

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV012420\
 Data File : VV014391.D
 Acq On : 24 Jan 2020 15:36
 Operator : SY/MD
 Sample : L1253-01
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 H0AB0

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\SOMVTR010220WMA.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	1.319	63	71	87	rVB2	436971	488694	1.43%	0.532%
2	1.479	113	121	144	rBV	3138909	4282919	12.49%	4.662%
3	2.129	316	323	336	rVB2	506738	755716	2.20%	0.823%
4	2.232	345	355	370	rVB	608832	937073	2.73%	1.020%
5	2.537	441	450	469	rVB	357556	629993	1.84%	0.686%
6	3.958	873	892	935	rBV	13940522	34280128	100.00%	37.312%
7	4.399	1013	1029	1048	rBV	537138	1277358	3.73%	1.390%
8	5.093	1229	1245	1276	rBV2	1175215	2888743	8.43%	3.144%
9	5.663	1410	1422	1445	rVB	1094849	2154839	6.29%	2.345%
10	5.955	1496	1513	1547	rBV	12106426	23308690	67.99%	25.370%
11	6.113	1550	1562	1579	rVB	718386	1434723	4.19%	1.562%
12	7.026	1837	1846	1860	rBV2	365265	639332	1.87%	0.696%
13	7.135	1865	1880	1920	rBV2	800751	2578838	7.52%	2.807%
14	7.357	1937	1949	1965	rBV	1289815	2211679	6.45%	2.407%
15	7.659	2028	2043	2062	rBV	226572	417619	1.22%	0.455%
16	8.132	2179	2190	2230	rBV	1678587	3490659	10.18%	3.799%
17	8.891	2412	2426	2442	rBV	1567045	2583444	7.54%	2.812%
18	10.257	2838	2851	2864	rBV	520739	836179	2.44%	0.910%
19	10.833	3019	3030	3047	rBV	544222	967513	2.82%	1.053%
20	10.977	3056	3075	3092	rBV	628870	1049182	3.06%	1.142%
21	11.289	3158	3172	3188	rBV	1641047	2538485	7.41%	2.763%
22	11.666	3277	3289	3307	rVB	1346218	2122356	6.19%	2.310%

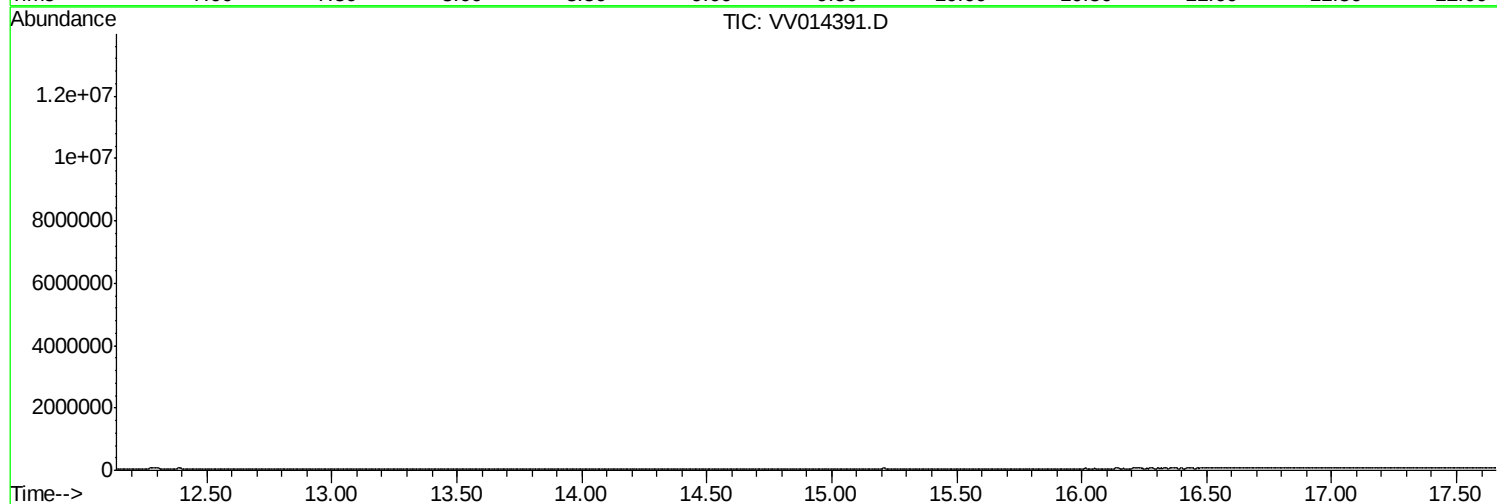
