

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081619\
 Data File : VX011581.D
 Acq On : 16 Aug 2019 15:14
 Operator : JC/SP
 Sample : K4368-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PH2-0137

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.398	36	40	58	rBV	7290398	7694015	4.35%	1.831%
2	1.995	133	138	148	rVB	1710733	2470136	1.40%	0.588%
3	4.397	521	532	551	rVB	1024138	3039343	1.72%	0.723%
4	5.574	716	725	734	rVV	1901264	6048482	3.42%	1.439%
5	6.147	808	819	830	rVB	15551906	41995349	23.77%	9.993%
6	7.464	1017	1035	1044	rBV	4042583	9129387	5.17%	2.172%
7	8.719	1236	1241	1246	rVV	915612	1788521	1.01%	0.426%
8	8.823	1246	1258	1263	rVV3	63453782	176699557	100.00%	42.047%
9	10.256	1486	1493	1499	rBV	19057335	26582431	15.04%	6.325%
10	10.372	1504	1512	1517	rVB2	47614005	78914456	44.66%	18.778%
11	10.701	1560	1566	1572	rVB	29934900	41532335	23.50%	9.883%
12	11.432	1679	1686	1693	rVV	4219349	7264518	4.11%	1.729%
13	11.505	1693	1698	1707	rVB	2341896	3075100	1.74%	0.732%
14	11.664	1719	1724	1733	rVB	1944413	2513221	1.42%	0.598%
15	11.804	1742	1747	1752	rBV	6058186	7078416	4.01%	1.684%
16	12.072	1786	1791	1796	rVB2	1365735	1838956	1.04%	0.438%
17	12.140	1796	1802	1807	rBV	2132744	2580202	1.46%	0.614%

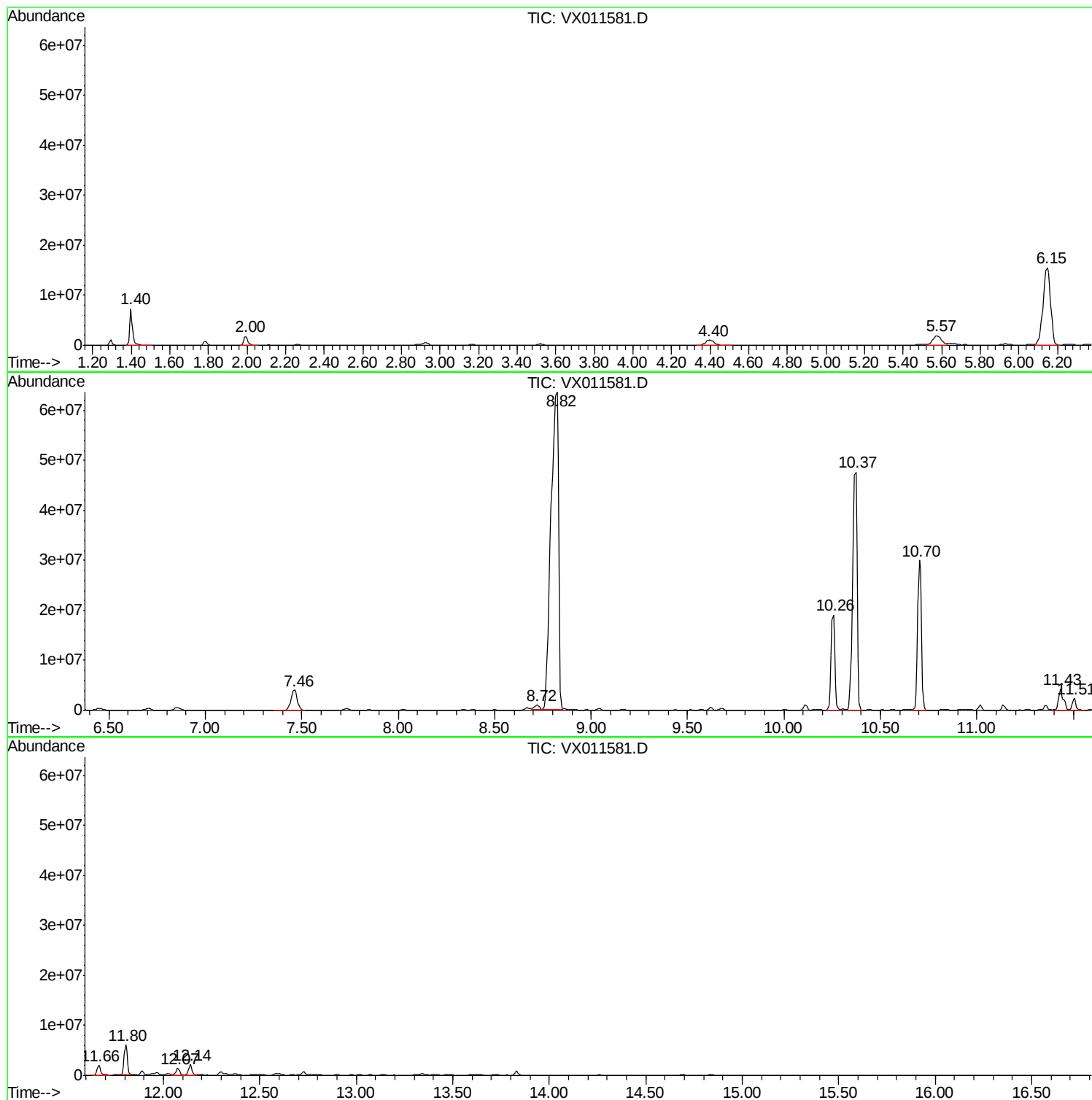
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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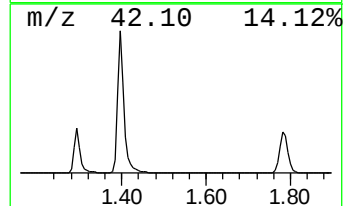
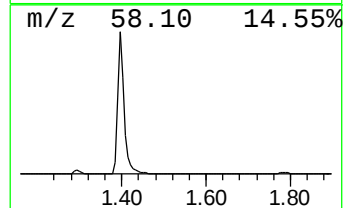
