

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100622\
 Data File : VN074789.D
 Acq On : 06 Oct 2022 17:28
 Operator : JC\MD
 Sample : N4910-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-2

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_N\methods\82N100522W.M

Title : SW846 8260

Signal : TIC: VN074789.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.306	38	43	52	rBV	349730	649495	24.03%	5.395%
2	2.418	59	62	65	rBV2	24301	46045	1.70%	0.382%
3	2.830	127	132	133	rBV2	127373	165197	6.11%	1.372%
4	5.530	582	591	602	rVB2	28593	98400	3.64%	0.817%
5	7.447	909	917	930	rBV2	86564	255847	9.47%	2.125%
6	8.177	1030	1041	1046	rBV	353755	860751	31.84%	7.150%
7	8.229	1046	1050	1060	rVB2	333033	756374	27.98%	6.283%
8	8.588	1102	1111	1124	rBV3	442236	1006093	37.22%	8.357%
9	9.112	1190	1200	1211	rBV	529458	1113842	41.21%	9.252%
10	10.571	1438	1448	1457	rBV	1453318	2702962	100.00%	22.452%
11	11.870	1661	1669	1681	rBV	819191	1489408	55.10%	12.372%
12	12.853	1829	1836	1845	rVB	833335	1420293	52.55%	11.798%
13	13.794	1987	1996	2004	rBV	874544	1473983	54.53%	12.244%

