

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050522\
 Data File : VN072341.D
 Acq On : 05 May 2022 13:41
 Operator : JC\MD
 Sample : N2641-04
 Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-24

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: VN072341.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	34	42	46	rBV4	32081	82732	5.87%	1.031%
2	2.810	120	140	141	rBV5	30404	111542	7.91%	1.390%
3	5.298	547	563	580	rBV2	18505	75566	5.36%	0.942%
4	7.351	901	912	922	rBV2	15052	50302	3.57%	0.627%
5	8.016	1013	1025	1030	rBV2	171351	426223	30.23%	5.312%
6	8.075	1030	1035	1049	rVB	294895	675095	47.88%	8.413%
7	8.428	1086	1095	1106	rBV	189345	448990	31.85%	5.595%
8	8.651	1125	1133	1142	rBV4	10673	27059	1.92%	0.337%
9	8.963	1177	1186	1202	rVB	472964	990114	70.23%	12.339%
10	10.439	1427	1437	1445	rBV	759362	1409845	100.00%	17.570%
11	10.504	1445	1448	1453	rVB2	9942	15658	1.11%	0.195%
12	11.739	1650	1658	1672	rBV	789472	1407983	99.87%	17.547%
13	12.727	1819	1826	1838	rBV	639067	1067922	75.75%	13.309%
14	13.668	1979	1986	1999	rVB	707750	1216838	86.31%	15.165%
15	15.504	2291	2298	2304	rVB2	8551	18323	1.30%	0.228%

