

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
 Data File : VN074702.D
 Acq On : 01 Oct 2022 10:04
 Operator : JC\MD
 Sample : N4882-15
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-127

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\82N092922W.M
 Title : SW846 8260

Signal : TIC: VN074705.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	39	45	53	rBV	462656	871963	11.51%	2.510%
2	2.234	53	59	60	rBV3	61037	112360	1.48%	0.323%
3	5.163	545	557	573	rBV2	528760	1882365	24.85%	5.419%
4	5.422	587	601	616	rBV	2125108	7575603	100.00%	21.811%
5	6.304	741	751	761	rBV2	41077	118948	1.57%	0.342%
6	6.910	844	854	865	rBV3	92744	279034	3.68%	0.803%
7	7.869	1005	1017	1023	rBV2	710126	1800041	23.76%	5.182%
8	7.933	1023	1028	1042	rVB	705626	1568845	20.71%	4.517%
9	8.292	1078	1089	1099	rBV	823413	1923078	25.39%	5.537%
10	8.392	1099	1106	1114	rVV3	42708	98074	1.29%	0.282%
11	8.492	1114	1123	1132	rVB3	294225	692024	9.13%	1.992%
12	8.827	1171	1180	1191	rBV2	1124981	2328407	30.74%	6.704%
13	10.310	1424	1432	1446	rBV	2944525	5354573	70.68%	15.416%
14	11.615	1647	1654	1668	rBV	1819153	3262573	43.07%	9.393%
15	12.604	1815	1822	1833	rBV	2163812	3668359	48.42%	10.561%
16	13.545	1975	1982	1990	rBV	1879794	3197438	42.21%	9.206%

