

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
 Data File : VU048693.D
 Acq On : 27 May 2022 15:04
 Operator : SY/MD
 Sample : N3056-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 MW-15

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_U\Method\82U052622W.M
 Title : SW846 8260

Signal : TIC: VU048693.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.488	34	46	58	rBV	37767	104596	8.59%	1.397%
2	5.089	1150	1166	1182	rBV	46488	100350	8.24%	1.341%
3	5.292	1210	1229	1242	rBV	205879	438753	36.03%	5.861%
4	5.375	1242	1255	1274	rVB	298910	609012	50.01%	8.136%
5	5.703	1342	1357	1379	rBV2	211521	434343	35.67%	5.803%
6	6.250	1511	1527	1551	rBV	422423	803374	65.97%	10.732%
7	7.899	2024	2040	2069	rBV	601292	1050533	86.26%	14.034%
8	8.555	2233	2244	2256	rBV	22480	37291	3.06%	0.498%
9	9.417	2499	2512	2541	rBV	604035	1014507	83.30%	13.553%
10	10.632	2877	2890	2913	rBV	556367	907937	74.55%	12.129%
11	11.472	3141	3151	3160	rBV2	10361	15999	1.31%	0.214%
12	11.812	3243	3257	3277	rBV	766136	1217828	100.00%	16.269%
13	12.095	3334	3345	3364	rVB2	16463	28621	2.35%	0.382%
14	14.089	3953	3965	3983	rBV	93211	158659	13.03%	2.120%
15	15.224	4305	4318	4335	rBV	72366	120312	9.88%	1.607%
16	15.410	4364	4376	4388	rBV	115024	186389	15.31%	2.490%
17	15.954	4534	4545	4557	rBV2	50886	87251	7.16%	1.166%
18	16.147	4596	4605	4611	rBV2	9230	14969	1.23%	0.200%
19	16.262	4631	4641	4651	rBV4	14503	25394	2.09%	0.339%
20	16.410	4677	4687	4695	rBV2	27225	47564	3.91%	0.635%
21	16.449	4696	4699	4713	rVB6	9453	12846	1.05%	0.172%
22	17.098	4890	4901	4913	rBV3	38074	68910	5.66%	0.921%

