

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111422\
 Data File : VX032793.D
 Acq On : 14 Nov 2022 14:41
 Operator : JC/MD
 Sample : N5551-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-14D

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\82X102622W.M
 Title : SW846 8260

Signal : TIC: VX032793.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	41	rVB	33363	32383	6.46%	0.835%
2	1.374	41	47	53	rBV	64704	70956	14.15%	1.829%
3	1.660	87	94	102	rVB	8492	11903	2.37%	0.307%
4	1.752	102	109	117	rVV	98646	130986	26.12%	3.377%
5	1.843	119	124	128	rVV	19114	26758	5.34%	0.690%
6	1.910	128	135	139	rVV2	14777	29253	5.83%	0.754%
7	1.965	139	144	154	rVB2	29682	61719	12.31%	1.591%
8	2.069	156	161	169	rBV	29222	41399	8.25%	1.067%
9	2.166	169	177	181	rVV	27631	41310	8.24%	1.065%
10	2.215	181	185	193	rVB	22673	34665	6.91%	0.894%
11	2.325	197	203	210	rBV	10755	18228	3.63%	0.470%
12	2.751	261	273	276	rBV2	11341	25447	5.07%	0.656%
13	2.788	277	279	282	rVV3	7376	10635	2.12%	0.274%
14	2.873	284	293	302	rVV2	24156	61697	12.30%	1.591%
15	2.934	302	303	315	rVB4	2953	5700	1.14%	0.147%
16	3.105	320	331	339	rBV2	5414	12160	2.42%	0.313%
17	3.325	358	367	374	rBV4	3199	7534	1.50%	0.194%
18	3.605	404	413	419	rBV5	3024	9892	1.97%	0.255%
19	3.843	444	452	457	rBV3	2593	6191	1.23%	0.160%
20	3.904	457	462	471	rVV4	5637	17974	3.58%	0.463%
21	3.989	474	476	484	rVB3	3091	5893	1.18%	0.152%
22	4.300	516	527	539	rBV3	15977	45643	9.10%	1.177%
23	4.489	550	558	566	rBV3	15521	43183	8.61%	1.113%
24	5.105	647	659	665	rBV2	2569	7498	1.50%	0.193%
25	5.385	695	705	715	rBV2	61373	182291	36.35%	4.699%
26	5.477	715	720	724	rVV4	5074	12991	2.59%	0.335%
27	5.556	724	733	747	rVB	97918	277535	55.34%	7.155%
28	5.958	789	799	806	rBV	65367	173330	34.56%	4.468%
29	6.044	806	813	826	rVB2	41764	111775	22.29%	2.882%
30	6.202	829	839	844	rBV3	5051	13488	2.69%	0.348%
31	6.763	920	931	952	rBV	147820	361951	72.17%	9.331%
32	7.129	982	991	1004	rVB	66139	144396	28.79%	3.722%
33	8.647	1234	1240	1249	rBV	319616	501503	100.00%	12.928%
34	8.720	1249	1252	1261	rVB2	2887	5148	1.03%	0.133%
35	8.958	1286	1291	1298	rVV2	7946	11918	2.38%	0.307%
36	9.049	1301	1306	1316	rVB	7644	12079	2.41%	0.311%

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Peak separation: 5

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37	9.275	1338	1343	1349	rVB	17924	25333	5.05%	0.653%
38	10.055	1465	1471	1483	rBV	320745	422677	84.28%	10.896%
39	10.195	1490	1494	1500	rVB	12927	16231	3.24%	0.418%
40	10.305	1506	1512	1521	rBV2	13634	19581	3.90%	0.505%
41	10.640	1563	1567	1572	rBV	14131	18986	3.79%	0.489%
42	11.079	1634	1639	1650	rBV	289298	376421	75.06%	9.704%
43	11.756	1745	1750	1754	rVB	5559	6959	1.39%	0.179%
44	12.024	1788	1794	1801	rBV	323291	405479	80.85%	10.453%
45	12.085	1801	1804	1817	rVB	14829	19974	3.98%	0.515%

