

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV080819\
 Data File : VV012138.D
 Acq On : 08 Aug 2019 22:09
 Operator : SY/MD
 Sample : K4214-03
 Misc : 25mL/MSVOA V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0JZ6

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.1
 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_V\METHOD\SOMVTR080819WMA.M
 Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.129	311	323	330	rBV	73466	106109	1.59%	0.939%
2	2.184	330	340	370	rVV	4588818	6658088	100.00%	58.914%
3	2.663	475	489	513	rBV	96880	190800	2.87%	1.688%
4	3.737	802	823	845	rBV2	209559	550192	8.26%	4.868%
5	3.965	873	894	900	rBV5	45438	136915	2.06%	1.211%
6	4.389	1010	1026	1055	rBV4	164833	437714	6.57%	3.873%
7	5.093	1227	1245	1269	rBV3	147440	350304	5.26%	3.100%
8	5.663	1402	1422	1445	rBV	131334	273492	4.11%	2.420%
9	6.116	1546	1563	1589	rBV2	78577	155137	2.33%	1.373%
10	6.579	1692	1707	1715	rBV	193127	387812	5.82%	3.432%
11	7.029	1834	1847	1864	rBV2	47064	80340	1.21%	0.711%
12	7.357	1937	1949	1968	rBV	186288	324156	4.87%	2.868%
13	8.132	2176	2190	2225	rBV3	148375	307802	4.62%	2.724%
14	8.894	2415	2427	2447	rBV	186307	304387	4.57%	2.693%
15	10.055	2769	2788	2809	rBV	114310	205624	3.09%	1.819%
16	10.257	2841	2851	2864	rBV2	62699	99935	1.50%	0.884%
17	11.293	3162	3173	3194	rVB	207293	327934	4.93%	2.902%
18	11.669	3279	3290	3307	rVB	199362	320385	4.81%	2.835%
19	15.164	4366	4377	4390	rBV2	55379	84338	1.27%	0.746%

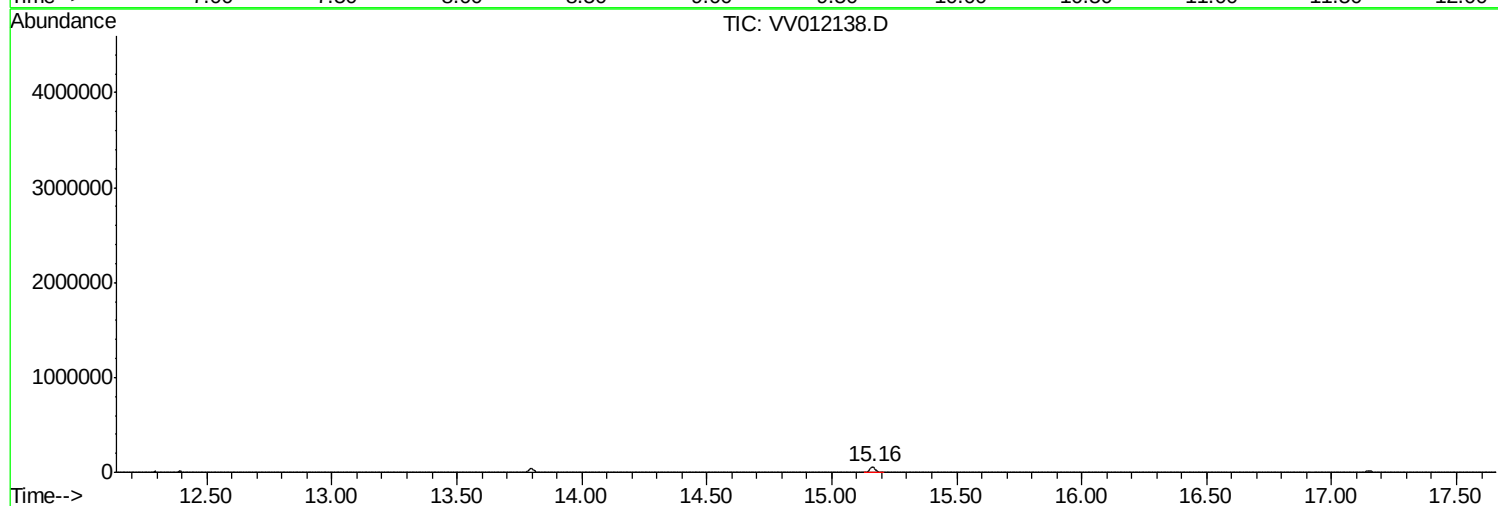
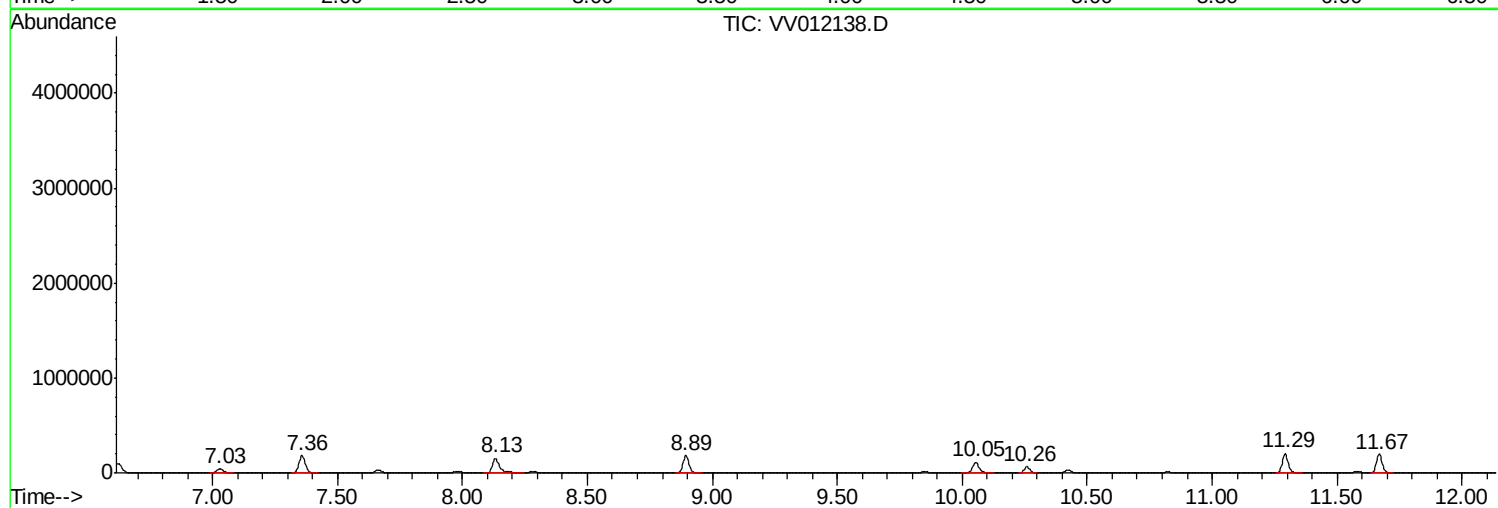
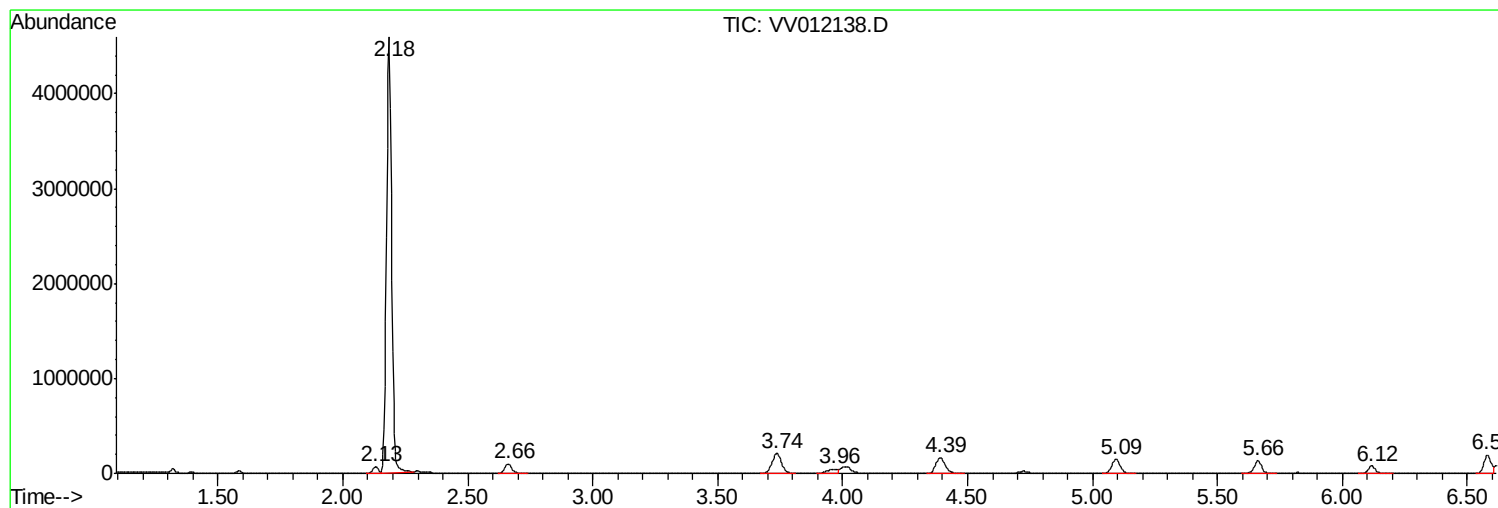