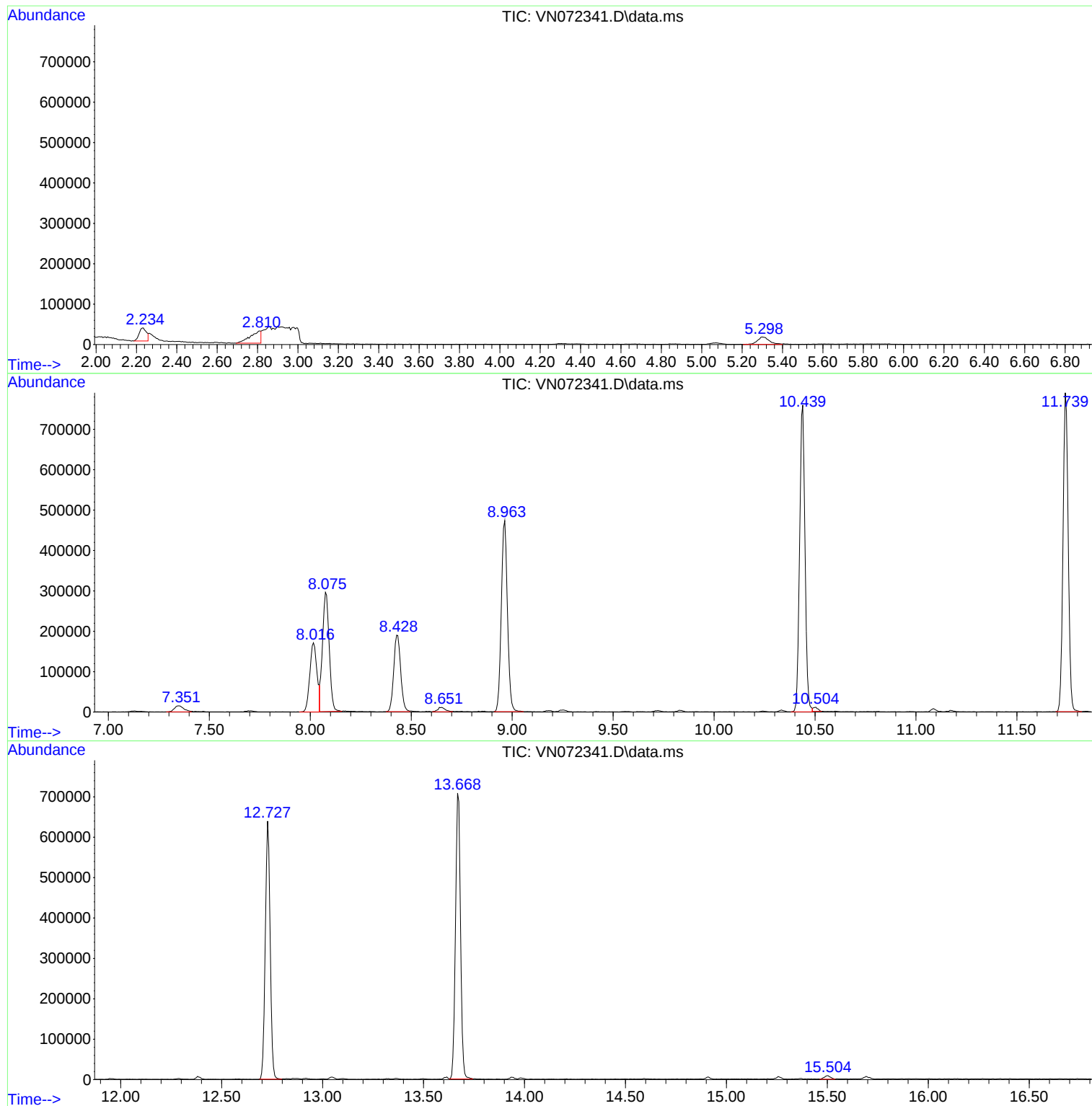
Sum of corrected areas: 8024192

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050522\
Data File : VN072341.D
Acq On : 05 May 2022 13:41
Operator : JC\MD
Sample : N2641-04
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-24

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050522\
Data File : VN072341.D
Acq On : 05 May 2022 13:41
Operator : JC\MD
Sample : N2641-04
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-24

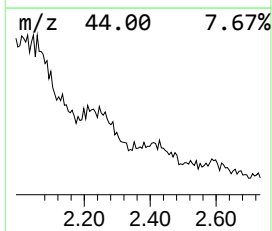
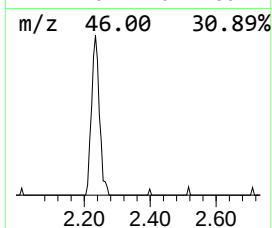
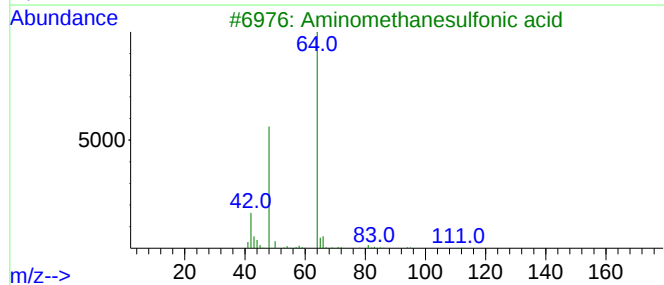
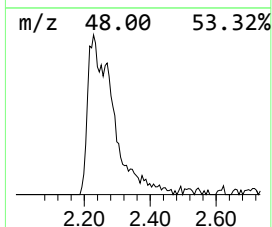
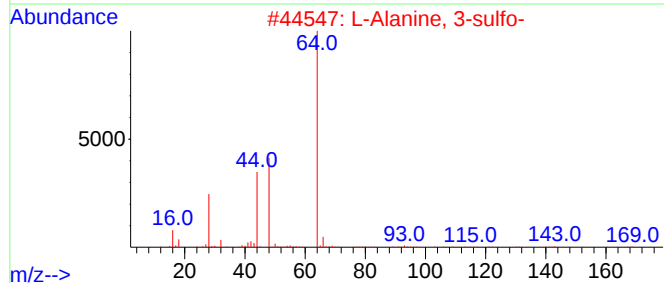
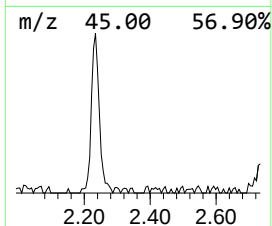
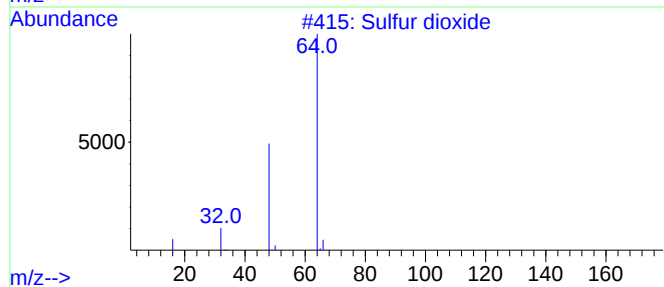
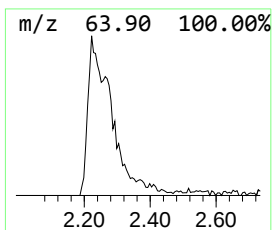
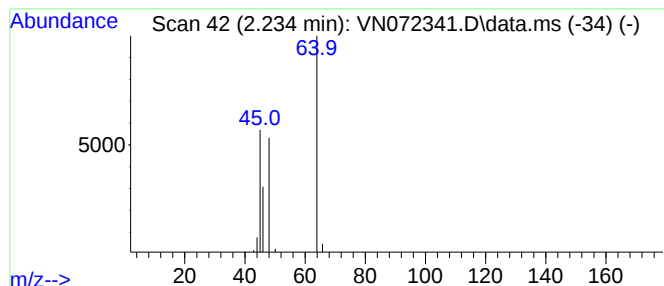
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	6.13 ug/l	82732	Pentafluorobenzene	8.080