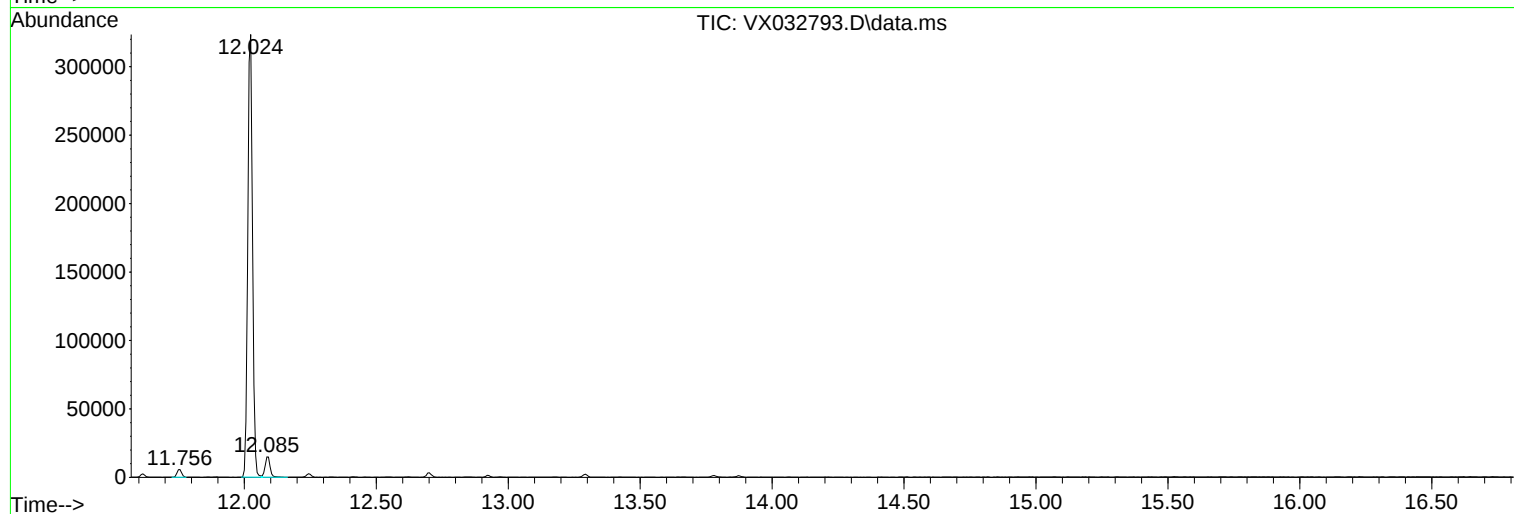
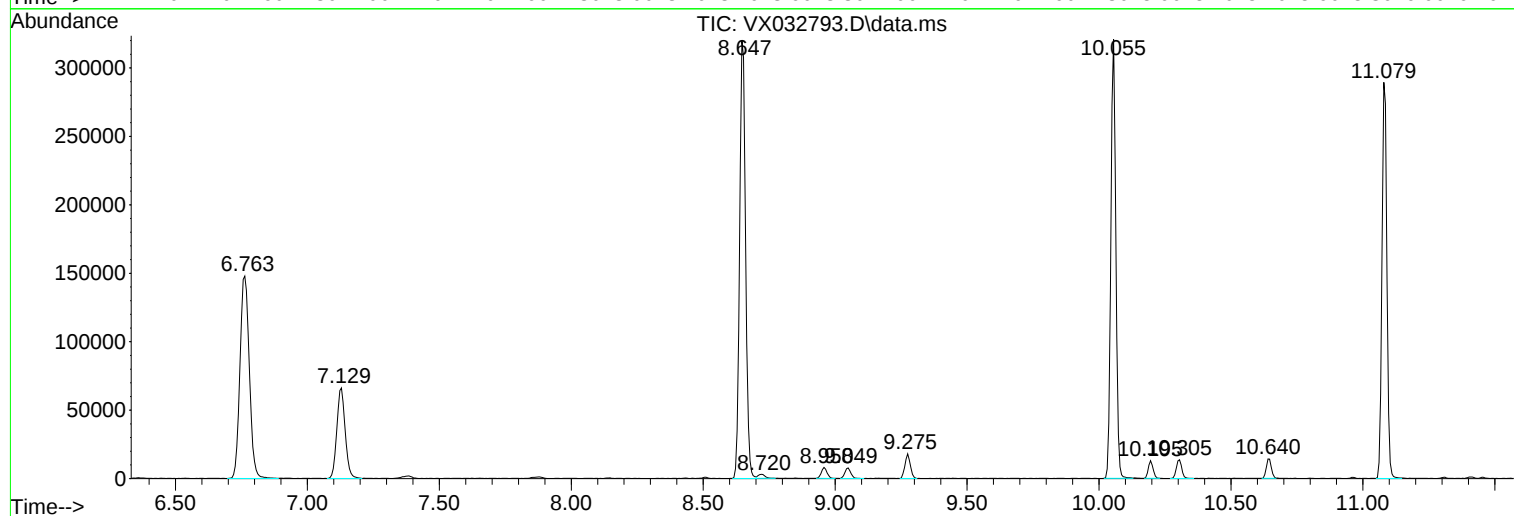
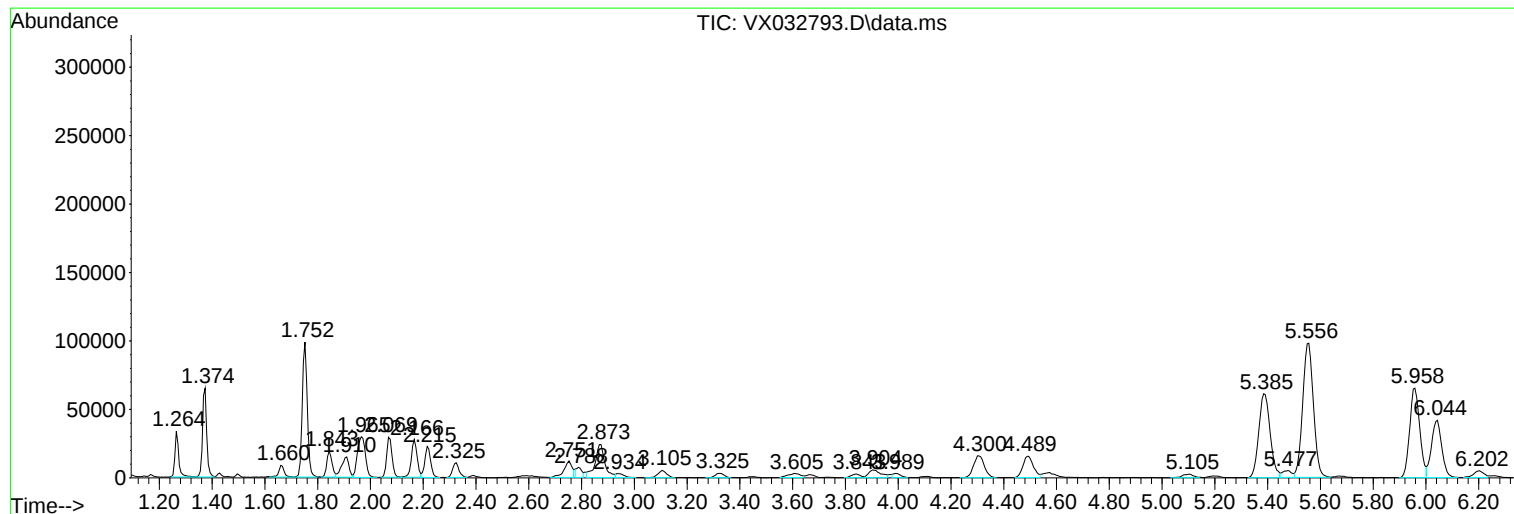
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