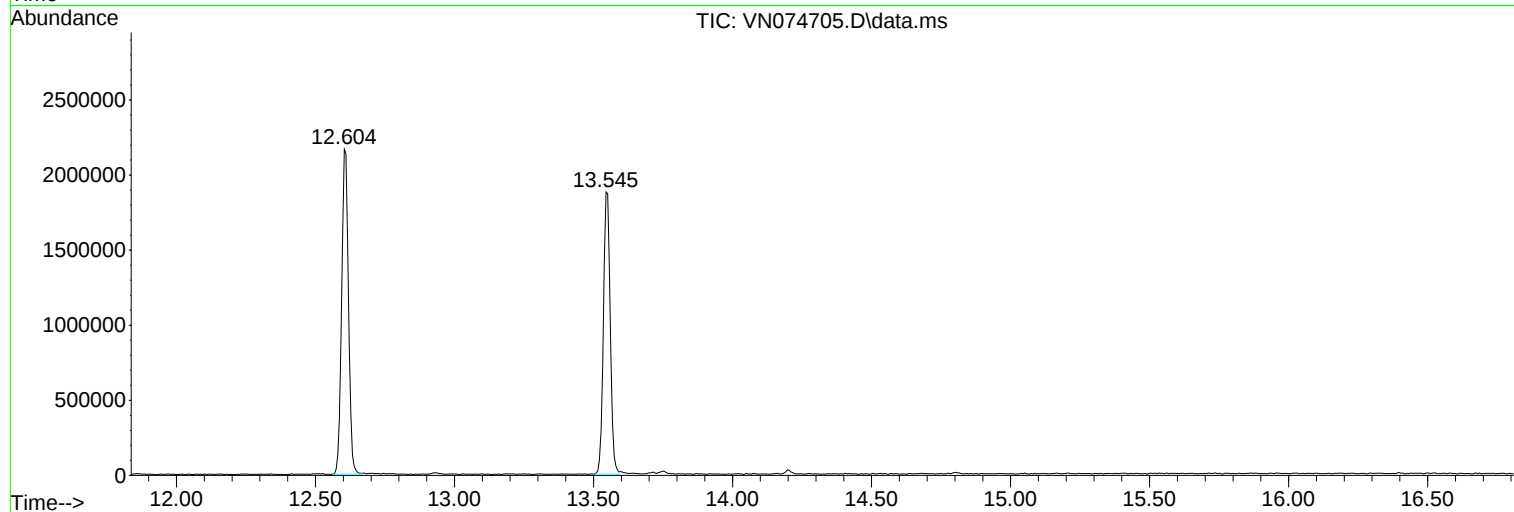
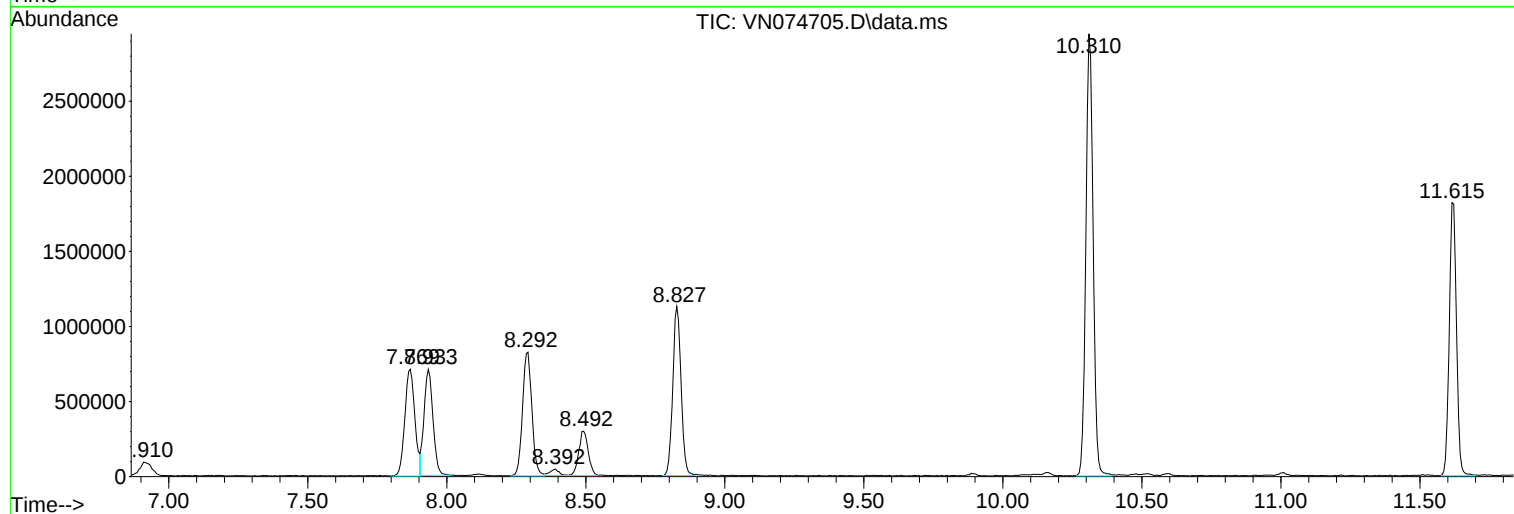
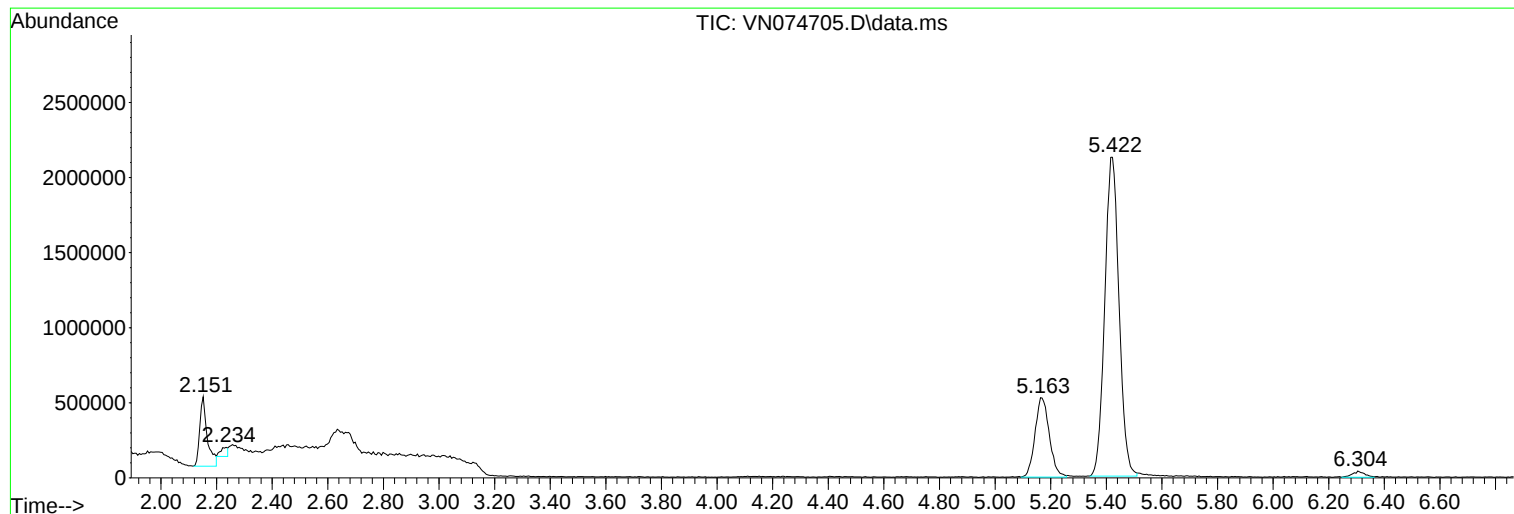
Sum of corrected areas: 34733685

