

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091922\
 Data File : VY010565.D
 Acq On : 19 Sep 2022 20:45
 Operator : KP/MD
 Sample : N4641-07
 Misc : 5.99g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 A1-8-17.5

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_Y\methods\82Y091922S.M

Title : SW846 8260

Signal : TIC: VY010565.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.070	32	41	57	rBV	213652	305327	6.74%	2.246%
2	2.241	59	69	78	rVV	346149	570120	12.59%	4.193%
3	2.893	167	176	194	rBV	268599	593913	13.11%	4.368%
4	3.942	338	348	362	rBV	50146	142865	3.15%	1.051%
5	4.704	464	473	479	rBV2	15805	48645	1.07%	0.358%
6	4.796	479	488	500	rVV3	50951	177908	3.93%	1.309%
7	4.948	500	513	531	rVB	57212	216462	4.78%	1.592%
8	5.210	539	556	588	rBV	1264965	4528997	100.00%	33.311%
9	6.112	689	704	716	rBV3	40477	137611	3.04%	1.012%
10	6.978	837	846	860	rBV2	20449	59283	1.31%	0.436%
11	7.527	926	936	950	rBV3	203680	557651	12.31%	4.102%
12	7.710	956	966	972	rBV	140110	336084	7.42%	2.472%
13	7.783	972	978	990	rVB	251183	573442	12.66%	4.218%
14	8.149	1025	1038	1046	rBV3	330649	868569	19.18%	6.388%
15	8.234	1046	1052	1064	rVB2	89099	212692	4.70%	1.564%
16	8.685	1117	1126	1140	rBV	376346	747730	16.51%	5.500%
17	9.971	1333	1337	1347	rVB	41391	77150	1.70%	0.567%
18	10.173	1362	1370	1379	rBV	570006	982920	21.70%	7.229%
19	10.289	1383	1389	1398	rVB	45248	78599	1.74%	0.578%
20	11.490	1578	1586	1598	rBV	535767	892261	19.70%	6.563%
21	12.477	1741	1748	1761	rBV2	429426	688561	15.20%	5.064%
22	13.422	1890	1903	1913	rBV	518535	799254	17.65%	5.879%

