

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100623\
 Data File : VX038124.D
 Acq On : 06 Oct 2023 12:38
 Operator : JC/MD
 Sample : 04723-03 200X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-6A

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\82X100523W.M
 Title : SW846 8260

Signal : TIC: VX038124.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	53	rBV	49901	52022	4.05%	0.825%
2	1.453	57	60	65	rVB	13303	13961	1.09%	0.221%
3	1.752	104	109	117	rBV	63731	84897	6.61%	1.346%
4	1.959	138	143	153	rVB3	33088	65682	5.11%	1.041%
5	2.069	156	161	169	rVV	20561	32710	2.55%	0.519%
6	2.166	172	177	180	rVV	14065	23269	1.81%	0.369%
7	2.215	180	185	196	rVB	48912	70190	5.46%	1.113%
8	2.751	266	273	277	rBV2	10621	19736	1.54%	0.313%
9	2.867	287	292	300	rVB3	13654	28179	2.19%	0.447%
10	4.306	519	528	541	rVB3	8870	23956	1.87%	0.380%
11	4.568	558	571	586	rBV	8414	29252	2.28%	0.464%
12	5.202	664	675	686	rVB2	4870	14120	1.10%	0.224%
13	5.391	694	706	717	rBV	69682	205324	15.99%	3.255%
14	5.556	723	733	749	rVB	111802	324371	25.25%	5.143%
15	5.958	788	799	806	rBV	79562	212318	16.53%	3.366%
16	6.043	806	813	829	rVB	72441	194056	15.11%	3.077%
17	6.763	918	931	957	rBV2	188887	459485	35.77%	7.285%
18	8.653	1234	1241	1246	rBV	393904	632945	49.28%	10.035%
19	8.720	1246	1252	1267	rVB	826707	1284445	100.00%	20.364%
20	10.055	1465	1471	1484	rBV	433067	594148	46.26%	9.420%
21	10.195	1489	1494	1503	rVV	108139	142377	11.08%	2.257%
