

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090216\
 Data File : BF089982.D
 Acq On : 2 Sep 2016 18:36
 Operator : UM/SJ
 Sample : H4675-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RAMP-A(0-2)-4

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-BF083116.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	1.644	3	5	11	rVB	54446	127841	2.47%	0.255%
2	1.747	13	14	25	rVB	518668	952562	18.40%	1.898%
3	4.776	276	279	288	rVB	856496	1345960	25.99%	2.682%
4	5.222	315	318	320	rBV	4381627	4820542	93.09%	9.605%
5	5.324	324	327	335	rVV	19251	51880	1.00%	0.103%
6	6.284	407	411	413	rBV	4349944	5178273	100.00%	10.317%
7	6.399	419	421	424	rBV	3539330	5085618	98.21%	10.133%
8	6.639	439	442	444	rBV	1223978	1191252	23.00%	2.374%
9	6.799	453	456	457	rBV	2737492	3810999	73.60%	7.593%
10	7.210	488	492	494	rBV	2369814	3422240	66.09%	6.819%
11	7.325	498	502	509	rBV	100288	192203	3.71%	0.383%
12	7.667	528	532	539	rBV3	63488	147807	2.85%	0.294%
13	7.919	552	554	557	rBV	1558533	1369759	26.45%	2.729%
14	9.005	646	649	651	rBV	3658537	4921260	95.04%	9.805%
15	9.119	658	659	661	rVB2	62444	75198	1.45%	0.150%
16	9.336	672	678	680	rBV2	38201	60657	1.17%	0.121%
17	9.393	681	683	686	rVB	1771519	1904951	36.79%	3.796%
18	9.588	698	700	701	rBV	73852	64831	1.25%	0.129%
19	9.622	701	703	704	rVV	76713	71236	1.38%	0.142%
20	9.668	704	707	709	rVV	1523648	1526809	29.48%	3.042%
21	9.793	716	718	720	rVV	73227	79275	1.53%	0.158%
22	9.828	720	721	724	rVV2	42801	62348	1.20%	0.124%
23	10.113	745	746	748	rVB	126001	117334	2.27%	0.234%
24	10.319	762	764	767	rBV2	49106	107527	2.08%	0.214%
25	10.445	772	775	778	rVV	2651925	2796433	54.00%	5.572%
26	10.491	778	779	781	rVV2	47440	55764	1.08%	0.111%