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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



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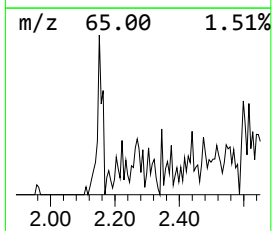
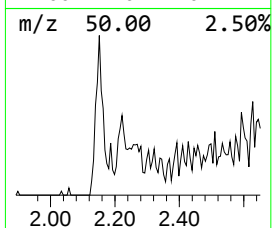
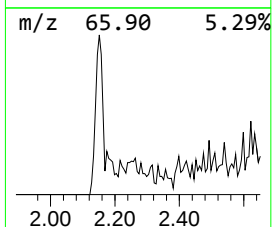
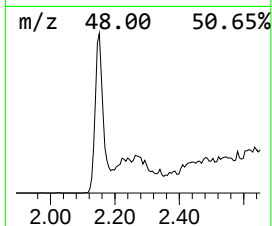
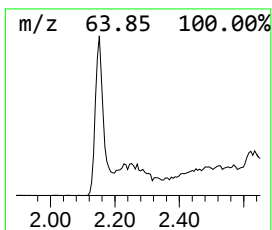
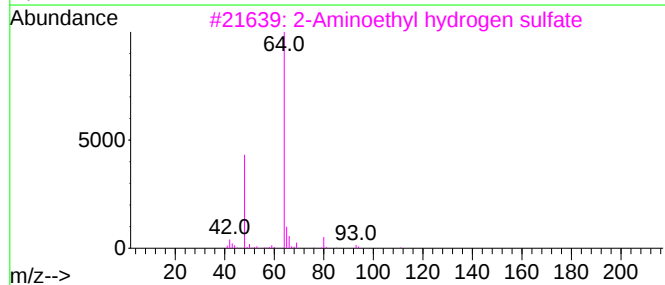
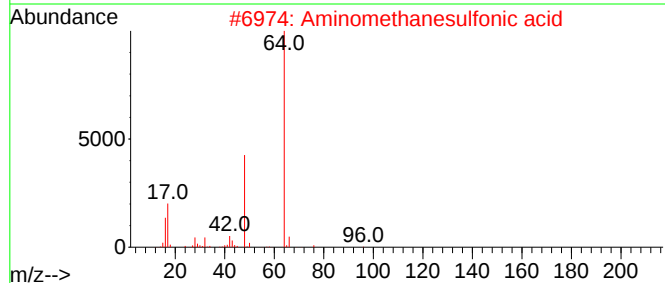
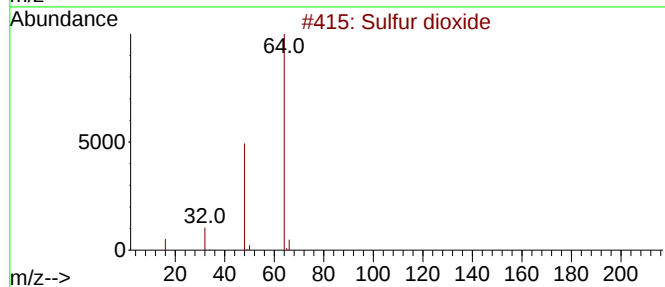
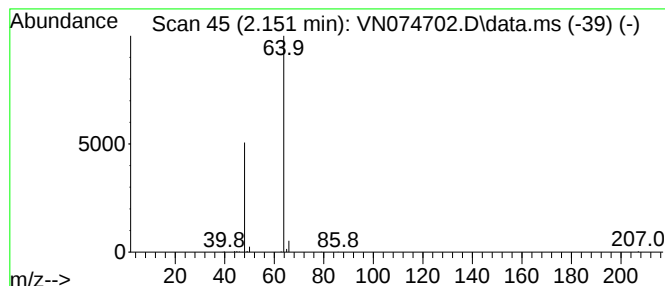
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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.
2.151	27.79 ug/l	871963	Pentafluorobenzene	7.933