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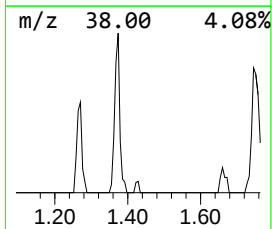
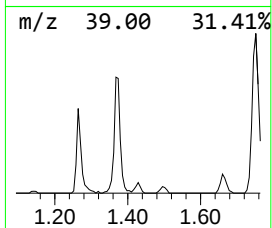
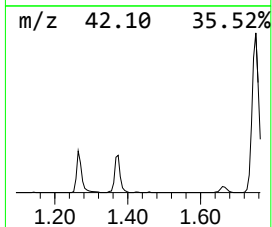
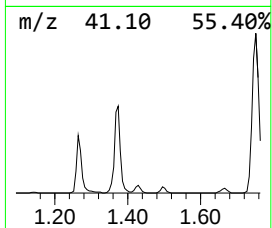
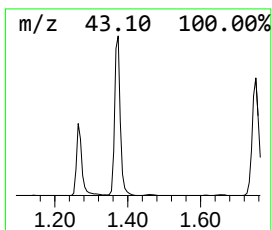
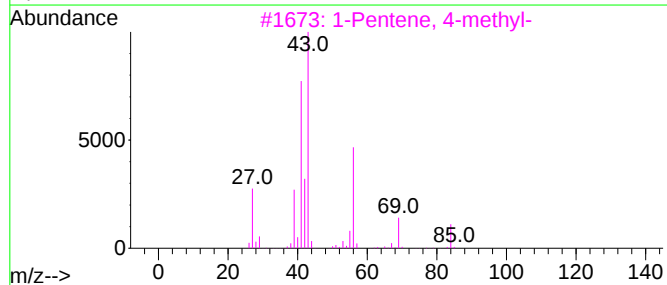
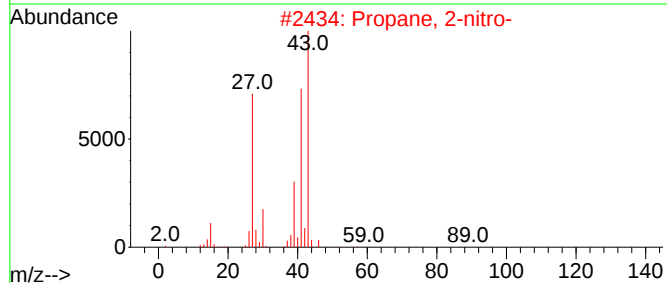
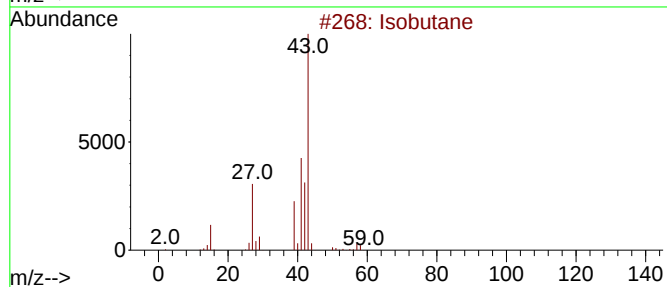
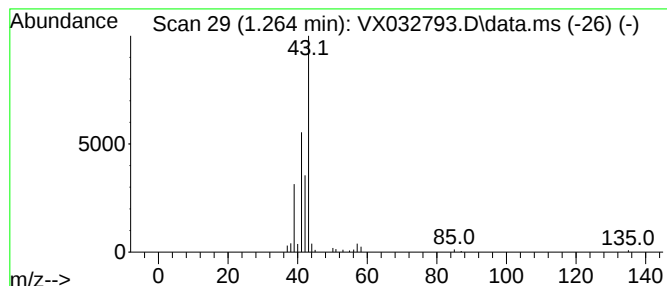
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	5.83 ug/l	32383	Pentafluorobenzene	5.556

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			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	9
4			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	9
5			5-Methyloxazolidine	87	C4H9NO	058328-22-6	7



