

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051717\
 Data File : BF095201.D
 Acq On : 17 May 2017 23:52
 Operator : SJ/MA
 Sample : I3172-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-04

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.125	539	542	561	rBV	118091	279739	12.61%	1.441%
2	5.737	643	646	680	rBV	688480	1636553	73.79%	8.430%
3	7.313	910	914	930	rBV	962793	1747567	78.80%	9.002%
4	7.436	930	935	954	rVB	1180291	1810079	81.61%	9.324%
5	7.772	988	992	1004	rBV	354051	429519	19.37%	2.212%
6	8.007	1027	1032	1045	rBV	1144870	1361942	61.41%	7.015%
7	8.666	1140	1144	1162	rBV	665963	1088864	49.10%	5.609%
8	9.789	1331	1335	1355	rBV	451898	696924	31.42%	3.590%
9	11.560	1631	1636	1652	rBV	1712755	2217856	100.00%	11.424%
10	12.077	1721	1724	1733	rBV3	34654	41447	1.87%	0.213%
11	12.260	1751	1755	1765	rBV	129537	211078	9.52%	1.087%
12	12.618	1811	1816	1831	rBV2	498908	782909	35.30%	4.033%
13	13.454	1953	1958	1965	rVB	28146	37778	1.70%	0.195%
14	13.918	2032	2037	2051	rBV	719081	1131106	51.00%	5.826%
15	14.224	2085	2089	2092	rBV	35710	45602	2.06%	0.235%
