

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111621\
 Data File : VY006763.D
 Acq On : 16 Nov 2021 15:50
 Operator : SY/MD
 Sample : M4674-03
 Misc : 5.03G/5ML/MSVOA_Y/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 MF-SOIL-P2

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_Y\methods\82Y111521S.M

Title : SW846 8260

Signal : TIC: VY006763.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.204	384	391	400	rVB2	2580	6692	1.91%	0.339%
2	4.728	468	477	489	rBV2	4908	14158	4.03%	0.717%
3	7.002	841	850	861	rBV3	4846	20762	5.91%	1.051%
4	7.728	960	969	974	rBV	36549	87397	24.89%	4.423%
5	7.801	974	981	993	rVB	70654	160662	45.76%	8.131%
6	8.130	1023	1035	1049	rBV2	78531	257541	73.35%	13.034%
7	8.697	1119	1128	1138	rVB	109636	212792	60.61%	10.769%
8	10.185	1365	1372	1380	rBV	170347	287274	81.82%	14.539%
9	10.581	1429	1437	1444	rBV	33956	60099	17.12%	3.042%
10	10.959	1493	1499	1503	rBV	3942	6975	1.99%	0.353%
11	11.325	1552	1559	1566	rBV	36605	62040	17.67%	3.140%
12	11.496	1580	1587	1596	rBV	135222	215891	61.49%	10.926%
13	12.337	1720	1725	1733	rVB	25187	40547	11.55%	2.052%
14	12.489	1743	1750	1757	rBV2	192801	351106	100.00%	17.769%
15	13.148	1854	1858	1861	rBV3	5610	9004	2.56%	0.456%
16	13.190	1861	1865	1871	rVB2	8486	13502	3.85%	0.683%
17	13.428	1898	1904	1910	rVB	96217	149022	42.44%	7.542%
18	13.965	1987	1992	2001	rVB2	12570	20482	5.83%	1.037%