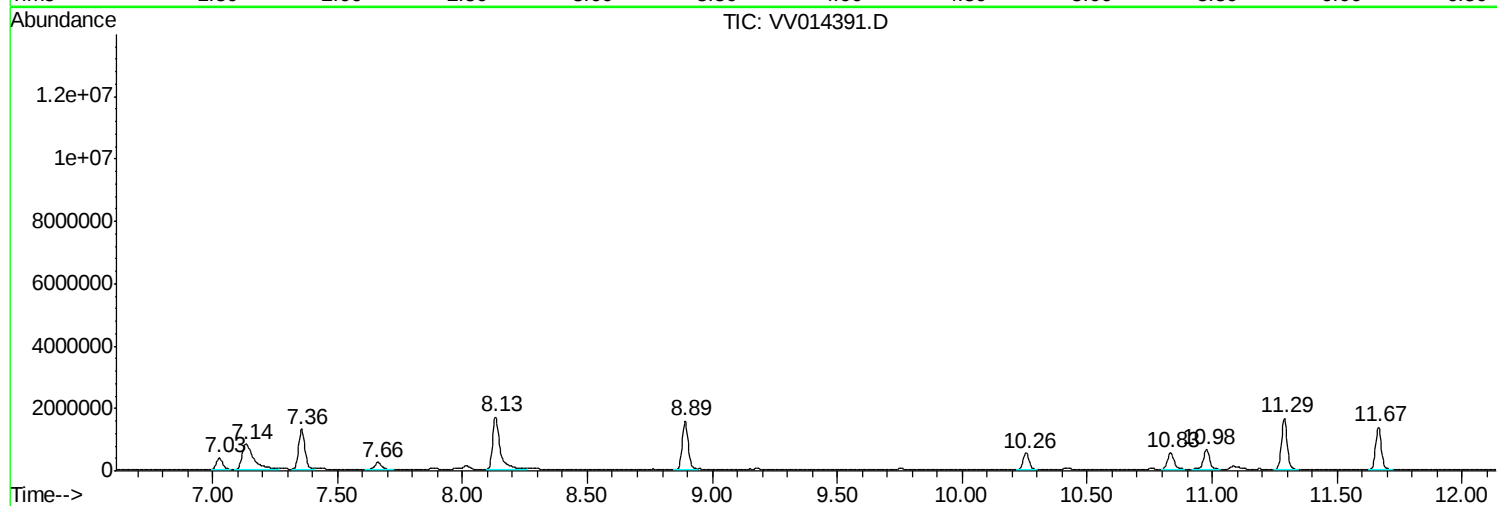
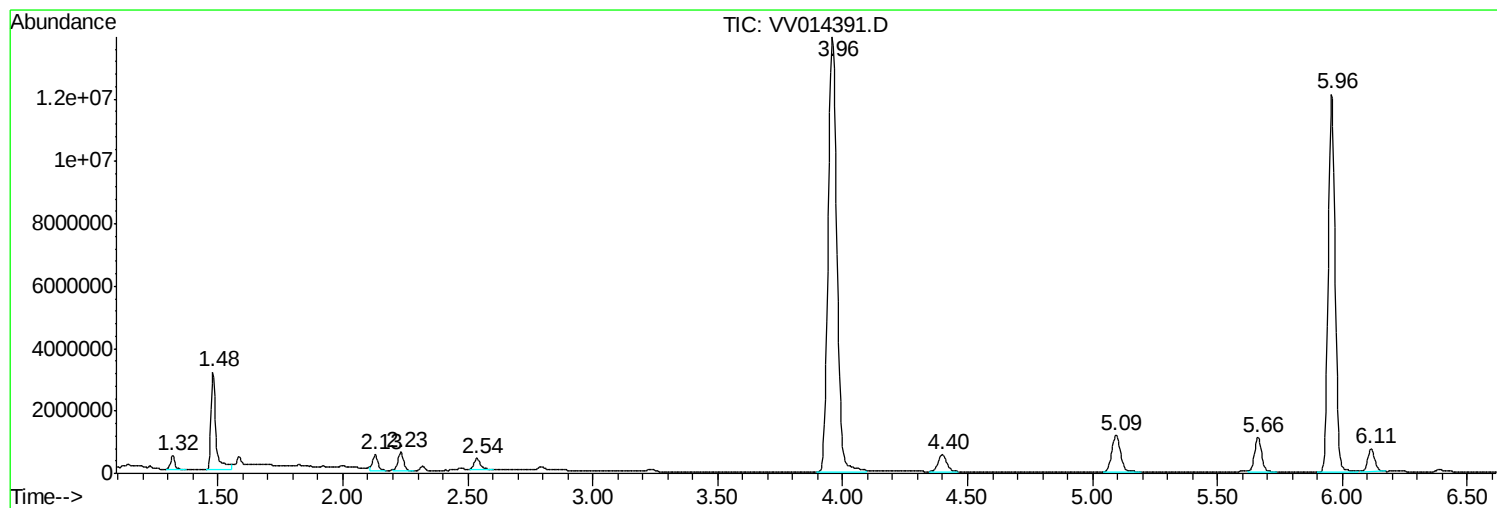
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR010220WMA.M
Quant Title : TRACE VOA SOM01.0

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



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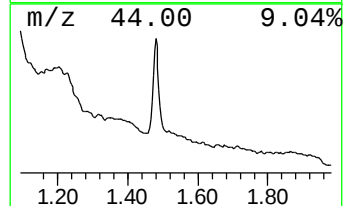
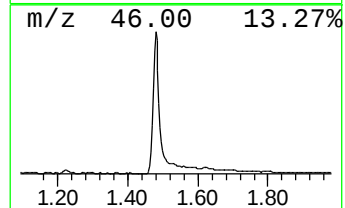
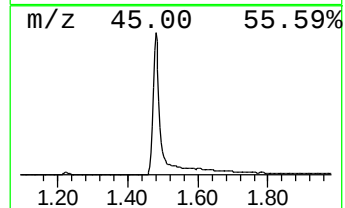
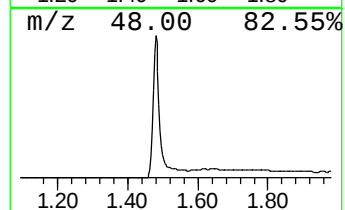
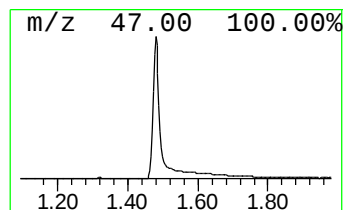
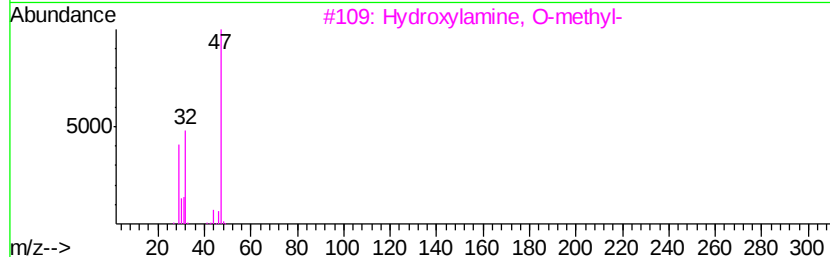
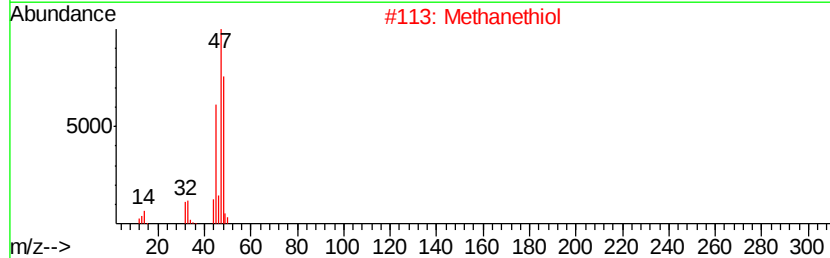
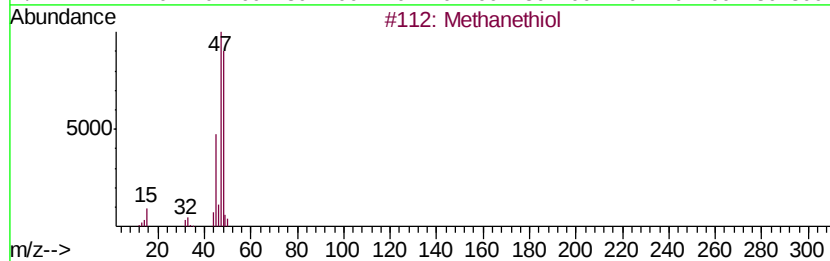
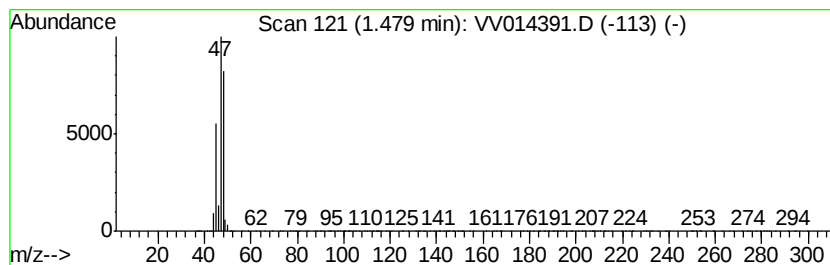
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Methanethiol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	9.94 ug/L	4282920	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethiol	48	CH4S	000074-93-1	90