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Instrument :
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ClientSampleId :
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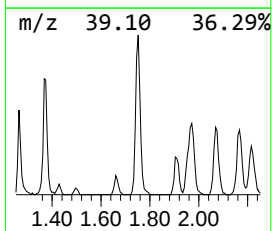
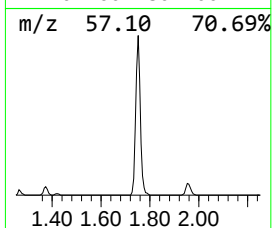
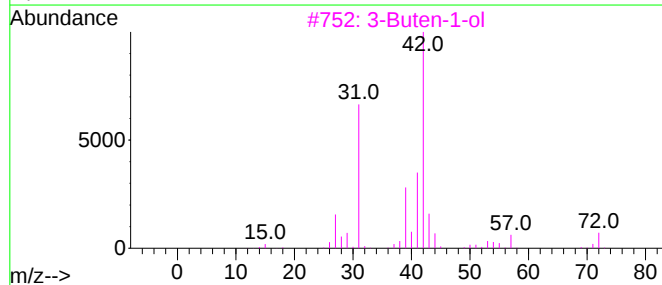
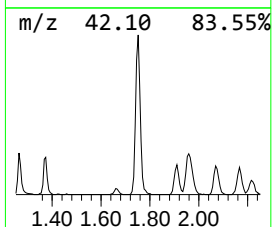
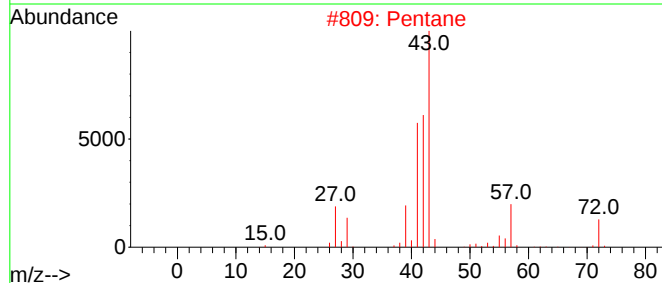
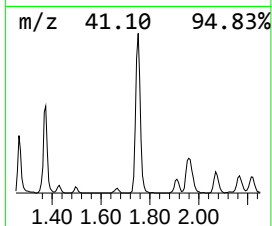
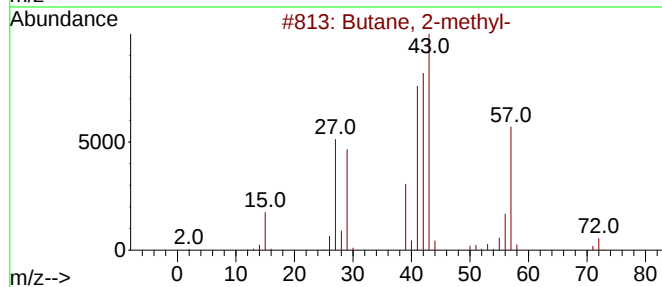
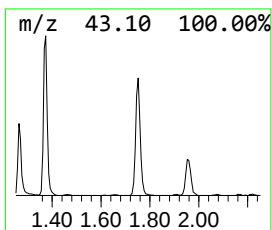
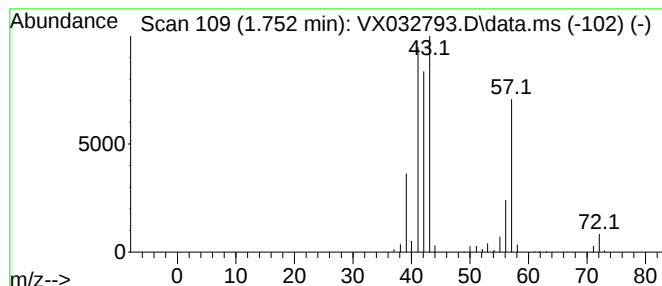
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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	23.60 ug/l	130986	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	36
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			1-Butene	56	C4H8	000106-98-9	9
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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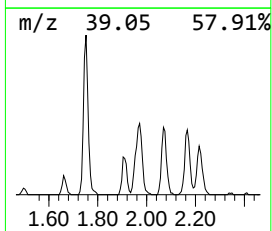
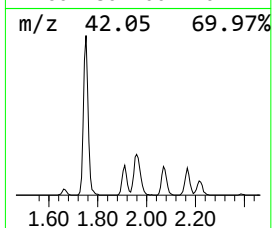
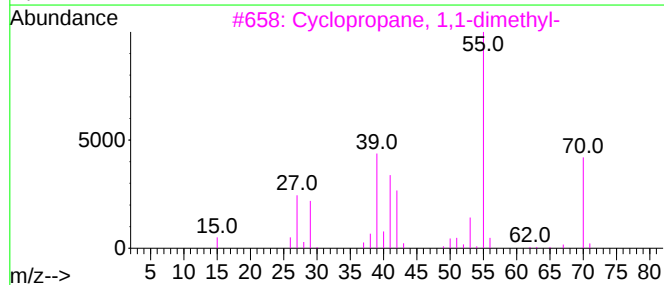
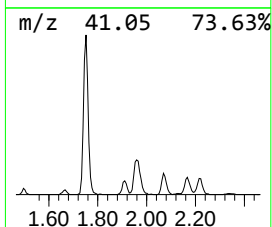
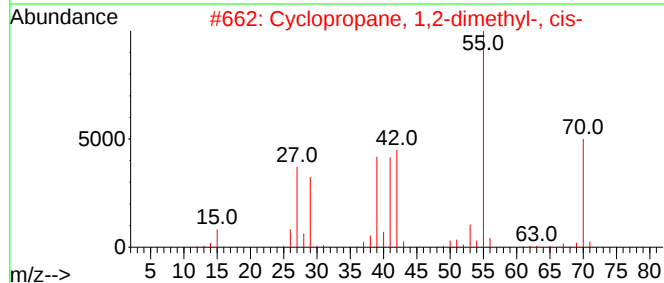
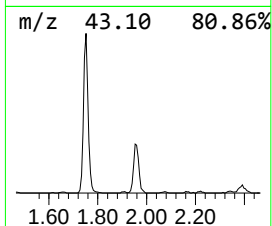
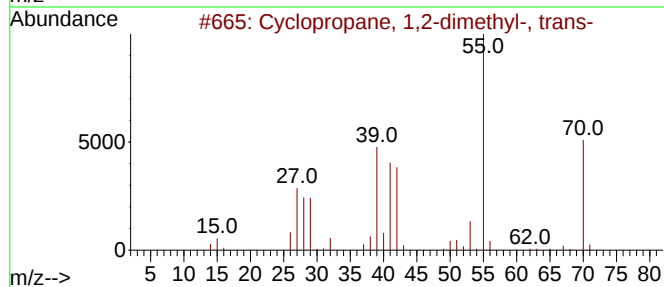
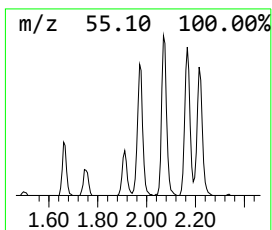
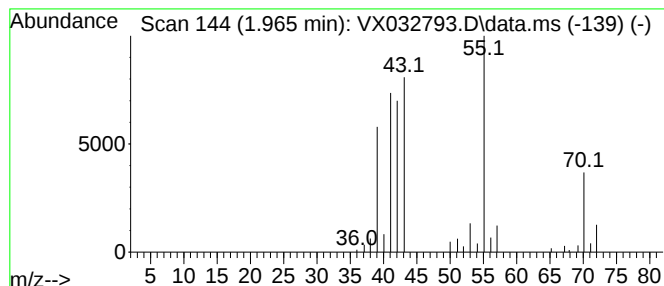
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopropane, 1,2-dimethyl-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.965	11.12 ug/l	61719	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	59
2			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	58
3			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	46
4			2-Pentene, (Z)-	70	C5H10	000627-20-3	43
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	43