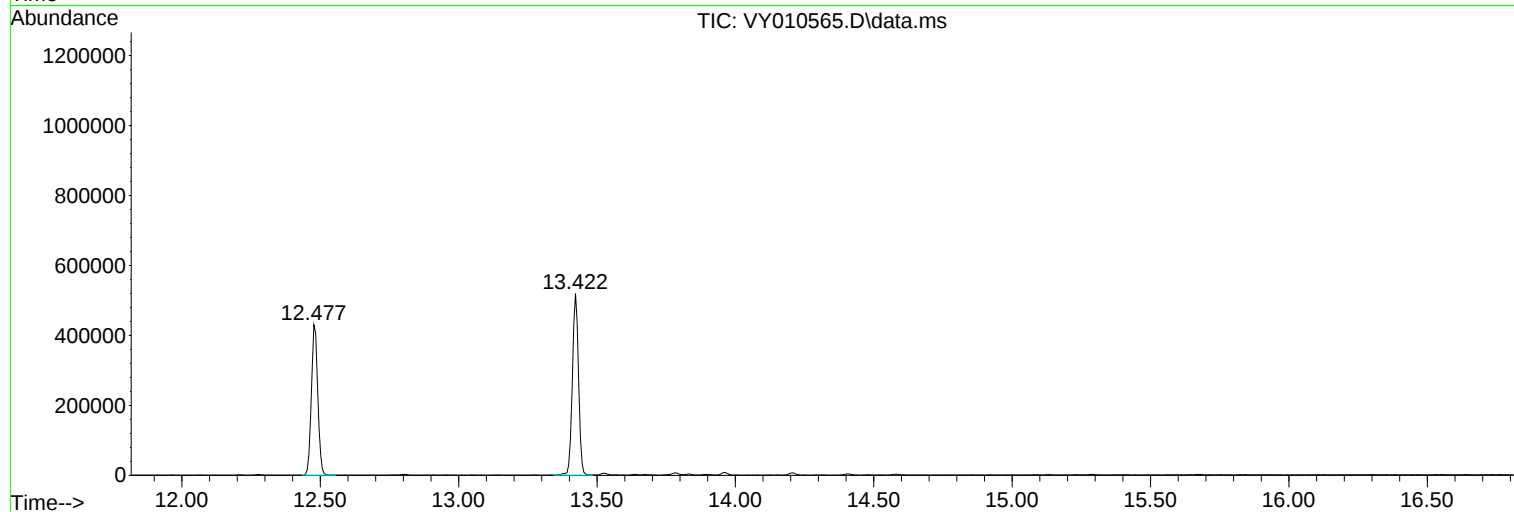
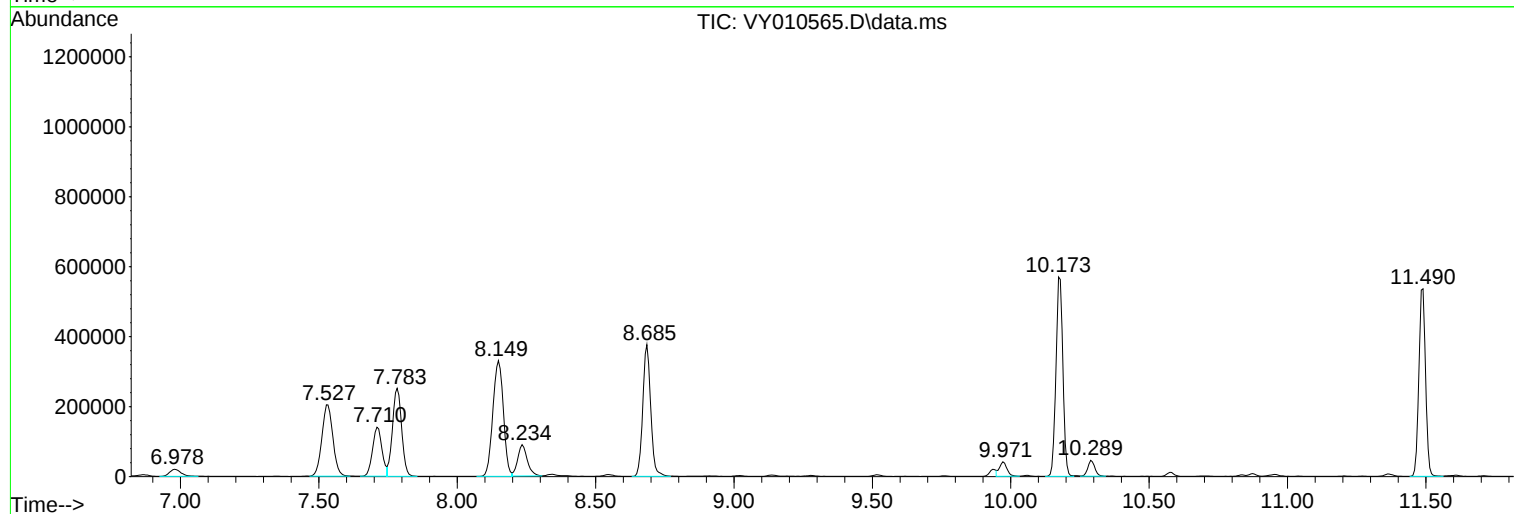
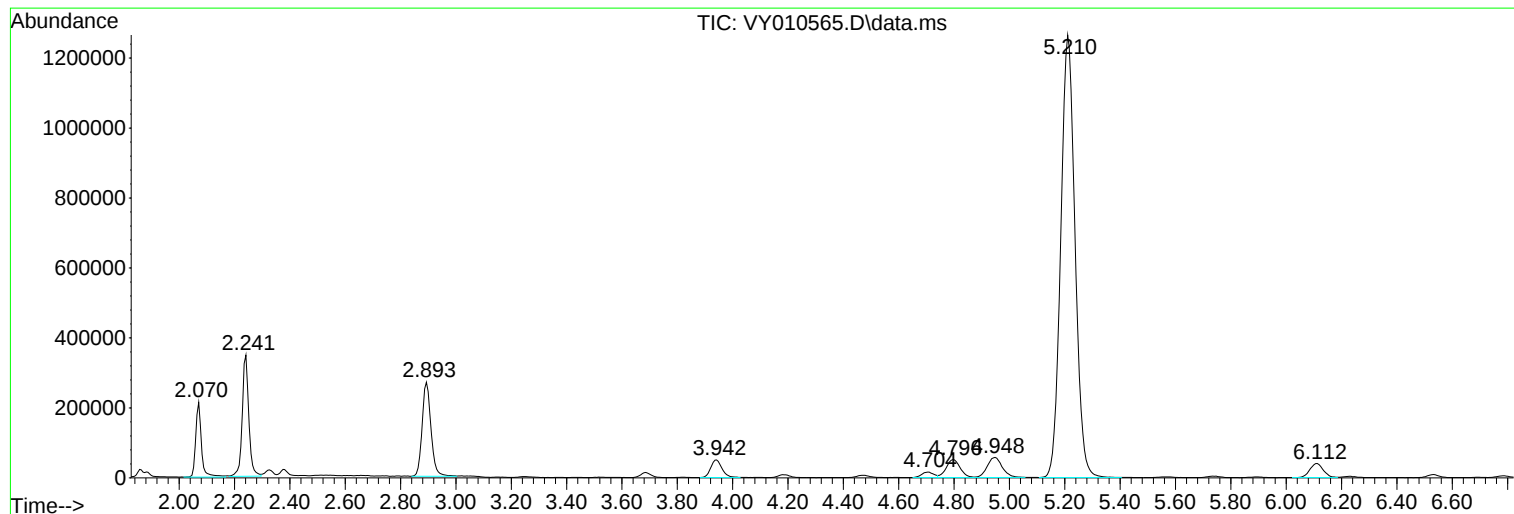
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091922S.M
Quant Title : SW846 8260

