

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050422\
 Data File : VN072329.D
 Acq On : 04 May 2022 15:38
 Operator : JC\MD
 Sample : N2602-03
 Misc : 5.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 12-15-SB4-BK-PRISON

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\82N042622W.M
 Title : SW846 8260

Signal : TIC: VN072329.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	34	41	62	rVB3	50834	187175	10.92%	1.865%
2	2.410	68	72	76	rVB3	10263	17547	1.02%	0.175%
3	2.822	119	142	143	rBV7	34528	148033	8.64%	1.475%
4	5.304	551	564	576	rBV2	18687	69883	4.08%	0.696%
5	7.345	901	911	922	rBV2	15018	47714	2.78%	0.475%
6	8.016	1015	1025	1030	rBV	202071	505064	29.47%	5.032%
7	8.075	1030	1035	1046	rVB	347634	791909	46.21%	7.890%
8	8.428	1085	1095	1108	rBV	231285	542017	31.63%	5.400%
9	8.645	1125	1132	1143	rBV3	11710	28800	1.68%	0.287%
10	8.963	1177	1186	1197	rBV	580487	1208060	70.49%	12.036%
11	10.433	1428	1436	1445	rBV	905876	1713721	100.00%	17.074%
12	10.498	1445	1447	1455	rVB2	28964	43936	2.56%	0.438%
13	11.739	1650	1658	1672	rBV	934468	1682990	98.21%	16.768%
14	12.727	1818	1826	1839	rBV	785860	1283074	74.87%	12.784%
15	13.045	1875	1880	1888	rVB6	10394	20023	1.17%	0.199%
16	13.668	1979	1986	1996	rBV	892544	1498829	87.46%	14.933%
17	13.992	2036	2041	2047	rVB3	13256	18952	1.11%	0.189%
18	14.645	2145	2152	2159	rVB5	7685	19396	1.13%	0.193%
19	16.315	2428	2436	2447	rBV2	90272	209637	12.23%	2.089%

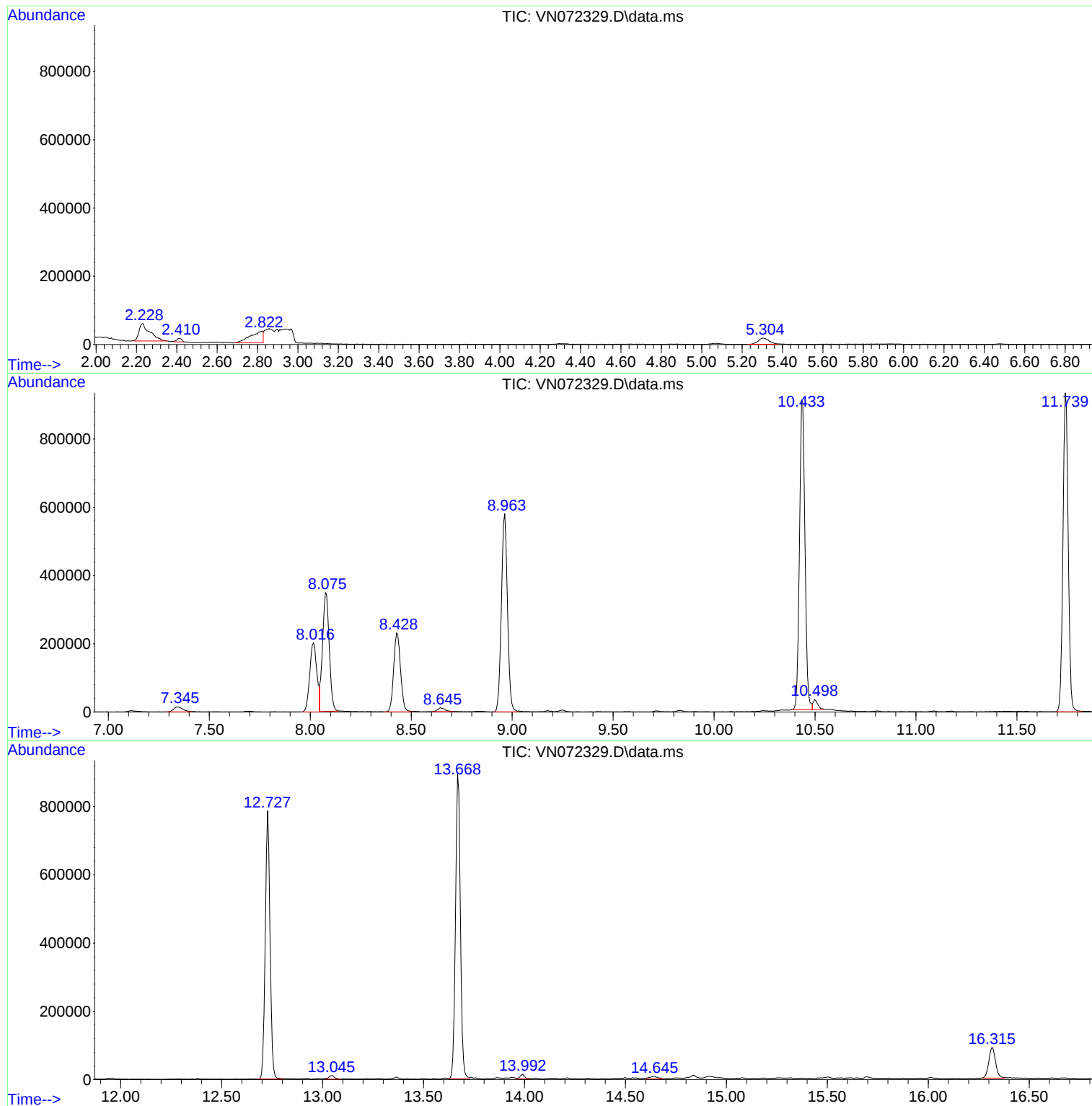
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