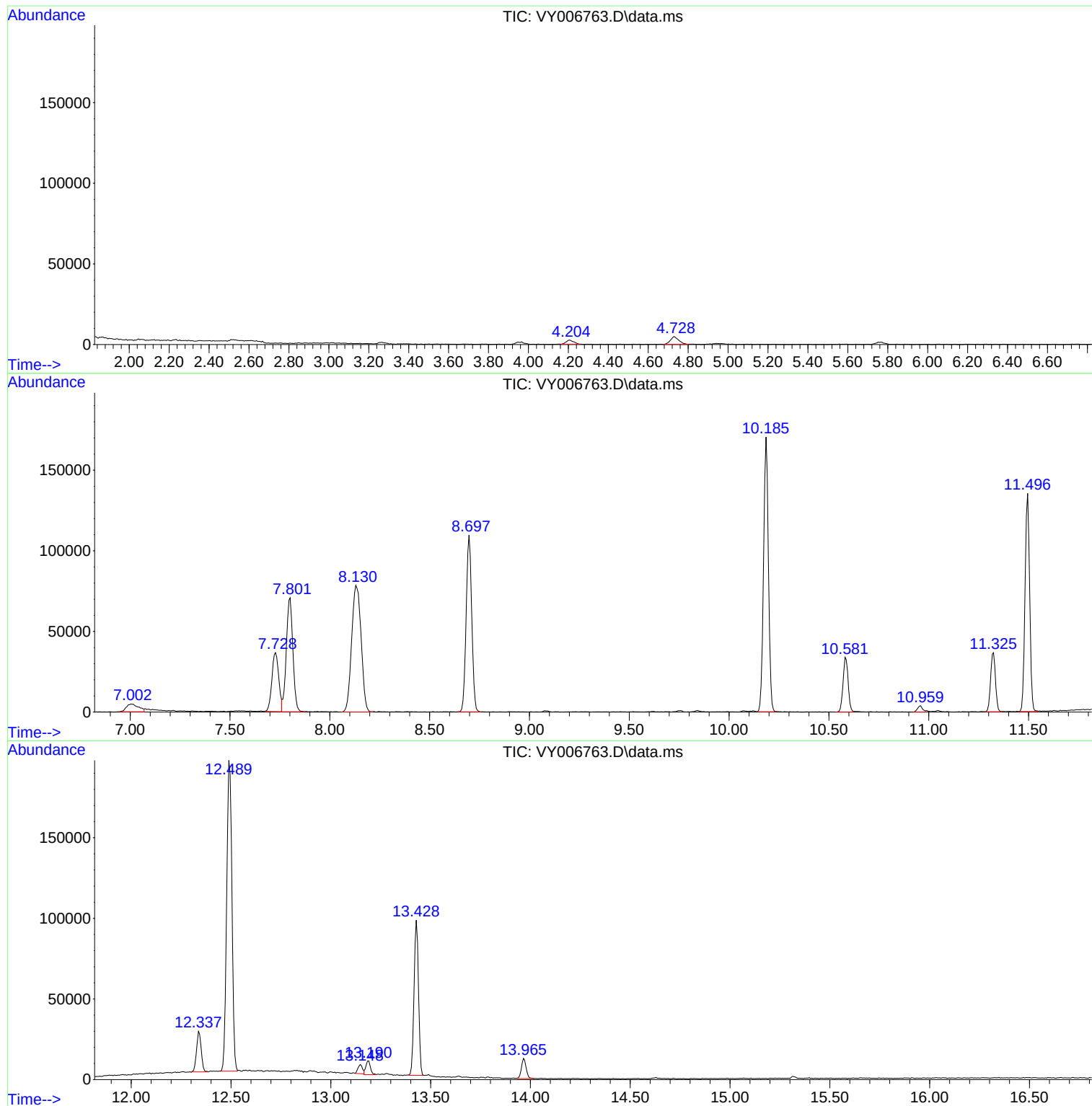
Sum of corrected areas: 1975946

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Instrument :
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ClientSampleId :
MF-SOIL-P2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