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			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4			1,1,1,2,2,3,3,4,4,5,5-Undecafluorooctane	602	C10F22O2S	1000486-78-5	64
5			4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	9



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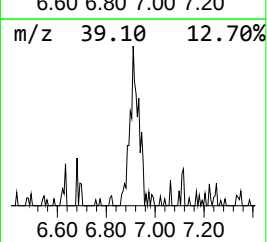
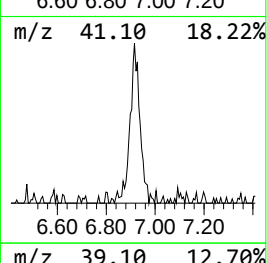
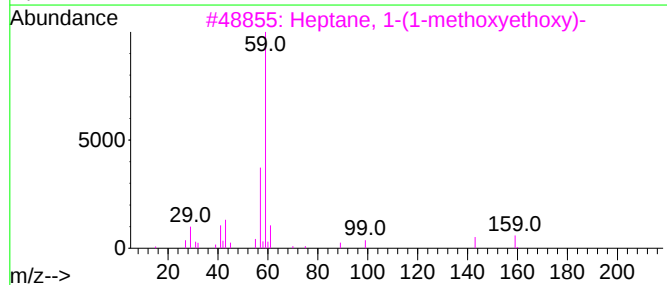
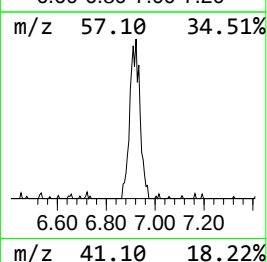
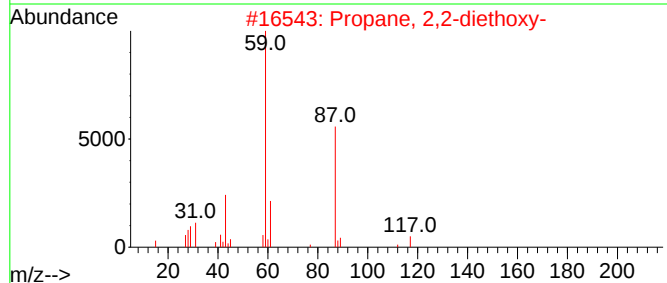
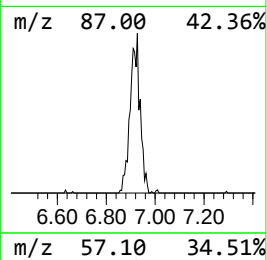
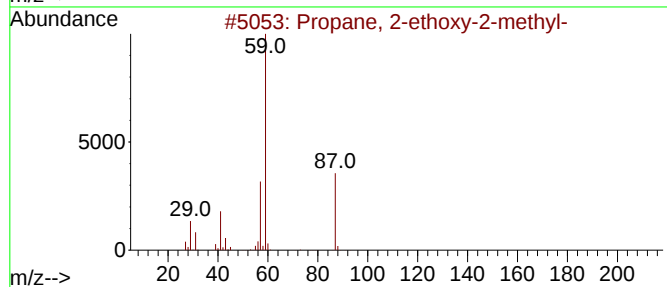
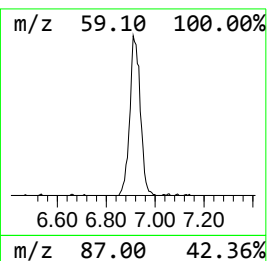
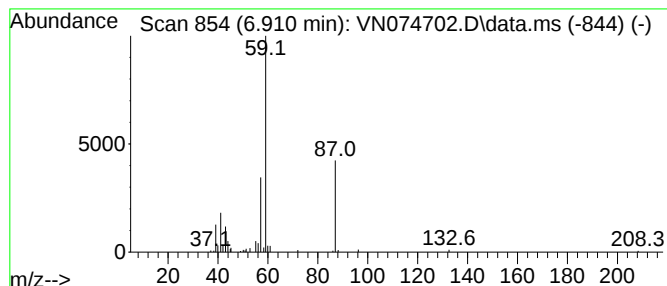
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Peak Number 2 Propane, 2-ethoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.910	8.89 ug/l	279034	Pentafluorobenzene	7.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	64
2			Propane, 2,2-diethoxy-	132	C7H16O2	000126-84-1	39
3			Heptane, 1-(1-methoxyethoxy)-	174	C10H22O2	054532-15-9	38
4			Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	33
5			2,4-Dimethyl-2,4-pentanedio1	132	C7H16O2	024892-49-7	33