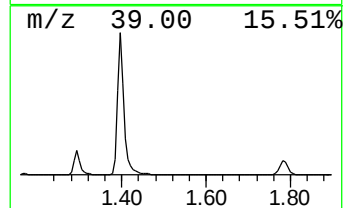
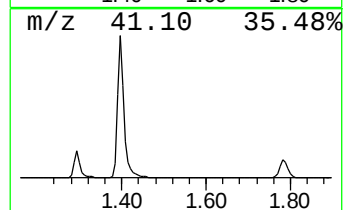
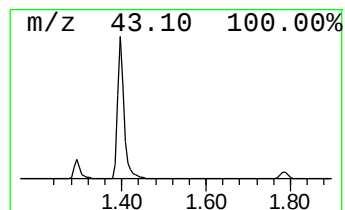
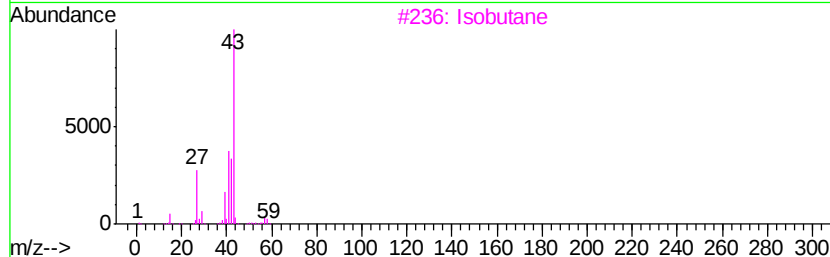
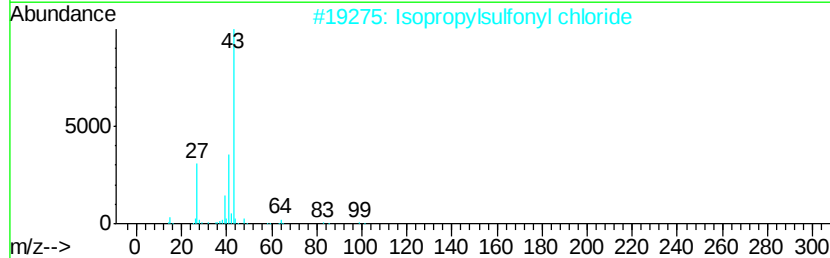
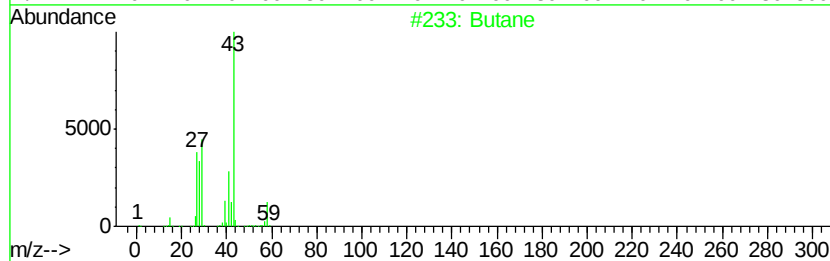
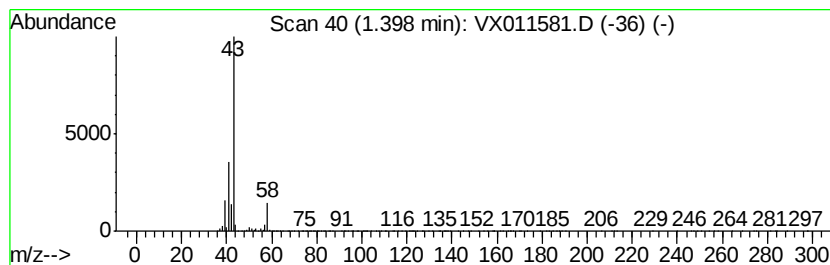
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.40	63.60 ug/l	7694020	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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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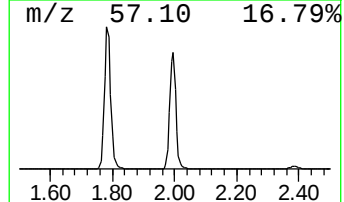
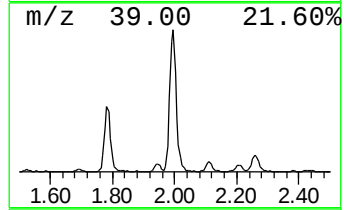
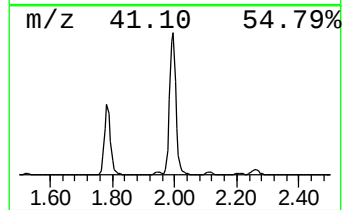
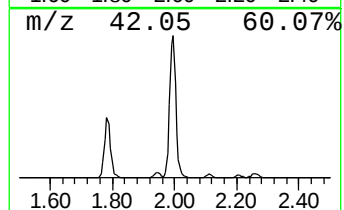
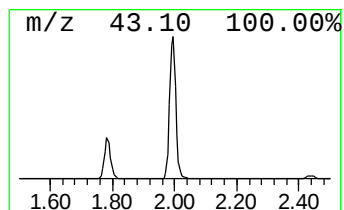
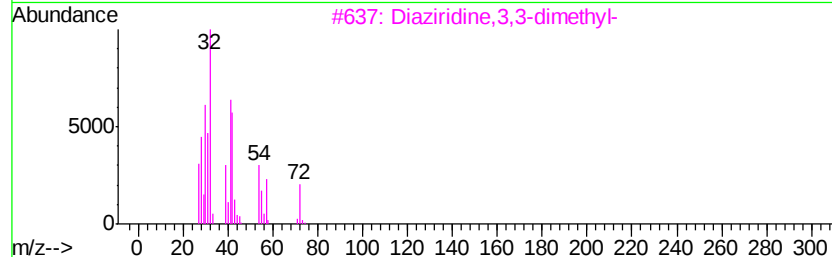