16	14.954	2207	2213	2217	rBV2	18312	25442	1.15%	0.131%
17	15.024	2217	2225	2230	rBV	463590	638788	28.80%	3.290%
18	15.977	2381	2387	2403	rBV4	93974	173658	7.83%	0.895%
19	16.806	2524	2528	2538	rVB	94484	129679	5.85%	0.668%
20	17.065	2569	2572	2575	rBV4	29412	36446	1.64%	0.188%
21	17.112	2576	2580	2586	rVB	102215	148205	6.68%	0.763%
22	17.342	2614	2619	2629	rBV	1318259	1493824	67.35%	7.695%
23	17.718	2679	2683	2690	rBV6	25085	46759	2.11%	0.241%
24	17.995	2725	2730	2735	rBV	42032	61550	2.78%	0.317%
25	18.600	2828	2833	2839	rBV9	35436	96685	4.36%	0.498%
26	18.689	2844	2848	2853	rVV2	434456	670912	30.25%	3.456%
27	18.730	2853	2855	2861	rVB2	132249	178874	8.07%	0.921%
28	18.989	2895	2899	2902	rBV5	35955	49516	2.23%	0.255%
29	19.206	2933	2936	2940	rBV5	32155	39623	1.79%	0.204%
30	19.406	2968	2970	2974	rBV5	23837	32670	1.47%	0.168%
31	19.518	2985	2989	2992	rBV6	21306	40864	1.84%	0.210%
32	19.965	3061	3065	3068	rBV	237697	354096	15.97%	1.824%
33	20.253	3111	3114	3118	rBV	146509	163898	7.39%	0.844%
34	20.312	3121	3124	3130	rVV	196163	259884	11.72%	1.339%

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35	20.365	3130	3133	3146	rVV	345216	548391	24.73%	2.825%