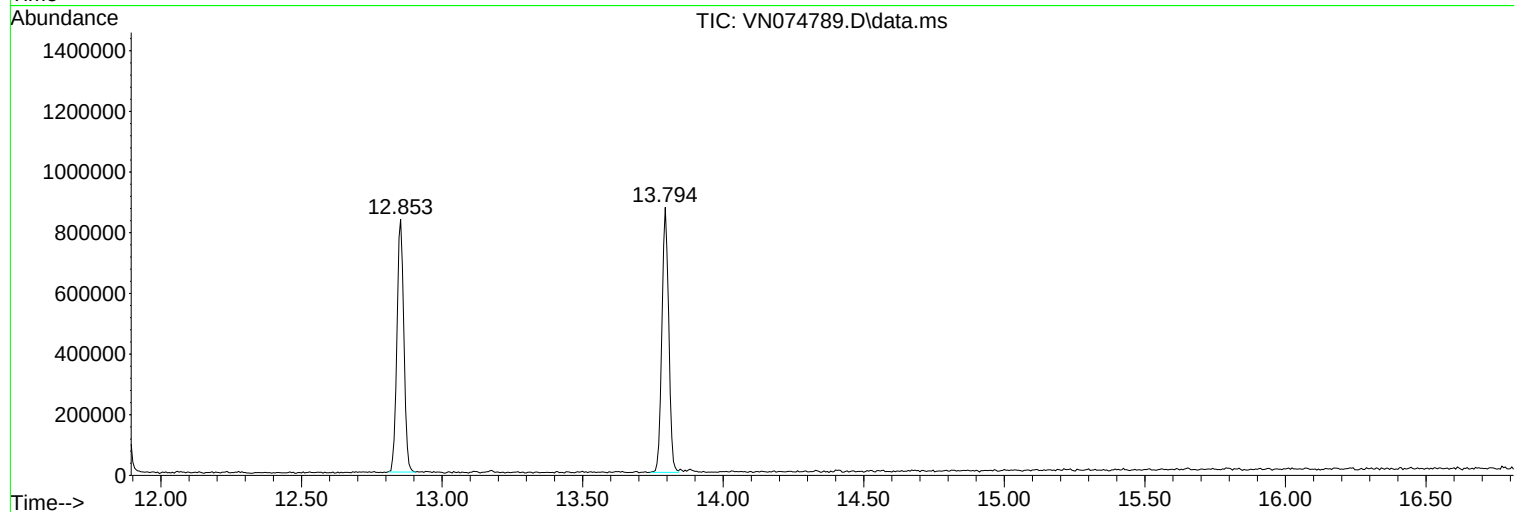
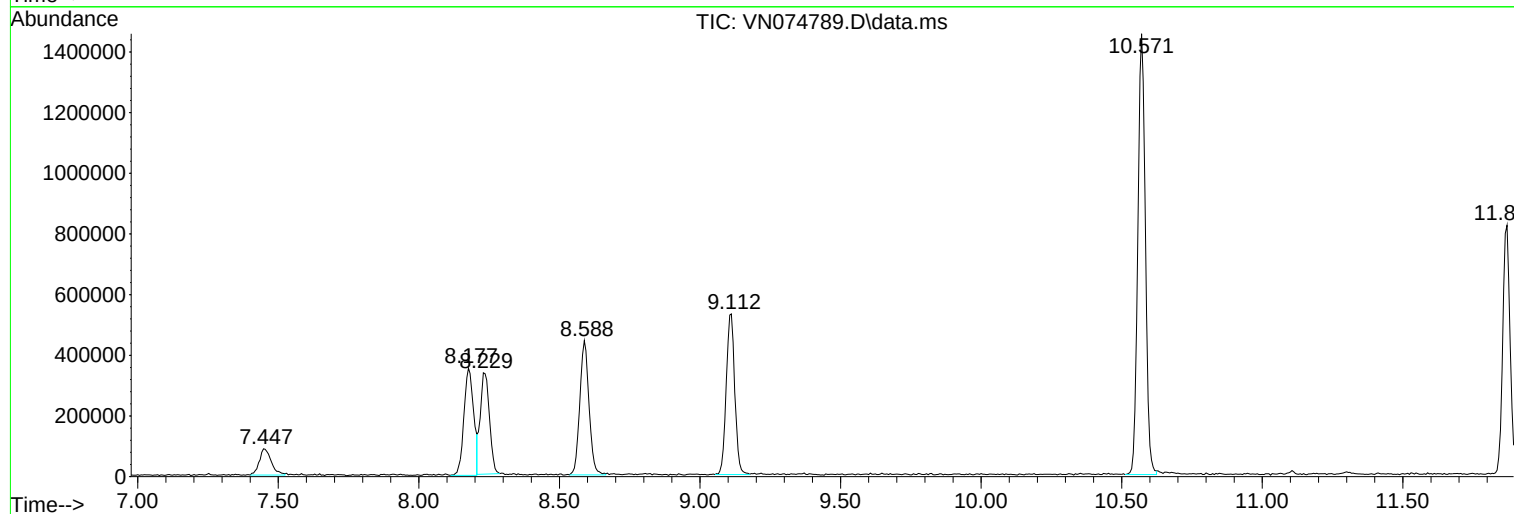
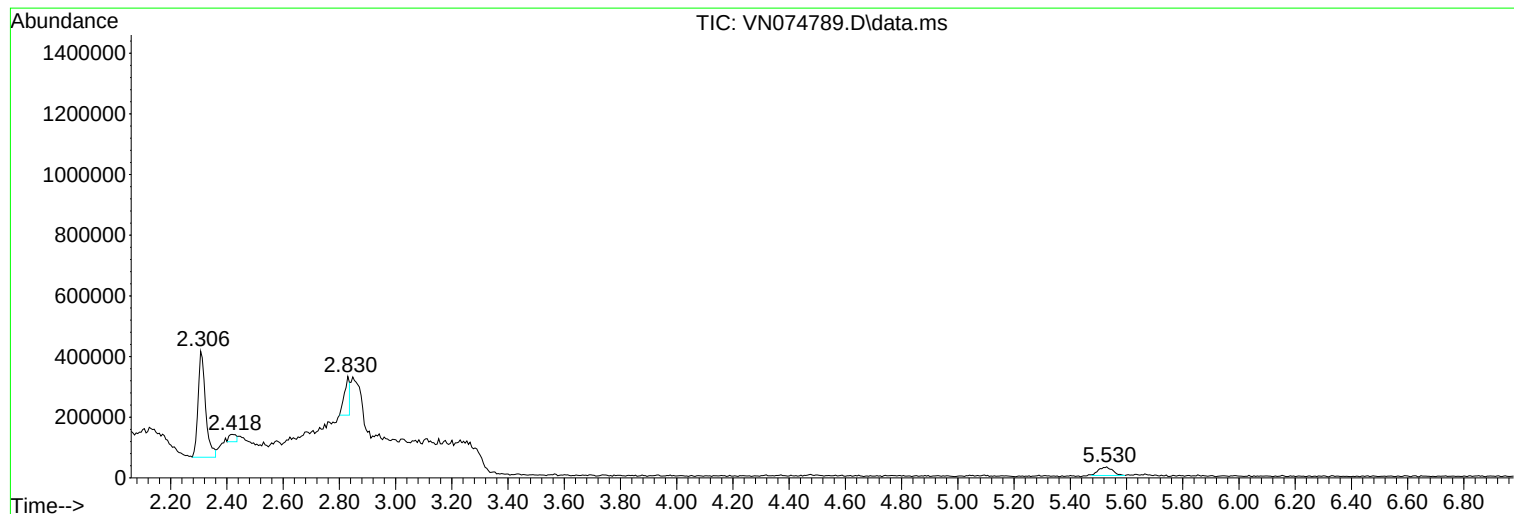
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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