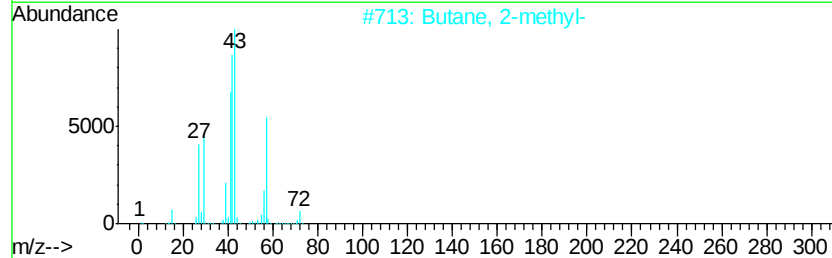
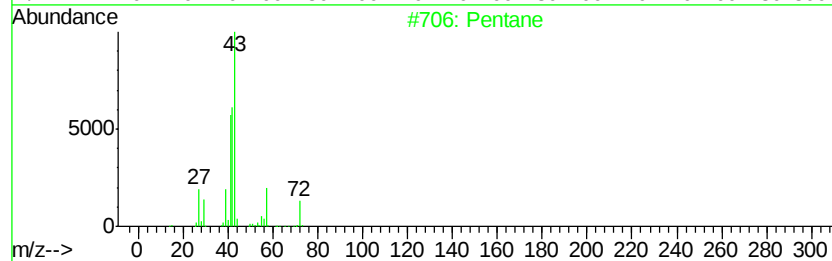
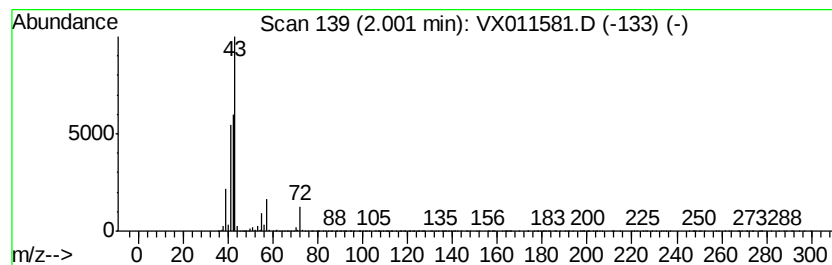
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	20.42 ug/l	2470140	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	91
2		Butane, 2-methyl-	72	C5H12	000078-78-4	38
3		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
4		Tetrahydrofuran	72	C4H8O	000109-99-9	9
5		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9



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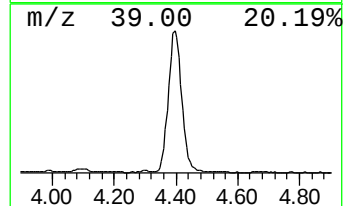
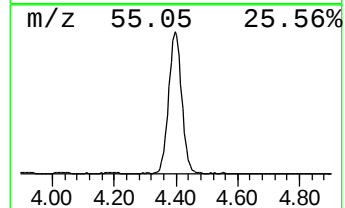
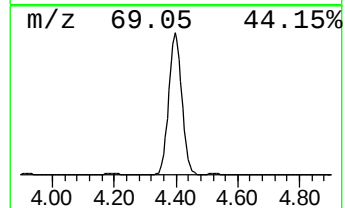
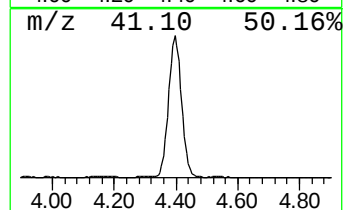
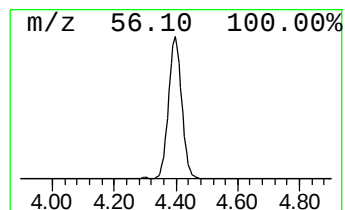