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



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ClientSampleId :
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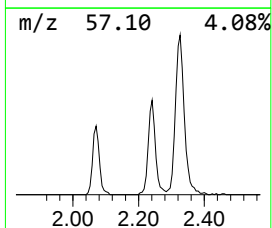
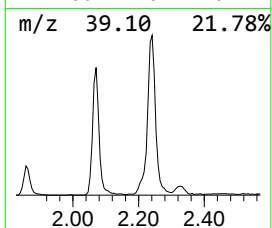
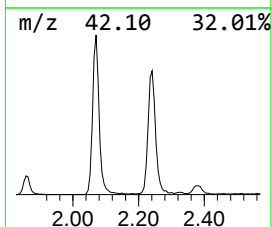
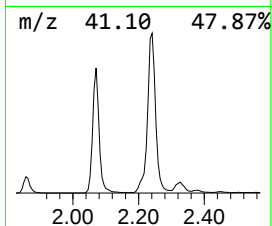
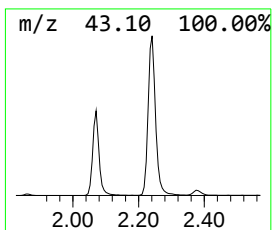
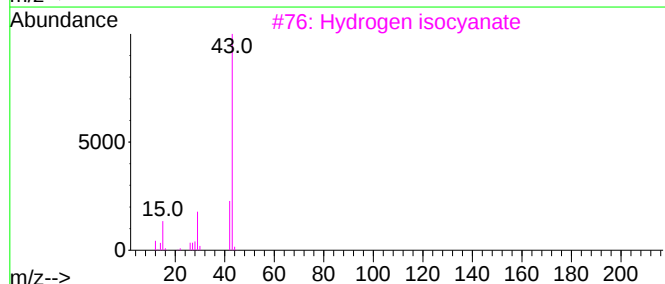
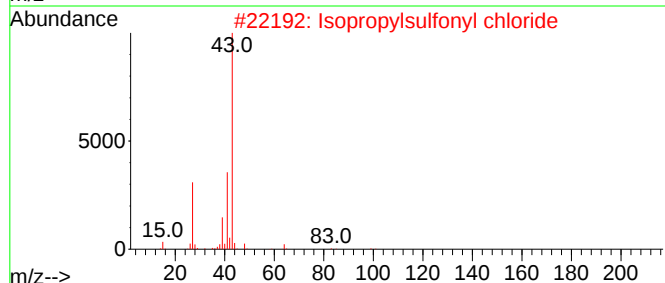
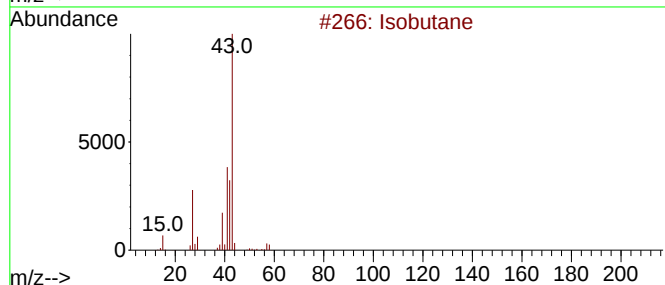
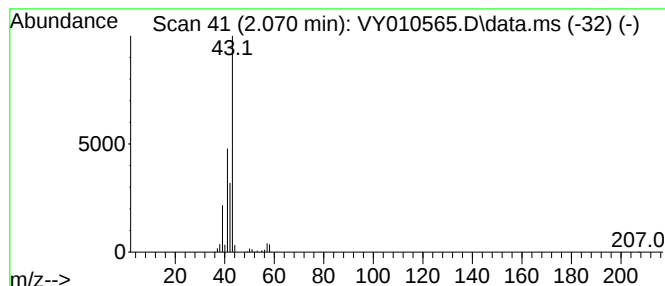
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091922S.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.070	26.62 ug/l	305327	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	72
2			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3			Hydrogen isocyanate	43	CHNO	000075-13-8	4
4			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4
5			Cyclobutylamine	71	C4H9N	002516-34-9	4



