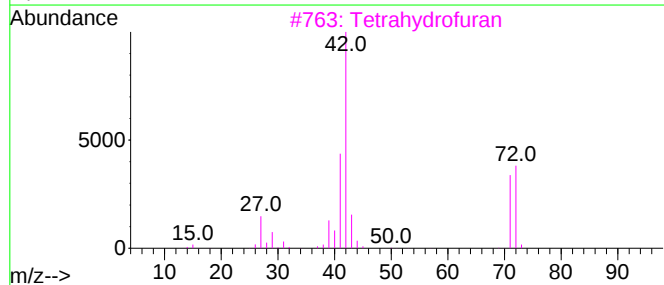
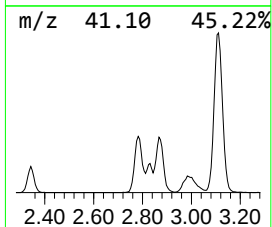
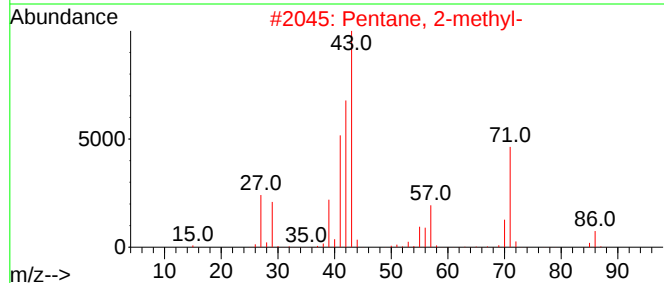
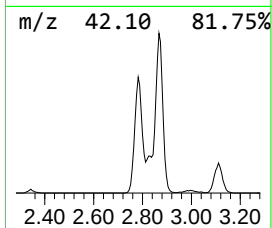
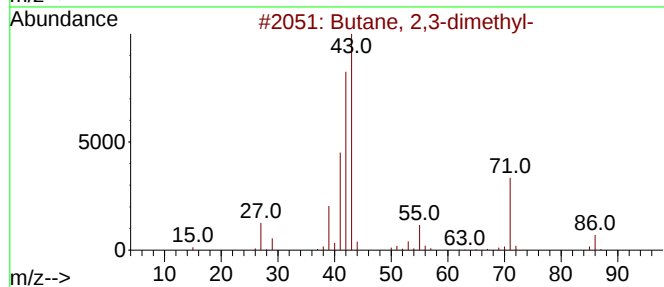
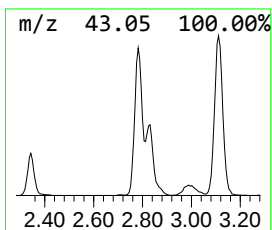
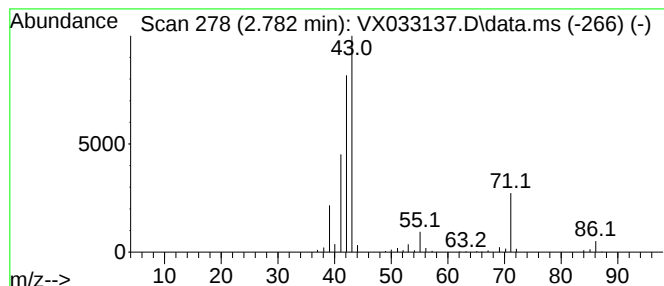
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Quant Title : SW846 8260

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

Peak Number 6 Butane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	36.51 ug/l	250823	Pentafluorobenzene	5.550

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	78
3			Tetrahydrofuran	72	C4H8O	000109-99-9	38
4			Pentane	72	C5H12	000109-66-0	36
5			1-Pentene	70	C5H10	000109-67-1	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033137.D
Acq On : 30 Nov 2022 17:14
Operator : JC/MD
Sample : N5815-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-01