36	21.600	3335	3343	3349	rBV5	102178	203807	9.19%	1.050%
37	21.706	3358	3361	3369	rVB	106374	188612	8.50%	0.972%
38	22.100	3423	3428	3437	rBV	63673	149209	6.73%	0.769%
39	23.571	3672	3678	3679	rBV6	16740	35938	1.62%	0.185%
40	23.659	3687	3693	3700	rVB5	55769	127229	5.74%	0.655%

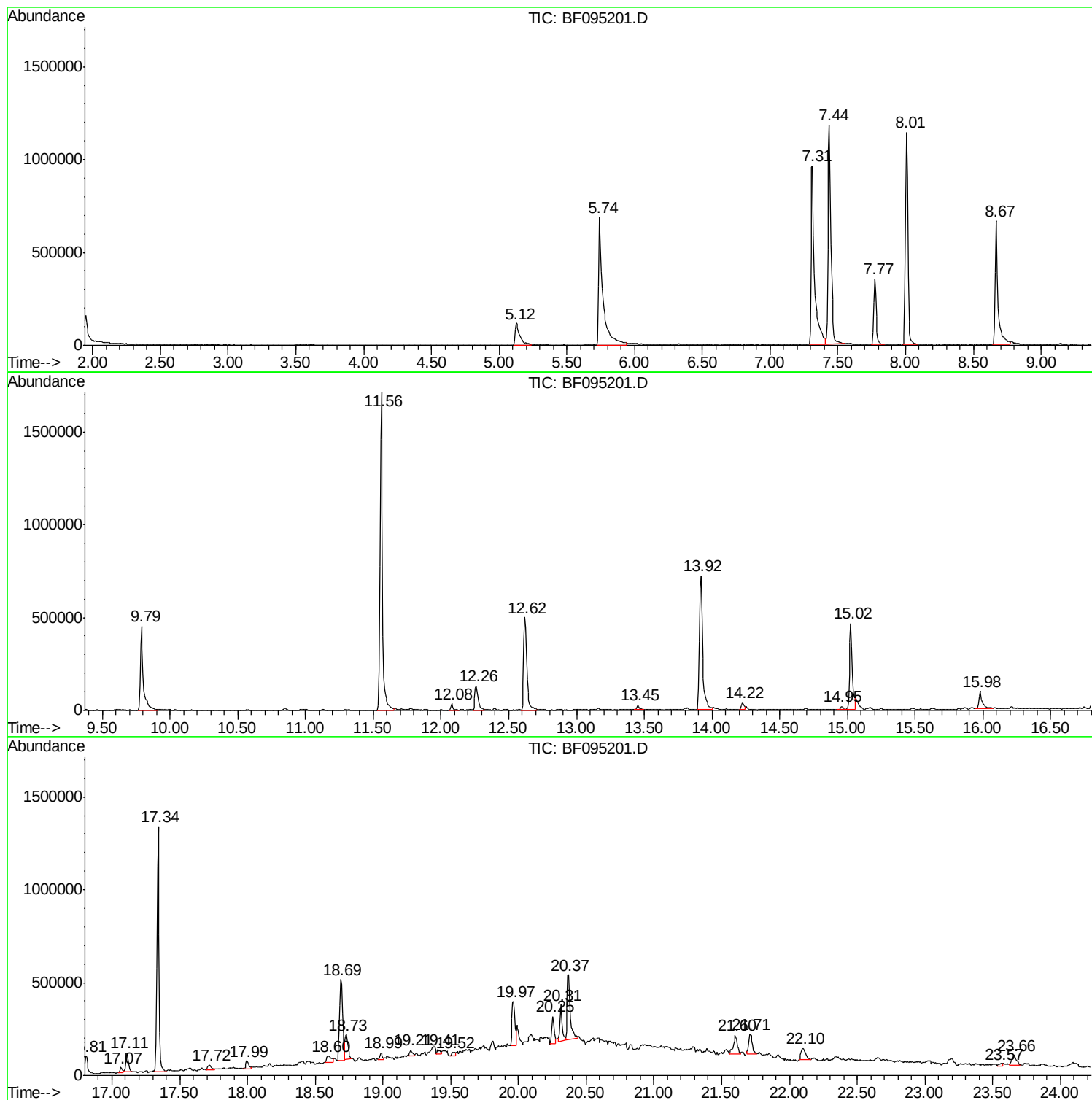
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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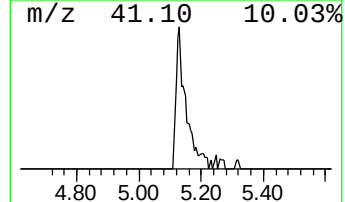
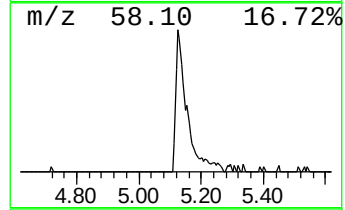
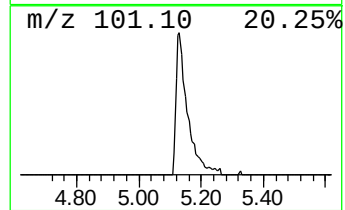
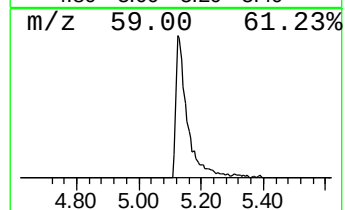
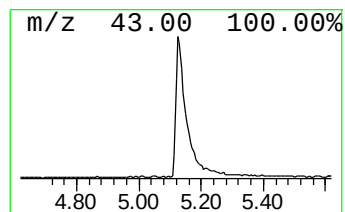
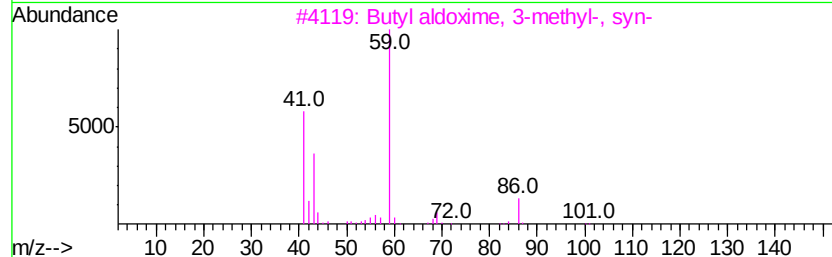
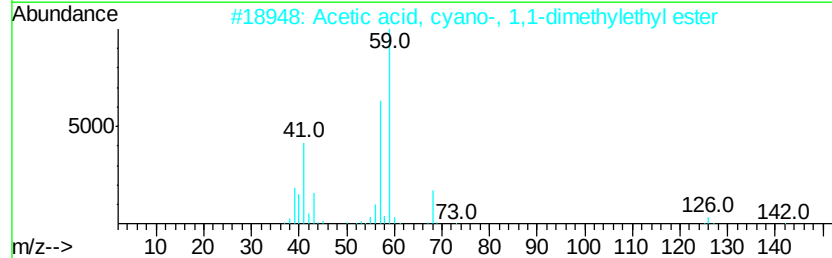
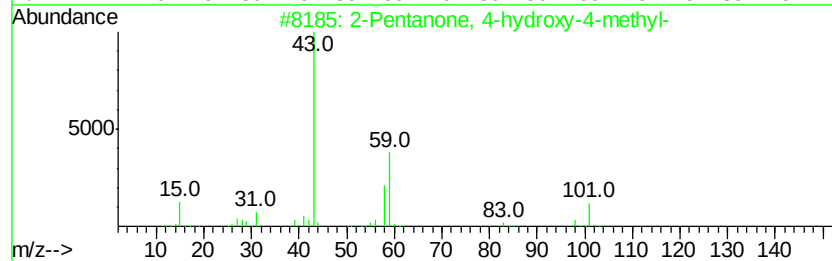
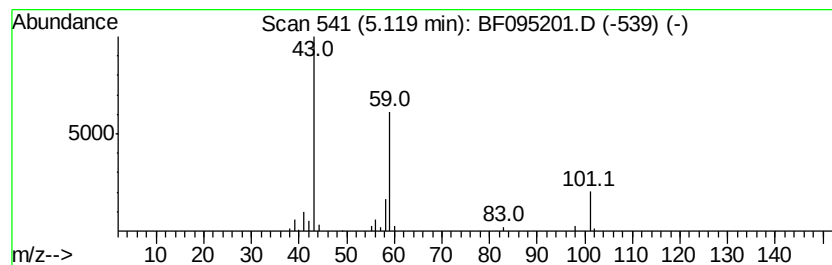
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	13.03 ng	279739	1,4-Dichlorobenzene-d4	7.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25	
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	