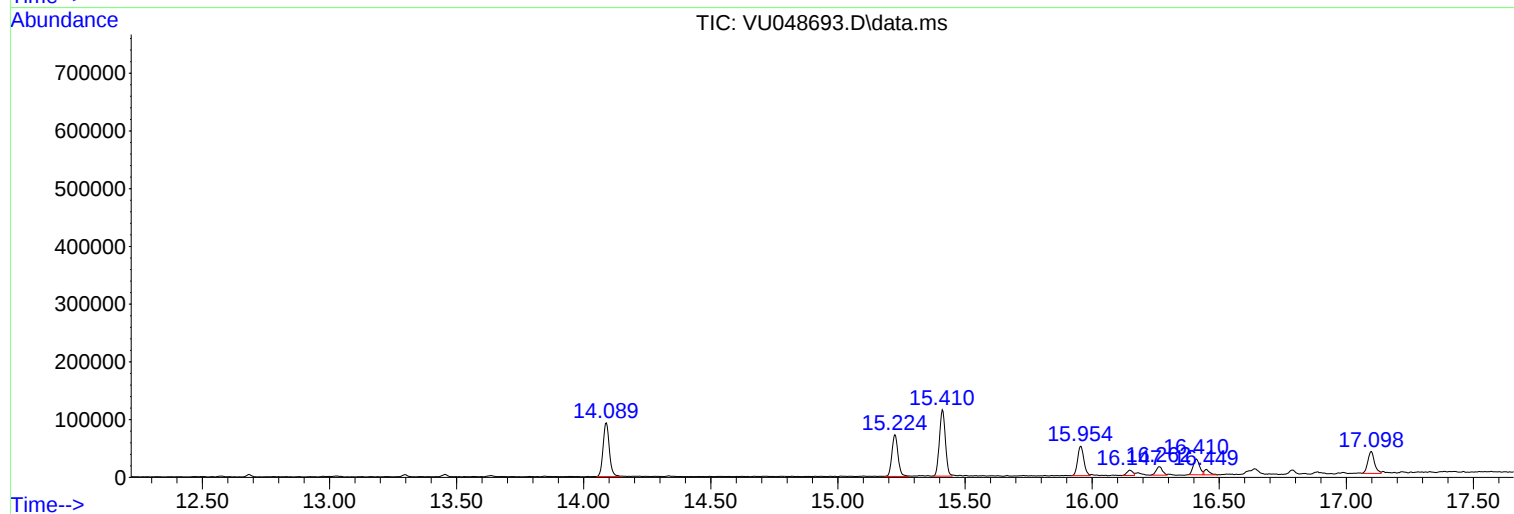
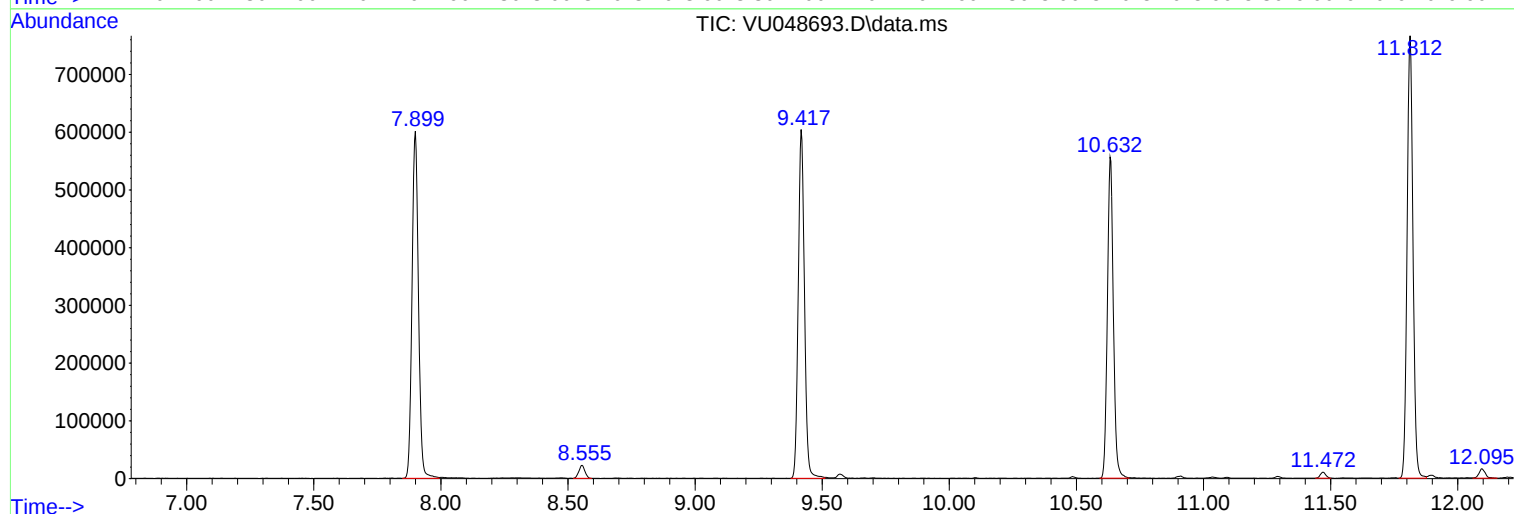
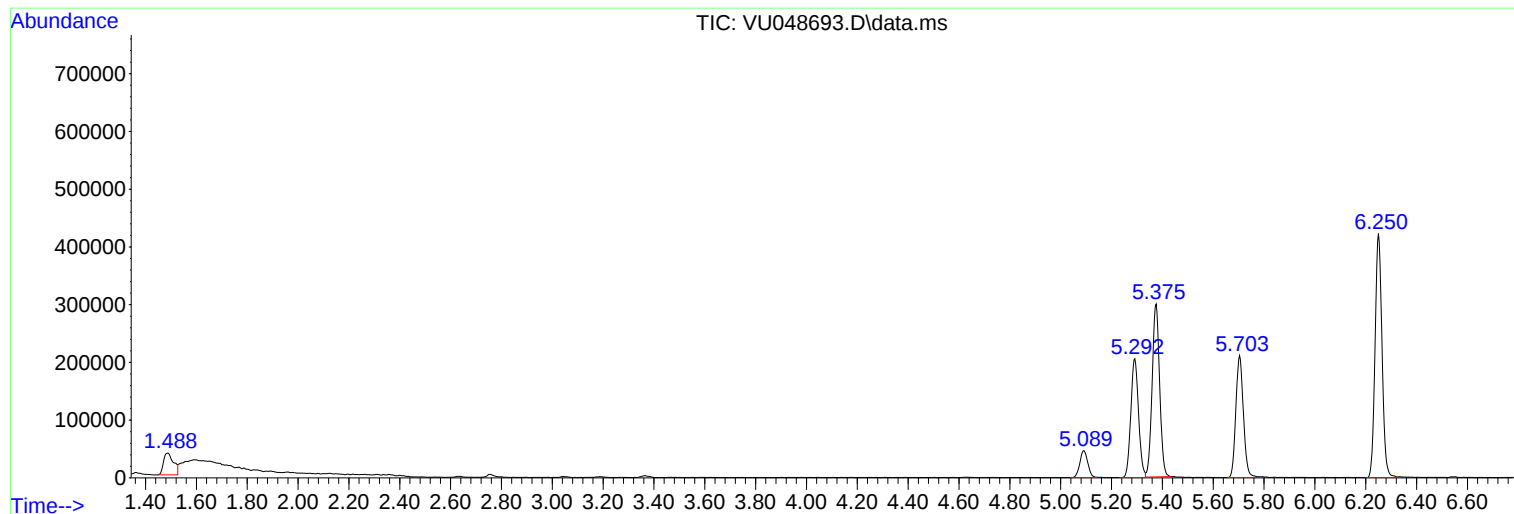
Sum of corrected areas: 7485438