2		Methanethiol	48	CH4S	000074-93-1	86
3		Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4		Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5		Methane, nitroso-	45	CH3NO	000865-40-7	5



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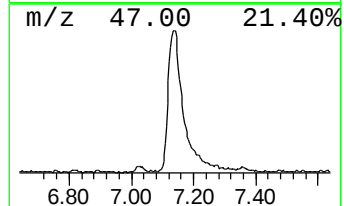
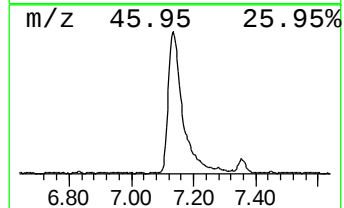
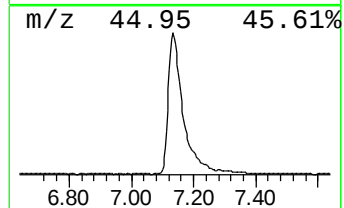
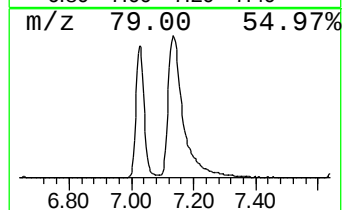
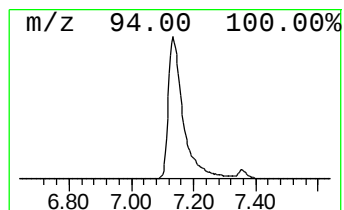
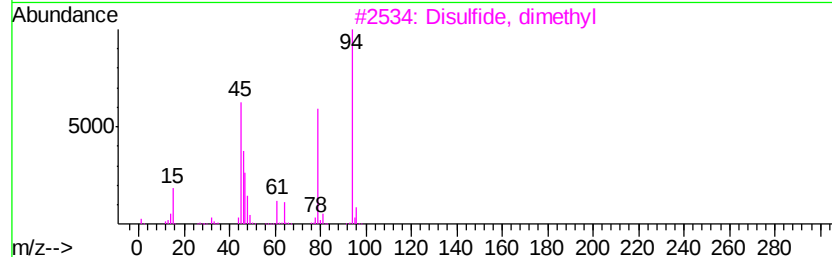
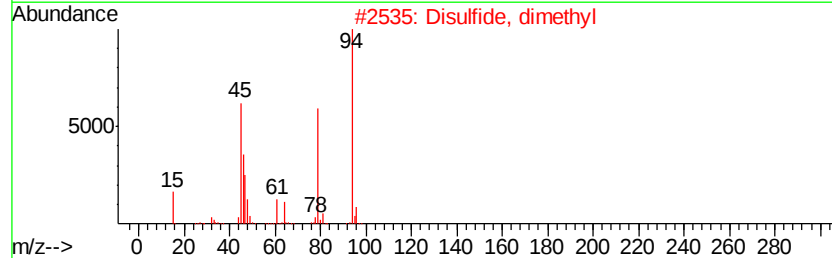
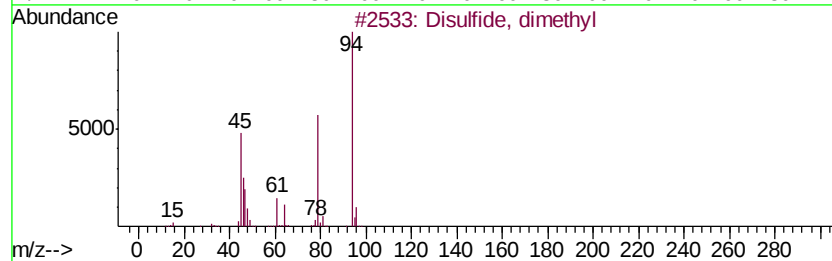
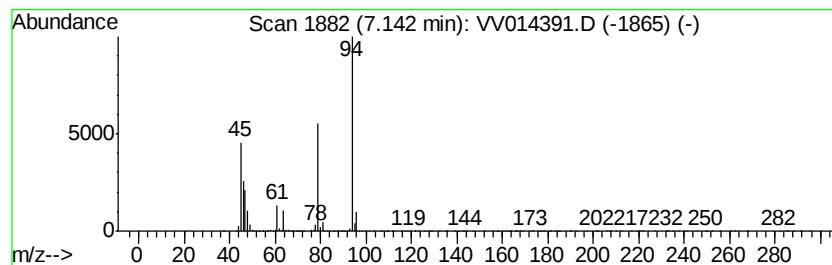