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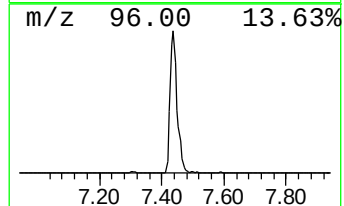
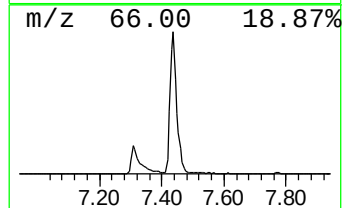
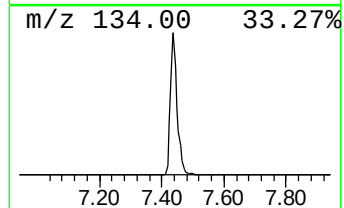
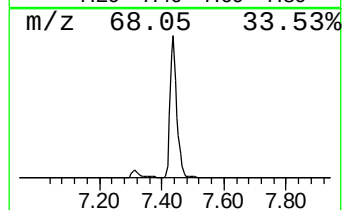
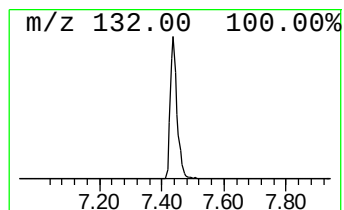
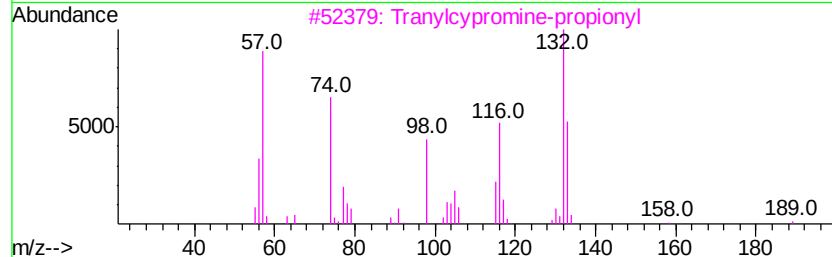
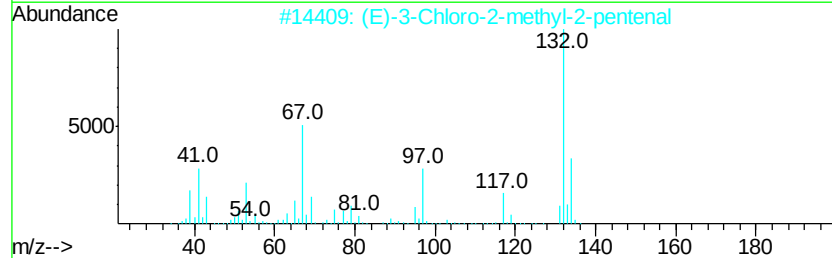
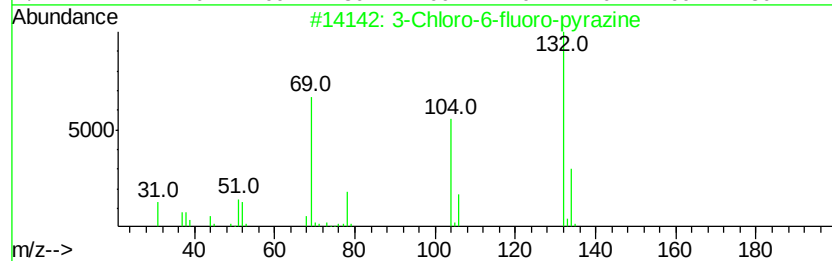
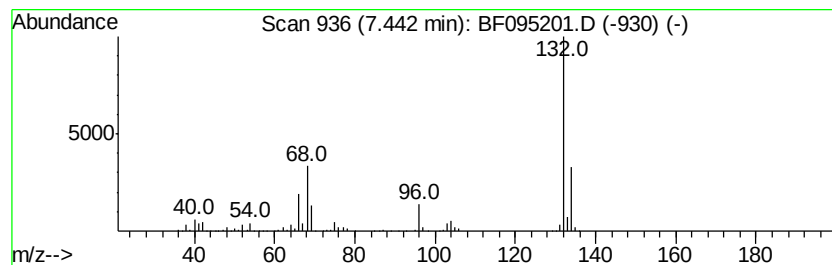
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Peak Number 2 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	84.28 ng	1810080	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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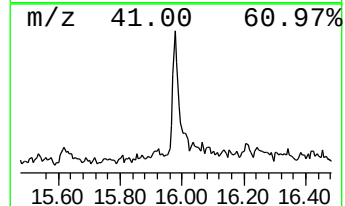
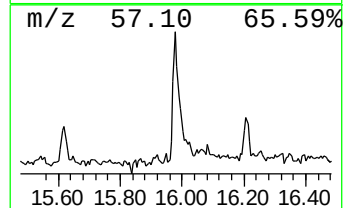
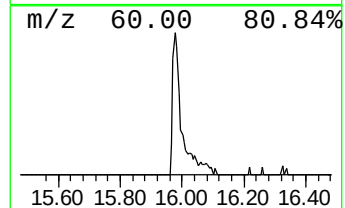
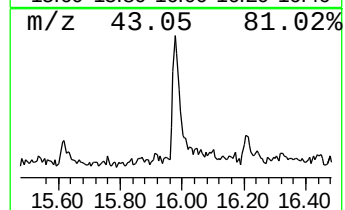
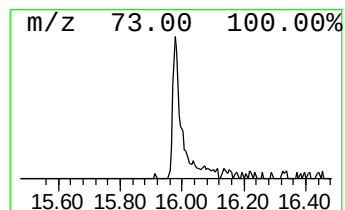
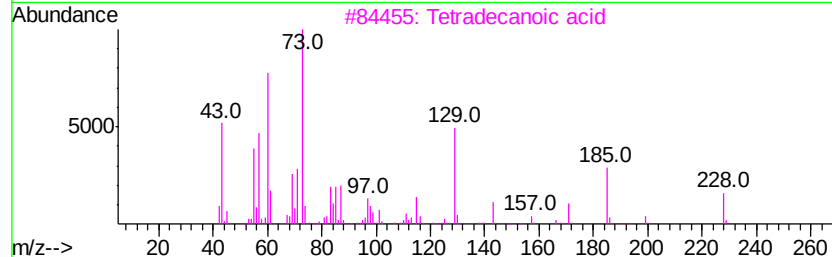
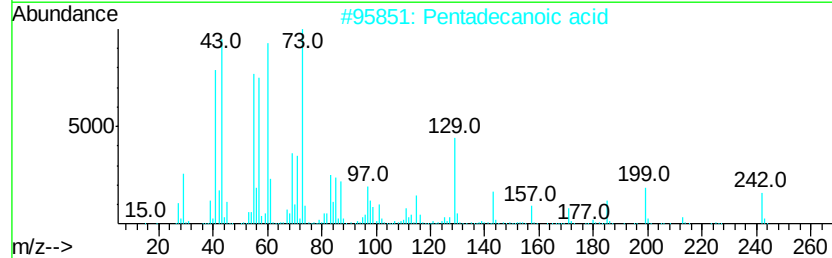
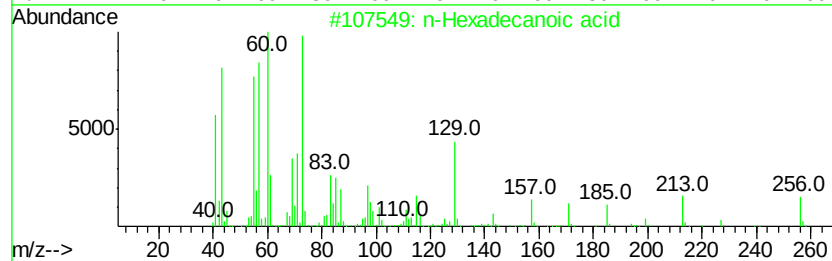
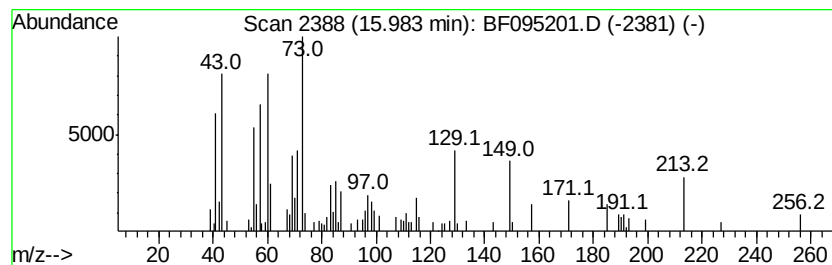
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.98	5.44 ng	173658	Phenanthrene-d10	15.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53
