

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042121\
 Data File : BF123666.D
 Acq On : 21 Apr 2021 14:33
 Operator : JU/CG
 Sample : M2077-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-21-0-2.0

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.469	571	575	590	rBV	5287258	4605961	97.64%	14.290%
2	6.481	743	747	763	rBV	4935327	4717071	100.00%	14.634%
3	6.851	806	810	813	rBV	1484011	1227022	26.01%	3.807%
4	7.410	900	905	908	rBV	3599436	3037549	64.39%	9.424%
5	8.133	1024	1028	1032	rBV	1946400	1546831	32.79%	4.799%
6	9.210	1207	1211	1215	rBV	5025266	4397319	93.22%	13.642%
7	9.604	1275	1278	1282	rBV	164178	145857	3.09%	0.453%
8	9.892	1323	1327	1336	rBV	1917047	1573368	33.35%	4.881%
9	10.680	1457	1461	1469	rBV	3168608	2729802	57.87%	8.469%
10	10.739	1469	1471	1475	rVB2	67295	64961	1.38%	0.202%
11	11.380	1576	1580	1584	rBV	1913884	1571963	33.32%	4.877%
12	12.968	1846	1850	1854	rBV	3829134	3629831	76.95%	11.261%
13	13.945	2007	2016	2024	rBV7	102698	362356	7.68%	1.124%
14	14.027	2025	2030	2037	rVB	1273055	1207604	25.60%	3.747%
15	14.504	2107	2111	2114	rBV	73779	72128	1.53%	0.224%
16	14.962	2185	2189	2193	rBV5	64494	71742	1.52%	0.223%
17	15.157	2218	2222	2226	rBV	103305	117368	2.49%	0.364%
18	15.509	2277	2282	2286	rBV	782525	1005714	21.32%	3.120%
19	15.986	2359	2363	2368	rVB	96725	148336	3.14%	0.460%

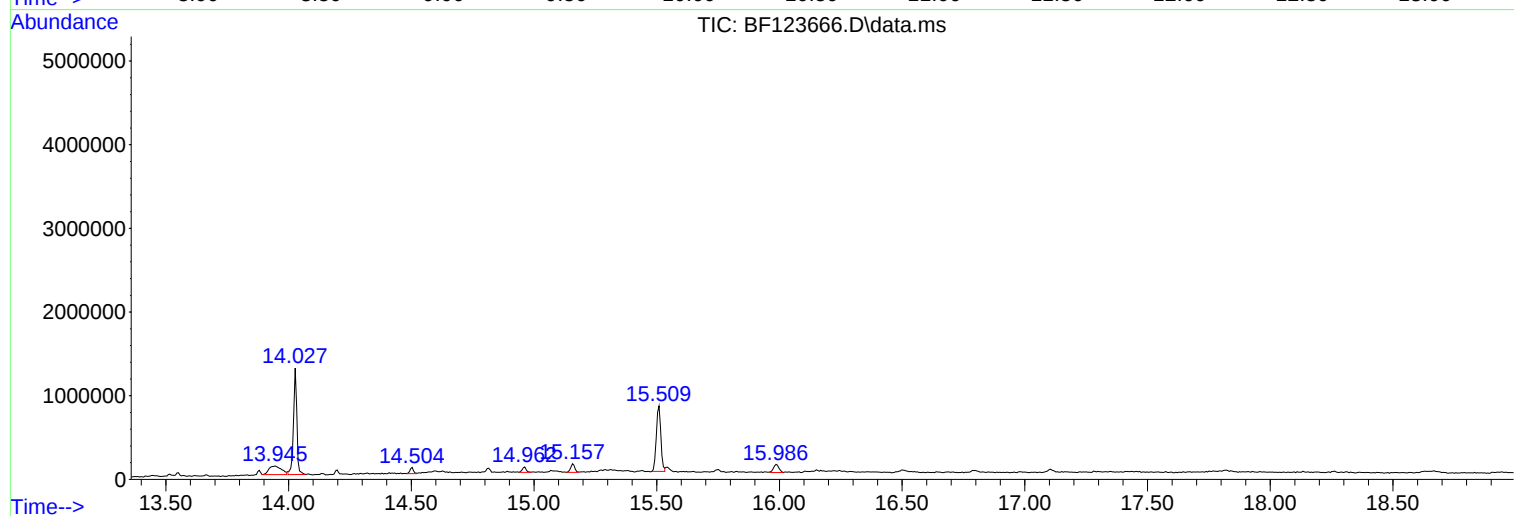
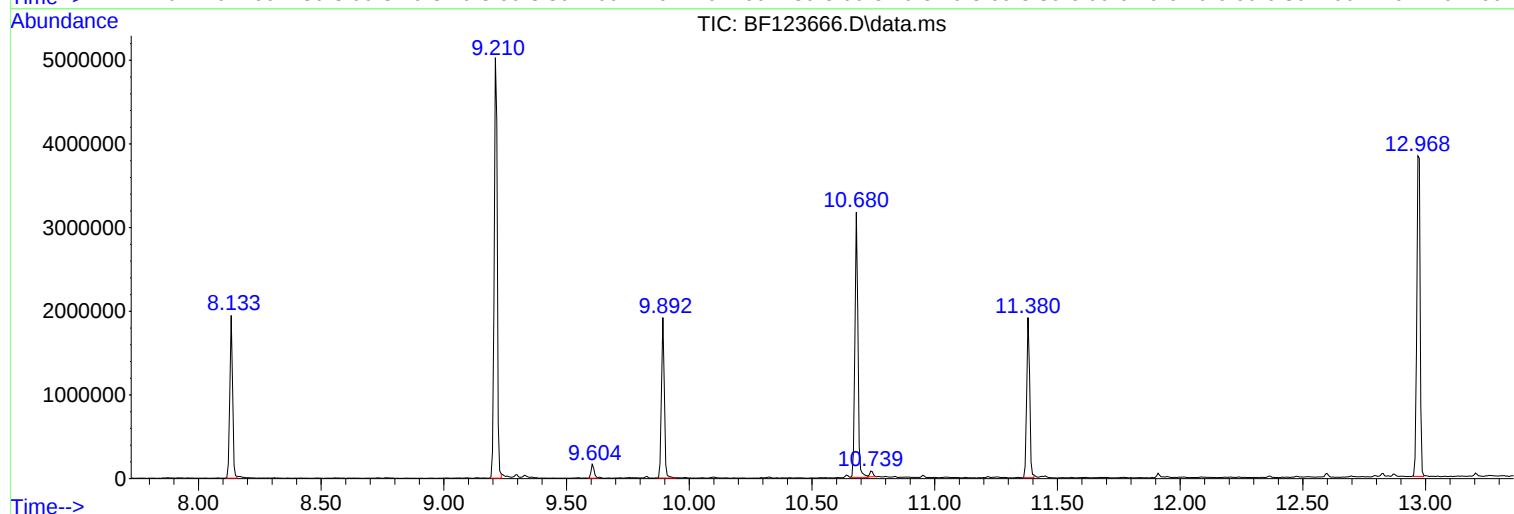
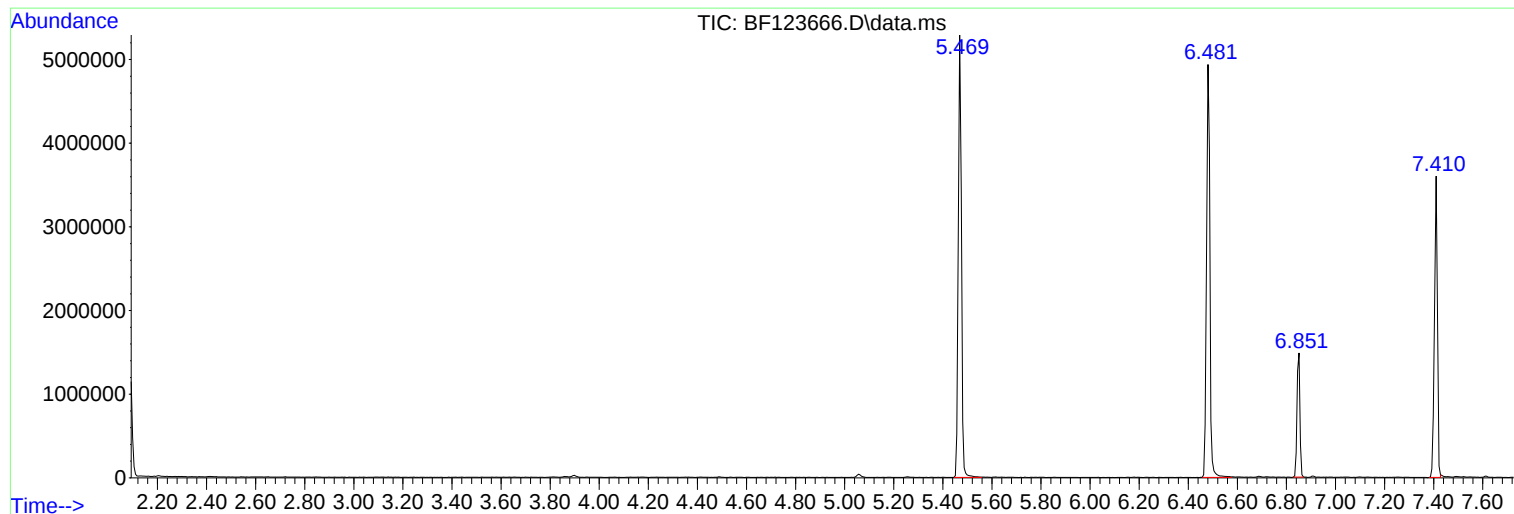
Sum of corrected areas: 32232783

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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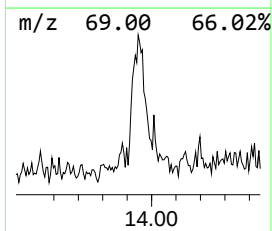
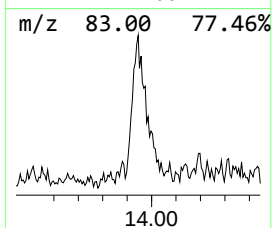
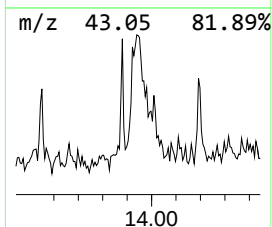