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Quant Title : TRACE VOA SOM01.0

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



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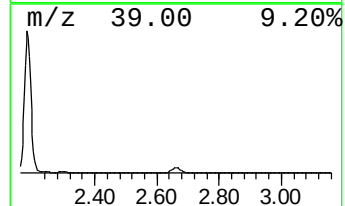
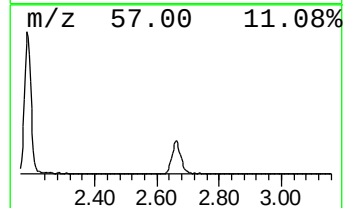
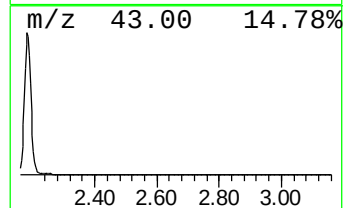
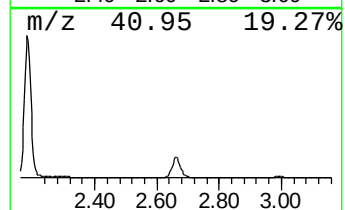
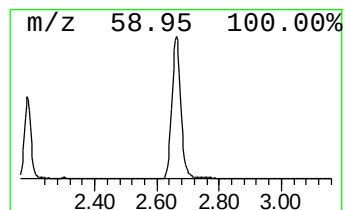
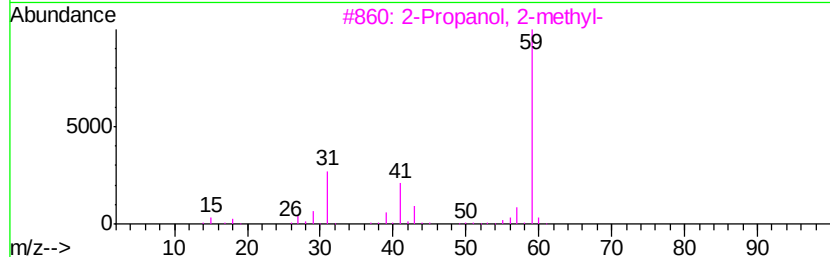
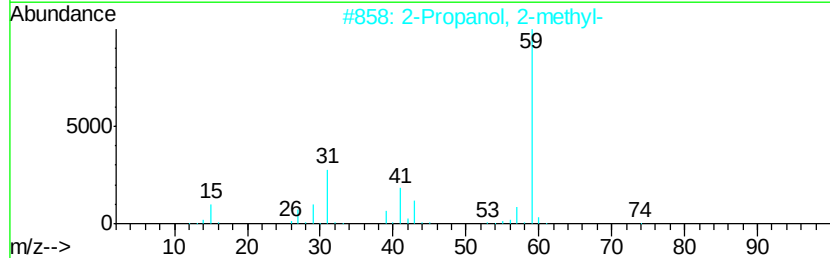
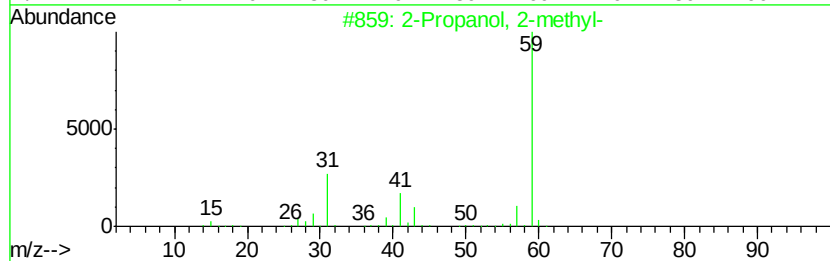
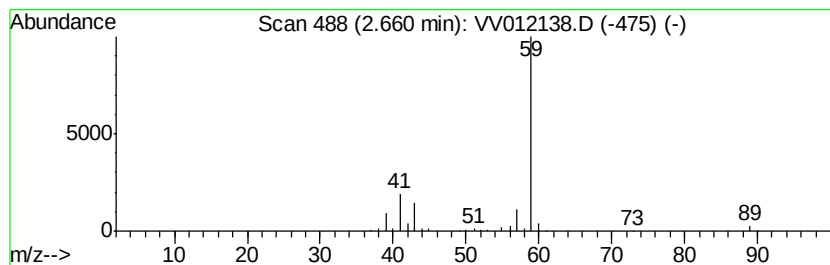
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR080819WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.66	3.49 ug/L	190800	1,4-Difluorobenzene	5.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	78