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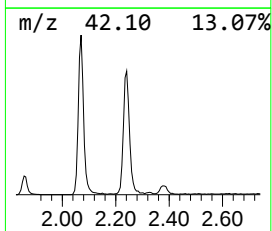
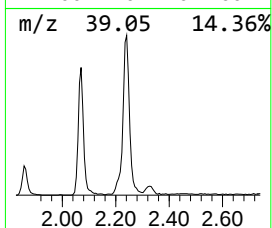
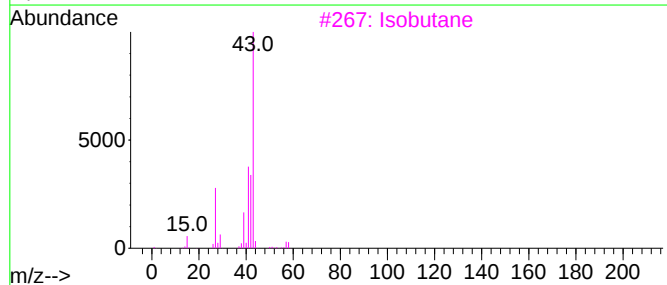
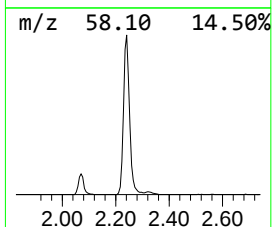
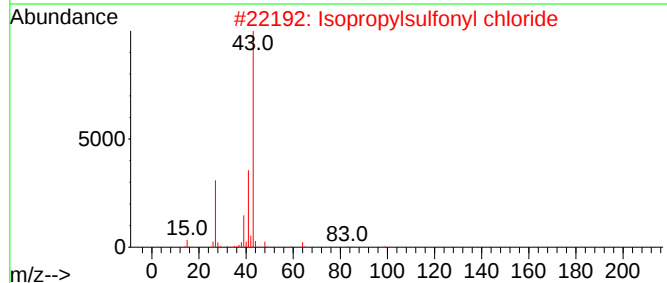
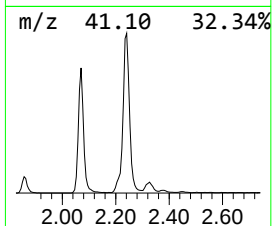
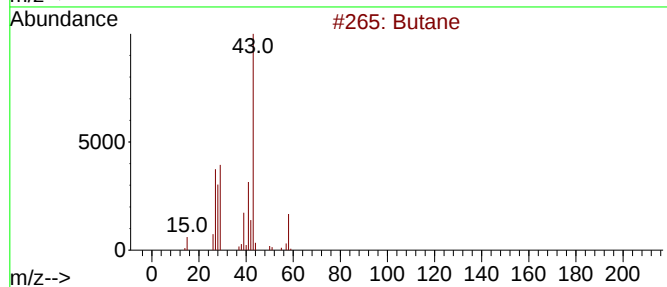
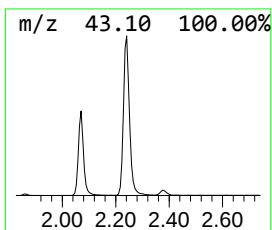
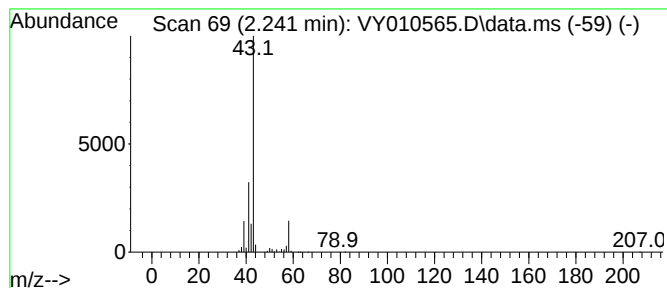
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091922S.M
Quant Title : SW846 8260