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048693.D
Acq On : 27 May 2022 15:04
Operator : SY/MD
Sample : N3056-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-15

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048693.D
Acq On : 27 May 2022 15:04
Operator : SY/MD
Sample : N3056-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-15

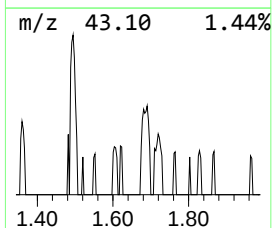
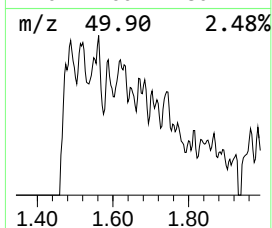
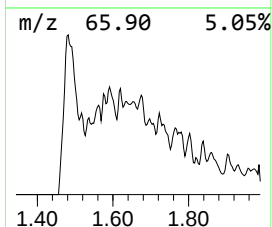
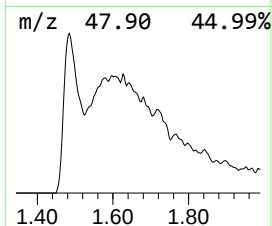
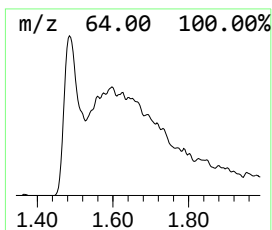
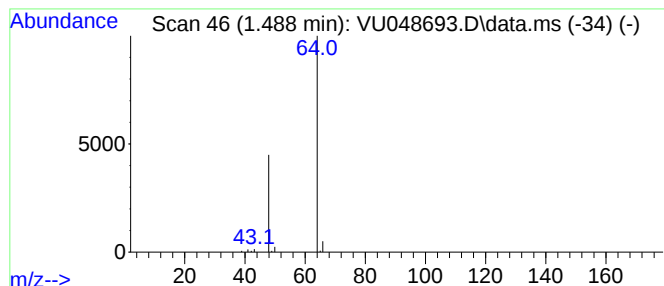
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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.
1.488	8.59 ug/l	104596	Pentafluorobenzene	5.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048693.D
Acq On : 27 May 2022 15:04
Operator : SY/MD
Sample : N3056-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-15

