

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
 Data File : BP007061.D
 Acq On : 20 Sep 2021 21:25
 Operator : CG/JU
 Sample : M3817-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SW-CB-03-(1.0)

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_P\Methods\8270E-BP091621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007061.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.217	356	362	371	rBV	196847	302284	1.71%	0.390%
2	5.481	400	407	417	rBV	2285360	3376299	19.09%	4.361%
3	7.069	670	677	687	rBV	1235977	1971591	11.14%	2.547%
4	7.905	812	819	835	rBV	1106005	1802723	10.19%	2.329%
5	9.069	1008	1017	1028	rBV	3139729	5377204	30.40%	6.946%
6	10.487	1252	1258	1268	rBV	213331	395205	2.23%	0.511%
7	10.705	1287	1295	1306	rBV	1444145	2393835	13.53%	3.092%
8	13.163	1705	1713	1728	rBV	8641897	13158088	74.38%	16.997%
9	14.375	1913	1919	1936	rVB2	73977	190631	1.08%	0.246%
10	14.534	1938	1946	1954	rBV	2159722	3243179	18.33%	4.189%
11	16.022	2192	2199	2211	rBV	6786870	9897520	55.95%	12.785%
12	16.222	2224	2233	2245	rBV	2373345	4066191	22.99%	5.252%
13	17.281	2406	2413	2419	rBV	2835185	3836769	21.69%	4.956%
14	18.169	2559	2564	2573	rBV	308076	517254	2.92%	0.668%
15	19.398	2768	2773	2783	rBV2	169073	307335	1.74%	0.397%
16	19.839	2842	2848	2853	rBV	14073616	17690570	100.00%	22.852%
17	21.075	3054	3058	3062	rBV2	176973	248532	1.40%	0.321%
18	21.357	3102	3106	3117	rBV	3207144	4203552	23.76%	5.430%
19	23.774	3510	3517	3533	rVB2	2168038	4436248	25.08%	5.730%

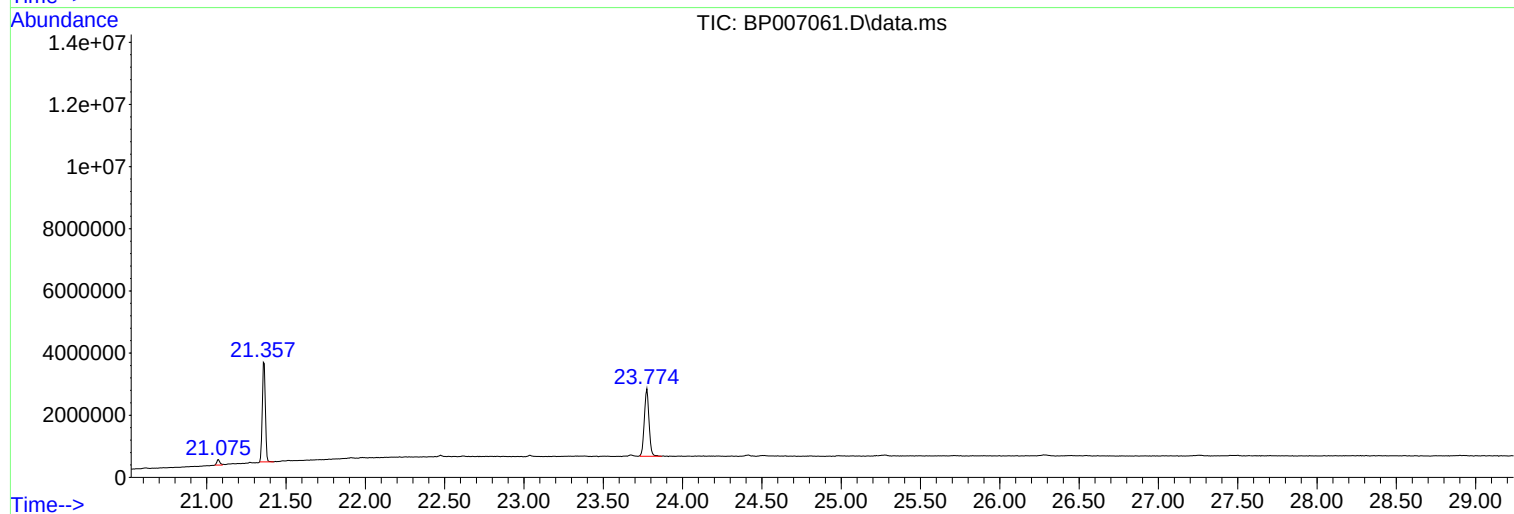
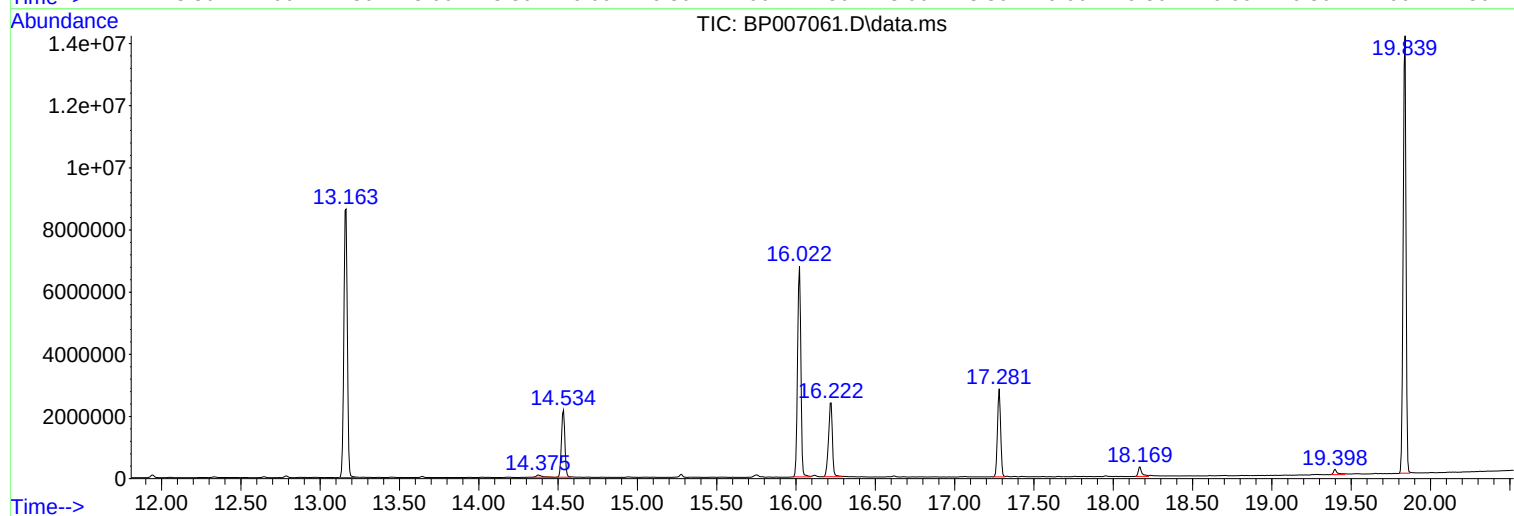
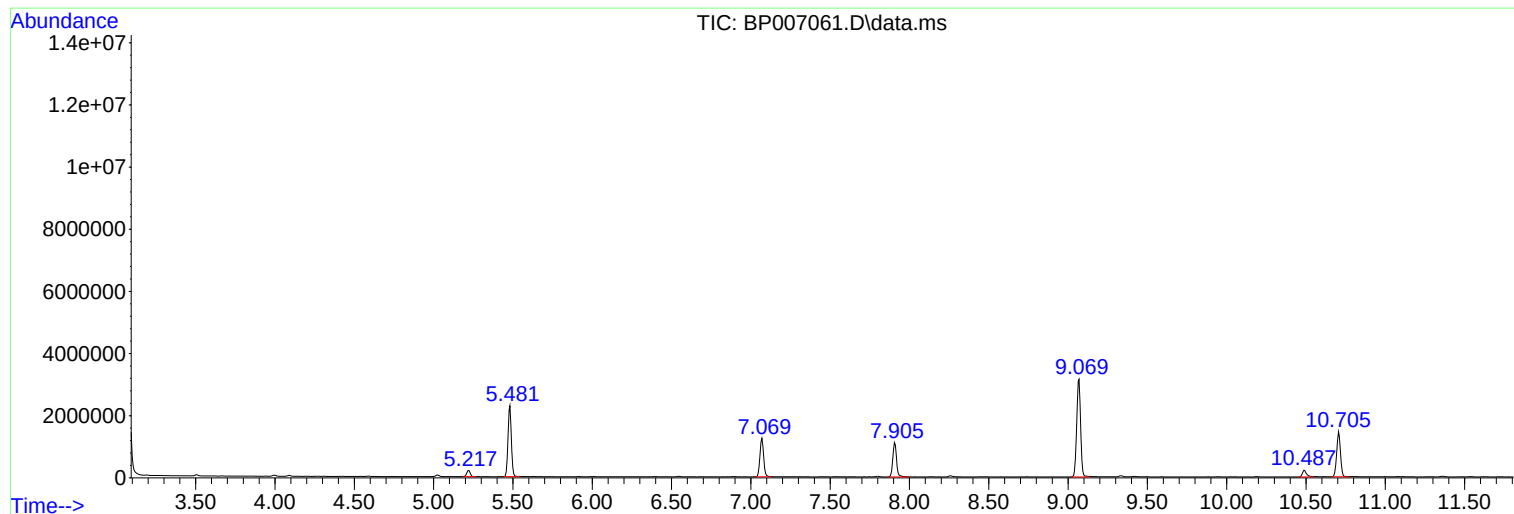
Sum of corrected areas: 77415010