27	10.582	785	787	793	rVB	131580	203882	3.94%	0.406%
28	11.028	821	826	828	rBV2	79587	133310	2.57%	0.266%
29	11.131	833	835	839	rVB	1336030	1409805	27.23%	2.809%
30	11.211	839	842	846	rBV2	33760	66455	1.28%	0.132%
31	11.382	855	857	862	rVV	315615	374378	7.23%	0.746%
32	11.462	862	864	870	rVB	65737	105051	2.03%	0.209%
33	11.691	880	884	885	rBV	135003	167847	3.24%	0.334%
34	11.714	885	886	889	rVV	52492	95413	1.84%	0.190%

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Integrator: RTE
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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 >
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35	12.205	925	929	931	rBV2	44332	64615	1.25%	0.129%
36	12.331	939	940	943	rVB	73487	75315	1.45%	0.150%
37	12.559	957	960	962	rBV	88300	86682	1.67%	0.173%
38	12.719	971	974	976	rBV	3566781	3368428	65.05%	6.711%
39	12.971	990	996	997	rBV3	24494	54739	1.06%	0.109%
40	13.634	1051	1054	1061	rBV	248893	362407	7.00%	0.722%
41	13.748	1061	1064	1069	rBV	1304921	1395967	26.96%	2.781%
42	13.954	1080	1082	1088	rBV4	29676	61266	1.18%	0.122%
43	14.262	1106	1109	1114	rBV2	176264	318015	6.14%	0.634%
44	14.617	1138	1140	1141	rBV	61123	87504	1.69%	0.174%
45	14.731	1148	1150	1155	rBV	54186	124376	2.40%	0.248%
46	14.845	1158	1160	1161	rBV	38725	68659	1.33%	0.137%
47	14.994	1171	1173	1175	rBV	33332	52983	1.02%	0.106%
48	15.097	1179	1182	1185	rBV	1040543	1112660	21.49%	2.217%
49	15.337	1201	1203	1207	rVB3	52726	88039	1.70%	0.175%
50	15.531	1218	1220	1222	rBV	68061	106323	2.05%	0.212%
51	15.577	1222	1224	1227	rVB2	61009	108878	2.10%	0.217%
52	16.480	1300	1303	1306	rVB	120094	214489	4.14%	0.427%
53	16.834	1331	1334	1341	rBV5	72404	161312	3.12%	0.321%