2	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	64
3	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	56
4	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	43
5	3-Pentanol			88	C5H12O	000584-02-1	40



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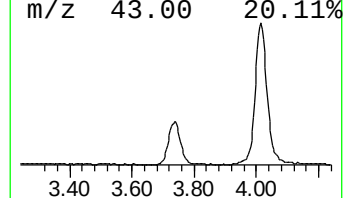
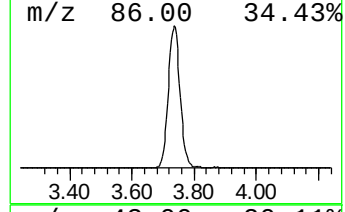
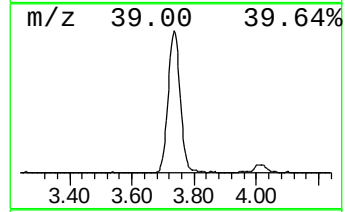
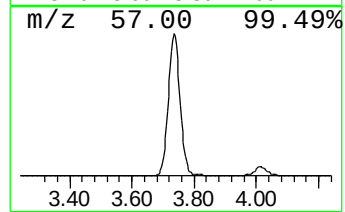
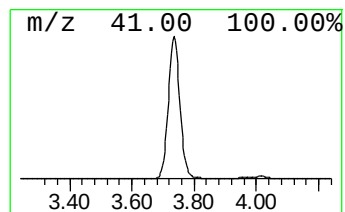
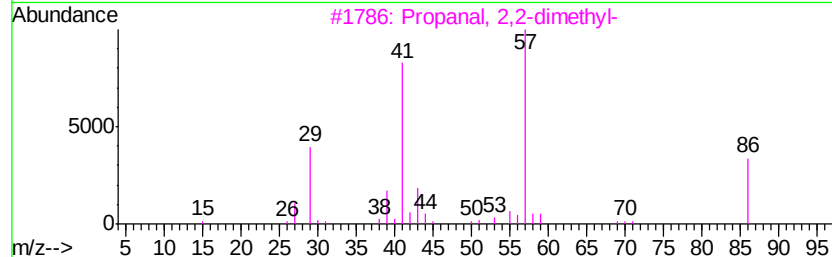
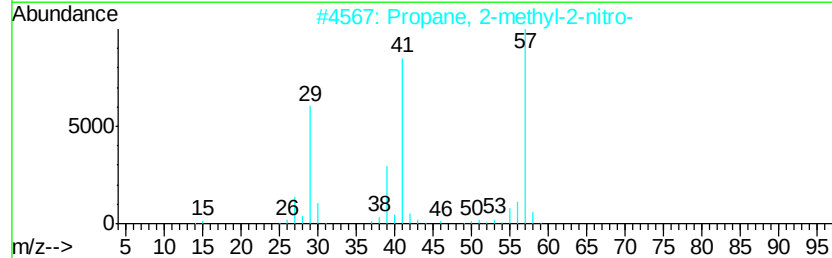
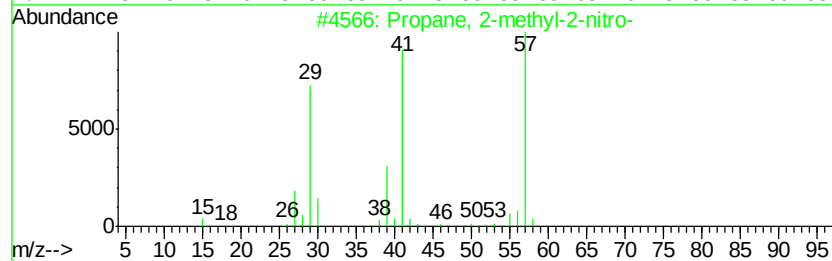
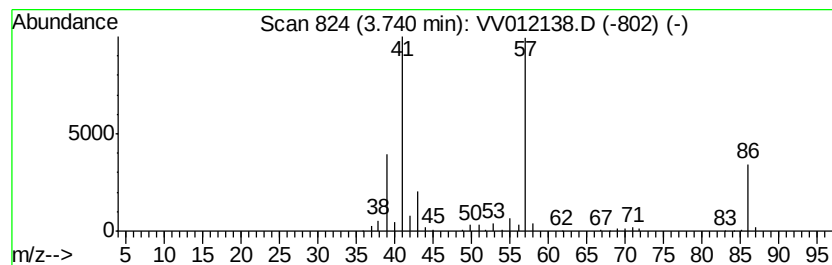
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Propane, 2-methyl-2-nitro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.74	10.06 ug/L	550192	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