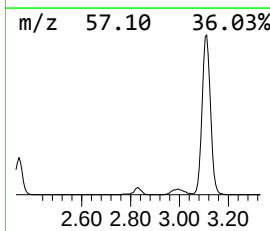
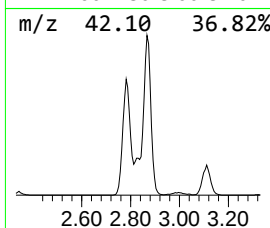
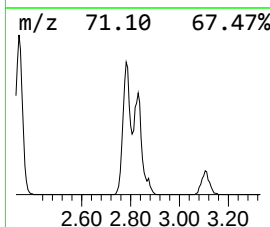
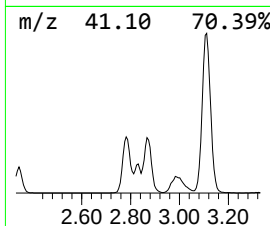
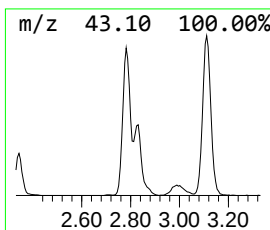
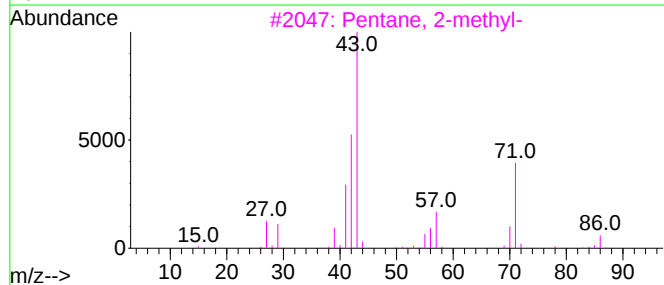
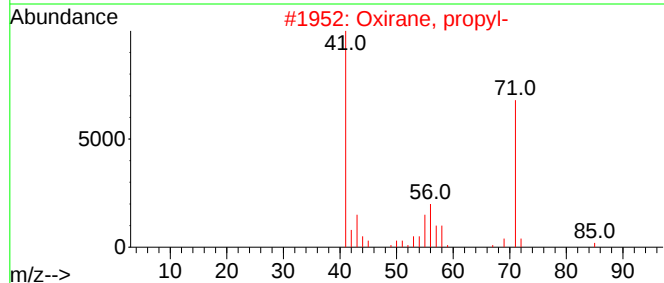
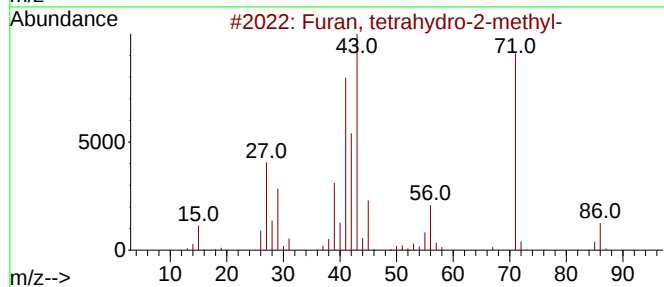
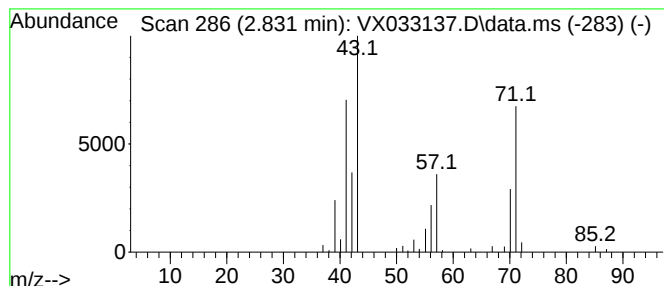
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Quant Title : SW846 8260

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

Peak Number 7 Furan, tetrahydro-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.831	13.50 ug/l	92713	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	53
2			Oxirane, propyl-	86	C5H10O	001003-14-1	38
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	38
4			Oxirane, butyl-	100	C6H12O	001436-34-6	32
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033137.D
Acq On : 30 Nov 2022 17:14
Operator : JC/MD
Sample : N5815-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-01