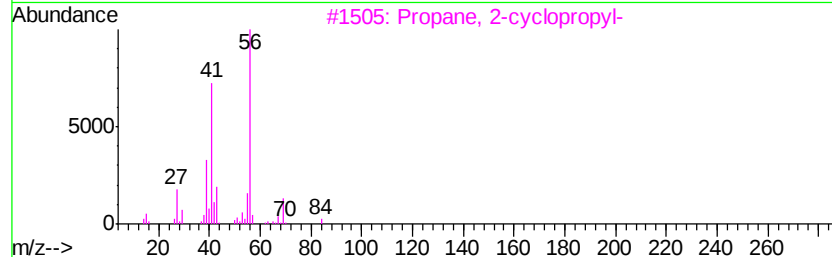
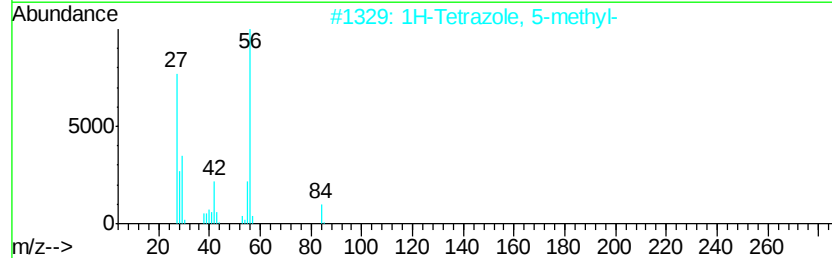
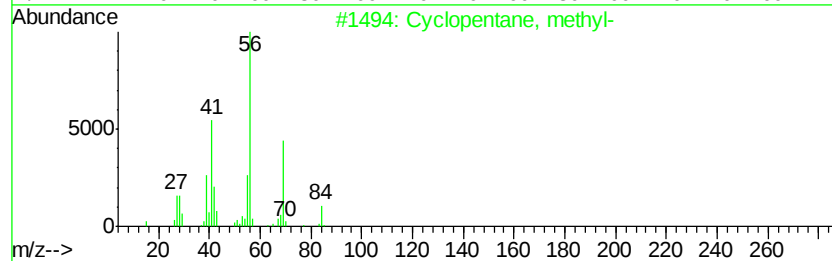
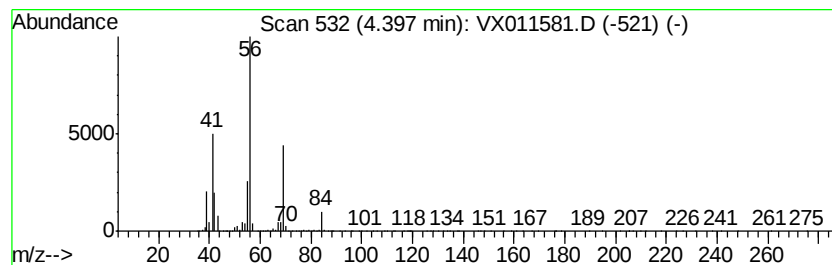
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Peak Number 3 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	25.12 ug/l	3039340	Pentafluorobenzene	5.66

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		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5		Cyclohexane	84	C6H12	000110-82-7	56



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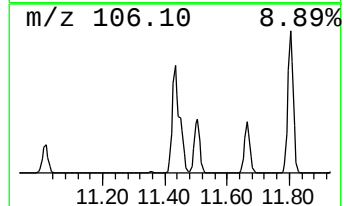
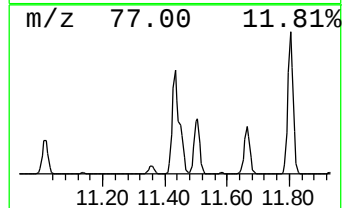
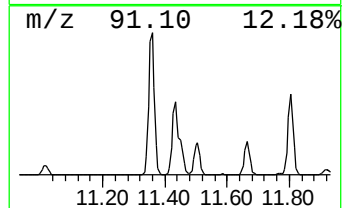
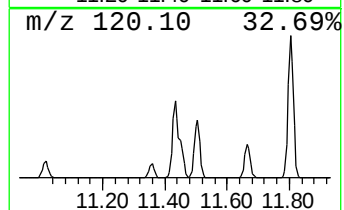
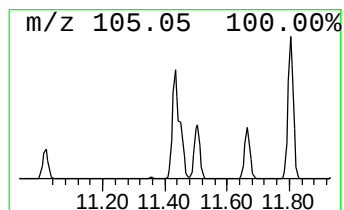