2		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38
3		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	37
4		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	35
5		2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	33



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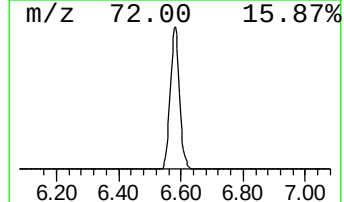
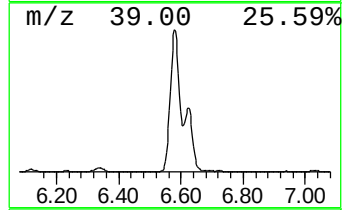
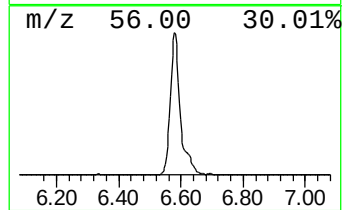
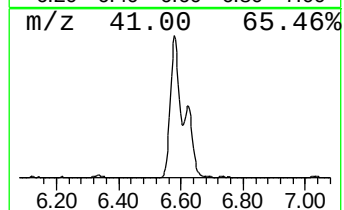
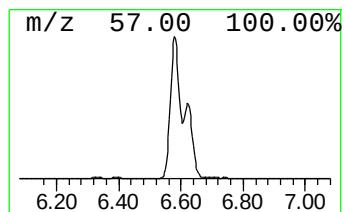
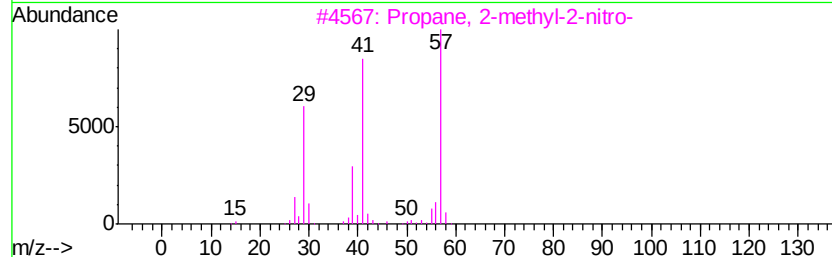
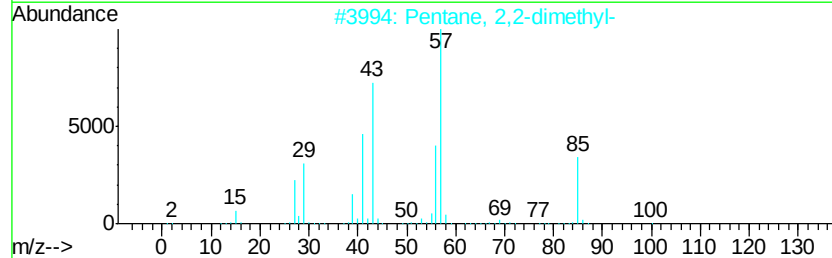
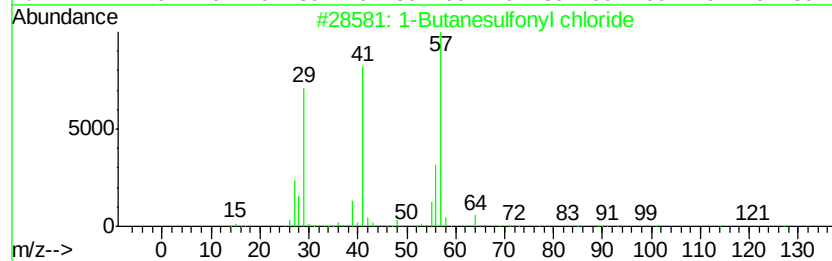
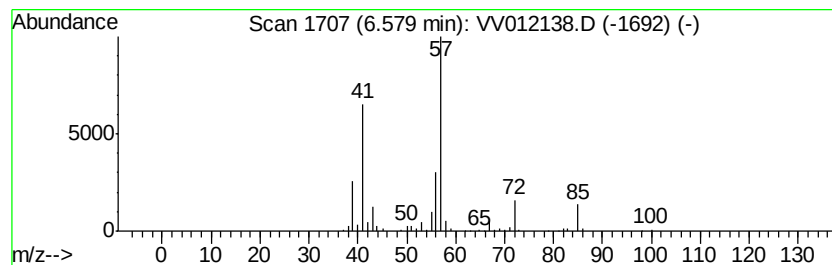