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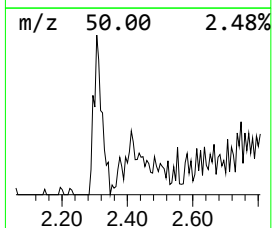
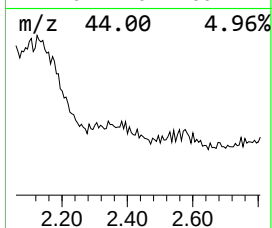
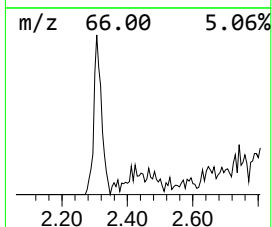
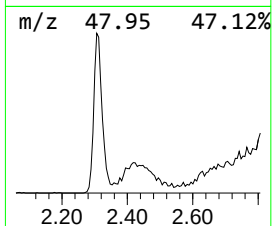
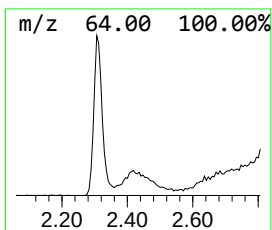
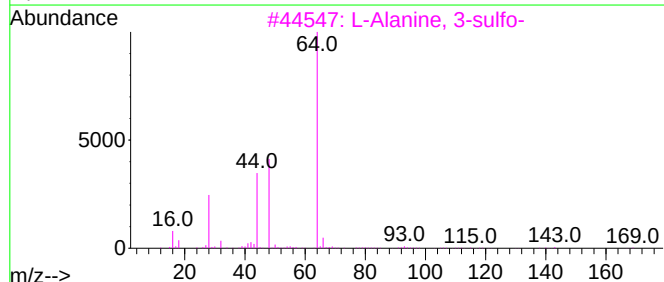
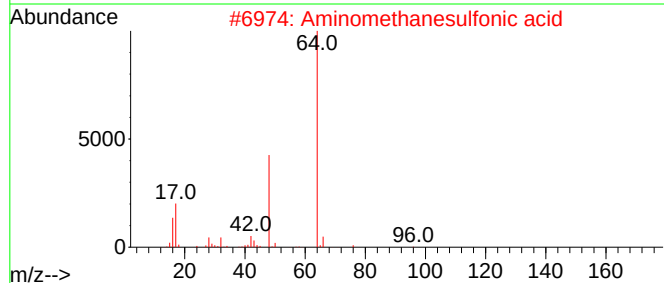
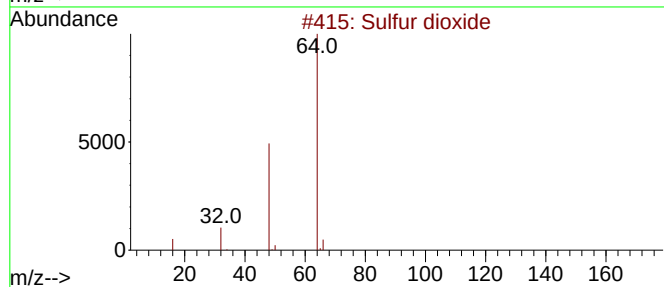
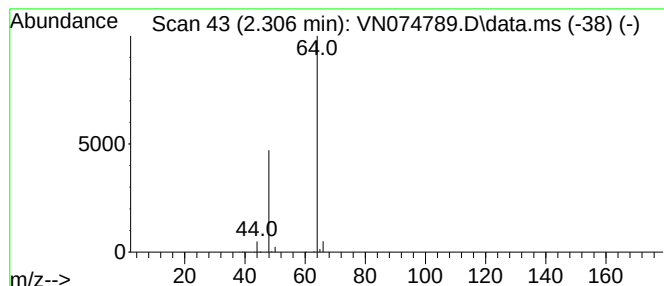
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.306	42.93 ug/l	649495	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	4