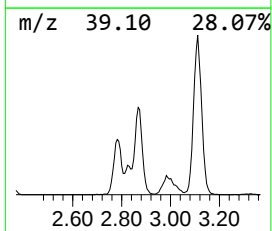
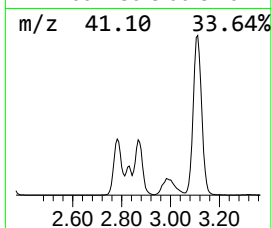
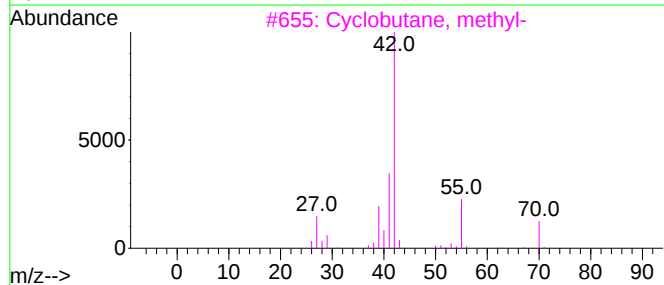
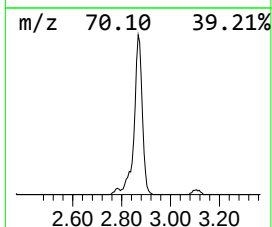
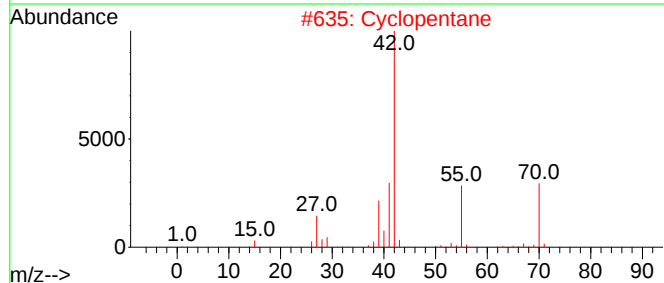
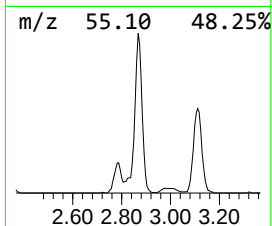
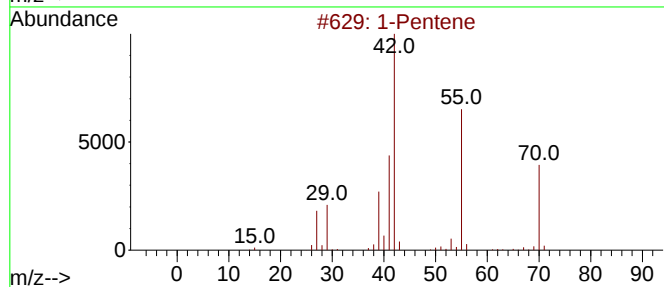
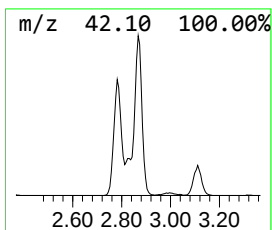
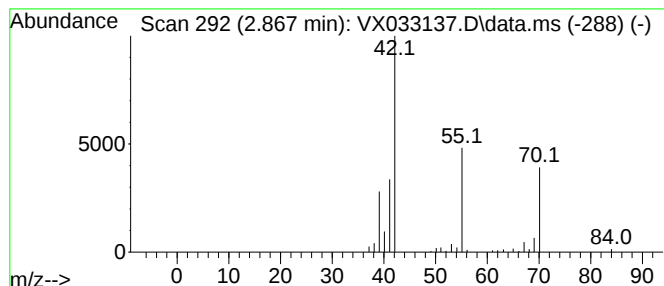
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Quant Title : SW846 8260

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

Peak Number 8 1-Pentene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	35.62 ug/l	244707	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene	70	C5H10	000109-67-1	80
2			Cyclopentane	70	C5H10	000287-92-3	78
3			Cyclobutane, methyl-	70	C5H10	000598-61-8	72
4			3-Buten-1-ol	72	C4H8O	000627-27-0	38
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033137.D
Acq On : 30 Nov 2022 17:14
Operator : JC/MD
Sample : N5815-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-01