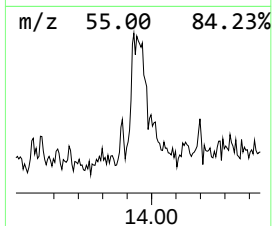
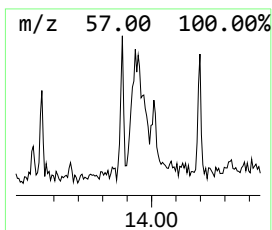
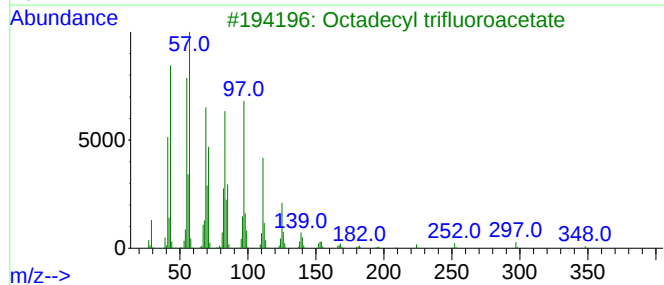
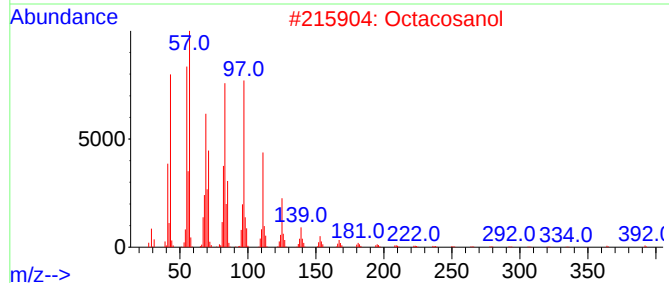
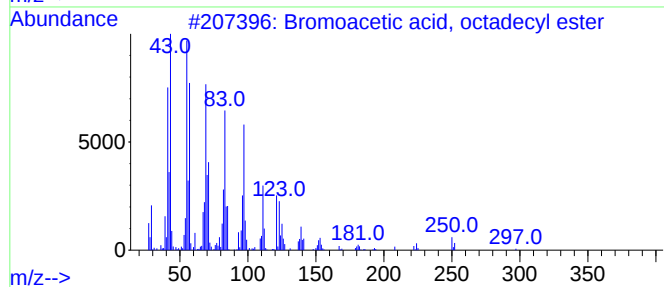
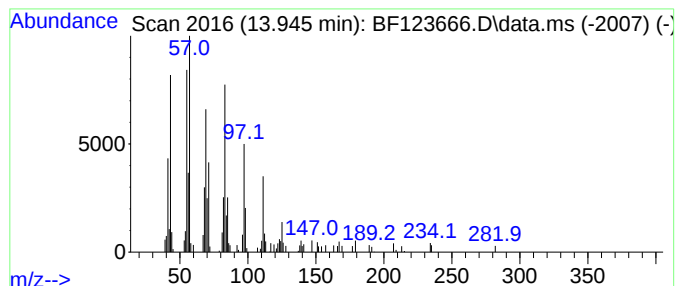
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Bromoacetic acid, octadecyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	6.00 ng	362356	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
2			Octacosanol	410	C28H58O	000557-61-9	83
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81
4			17-Pentatriacontene	491	C35H70	006971-40-0	80
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	74



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ClientSampled :
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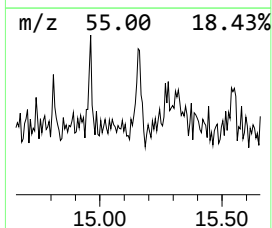
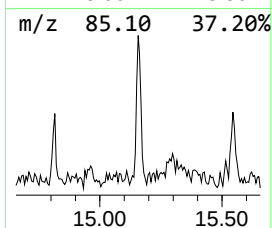