54	18.400	1467	1471	1479	rVB5	62358	180099	3.48%	0.359%

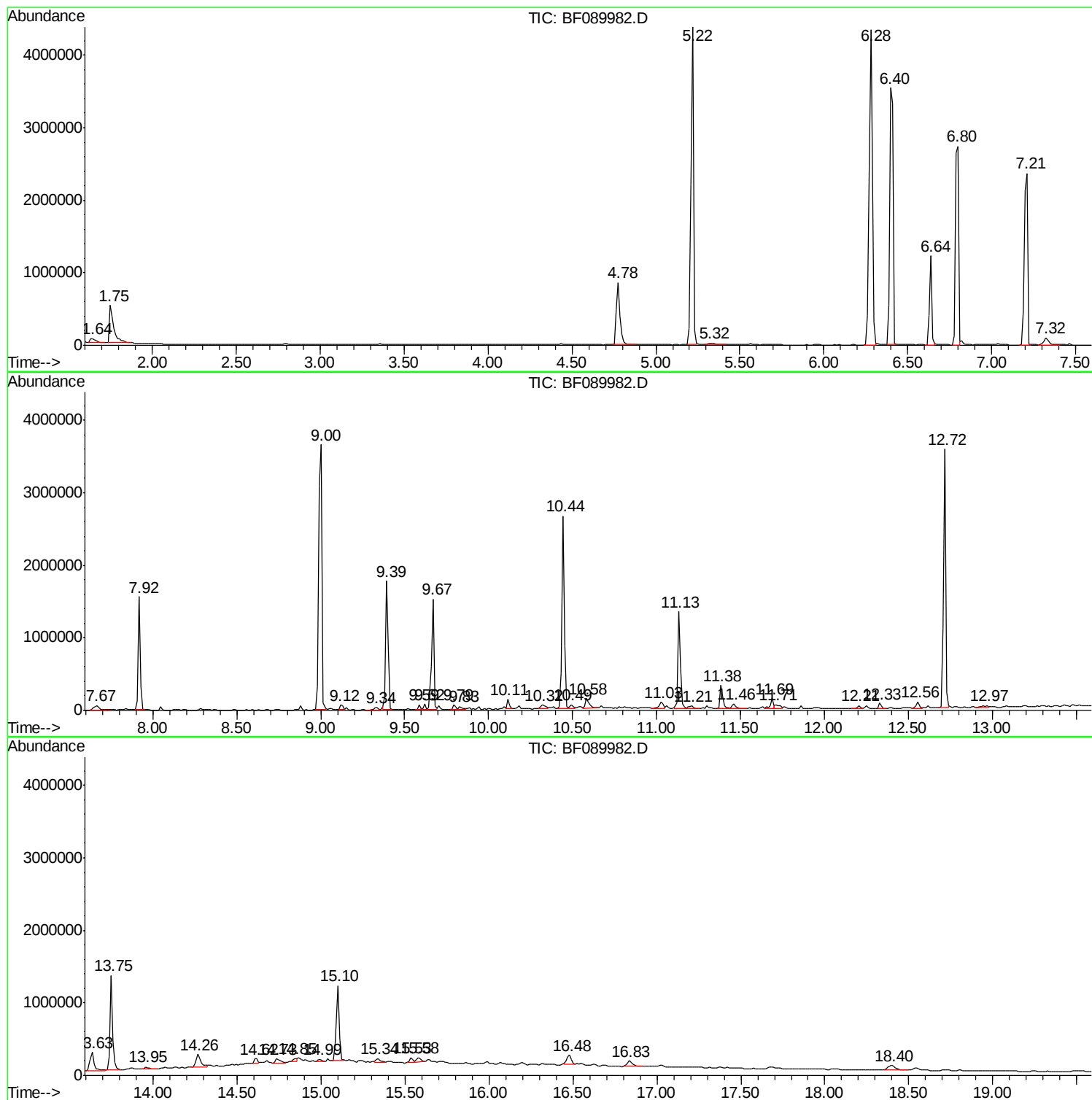
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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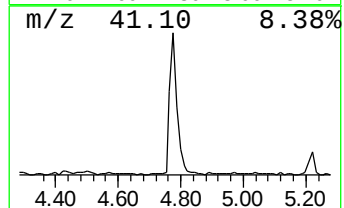
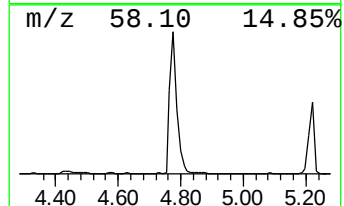
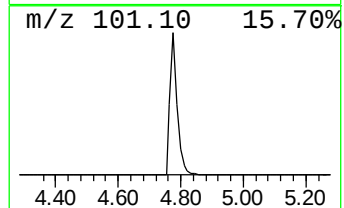
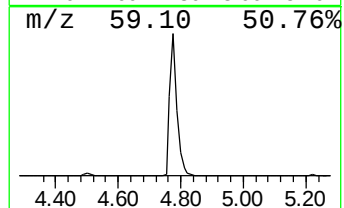
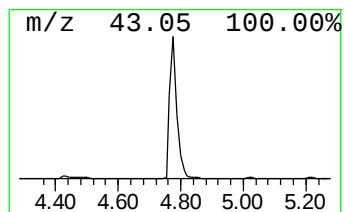
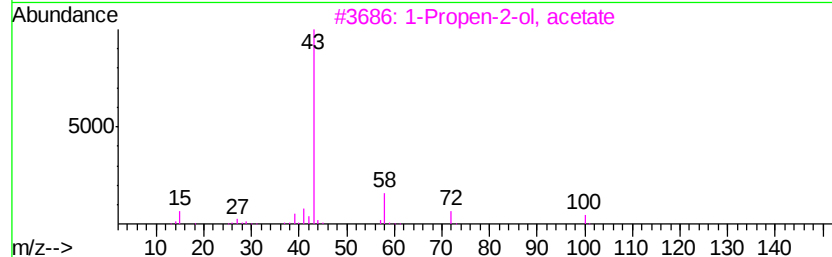
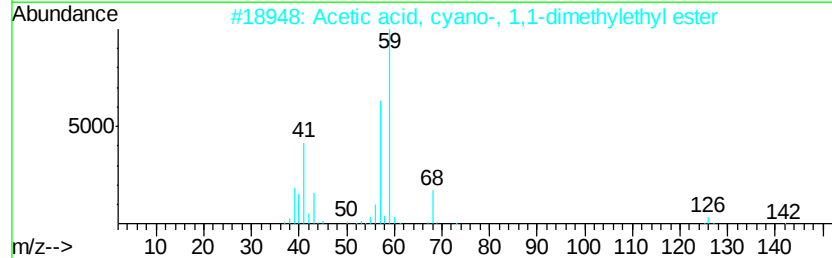
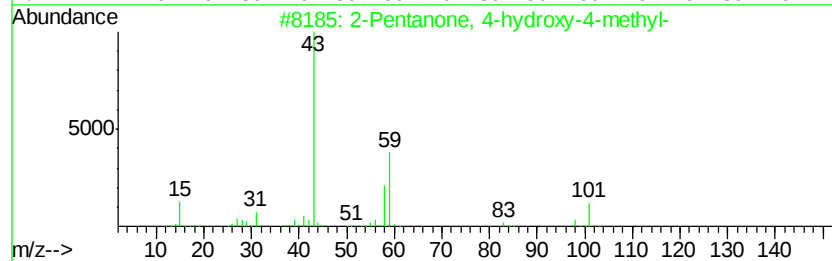
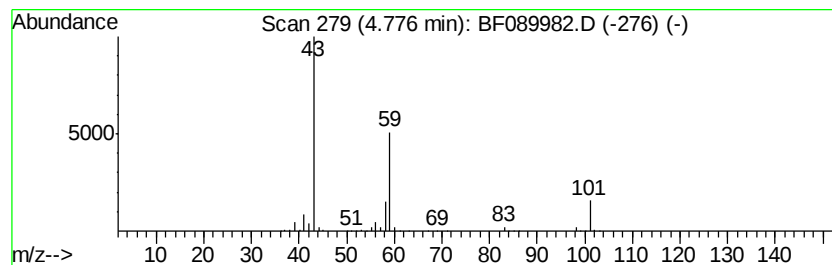
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	22.60 ng	1345960	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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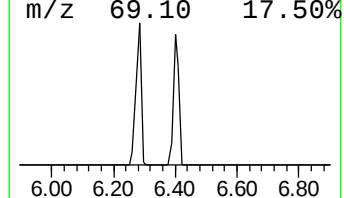
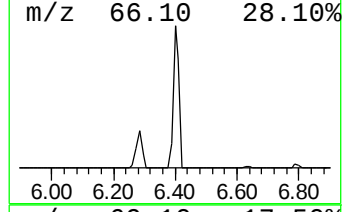
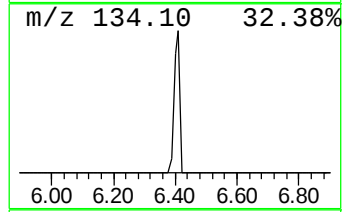
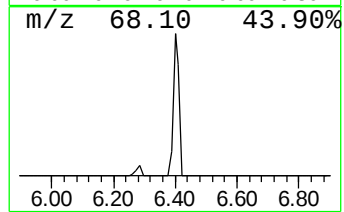
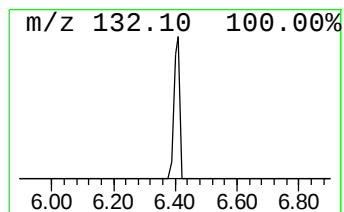
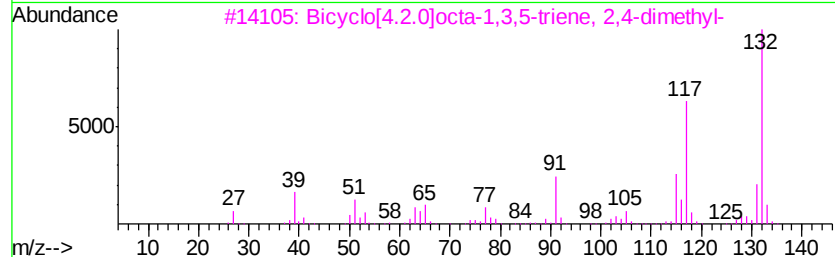
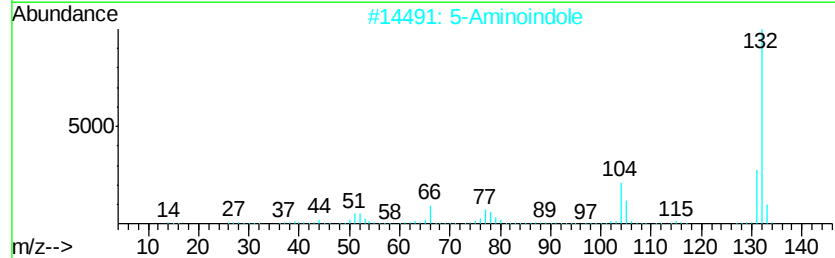
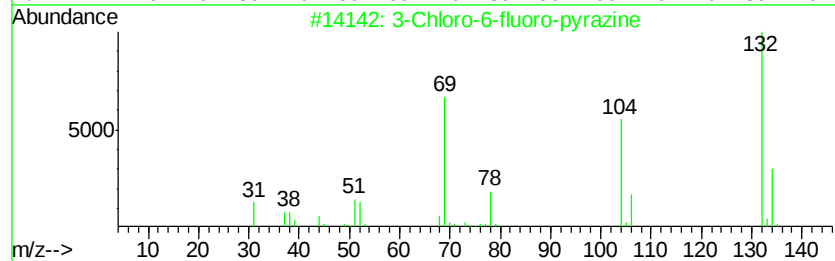
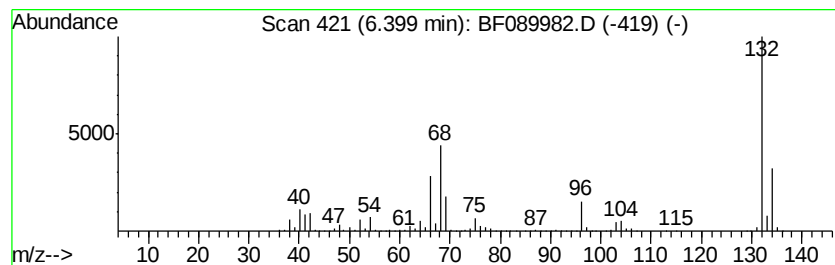
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	85.38 ng	5085620	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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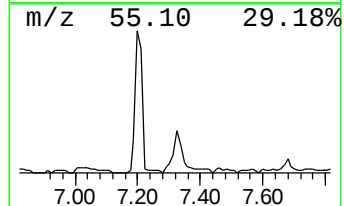
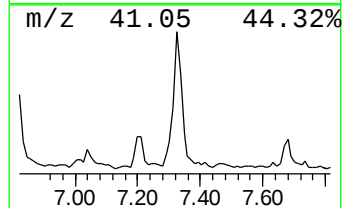
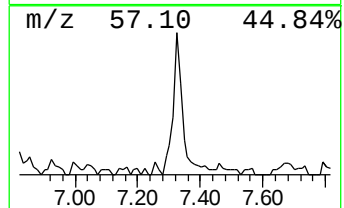
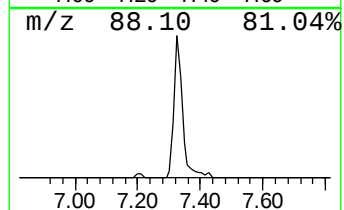
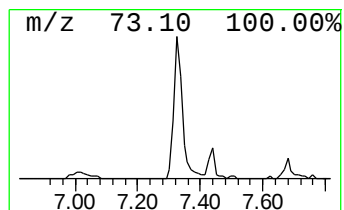
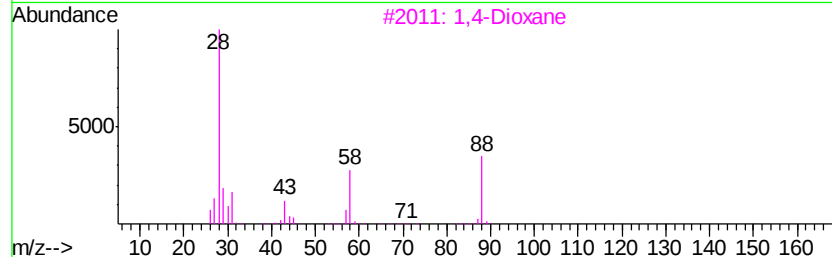
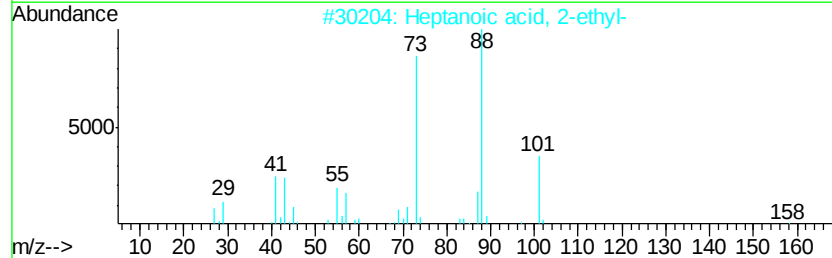
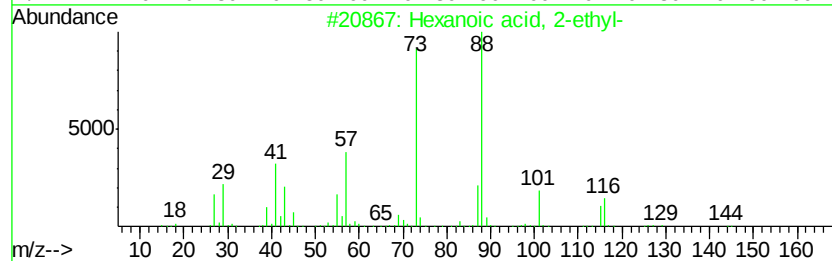
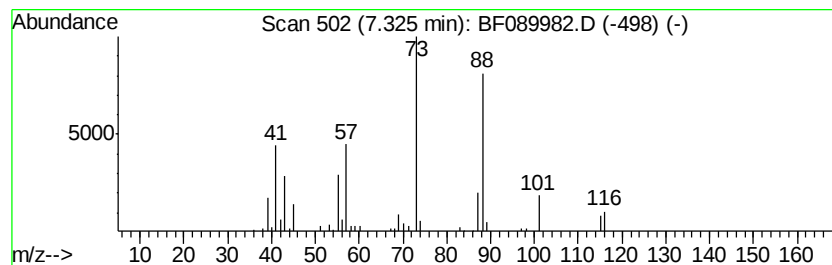