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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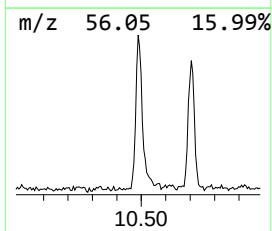
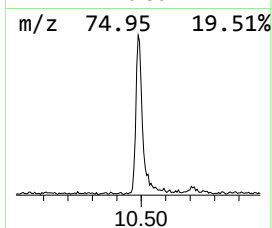
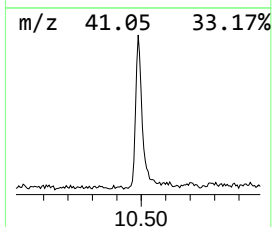
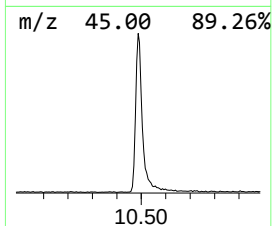
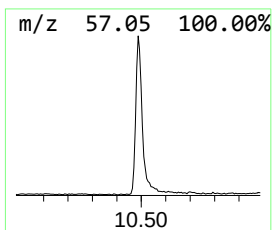
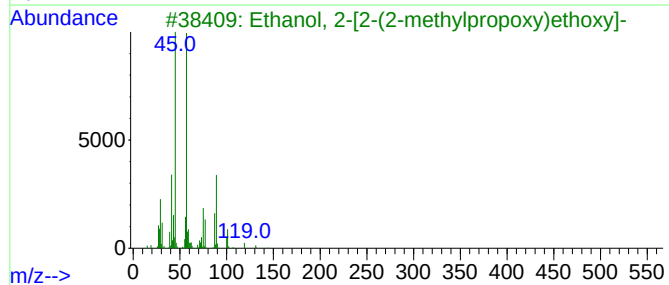
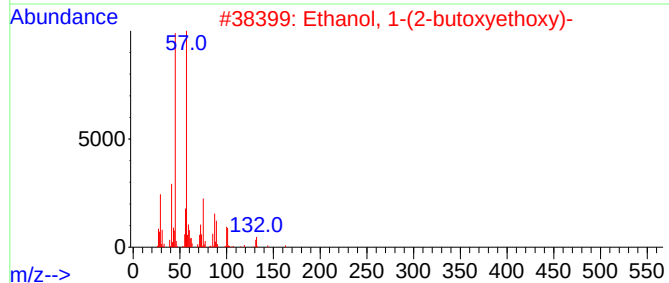
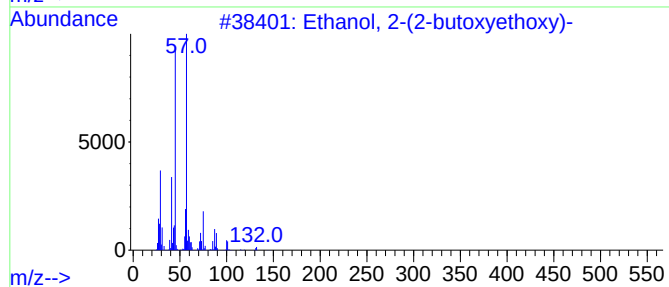
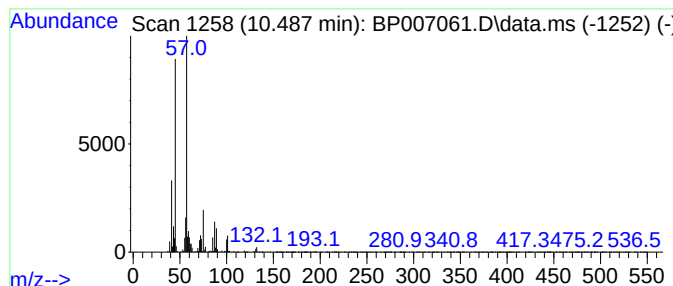
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.487	3.30 ng	395205	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	50



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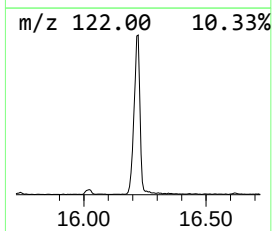
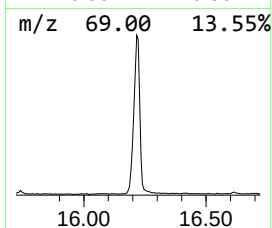
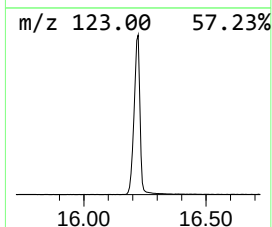
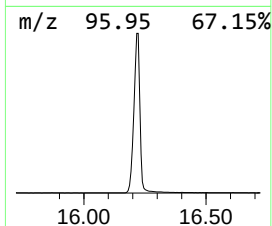