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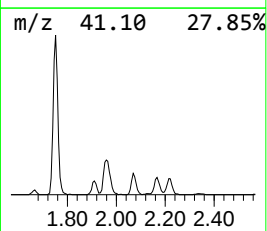
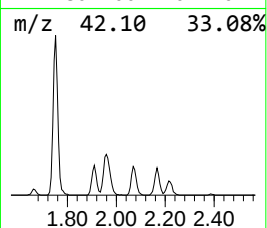
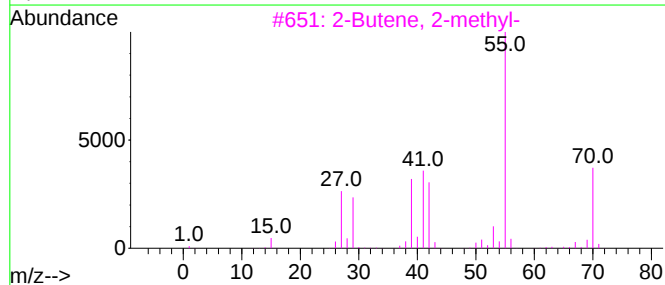
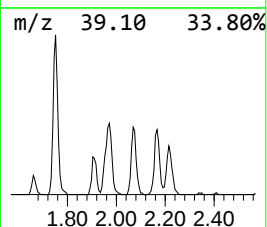
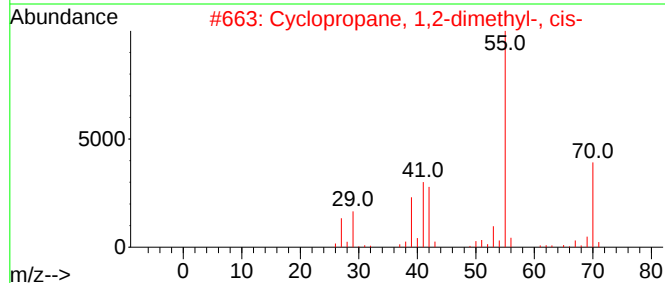
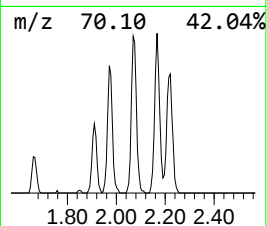
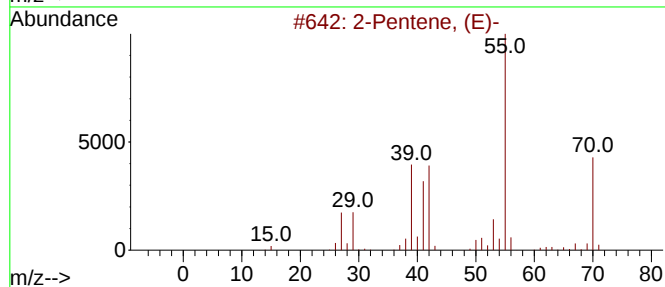
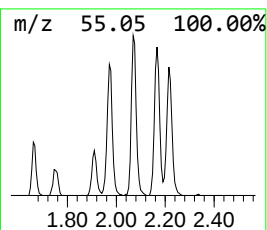
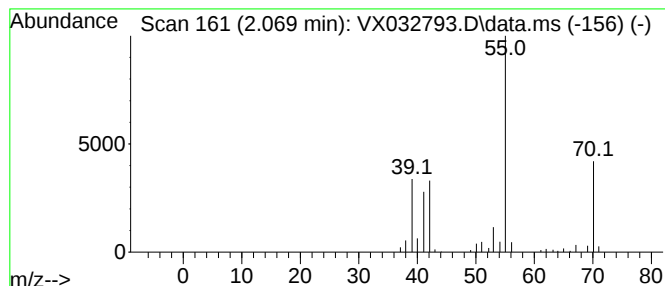
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Quant Title : SW846 8260

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

Peak Number 4 2-Pentene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	7.46 ug/l	41399	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-Butene, 2-methyl-	70	C5H10	000513-35-9	90
4			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	90
5			2-Methyl-1-butene	70	C5H10	000563-46-2	87