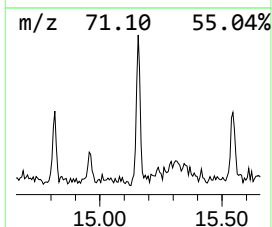
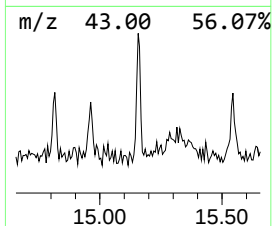
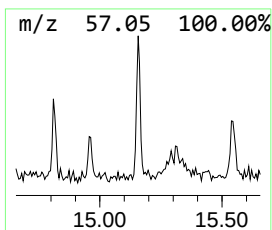
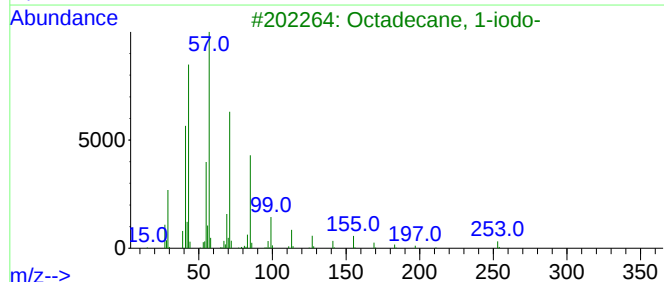
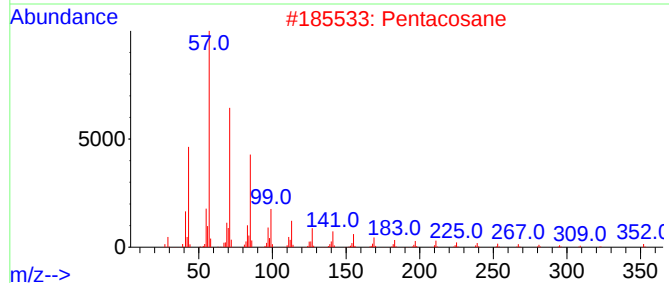
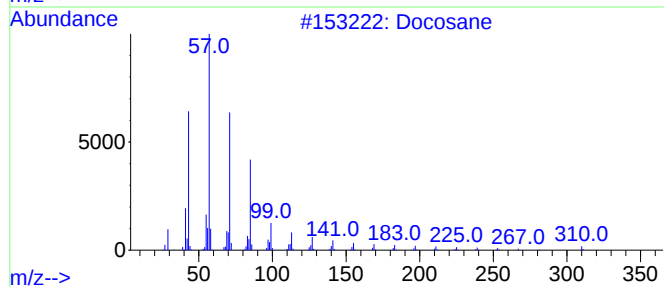
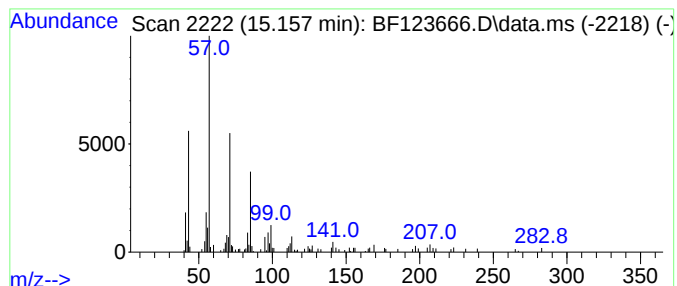
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Peak Number 2 Docosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.157	2.33 ng	117368	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	78
2			Pentacosane	352	C25H52	000629-99-2	72
3			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
4			Hexacosane	366	C26H54	000630-01-3	72
5			triacontane	422	C30H62	000638-68-6	72



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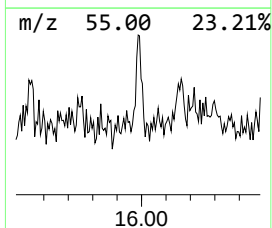
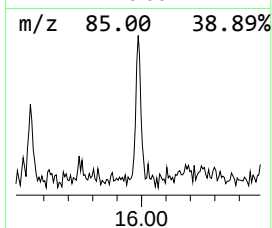
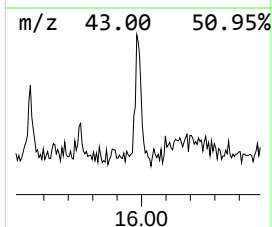
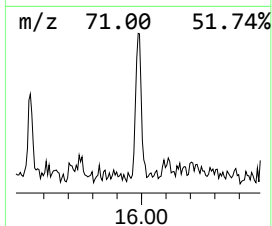