22	10.299	1505	1511	1526	rVB	256097	347554	27.06%	5.510%
23	10.640	1562	1567	1578	rVB	85159	111178	8.66%	1.763%
24	11.079	1634	1639	1651	rBV	358397	468290	36.46%	7.425%
25	11.378	1682	1688	1697	rVV	27532	52858	4.12%	0.838%
26	11.451	1697	1700	1706	rVB2	12567	15851	1.23%	0.251%
27	11.616	1721	1727	1736	rBV	14531	19157	1.49%	0.304%
28	11.750	1745	1749	1755	rBV	58201	75666	5.89%	1.200%
29	12.024	1788	1794	1800	rBV	484250	631132	49.14%	10.006%
30	12.085	1800	1804	1810	rVB	18471	23227	1.81%	0.368%
31	12.244	1824	1830	1838	rBV	21253	28006	2.18%	0.444%
32	13.774	2076	2081	2087	rBV	20217	26996	2.10%	0.428%

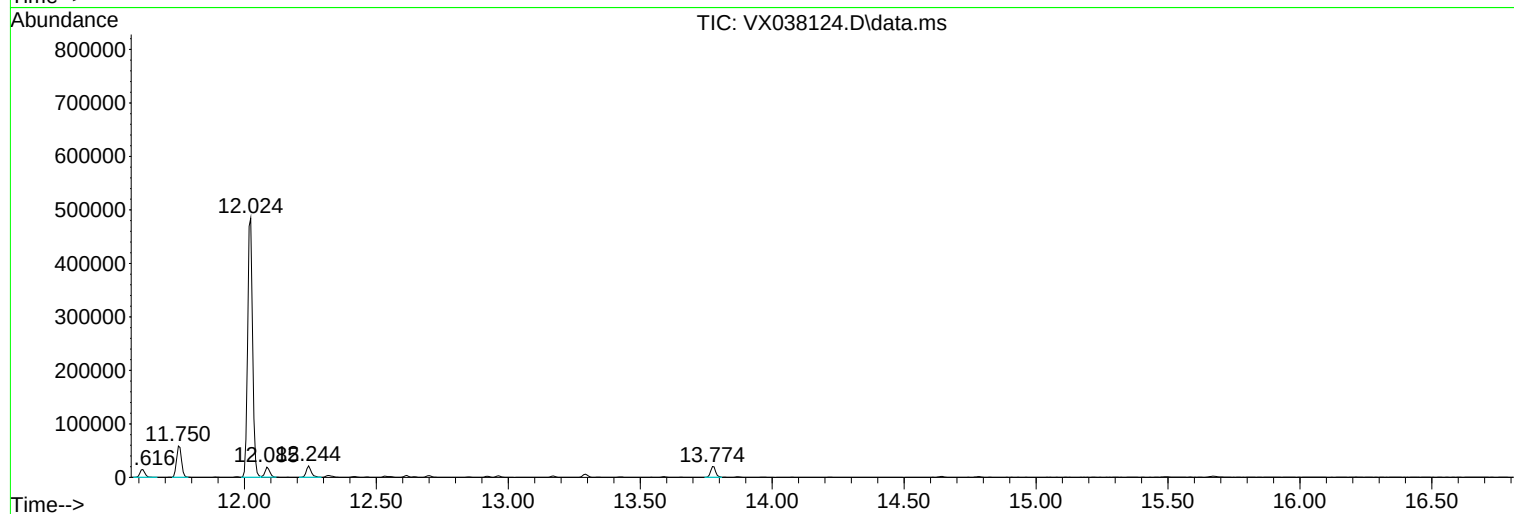
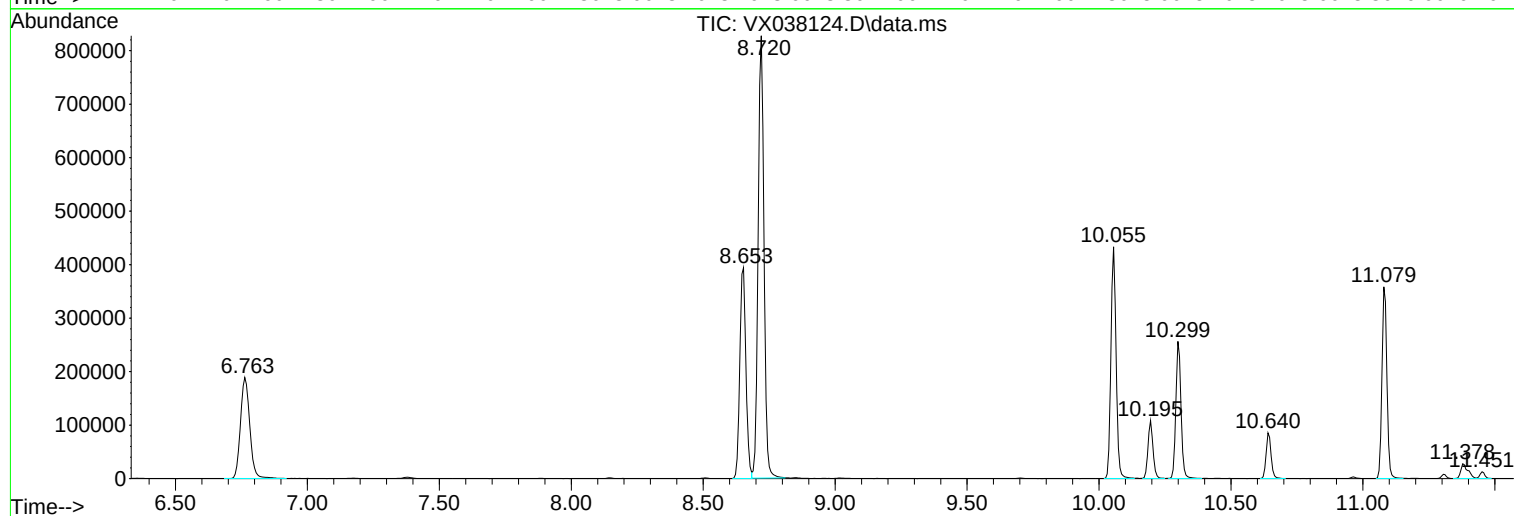