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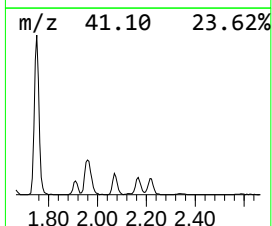
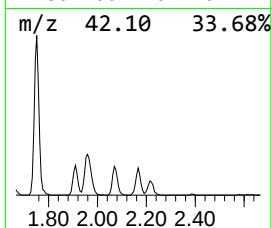
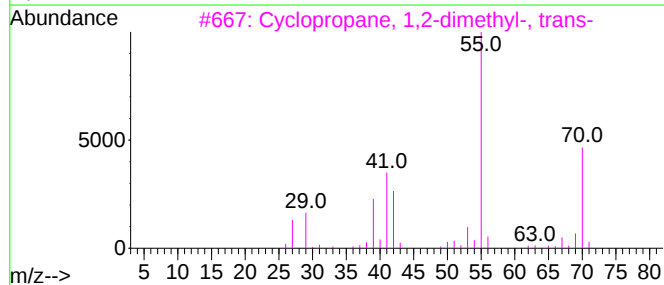
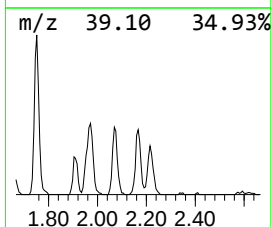
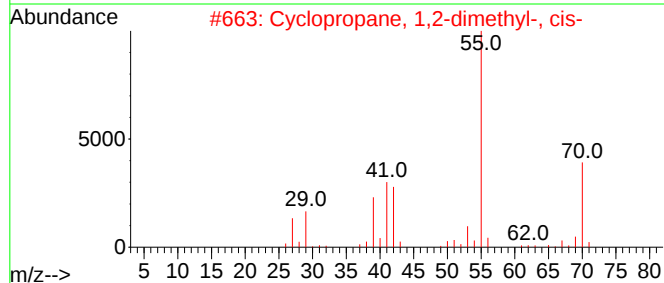
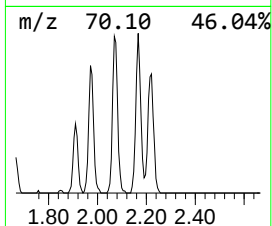
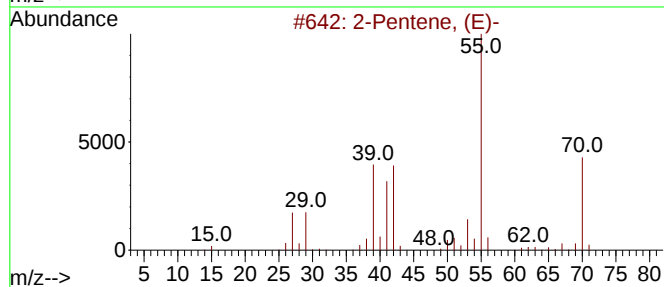
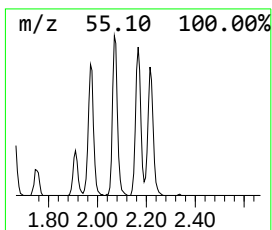
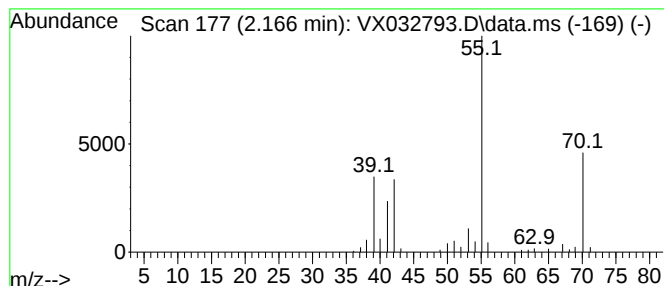
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.166	7.44 ug/l	41310	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	91
3	Cyclopropane, 1,2-dimethyl-, trans-			70	C5H10	002402-06-4	91
4	2-Butene, 2-methyl-			70	C5H10	000513-35-9	87
5	2-Methyl-1-butene			70	C5H10	000563-46-2	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111422\
Data File : VX032793.D
Acq On : 14 Nov 2022 14:41
Operator : JC/MD
Sample : N5551-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14D

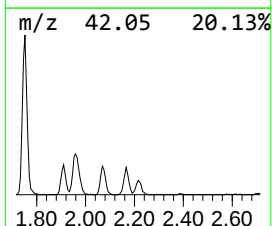
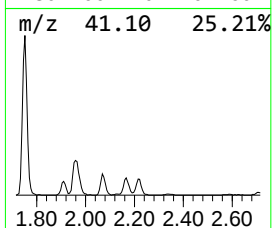
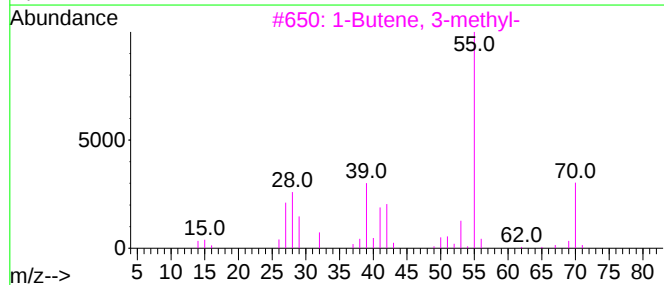
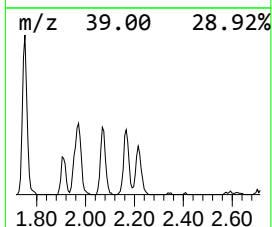
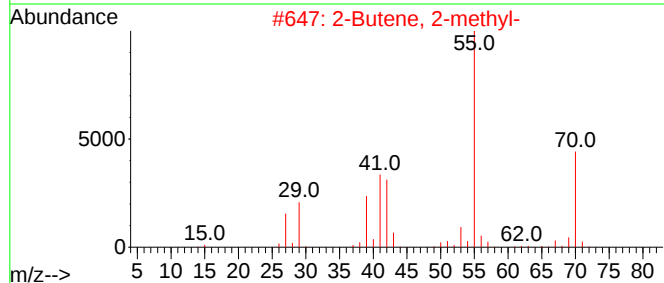
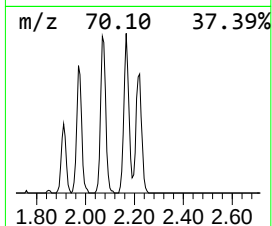
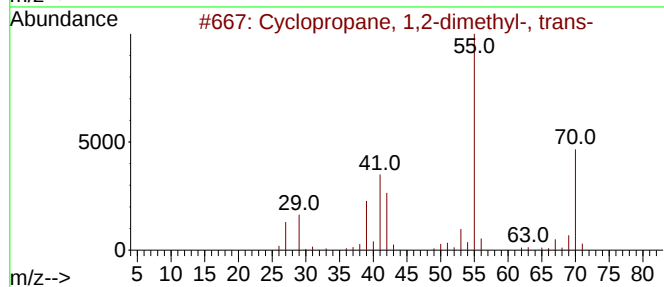
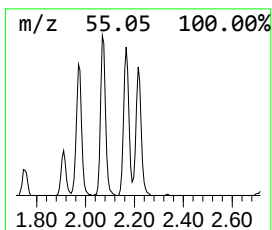
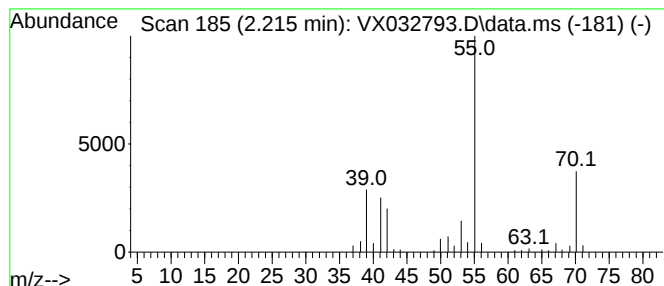
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Quant Title : SW846 8260