5	Lactose	342	C12H22O11	000063-42-3	38



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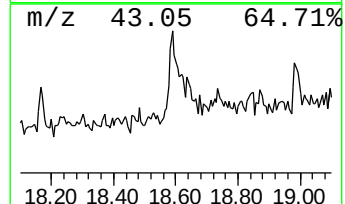
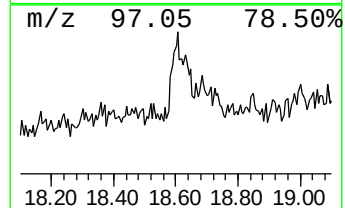
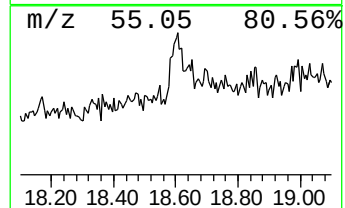
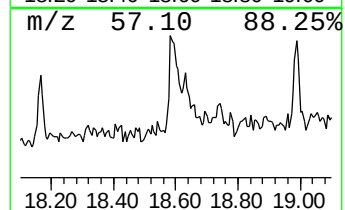
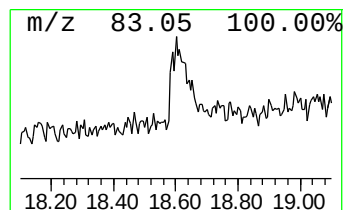
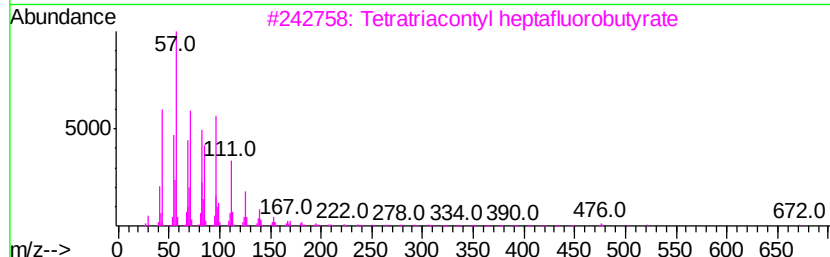
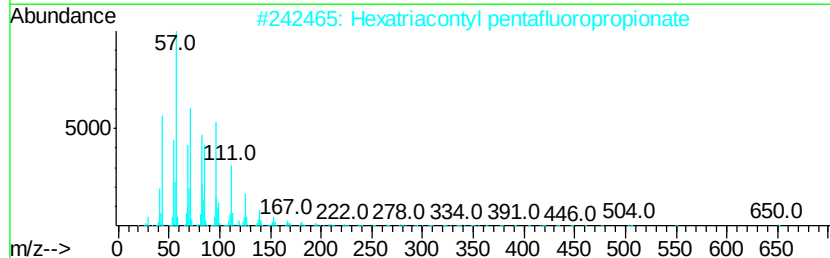
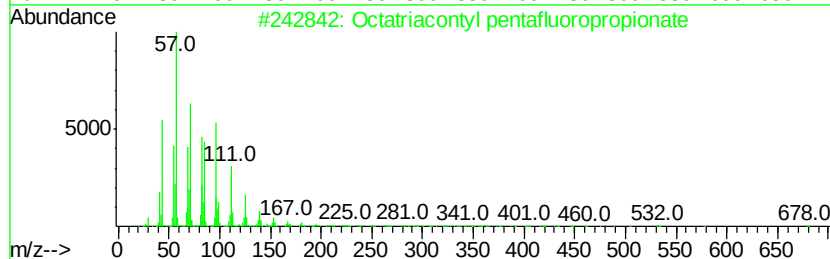
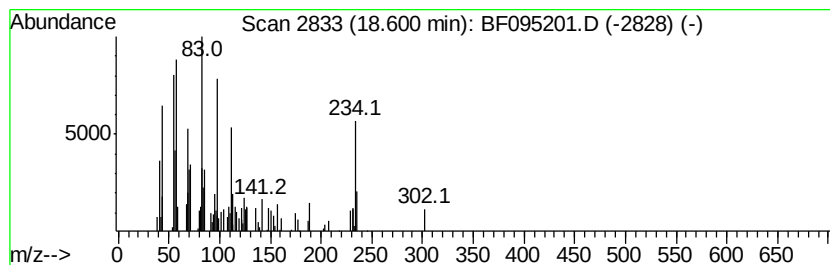
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Peak Number 5 unknown18.60 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.60	2.88 ng	96685	Chrysene-d12	18.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	47
2		Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	43
3		Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	43
4		Cyclohexanecarboxylic acid, 4-oc...	240	C15H28O2	1000279-52-2	27
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	25



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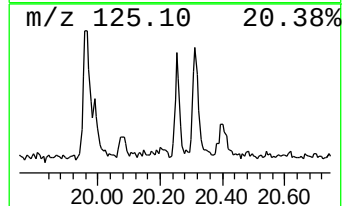
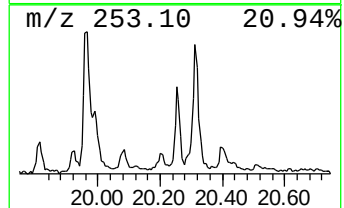