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



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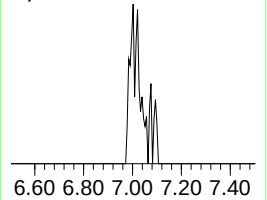
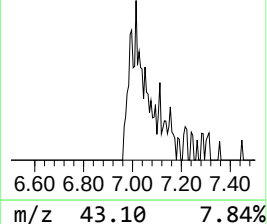
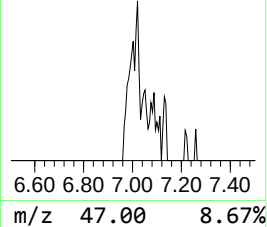
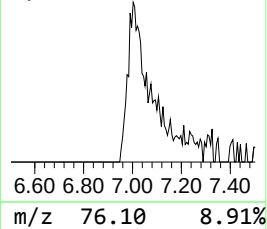
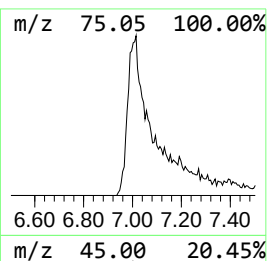
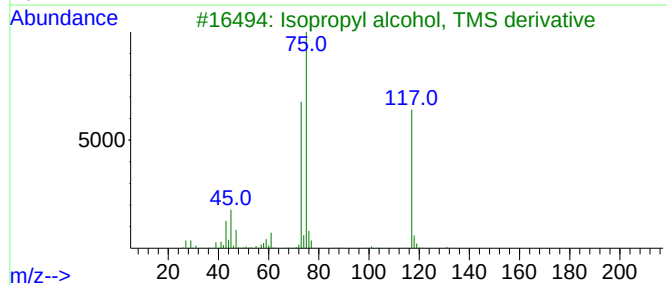
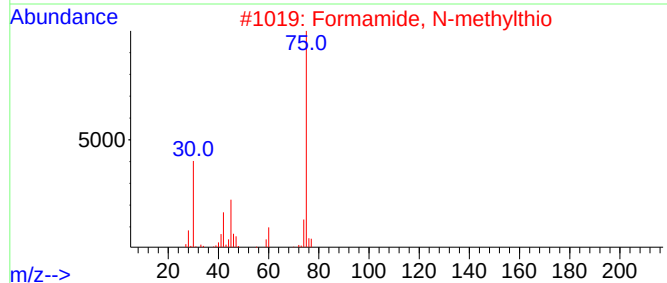
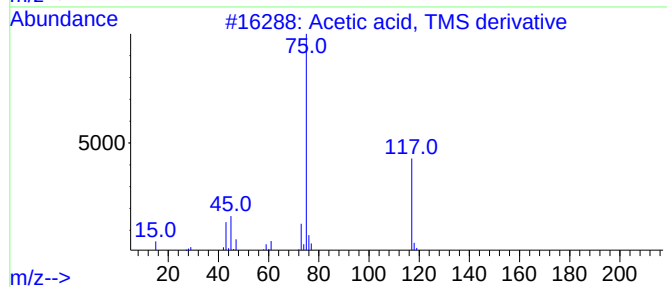
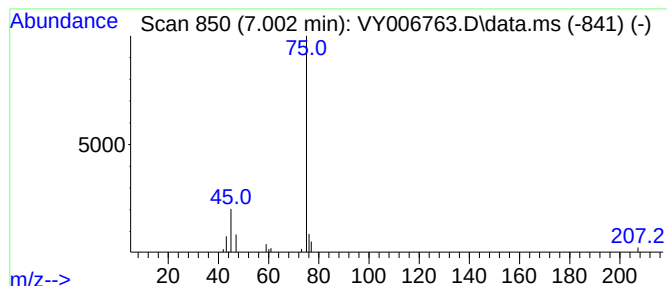
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetic acid, TMS derivative Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.002	6.46 ug/l	20762	Pentafluorobenzene	7.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, TMS derivative	132	C5H12O2Si	002754-27-0	83
2			Formamide, N-methylthio	75	C2H5NS	018952-41-5	83
3			Isopropyl alcohol, TMS derivative	132	C6H16OSi	001825-64-5	74
4			Propanoic acid, TMS derivative	146	C6H14O2Si	016844-98-7	74
5			2-Methylpropanoic acid, TBDMS de...	202	C10H22O2Si	111864-21-2	72