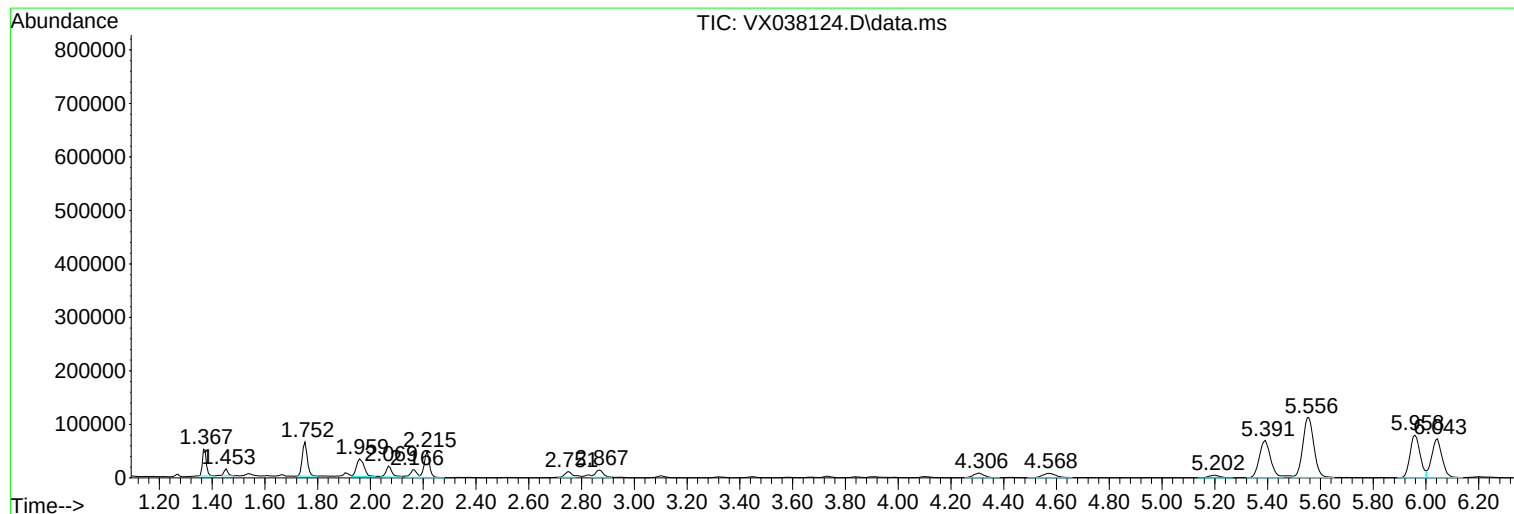
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Instrument :
MSVOA_X
ClientSampleId :
MW-6A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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



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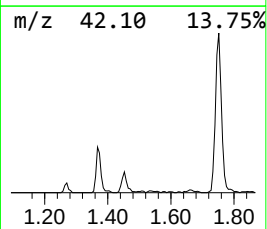
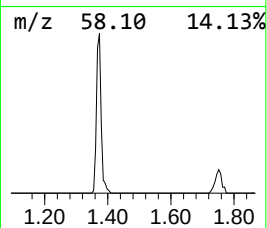
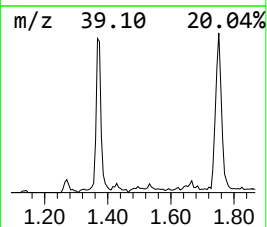
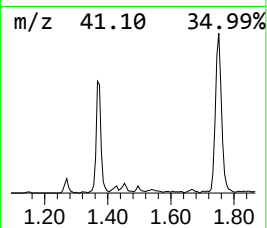
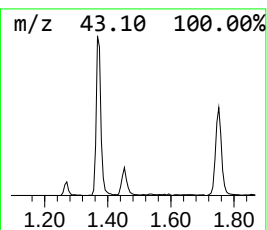
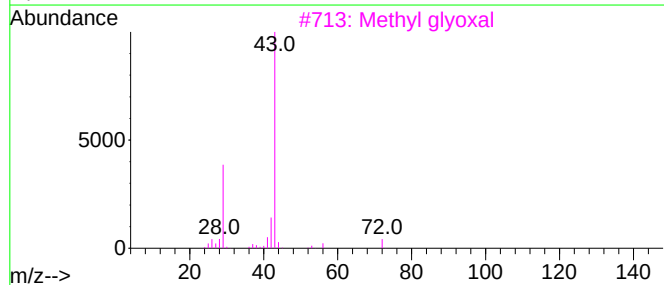
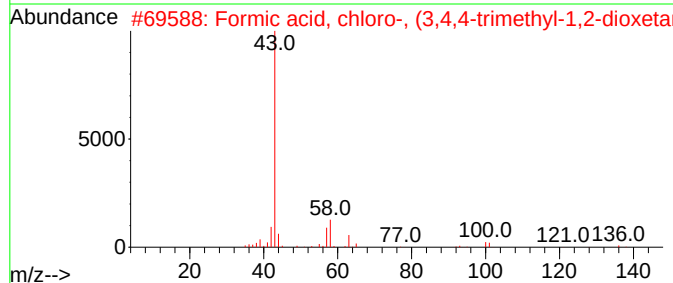
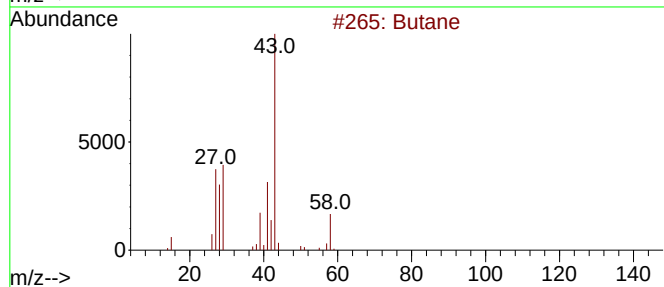
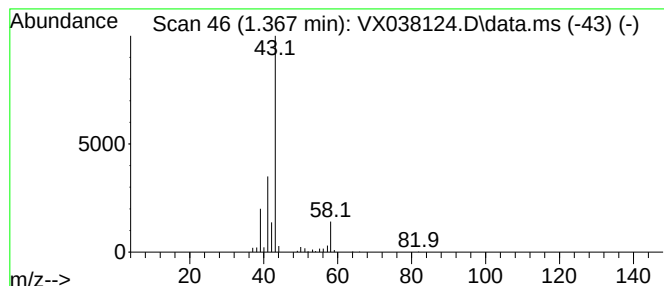