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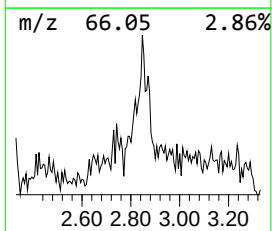
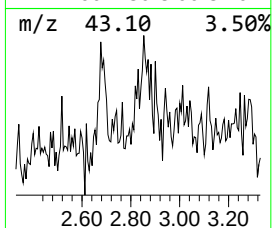
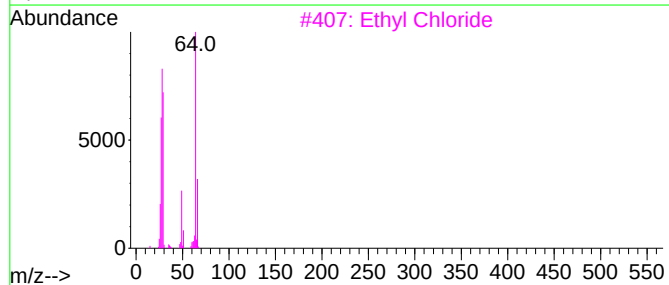
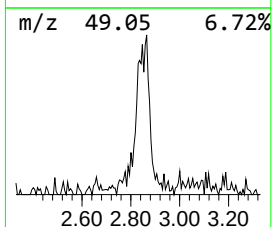
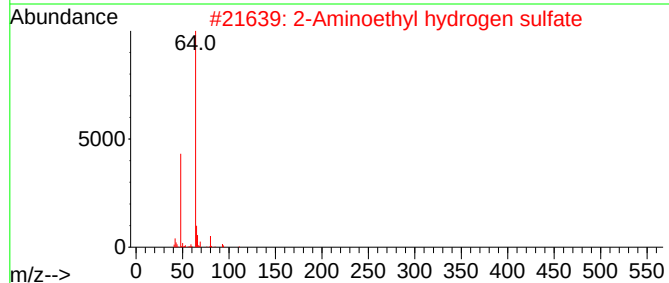
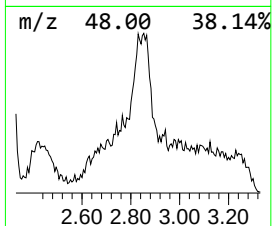
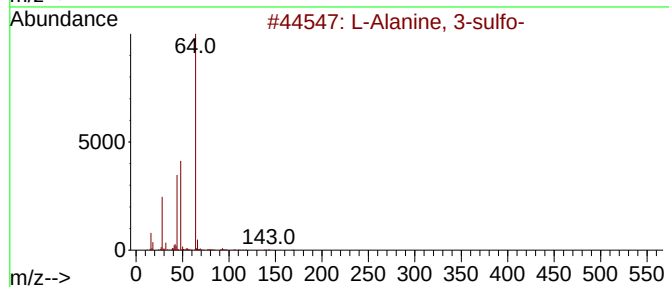
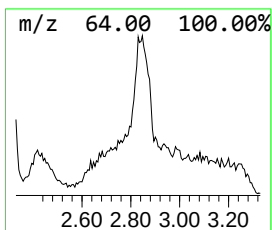
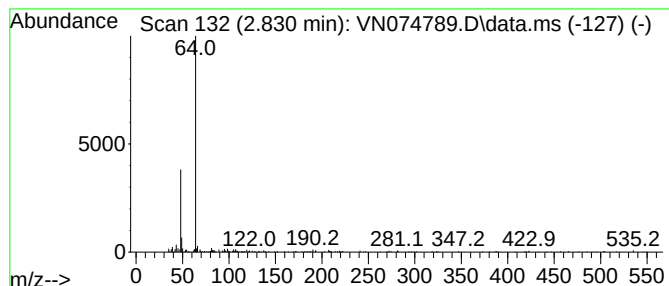
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Quant Title : SW846 8260

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

Peak Number 2 L-Alanine, 3-sulfo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.830	10.92 ug/l	165197	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	74
2			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	64
3			Ethyl Chloride	64	C2H5Cl	000075-00-3	9
4			6-Amino-2,3-diphenyl-8-[p-sulfam...	482	C26H22N6O2S	021271-90-9	9
5			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	9