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Disulfide, dimethyl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.14	5.98 ug/L	2578840	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2		Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
3		Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
4		Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
5		Disulfide, dimethyl	94	C2H6S2	000624-92-0	96



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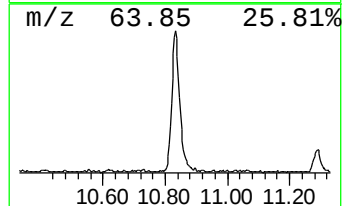
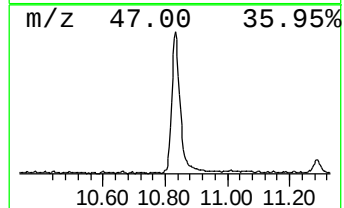
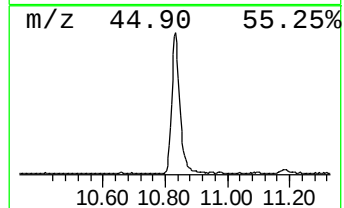
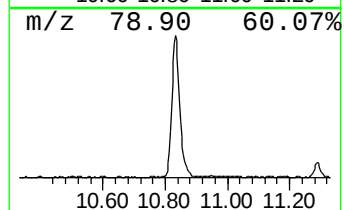
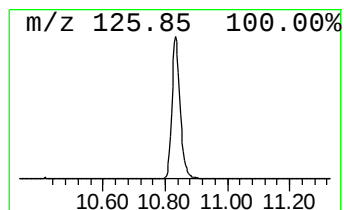
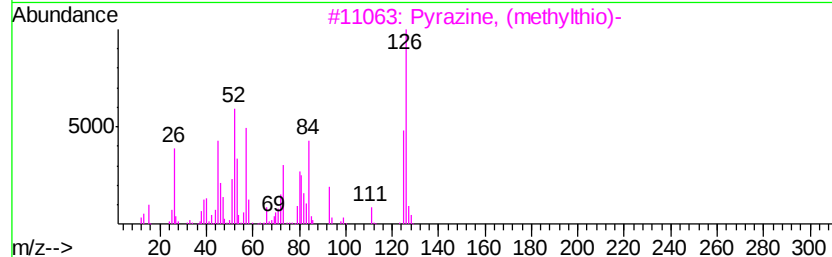
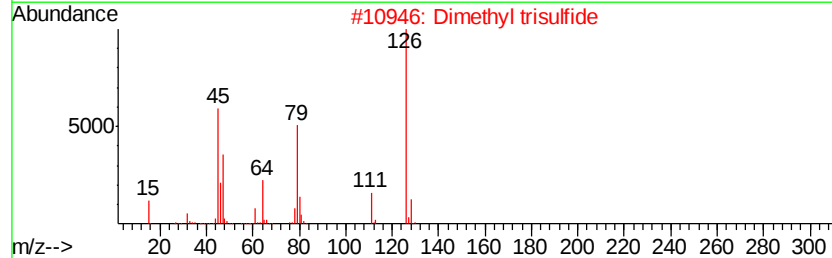
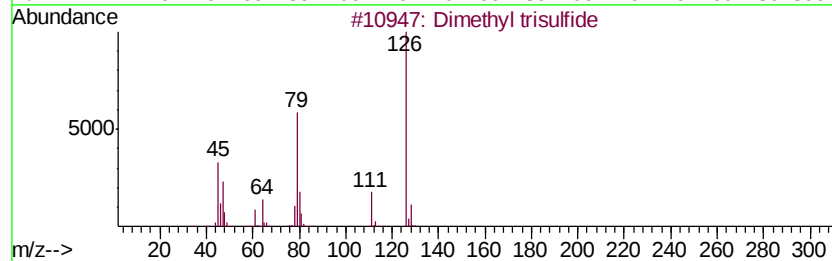
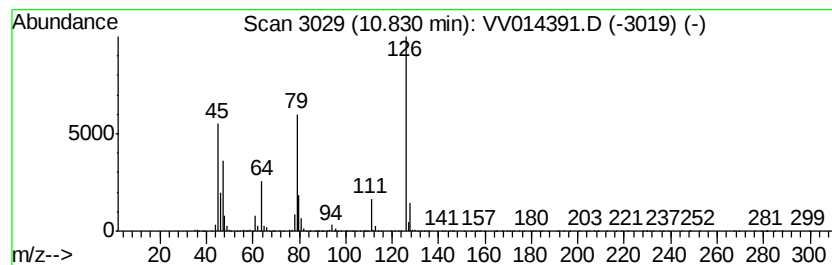