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexanoic acid, 2-ethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.32	2.81 ng	192203	Naphthalene-d8	7.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3	1,4-Dioxane	88	C4H8O2	000123-91-1	47
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
5	Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	36



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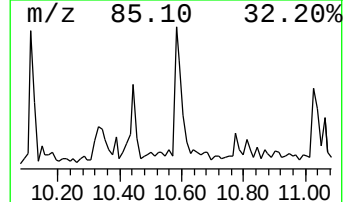
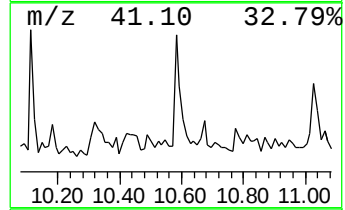
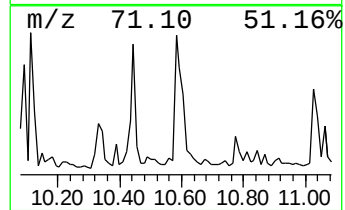
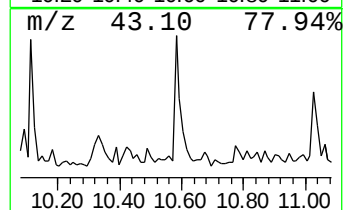
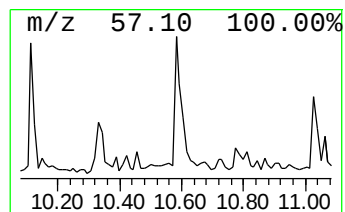
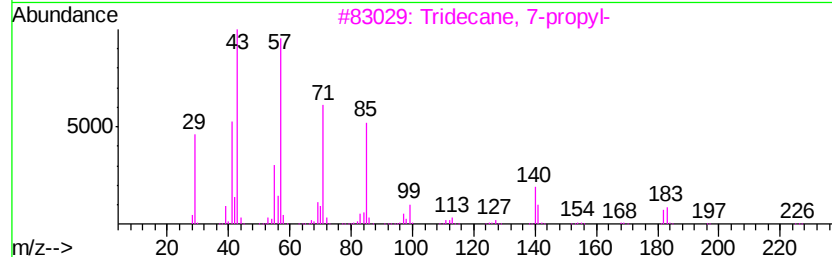
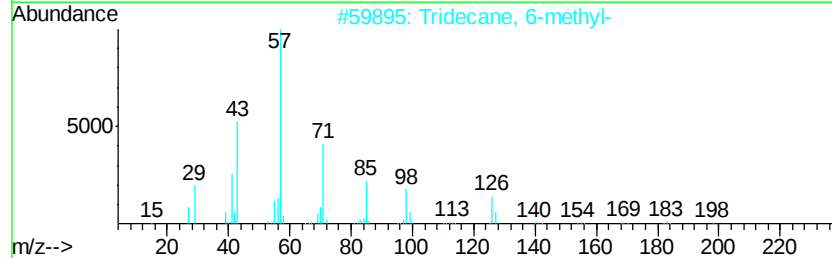
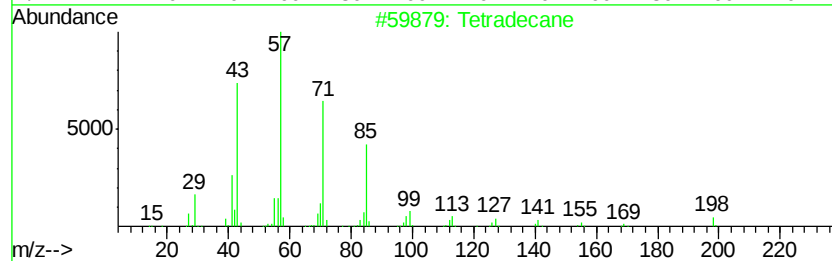
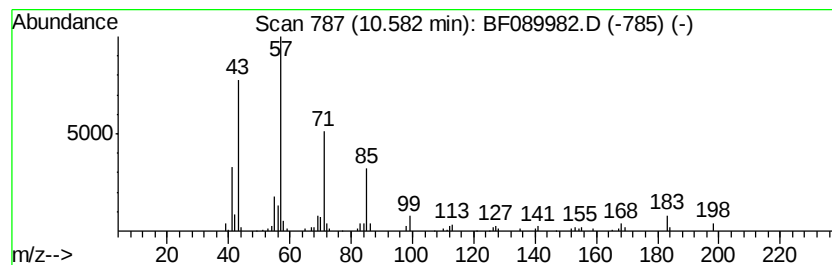
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Peak Number 7 Tetradecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.58	2.89 ng	203882	Phenanthrene-d10		11.13
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Tridecane, 6-methyl-	198	C14H30	013287-21-3	72
3	Tridecane, 7-propyl-	226	C16H34	055045-09-5	72
4	Hexadecane	226	C16H34	000544-76-3	72
5	Tridecane	184	C13H28	000629-50-5	70



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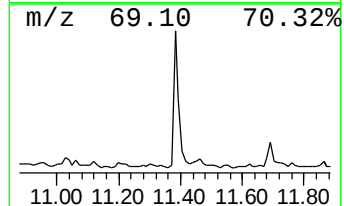
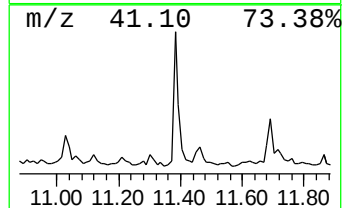
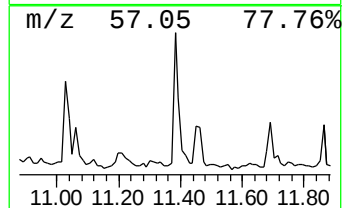
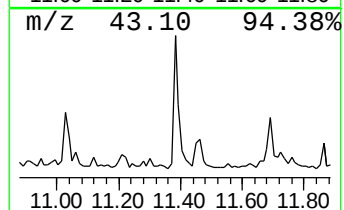
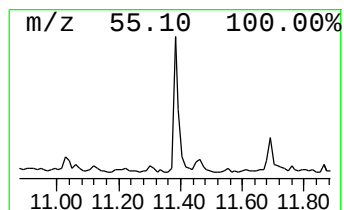
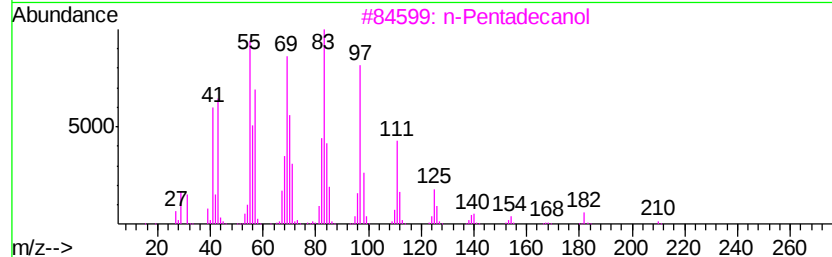
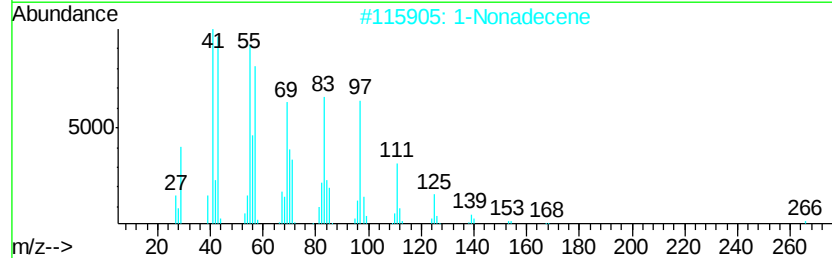
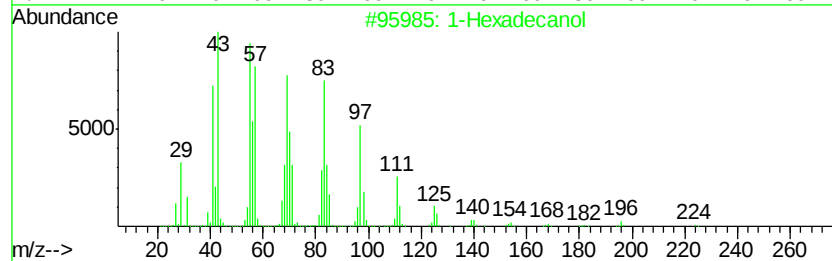
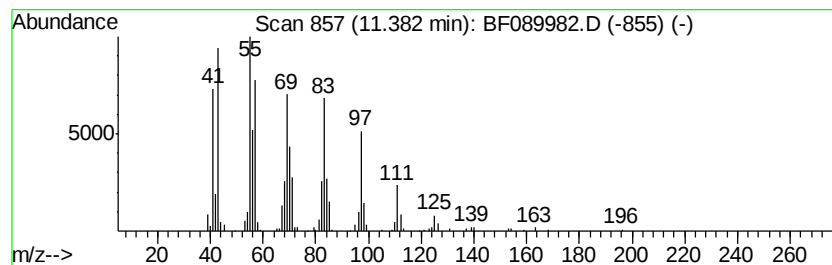
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Hexadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.38	5.31 ng	374378	Phenanthrene-d10		11.13