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050522\
Data File : VN072341.D
Acq On : 05 May 2022 13:41
Operator : JC\MD
Sample : N2641-04
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-24

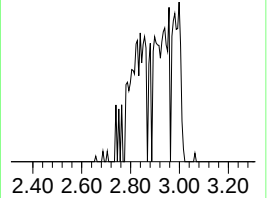
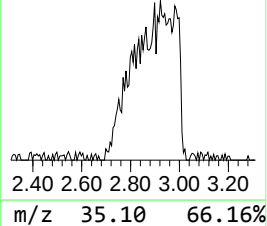
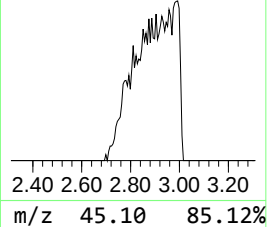
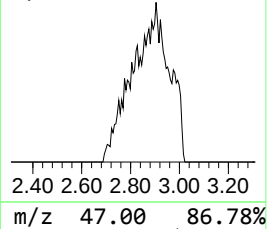
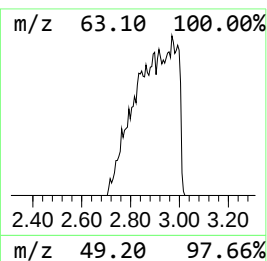
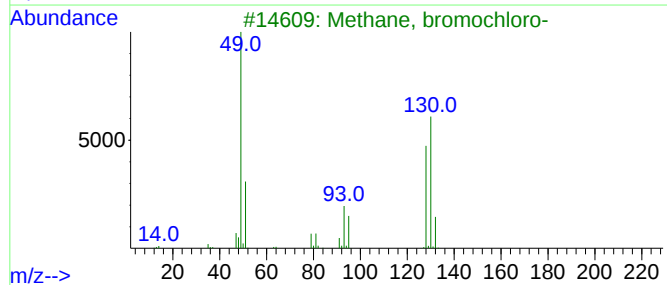
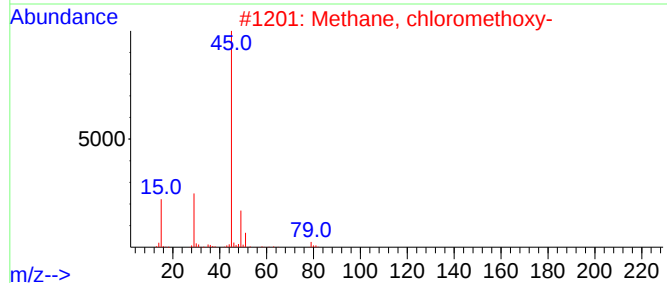
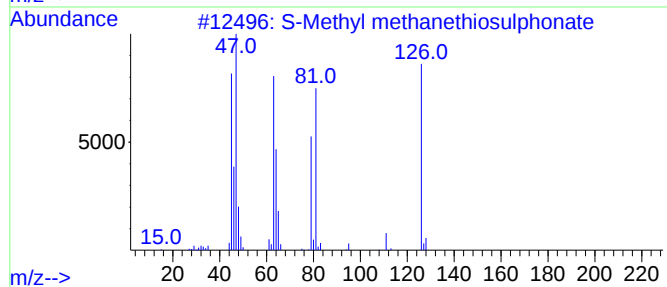
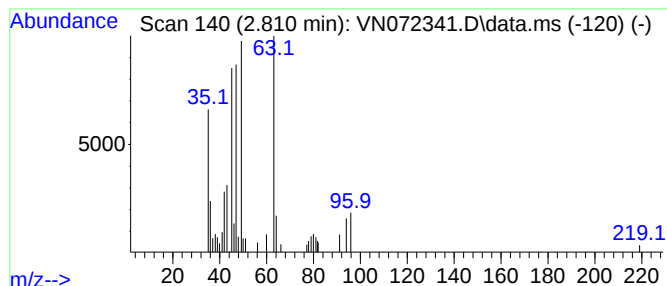
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown2.810 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.810	8.26 ug/l	111542	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			S-Methyl methanethiosulphonate	126	C2H6O2S2	002949-92-0	13
2			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	12
3			Methane, bromochloro-	128	CH2BrCl	000074-97-5	9
4			Chloromethyl thiocyanate	107	C2H2ClNS	003268-79-9	9
5			bis(chloromethyl) carbonate	158	C3H4Cl2O3	1000404-37-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050522\
Data File : VN072341.D
Acq On : 05 May 2022 13:41
Operator : JC\MD
Sample : N2641-04
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-24