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	7.09 ug/L	387812	1,4-Difluorobenzene	5.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	38
2		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	36
3		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	35
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	28
5		1-Hepten-3-ol	114	C7H14O	004938-52-7	28



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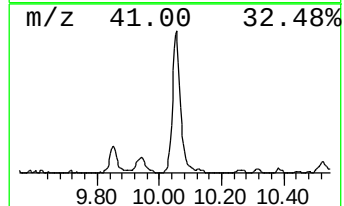
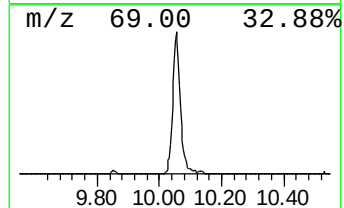
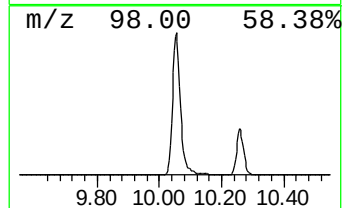
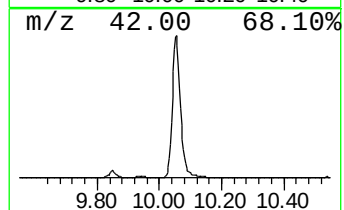
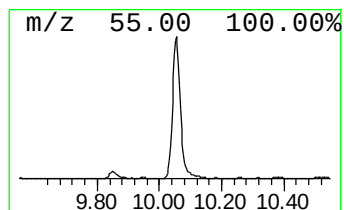
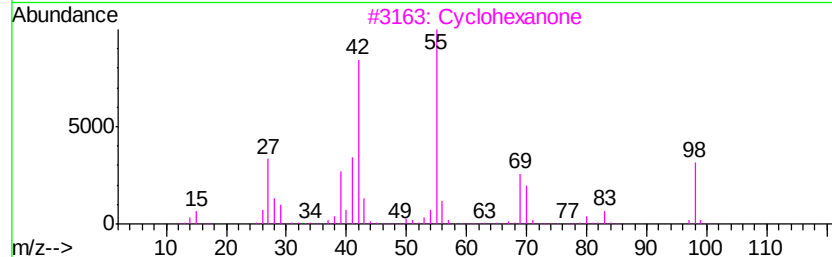
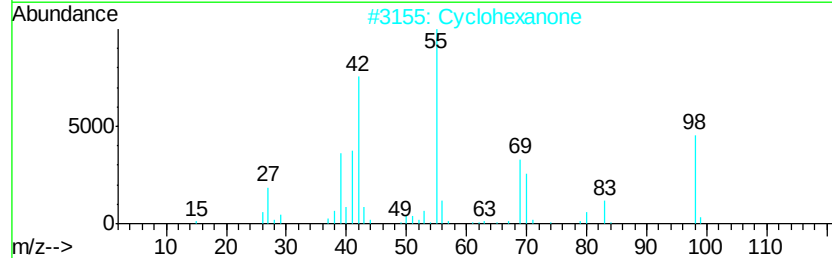
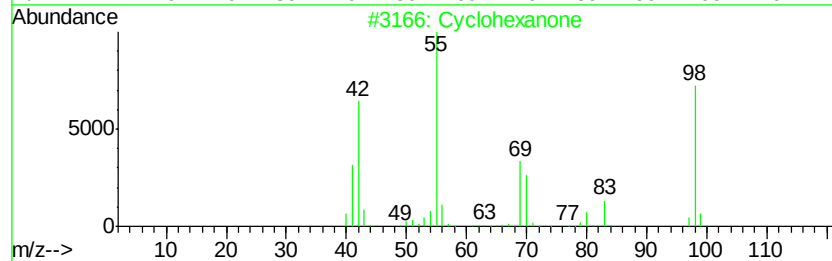
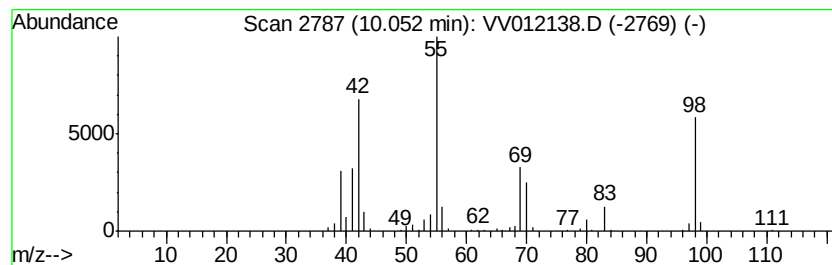