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	n-Pentadecanol	228	C15H32O	000629-76-5	91
4	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090216\
Data File : BF089982.D
Acq On : 2 Sep 2016 18:36
Operator : UM/SJ
Sample : H4675-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

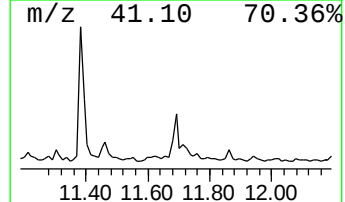
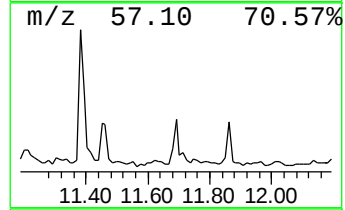
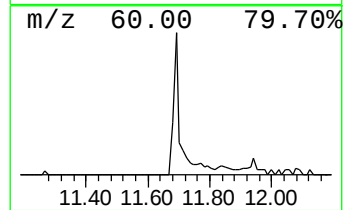
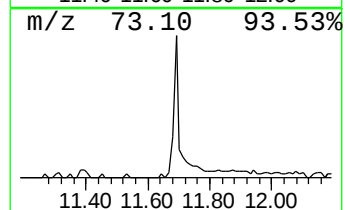
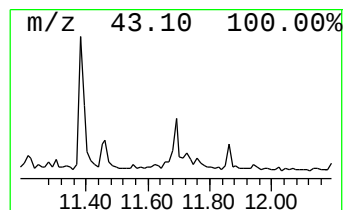
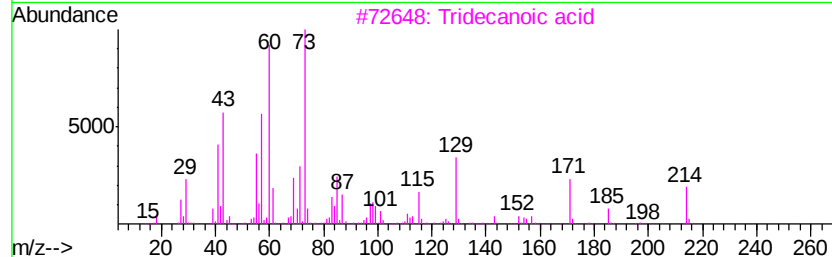
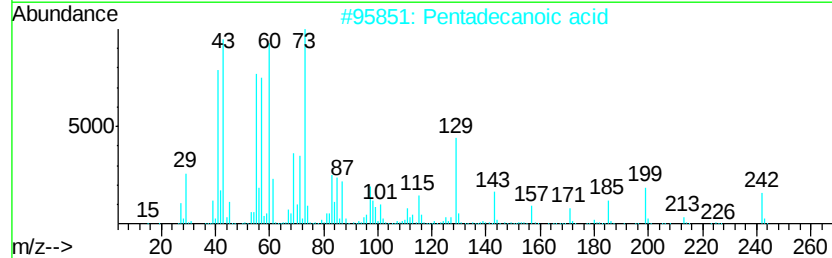
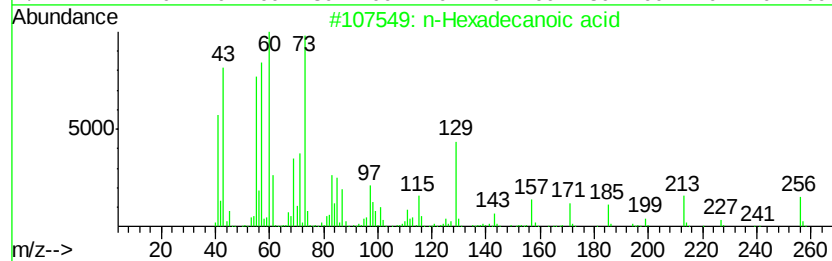
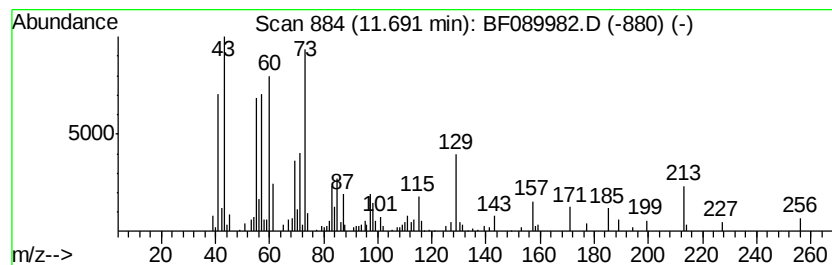
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.69	2.38 ng	167847	Phenanthrene-d10	11.13		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090216\
Data File : BF089982.D
Acq On : 2 Sep 2016 18:36
Operator : UM/SJ
Sample : H4675-07
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Instrument :
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ClientSampleId :
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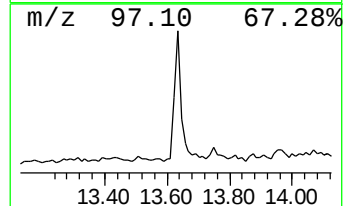
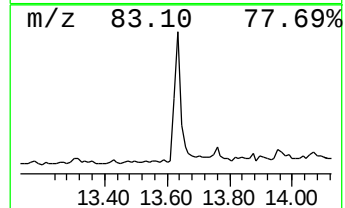
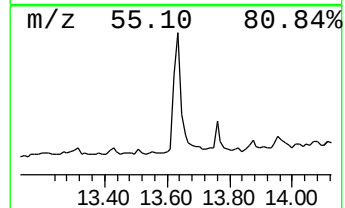
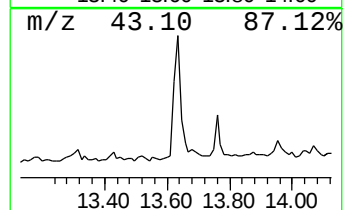
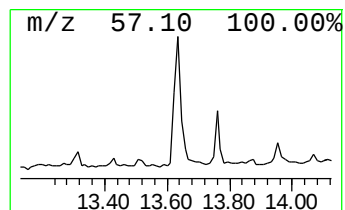
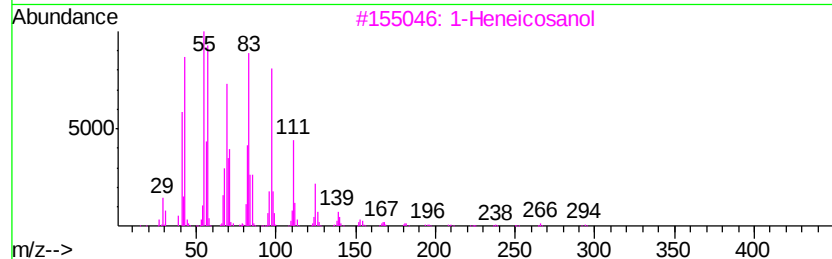
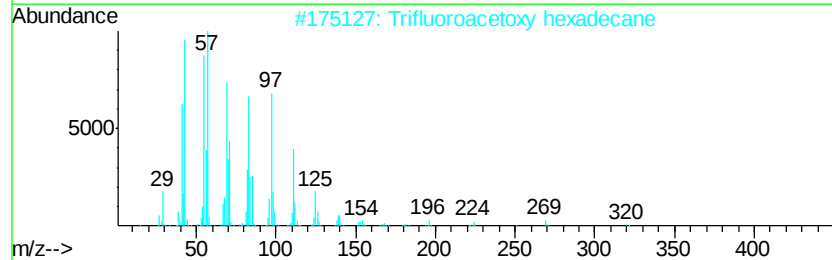
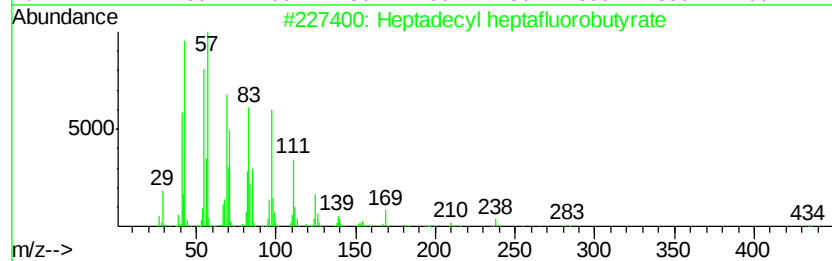
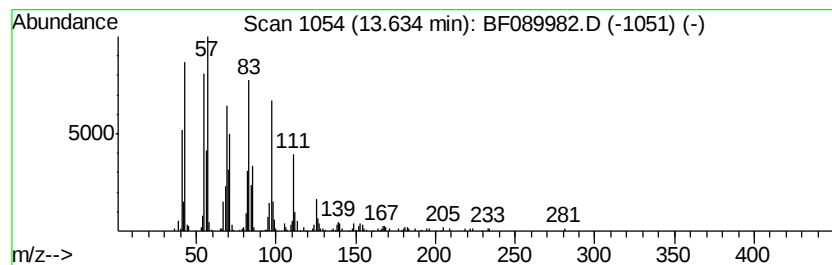
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	5.19 ng	362407	Chrysene-d12	13.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090216\
Data File : BF089982.D
Acq On : 2 Sep 2016 18:36
Operator : UM/SJ