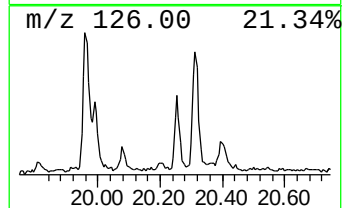
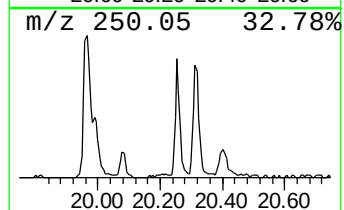
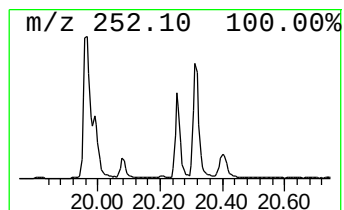
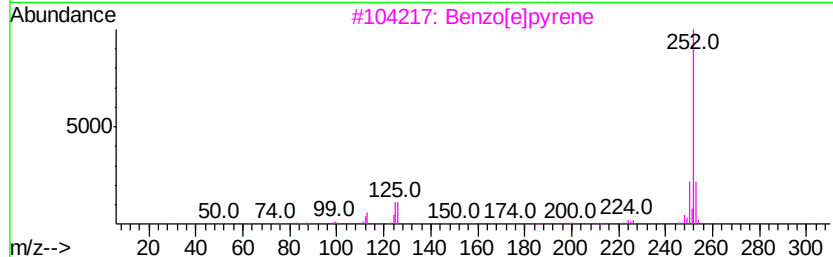
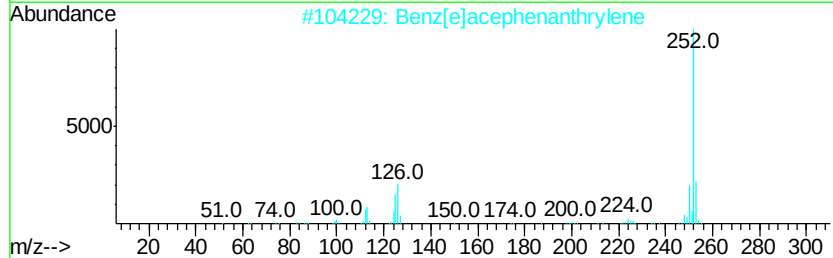
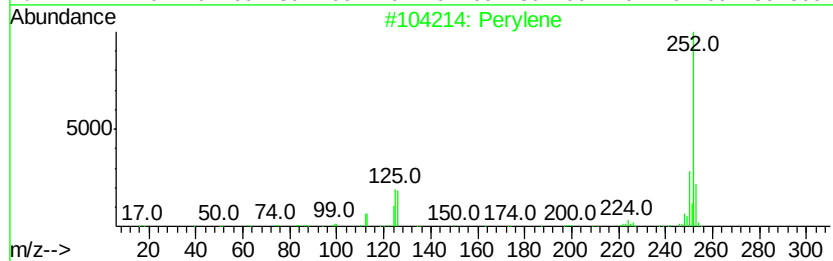
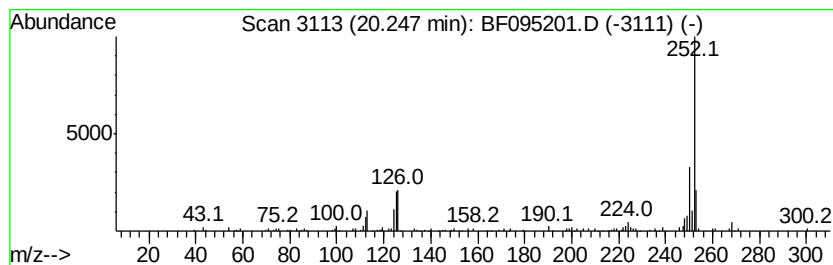
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Peak Number 6 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.25	5.98 ng	163898	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	95
2		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
3		Benzo[e]pyrene	252	C20H12	000192-97-2	91
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	81



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Data File : BF095201.D
Acq On : 17 May 2017 23:52
Operator : SJ/MA
Sample : I3172-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-04

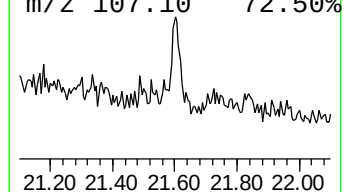
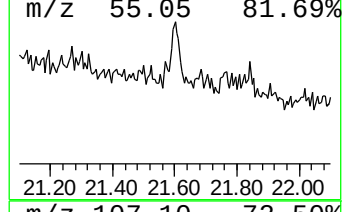
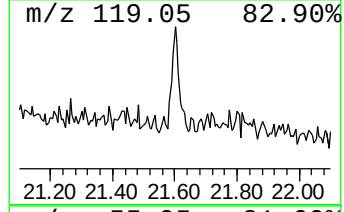
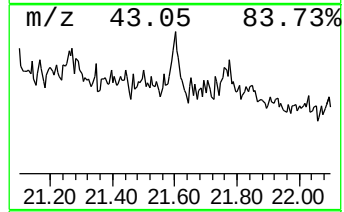
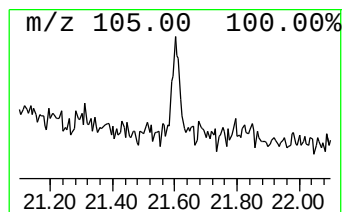
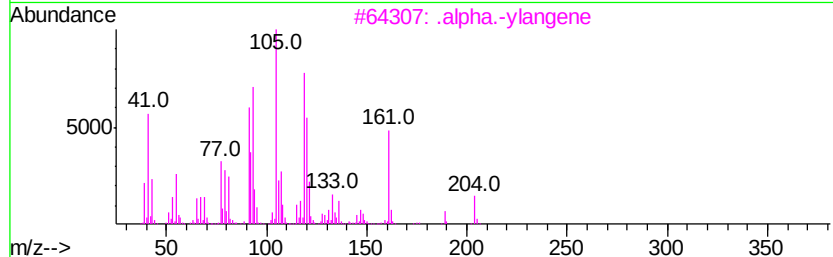