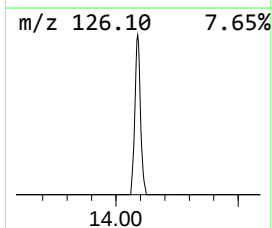
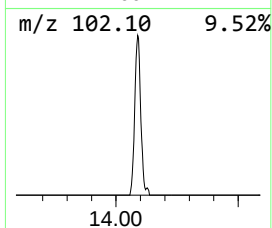
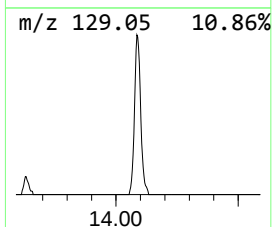
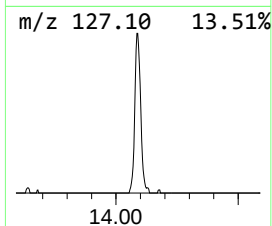
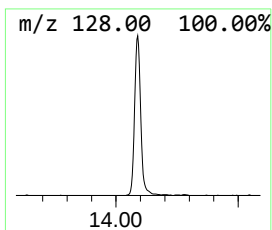
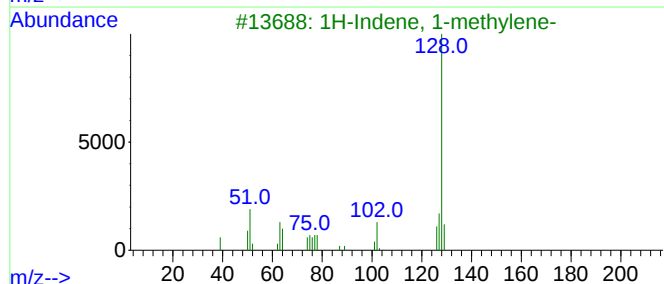
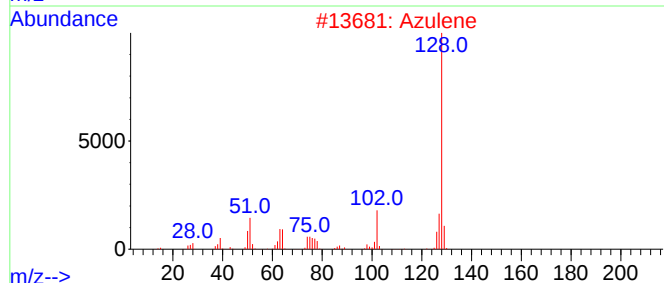
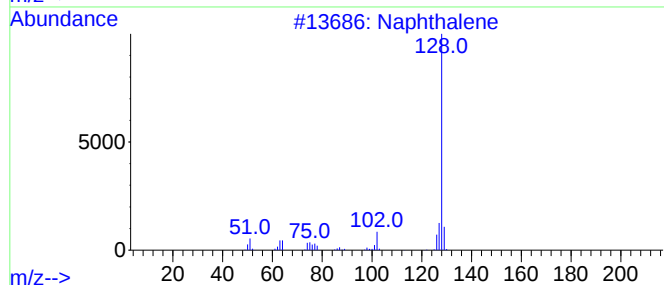
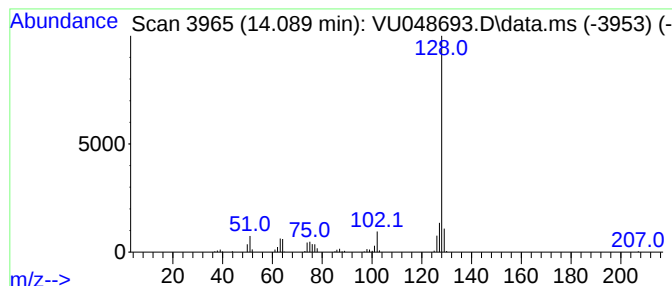
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 2 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	6.51 ug/l	158659	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	94
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
4			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	83
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048693.D
Acq On : 27 May 2022 15:04
Operator : SY/MD
Sample : N3056-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-15