Sample : H4675-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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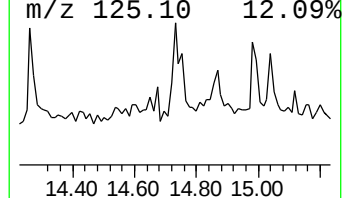
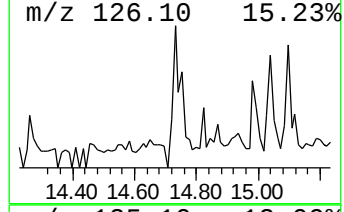
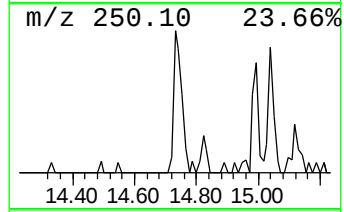
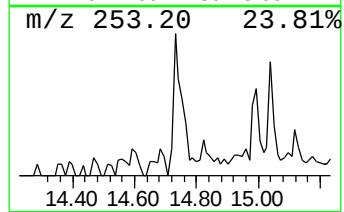
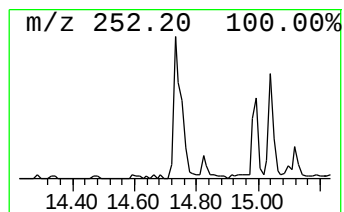
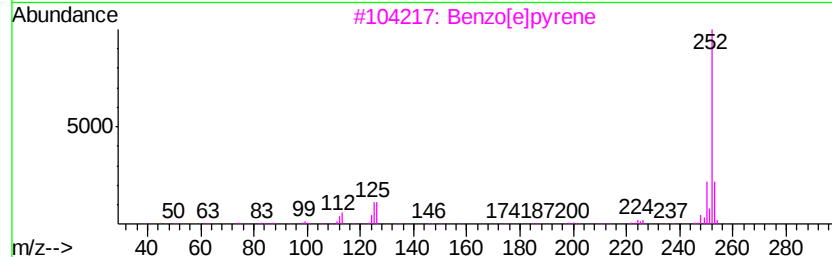
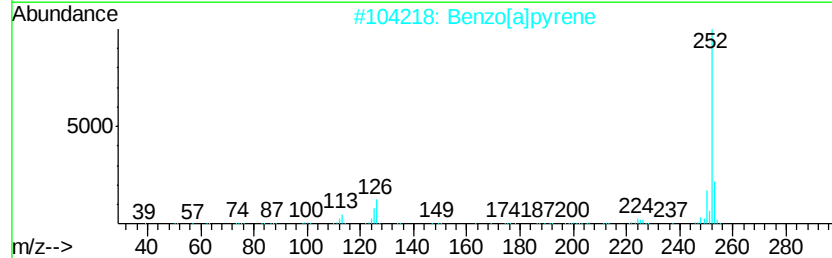
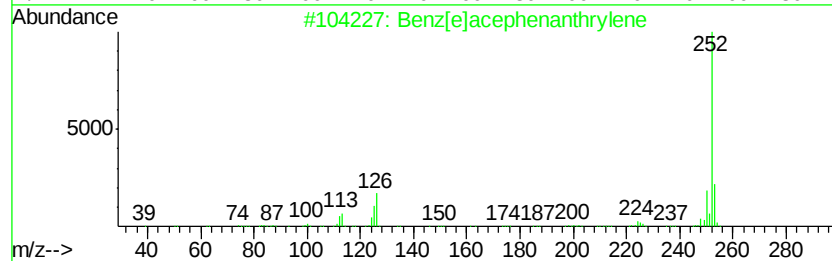
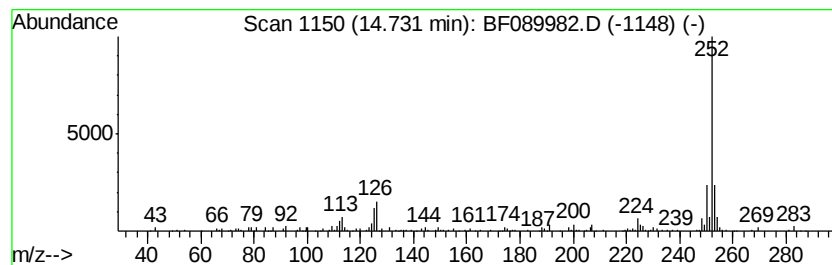
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benz[e]acephenanthrylene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.24 ng	124376	Perylene-d12	15.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
2		Benzo[a]pyrene	252	C20H12	000050-32-8	96
3		Benzo[e]pyrene	252	C20H12	000192-97-2	95
4		Perylene	252	C20H12	000198-55-0	94
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090216\
Data File : BF089982.D
Acq On : 2 Sep 2016 18:36
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Sample : H4675-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

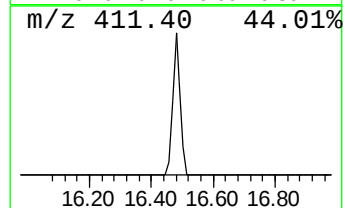
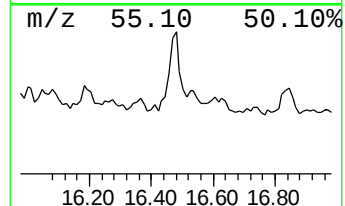
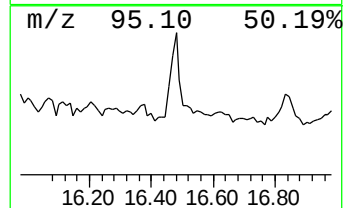
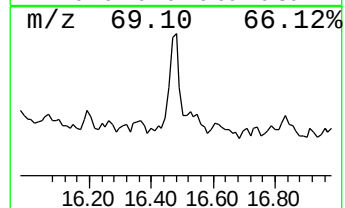
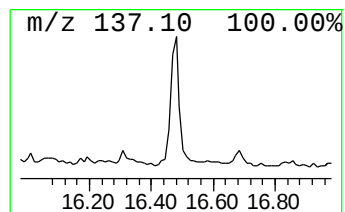
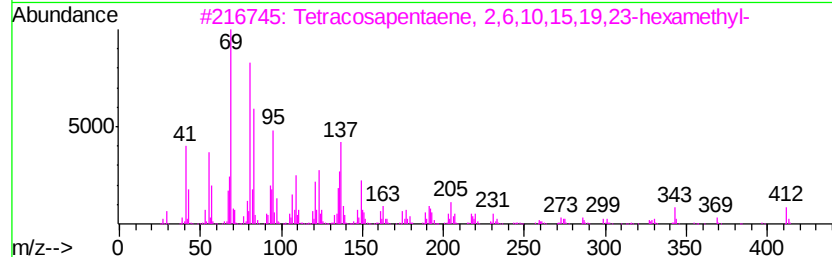
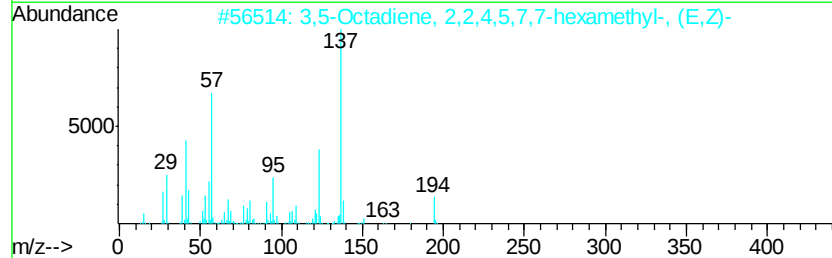
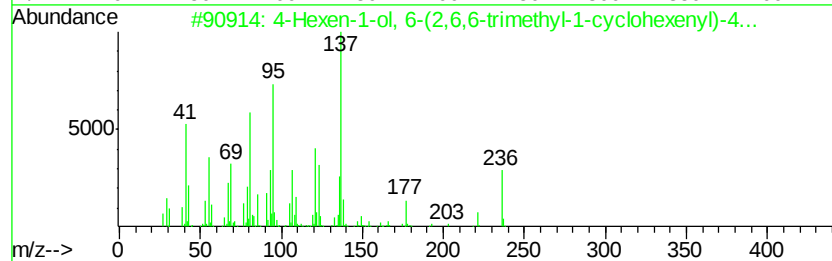
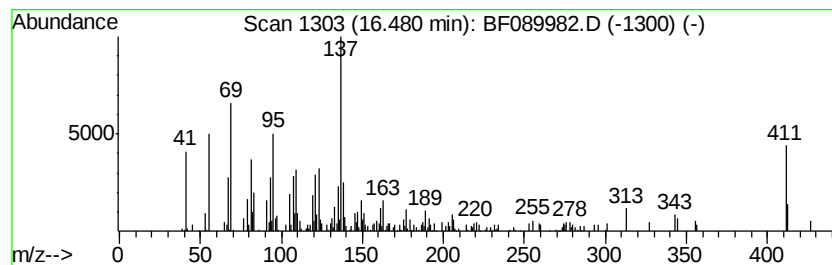
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 4-Hexen-1-ol, 6-(2,6,6-trimethyl-1-cyclohexenyl)-4... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.48	3.86 ng	214489	Perylene-d12	15.10	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Hexen-1-ol, 6-(2,6,6-trimethyl-1-cyclohexenyl)-4-methyl-	236	C16H28O	1000221-57-6	50