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.367	8.02 ug/l	52022	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	39
3			Methyl glyoxal	72	C3H4O2	000078-98-8	9
4			Isobutane	58	C4H10	000075-28-5	5
5			Acetone	58	C3H6O	000067-64-1	5



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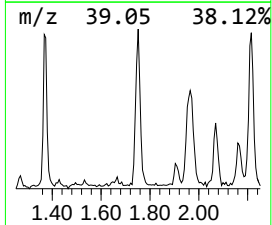
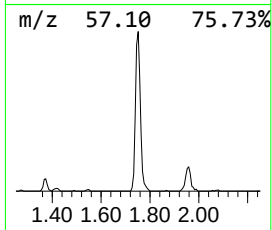
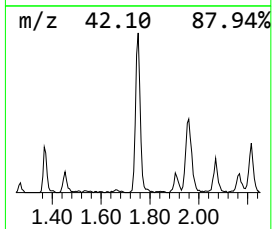
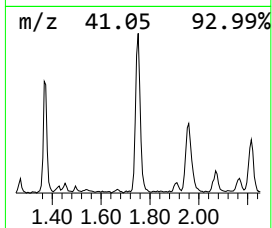
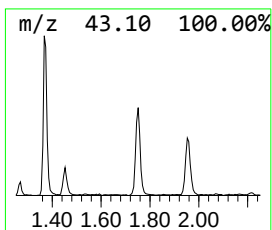
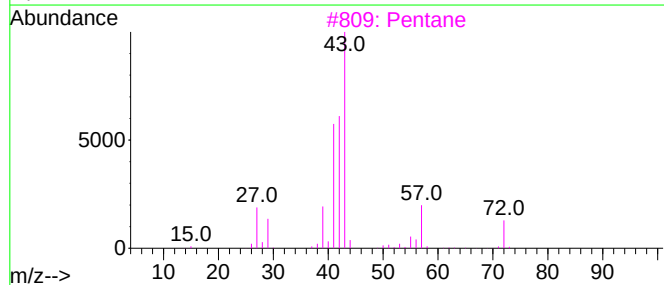
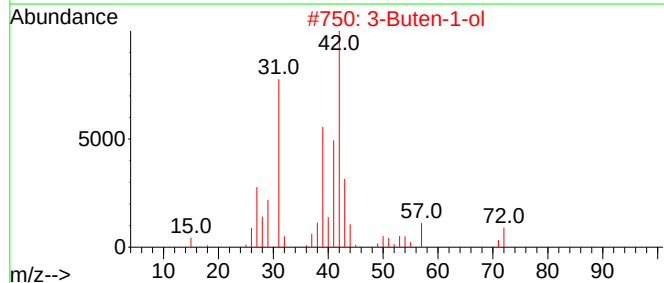
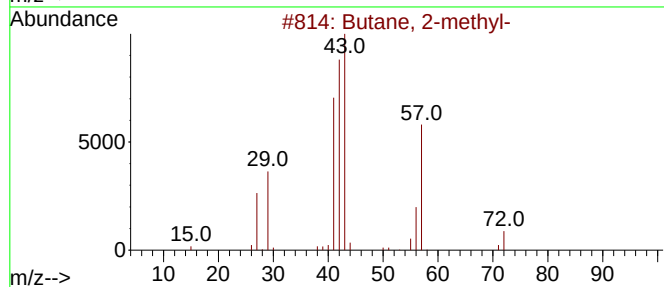
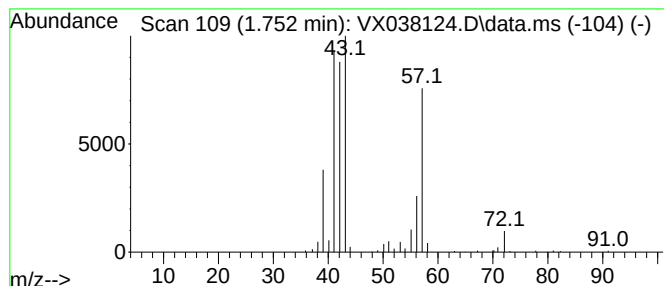
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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.