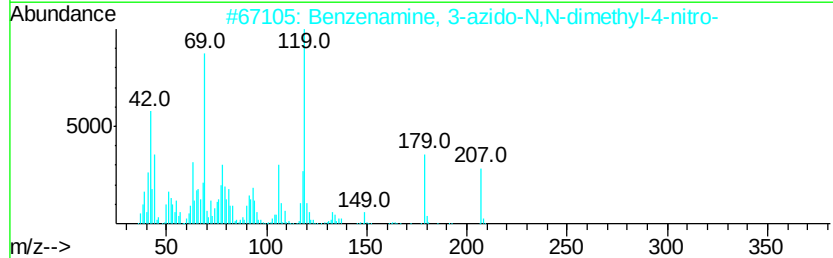
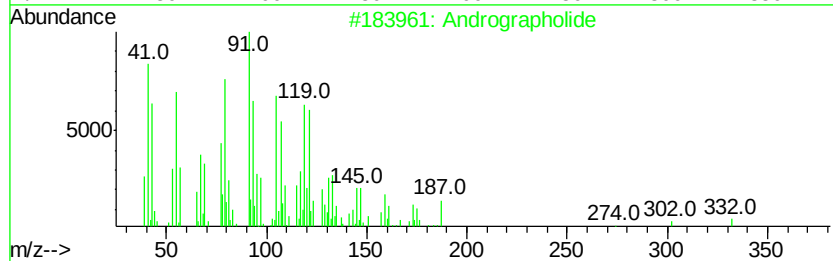
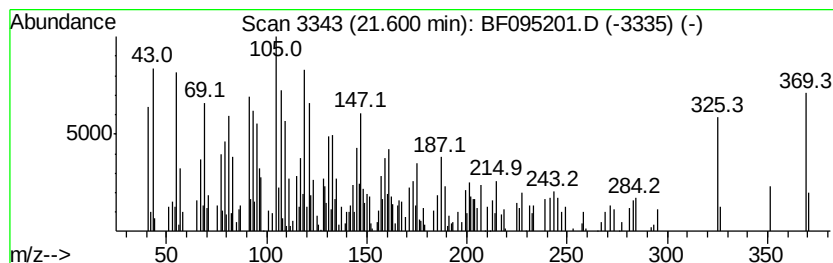
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown21.60 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.60	7.43 ng	203807	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Andrographolide	350	C20H30O5	005508-58-7	49
2		Benzenamine, 3-azido-N,N-dimethyl...	207	C8H9N5O2	001437-65-6	25
3		.alpha.-ylangene	204	C15H24	1000374-19-0	20
4		benz[d]isoxazole, 3-ethyl-	147	C9H9NO	066033-77-0	18
5		Caryophyllene	204	C15H24	000087-44-5	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051717\
Data File : BF095201.D
Acq On : 17 May 2017 23:52
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Sample : I3172-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

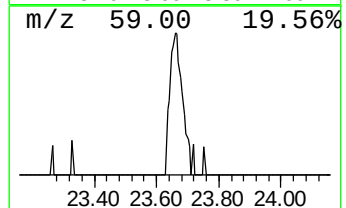
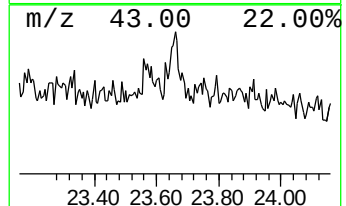
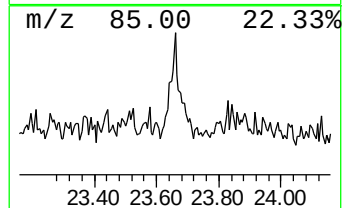
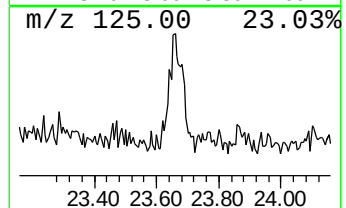
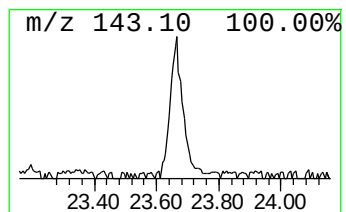
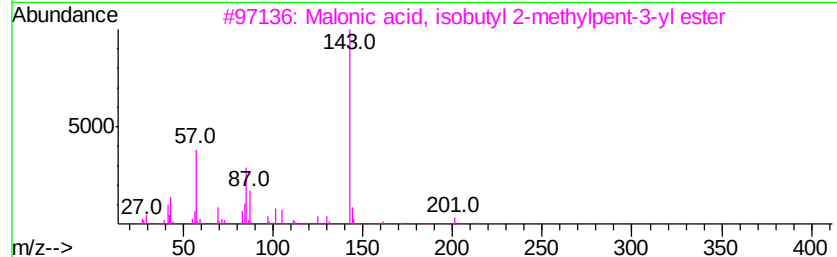
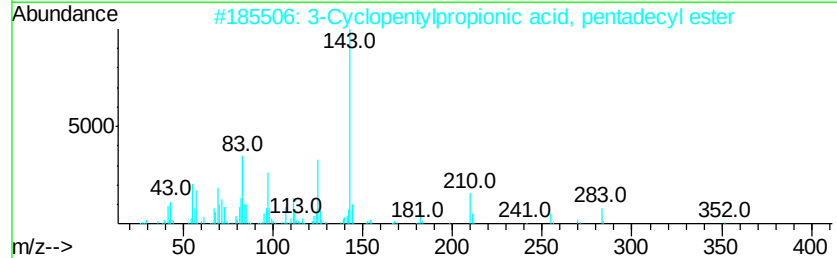
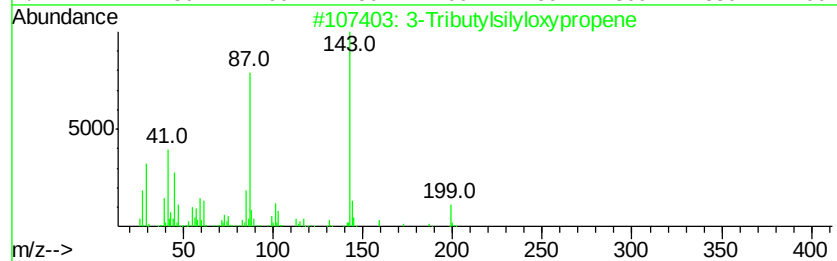