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Cyclohexanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.05	3.38 ug/L	205624	Chlorobenzene-d5	8.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanone	98	C6H10O	000108-94-1	96
2		Cyclohexanone	98	C6H10O	000108-94-1	94
3		Cyclohexanone	98	C6H10O	000108-94-1	91
4		Cyclohexanone	98	C6H10O	000108-94-1	91
5		Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	87



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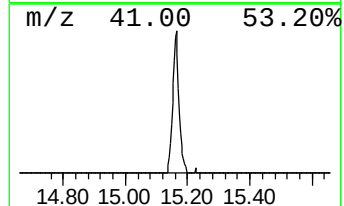
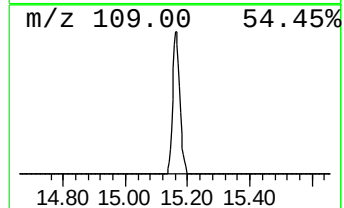
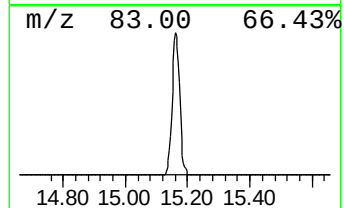
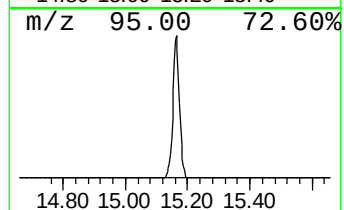
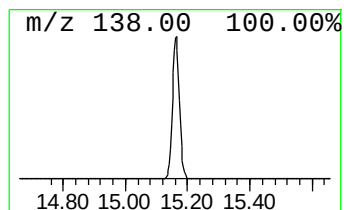
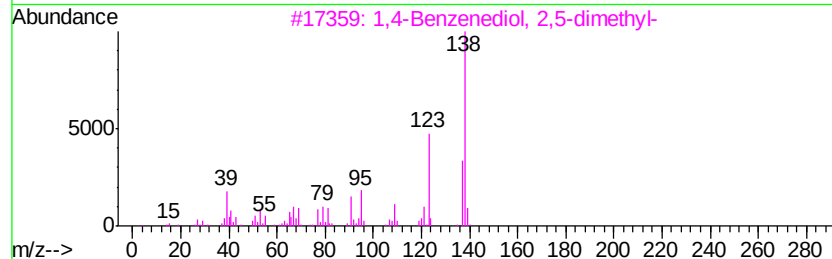
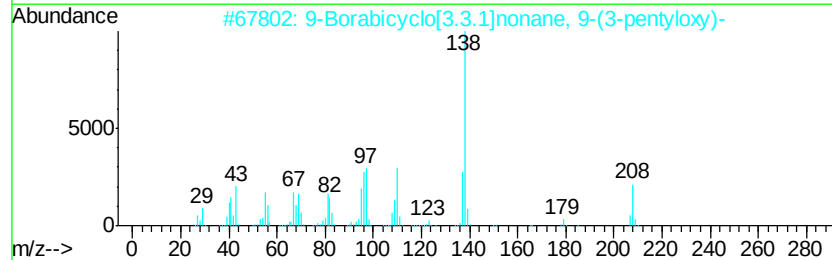
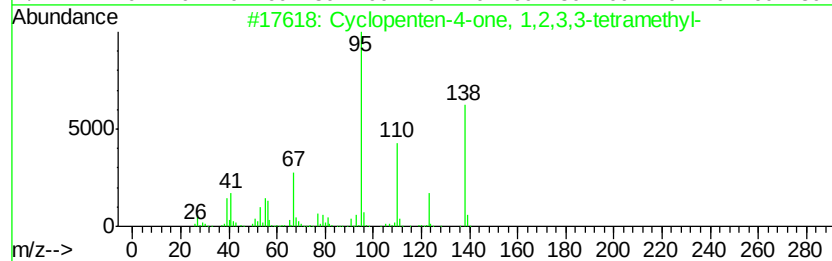