1.752	13.09 ug/l	84897	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	64
2			3-Buten-1-ol	72	C4H8O	000627-27-0	33
3			Pentane	72	C5H12	000109-66-0	33
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	25
5			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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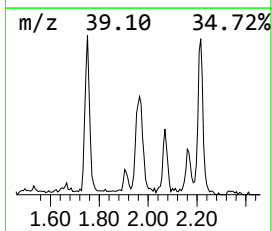
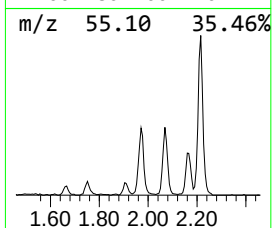
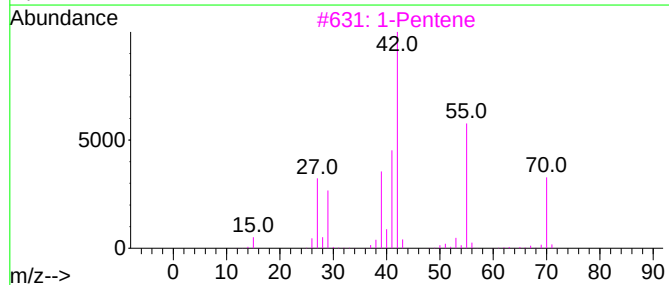
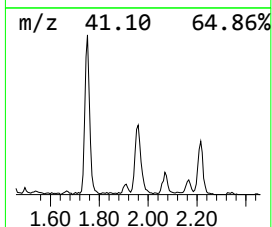
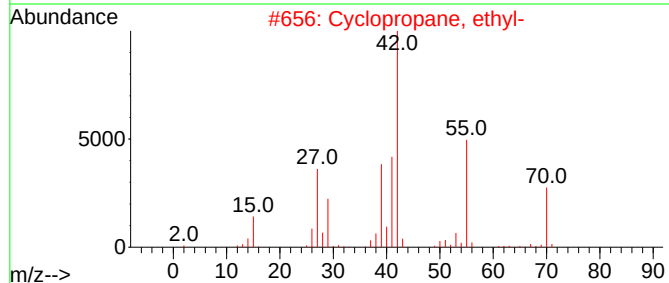
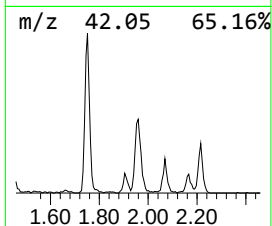
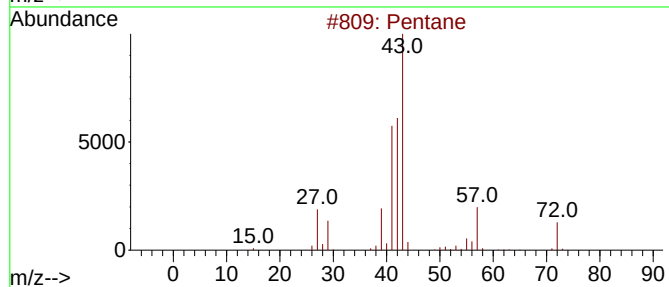
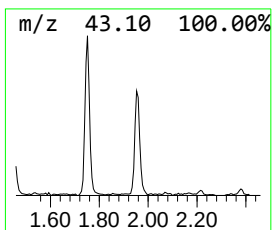
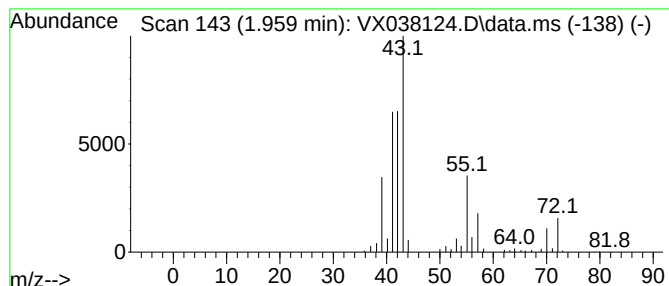
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	10.12 ug/l	65682	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	80
2			Cyclopropane, ethyl-	70	C5H10	001191-96-4	43
3			1-Pentene	70	C5H10	000109-67-1	43
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	43