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



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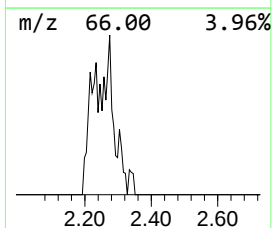
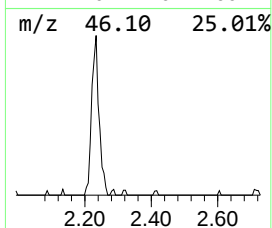
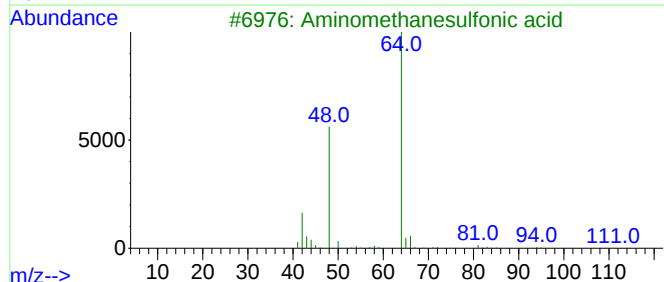
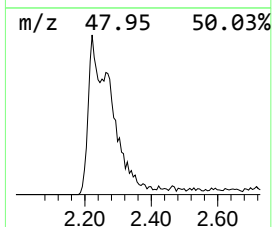
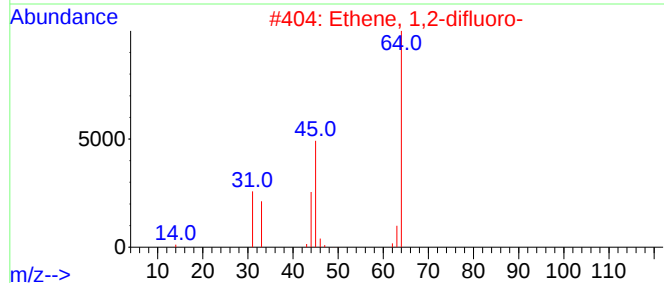
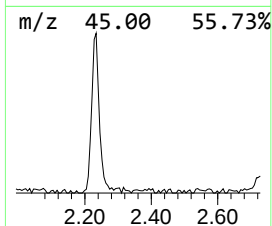
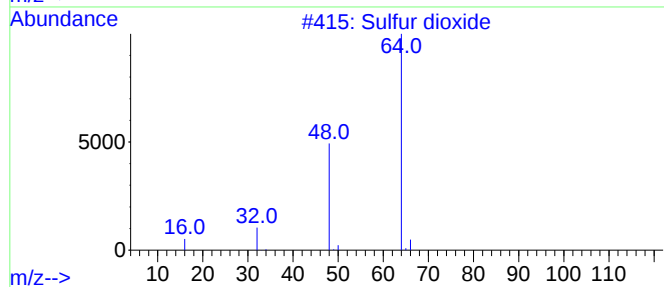
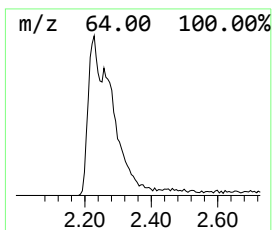
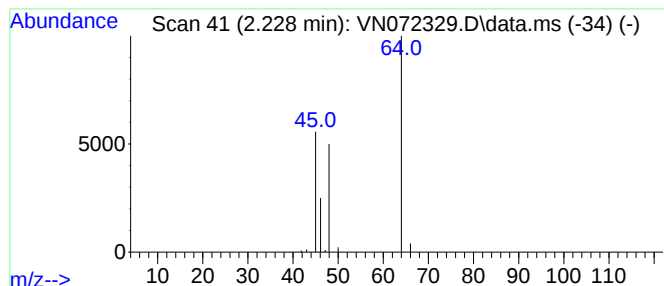
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