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.
2.241	49.71 ug/l	570120	Pentafluorobenzene	7.783

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			Acetone	58	C3H6O	000067-64-1	4



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
A1-8-17.5

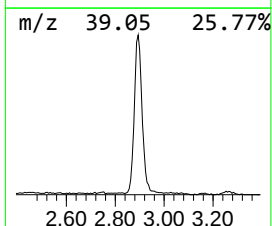
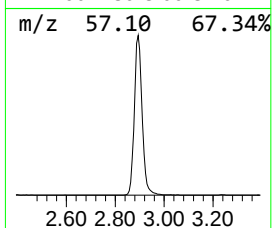
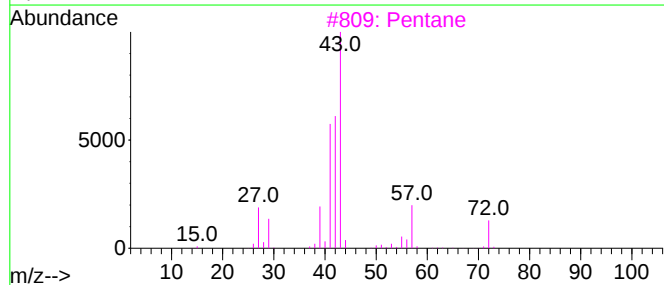
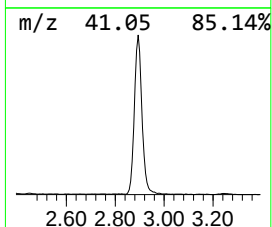
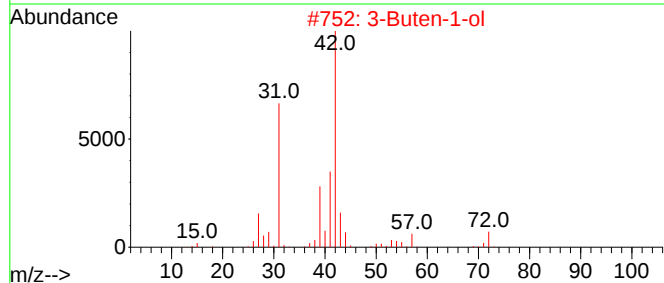
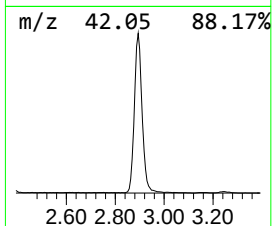
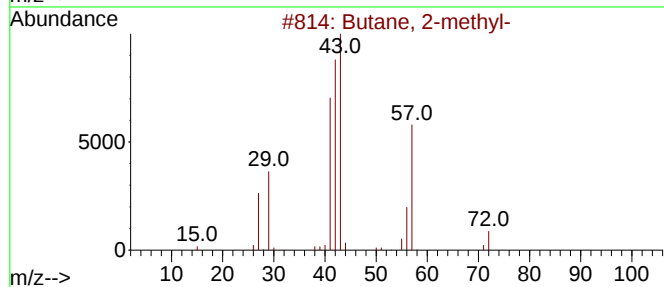
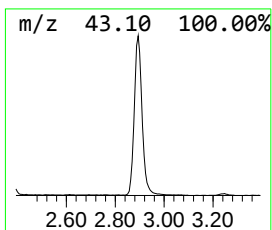
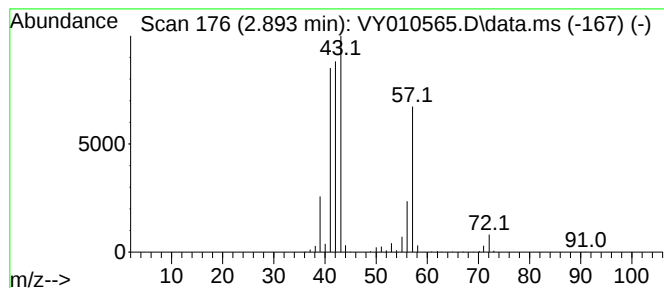
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Quant Title : SW846 8260