5			Oxirane, ethyl-	72	C4H8O	000106-88-7	37



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

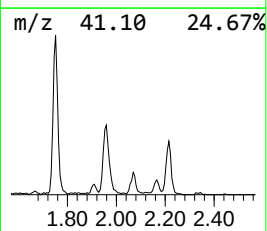
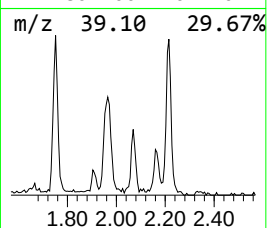
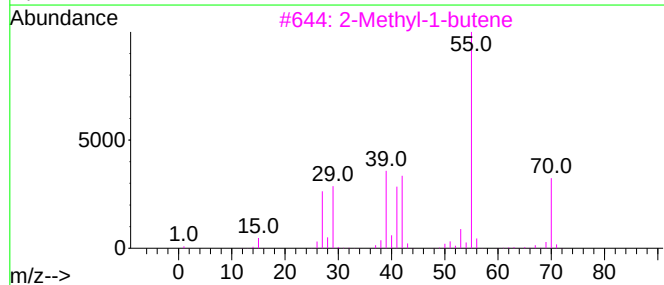
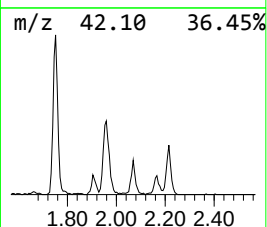
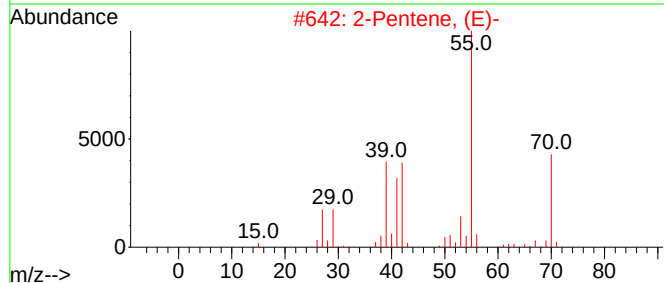
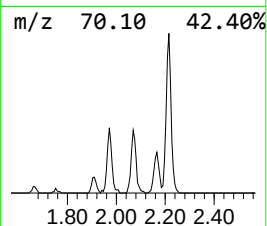
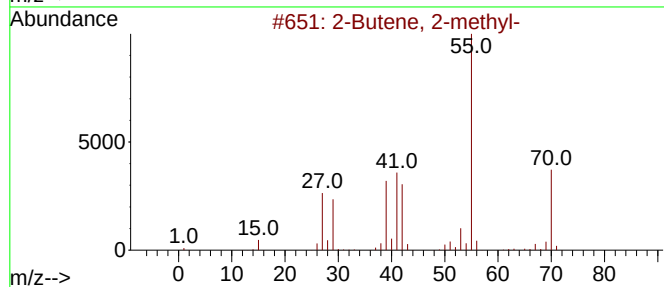
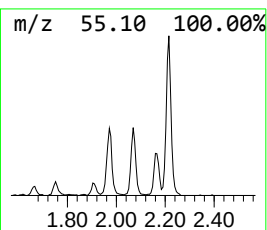
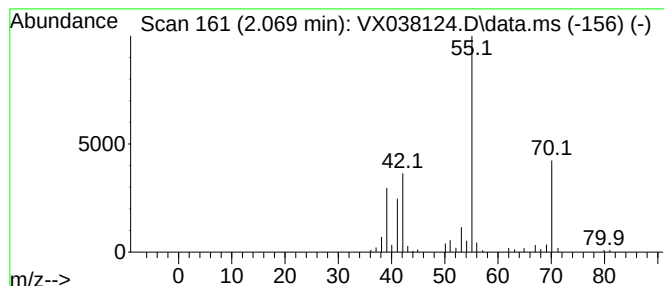
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	5.04 ug/l	32710	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
2		2-Pentene, (E)-	70	C5H10	000646-04-8	90
3		2-Methyl-1-butene	70	C5H10	000563-46-2	87
4		2-Pentene, (Z)-	70	C5H10	000627-20-3	87
5		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	86



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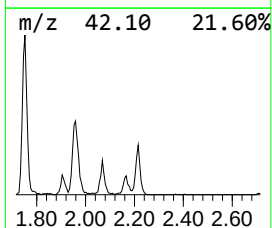
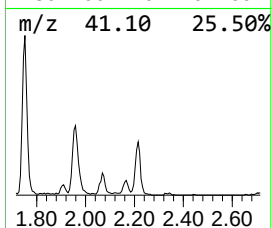
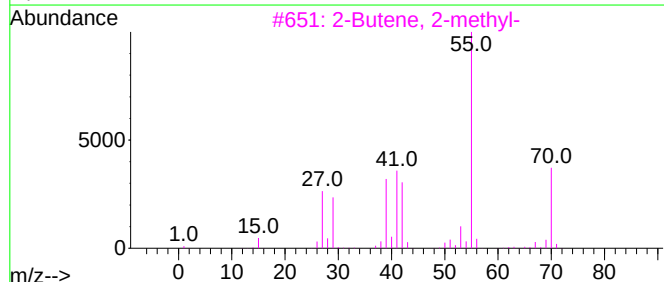