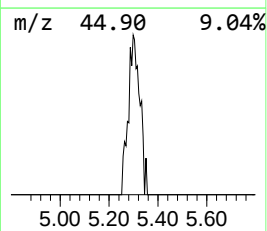
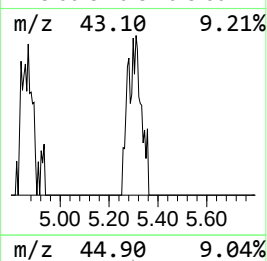
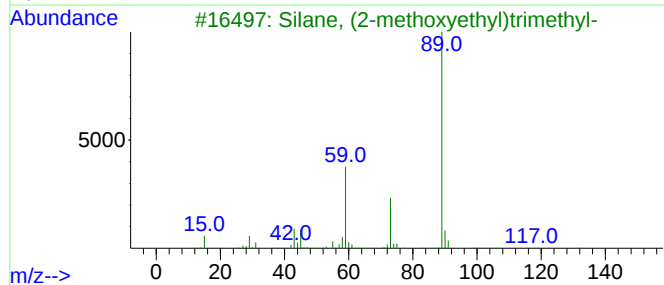
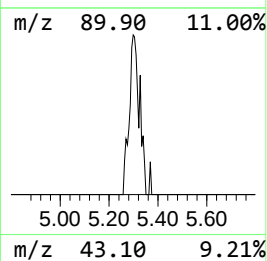
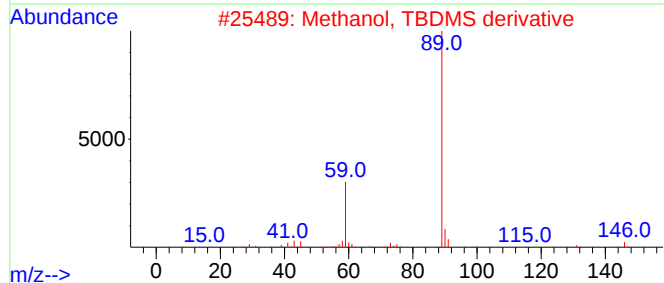
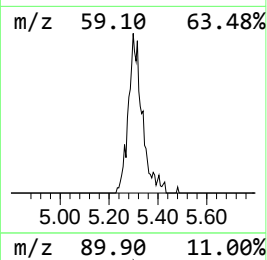
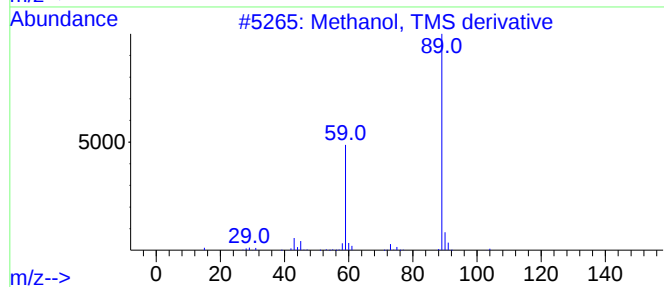
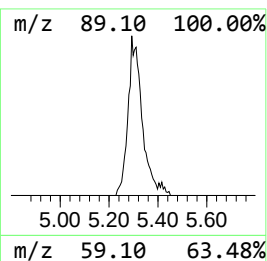
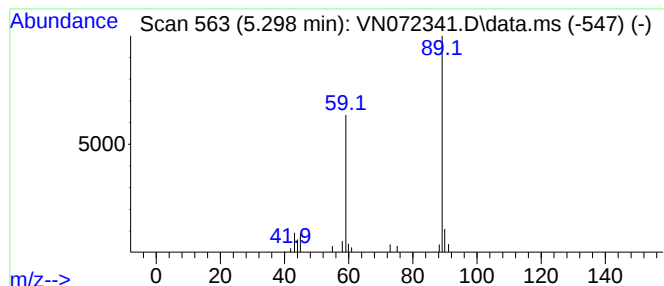
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

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

Peak Number 3 Methanol, TMS derivative Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.298	5.60 ug/l	75566	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
2			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	83
3			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	78
4			Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	72
5			Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050522\
Data File : VN072341.D
Acq On : 05 May 2022 13:41
Operator : JC\MD
Sample : N2641-04
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-24

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.234	6.1	ug/l	82732	1	8.080	675095	50.0
unknown2.810	2.810	8.3	ug/l	111542	1	8.080	675095	50.0
Methanol, TMS d...	5.298	5.6	ug/l	75566	1	8.080	675095	50.0