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.
2.893	51.78 ug/l	593913	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			1-Butene	56	C4H8	000106-98-9	10
5			Methane, isocyanato-	57	C2H3NO	000624-83-9	9



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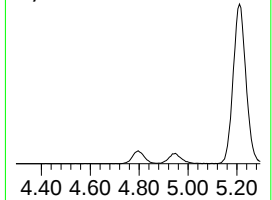
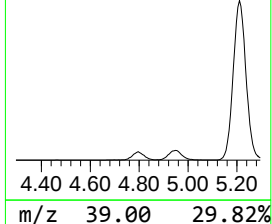
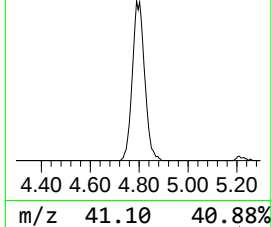
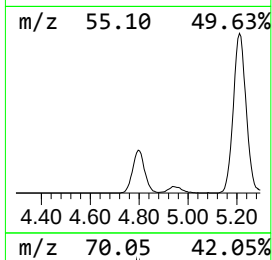
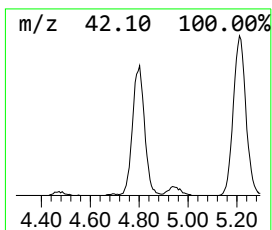
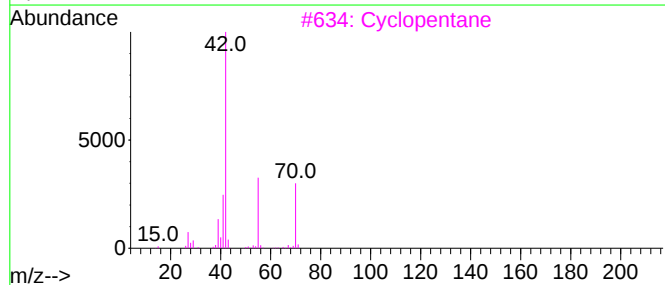
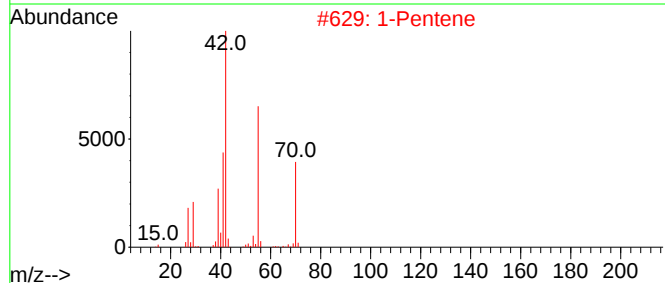
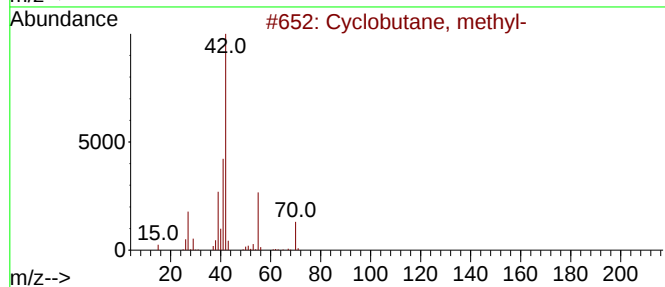
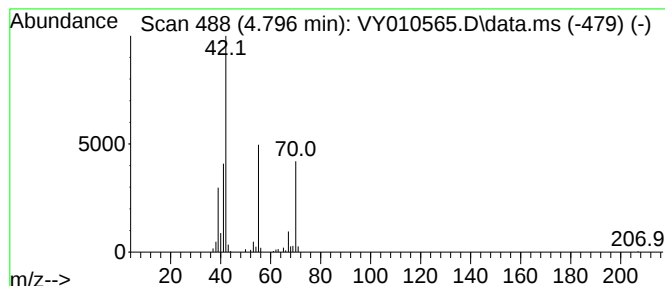
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclobutane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.796	15.51 ug/l	177908	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	86
2			1-Pentene	70	C5H10	000109-67-1	80
3			Cyclopentane	70	C5H10	000287-92-3	72
4			3-Buten-1-ol	72	C4H8O	000627-27-0	38
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	23