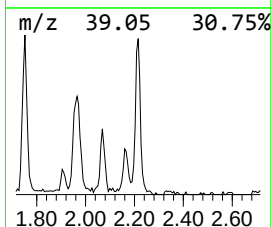
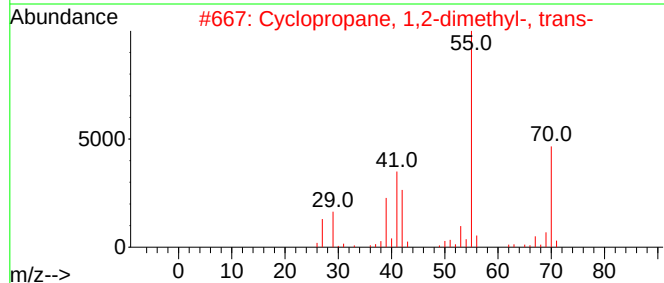
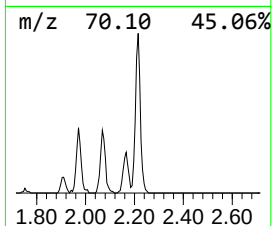
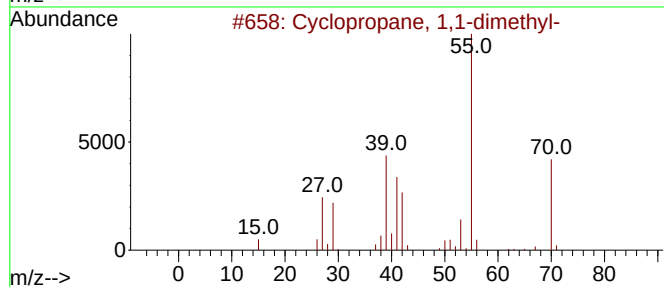
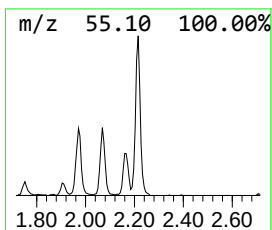
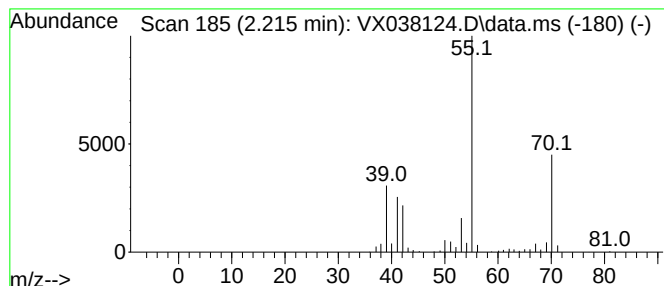
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclopropane, 1,1-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	10.82 ug/l	70190	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	72
2			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	72
3			2-Butene, 2-methyl-	70	C5H10	000513-35-9	72
4			1-Butene, 3-methyl-	70	C5H10	000563-45-1	72
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	62



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	1.367	8.0	ug/l	52022	1	5.556	324371	50.0
Butane, 2-methyl-	1.752	13.1	ug/l	84897	1	5.556	324371	50.0
Pentane	1.959	10.1	ug/l	65682	1	5.556	324371	50.0
2-Butene, 2-met...	2.069	5.0	ug/l	32710	1	5.556	324371	50.0
Cyclopropane, 1...	2.215	10.8	ug/l	70190	1	5.556	324371	50.0