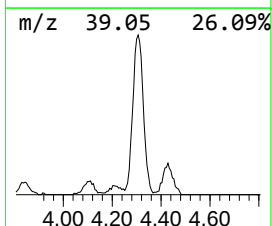
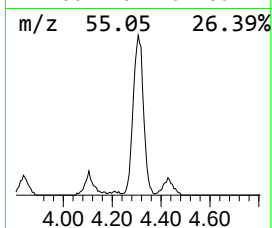
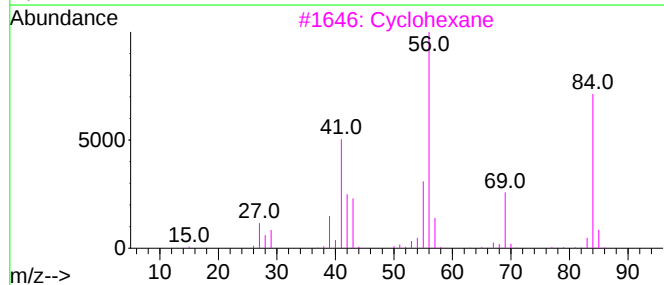
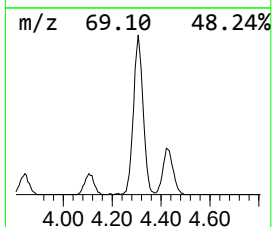
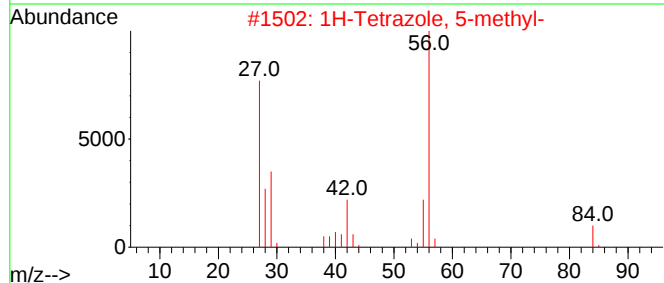
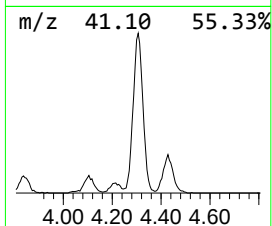
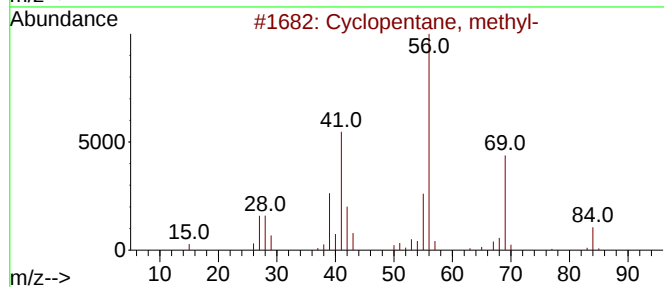
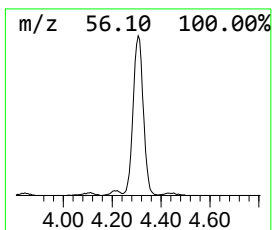
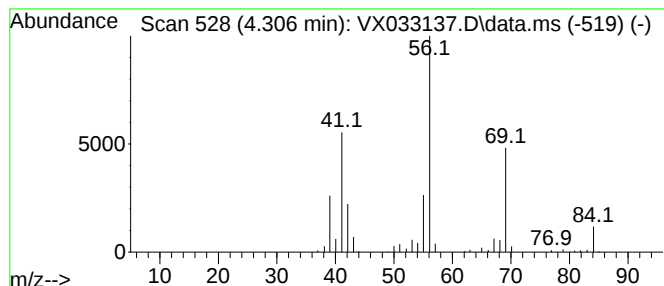
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Quant Title : SW846 8260

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

Peak Number 9 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	39.70 ug/l	272758	Pentafluorobenzene	5.550

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			Cyclohexane	84	C6H12	000110-82-7	78
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5			Cyclobutane	56	C4H8	000287-23-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033137.D
Acq On : 30 Nov 2022 17:14
Operator : JC/MD
Sample : N5815-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-01