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

Peak Number 6 2-Butene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	6.25 ug/l	34665	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
3			1-Butene, 3-methyl-	70	C5H10	000563-45-1	80
4			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
5			2-Methyl-1-butene	70	C5H10	000563-46-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111422\
Data File : VX032793.D
Acq On : 14 Nov 2022 14:41
Operator : JC/MD
Sample : N5551-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14D

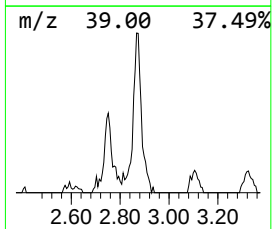
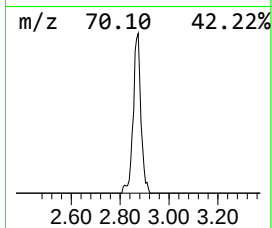
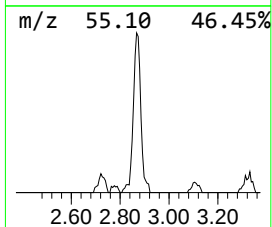
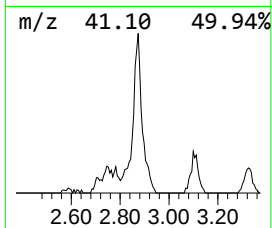
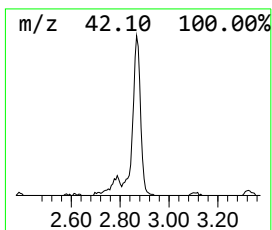
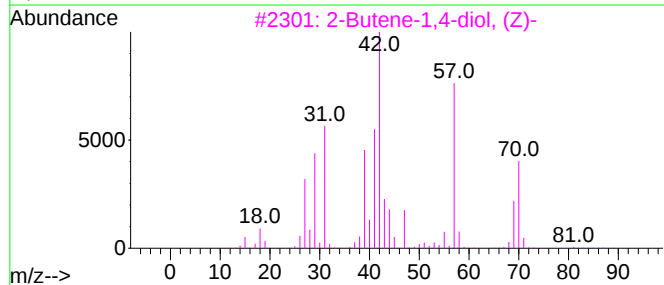
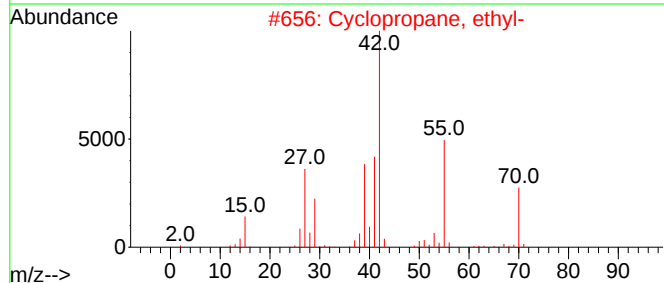
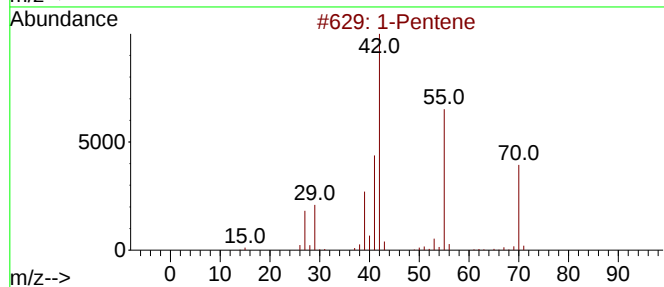
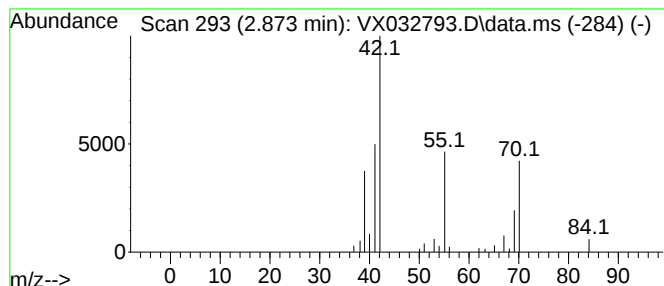
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Quant Title : SW846 8260