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Peak Number 4 Dimethyl trisulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	1.91 ug/L	967513	1,4-Dichlorobenzene-d4	11.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Dimethyl trisulfide	126 C2H6S3	003658-80-8 96
2		Dimethyl trisulfide	126 C2H6S3	003658-80-8 96
3		Pyrazine, (methylthio)-	126 C5H6N2S	021948-70-9 43
4		Pentasulfide, dimethyl	190 C2H6S5	007330-31-6 37
5		S-(2,2,2-Trifluoroethyl) methane...	194 C3H5F3O2S2	069466-44-0 35



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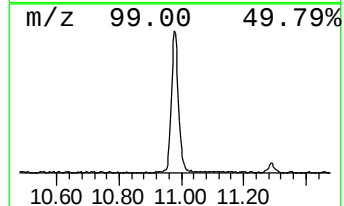
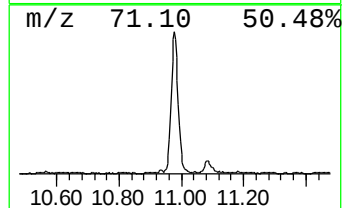
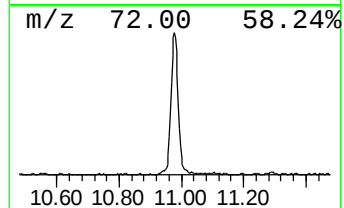
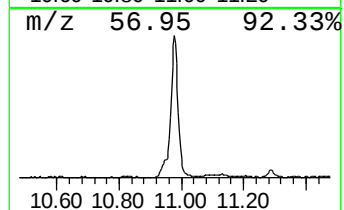
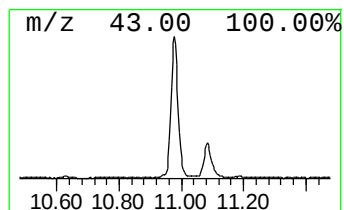
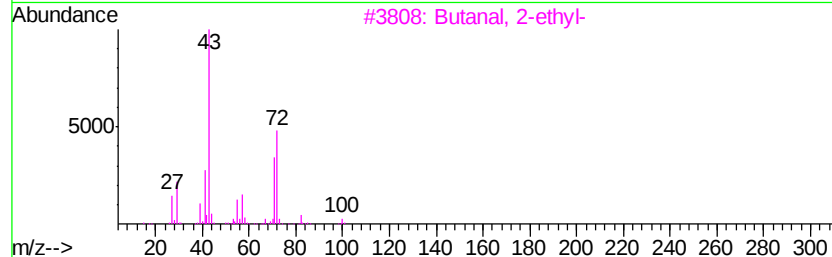
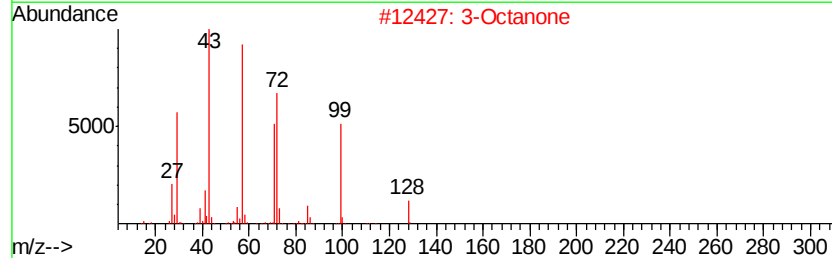