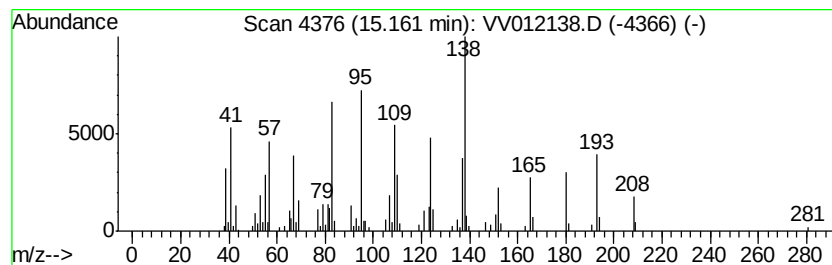
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	1.29 ug/L	84338	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopenten-4-one, 1,2,3,3-tetra...	138	C9H14O	1000163-38-6	38
2		9-Borabicyclo[3.3.1]nonane, 9-(3...	208	C13H25BO	1000160-84-8	35
3		1,4-Benzenediol, 2,5-dimethyl-	138	C8H10O2	000615-90-7	30
4		(2Z,4E)-3,7-Dimethyl-2,4-octadiene	138	C10H18	1000374-08-4	30
5		1,3-Diazadamantan-6-one, 5,7-dim...	180	C10H16N2O	080808-86-2	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanol, 2-met...	2.66	3.5	ug/L	190800	1	5.66	273492	5.0
Propane, 2-methyl...	3.74	10.1	ug/L	550192	1	5.66	273492	5.0
unknown-01	6.58	7.1	ug/L	387812	1	5.66	273492	5.0
Cyclohexanone	10.05	3.4	ug/L	205624	2	8.89	304387	5.0
unknown-02	15.16	1.3	ug/L	84338	3	11.29	327934	5.0