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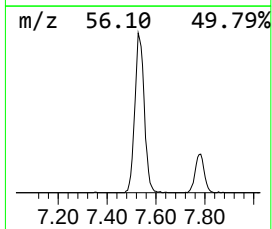
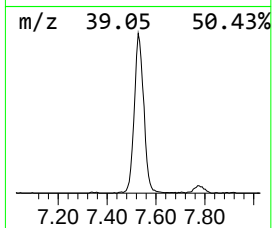
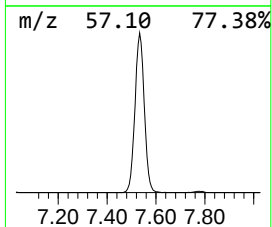
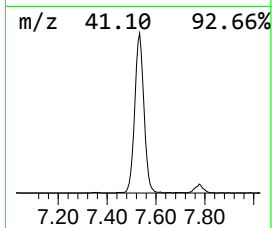
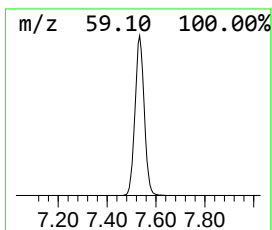
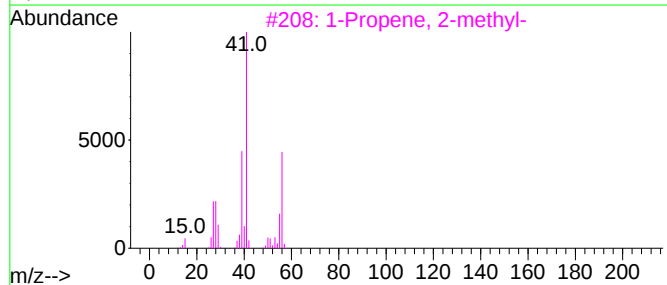
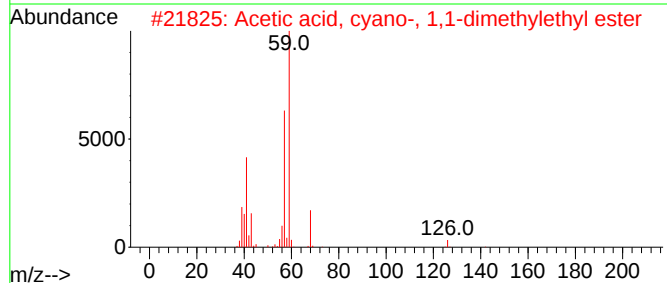
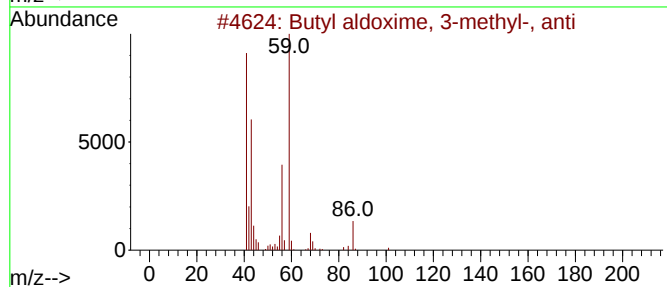
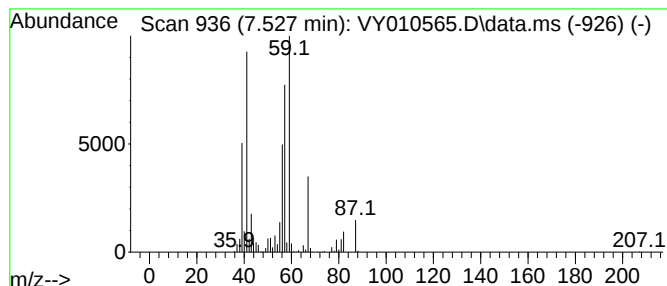
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.527 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.527	48.62 ug/l	557651	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl aldoxime, 3-methyl-, anti	101	C5H11NO	005775-74-6	42
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3			1-Propene, 2-methyl-	56	C4H8	000115-11-7	30
4			2-Butene, (E)-	56	C4H8	000624-64-6	25
5			Formic acid, 1,1-dimethylethyl e...	102	C5H10O2	000762-75-4	25