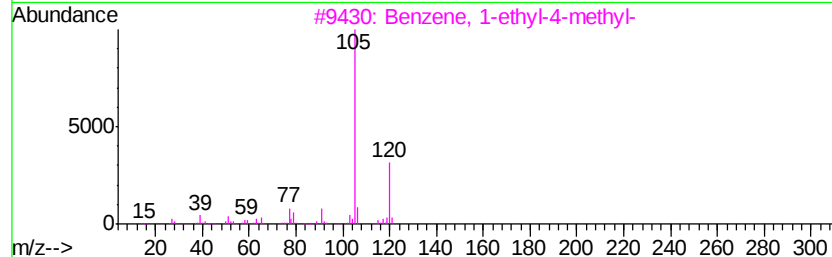
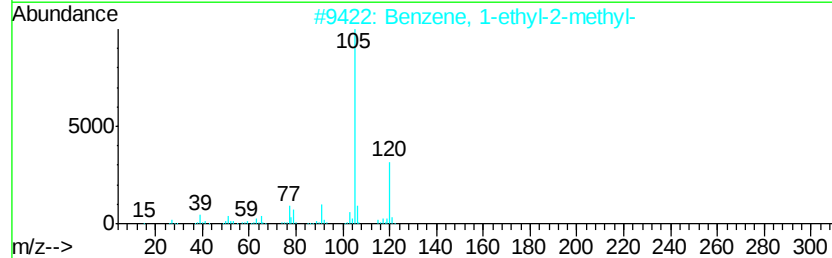
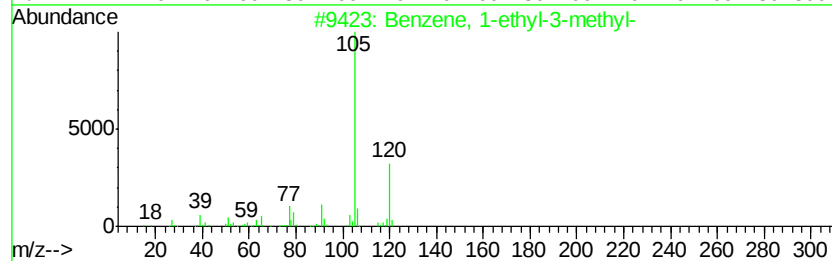
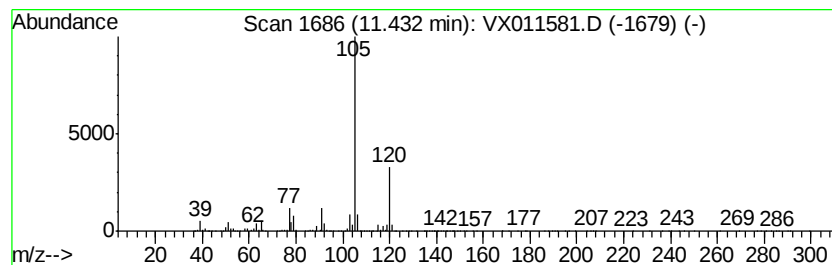
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	197.52 ug/l	7264520	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Mesitylene	120	C9H12	000108-67-8	91



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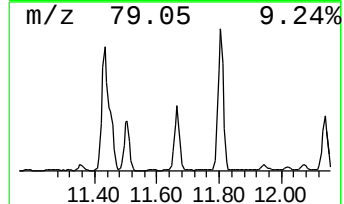
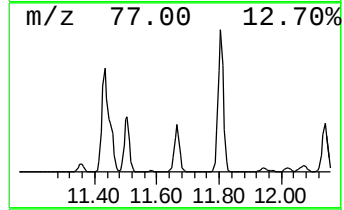
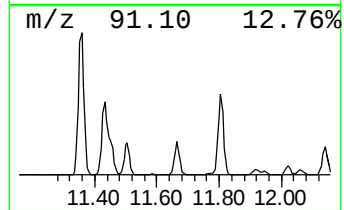
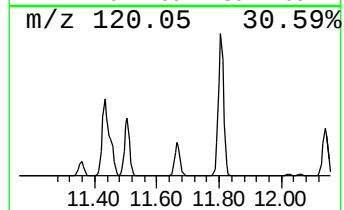
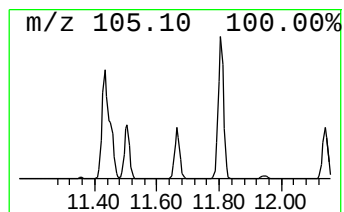
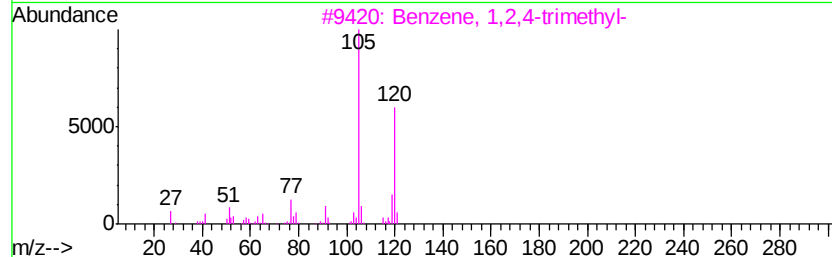
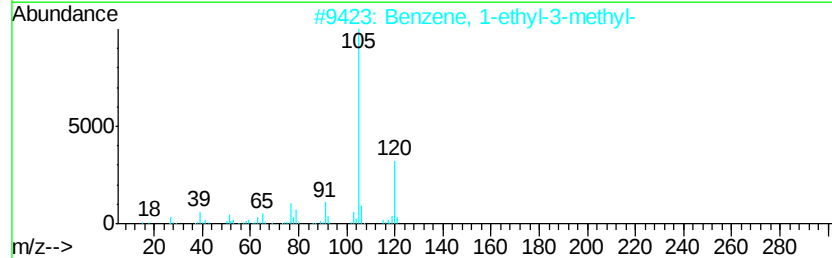
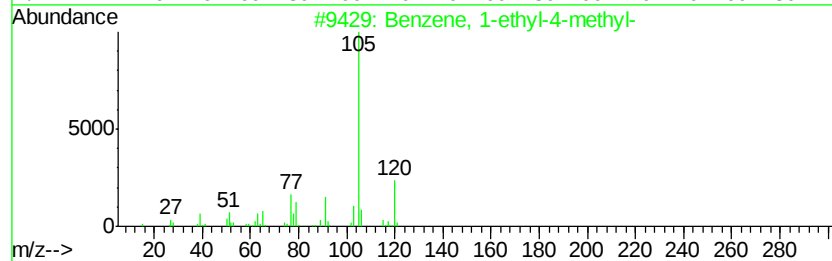
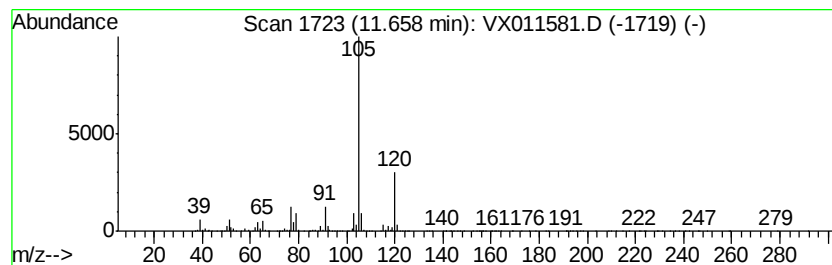