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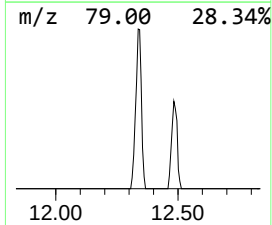
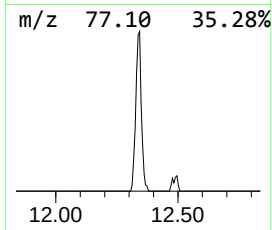
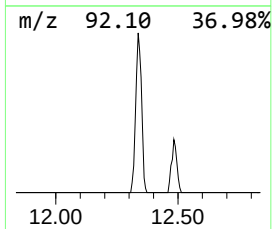
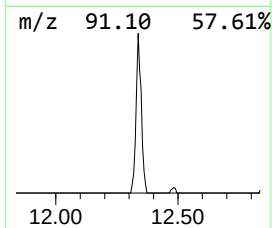
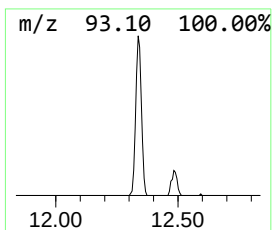
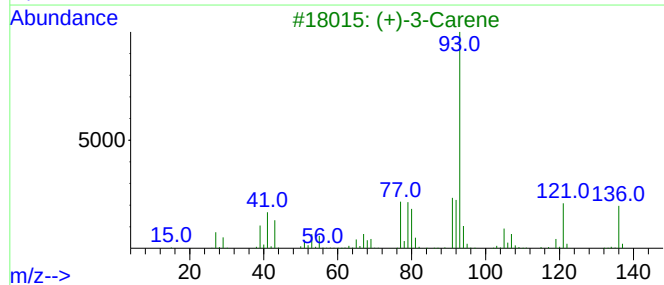
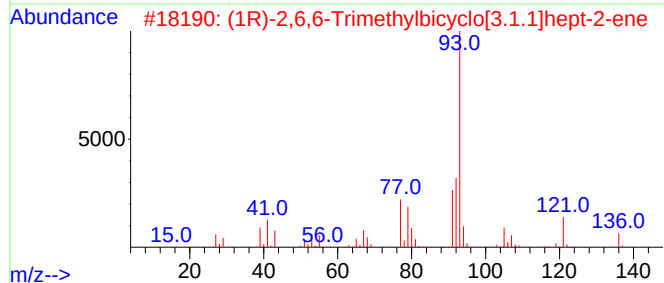
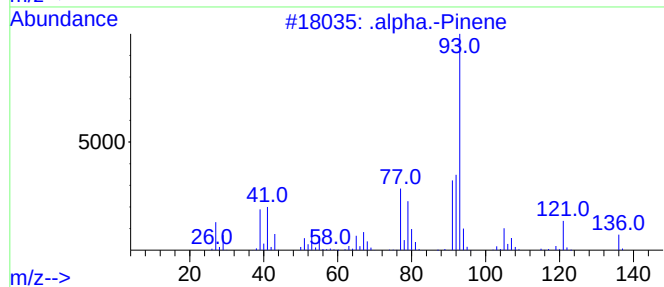
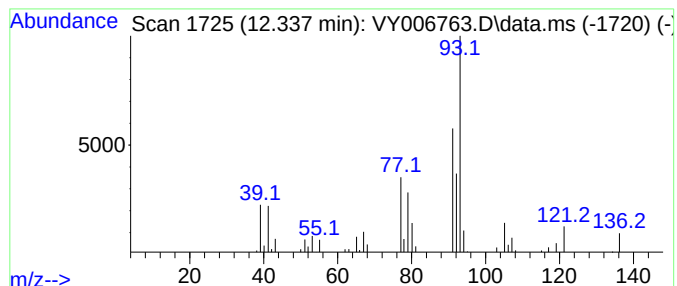
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Peak Number 4 .alpha.-Pinene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.337	9.39 ug/l	40547	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Pinene	136	C10H16	000080-56-8	95
2			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
3			(+)-3-Carene	136	C10H16	000498-15-7	91
4			(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	91
5			Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	91