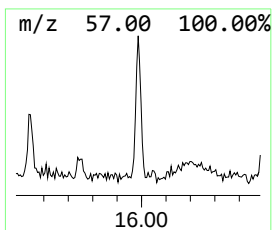
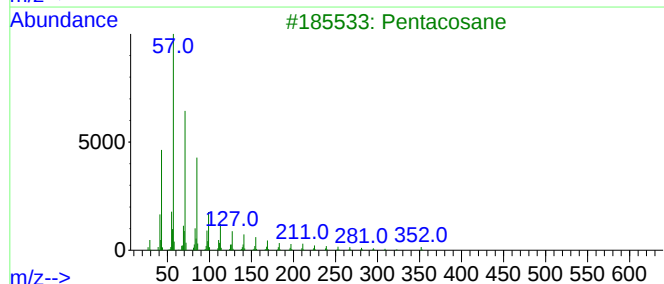
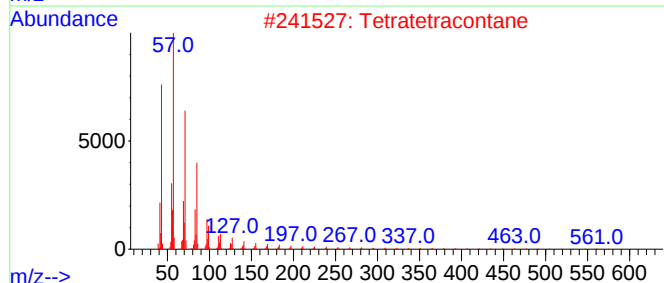
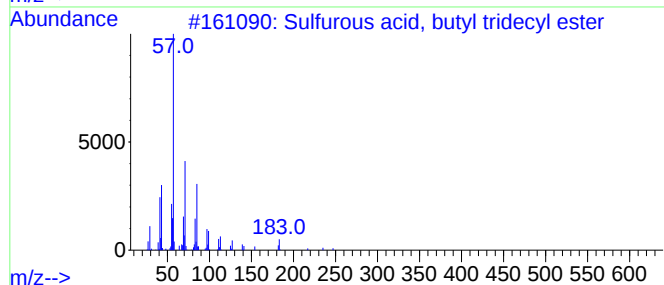
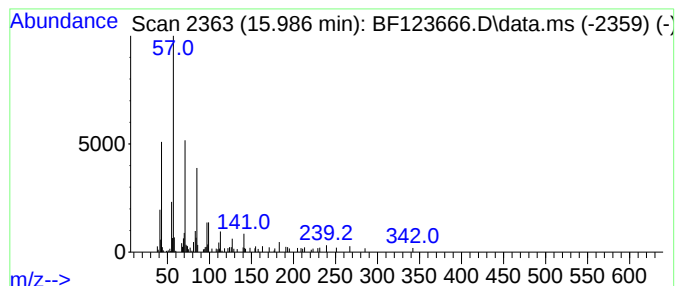
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Peak Number 3 Sulfurous acid, butyl tridecyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.986	2.95 ng	148336	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	90
2			Tetratetracontane	619	C44H90	007098-22-8	86
3			Pentacosane	352	C25H52	000629-99-2	86
4			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	86
5			2-methyloctacosane	408	C29H60	1000376-72-8	80



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Bromoacetic aci...	13.945	6.0	ng	362356	5	14.027	1207600	20.0
Docosane	15.157	2.3	ng	117368	6	15.509	1005710	20.0
Sulfurous acid,...	15.986	3.0	ng	148336	6	15.509	1005710	20.0