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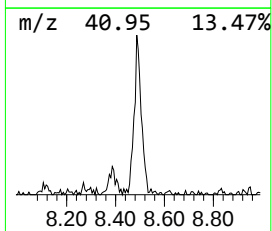
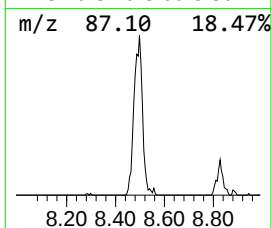
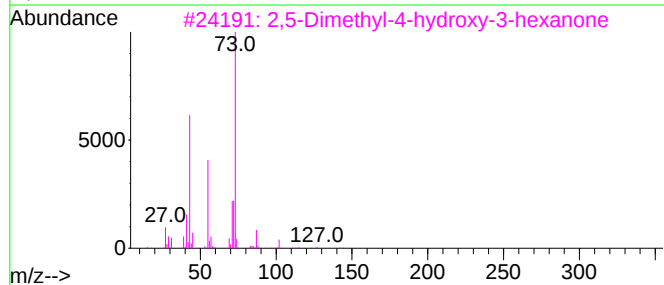
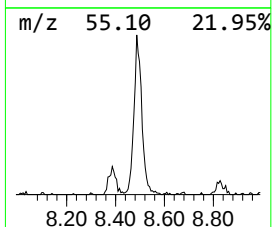
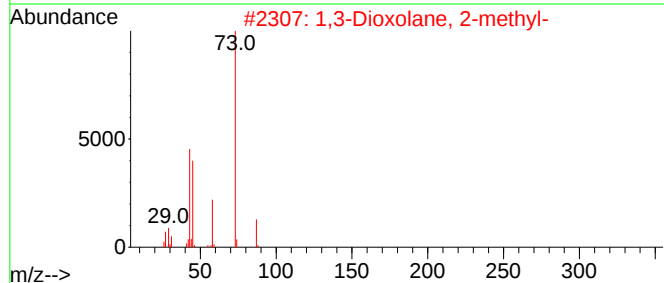
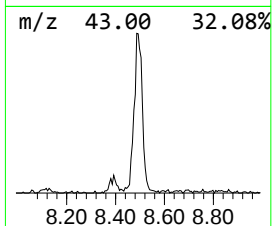
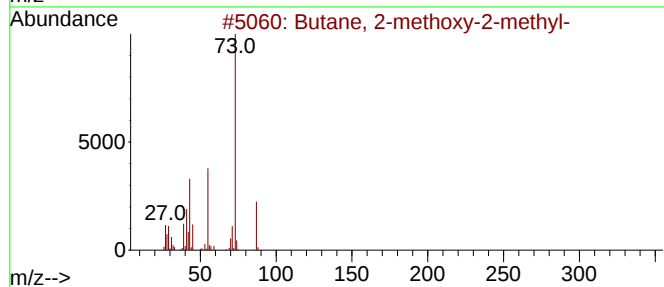
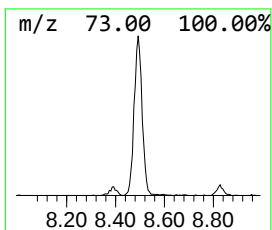
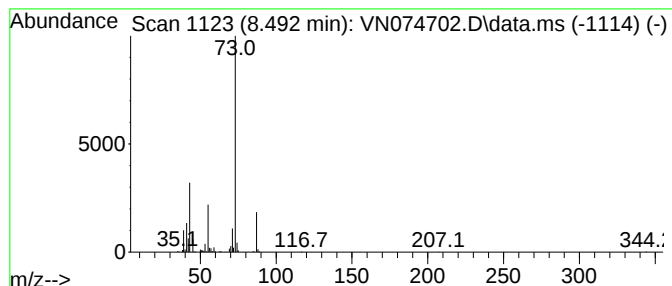
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Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.492	14.86 ug/l	692024	1,4-Difluorobenzene	8.827

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	47
3			2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	33
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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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	2.151	27.8	ug/l	871963	1	7.933	1568850	50.0
Propane, 2-etho...	6.910	8.9	ug/l	279034	1	7.933	1568850	50.0
Butane, 2-metho...	8.492	14.9	ug/l	692024	2	8.827	2328410	50.0