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.
2.228	11.82 ug/l	187175	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	56
2			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7



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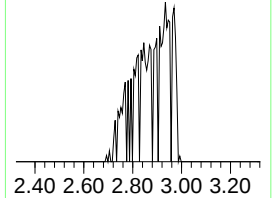
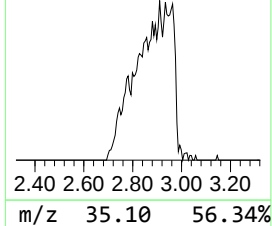
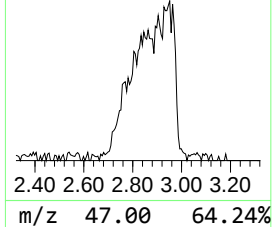
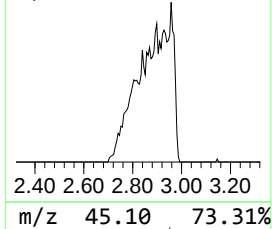
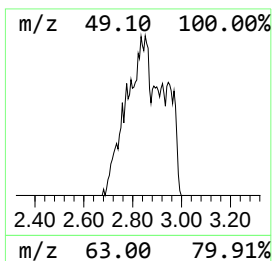
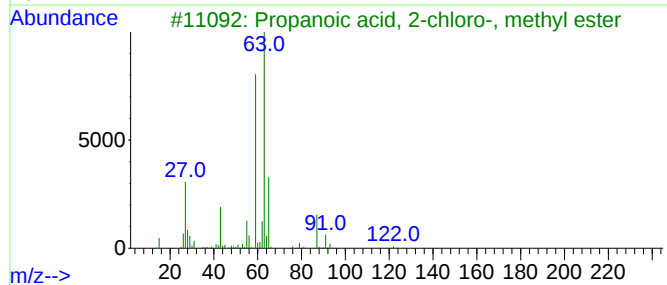
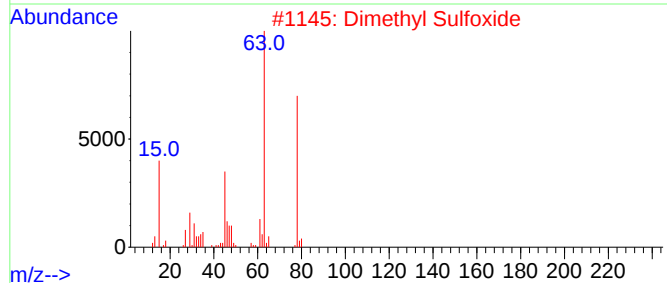
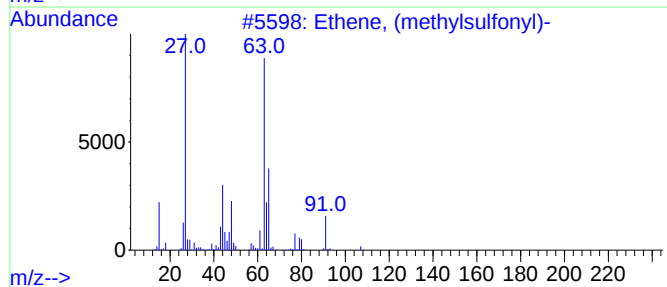
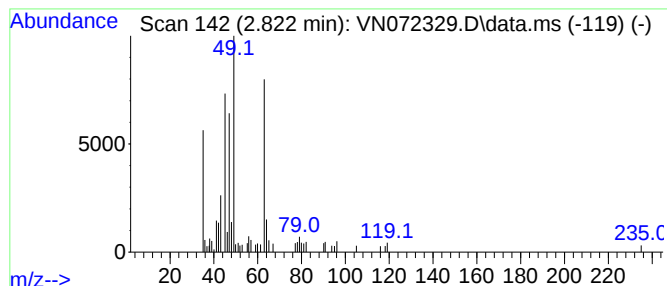
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Peak Number 2 unknown2.822 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.822	9.35 ug/l	148033	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	12
2			Dimethyl Sulfoxide	78	C2H6OS	000067-68-5	10
3			Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	017639-93-9	9
4			1-Chloro-2-(ethanesulfonyl)ethane	156	C4H9ClO2S	025027-40-1	9
5			1,3-Dioxonane, 5,5,6,6,7,7,8,8-o...	274	C7H6F8O2	036301-47-0	9