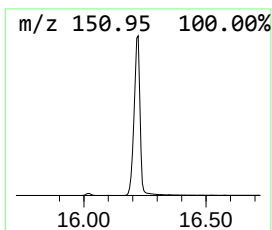
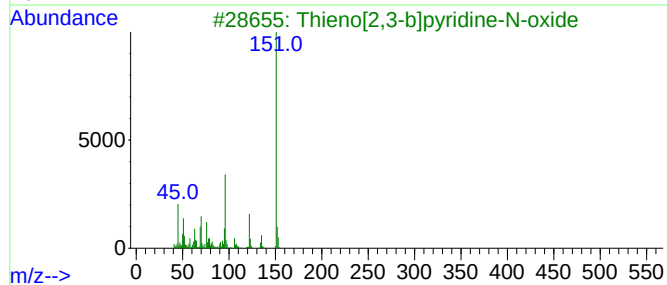
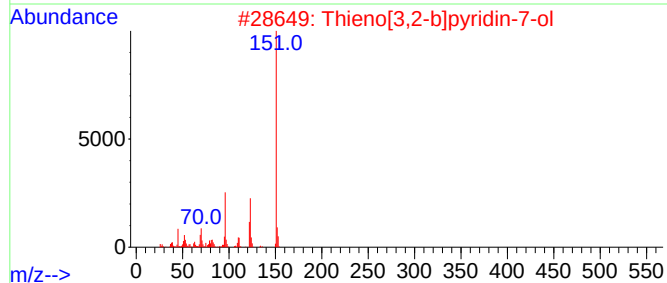
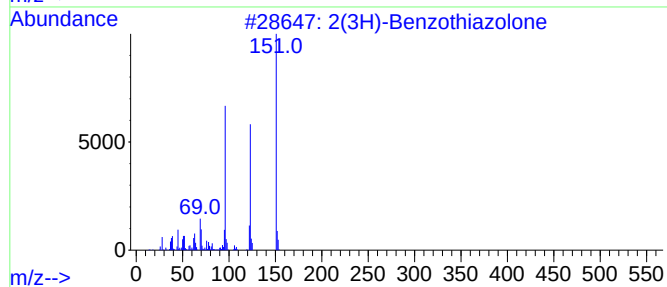
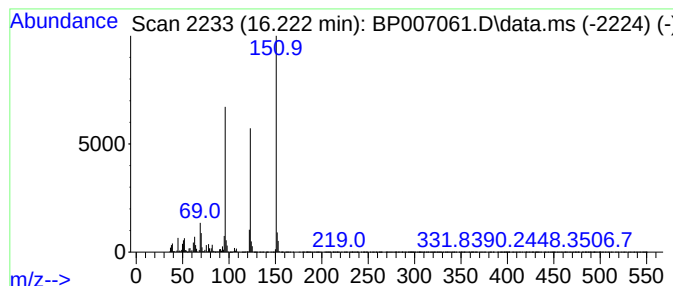
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Peak Number 3 2(3H)-Benzothiazolone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.222	21.20 ng	4066190	Phenanthrene-d10		17.281	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone		151	C7H5NOS	000934-34-9	94
2	Thieno[3,2-b]pyridin-7-ol		151	C7H5NOS	107818-20-2	64
3	Thieno[2,3-b]pyridine-N-oxide		151	C7H5NOS	025557-50-0	53
4	6-Methyl-7-oxo-4,7-dihydro-triaz...		151	C5H5N5O	057250-39-2	53
5	1,2-Benzisothiazol-3(2H)-one		151	C7H5NOS	002634-33-5	42



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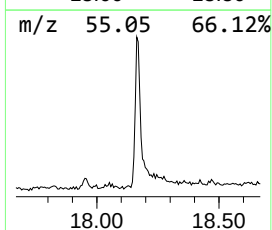