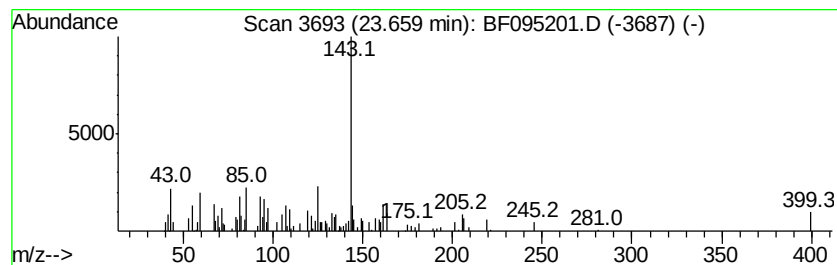
Instrument :
BNA_F
ClientSampled :
SS-04

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3-Tributylsilyloxypropene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.66	4.64 ng	127229	Perylene-d12	20.37
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	3-Tributylsilyloxypropene	256 C15H32OSi	017922-05-3	50
2	3-Cyclopentylpropionic acid, pen...	352 C23H44O2	1000292-33-9	47
3	Malonic acid, isobutyl 2-methylp...	244 C13H24O4	1000349-04-6	47
4	3-Cyclopentylpropionic acid, tet...	338 C22H42O2	1000292-33-8	47
5	1-(1-Butoxypropan-2-yloxy)propan...	274 C15H30O4	1000367-12-9	40



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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	13.0	ng	279739	1	7.77	429519	20.0
unknown7.44	7.44	84.3	ng	1810080	1	7.77	429519	20.0
n-Hexadecanoic acid	15.98	5.4	ng	173658	4	15.02	638788	20.0
unknown18.60	18.60	2.9	ng	96685	5	18.69	670912	20.0
Perylene	20.25	6.0	ng	163898	6	20.37	548391	20.0
unknown21.60	21.60	7.4	ng	203807	6	20.37	548391	20.0
3-Tributylsilylox...	23.66	4.6	ng	127229	6	20.37	548391	20.0