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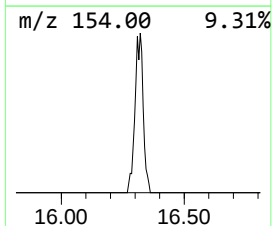
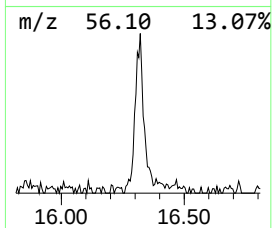
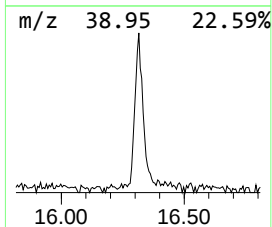
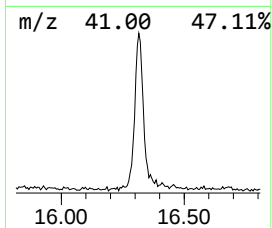
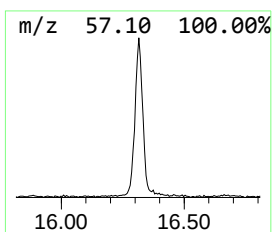
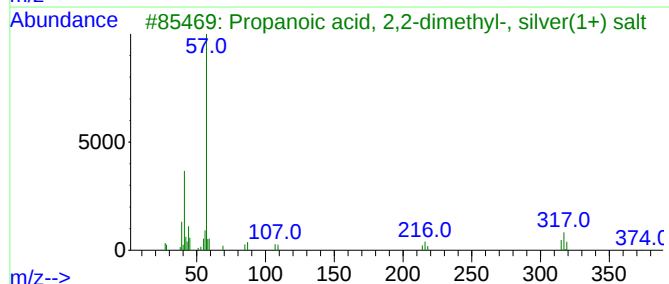
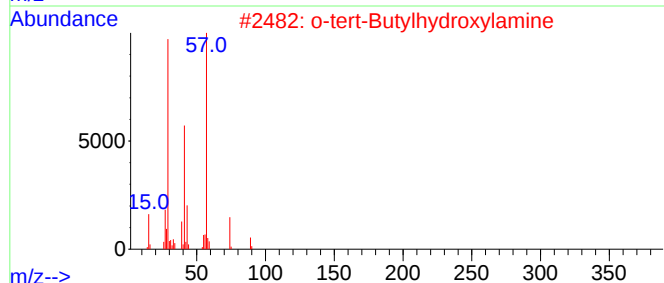
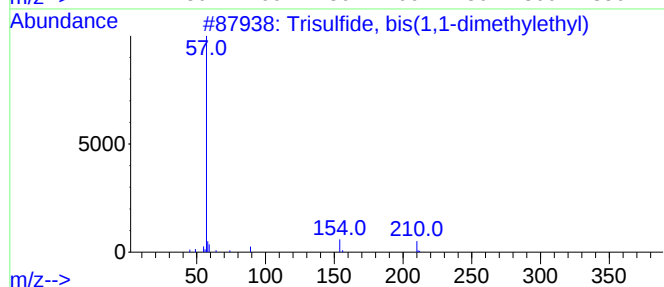
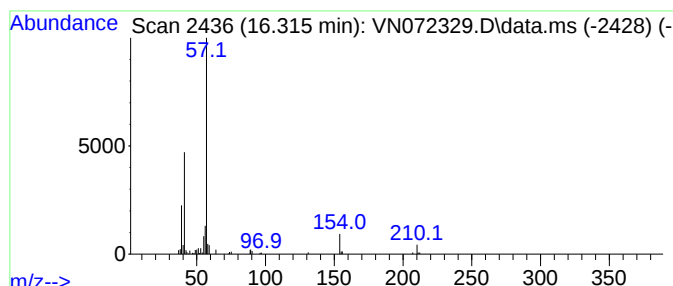
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Trisulfide, bis(1,1-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.315	6.99 ug/l	209637	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	83
2			o-tert-Butylhydroxylamine	89	C4H11NO	1000322-43-1	38
3			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	32
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	25
5			Propane, 2,2'-[methylenebis(oxy)...]	160	C9H20O2	002568-93-6	23



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.228	11.8	ug/l	187175	1	8.081	791909	50.0
unknown2.822	2.822	9.3	ug/l	148033	1	8.081	791909	50.0
Trisulfide, bis...	16.315	7.0	ug/l	209637	4	13.668	1498830	50.0