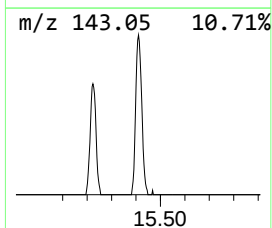
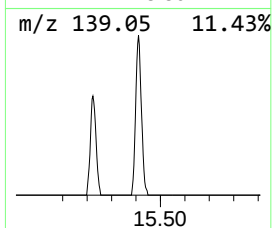
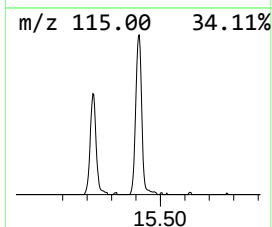
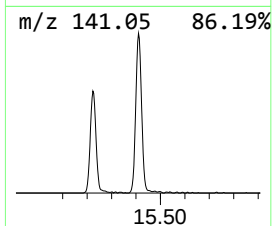
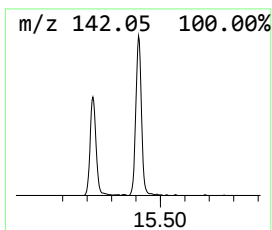
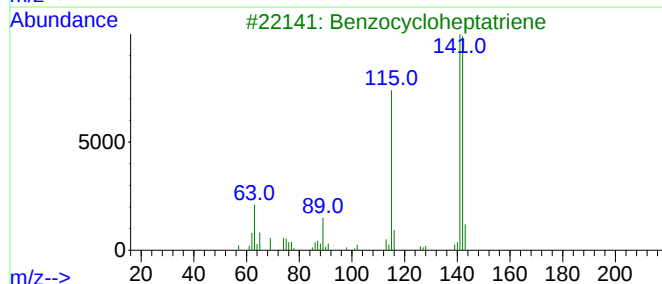
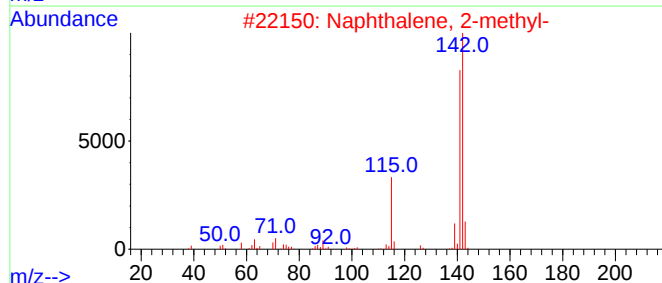
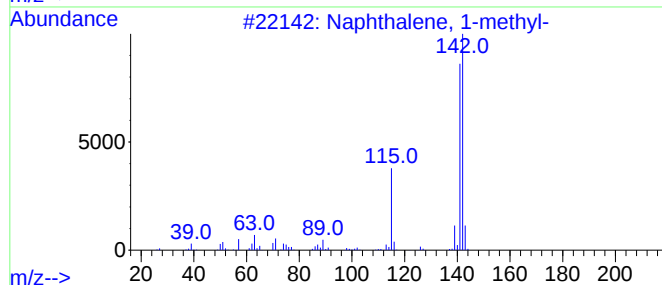
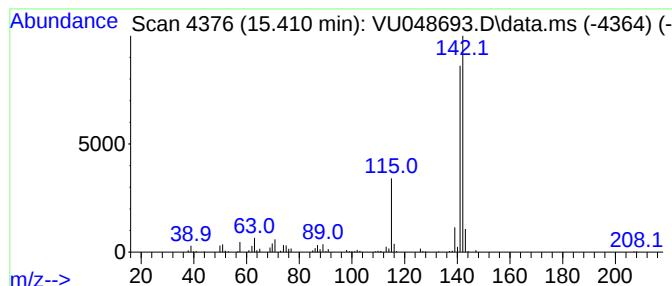
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	7.65 ug/l	186389	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1-Naphthaleneacetamide	185	C12H11NO	000086-86-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048693.D
Acq On : 27 May 2022 15:04
Operator : SY/MD
Sample : N3056-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-15

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.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	1.488	8.6	ug/l	104596	1	5.375	609012	50.0
Azulene	14.089	6.5	ug/l	158659	4	11.812	1217830	50.0
Benzocyclohepta...	15.410	7.7	ug/l	186389	4	11.812	1217830	50.0