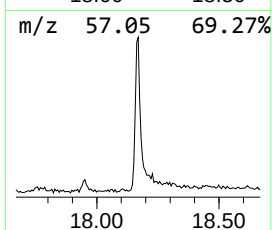
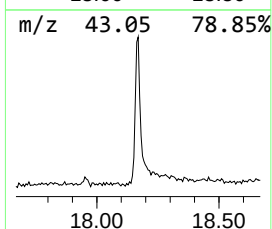
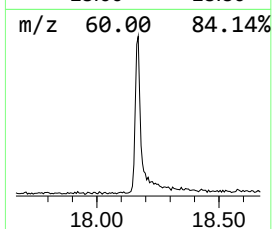
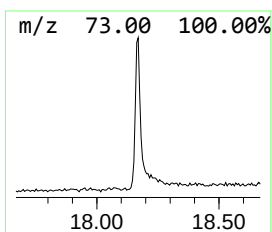
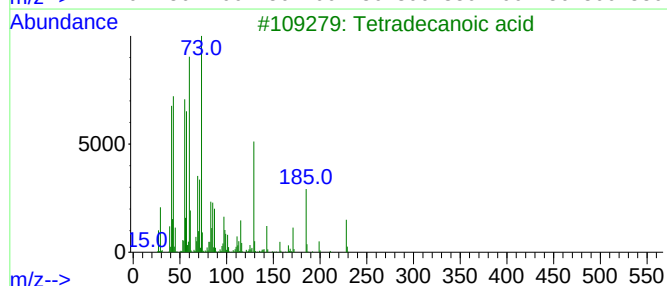
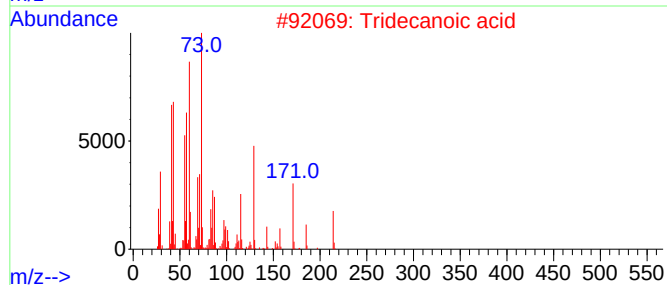
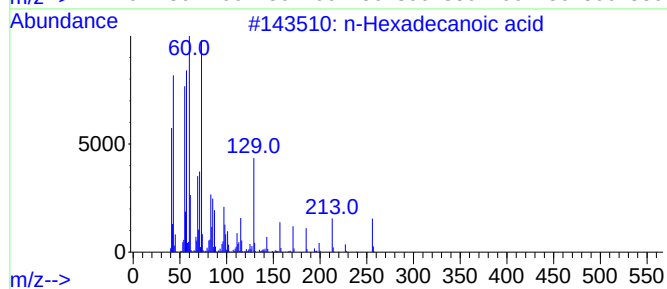
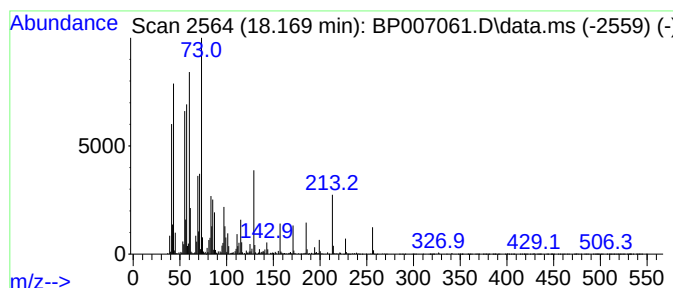
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	2.70 ng	517254	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			Octadecanoic acid	284	C18H36O2	000057-11-4	83



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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
Ethanol, 2-(2-b...	10.487	3.3	ng	395205	2	10.704	2393840	20.0
2(3H)-Benzothia...	16.222	21.2	ng	4066190	4	17.281	3836770	20.0
n-Hexadecanoic ...	18.169	2.7	ng	517254	4	17.281	3836770	20.0