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	68.33 ug/l	2513220	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
2		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4		Mesitylene	120	C9H12	000108-67-8	91
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91



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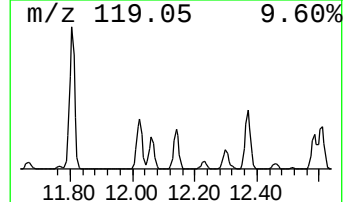
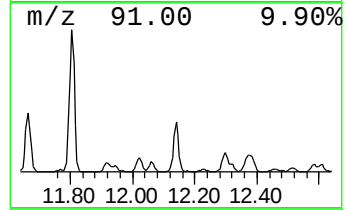
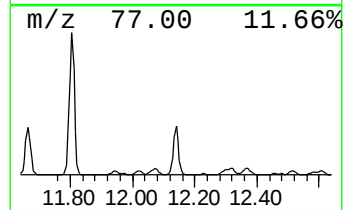
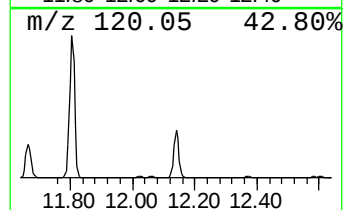
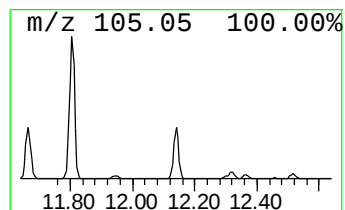
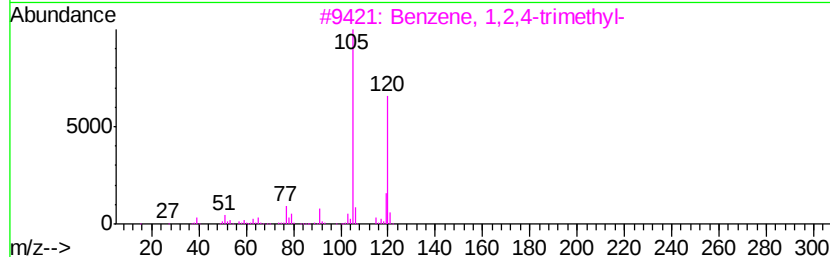
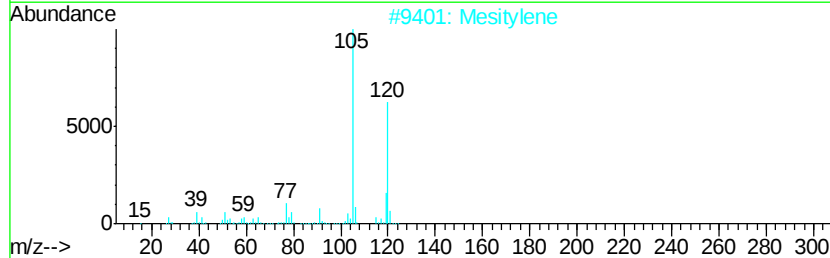
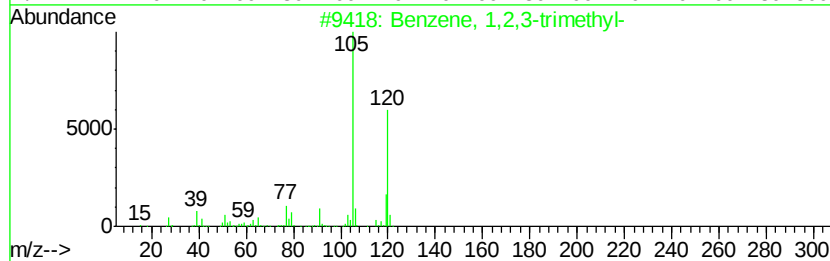
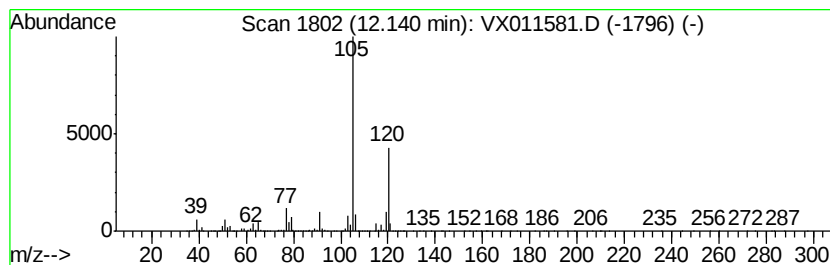
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	70.15 ug/l	2580200	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2		Mesitylene	120	C9H12	000108-67-8	94
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX081619\
Data File : VX011581.D
Acq On : 16 Aug 2019 15:14
Operator : JC/SP
Sample : K4368-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PH2-0137

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	1.40	63.6	ug/l	7694020	1	5.66	6048480	50.0
Pentane	2.00	20.4	ug/l	2470140	1	5.66	6048480	50.0
Cyclopentane, met...	4.40	25.1	ug/l	3039340	1	5.66	6048480	50.0
Benzene, 1-ethyl-...	11.43	197.5	ug/l	7264520	4	12.07	1838960	50.0
Benzene, 1-ethyl-...	11.66	68.3	ug/l	2513220	4	12.07	1838960	50.0
Benzene, 1,2,3-tr...	12.14	70.2	ug/l	2580200	4	12.07	1838960	50.0