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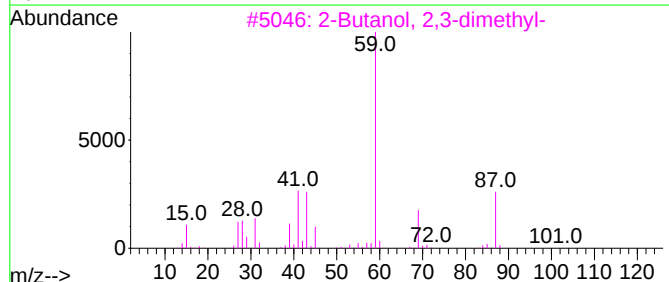
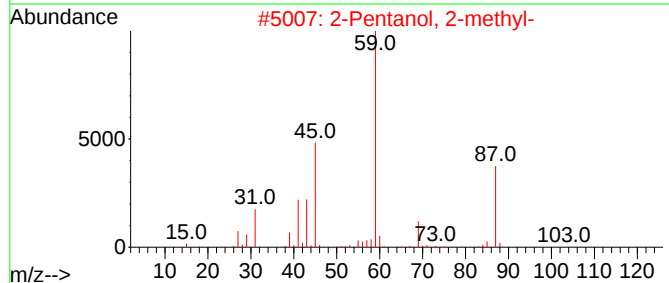
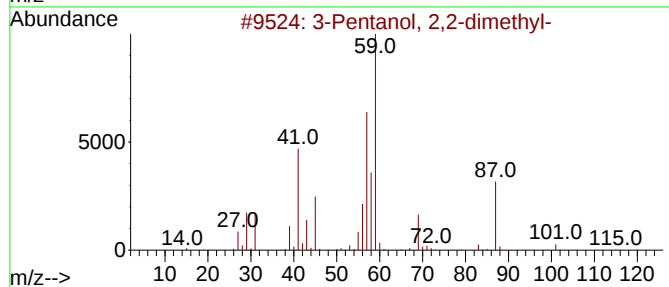
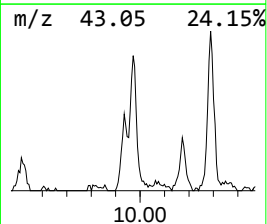
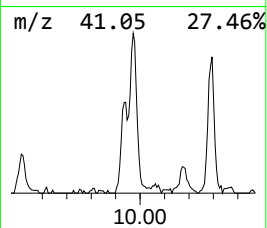
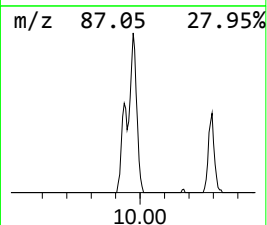
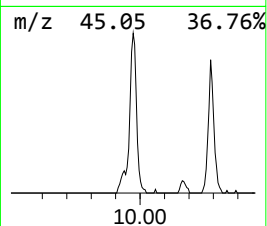
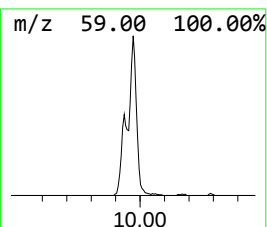
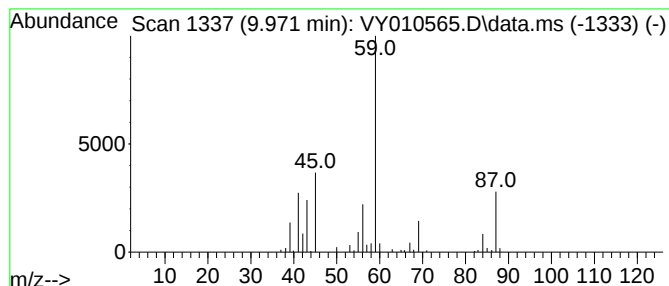
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091922S.M
Quant Title : SW846 8260

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

Peak Number 6 3-Pentanol, 2,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.971	5.16 ug/l	77150	1,4-Difluorobenzene	8.685

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	78		
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64		
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	59		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	39		
5	3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	38		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091922\
Data File : VY010565.D
Acq On : 19 Sep 2022 20:45
Operator : KP/MD
Sample : N4641-07
Misc : 5.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
A1-8-17.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091922S.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	2.070	26.6	ug/l	305327	1	7.783	573442	50.0
Butane	2.241	49.7	ug/l	570120	1	7.783	573442	50.0
Butane, 2-methyl-	2.893	51.8	ug/l	593913	1	7.783	573442	50.0
Cyclobutane, me...	4.796	15.5	ug/l	177908	1	7.783	573442	50.0
unknown7.527	7.527	48.6	ug/l	557651	1	7.783	573442	50.0
3-Pentanol, 2,2...	9.971	5.2	ug/l	77150	2	8.685	747730	50.0