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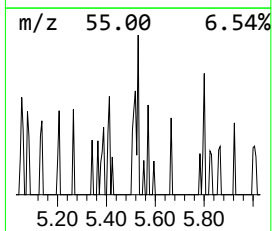
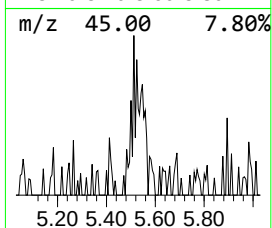
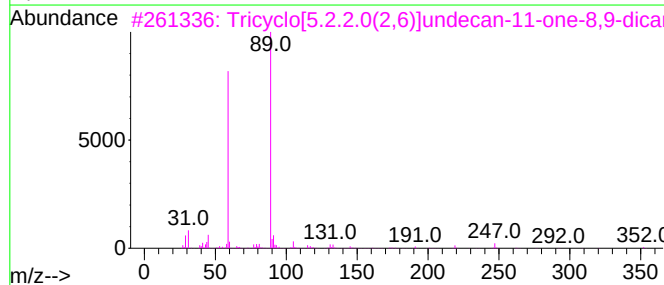
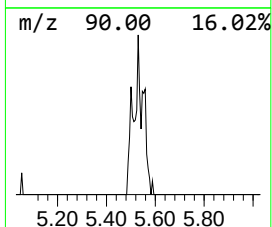
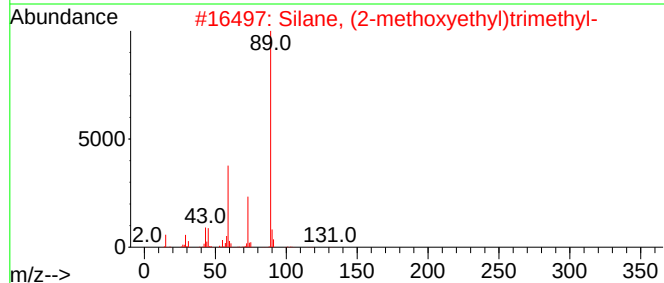
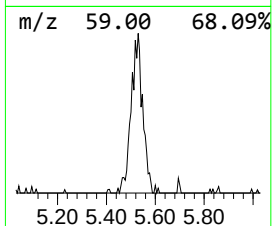
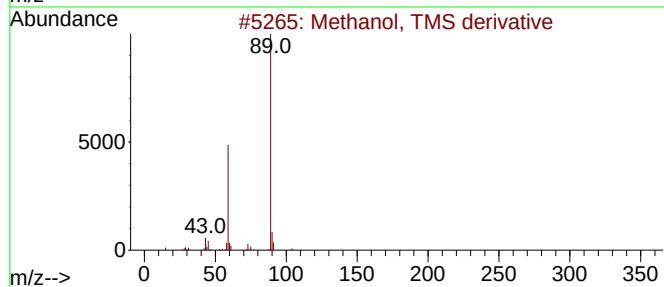
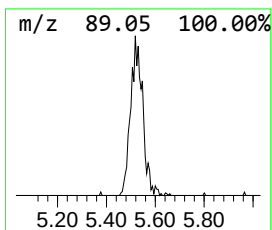
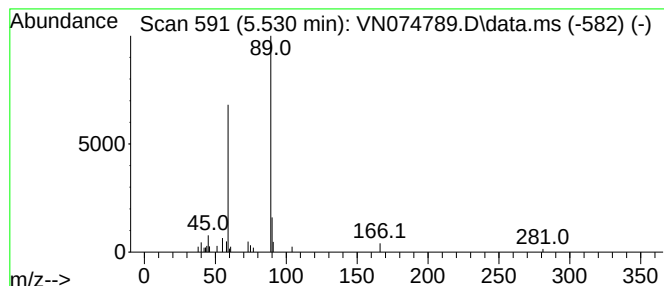
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Peak Number 3 Methanol, TMS derivative Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.530	6.50 ug/l	98400	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
2			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	74
3			Tricyclo[5.2.2.0(2,6)]undecan-11...	352	C18H24O7	1000155-17-7	43
4			2-Methoxyethanol, TBDMS derivative	190	C9H22O2Si	1000352-09-4	40
5			Dimethyloctylmethoxysilane	202	C11H26OSi	093804-29-6	40