2	3,5-Octadiene, 2,2,4,5,7,7-hexamethyl-, (E,Z)-	194	C14H26	055712-52-2	43
3	Tetracosapentaene, 2,6,10,15,19,23-hexamethyl-, (E,Z)-	412	C30H52	026266-08-0	43
4	2-Propanone, 1-phenylthio-1-methyl-, (E)-	214	C10H11ClOS	087231-12-7	35
5	2,6,10,14,18-Pentamethyl-2,6,10,14,18-pentacosane	342	C25H42	075581-03-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090216\
Data File : BF089982.D
Acq On : 2 Sep 2016 18:36
Operator : UM/SJ
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Instrument :
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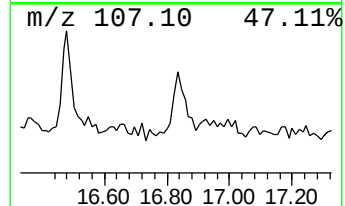
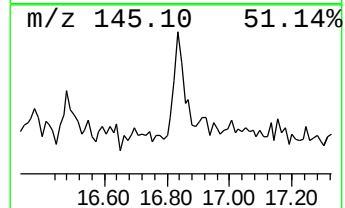
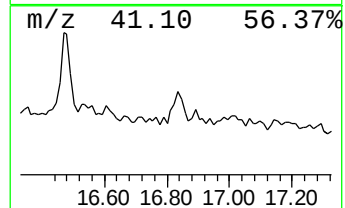
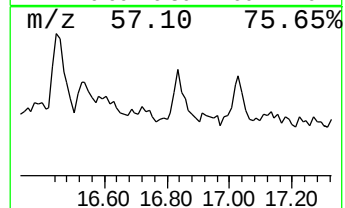
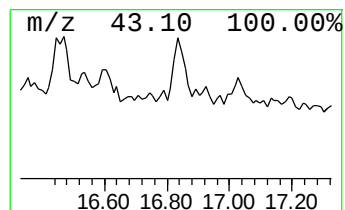
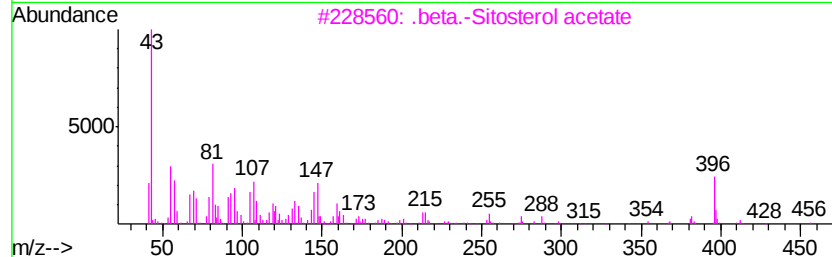
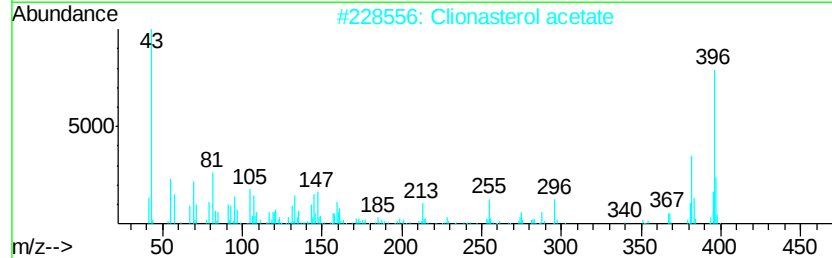
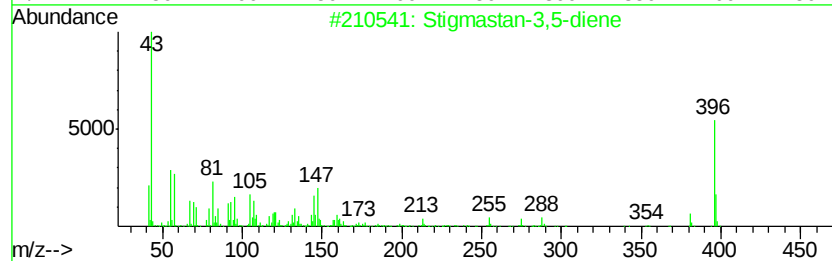
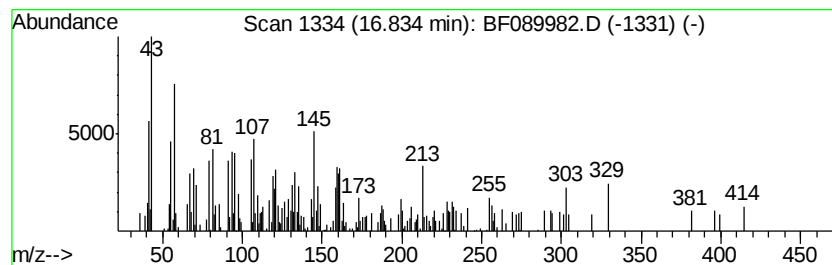
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown16.83 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	2.90 ng	161312	Perylene-d12	15.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stigmastan-3,5-diene	396	C29H48	1000214-16-4	46
2		Clionasterol acetate	456	C31H52O2	004651-54-1	40
3		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	38
4		9.beta.,10.alpha.-Androst-4-en-3...	408	C21H29BrO3	006765-86-2	25
5		(3E,5E,7E)-6-Methyl-8-(2,6,6-tri...	258	C18H26O	017974-57-1	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090216\
Data File : BF089982.D
Acq On : 2 Sep 2016 18:36
Operator : UM/SJ
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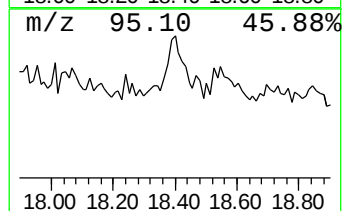
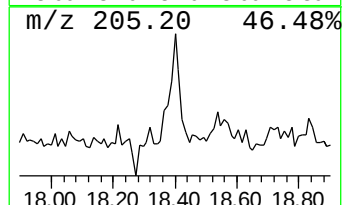