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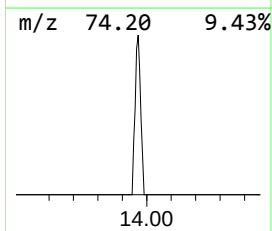
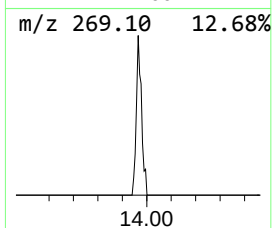
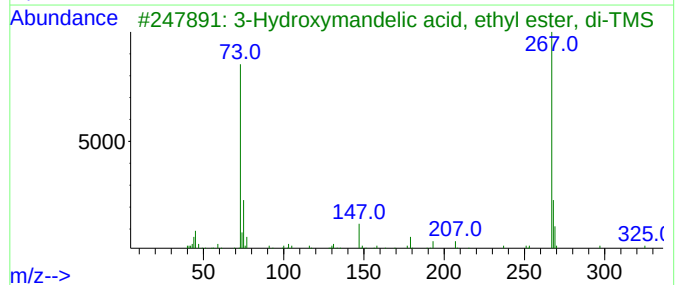
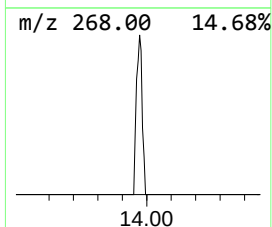
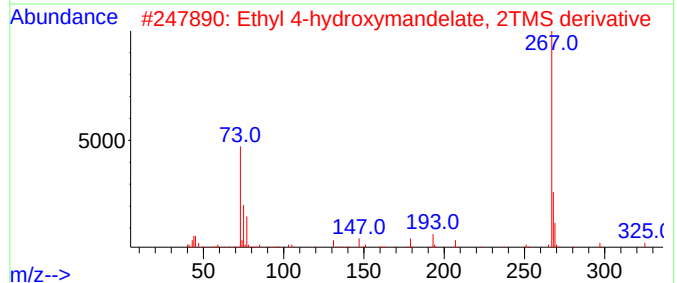
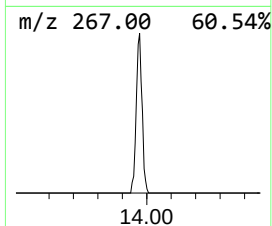
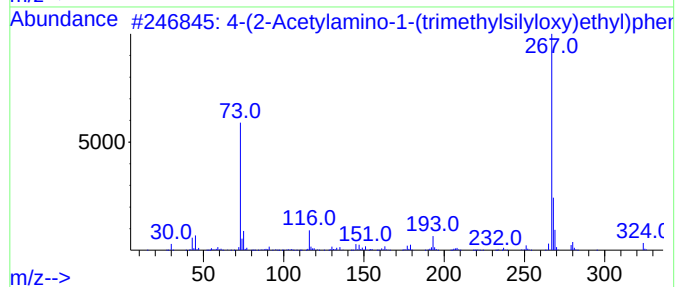
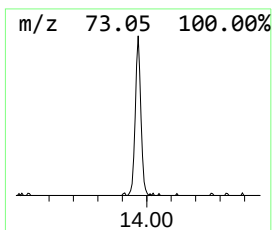
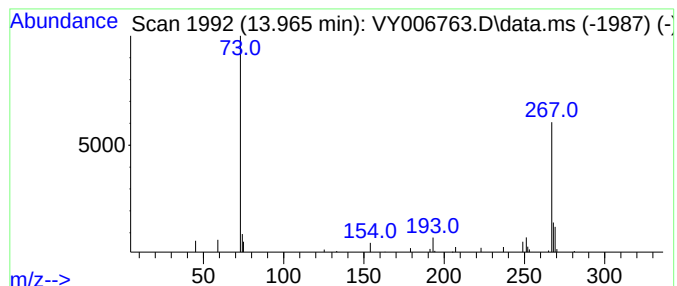
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Peak Number 5 4-(2-Acetylamino-1-(trimeth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	6.87 ug/l	20482	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(2-Acetylamino-1-(trimethylsil...	339	C16H29NO3Si2	1000373-43-5	59
2			Ethyl 4-hydroxymandelate, 2TMS d...	340	C16H28O4Si2	1010071-53-3	50
3			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	50
4			4-(4-Fluorophenyl)-2,3-dihydro-1...	267	C12H14FN0SSi	1010501-61-0	47
5			Benzonitrile, 2-(2-hydroxy-5-nit...	267	C14H9N3O3	303768-30-1	46



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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
Acetic acid, TM...	7.002	6.5	ug/l	20762	1	7.801	160662	50.0
.alpha.-Pinene	12.337	9.4	ug/l	40547	3	11.496	215891	50.0
4-(2-Acetylamin...	13.965	6.9	ug/l	20482	4	13.428	149022	50.0