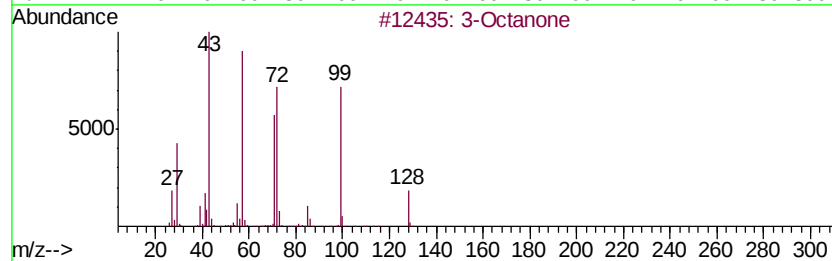
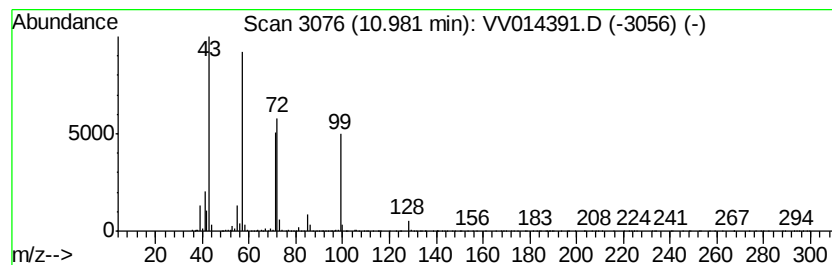
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 Peak Number 5 3-Octanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	2.07 ug/L	1049180	1,4-Dichlorobenzene-d4	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone		128	C8H16O	000106-68-3	94
2	3-Octanone		128	C8H16O	000106-68-3	59
3	Butanal, 2-ethyl-		100	C6H12O	000097-96-1	50
4	Ethanone, 1-(3,3-dimethyloxiranyl)-		114	C6H10O2	004478-63-1	50
5	2-Buten-1-ol, acetate		114	C6H10O2	000628-08-0	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanethiol	1.48	9.9	ug/L	4282920	1	5.66	2154840	5.0
Disulfide, dimethyl	7.14	6.0	ug/L	2578840	1	5.66	2154840	5.0
Dimethyl trisulfide	10.83	1.9	ug/L	967513	3	11.29	2538490	5.0
3-Octanone	10.98	2.1	ug/L	1049180	3	11.29	2538490	5.0