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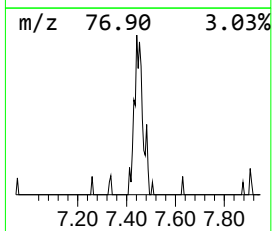
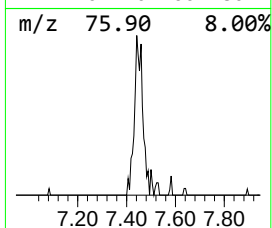
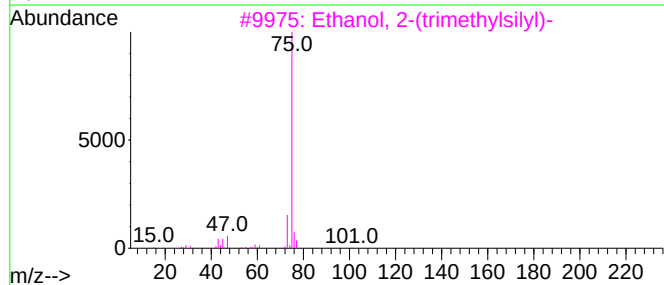
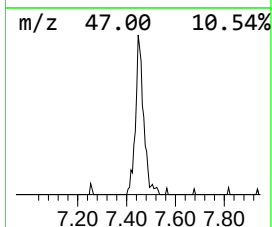
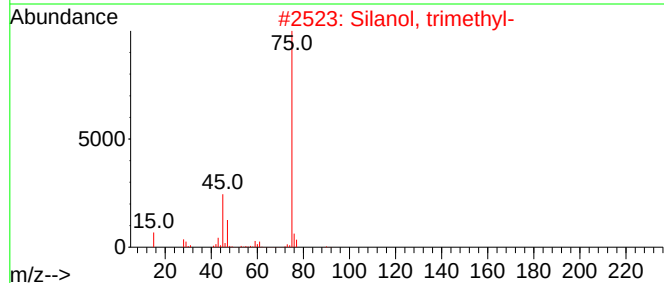
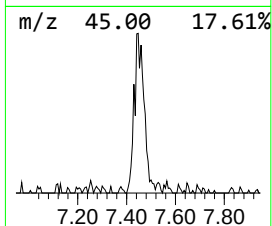
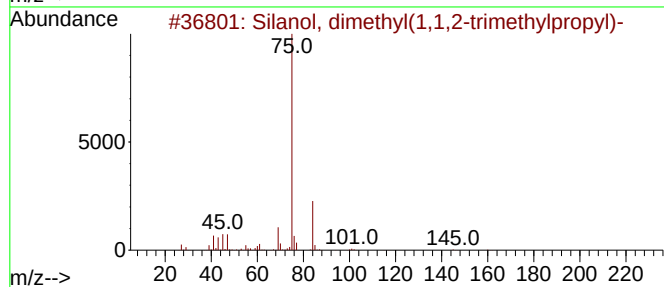
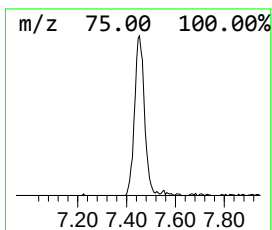
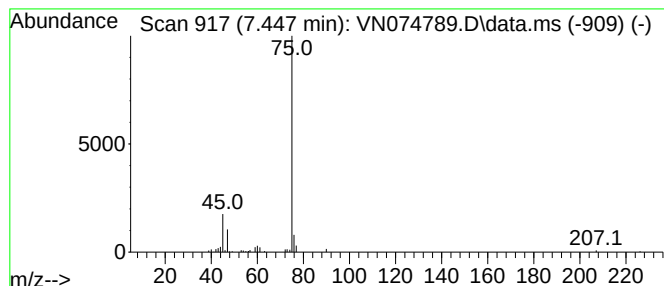
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Silanol, dimethyl(1,1,2-tri... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.447	16.91 ug/l	255847	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silanol, dimethyl(1,1,2-trimethy...	160	C8H20OSi	055644-10-5	78
2			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	64
3			Ethanol, 2-(trimethylsilyl)-	118	C5H14OSi	002916-68-9	50
4			4-Dimethyl(isopropyl)silyloxyoctane	230	C13H30OSi	1000278-74-6	43
5			Hexanal dimethyl acetal	146	C8H18O2	001599-47-9	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.306	42.9	ug/l	649495	1	8.235	756374	50.0
L-Alanine, 3-su...	2.830	10.9	ug/l	165197	1	8.235	756374	50.0
Methanol, TMS d...	5.530	6.5	ug/l	98400	1	8.235	756374	50.0
Silanol, dimeth...	7.447	16.9	ug/l	255847	1	8.235	756374	50.0