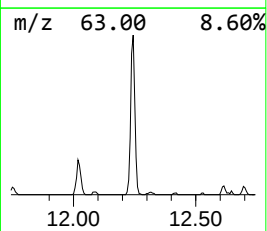
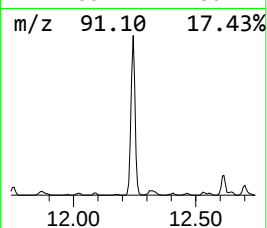
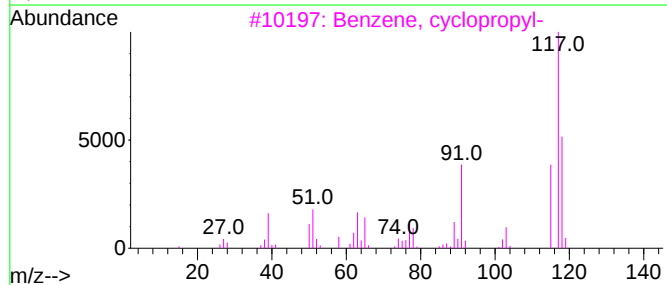
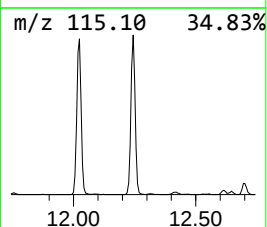
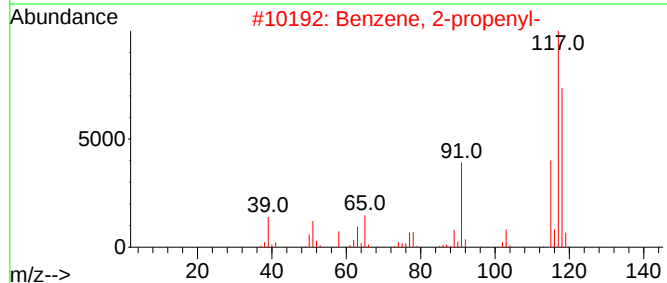
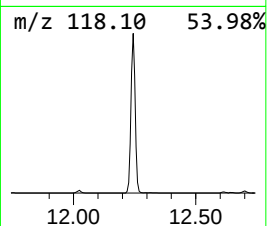
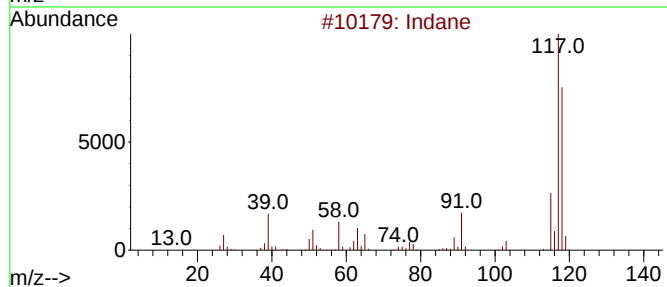
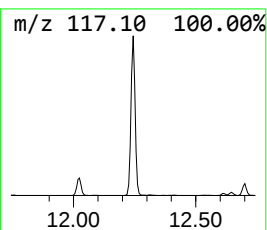
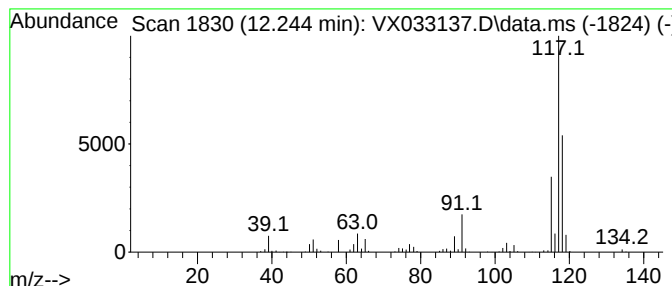
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Quant Title : SW846 8260

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.
12.244	44.08 ug/l	469071	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	81
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	72
5			Deltacyclene	118	C9H10	007785-10-6	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033137.D
Acq On : 30 Nov 2022 17:14
Operator : JC/MD
Sample : N5815-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.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	1.374	64.5	ug/l	443149	1	5.550	343502	50.0
Butane, 2-methyl-	1.752	286.9	ug/l	1970700	1	5.550	343502	50.0
Cyclopropane, 1...	2.215	8.6	ug/l	58780	1	5.550	343502	50.0
Butane, 2,2-dim...	2.343	15.3	ug/l	104861	1	5.550	343502	50.0
Butane, 2,3-dim...	2.782	36.5	ug/l	250823	1	5.550	343502	50.0
Furan, tetrahyd...	2.831	13.5	ug/l	92713	1	5.550	343502	50.0
1-Pentene	2.867	35.6	ug/l	244707	1	5.550	343502	50.0
Cyclopentane, m...	4.306	39.7	ug/l	272758	1	5.550	343502	50.0
Indane	12.244	44.1	ug/l	469071	4	12.024	532011	50.0