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

Peak Number 7 1-Pentene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.873	11.12 ug/l	61697	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene		70	C5H10	000109-67-1	72
2	Cyclopropane, ethyl-		70	C5H10	001191-96-4	64
3	2-Butene-1,4-diol, (Z)-		88	C4H8O2	006117-80-2	39
4	3-Buten-1-ol		72	C4H8O	000627-27-0	25
5	Cyclopentane		70	C5H10	000287-92-3	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111422\
Data File : VX032793.D
Acq On : 14 Nov 2022 14:41
Operator : JC/MD
Sample : N5551-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14D

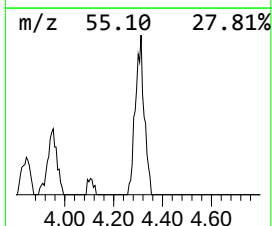
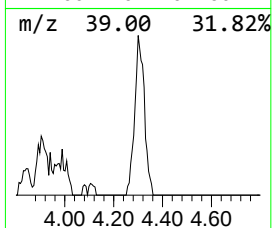
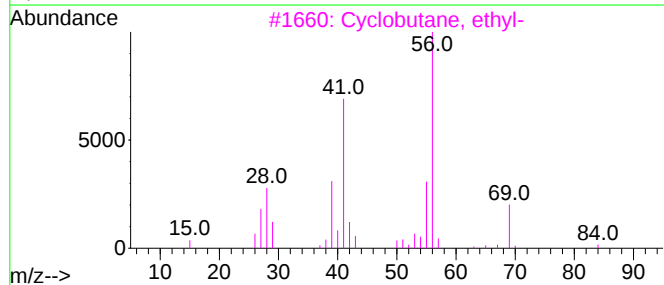
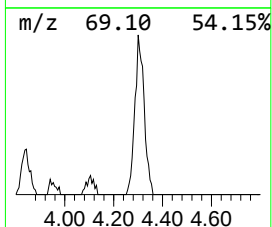
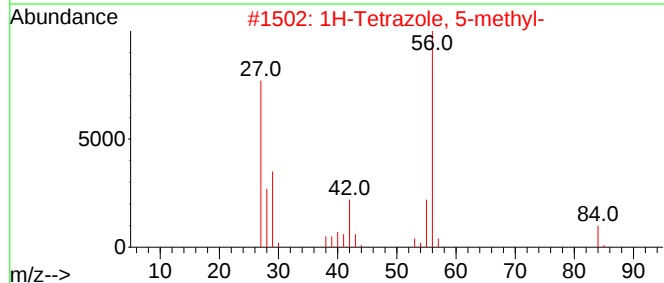
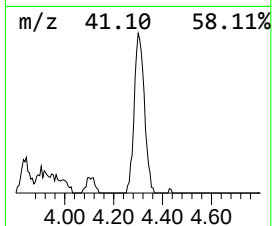
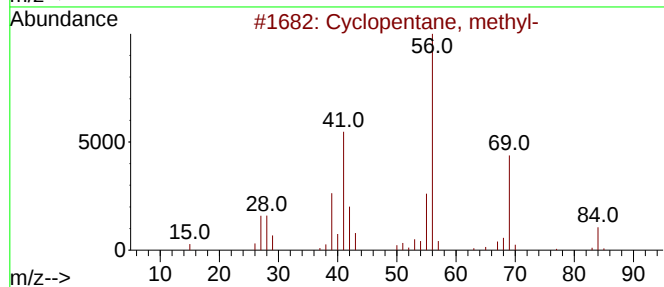
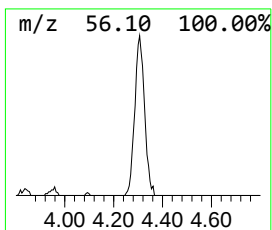
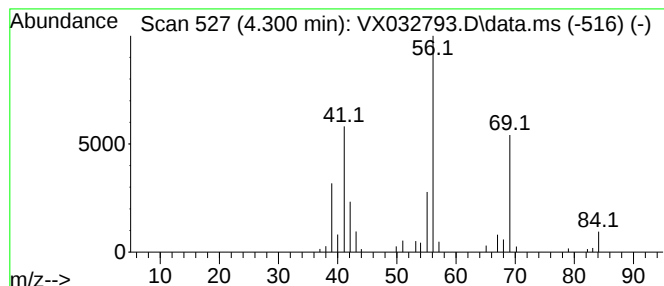
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	8.22 ug/l	45643	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4			2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	50
5			Aziridine, 1-(2-buten-2-yl)-	97	C6H11N	1000158-95-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111422\
Data File : VX032793.D
Acq On : 14 Nov 2022 14:41
Operator : JC/MD
Sample : N5551-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.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
Isobutane	1.264	5.8	ug/l	32383	1	5.556	277535	50.0
Butane, 2-methyl-	1.752	23.6	ug/l	130986	1	5.556	277535	50.0
Cyclopropane, 1...	1.965	11.1	ug/l	61719	1	5.556	277535	50.0
2-Pentene, (E)-	2.069	7.5	ug/l	41399	1	5.556	277535	50.0
Cyclopropane, 1...	2.166	7.4	ug/l	41310	1	5.556	277535	50.0
2-Butene, 2-met...	2.215	6.3	ug/l	34665	1	5.556	277535	50.0
1-Pentene	2.873	11.1	ug/l	61697	1	5.556	277535	50.0
Cyclopentane, m...	4.300	8.2	ug/l	45643	1	5.556	277535	50.0