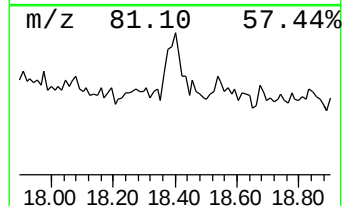
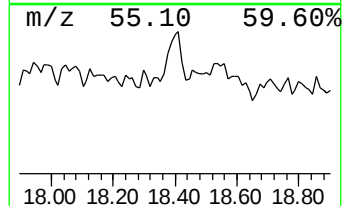
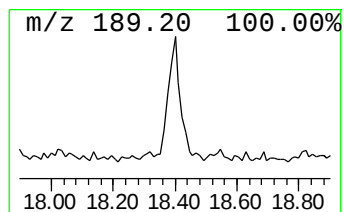
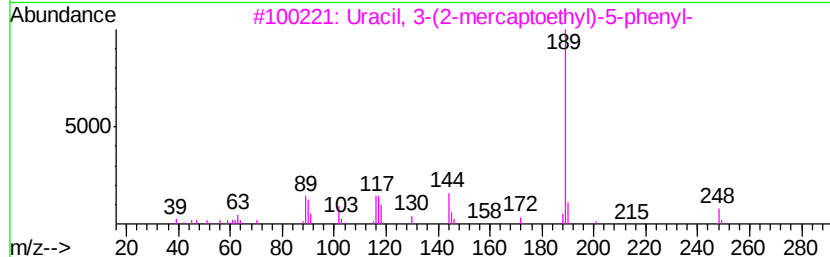
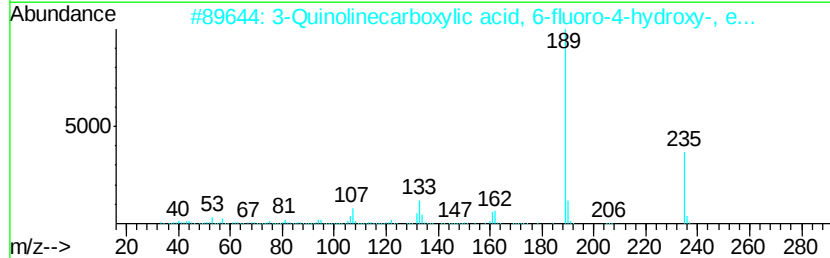
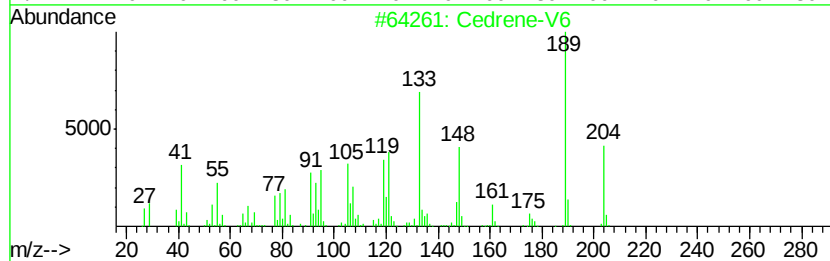
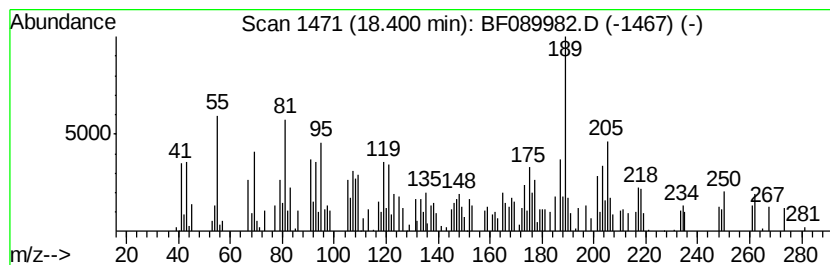
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown18.40 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	3.24 ng	180099	Perylene-d12	15.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cedrene-V6	204	C15H24	1000162-76-8	38
2		3-Quinolinecarboxylic acid, 6-fl...	235	C12H10FN03	1000350-64-5	30
3		Uracil, 3-(2-mercaptoethyl)-5-ph...	248	C12H12N2O2S	029558-47-2	25
4		2-(4-Fluorophenoxy)nicotinic acid	233	C12H8FN03	054629-13-9	25
5		Acetamide, N-[1-(4,6-dimethyl-2-...	248	C13H20N4O	1000362-37-5	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090216\
Data File : BF089982.D
Acq On : 2 Sep 2016 18:36
Operator : UM/SJ
Sample : H4675-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RAMP-A(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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...	4.78	22.6	ng	1345960	1	6.64	1191250	20.0
unknown6.40	6.40	85.4	ng	5085620	1	6.64	1191250	20.0
Hexanoic acid, 2-...	7.32	2.8	ng	192203	2	7.92	1369760	20.0
Tetradecane	10.58	2.9	ng	203882	4	11.13	1409810	20.0
1-Hexadecanol	11.38	5.3	ng	374378	4	11.13	1409810	20.0
n-Hexadecanoic acid	11.69	2.4	ng	167847	4	11.13	1409810	20.0
Heptadecyl hepta...	13.63	5.2	ng	362407	5	13.75	1395970	20.0
Benz[e]acephenant...	14.73	2.2	ng	124376	6	15.10	1112660	20.0
4-Hexen-1-ol, 6-(...	16.48	3.9	ng	214489	6	15.10	1112660	20.0
unknown16.83	16.83	2.9	ng	161312	6	15.10	1112660	20.0
unknown18.40	18.40	3.2	ng	180099	6	15.10	1112660	20.0